VSim Examples

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CONTENTS

CHAPTER

ONE

OVERVIEW

These are examples for illustrating the capabilities of VSim.

VSim [VSi] is an arbitrary dimensional, electromagnetics and plasma simulation code consisting of two major components:

- VSimComposer, the graphical user interface.
- Vorpal [NC04], the VSim Computational Engine.

VSim also includes many more items such as Python, MPI, data analyzers, and a set of input simplifying macros.

CHAPTER

TWO

VSIM FOR BASIC PHYSICS EXAMPLES

These examples demonstrate the basic solvers for simple, grid-aligned boundary conditions.

These examples can be run with any license.

2.1 Basic Examples

2.1.1 Cylindrical Capacitor (cylindricalCapacitor.sdf)

Keywords:

`cylindrical, capacitor, electrostatic`

Problem description

The Cylindrical Capacitor simulation solves for the potential between two cylinders with a ring of charge.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Cylindrical Capacitor example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Cylindrical Capacitor* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.1. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

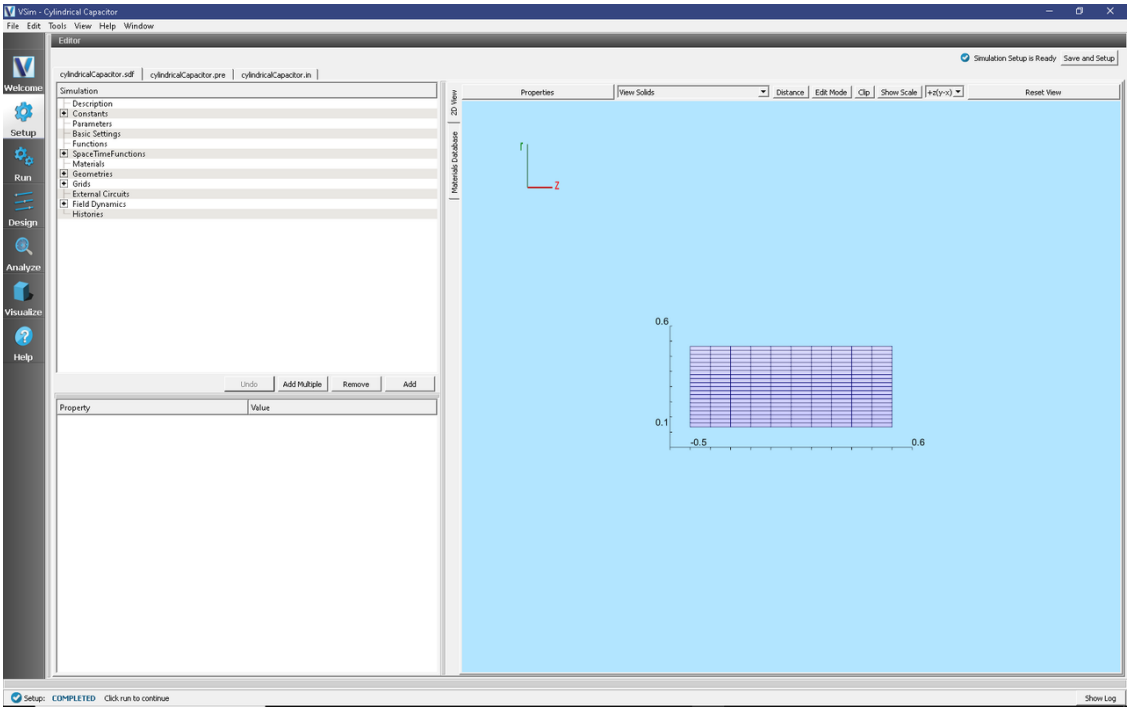


Fig. 2.1: Setup Window for the Cylindrical Capacitor example.

Simulation Properties

In this simulation there is a backgroundChargeDensity0 field which is given by an expression, chargedDist. That expression is defined as a SpaceTimeFunction. The variables x and y in the expression are place holders for the actual variables, Z and R, in the simulation. So this is a ring of charge, centered at R = 0.3, with a Gaussian fall off.

There are Dirichlet boundary conditions on the lower and upper R boundaries, with the lower bound set to 10 volts.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, “Engine completed successfully”. This result is shown in Fig. 2.2.

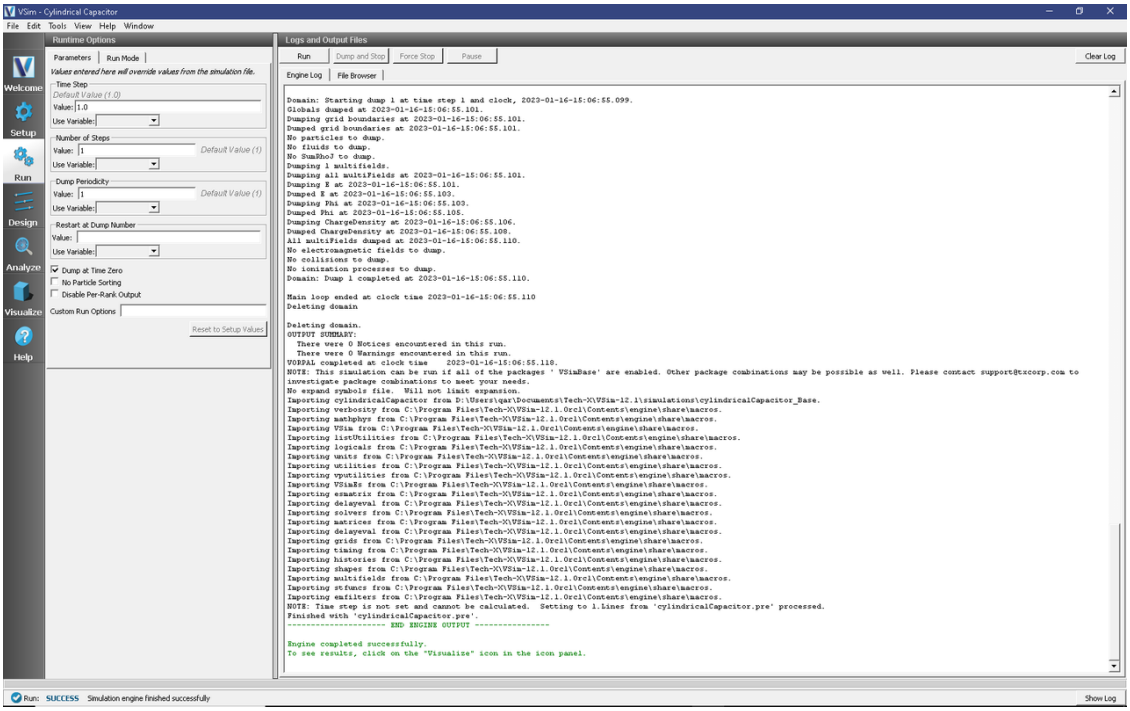


Fig. 2.2: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

This particular run computes the electrostatic potential, which we see by opening the scalar data and checking the box next to Phi, which is shown in the right of the visualization tab. See Fig. 2.3.

Further Experiments

Looking inside the field boundary conditions, and highlighting dirichlet0, you can see that 10V was put on the lower R boundary. You can try experimenting with this, going to run and visualize with each change. The more voltage, the less the background charge should matter.

You can take the charge out of the system. Highlight the backgroundChargeDensity0 label. In the property editor below, double click on chargedDist, hit delete, and type 0.0. Then run and viz, and you will see a potential that is independent of Z.

Click the *Add a Data View* dropdown below the menu bar and select Field Analysis. For the Field, choose E_r with the Vertical Lineout Settings, then hit "Perform Lineout". You will see, as expected, that the radial electric field is positive (pointing outward) and falling off with the expected 1/r behavior.

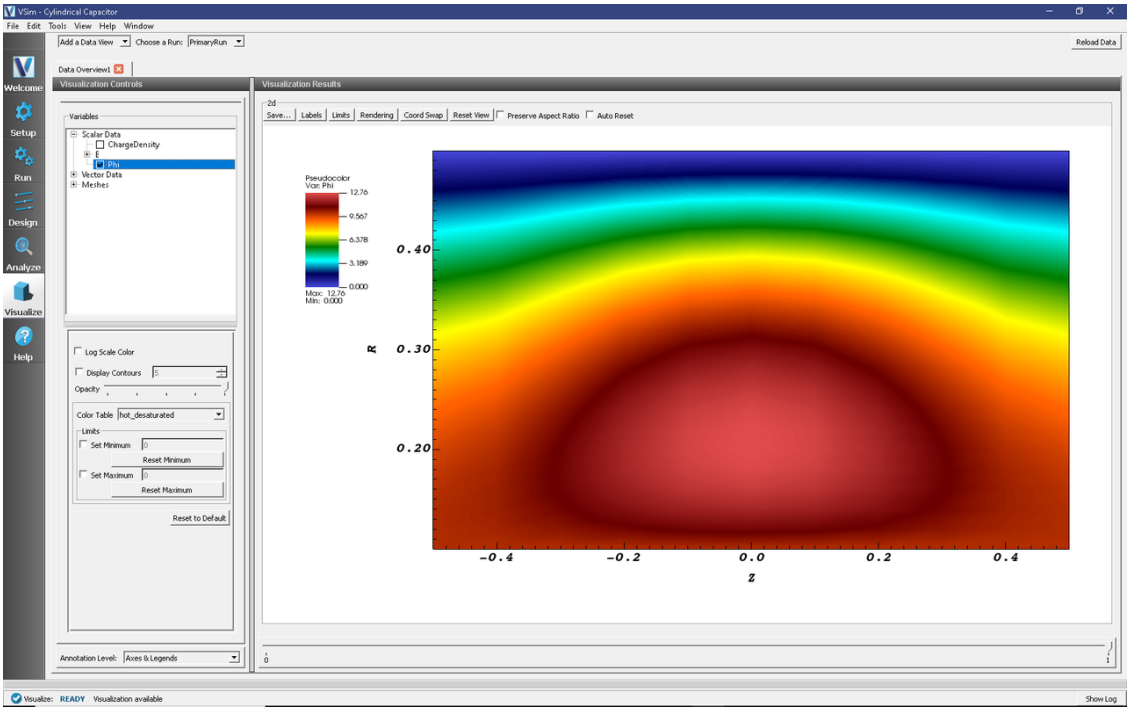


Fig. 2.3: Visualization of the electrostatic potential

2.1.2 Oscillating Dipole Above Conducting Plane (emOscDipoleAboveConductor.sdf)

Keywords:

`emOscDipoleAboveConductor, radiation`

Problem Description

This problem consists of an infinitesimally short dipole located at a variable height and orientation above a conducting plane. The simulation computes the electric and magnetic fields that can be visualized to show how the distance between, and orientation of the dipole relative to the conducting plane affects these fields.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Dipole Above Conducting Plane example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Oscillating Dipole Above Conducting Plane* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.4. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

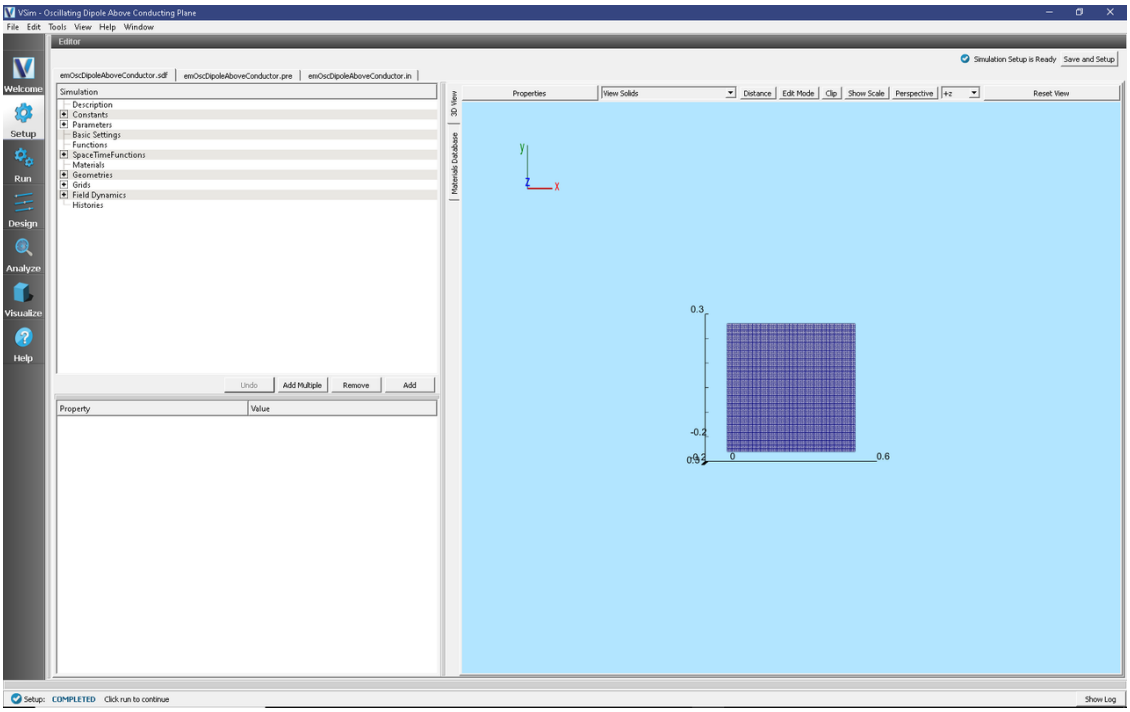


Fig. 2.4: Setup Window for the Dipole Above Conducting Plane example.

Simulation Properties

This example includes several constants for easy adjustment of simulation properties, Including:

- AMPLITUDE: The amplitude of the dipole current
- FREQUENCY: The operating frequency

There is also a SpaceTimeFunction to define the current driver of the dipole source

Other properties of the simulation include open boundaries on all sides except for the lower x boundary, which is a perfect electric conductor. A *Dipole Current* source is used to set the location of the dipole source.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.08e-11
  - *Number of Steps*: 400
  - *Dump Periodicity*: 50

  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.5.

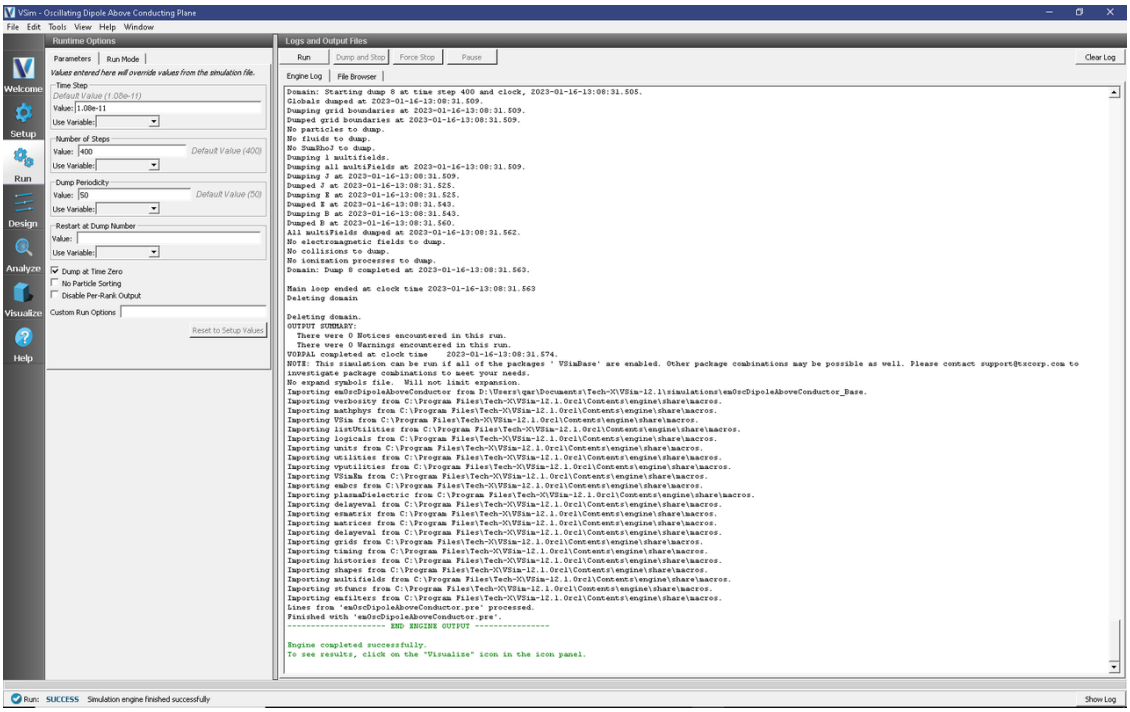


Fig. 2.5: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The electric and magnetic field components can be found in the scalar data variables of the data overview tab. To create the plot shown in Fig. 2.6 do the following:

- Expand *Scalar Data*
- Expand *E*
- Select *E_y*
- Select the box next to *Display Contours* and set the # of contours to 12
- Select the box next to *Clip All Plots*
- Drag the slider at the bottom of the *Visualization Results* pane to the right to show the 8th data dump
- If desired, rotate the plot by clicking and dragging your mouse

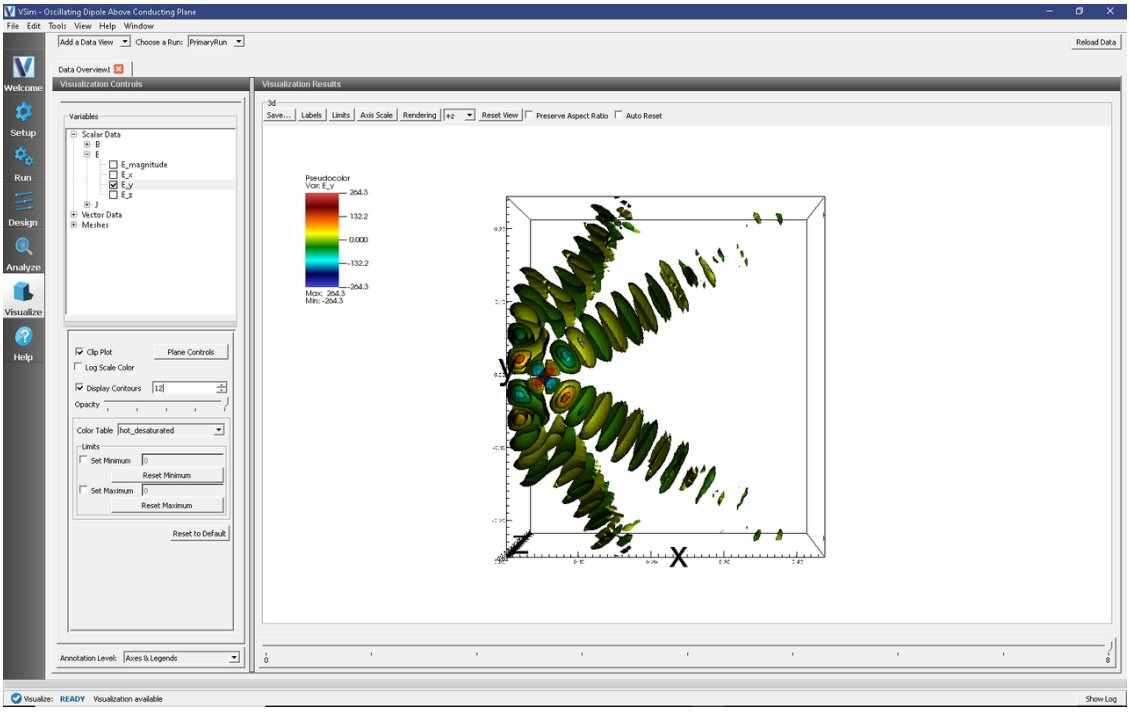


Fig. 2.6: The electric field

Further Experiments

In this example the "infinite" electric conductor is simulated by a physical conducting boundary at the bottom of the simulation. It would be possible to achieve the same results by having a second, equal infinitesimal dipole placed the same height "below" the conducting plane.

The number of "lobes" visible in the far field is dependent on Antenna Orientation and height. If vertically oriented there will be 2*Height/Wavelength +1 lobes.A horizontally oriented dipole will produce 2*Height/Wavelength lobes. This can be a bit difficult to visualize using just E-field data as it must be properly thresholded. The lobes will be easier to see in the example Advanced Dipole Above Conductor, a part of the VSimEM package.

2.1.3 Electromagnetic Plane Wave (emPlaneWave.sdf)

Keywords:

`electromagnetics, plane wave, periodic boundary conditions, wave launcher`

Problem Description

A linearly-polarized (with electric field in the z-direction) continuous electromagnetic plane wave with a sinusoidal amplitude is launched from the left side (x=0) to propagate in the x-direction. The transverse (y,z) boundary conditions are periodic.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Electromagnetic Plane Wave example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Electromagnetic Plane Wave* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.7. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

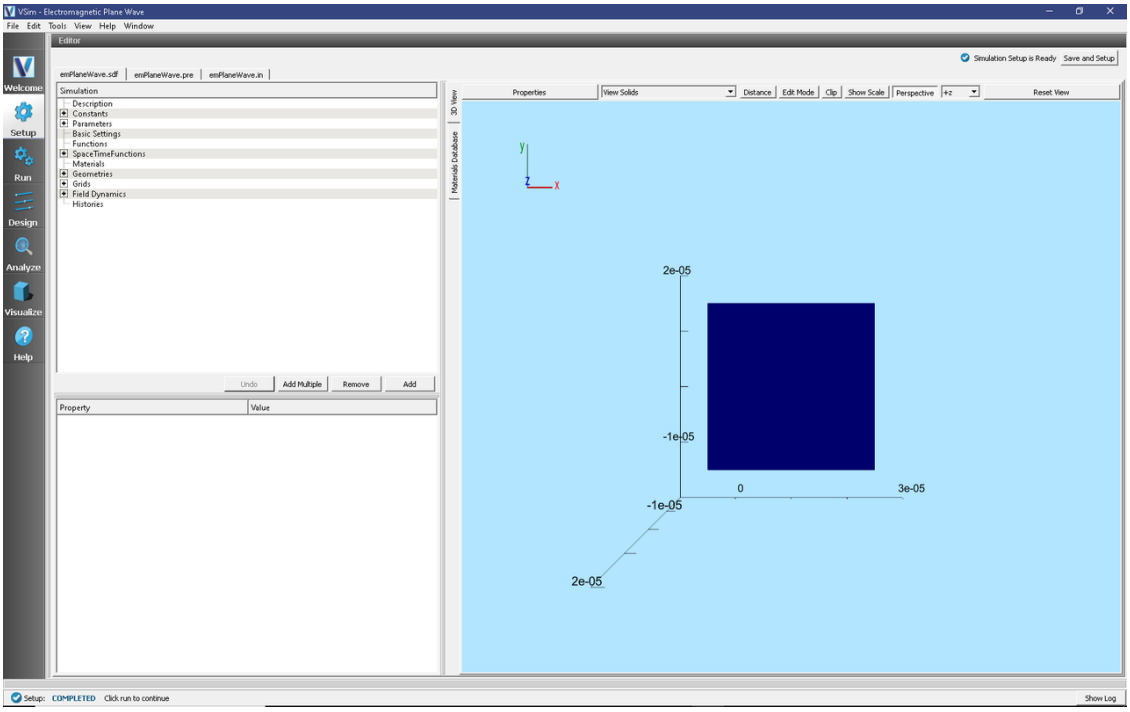


Fig. 2.7: Setup Window for the Electromagnetic Plane Wave example.

Simulation Properties

This example includes several constants for easy adjustment of simulation properties. Those include:

- AMPLITUDE: The amplitude of the plane wave
- WAVELENGTHS: The number of wavelengths inside the domain

There is a SpaceTimeFunction to define the plane wave that is launched with a *Port Launcher* boundary condition.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.6590830829382937e-16
  - *Number of Steps*: 100
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.8.

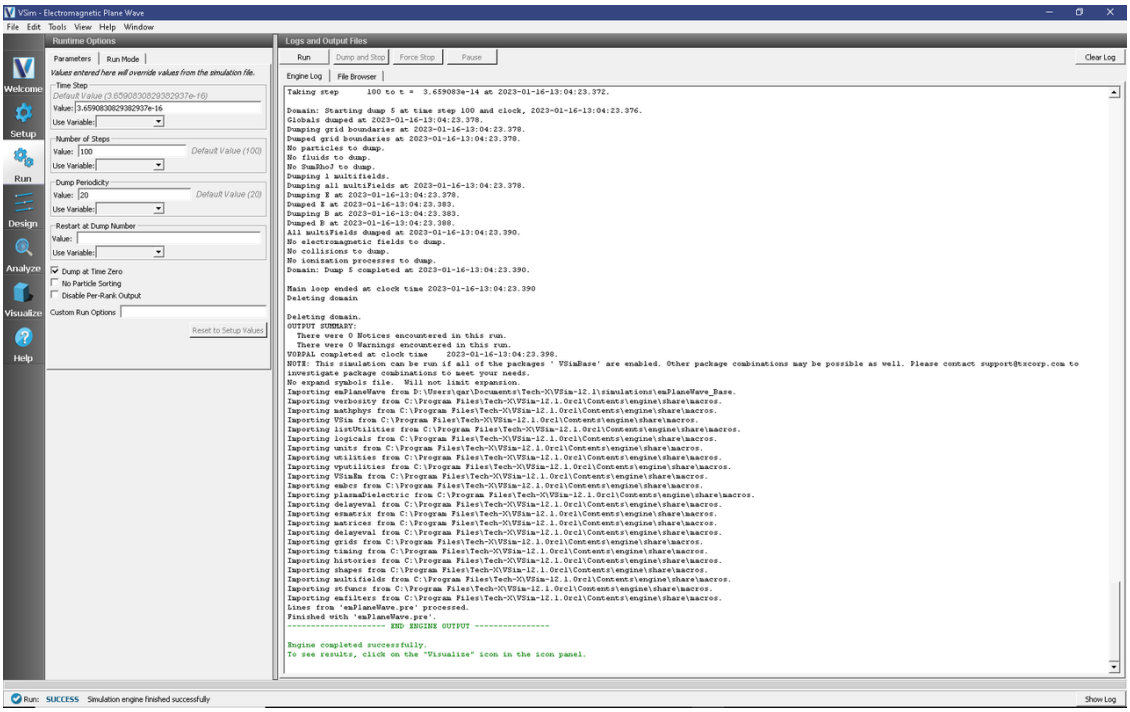


Fig. 2.8: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The electric and magnetic field components can be found in the scalar data variables of the data overview tab.

- The Data Overview tab should be active. If it is not, click the *Add a Data View* dropdown below the toolbar and select *Data Overview*.
- Here you can see *Variables*. Expand the *Scalar Data*.

- Expand E
- Select E_z

Initially, no field will be seen, as one is looking at Dump 0, the initial dump, when no fields are yet in the simulation. Move the slider at the bottom of the right pane to see the electric field at different times. The final time is shown in Fig. 2.9.

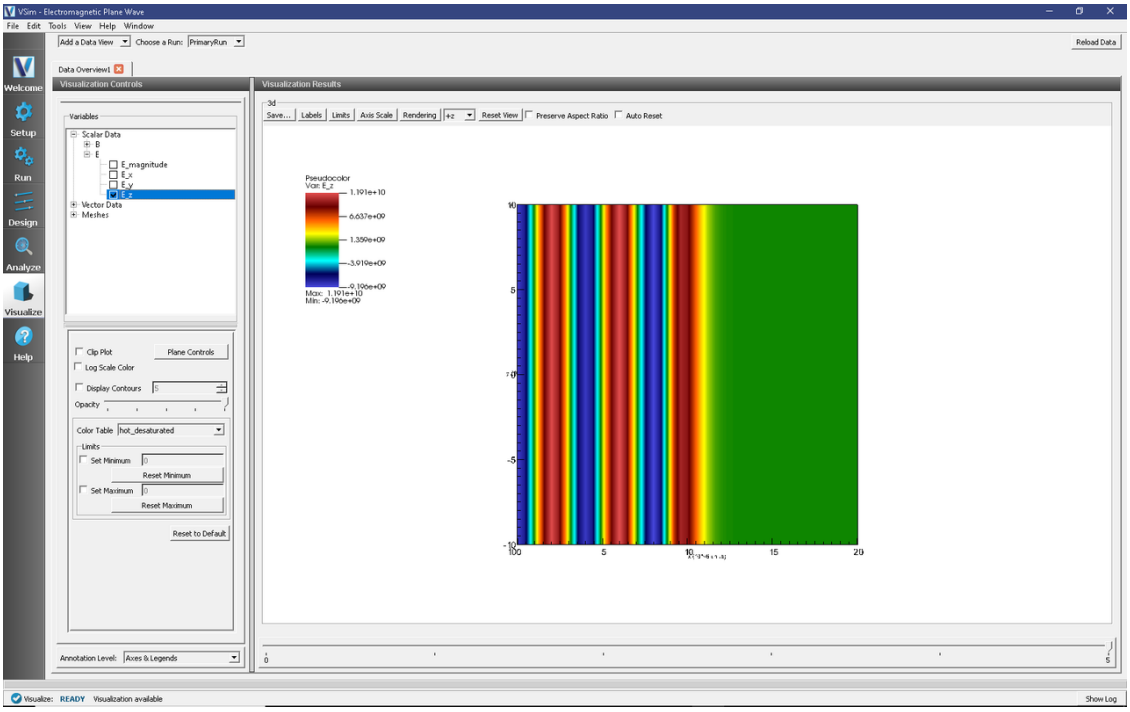


Fig. 2.9: Visualization of plane wave as a color contour plot.

Further Experiments

To see more wavelengths, change the value of the WAVELENGTHS variable. What happens to the waves when there are very few cells in a wavelength?

See the wave reflect off the right boundary by running for more time steps.

Try rotating the visualization by left-clicking and dragging with the mouse to see how the simulation is uniform across the z- dimension.

2.1.4 Electromagnetic Particle in Cell (emPtclInCell.sdf)

Keywords:

`electromagnetics, particle in cell, sheath`

Problem description

A dipole antenna launches a wave from a point that is midway in x and y. The simulation is periodic in y and open in x. The electromagnetic field and plasma respond self consistently to the antenna current.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Electromagnetic Particle In Cell example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select "Electromagnetic Particle In Cell" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.10. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

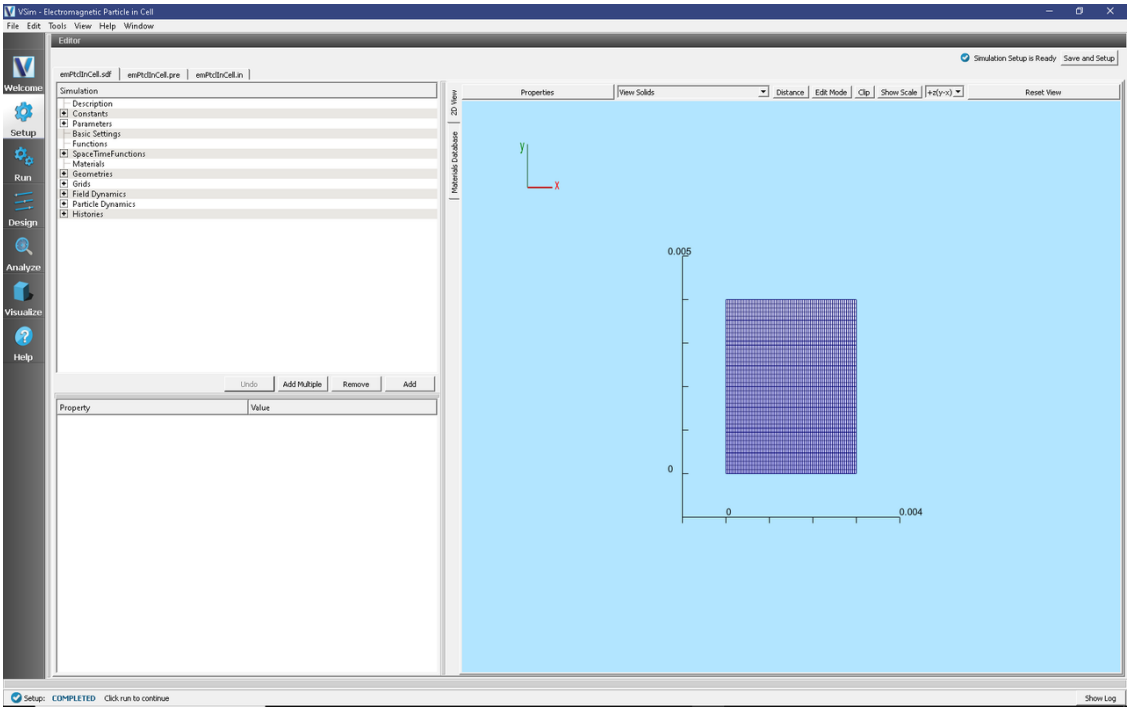


Fig. 2.10: Setup Window for Electromagnetic Particle in Cell.

Simulation Properties

This simulation includes several constants for easy adjustment of simulation properties including:

- N_X, N_Y: The number of cells in each direction
- LEN_X, LEN_Y: The length of the domain in each direction
- PPC: The number of macroparticles per cell
- FREQUENCY: The frequency of the dipole antenna

The *Parameters* element contains several parameters useful for calculating basic plasma physics properties such as the plasma frequency and Debye length.

There are 2 SpaceTimeFunctions that are used later in the setup to describe the thermal velocity of the electrons and the antenna current profile.

The simulation has open boundary conditions in x, and periodic in y.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.580718045498294e-14
  - *Number of Steps*: 200
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.11.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric field and particles as shown in Fig. 2.12, do the following:

- Expand *Particle Data*
- Expand *electrons0*
- Select *electrons0*
- Expand *Scalar Data*
- Expand *E*
- Select *E_z*

Initially the field is at zero and particles are evenly distributed throughout the simulation. Move the dump slider forward in time to view the results.

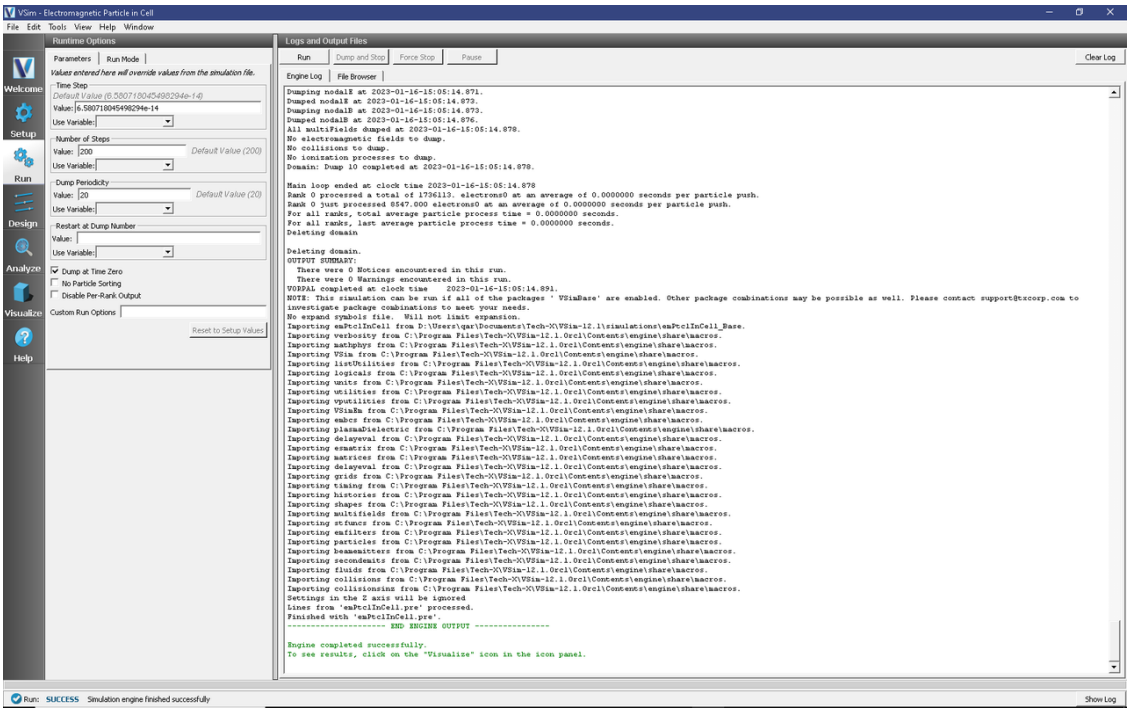


Fig. 2.11: The Run Window at the end of execution of Electromagnetic Particle in Cell.

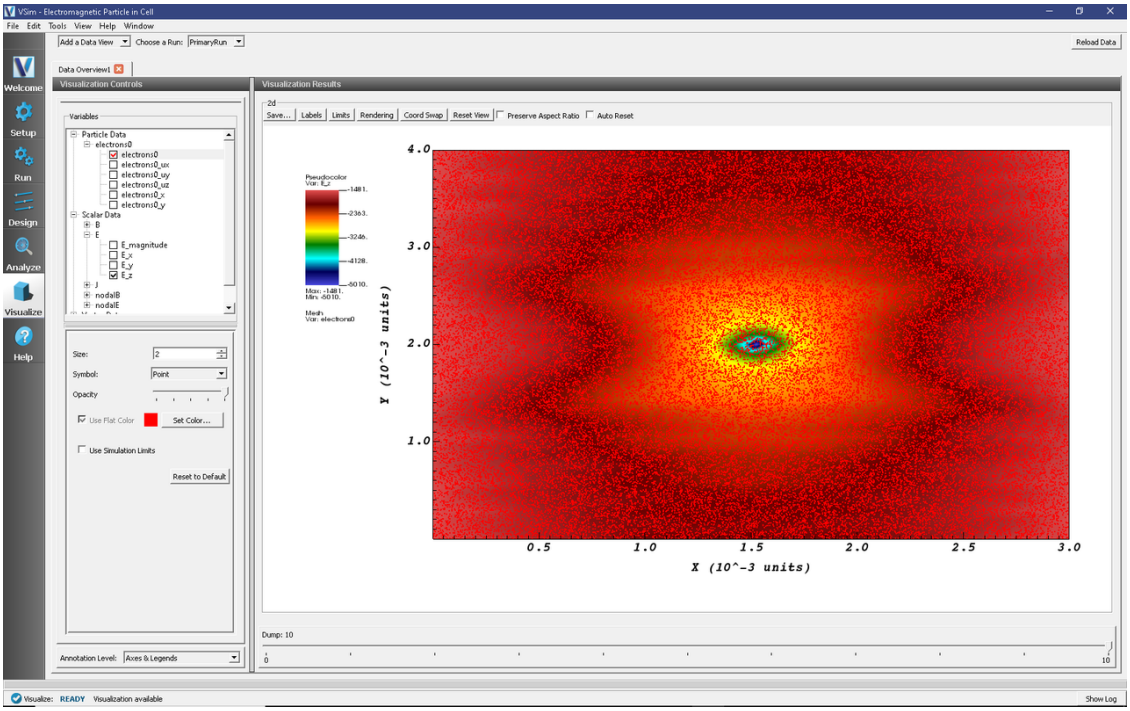


Fig. 2.12: Visualize Window with electric field and particles

Further Experiments

Vary the antenna amplitude, to find out how low it can be before the signal is swamped by the plasma noise.

Add in a magnetic field in the plane.

2.1.5 Vacuum Electromagnetic Pulse (emPulseInVacuum.sdf)

Keywords:

electromagnetics, laser, plane wave pulse, field energy monitoring

Problem description

A linearly-polarized (with electric field in the z-direction) electromagnetic pulse with a sinusoidal amplitude on a plane wave is launched from the left side (x=0). The transverse (y, z) boundary conditions are periodic, but the pulse has finite transverse extent.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Vacuum Electromagnetic Pulse example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Vacuum Electromagnetic Pulse* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.13. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

Simulation Properties

The Vacuum Electromagnetic Pulse example includes several constants for easy adjustment of simulation properties. Those include:

- AMPLITUDE: The amplitude of the pulse
- WAVELENGTH: The wavelength of the pulse
- PULSELENGTH: The length of the pulse in the propagation direction
- PULSEWIDTH: The width of the pulse in the transverse direction

There is also a SpaceTimeFunction defined for the pulse shape and is used in the *Port Launcher* boundary condition.

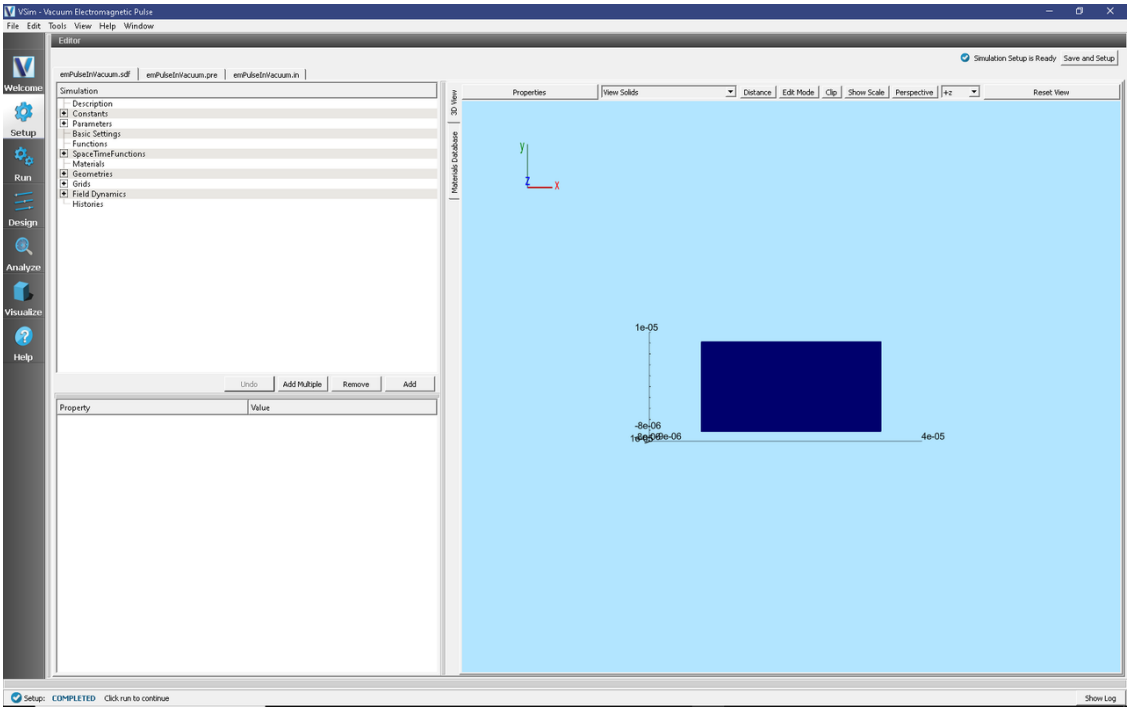


Fig. 2.13: The Setup Window for the electromagnetic pulse.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.865974429602727e-16
  - *Number of Steps*: 300
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.14.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The electric and magnetic field components can be found in the scalar data variables of the data overview tab.

- Make sure the *Data View* drop down is set to *Data Overview*.
- Here you can see *Variables*. Expand the *Scalar Data*.
- Expand E

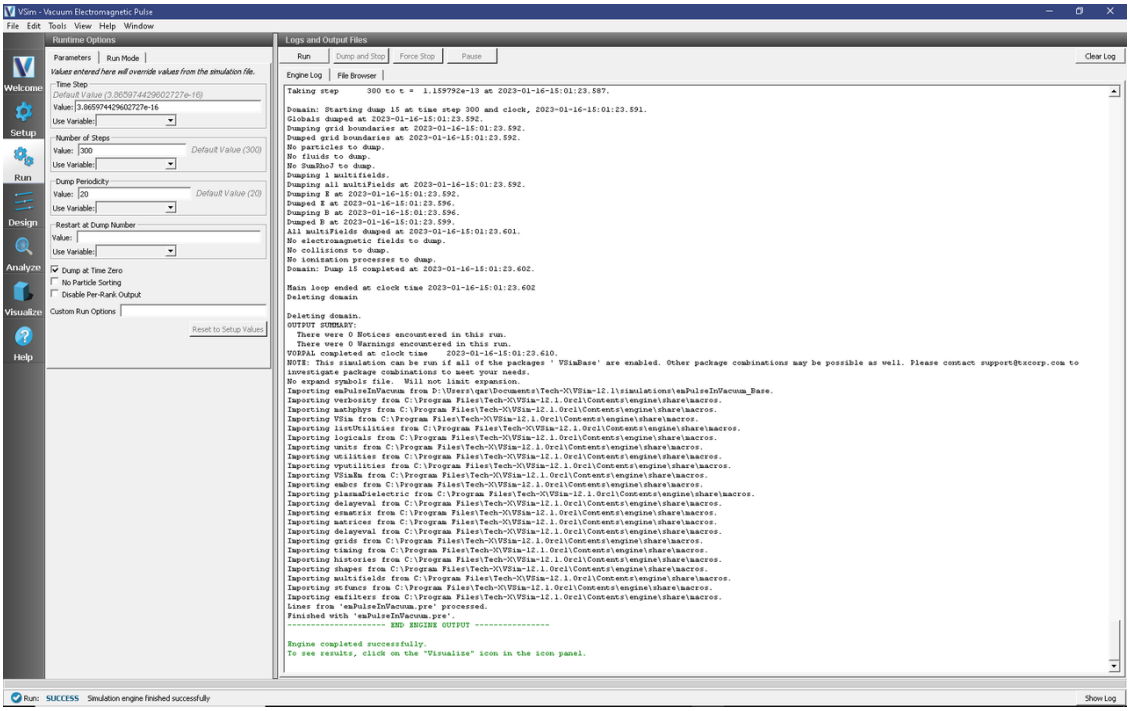


Fig. 2.14: The Run Window for the electromagnetic pulse.

- Select E_z
- Check the box next to *Clip Plot*
- Check the box next to *Display Contours* and set the # of contours to 5
- Click and drag with your mouse to rotate the view

Initially, no field will be seen, as one is looking at Dump 0, the initial dump, when no fields are yet in the simulation. Move the slider at the bottom of the right pane to see the magnetic field at different times.

Further Experiments

Increase NX to better resolve the wave and see whether it slips less with respect to the box.

Increase the pulse and box widths (you will also need to increase the number of cells in the transverse directions) to reduce diffraction.

2.1.6 Electrostatic Particle in Cell (esPtclInCell.sdf)

Keywords:

`electrostatics, particle in cell, sheath`

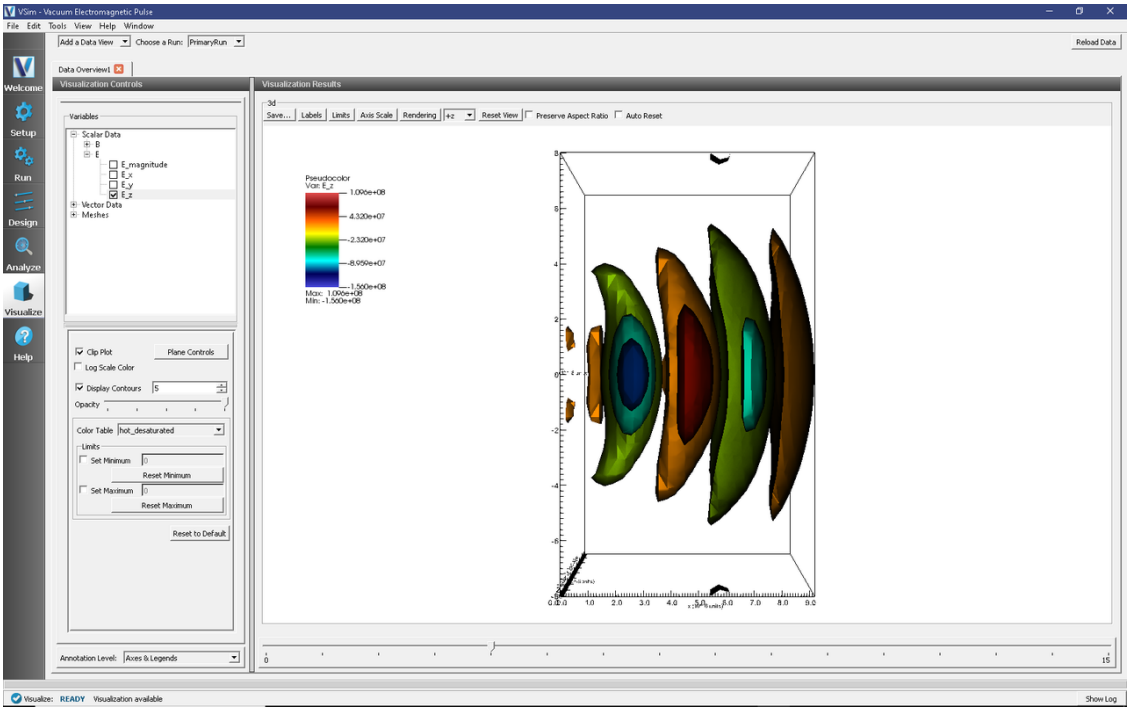


Fig. 2.15: Ez field at Dump 5.

Problem description

This Electrostatic Particle in Cell example computes the electrostatic potential and field in a box with conducting walls and particle absorbers and with an immobile, background neutralizing charge density. The electrons move to the wall by the potential, creating a sheath.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The electrostatic particle in cell example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Electrostatic Particle in Cell* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.16. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

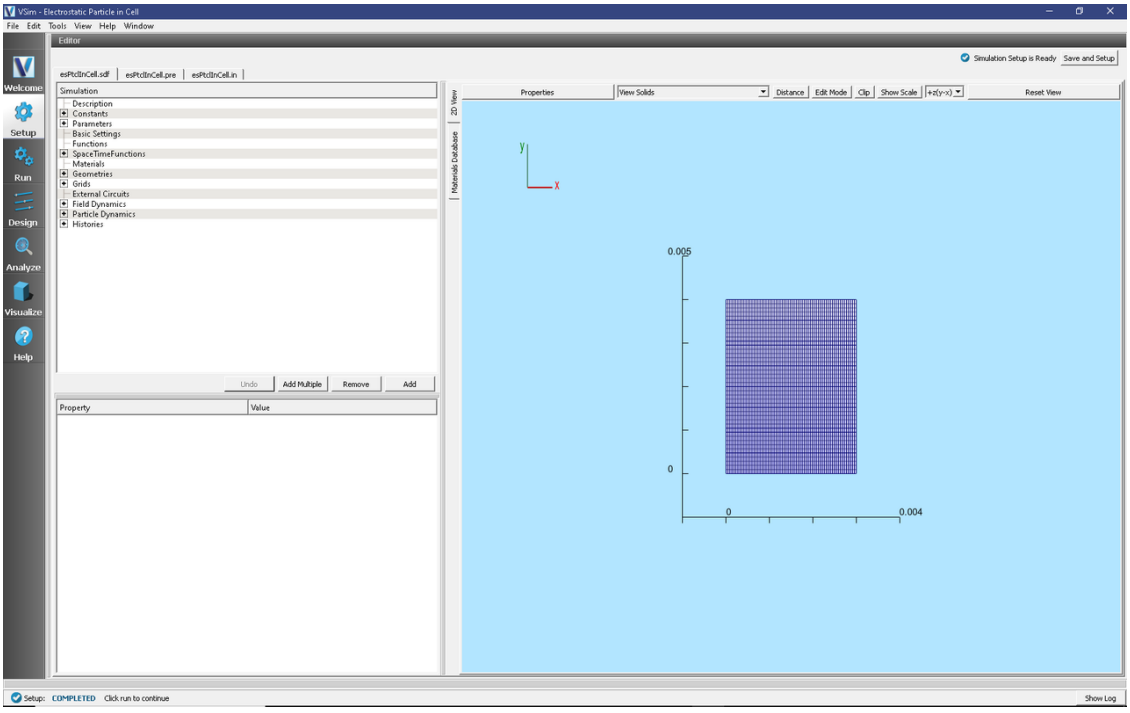


Fig. 2.16: Setup Window for the electrostatic particle in cell example.

Simulation Properties

This simulation includes several constants for easy adjustment of simulation properties including:

- N_X, N_Y: The number of cells in each direction
- W_X, W_Y: The length of the domain in each direction
- PPC: The number of macroparticles per cell

The Parameters element contains several parameters useful for calculating basic plasma physics properties such as the plasma frequency and Debye length.

There is a SpaceTimeFunction used later in the setup to describe the thermal velocity of the electrons.

The simulation is periodic in y with Dirichlet boundary conditions in x set to zero.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.3342825598992326e-12
  - *Number of Steps*: 400
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.17.

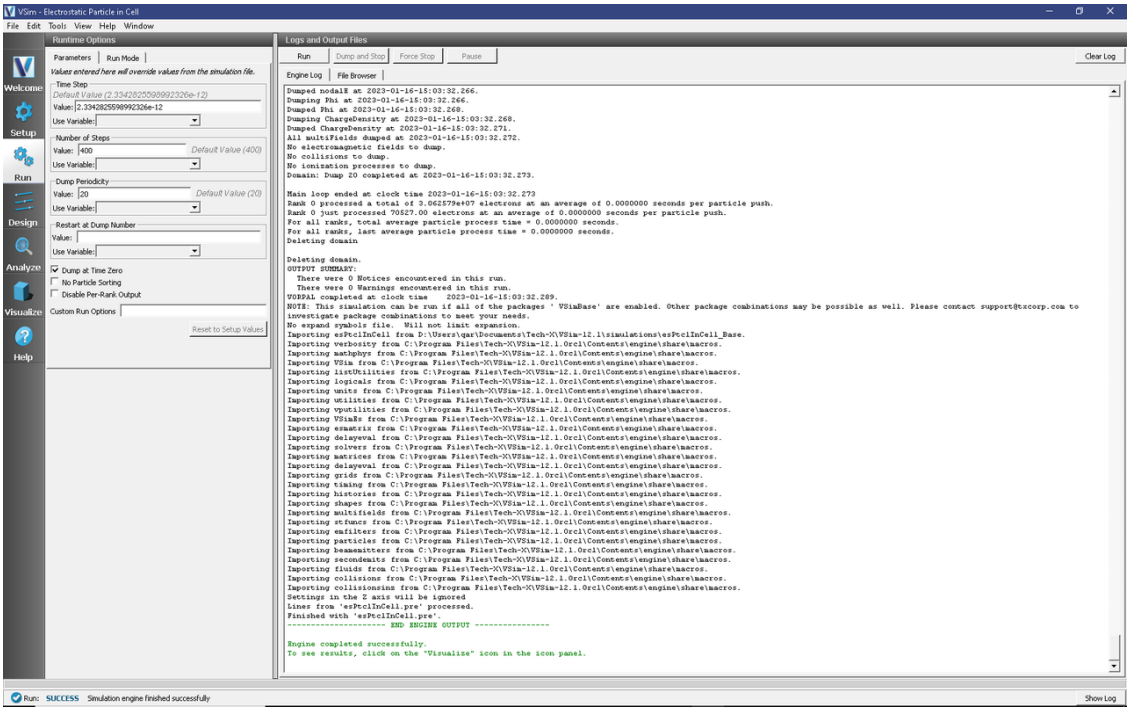


Fig. 2.17: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric potential as shown in Fig. 2.18, do the following:

- Expand *Scalar Data*
- Select *Phi*

Move the dump slider forward in time to see the evolution of the field.

Further Experiments

Change the plasma density and see whether the frequency in the histories changes.

Use the computePtclNumDensity analysis script in the *Analyze* Tab to calculate the electron density at each dump and view the sheath formation.

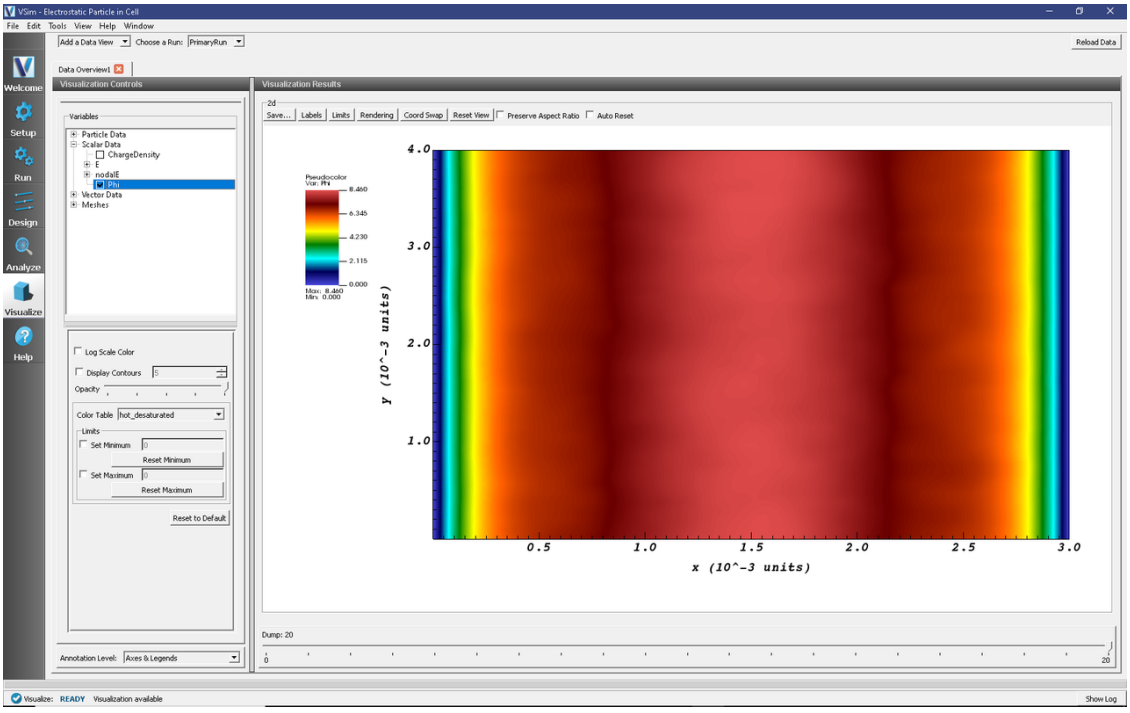


Fig. 2.18: The Visualize Window showing the electric potential, *Phi*, at dump 20.

2.1.7 Half-Wave Antenna (halfWaveAntenna.sdf)

Keywords:

`electromagnetics, antennas`

Problem Description

The half wave antenna example describes a simple box source in a vacuum.

This simulation can be performed with any license.

Opening the Simulation

The Half Wave Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Half Wave Antenna* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.19. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

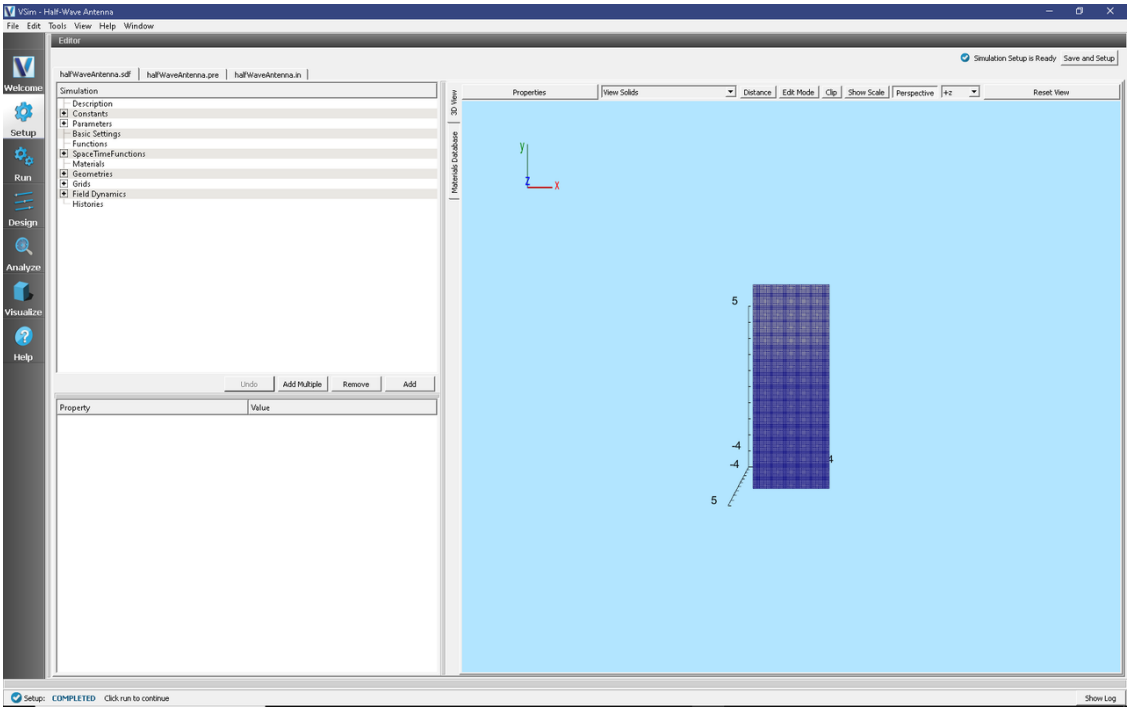


Fig. 2.19: Setup Window for the Half Wave Antenna example.

Simulation Properties

This example includes several constants for easy adjustment of simulation properties, Including:

- WAVELENGTH: The wavelength of the antenna

There is also a SpaceTimeFunction to define the current driver of the half wavelength source.

Other properties of the simulation include port boundaries on all sides except for the lower x boundary, which is a perfect electric conductor. A Distributed Current source is used to set the current of the half wavelength source.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.0312392390401535e-11
  - *Number of Steps*: 100
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.20.

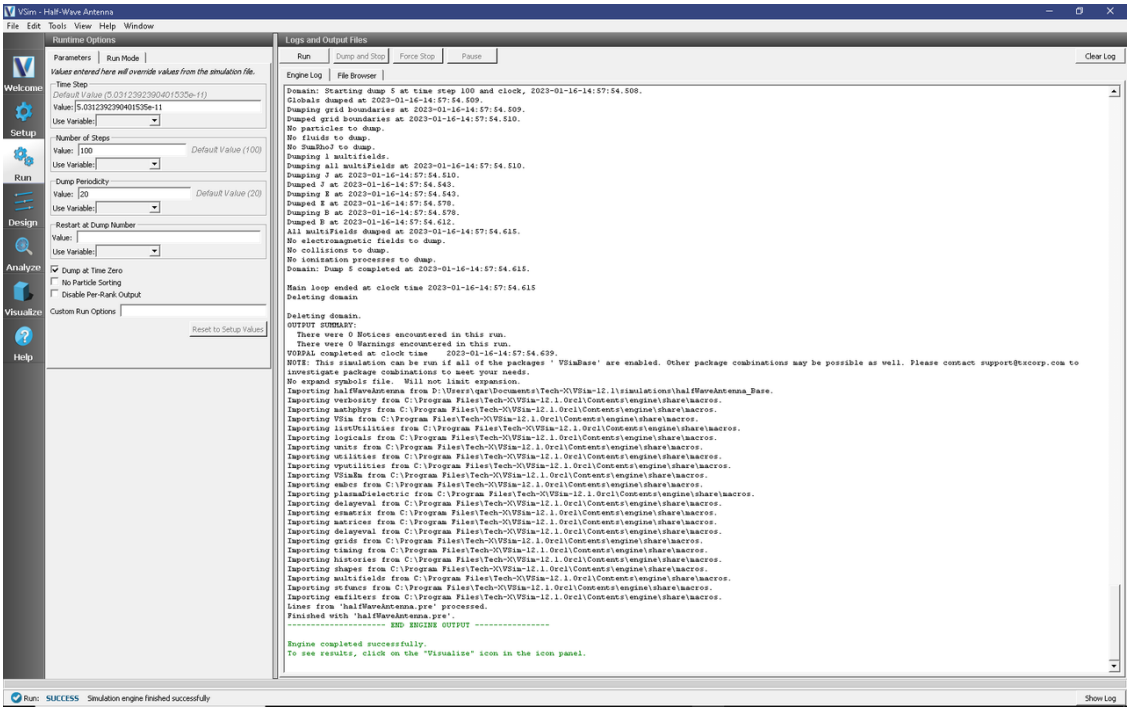


Fig. 2.20: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the field pattern as shown in Fig. 2.21, do the following:

- Expand *Scalar Data*
- Expand *B*
- Select *B_y*
- Select *Display Contours* and set the # of Contours to 10
- Move the dump slider forward in time to the last dump
- Rotate the plot by clicking and dragging with your mouse

Further Experiments

Additional experiments worth investigating are:

- Change the frequency of the source.

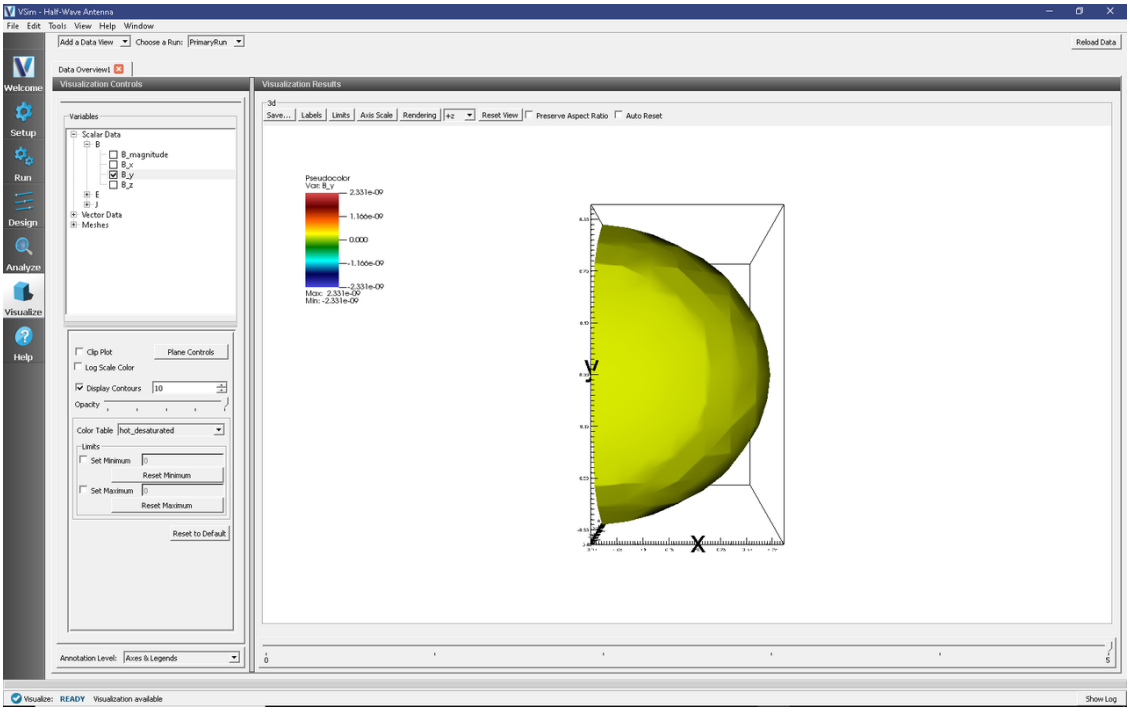


Fig. 2.21: Visualization of the wave pattern as a color contour plot.

2.1.8 Kelvin-Helmholtz Instability (kelvinHelmholtz.sdf)

Keywords:

`fluid, periodic boundary`

Problem description

This example demonstrates the Kelvin-Helmholtz instability that occurs in the presence of a velocity shear in a single, continuous fluid. The instability results in swirling eddies of fluid.

In this simulation, the density, flux, and energy density of a fluid are modeled via the Euler equations:

$$‘\frac{\partial n}{\partial t} = -\nabla \cdot (nv)‘$$

$$‘\frac{\partial nv}{\partial t} = -\nabla \cdot (nv \cdot v + Ip)‘$$

$$‘\frac{\partial nE}{\partial t} = -\nabla \cdot (vE)‘$$

This problem demonstrates the Kelvin-Helmholtz instability for the case of a velocity difference across the interface between two different fluids that differ in density by a factor 2. A finite-width shear layer is used to ensure results converge at finite resolution. For the two-dimensional version of the problem setup considered here, we use a domain with periodic boundary conditions.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Kelvin Helmholtz example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select "Kelvin-Helmholtz" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.22.

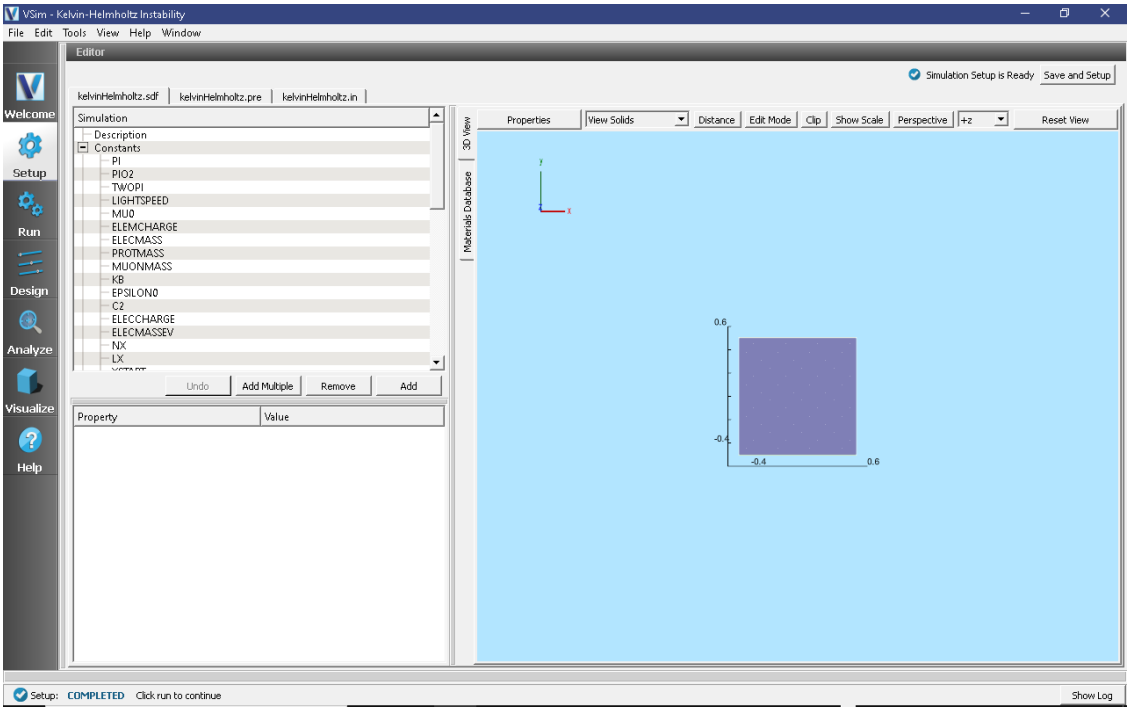


Fig. 2.22: Setup Window for the Kelvin-Helmholtz example.

Simulation Properties

Constants are set up to allow setting the number of cells (RESOLUTION), box length (BOX_LENGTH), CFL condition factor (CFL_FACTOR), number of timesteps (NSTEPS), pressure (P0), width of the initial perturbation (SWIDTH), initial density floor (D0), amplitude of the initial pressure perturbation (PAMP), and initial minimum flux (VFLOW).

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 0.0013703619790437
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 400
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.23.

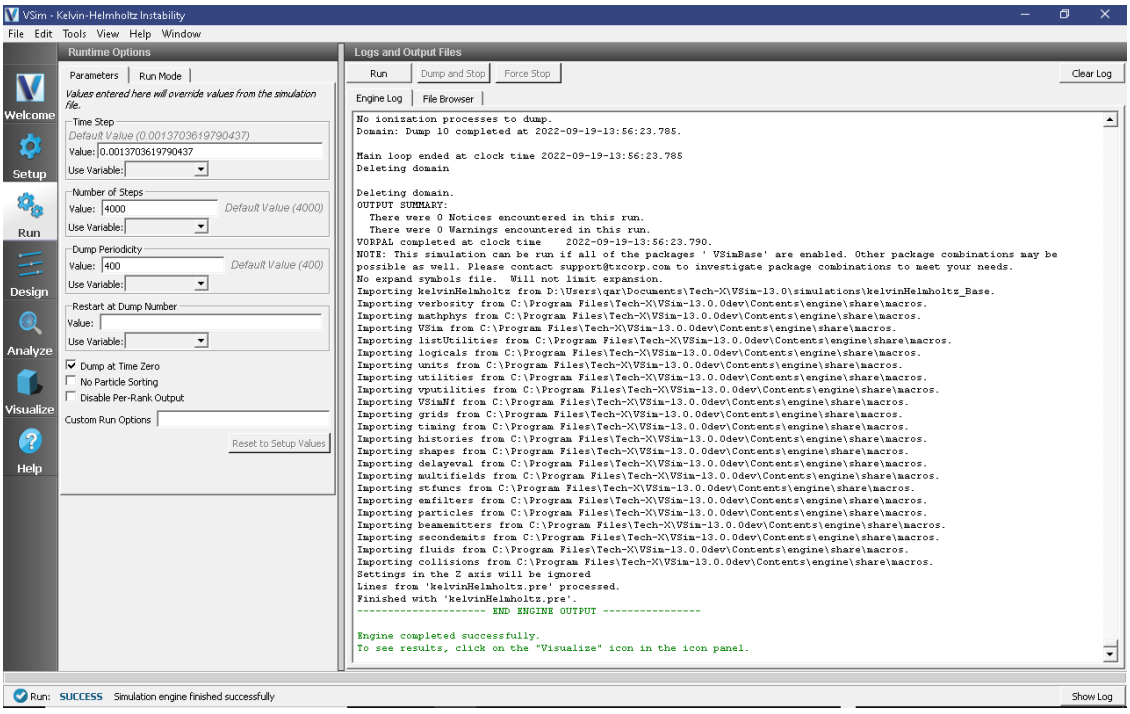


Fig. 2.23: The Run Window at the end of execution.

Visualizing the Results

The density shown in Fig. 2.24 shows the classic swirling structure that develops due to the Kelvin-Helmholtz instability.

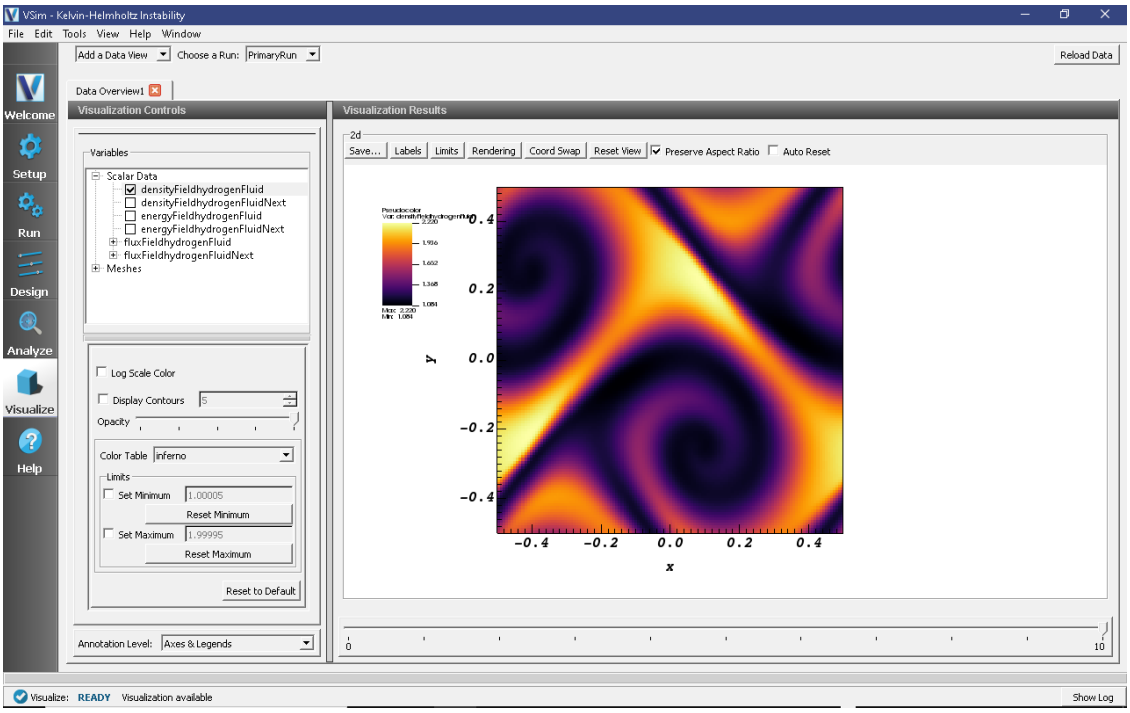


Fig. 2.24: The fluid density.

Further Experiments

2.1.9 Parallel Plate Capacitor (parPlateCapacitor.sdf)

Keywords:

electrostatics, parallel plate capacitor

Problem description

This Parallel Plate Capacitor simulation computes the electrostatic potential and field for a parallel plate capacitor. It can be run in any number of dimensions. It is periodic in the y and z directions when they are present.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Parallel Plate Capacitor example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Parallel Plate Capacitor* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.25. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`

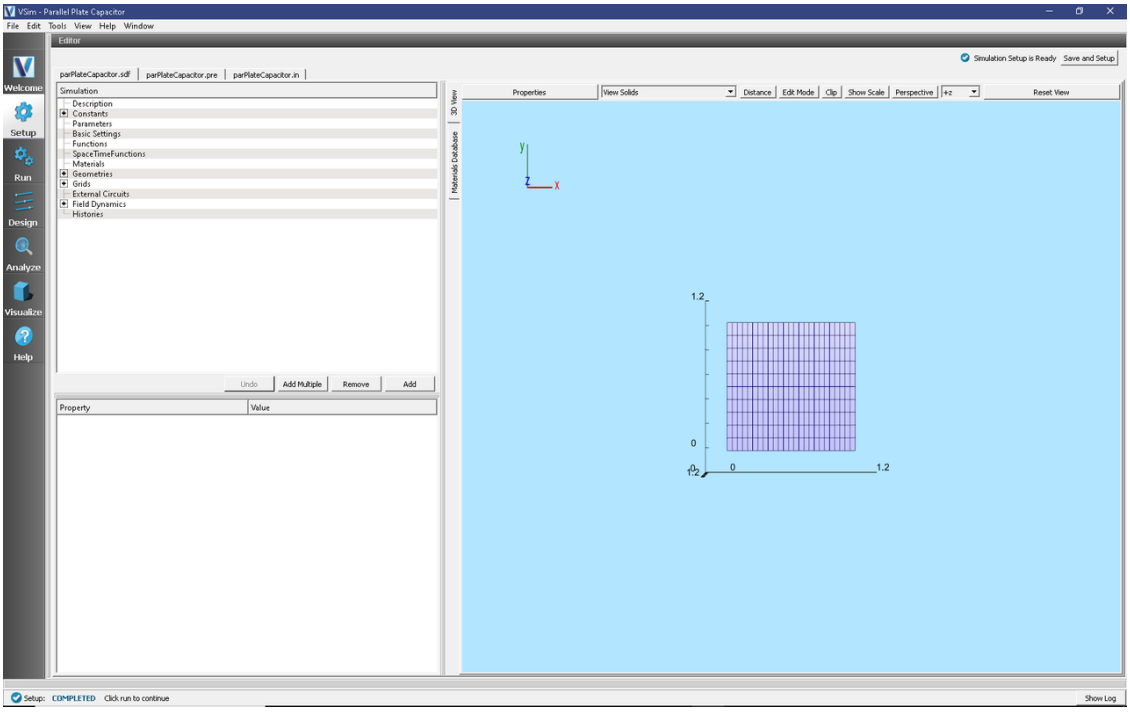


Fig. 2.25: Setup Window for the Parallel Plate Capacitor example.

Simulation Properties

The Simulation Elements Tree and Property Editor allow one to choose the distance between the plates, width of the plates, voltage of the positive plate and the length of a time step (which is irrelevant as this is an electrostatic simulation)

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.26.

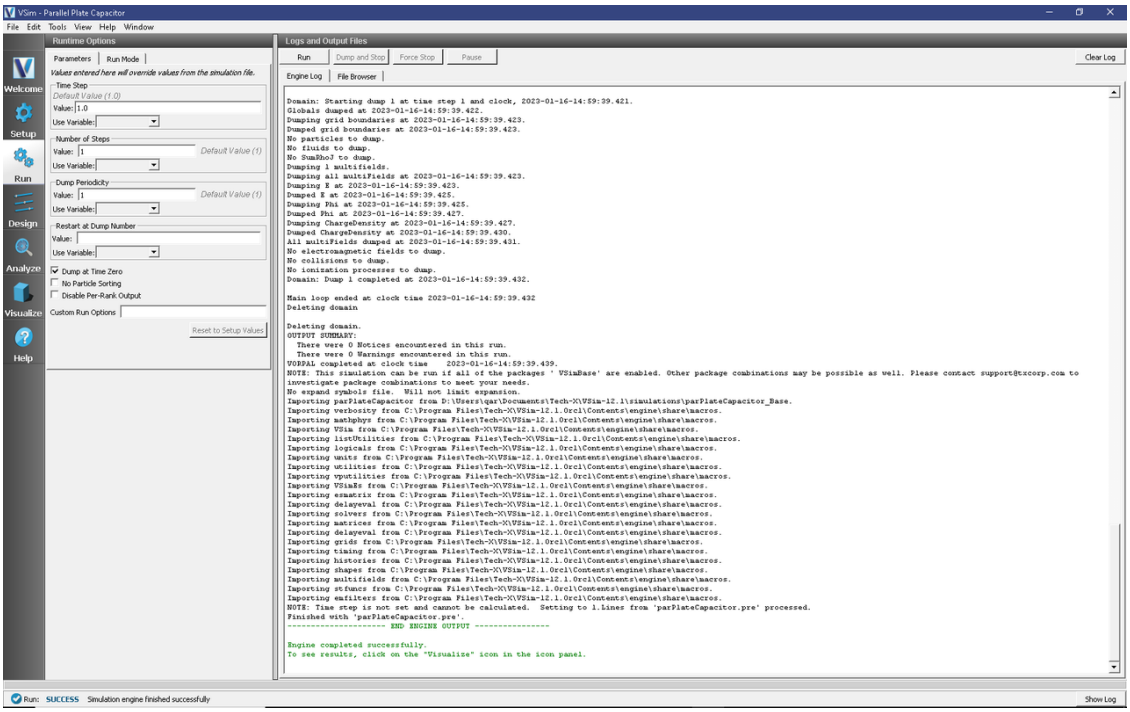


Fig. 2.26: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To create the image shown in Fig. 2.27, proceed as follows:

- Expand *Scalar Data* and select the box next to *Phi*

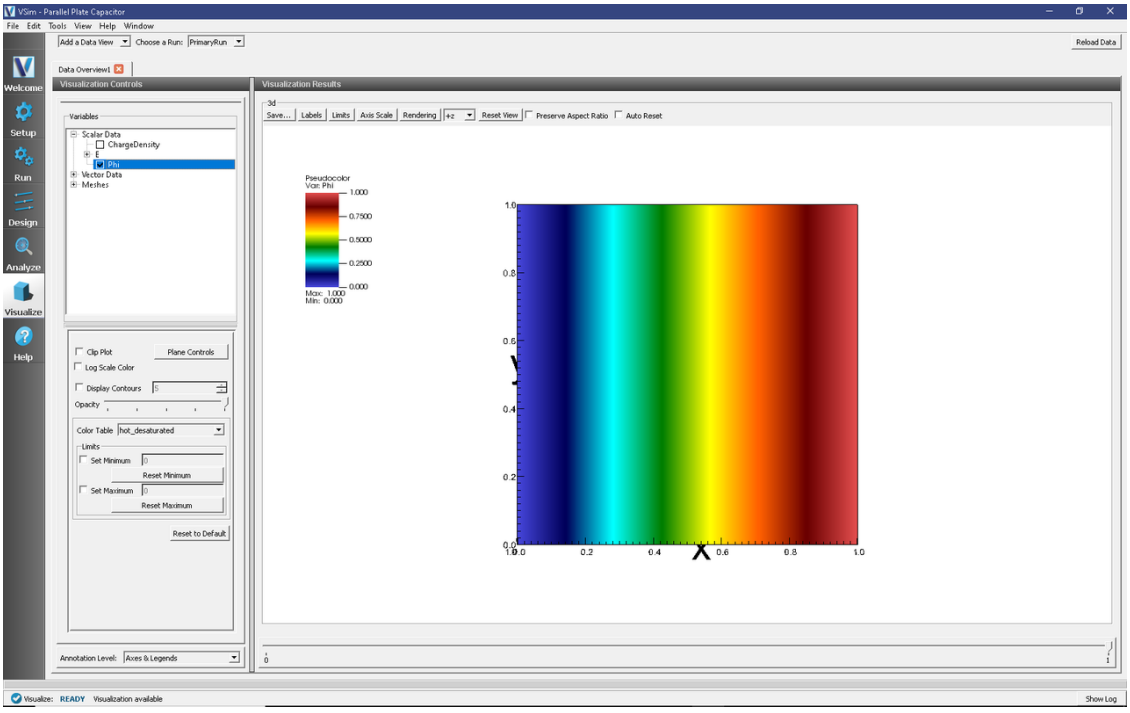


Fig. 2.27: Visualization of plane wave as a color contour plot.

Further Experiments

Change the gap between the plates by changing the length of the grid in the z direction and see how the electric field changes.

Change a width, e.g., LY and see whether it has an effect on the electric field.

Change the voltage on the right plate and see if it affects the electric field.

Set the periodic directions under *BasicSettings* to *none*, add boundary conditions on those directions and see how the field changes.

2.1.10 Two-Stream Instability (twoStream.sdf)

Keywords:

`electromagnetics, two-stream instability`

Problem Description

The two-stream instability is a rapidly growing collisionless plasma instability arising from small charge imbalances. A local imbalance leads to the acceleration or deceleration of particles in its vicinity, which in turn leads to an even stronger imbalance. One setup that allows one to easily observe the instability is two counter-streaming beams of identical charge in a periodic system. The advantage of this configuration is that the generated plasma wave becomes a standing wave, thus allowing us to easily observe the formation of the phase space vortices.

In this example, we use two electron streams. At $t = 0$ the streams have drift velocities of magnitude 7.78×10^6 m/s. In order to accelerate the onset of the instability, the two particle beams are given a small sinusoidal perturbation in velocity space.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Two-Stream Instability example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples* option.
- Select *Two-Stream Instability* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 2.28. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

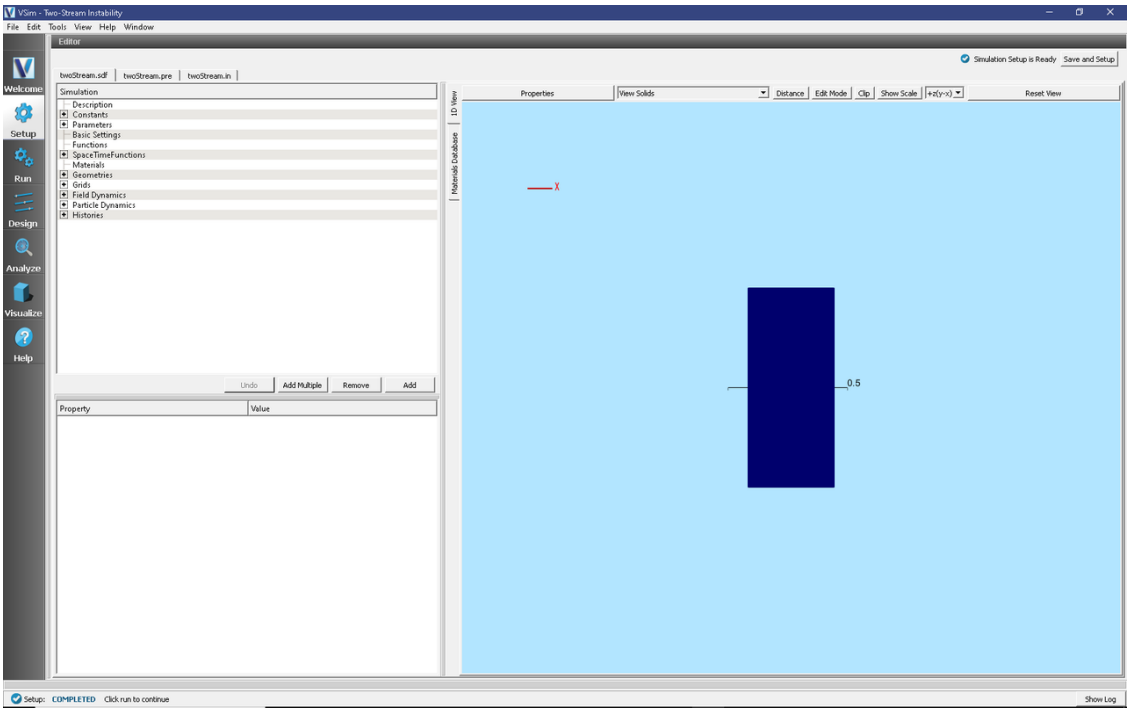


Fig. 2.28: Setup Window for the Two-Stream Instability example.

Simulation Properties

There are a number of *Constants* in this simulation to help make modifying the simulation even easier. Those include:

- XCELLS: The number of cells
- NOM_DEN_E: The electron density
- VBAR: The average velocity
- WAVELENGTHS: The number of wavelengths in the domain to simulate
- PPC: The number of particles per cell.

SpaceTimeFunctions are used to set the velocities of each particle stream.

The simulation is 1 dimensional and periodic in x.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.8602663991105245e-12
  - *Number of Steps*: 10000
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.29.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the instability as shown in Fig. 2.30, do the following:

- Select the *Phase Space* option from the *Data View* menu
- In the Plot 1 box, change the *X-axis* to *electrons0_x*, and the *Y-axis* to *electrons0_ux*
- Click the *Enable Second Plot* box
- In the Plot 2 box, change the *Base Variable* to *electrons1*, the *X-axis* to *electrons1_x*, and the *Y-axis* to *electrons1_ux*
- Click the *DRAW* button at the bottom, then move the *Dump* slider forward in time.

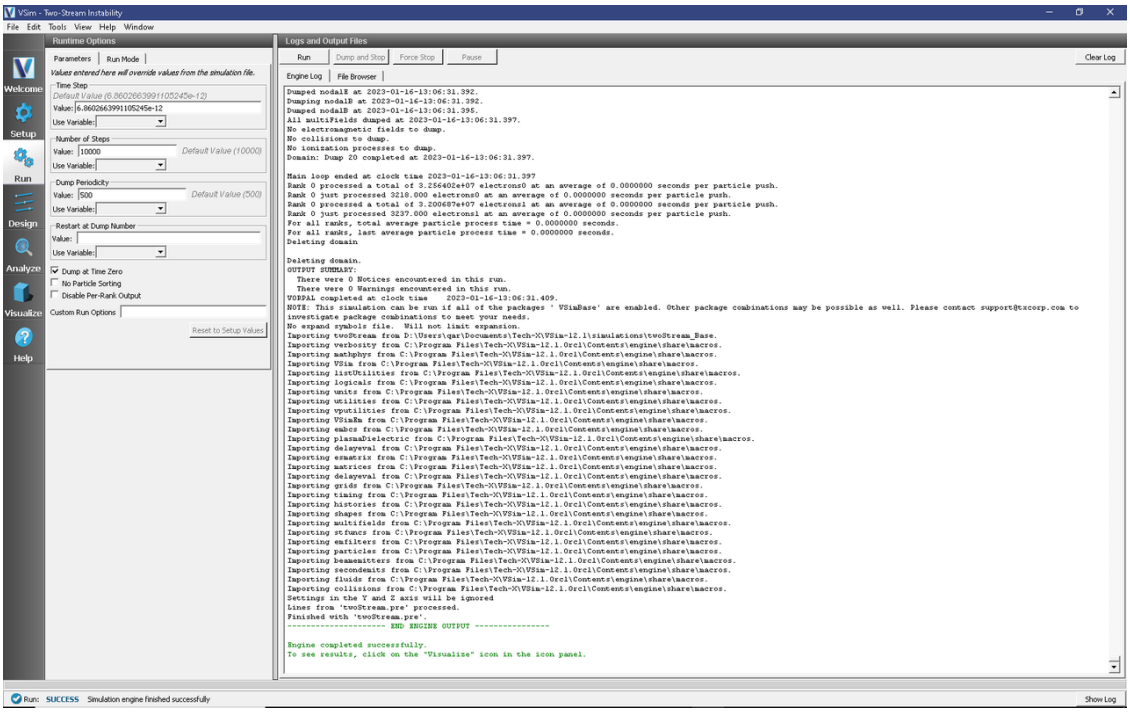


Fig. 2.29: The Run Window at the end of execution.

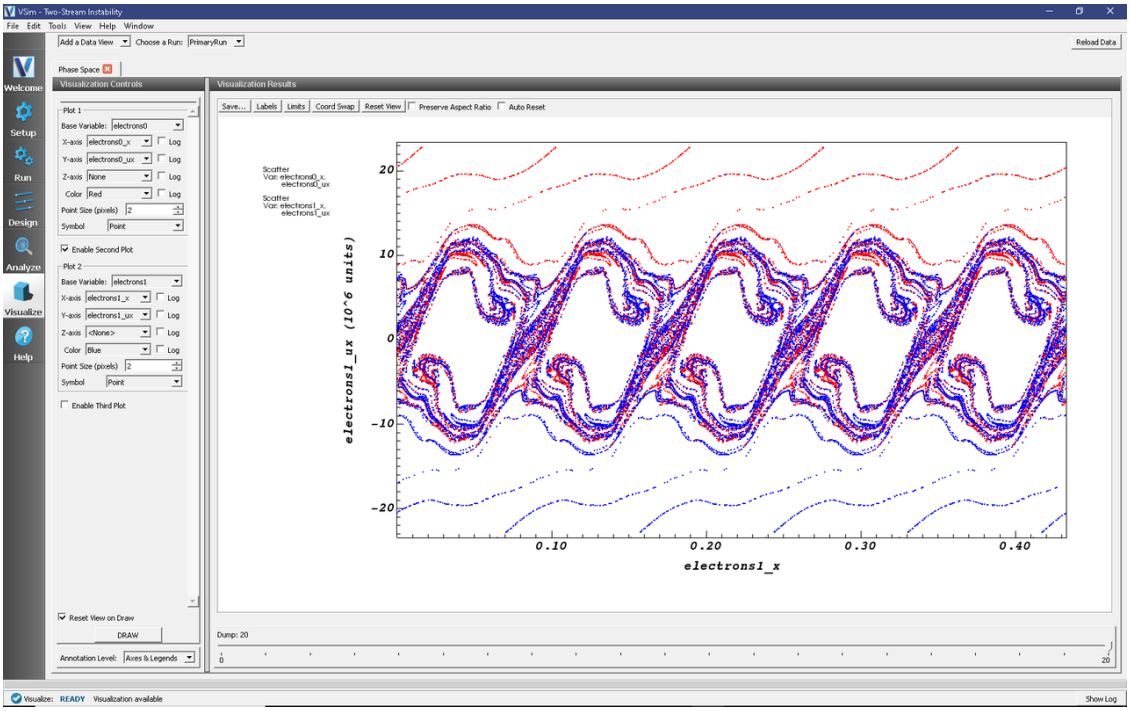


Fig. 2.30: Visualization of the two-stream instability developing in particle phase space.

Further Experiments

Change the average velocity and velocity modulation and see how the speed at which the instability sets in depends on the modulation.

View the particle density by using the *computePtclNumDensity* script in the Analyze Window.

2.2 Basic Examples (text-based setup)

2.2.1 Magnetic Fields of Wire (bFieldByJT.pre)

Keywords:

`Calculating A vector by a current-carrying long linear wire.`

Problem description

This simulation illustrates how to model magnetostatics. A straight current, J_o, is directed along the z-axis. The example solves Poisson's equation for the vector potential, A. The 0th dump of the simulation is the analytical solution for the purpose of comparison.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The magnetic field by a current example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Basic Physics* option.
- Expand the *Basic Examples (text-based setup)* option.
- Select "Magnetic Fields of Wire (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 2.31.

Input File Features

VSimComposer allows the user to vary the applied current and a radius of the wire. These are the main parameters that affect the A vector. By changing these parameters, a user can run simulations to explore how the A vector depends on the applied current and radius. The input file, when viewed in the editor, also exposes all the grid sizes of the simulation that are used by the implemented models.

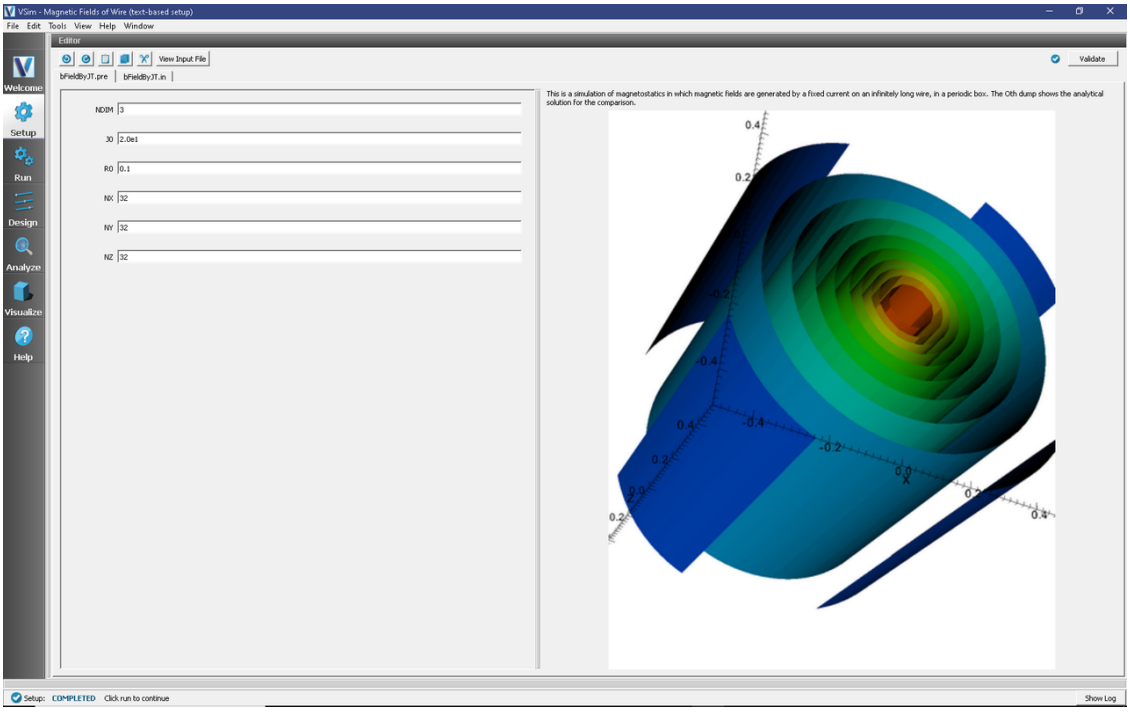


Fig. 2.31: Setup Window for the magnetic field by a current.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 2.32.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

For this example, one can see the A vector fields. To see the A vector, continue as follows:

- Make sure the *Data View* drop down is set to *Data Overview*.
- Here you can see *Variables*. Expand the *Scalar Data*. Then expand *A*
- Four variables are available, the three components of *A* and the magnitude of the vector. Select A_magnitude.

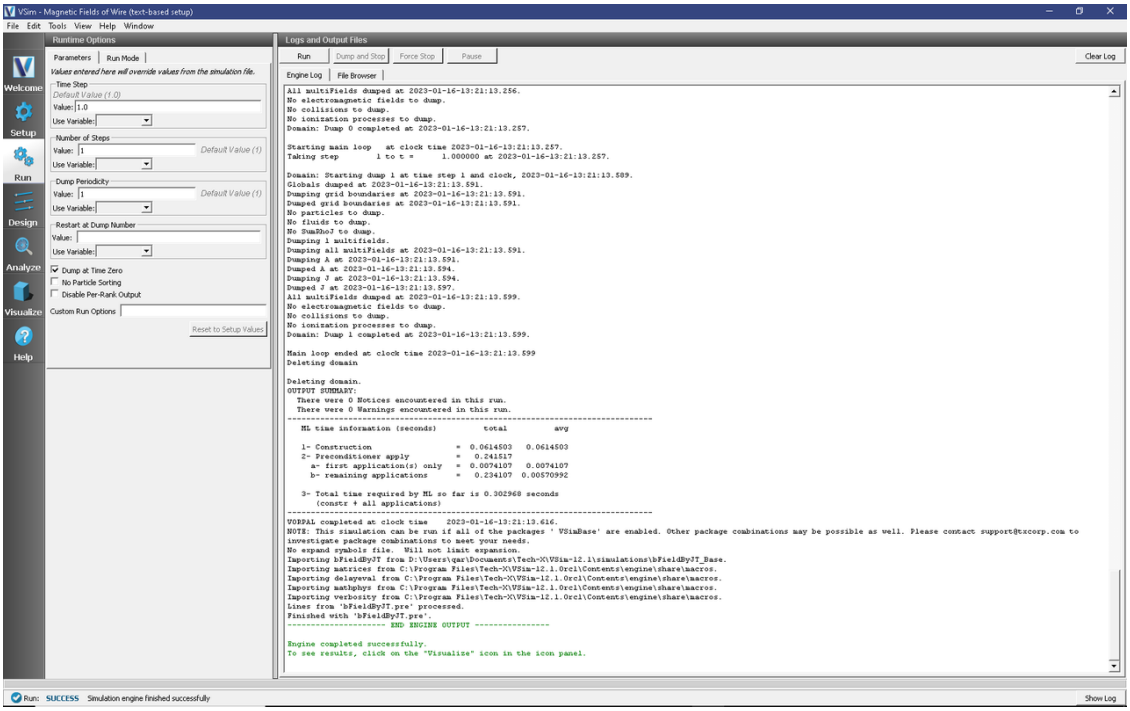


Fig. 2.32: The Run Window at the end of execution.

- Check the box next to *Display Contours*
- Rotate the view by clicking and dragging your mouse.

Fig. 2.33 shows the visualization seen for A_magnitude.

Further Experiments

This input file can be modified to test different current, and wire radius. This will allow users to study how to use the magnetostatics capability in Vorpal.

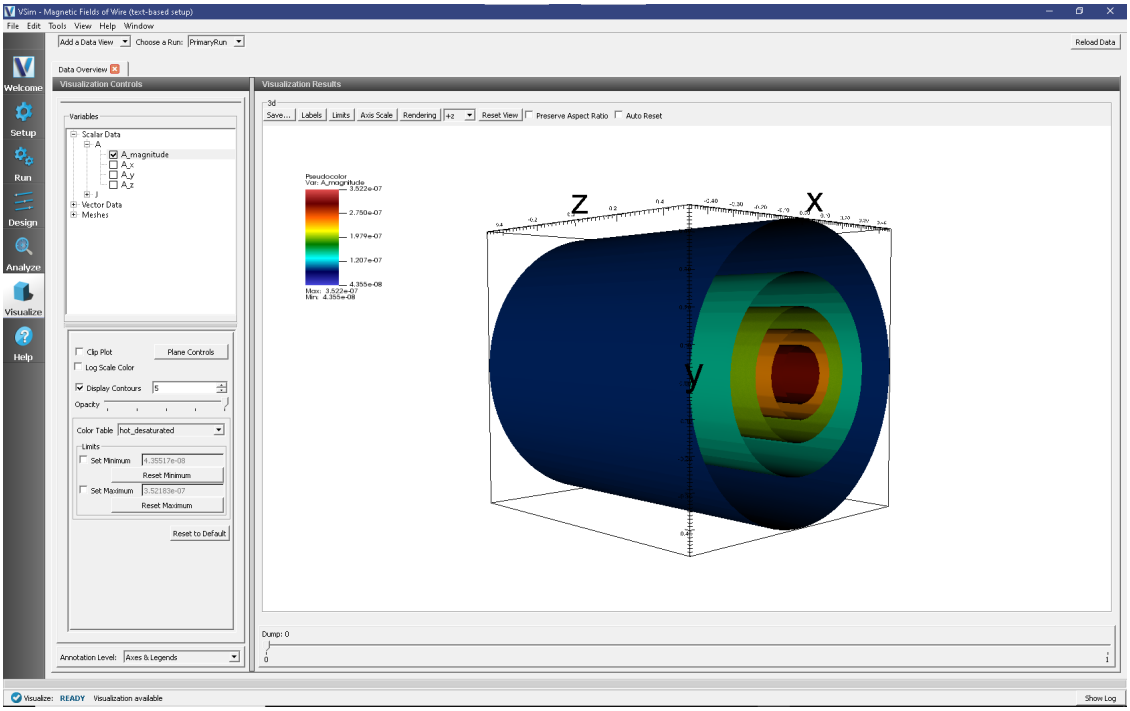


Fig. 2.33: Visualization of magnetic fields by the current as a color contour plot.

CHAPTER

THREE

VSIM FOR ELECTROMAGNETICS EXAMPLES

These examples illustrate how to solve complex problems in electromagnetics.

These examples can be run with a VSimEM license.

3.1 Antennas

3.1.1 2.4 GHz Yagi Uda Antenna (YagiUda2p4.sdf)

Keywords:

`yagiUdaArrayWireModel, yagiT, far field, radiation`

Problem description

A Yagi-Uda array is a directional antenna consisting of several parallel dipole elements. Only one of these dipole elements is driven, the other elements being parasitic . Directionality is achieved by requiring that there be one longer element adjacent to the source element, which is referred to as the reflector. The rest of the elements being adjacent to the source but opposite to the reflector, and shorter than the source element, are referred to as directors. Yagi antennas are ubiquitous, and as such optimal parameters for dipole lengths and separations have been established. We go with values one would typically find in any text covering the matter. This example illustrates how to obtain the far field radiation pattern of a Yagi-Uda array.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Yagi-Uda example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select *2.4 GHz Yagi Uda Antenna* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.1. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grids element and select or deselect the box next to `Grid`.

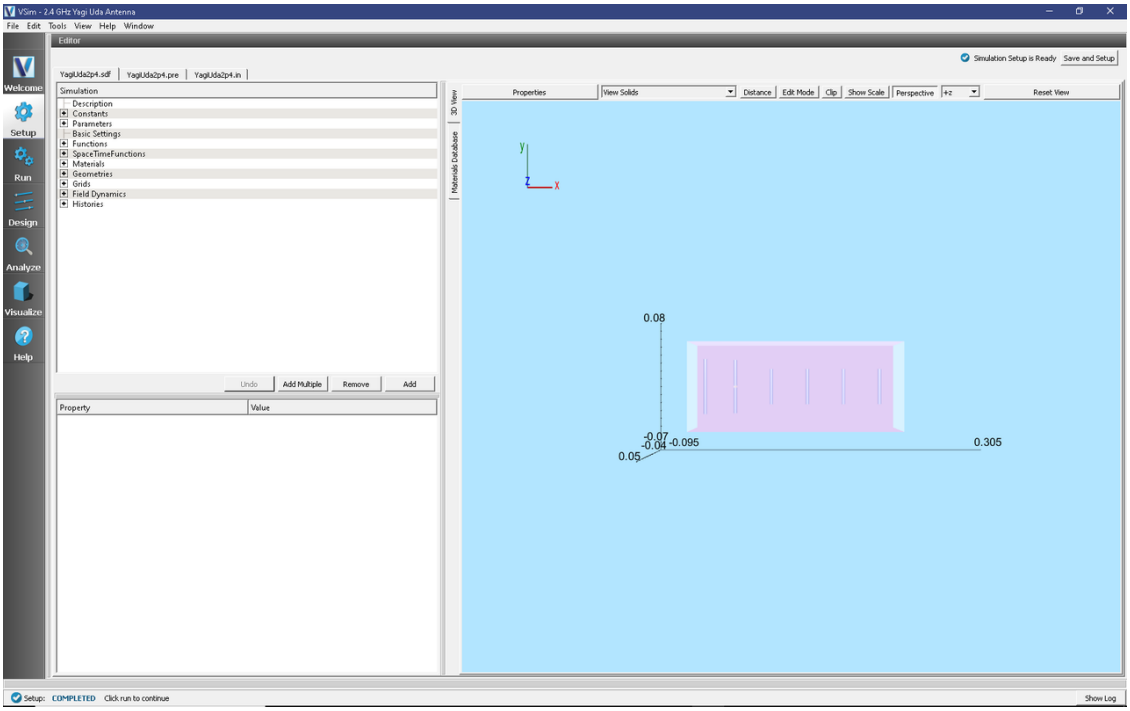


Fig. 3.1: Setup Window for the Yagi-Uda example.

Simulation Properties

This file allows the modification of the antenna operating frequency, antenna dimensions, and simulation domain size.

By adjusting the dimensions any sized Yagi-Uda array can be simulated.

Note: To obtain good far field resolution generally four or more antenna elements is desirable (One source, one reflector, two or more directors).

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.655996046470038e-13
  - *Number of Steps*: 6000
  - *Dump Periodicity*: 200
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.2.

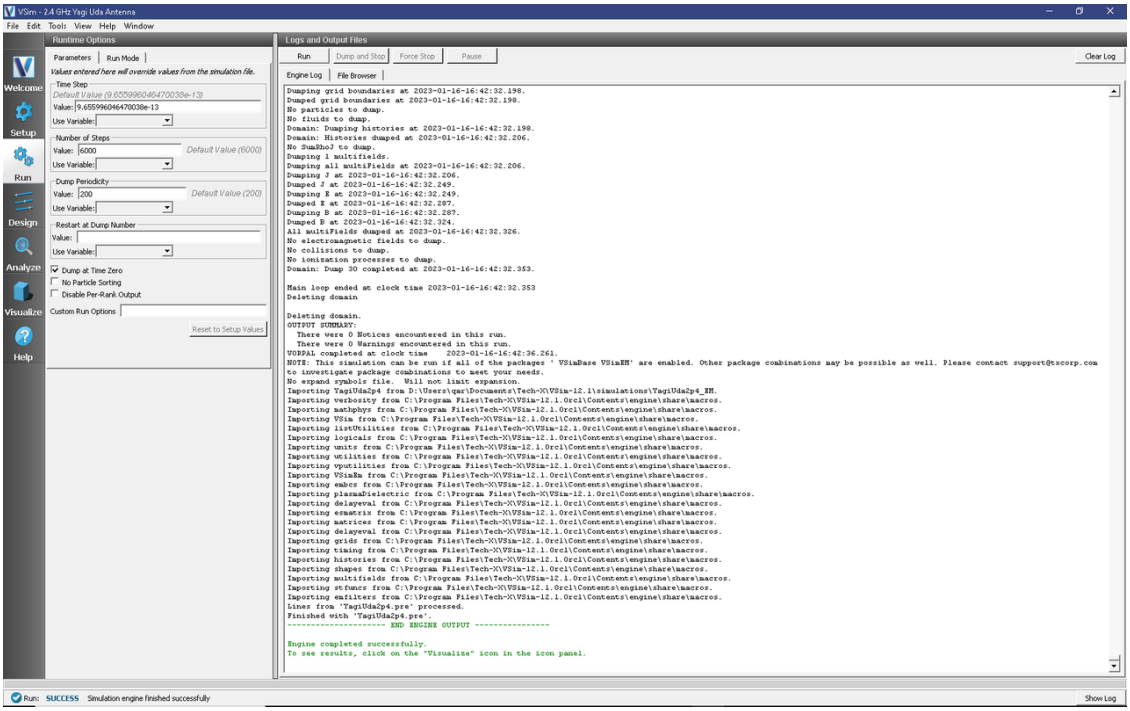


Fig. 3.2: The Run Window at the end of execution.

Analyzing the Results

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- Select computeFarFieldFromKirchhoffBox.py from the list and select “Open” (Fig. 3.3)
- Input values for the analyzer parameters. The analyzer may be run multiple times, allowing the user to experiment with different values.
  - simulationName - yagiUda2p4
  - fieldLabel - E
  - farFieldRadius - 1024.0
  - numPeriods - 0.25
  - numFarFieldTimes - 2
  - frequency - 2.4e9
  - numTheta - 45
  - numPhi - 60
  - zeroThetaDirection - (0,1,0)
  - zeroPhiDirection - (0,0,1)
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 1024.0
  - principalPlanesOnly - checked

- Click “Analyze”
- Depending on the values of numTheta, numPhi, and numFarFieldTimes, the script may need to run for several minutes.

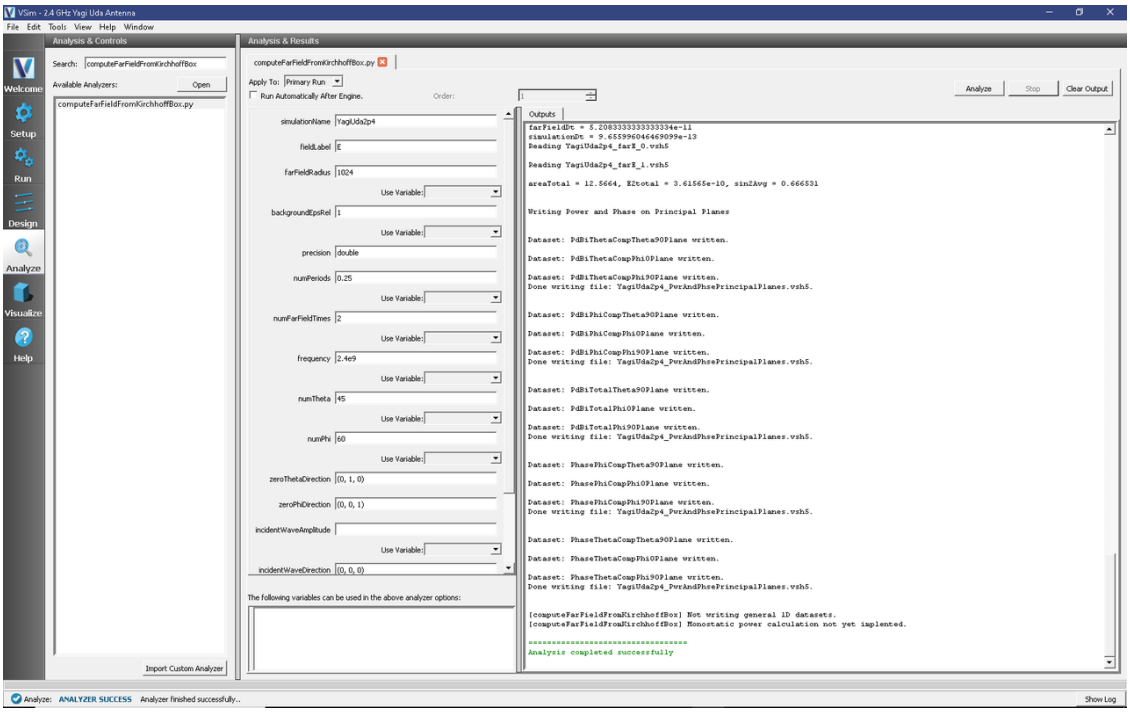


Fig. 3.3: The Analysis Window.

Visualizing the results

Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the near field pattern, do the following:

- Expand *Scalar Data*
- Expand *E*
- Select *E_x*
- Check the *Set Minimum* box and set the value to -0.1
- Check the *Set Maximum* box and set the value to 0.1
- Check the *Clip Plot* box
- Expand *Geometries*
- Select *poly (YagiUda2p4PecShapes)*
- Move the dump slider forward in time

The far field radiation pattern can be found in the scalar data variables of the data overview tab underneath the farE field. Uncheck the E_x dataset and check the farE_magnitude box under *farE*.

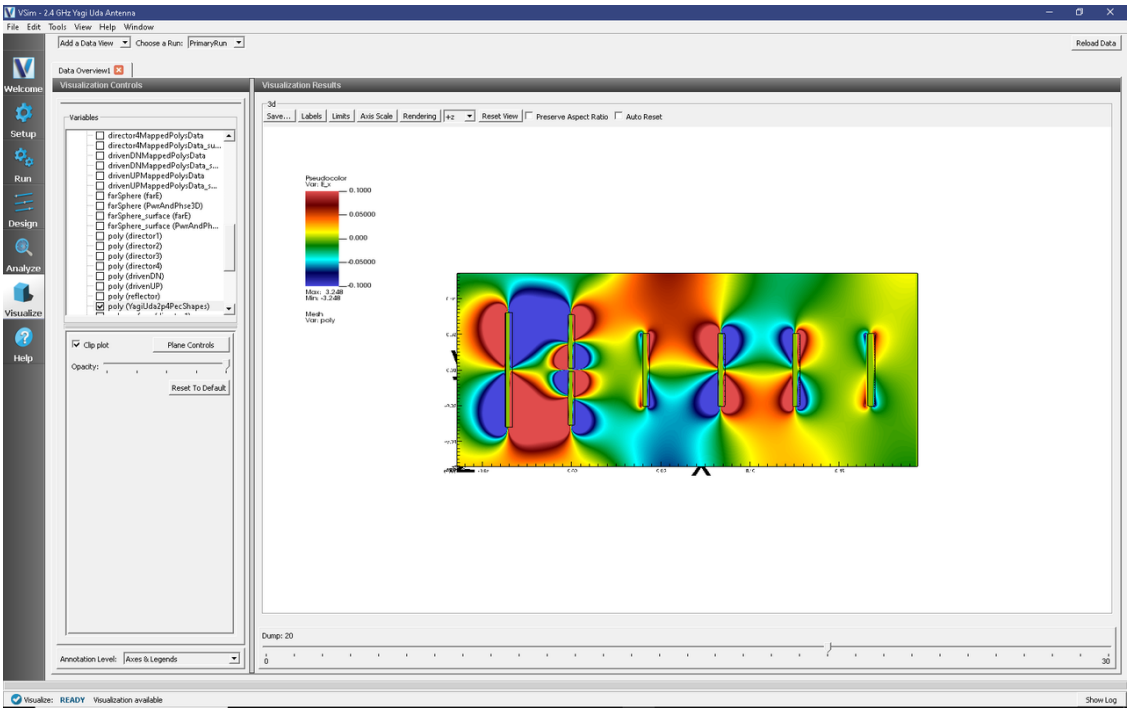


Fig. 3.4: The electric field near-field pattern.

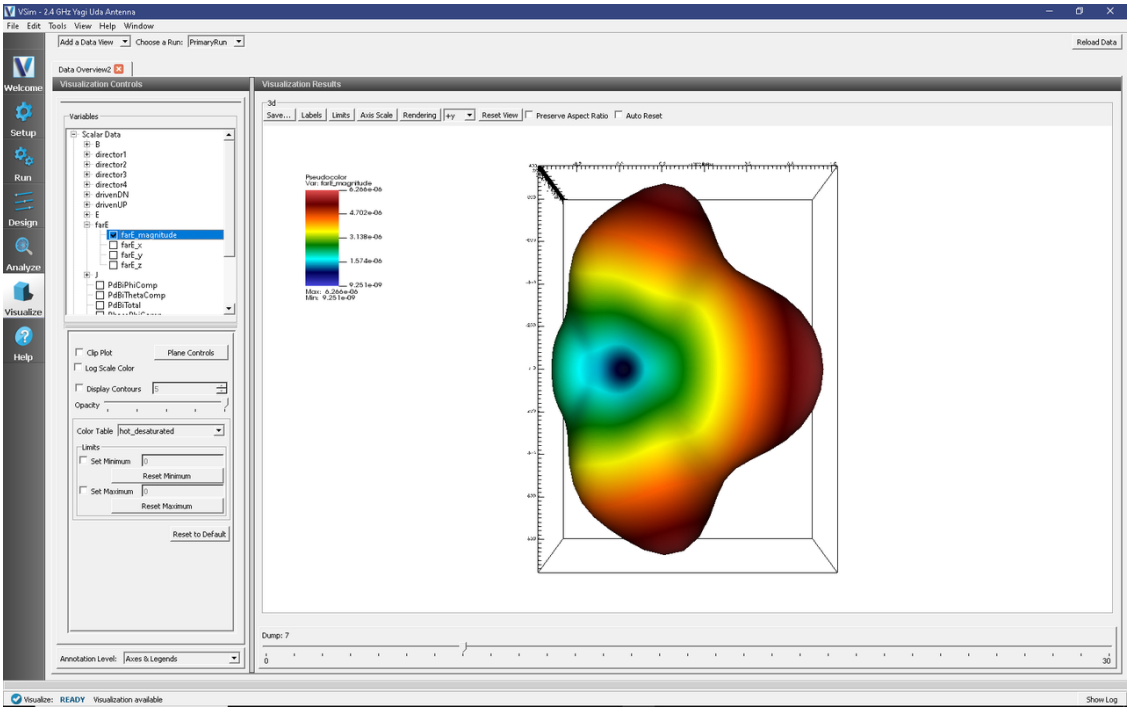


Fig. 3.5: The electric field manifestation of the far field pattern.

Further Experiments

Try adding more directors and changing their dimensions to see the effect on the far field pattern.

3.1.2 Antenna Array 2D (antennaArray2D.sdf)

Keywords:

`antennaArray2D, far field, radiation, s-parameters`

Problem Description

This set of 2-D VSimEM simulations shows how to obtain the far fields, S11 parameter, gain, and phase shift of a one-element antenna as well as the far fields, gain, S parameters, and phase shift of a multiple-element antenna array with one excited element. These simulations can be used as a basis for measuring coupling in phased array antennas. The analyzer compute2DantennaGainAndPhase.py is set up to calculate the S parameter for the excited element and any other reference element defined by the constant *S_PARAM_ELEM*.

Opening the Simulation

The Antenna Array 2D example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select *Antenna Array 2D* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 3.6.

Simulation Properties

The antennas are waveguide apertures excited with a frequency of 1 GHz and the aperture width is 0.1λ (see the parameter GAP in the element tree). The distance between the gaps is 0.4λ.

A different array of geometries can be created using input parameters such as number of elements in the array (N_ELEM) and the distance between the elements in each direction. To recreate a different antenna array, expand *Geometries*, expand CSG, right-click on *gap* → Create Array. In the *Array Description* window, select the "Union elements" checkbox, type in the number of elements to the value under N_ELEM, and the distance between elements to the value under DIST_ELEM. Then select the CSG "metal", hold down Ctrl and select *gapElemUnion* located at the end of the gap array elements → Boolean Operation → select *metal_gapElemUnion*. Rename accordingly and assign the material PEC to the newly created geometry.

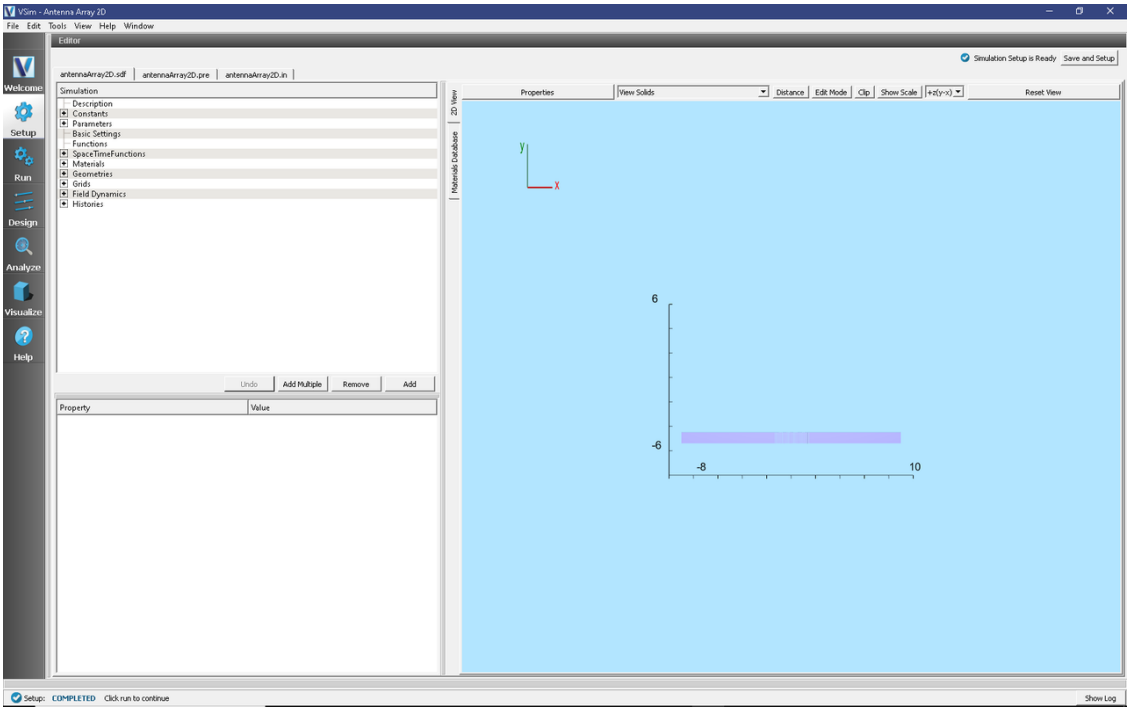


Fig. 3.6: Setup Window for the Antenna Array 2D example.

Running the Simulation

Once finished with the setup, continue as follows:

- Proceed to the Run Window by pressing the *Run* button in the navigation column out left.
- To run the file, click on the *Run* button in the upper left corner of the *Logs and Output Files* pane. You will see the output of the run in that pane. The run has completed successfully when you see the output, "Engine completed successfully."
- First run settings (default):
  - *Number of Steps*: 6000
  - *Dump Periodicity*: 3000
  - *Dump at Time Zero*: box checked

After the first run completes, proceed as follows:

- Second run settings:
  - *Number of Steps*: 1800
  - *Dump Periodicity*: 45 (Value taken from the parameter DUMP_PER_SECOND_RUN)
  - Set *Restart at Dump Number* to 2

Note: If the grid properties change, these values will have to be adjusted.

The end of the second run is shown in Fig. 3.7.

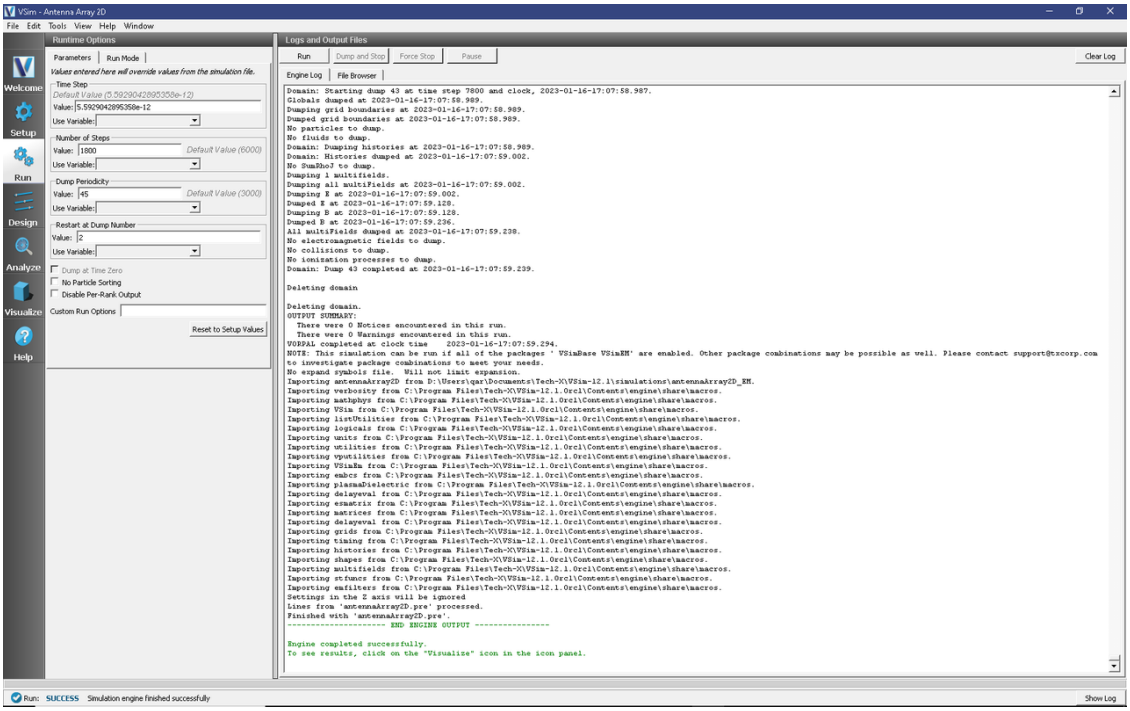


Fig. 3.7: The Run Window at the end of the second run execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column
- Expand *Scalar Data* in the *Visualization Controls* pane
- Expand *E*
- Select *E_x*
- Check the box for *Set Minimum* and set it to -100
- Check the box for *Set Maximum* and set it to 100
- Select the dump slider and move it to higher dump numbers to see the evolution of the electric field in time.

The resulting visualization is shown in Fig. 3.8.

Figure Fig. 3.8 shows the near and far electric fields at the end of the simulation run. The dispersion of the electric field through the non-excited waveguides can also be seen.

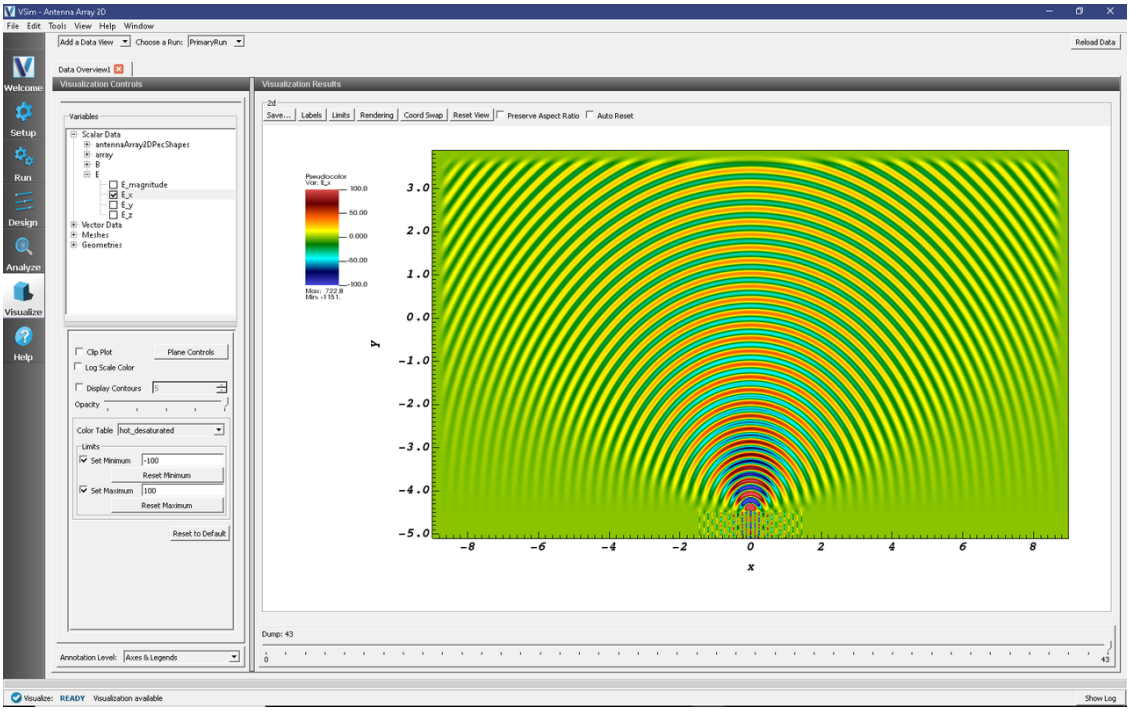


Fig. 3.8: The near and far electric fields in the x-direction at the end of the simulation.

Single Element Antenna

- Expand Constants
- Change constants N_ELEM to 1
- Change N_EXCITED_ELEM to 1
- Expand Geometries
- Expand CSG
- Deactivate *array*
- Deactivate *gapArray*
- Select *metal*, hold Ctrl, select *gap*, right click → *Boolean Operation* → select *metal - gap*
- Select *metalMinusgap*
- For *material* select *PEC* from the drop-down menu

You can now assign any name of your choice to the *metalMinusgap* geometry (e.g., aperture). Save and proceed to the Run tab. Follow the same run steps as described above in the section *Running the Simulation*.

Second viz is shown in Fig. 3.9.

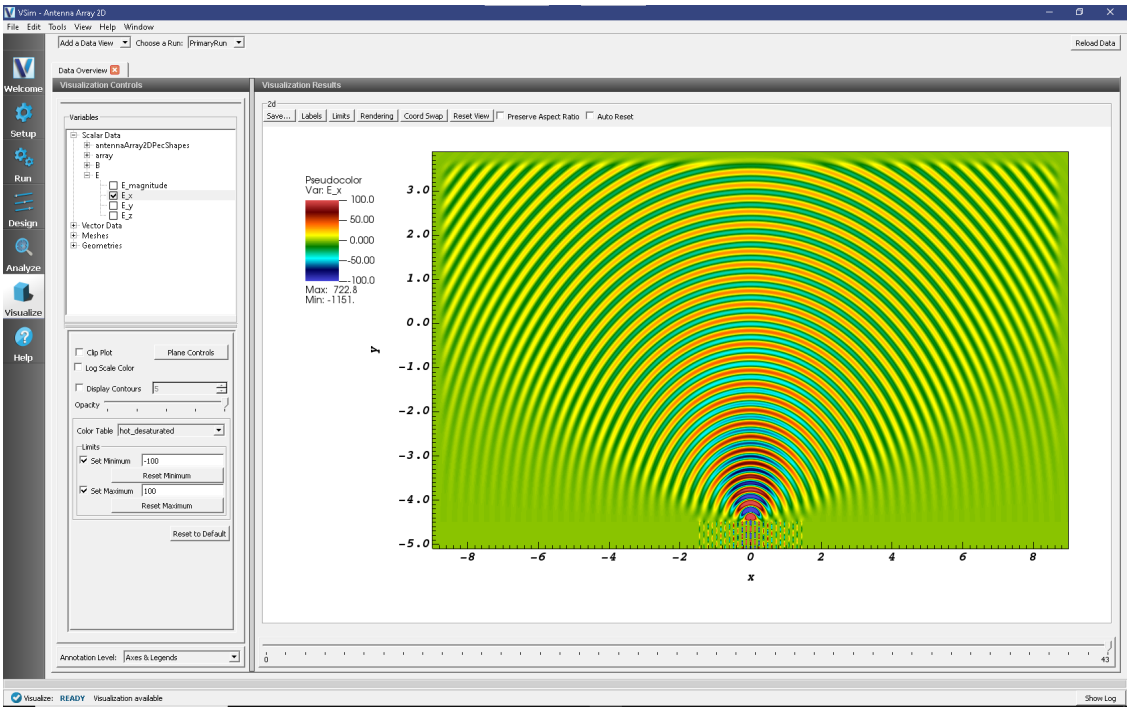


Fig. 3.9: The near and far electric fields in the x-direction for a 1-element antenna.

Calibration Runs

For both the multiple-element and single-element antenna simulations, calibration runs are needed for the analyzer.

For the original multiple-element array setup, proceed as follows:

- Proceed to the Setup Window
- In the top left corner, select *File* → *Save Simulation As* . . .
- Rename the simulation to *antennaArray2DCalibration.sdf*

Note: If your simulation has a different name, add the word *Calibration* before *.sdf*

- Click *Save*
- Expand *Geometries*
- Expand *CSG*
- Deactivate *array*
- Deactivate *gapArray*
- Select *gap*
- Change the height to HEIGHT_METAL_CALIB
- Change the x position setting to XBGN_EXCITED_GAP
- Select *metal*
- Change the height to HEIGHT_METAL_CALIB

- Click on *metal*, hold down Ctrl button and select *gap* right click → Boolean Operation
- Select metal_gap
- Select metalMinusgap
- Select *PEC* under *material* from the drop-down menu.

You can now assign any name of your choice to the metalMinusgap geometry (e.g., myWaveguide).

- Expand *Field Dynamics*
- Expand *FieldBoundaryConditions*
- Remove *malUpperY*
- Right-click *FieldBoundaryConditions* → Add FIeldBoundaryCondition → select *Port*
- Select *upper y* for the boundary surface from the drop-down menu
- Save and proceed to the Run tab.
- Change *Number of Steps* to 7800

Note: The calibration number of steps must equal the total number of steps that the simulation ran for during the regular run.

Repeat the same steps for the single-element antenna simulation setup.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- Open the *compute2DantennaGainAndPhase.py* analyzer by selecting it and selecting "open".
- The default analyzer fields are the following:
  - *simulationName*: antennaArray2D
  - *dumpNr*: 30
  - *nlambda*: 15.0
  - *gapWidth*: 0.03
  - *center*: 0.0,-4.4969
  - *dt*: 5.59290428954e-12
  - *freq*: 1000000000.0
- The *overwrite* box should be checked
- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 3.10.

The S-parameters for the excited element as well as the reference element associated with the constant S_PARAM_ELEM in the simulation setup are shown at the end of the analyzer run.

This analyzer creates a text file with 5 columns. The first column is the theta direction in degrees, the second column is the analytical gain of the ISOLATED excited element in dB, the third column is the gain measured by VSim in dB, the

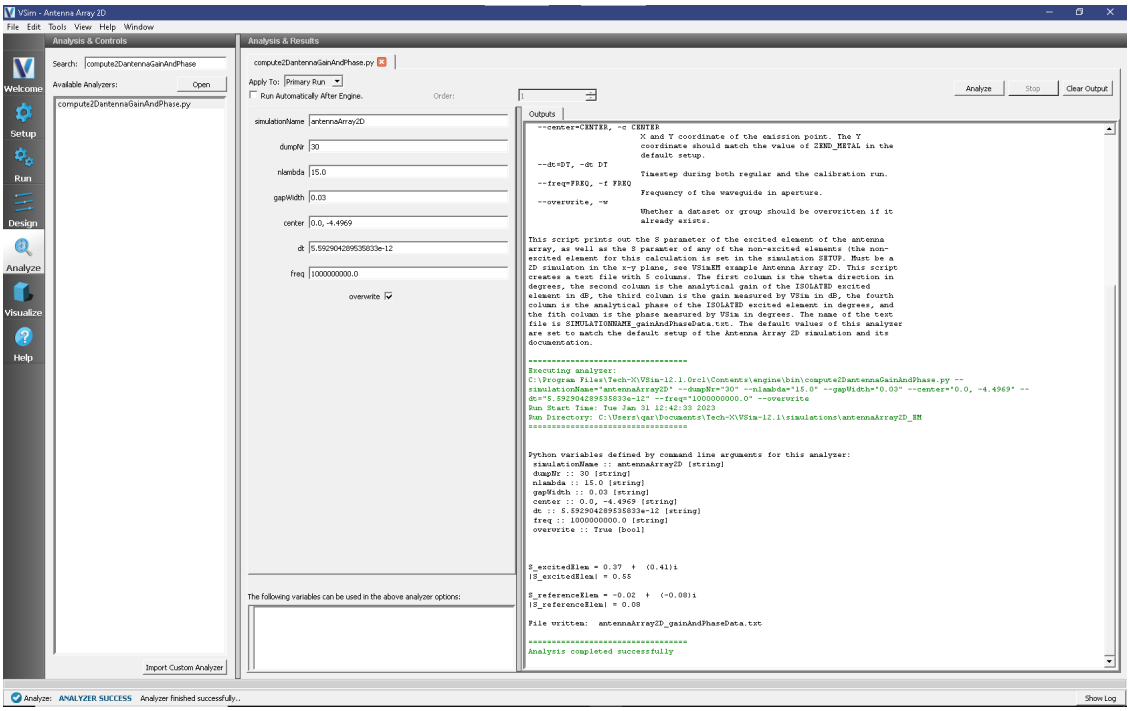


Fig. 3.10: The S-parameters for the excited element as well as the reference element associated with the constant S_PARAM_ELEM in the simulation setup are shown at the end of the analyzer run.

fourth column is the analytical phase of the ISOLATED excited element in degrees, and the fith column is the phase measured by VSim in degrees. The name of the text file is SIMULATIONNAME_gainAndPhaseData.txt.

For the default simulation settings (i.e., the center element of a 25-element array is excited while the other elements are turned off), plotting the second and third columns (analytical and measured gains) against the first column (as a function of theta) will give the results shown in Fig. 3.11.

Plotting the fourth and third columns (analytical and measured field phases) against the first column (as a function of theta) will give the results shown in Fig. 3.12.

Further Experiments

A different array of geometries can be created changing input parameters such as number of elements in the array (N_ELEM) and the distance between the elements in each direction (DIST_ELEM). After changing these *Constants*, to create a different antenna array, proceed as follows:

- Expand *Geometries*
- Expand CSG
- Right-click on *gap* → Create Array

In the *Array Description* window, select the "Union elements" checkbox, type in the number of elements to the value under N_ELEM, and the distance between elements to the value under DIST_ELEM. Then select the CSG "metal", hold down Ctrl and select *gapElemUnion* located at the end of the gap array elements → Boolean Operation → select *metal_gapElemUnion*. Rename accordingly and assign the material PEC to the newly created geometry.

Repeating the analysis steps for a 1-element antenna (N_ELEM = 1 in the simulation setup) will give the results shown in Fig. 3.13 and Fig. 3.14.

A different element can be excited by changing input parameter N_EXCITED_ELEM.

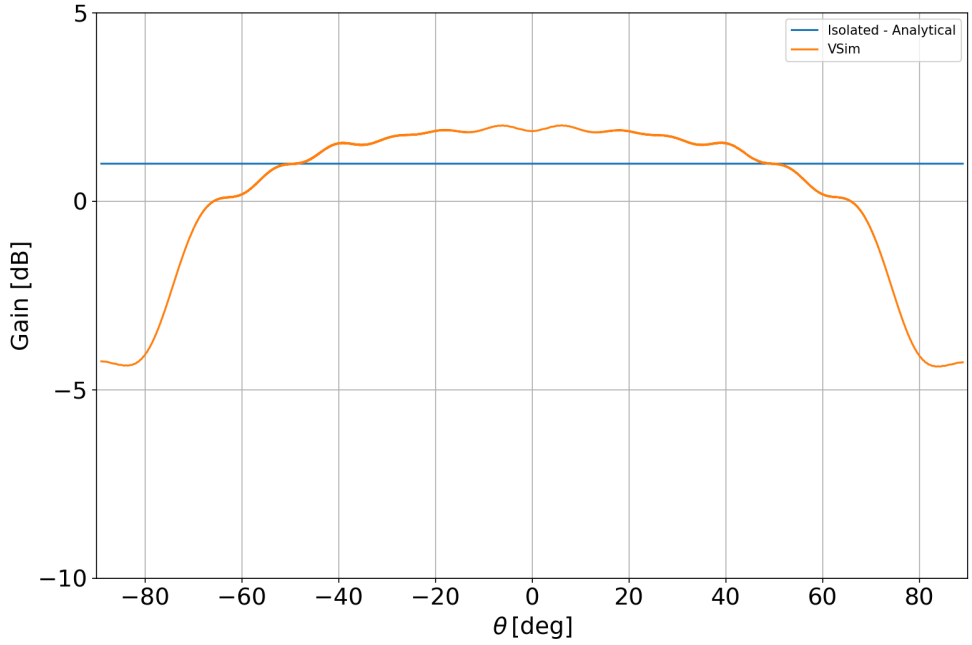


Fig. 3.11: The gain pattern of a 25-element array with the center excited element.

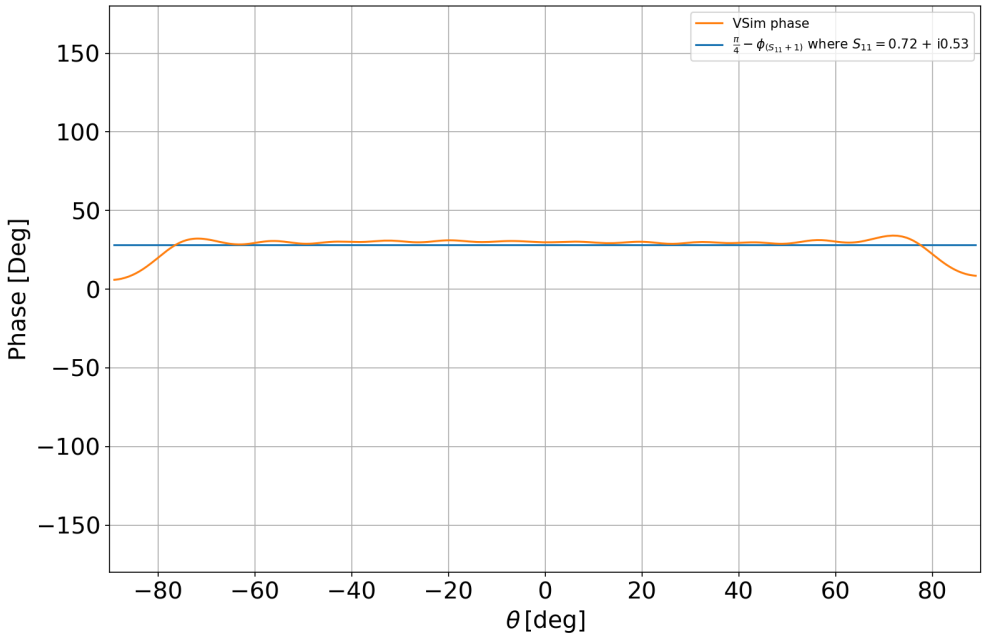


Fig. 3.12: The phase pattern of a 25-element array with the center excited element.

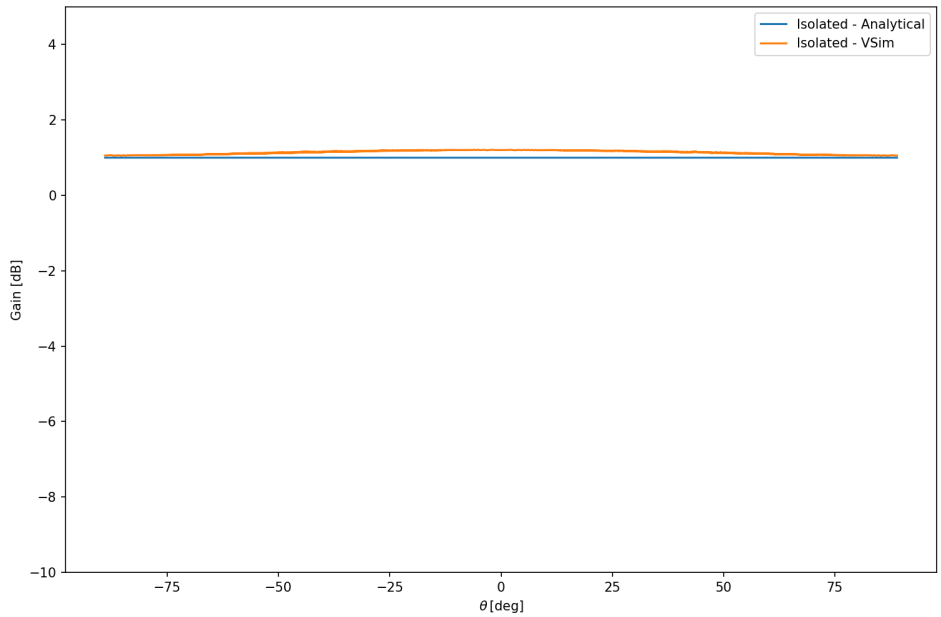


Fig. 3.13: The gain pattern of a 1-element array.

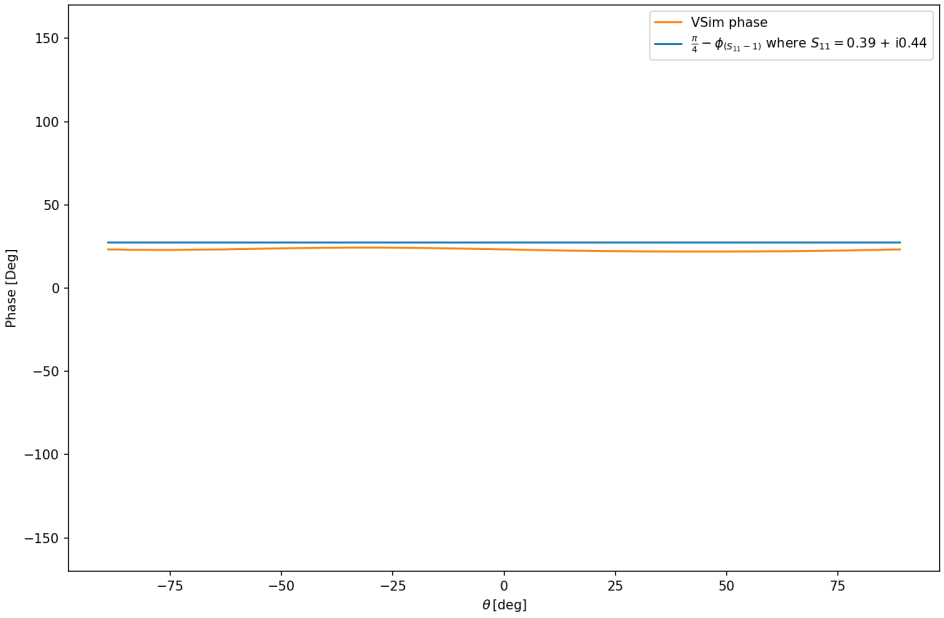


Fig. 3.14: The phase pattern of a 1-element array.

Repeating the analysis steps for a 25-element antenna with the edge element excited (N_EXCITED_ELEM = 25 in the simulation setup) will give the results shown in Fig. 3.15 and Fig. 3.16.

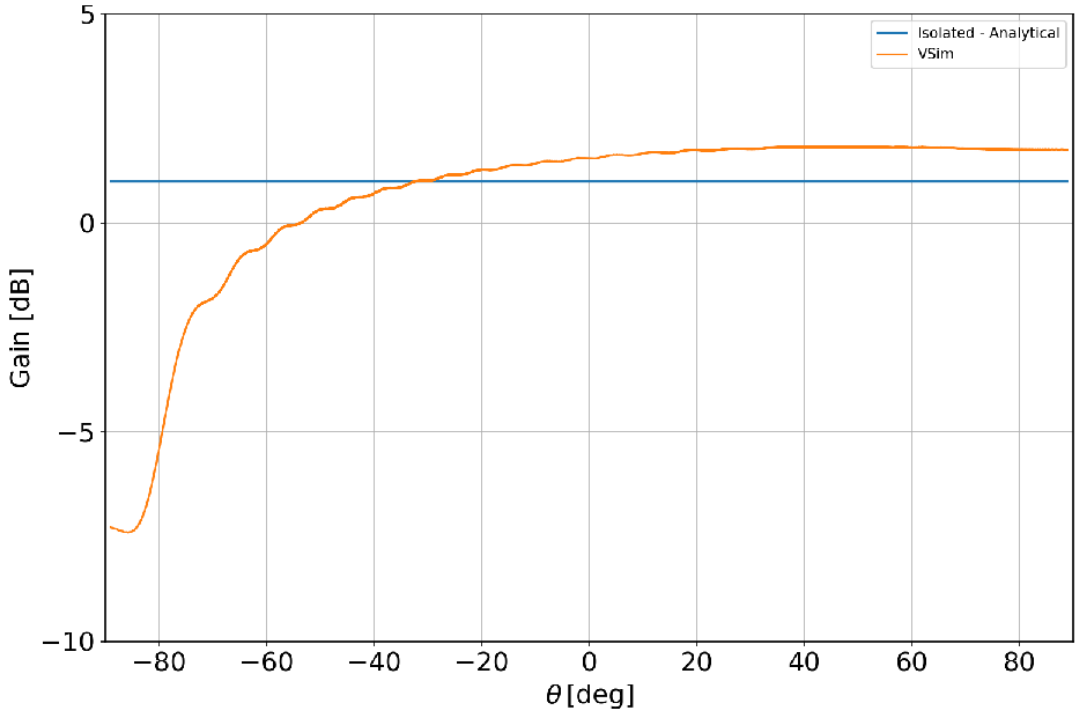


Fig. 3.15: The gain pattern of a 25-element array with the edge excited element.

3.1.3 Antenna on Human Hand with Dielectric (antennaOnHand.sdf)

Keywords:

antennaOnHand, far field, radiation

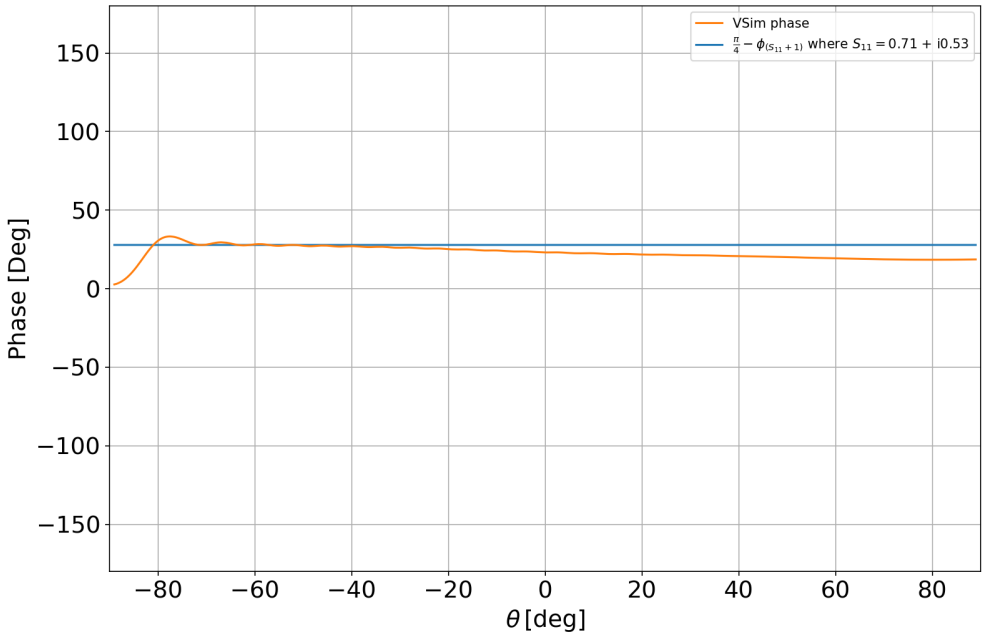


Fig. 3.16: The phase pattern of a 25-element array with the edge excited element.

Problem Description

This problem calculates the far-field radiation pattern of a small wifi antenna. The fields interact with the human hand for which the bone structure was approximated by long thin cylinders. The antenna frequency can be either 2.4 or 5 GHz, the two most common wifi bands.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Antenna on Human Hand with Dielectric example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Antenna on Human Hand with Dielectric" and press the *Choose* button.
- In the resulting dialog, create a new folder if desired, and press the *Save* button to create a copy of this example.

The **Setup** window is now shown with all the implemented physics and geometries. See Fig. 3.17.

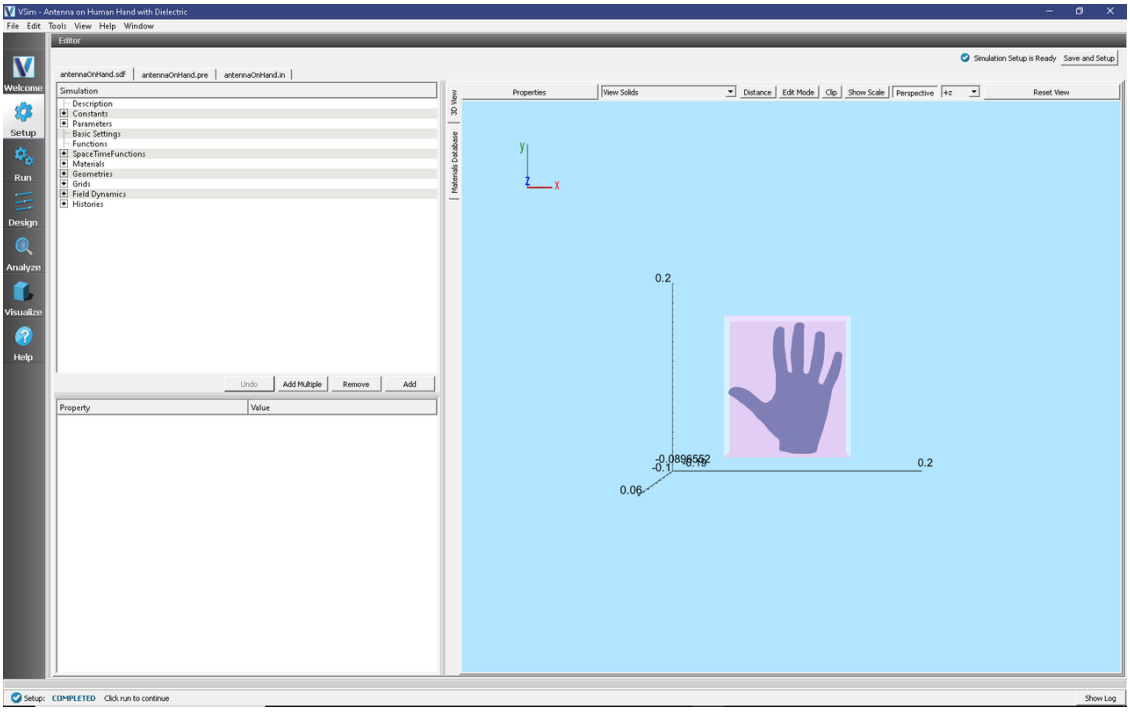


Fig. 3.17: Setup Window for the Antenna on Human Hand with Dielectric example, with Grid and farFieldBox History hidden.

Simulation Properties

This file allows the modification of antenna operating frequency, dimensions, orientation, and simulation domain size.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.659083082938264e-12
  - *Number of Steps*: 3000
  - *Dump Periodicity*: 300
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.18.

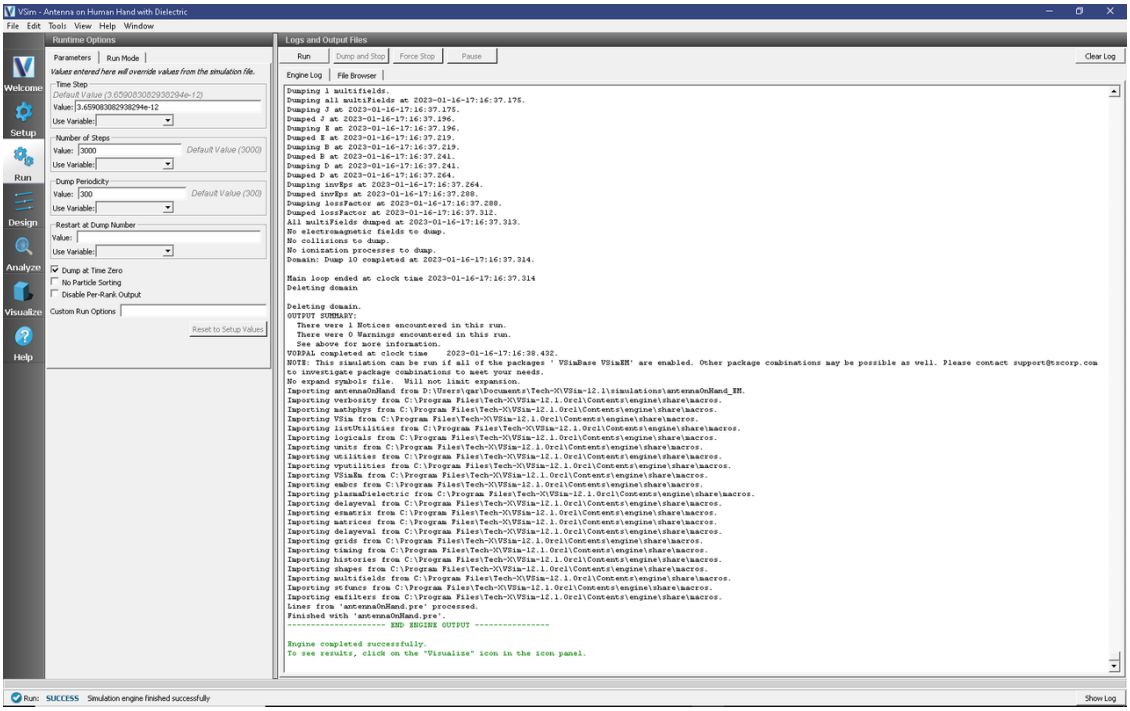


Fig. 3.18: The Run Window at the end of execution.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- Select computeFarFieldFromKirchhoffBox.py from the list and select “Open” (Fig. 3.19)
- Input values for the analyzer parameters. The analyzer may be run multiple times, allowing the user to experiment with different values.
  - simulationName - antennaOnHand
  - fieldLabel - E
  - farFieldRadius - 1024.0
  - numPeriods - 0.25
  - numFarFieldTimes - 2
  - frequency - 5.0e9
  - numTheta - 45
  - numPhi - 60
  - zeroThetaDirection - (1,0,0)
  - zeroPhiDirection - (0,0,1)
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 0.05

  - principalPlanesOnly - checked

- Click “Analyze”
- Depending on the values of numTheta, numPhi, and numFarFieldTimes, the script may need to run for several minutes or longer.

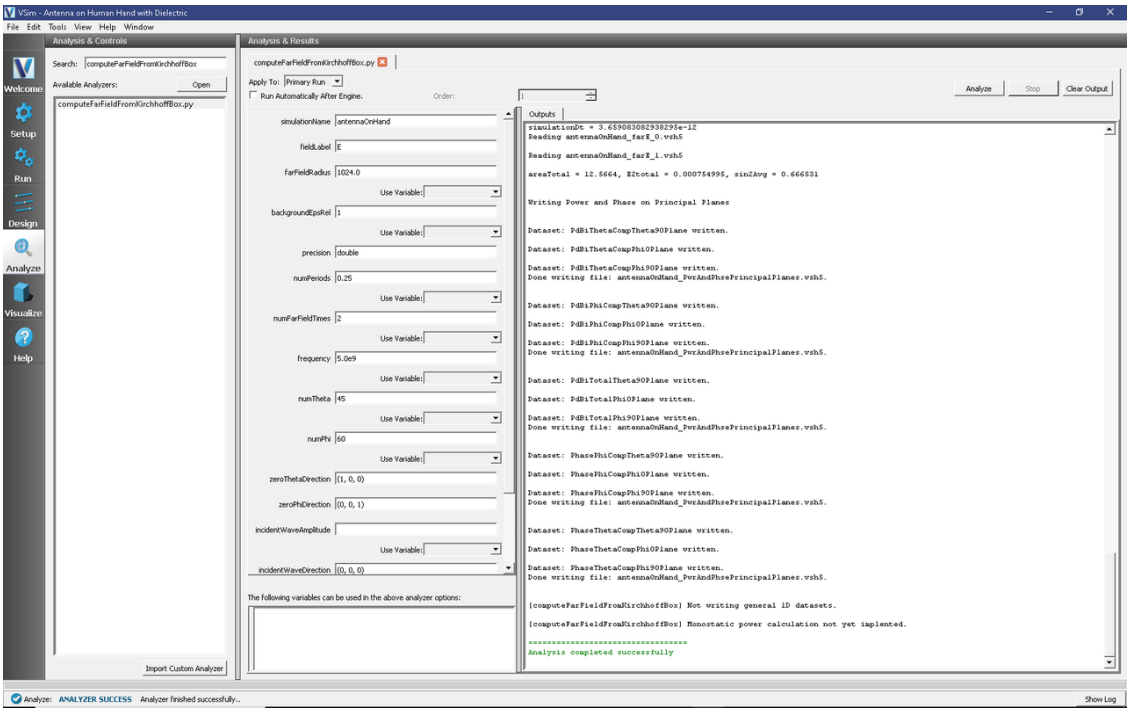


Fig. 3.19: The **Analyze** panel after running computeFarFieldFromKirchhoffBox.py.

Visualizing the Results

Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The far field radiation pattern can be found in the *Scalar Data* variables of the *Data Overview* tab. Expand *farE* and check the *farE_Magnitude* box. The poly_surface (HandGeomSolid) under *Geometries*, can also be plotted. Fig. 3.20 shows the visualization at last far-field time.

Further Experiments

The skin can be included as an additional geometry by simply importing the hand geometry a second time within the same set-up, but with a very slightly higher scaling factor and setting the *Skin* material for the hand geometry with the higher scaling factor. Some “by eye” adjustments of the x-, y-, and z- translation values may be needed.

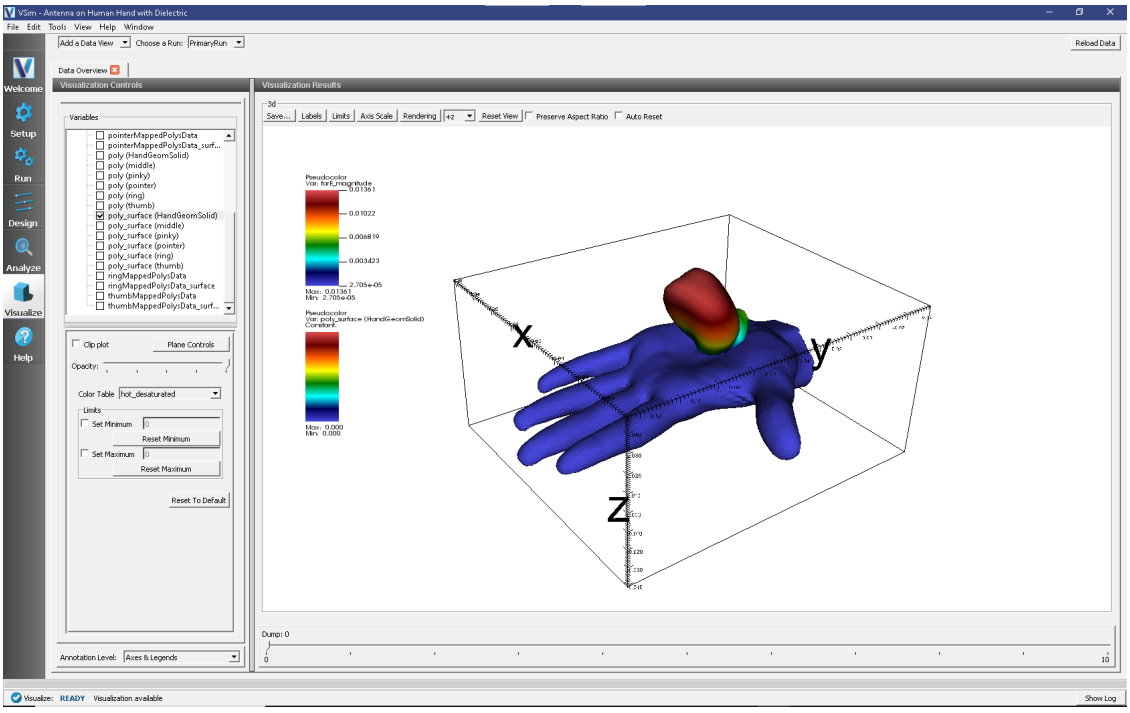


Fig. 3.20: The Far Field Radiation Pattern.

3.1.4 Loop Antenna from a Coaxial Cable (coaxialLoopAntenna.sdf)

Keywords:

coaxial, coaxial waveguide, coaxial cable

Problem description

This example illustrates how to use the coaxial cable Field Boundary Condition and Constructive Solid Geometry to create a coaxial loop antenna.

This simulation can be run with a VSimEM, VSimVE, VSimPD, or VSimPA license.

Opening the Simulation

The Coaxial Loop Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Loop Antenna From a Coaxial Cable" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is shown Fig. 3.21.

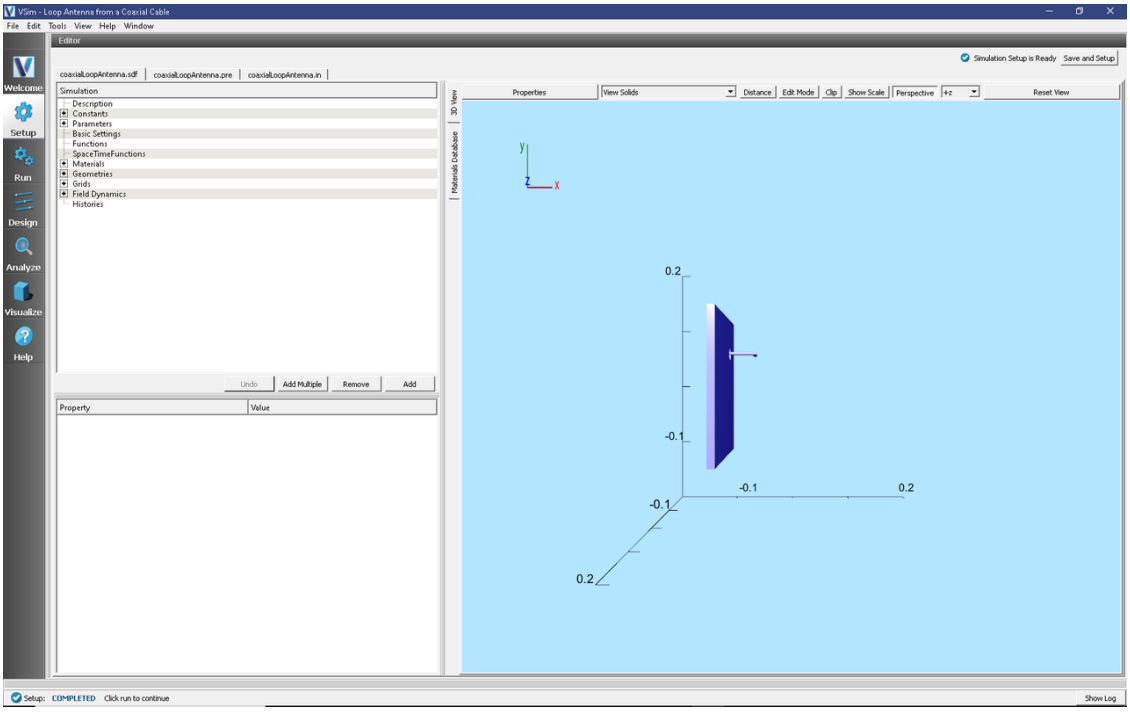


Fig. 3.21: Setup Window for the Coaxial Loop Antenna example.

Simulation Properties

This simulation makes use of the new coaxial waveguide Field Boundary Condition in VSim 8.1.

A coaxial waveguide is first constructed by creating a physical coaxial cable that enters the simulation domain. It is very important that this cable exists from at least 1 cell outside of the simulation boundary to 1 cell inside the simulation boundary. This is done by first creating a box primitive and setting it along the desired simulation boundary.

A cylinder corresponding to the outer diameter of the coaxial cable is then created, and subtracted from the plate.

A cylinder corresponding to the inner diameter of the coaxial cable is then created and extended into the simulation space.

It is then made into a loop antenna by adding a second, intersecting cylinder.

The wave itself is specified by a Field Boundary Condition.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.829541541469147e-12
  - *Number of Steps*: 400
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.22.

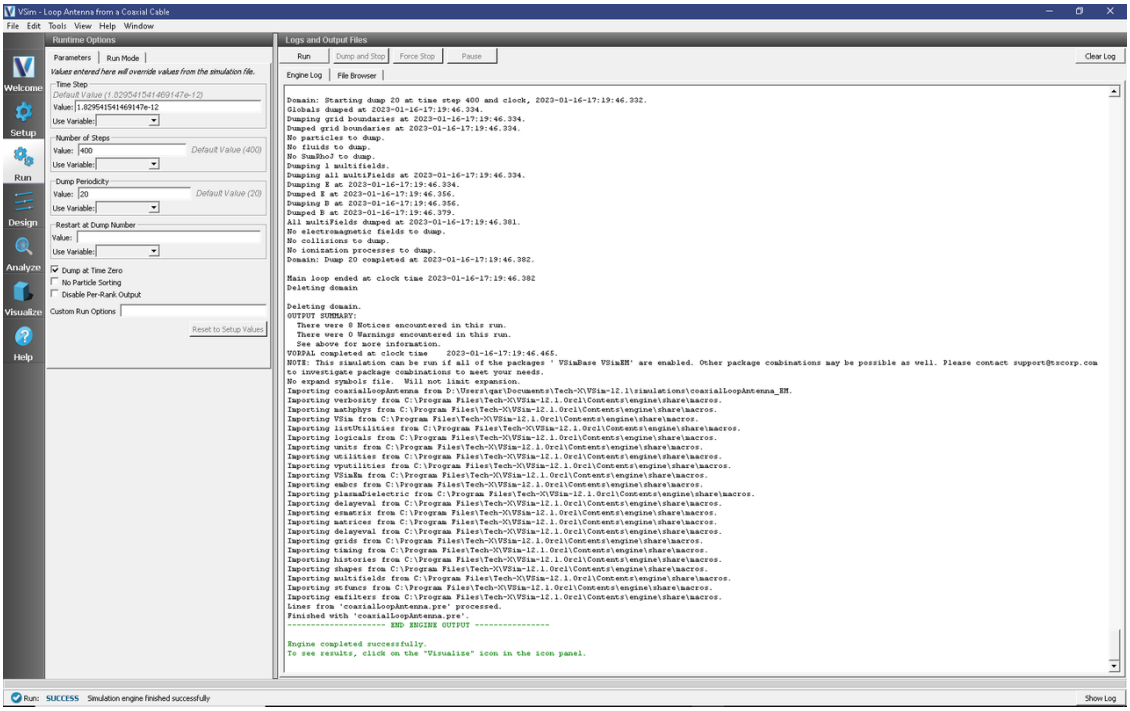


Fig. 3.22: The Run Window at the end of execution.

Visualizing the Results

After the run completes, the field may be visualized:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.
- Expand *Scalar Data*, expand *E*, and select *E_z*.
- To slice inside the field, select *Clip Plot* in the lower left hand corner, then click on *Plane Controls* and change the clip plane normal to Y instead of Z, and adjust the origin of the normal vector to Y = 0.05.
- To adjust the colors, check the *Set Minimum* and *Set Maximum* boxes, and set the minimum to -10 and the maximum to 10.
- Drag the *Dump* slider to the far right for dump 20.
- Finally, click and drag the visualization to rotate it so that you can see the field.

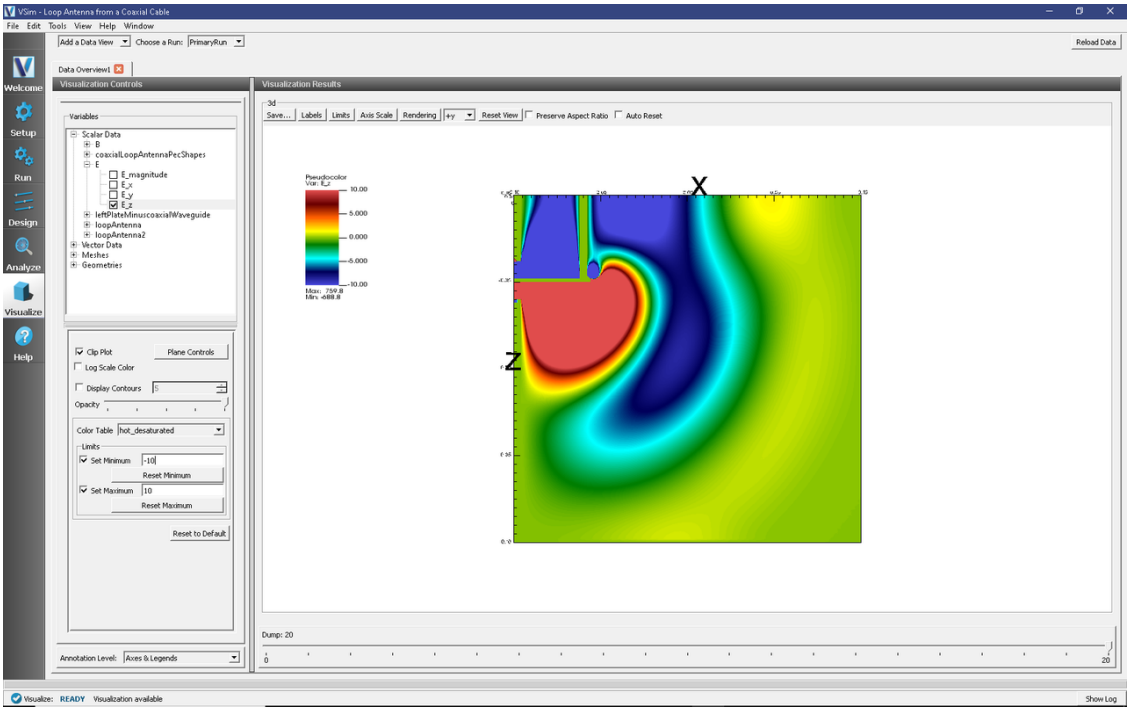


Fig. 3.23: The E_z field propagating off of the loop antenna.

3.1.5 Dipole Antenna (dipoleAntenna.sdf)

Keywords:

antenna, electromagnetics, current source

Problem Description

Dipole antennas are the simplest and most widely used type of antenna. In the most basic setup, a dipole antenna is composed of an oscillating current/voltage source in between two electrodes. The frequency of the source will determine the wavelength of the electromagnetic radiation emitted from the antenna according to the dispersion relation

$$\lambda = \frac{c}{f}.$$

Most commonly, the electrodes will be 1/4 of the emitted wavelength. In this example, the antenna will be driven with a current oscillating with a frequency of 1 GHz. Therefore, the emitted wavelength will be roughly 30 cm, meaning we will make each of the electrodes 7.5 cm. This will make the total length of the antenna 15 cm, which is why dipole antennas are sometimes called half-wave antennas. It is easiest to drive the antenna when the electrodes are a quarter wavelength.

For more background information on dipole antennas, visit the Wikipedia page: https://en.wikipedia.org/wiki/Dipole_antenna

This simulation can be run with a VSimEM, VSimVE, or VSimPD license.

Opening the Simulation

The Dipole Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select *Dipole Antenna* and press the *Choose* button.
- In the resulting dialog box, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 3.24.

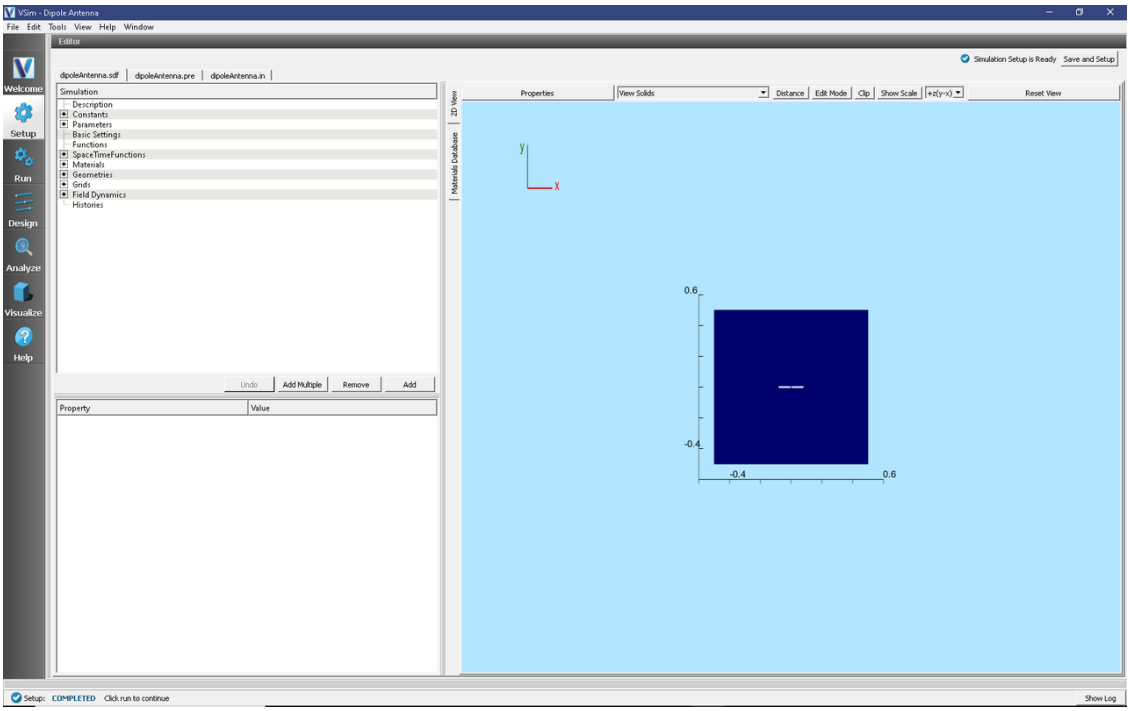


Fig. 3.24: Setup Window for the Dipole Antenna example.

Simulation Properties

In this simulation, we will excite the antenna and watch the dipole electromagnetic radiation emanate from the antenna. A *distributed current* source is used to apply the driving current. A volume for the current source and the functional form of the current is set under *Field Dynamics* → *CurrentDistributions* → *DrivingCurrent*. The user has the ability to set all three components of the current within the volume. In this example, we set the x-component of the current using the *drivingCurrent* spacetime function. The *drivingCurrent* function is a sine wave oscillating at 1 GHz to which a smooth turn on profile has been applied.

There are open boundaries on the walls of the simulation.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.7330431144652654e-12
  - *Number of Steps*: 1000
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.25.

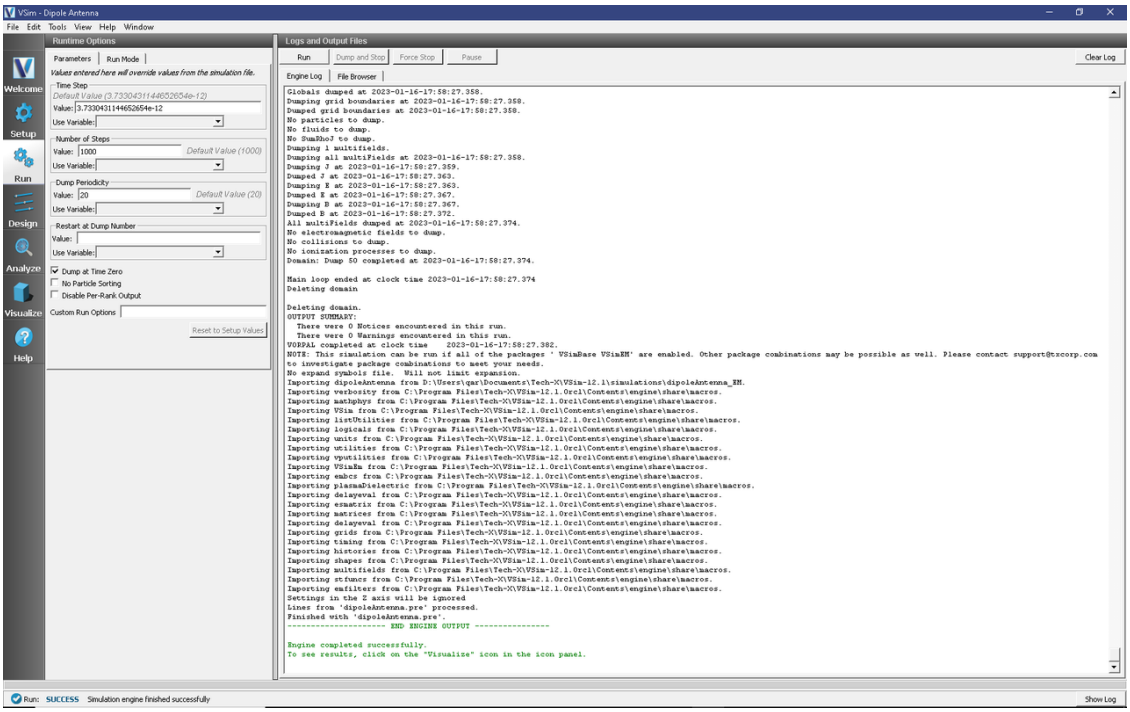


Fig. 3.25: The Run window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

1. Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
2. With the *Data Overview* open, expand *Scalar Data* then expand *E*.
3. Check the box for *E_y*. This will plot the y-component of the electric field.
4. For the color limits, set *Set Minimum* to -0.5, and *Set Maximum* to 0.5.

5. Scroll through the dumps to see how the y-component of the electric field changes with time. The last dump is shown in Fig. 3.26.

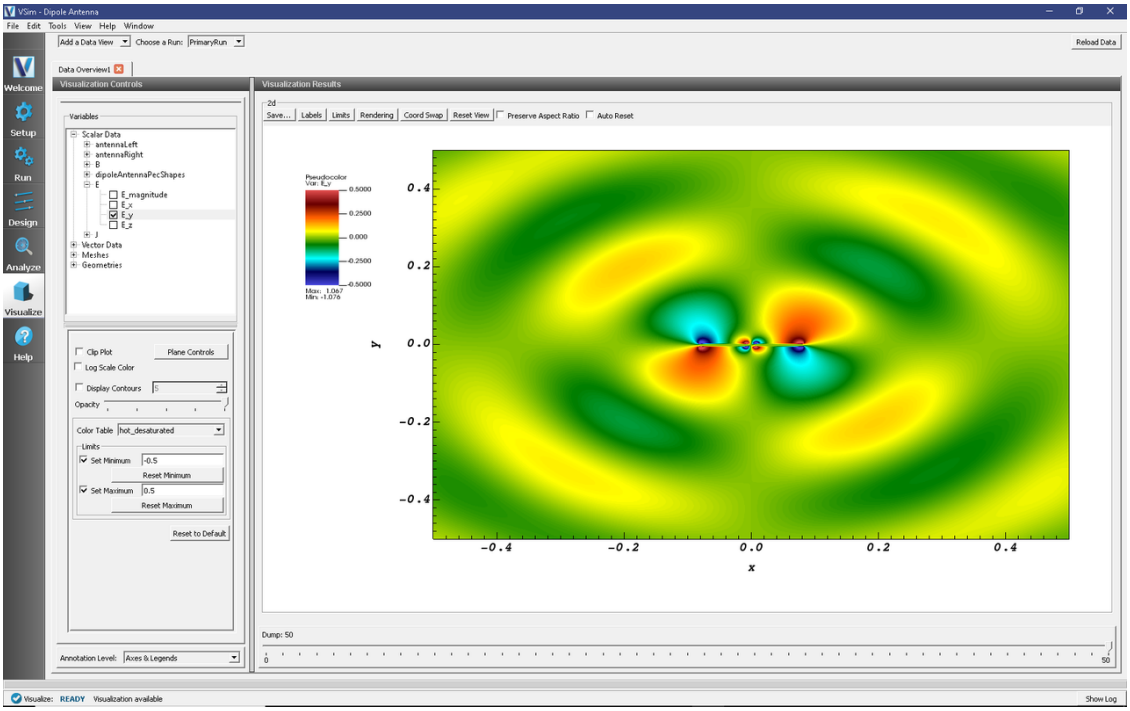


Fig. 3.26: The y-component of the Electric Field shows a 4-lobe pattern.

Un-check the *E_y* box, then check the box for *E_magnitude*. Then go back to the *Colors Options* and switch *Set Minimum* to -.1 and *Set Maximum* to 0.5. The magnitude of the electric field at the end of the simulation is shown in Fig. 3.27.

Further Experiments

1. Add an RCS Box around the antenna to measure the far field radiation pattern at a location of your choosing.
2. Modify the driving frequency or the dimensions of the electrodes.

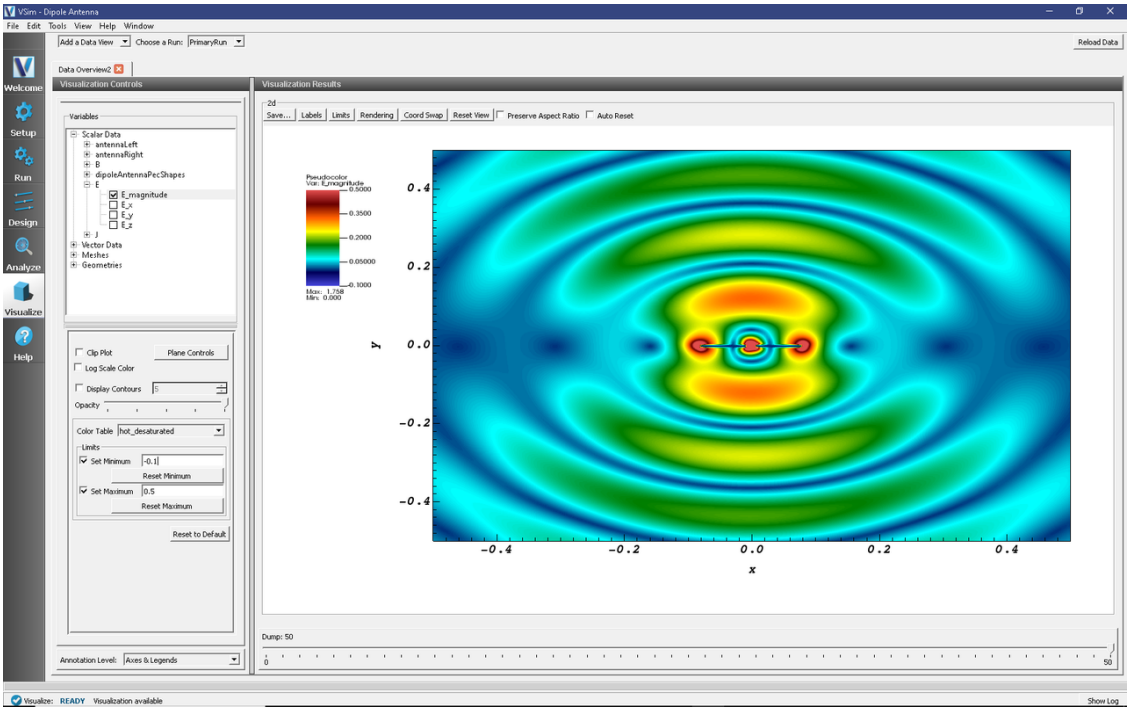


Fig. 3.27: The magnitude of the electric field shows the full 2-lobed dipole antenna pattern.

3.1.6 Dipole Above Conducting Plane (dipoleOnConductingPlane.sdf)

Keywords:

`dipoleOnConductingPlane, far field, radiation`

Problem Description

This problem illustrates how to obtain far fields within VSim by simulating an infinitesimally short dipole mounted a variable height above a conducting plane. The conducting plane is simulated by using the method of images and utilizes an equal magnitude dipole with direction rotated azimuthally by PI, on the opposite side of the plane. This example is similar to the Oscillating Dipole Above Conducting Plane of VSimBase, but modified with functionality available as part of the VSimEM package to obtain the far field radiation pattern. The number of lobes in the far field will vary as a function of height above the conducting plane. There will be 2*HEIGHT/WAVELENGTH + 1 lobes.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Dipole Above Conducting Plane example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select “Dipole Above Conducting Plane” and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

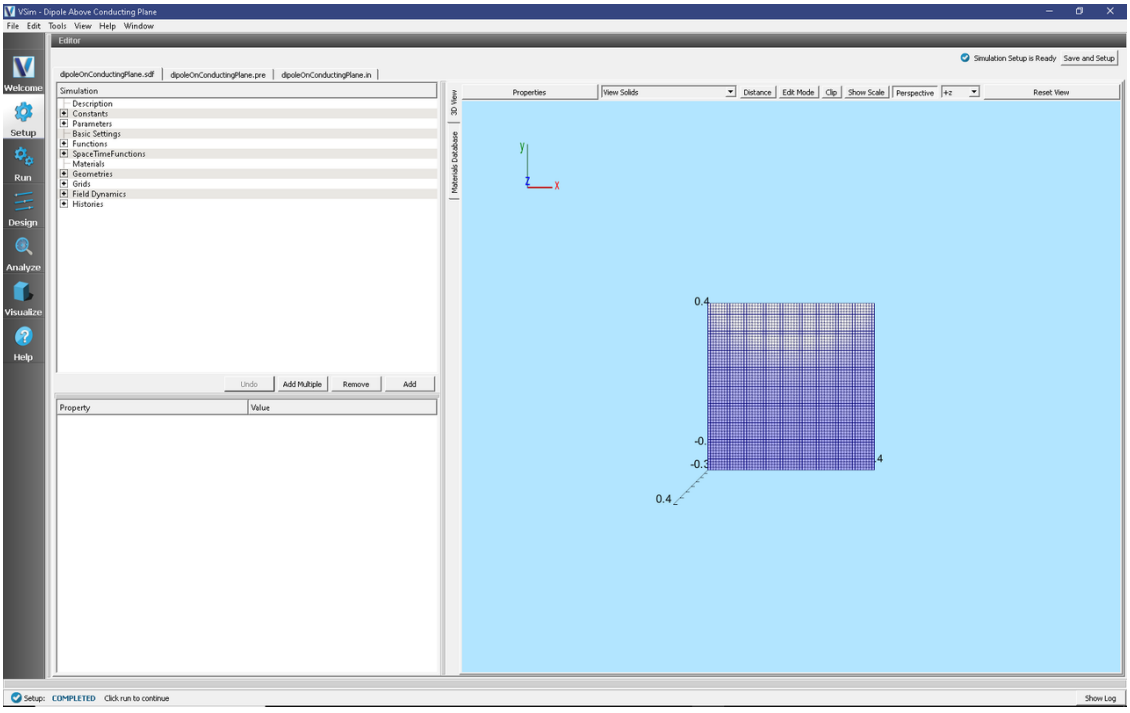


Fig. 3.28: Setup Window for the Dipole Above Conducting Plane example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.28. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

Simulation Properties

This setup includes several *Constants* and *Parameters* to help define the dipole signals, including the frequency and height of the antenna.

There are open boundary conditions on each side of the simulation domain.

The conducting plane is simulated by using the method of images and utilizes an equal magnitude dipole with direction rotated azimuthally by PI, on the opposite side of the plane.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.7380644643956894e-11
  - *Number of Steps*: 500
  - *Dump Periodicity*: 50
  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.29.

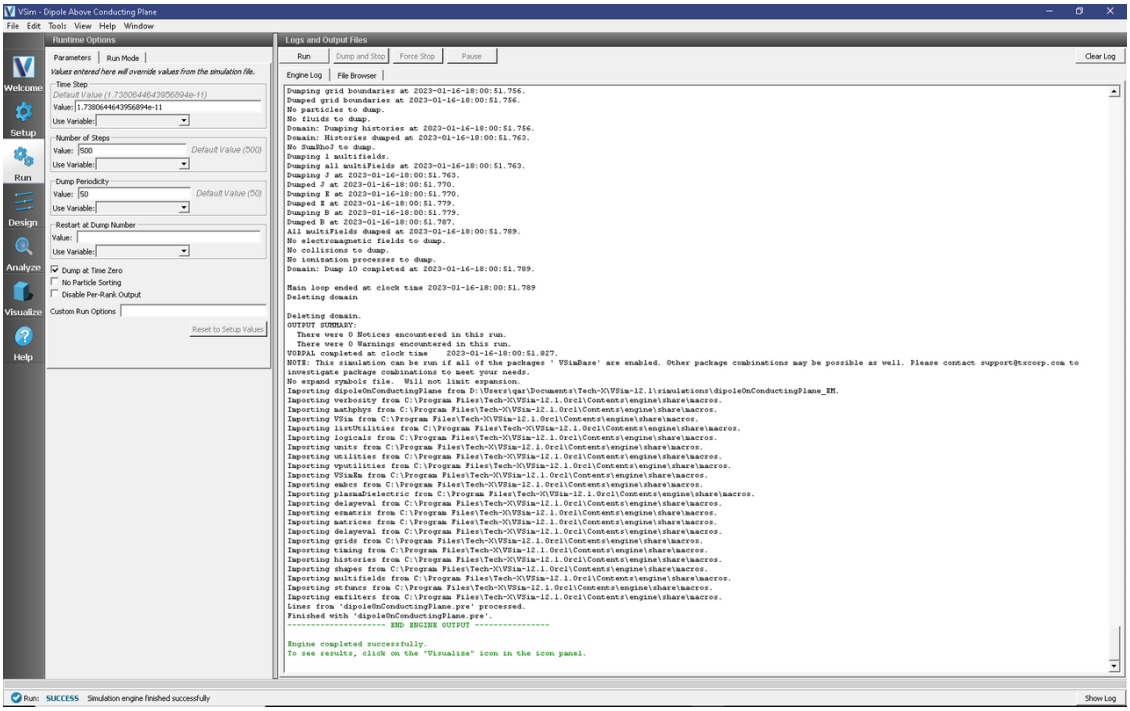


Fig. 3.29: The Run Window at the end of execution.

Analyzing the Results

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- Select the Default *computeFarFieldFromKirchhoffBox.py* Analyzer
- Input values for the variables given on the left hand side of the screen. Check that these have the following values:
  - simulationName - dipoleOnConductingPlane (name of the input file)
  - fieldLabel - E
  - farFieldRadius - 1024.0
  - numPeriods - 0.25
  - numFarFieldTimes - 2
  - frequency - 3.0e9
  - numTheta - 45 (number of points in the theta direction)
  - numPhi - 90 (number of points in the phi direction)
  - zeroThetaDirection - (0,0,1)
  - zeroPhiDirection - (1,0,0)
  - incidentWaveAmplitude - blank

  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 1024.0
  - principalPlanesOnly - checked

- Click the *Analyze* button near the top right of the window.

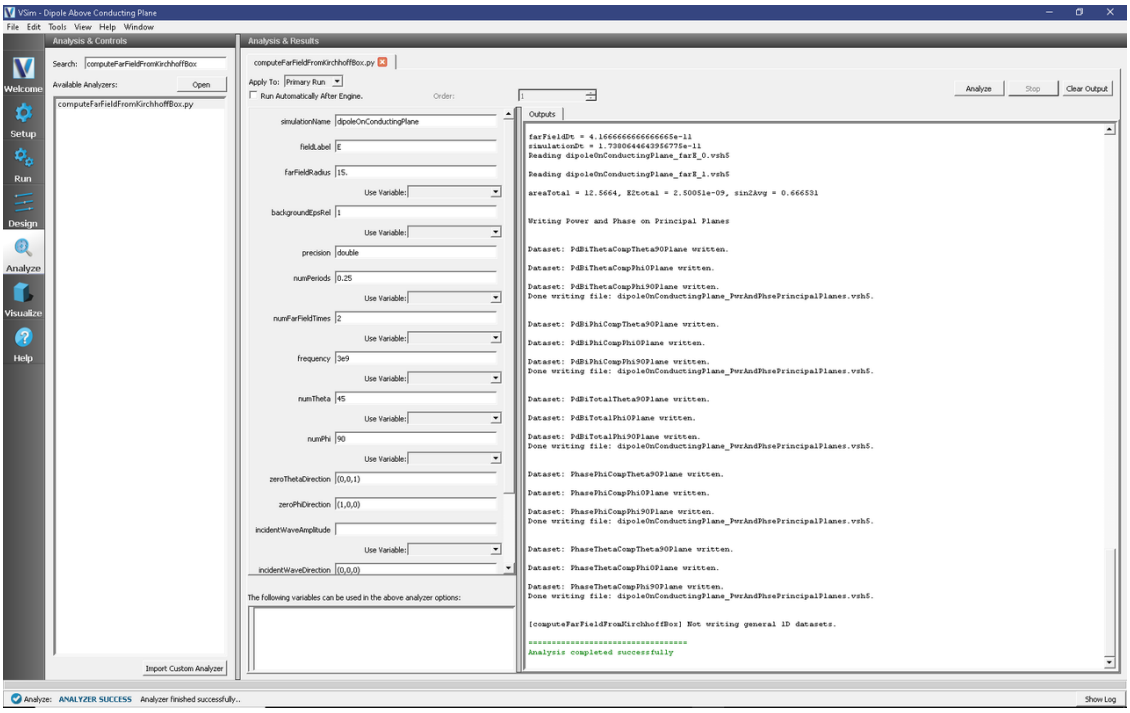


Fig. 3.30: The Analyze Window at the end of execution.

Visualizing the Results

The far field radiation pattern can be found in the Scalar Data variables of the data overview tab. Expand farE and then check the farE_magnitude box. You may need to rotate the view and check the *Clip Plot* box to hide the virtual far field pattern under the conducting plane.

Further Experiments

The number of lobes in the far field is dependent on Antenna Orientation and height. If vertically oriented there will be 2*Height/Wavelength +1 lobes. A horizontally oriented dipole will produce 2*Height/Wavelength lobes.

The resolution of the far field pattern can be changed by editing the number of theta and phi points in the analysis.

If the Simulation domain is made too small, the results will be distorted as the entire near field must be within the simulation domain in order to achieve a proper transformation to the far field.

Note that an infinite perfect electric conducting plane is simulated in the computational engine via image theory. An equal infinitesimal dipole is placed the same distance from the conducting "plane" in order to achieve the result of having an infinite electric conductor.

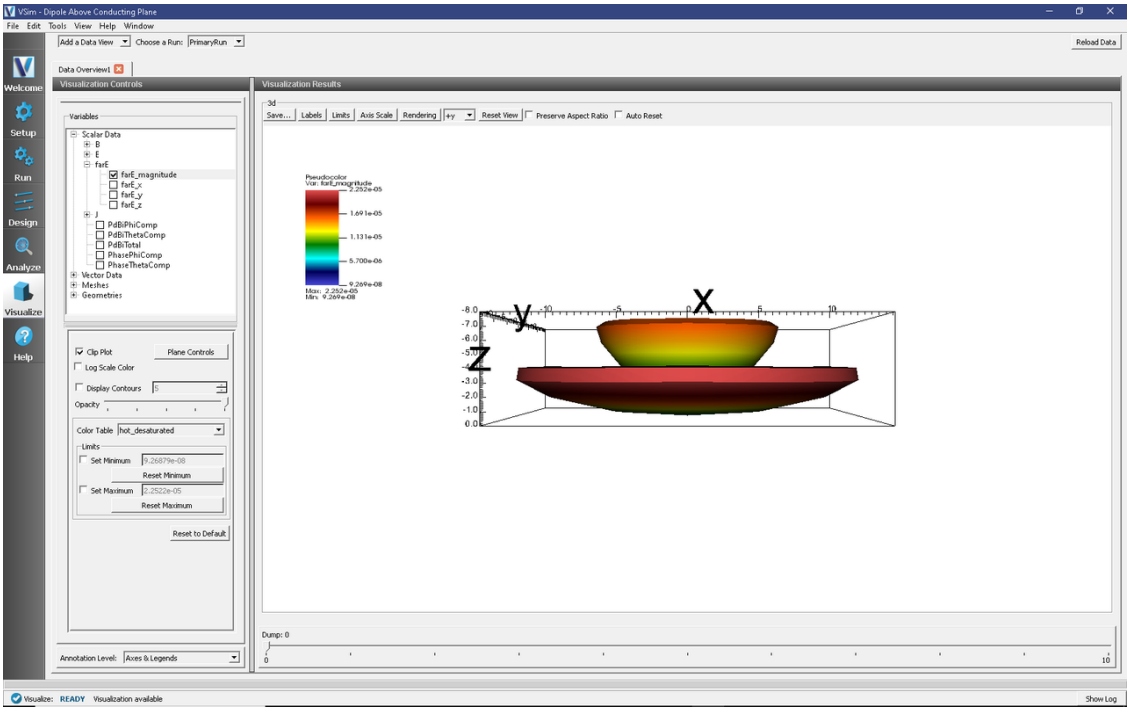


Fig. 3.31: The far field radiation pattern

3.1.7 Dish Antenna (dishAntenna.sdf)

Keywords:

`electromagnetics, antennas`

Problem Description

The Dish Antenna simulation illustrates how to get the radiation pattern from a source in the presence of a complex shape.

This simulation can be performed with a VSimEM, VSimVE or VSimPD license.

Opening the Simulation

The Dish Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Dish Antenna" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.32. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

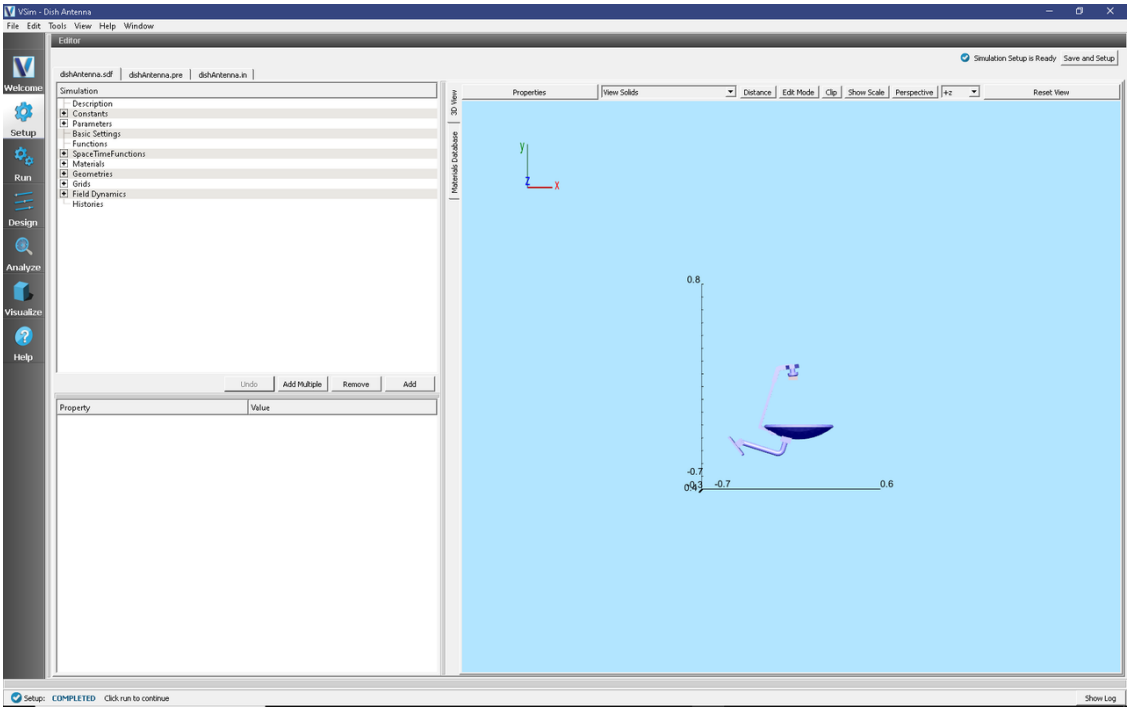


Fig. 3.32: Setup Window for the Dish Antenna example.

Simulation Properties

One can set the parameters of the grid and the source through the setup tree. The parameters are put under the Constants section.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.147707707345734e-12
  - *Number of Steps*: 1000
  - *Dump Periodicity*: 50
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.33.

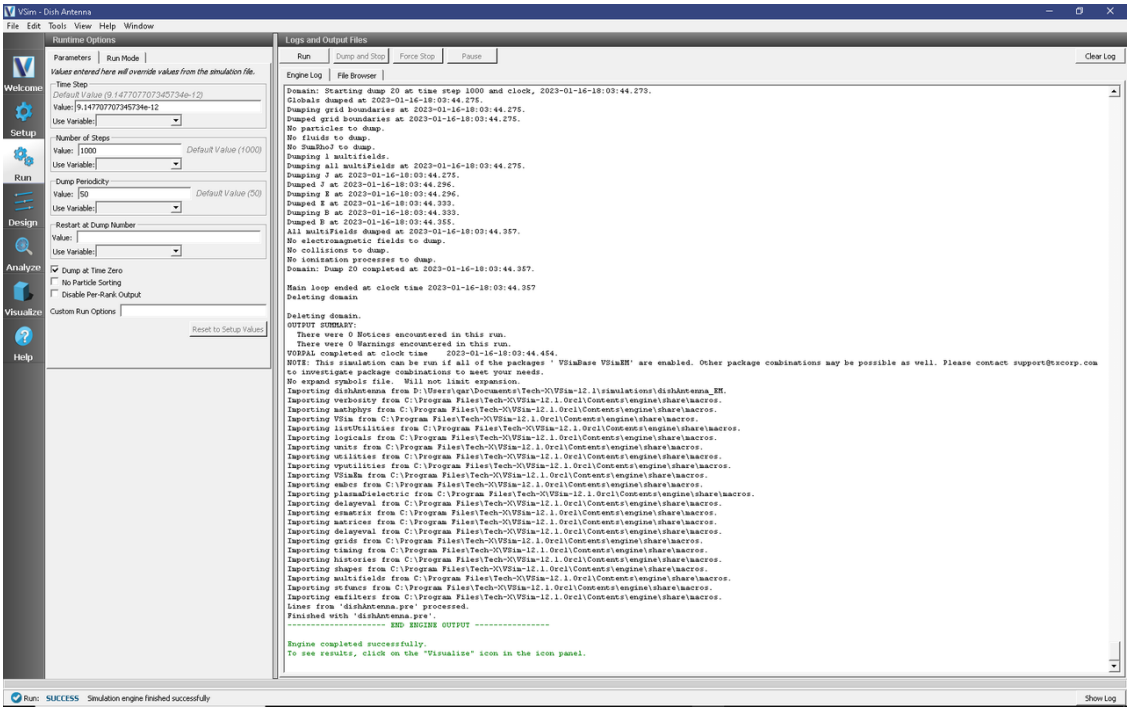


Fig. 3.33: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric field reflected from the dish antenna as shown in Fig. 3.34, do the following:

- Expand *Scalar Data*
- Expand *E*
- Select *E_x*
- Check *Clip Plot*
- Expand *Geometries*
- Select *poly (dishAntennaPecShapes)*
- Check *Clip Plot*

It is easier to see the fields if you change the color scale minimum and maximum. To do so, check the *Set Minimum* and *Set Maximum* boxes, and set a fixed minimum of -2 and a fixed maximum of 2.

Move the slider at the bottom of the right pane to see the electric field at different times.

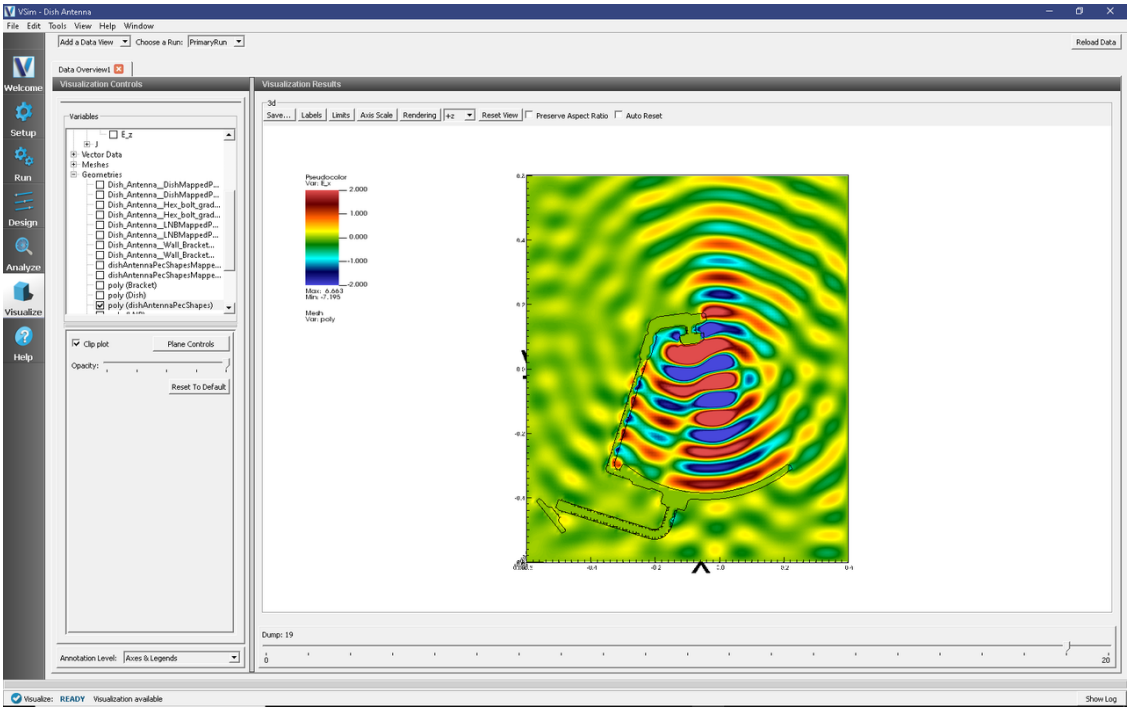


Fig. 3.34: Visualization of a slice of the electric field as a color contour plot at dump 19.

Further Experiments

Additional experiments worth investigating are:

- Change the resolution to see whether more resolution gives a different answer.
- Change the frequency of the source. Be careful, because at high frequencies with the chosen resolution, one will require a large amount of memory.

3.1.8 Half-Wave Dipole in Free Space (halfWaveDipoleAntenna.sdf)

Keywords:

`halfWaveDipoleAntenna, far field, radiation`

Problem Description

This problem illustrates how to obtain far field radiation patterns from VSim simulation data. The simulation itself consists of a half-wavelength long current source in free space.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Half Wave Dipole Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Half-Wave Dipole in Free Space" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.35. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

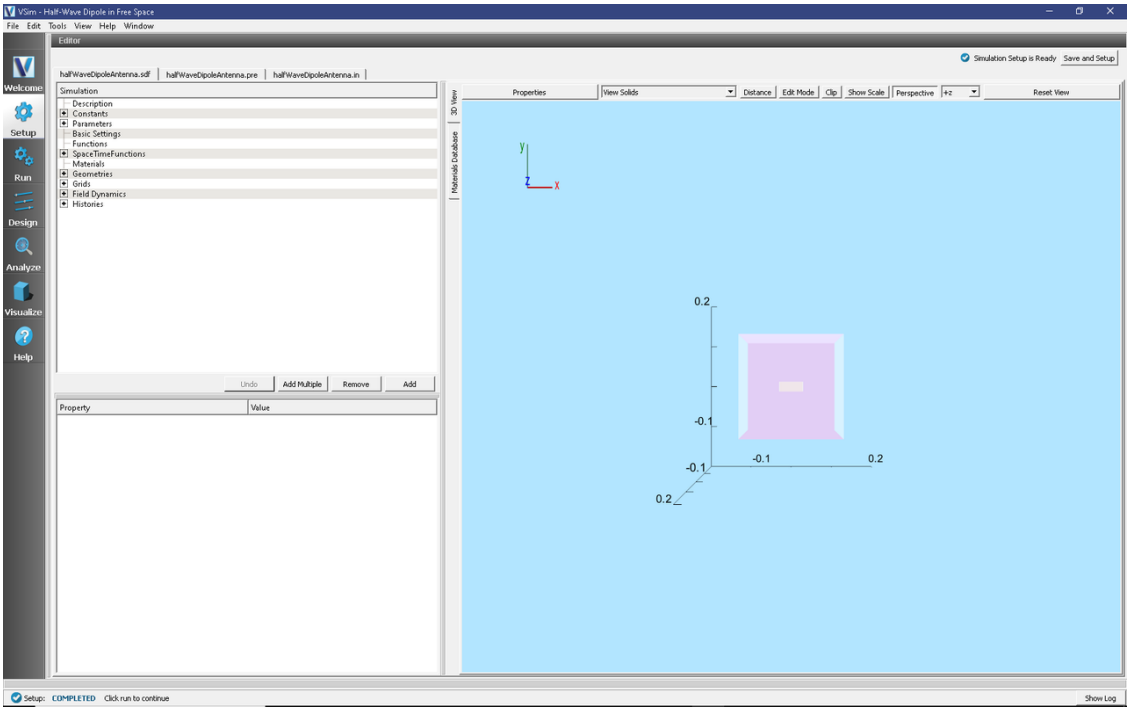


Fig. 3.35: Setup Window for the Half Wave Dipole Antenna example.

Simulation Properties

This example includes *Constants* for easy adjustment of simulation properties, Including:

- AMPLITUDE: The amplitude of the signal
- FREQUENCY: The frequency of the antenna

There are also *SpaceTimeFunctions* to define the current driver of the half wavelength source.

Other properties of the simulation include open boundaries on all sides. A Distributed Current source is used to set the current of the half wavelength antenna.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.147707707345734e-12
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.36.

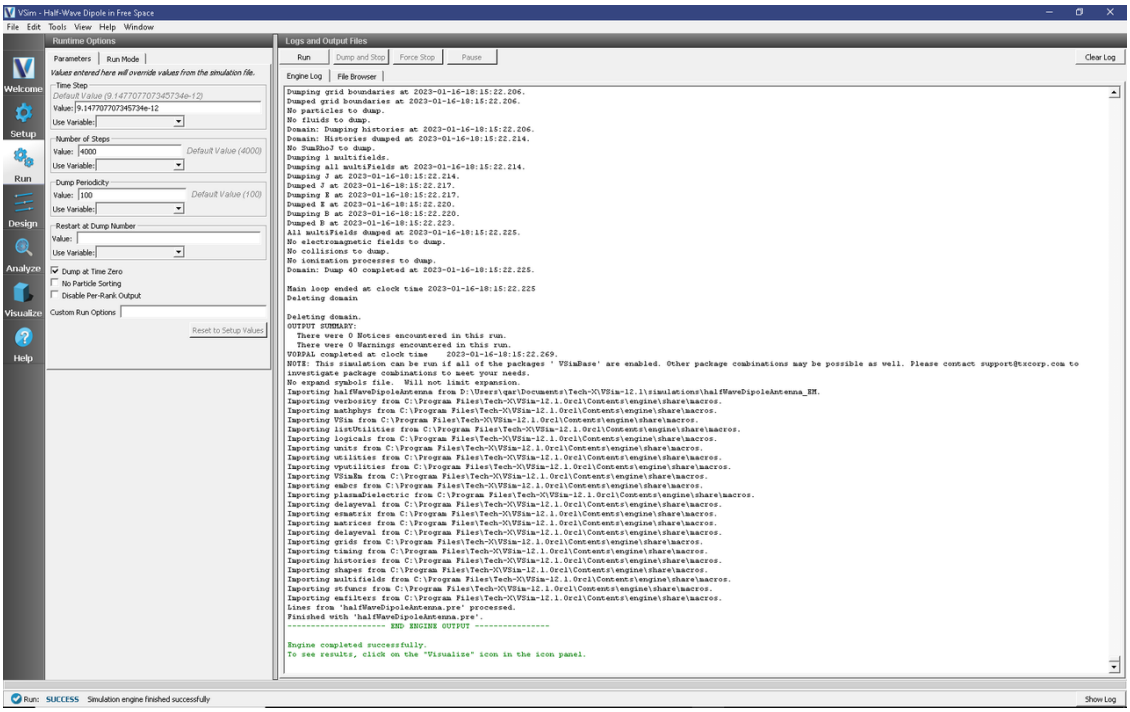


Fig. 3.36: The Run Window at the end of execution.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- Select *computeFarFieldFromKirchhoffBox.py (default)*. Then click *Open*.
- For this example, edit the following input parameters:
  - simulationName - halfWaveDipoleAntenna (name of the input file)
  - fieldLabel - E (name of the electromagnetic field)

- farFieldRadius - 10.0 (radius of the far sphere, i.e., distance to the far zone)
- numPeriods - 0.25
- numFarFieldTimes - 2
- frequency - 3.0e9
- numTheta - 45 (number of points in the theta direction)
- numPhi - 90 (number of points in the phi direction)
- zeroThetaDirection - (0,0,1) (determines orientation of far field coordinate system)
- zeroPhiDirection - (1,0,0) (determines orientation of far field coordinate system
- incidentWaveAmplitude - blank
- incidentWaveDirection - (0,0,0)
- varyingMeshMaxRadius - 10.0
- principalPlanesOnly - checked

- Click the *Analyze* button in the upper right corner.

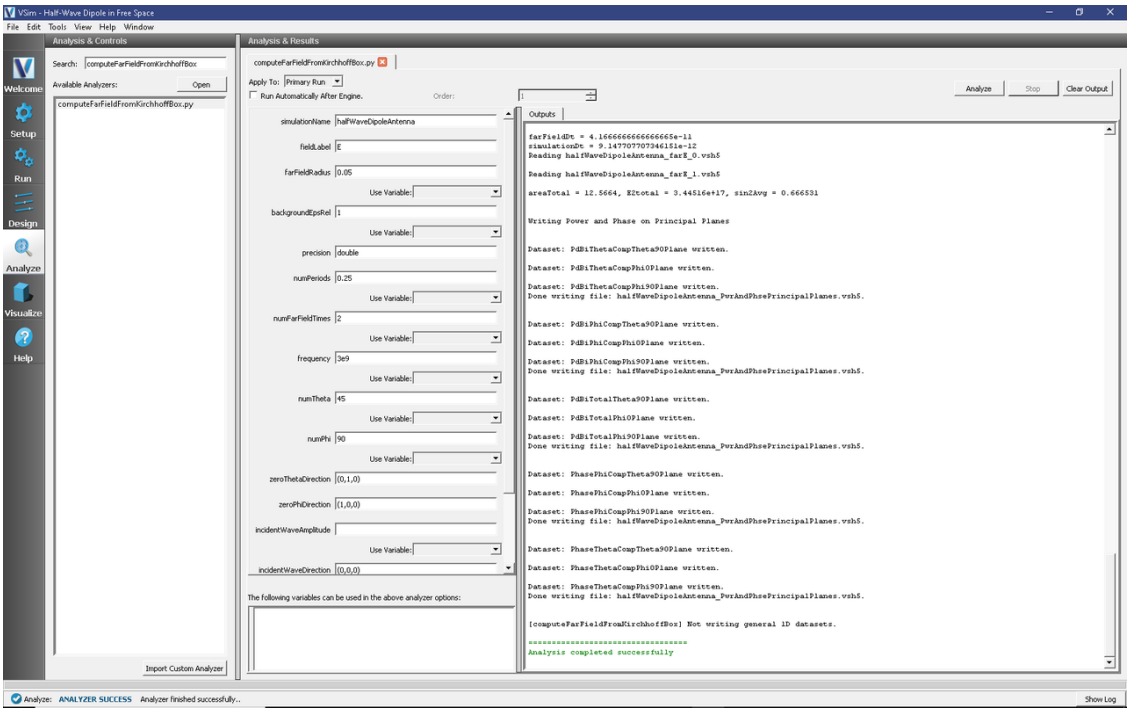


Fig. 3.37: The Analysis window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The far field radiation pattern can be found in the scalar data variables of the data overview tab:

- Expand *Scalar Data*
- Expand *farE*
- Select *farE_magnitude*
- Move the dump slider forward in time to see the evolution
- Click and drag to rotate the image

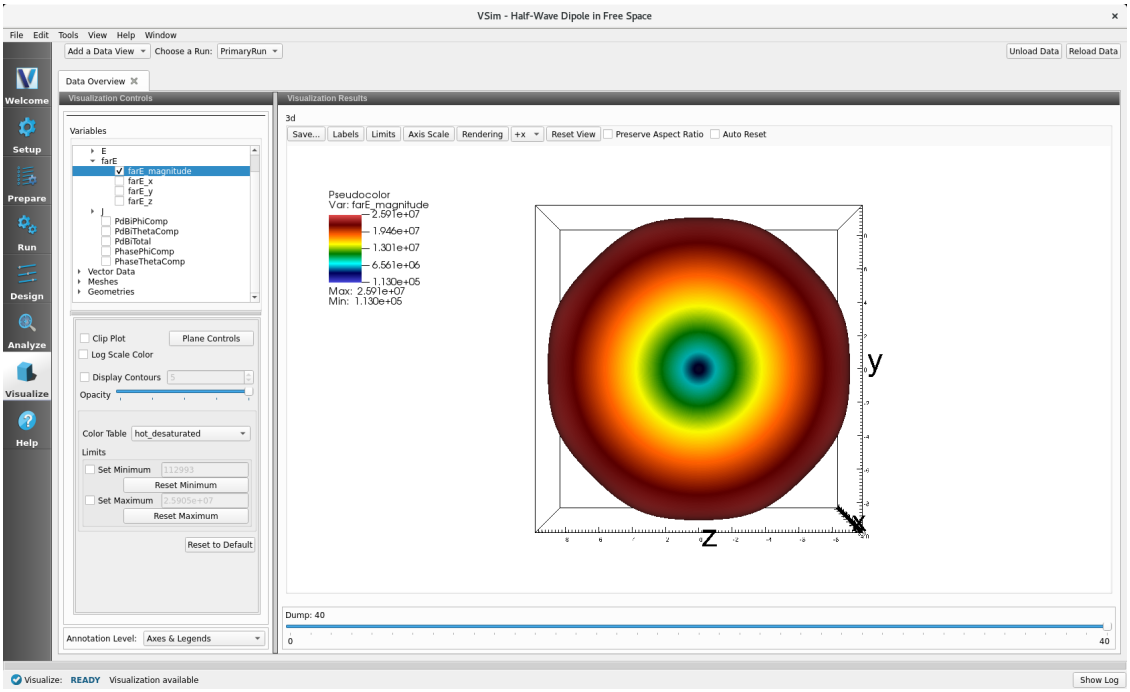


Fig. 3.38: The far field radiation pattern

Further Experiments

The resolution of the far field pattern can be changed by editing the number of theta, phi, and sphere points in the far field history.

Try implementing a conducting plane to see how it affects the far field.

If the Simulation domain is made too small, the results will be distorted as the entire near field must be within the simulation domain in order to achieve a proper transformation to the far field.

3.1.9 Horn Antenna (hornAntenna.sdf)

Keywords:

sectoral, horn antenna, far field, radiation

Problem description

This example illustrates how to obtain the far field radiation pattern of a sectoral horn antenna. A horn antenna consists of a flaring metal waveguide shaped like a horn that directs radio waves into a beam. Horns are widely used as antennas at UHF and microwave frequencies. A sectoral horn is only flared along one axis, the other horn axis has constant width and is equivalent to the width of the waveguide. Sectoral horns produce a fan shaped beam, wider in the plane of the narrow sides.

This simulation can be run with a VSimEM license.

Opening the Simulation

The Horn Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Horn Antenna" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is shown Fig. 3.39. One can click and unclick the grid, the farFieldBox0 in the histories, the current distribution, and so forth to see where those objects are. One can change locations through changing the values under Constants or, in some cases, the numbers directly in the objects.

Simulation Properties

The antenna geometry in this example has been set up using CSG in the graphical setup interface. The dimensions of the antenna can be adjusted by tuning the sizes of the various wedges and cubes used in the antenna's construction. Under *Constants*, the wavelength may be modified, as well as the grid size and resolution. The polarization of the antenna may be altered by going into *CurrentDistributions* and changing the components of the driving current source.

There are two scales that we need to resolve in this simulation. One is the wavelength and one is the smallest geometric scale to resolve (i.e. in this simulation it is the wall width). So, NX, NY, and NZ have been set up to resolve both scales.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 8.928466081792827e-12
  - *Number of Steps*: 1300
  - *Dump Periodicity*: 100

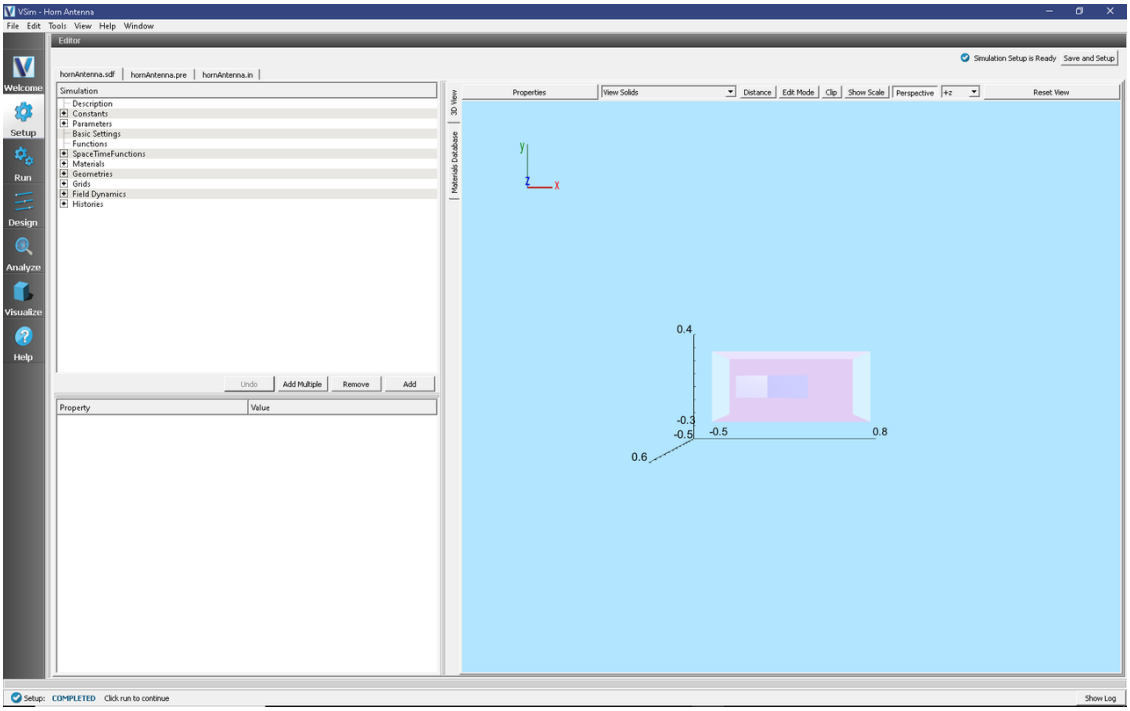


Fig. 3.39: Setup Window for the Horn Antenna example.

  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.40.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- In the resulting dialog, select computeFarFieldFromKirchhoffBox.py and press Open.
- Input values for the analyzer parameters. The analyzer may be run multiple times, allowing the user to experiment with different values.
  - simulationName - hornAntenna (name of the input file)
  - fieldLabel - E (name of the electric field)
  - farFieldRadius - 10.0 (distance to far field in m, 10.0 is a good value)
  - numPeriods - 0.25
  - numFarFieldTimes - 2
  - frequency - 2.0e9
  - numTheta - 45 (number of theta points in the far field, 18 for a quick calculation, 45 for finer resolution)
  - numPhi - 90 (number of phi points in the far field, 36 for a quick calculation, 90 for finer resolution)
  - zeroThetaDirection - (0,0,1) (determines orientation of far field coordinate system)

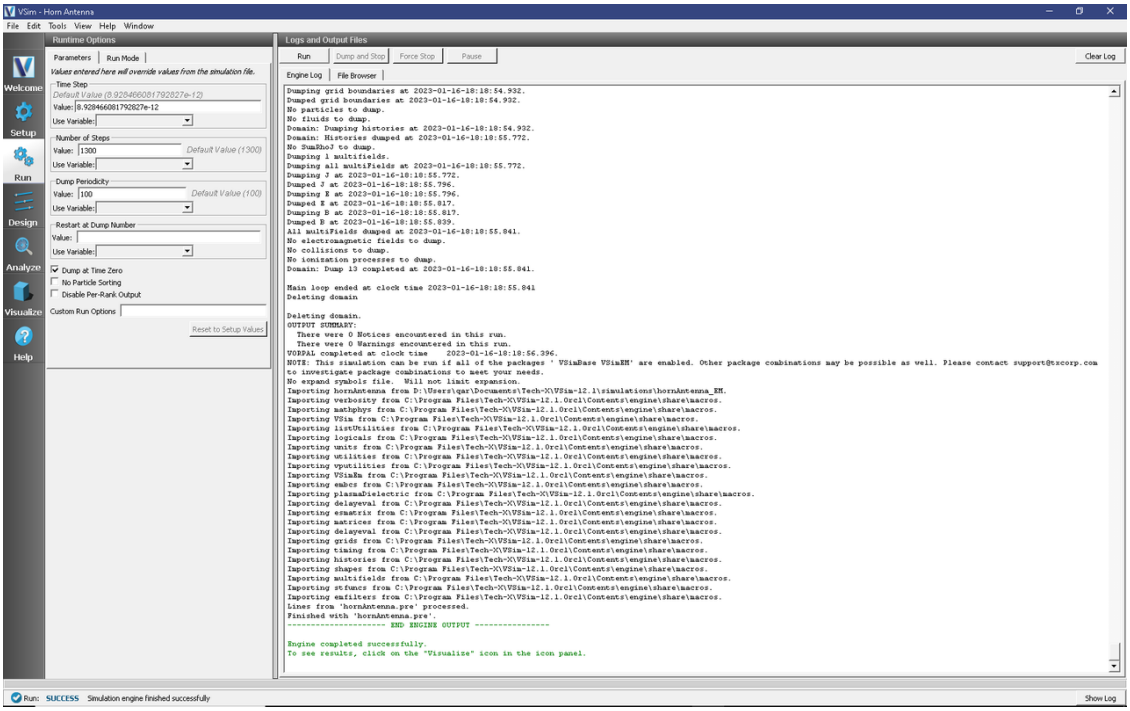


Fig. 3.40: The Run Window at the end of execution.

  - zeroPhiDirection - (1,0,0) (determines orientation of far field coordinate system
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 10.0
  - principalPlanesOnly - checked
- Click Analyze
- The analysis is completed when you see "Analysis completed successfully" in the Outputs. Depending on the values of numTheta, numPhi, and timeStepStride, the script may need to run for several minutes or longer.

Visualizing the Results

Under *Scalar Data* plot $E_{magnitude}$. To slice inside the horn, select *Clip Plot* in the lower left hand corner. Click on *Plane Controls* and change the cut-plane normal to lie along Y instead of Z. Move the dump slider to view the electric field emanating from the horn. You can get a better look by adjusting the color scale. Select *Log Scale Color* in the lower left hand corner. Try adjusting the min and max until the signal is well resolved (see Fig. 3.42).

The far field radiation pattern can be found in the *Scalar Data* variables of the *Data Overview* tab. Open the farE tree element and check the *farE_magnitude* box. The far field mesh can also be plotted; it can be found under *Geometries*.

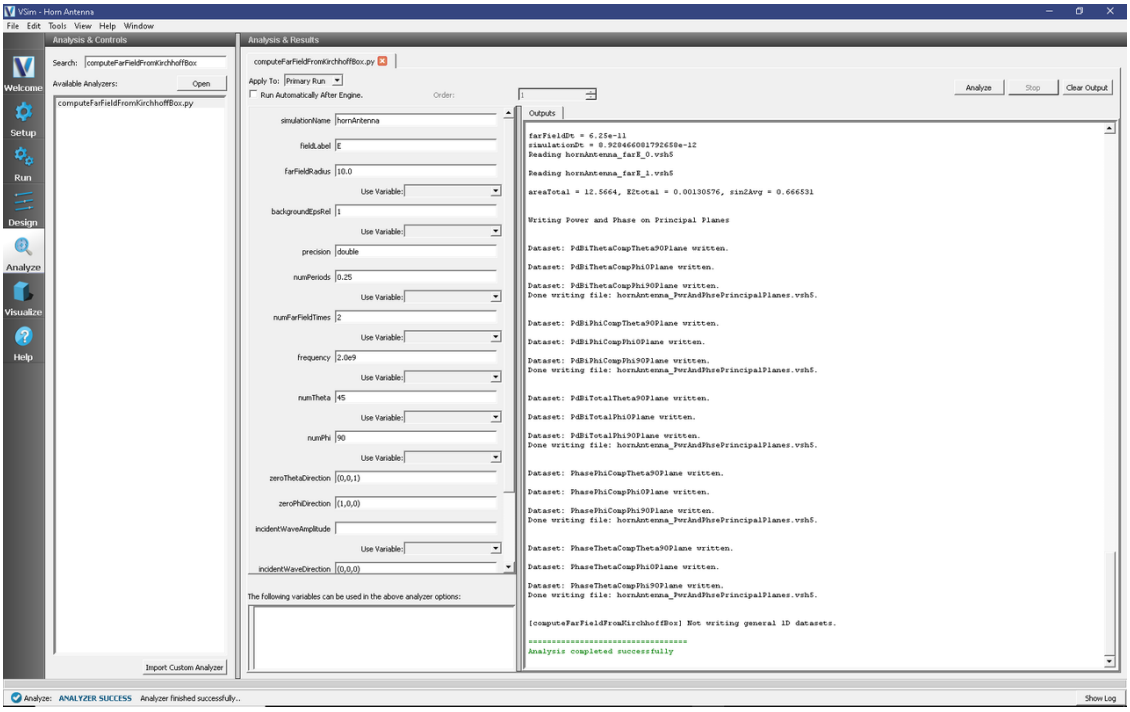


Fig. 3.41: The **Analyze** panel after running computeFarFieldFromKirhhoffBox.py.

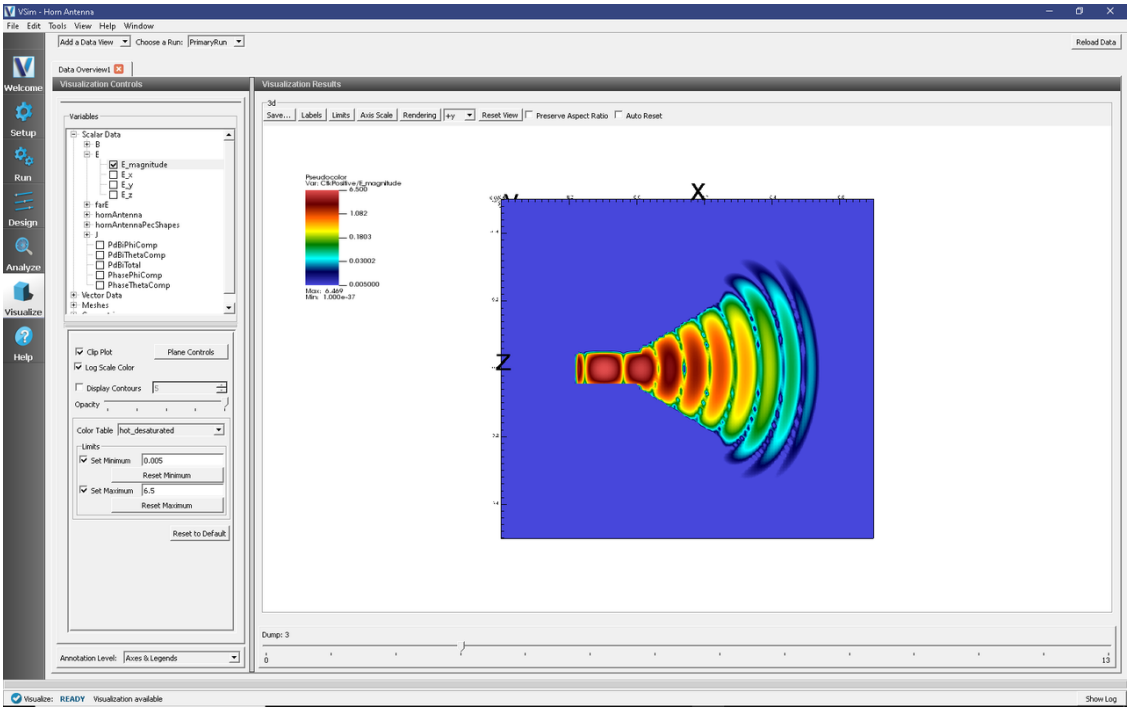


Fig. 3.42: The $E_{magnitude}$ field propagating out of the horn at dump 3. The color scale has been log scaled and the min and max have been fixed to 0.005 and 6.5, respectively. The optimal min/max values will depend on the dump selected. The view has been rotated to show the x-z plane.

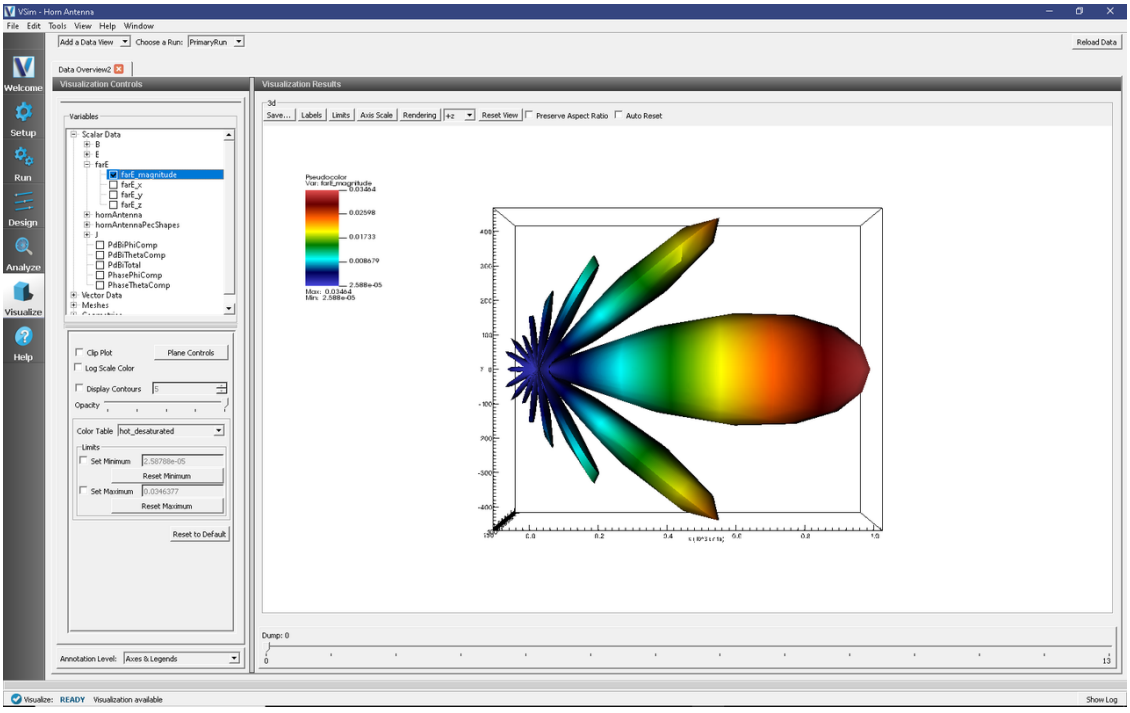


Fig. 3.43: The far field radiation pattern.

Further Experiments

The physical dimensions of the pyramidal horn can be modified in the GUI.

To turn the antenna into an E-plane sectoral horn, try changing the polarization to lie along the flared direction (z).

Try experimenting with different far field resolutions by changing the values of numTheta and numPhi during the *Analyze* step. You can also experiment with different far field distances by changing the value of farFieldRadius.

Try making the domain and the size of the Kirchhoff box larger or smaller (size of the Kirchhoff box is tied to the domain size by default). If the simulation domain is made too small, the results may appear distorted because the entire near field must be resolved within the simulation domain in order to achieve a proper transformation to the far field.

3.1.10 Patch Antenna Far Field (patchAntennaFarField.sdf)

Keywords:

`patchAntenna, far field, radiation`

Problem Description

This problem takes the same patch antenna from the *Patch Antenna* example (currently text-based only, visual setup coming soon) and modifies it to calculate the far-field radiation pattern. It is fed with a 5.5GHz source on a microstrip feed line. The patch itself is mounted on a dielectric substrate made of alumina.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Patch Antenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Patch Antenna with Far Fields" and press the *Choose* button.
- In the resulting dialog, create a new folder if desired, and press the *Save* button to create a copy of this example.

The **Setup** window is now shown with all the implemented physics and geometries. See Fig. 3.44.

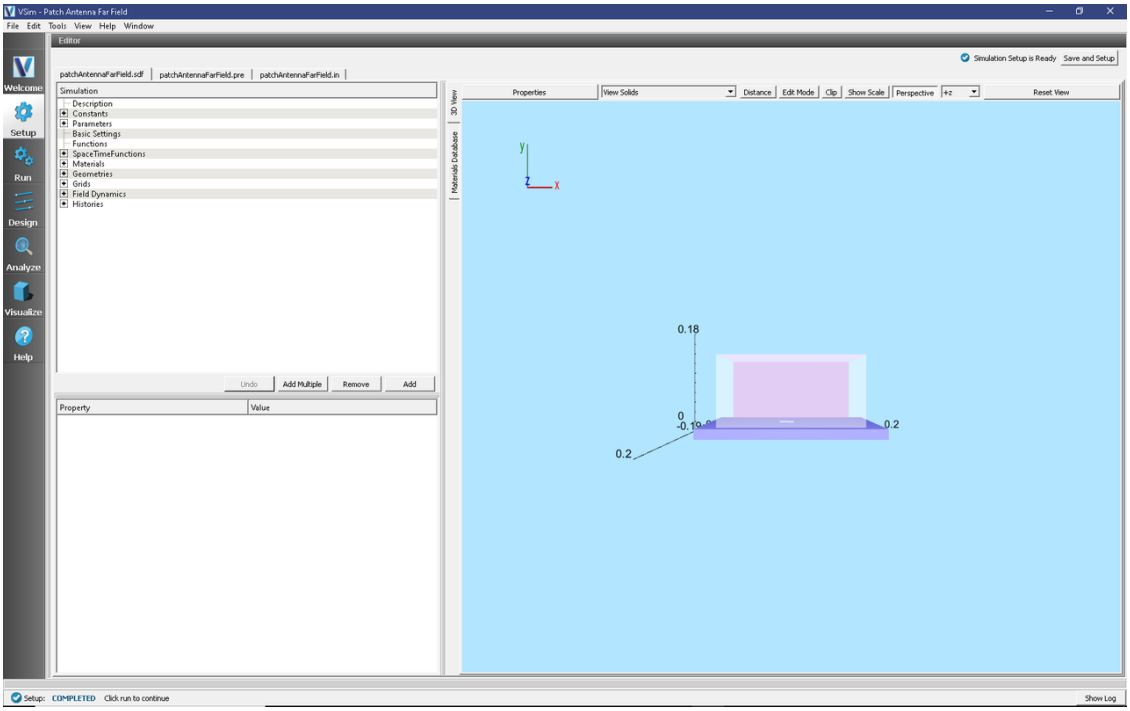


Fig. 3.44: Setup Window for the Patch Antenna example.

Simulation Properties

This file allows the modification of antenna operating frequency, dimensions, orientation, simulation domain size.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.8776873715078086e-12
  - *Number of Steps*: 2343
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.45.

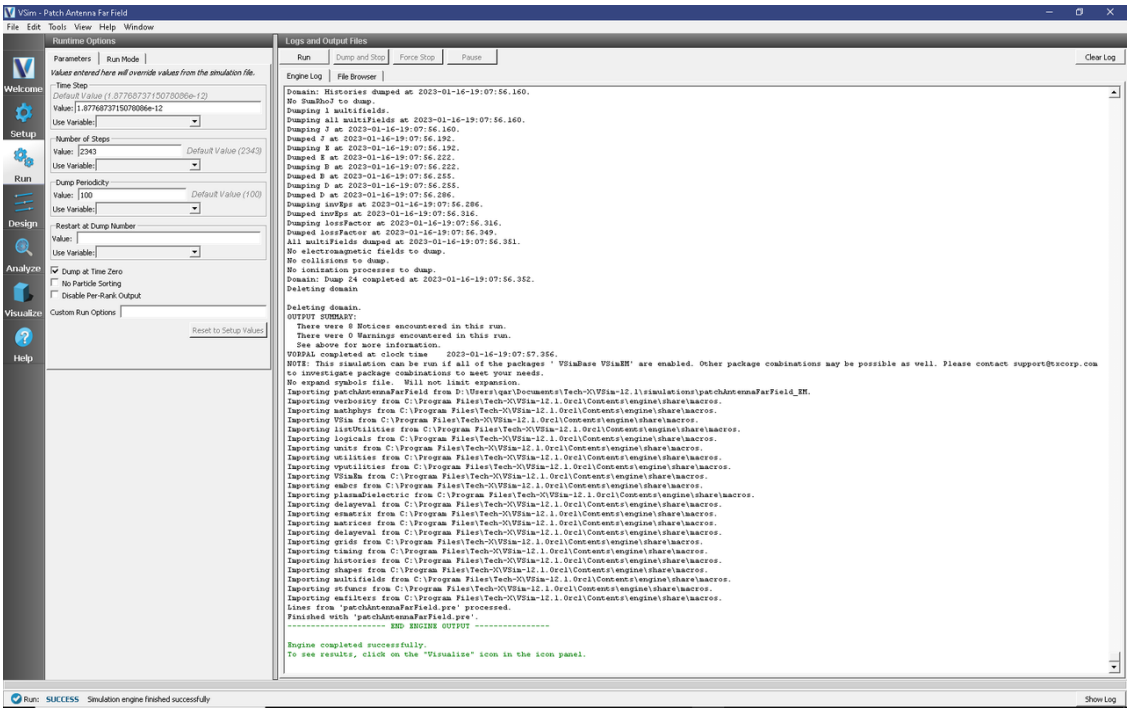


Fig. 3.45: The Run Window at the end of execution.

Analyzing the Results

After performing the above actions continue as follows to compute the far field radiation pattern:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list, select *computeFarFieldFromKirchhoffBox* and press *Open*
- The analyzer fields should be filled as below:
  - *simulationName*: patchAntennaFarField
  - *fieldLabel*: E
  - *farFieldRadius*: 1024.0
  - *numPeriods*: 0.25
  - *numFarFieldTimes*: 2
  - *frequency*: 5.5e9
  - *numTheta*: 45
  - *numPhi*: 60
  - *zeroThetaDirection*: (0,0,1)
  - *zeroPhiDirection*: (1,0,0)
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 1024.0
  - principalPlanesOnly - checked
- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 3.46.

Visualizing the Results

The far field radiation pattern can be found in the *Scalar Data* variables of the *Data Overview* tab. Check the *farE* box. The far field mesh can also be plotted; it can be found under *Geometries*.

Further Experiments

The physical dimensions of the patch can be modified to turn it into any rectangular patch. This model can in fact be used to simulate any form of patch antenna, simply modify the geometry in the Setup Window by expanding the *Parameters* tree node and adjusting the values of PATCH_WIDTH, PATCH_LENGTH, PATCH_THICKNESS, FEED_WIDTH, FEED_LENGTH, and FEED_OFFSET. The thickness of the alumina die may also be adjusted by modifying DIE_THICKNESS.

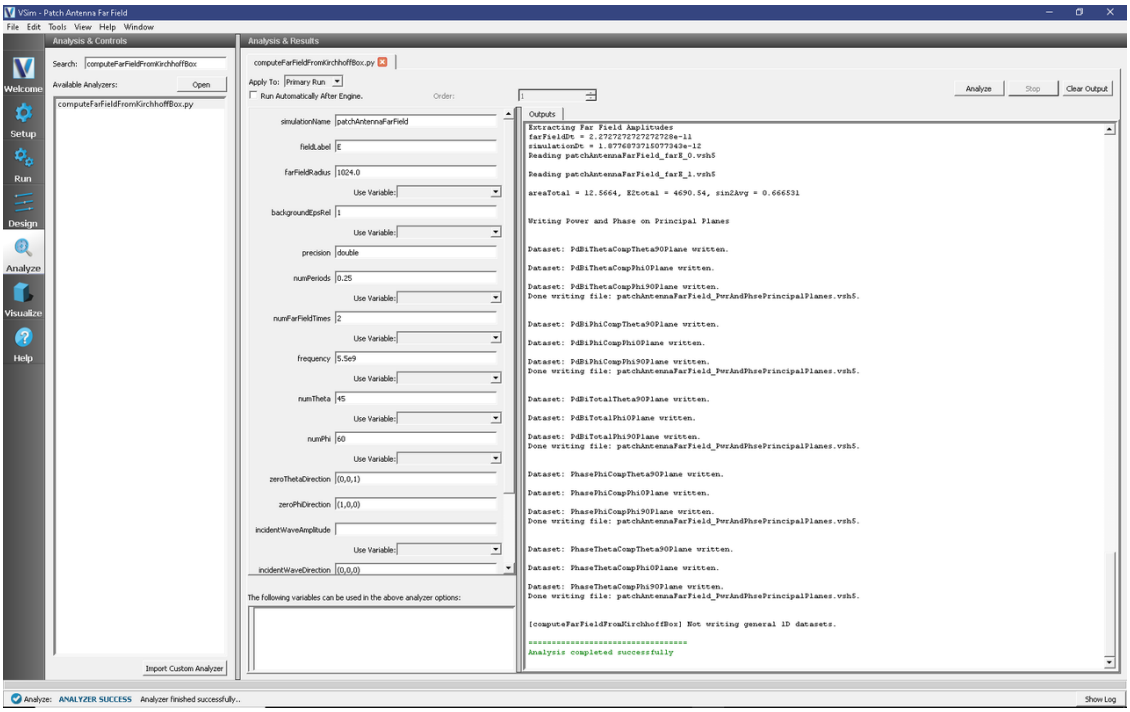


Fig. 3.46: Add the computeFarFieldFromKirhhoffBox.py script to your simulation.

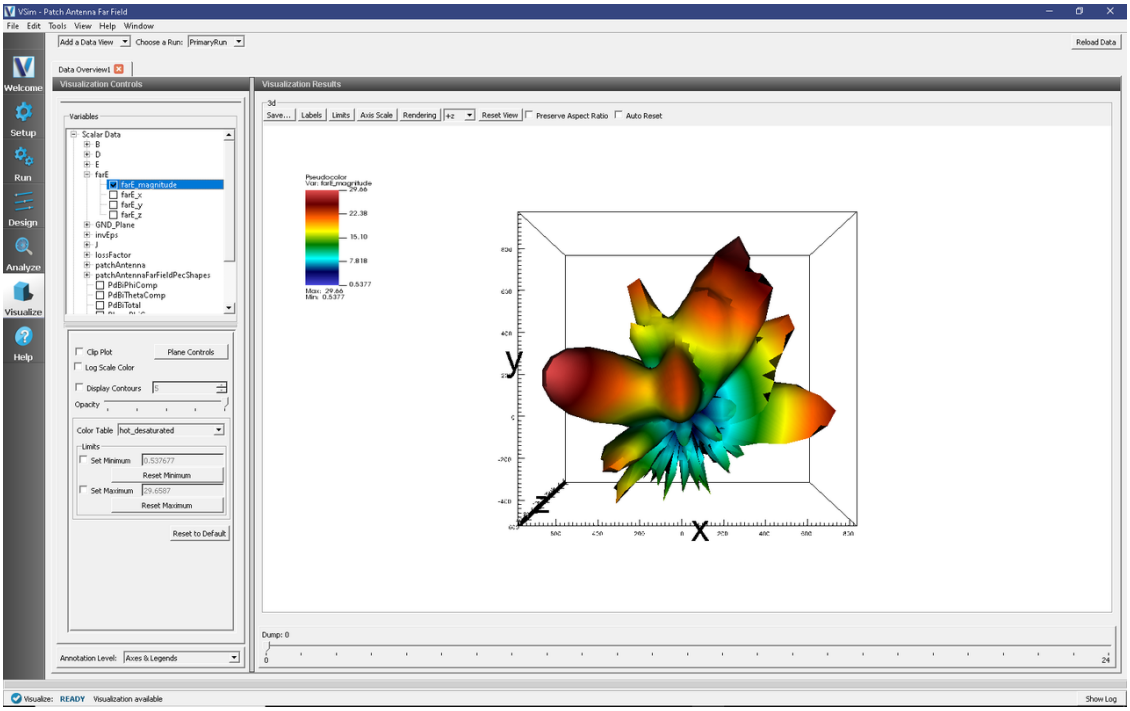


Fig. 3.47: The Far Field Radiation Pattern

3.1.11 Phased Array Antenna (phasedArrayAntenna.sdf)

Keywords:

phasedArrayAntenna, far field, radiation

Problem Description

This VSimEM example illustrates how to setup a phased array simulation and analyze the far field results. Phased array antennas are a vastly-expanding field of research and development due to the fact that going from a one element antenna to an N-element antenna provides more directive beamforming characteristics and, most importantly, non-mechanical steering. Creating a multiple-element antenna results in an array pattern composed of wires, apertures, or other element types. Directive patterns are obtained via constructive interference in the desired direction and destructive in the other directions. Applications of phased array antennas range from commercial (5G, wireless & mobile, satellite telecommunication), military & defense (RADAR, acoustics) to research: atmospheric, space.

For a full walkthrough of this example see the video below: https://www.youtube.com/watch?v=5-I8dmHv8qU&list=PLottQ0Bg2M-3ATV5O9IP-3TEC4toVYPAK&index=12

This simulation can be run with a VSimEM license.

Opening the Simulation

The phasedArrayAntenna example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select *Phased Array* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 3.48.

Simulation Properties

This example consist of 15×15 array of small metal antenna elements excited by a distributed current source. The separation between the elements is $\frac{\lambda}{6}$.

Note that the SPACING parameter CANNOT be used in the CSG array setup settings. To recreate an array with a different spacing between elements, the spacing needs to first be calculated and then typed into the array setup window.

The current source is results in an outging wave centered at $(x, y) = (0, 0)$. The wave amplitude has a Gaussian profile with the standard deviation σ. The phase and amplitude are tied to the azimuthal angle θ, and polar angle ϕ. In this example, the azimuthal angle θ is fixed at $\pi/4$ via the Function dphiFunc. The polar angle ϕ goes from 0 to 2π throughout the simulation via the Function thetaFunc.

The simulation domain contains a far field box history that is later used for the computeFarFieldFromKirchhoffBox analyser.

The current excitation formula, $F(x, y, \phi, \theta, t)$, is:

$$F(x, y, \phi, \theta, t) = A(x, y, \phi, \theta) \times \sin \Phi(x, y, \phi, \theta) \times X(x) \times Y(y)$$

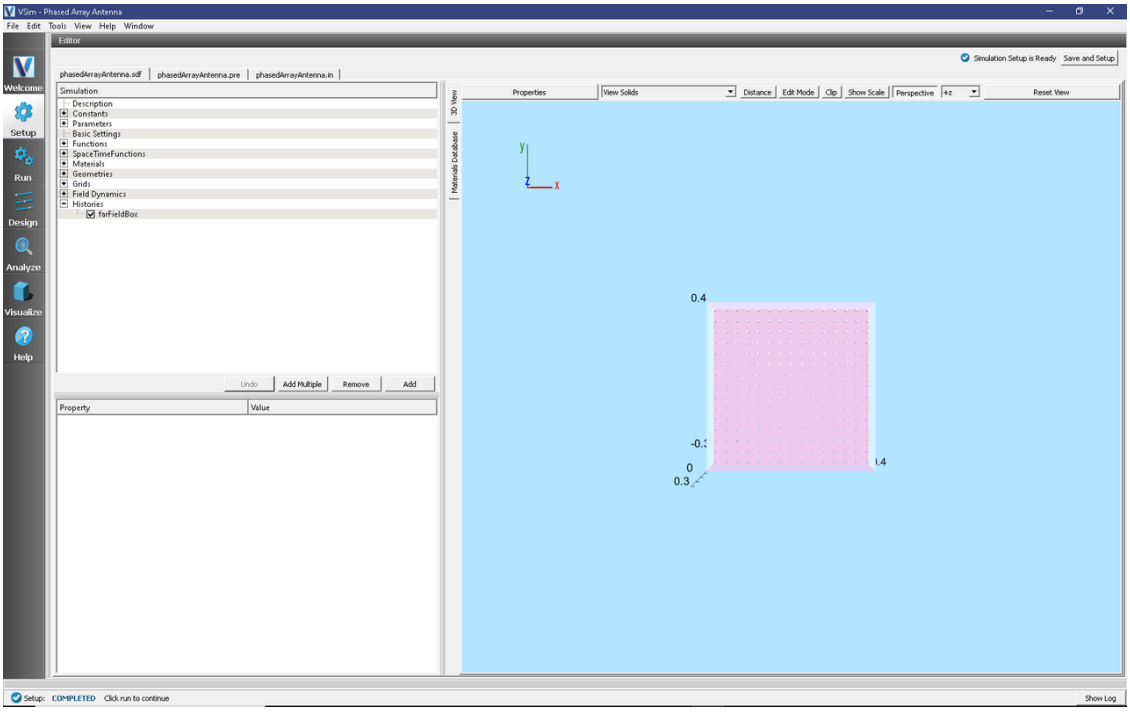


Fig. 3.48: Setup Window for the Phased Array example.

Where the aplitude $A(x, y, \phi, \theta)$, the phase $\Phi(x, y, \phi, \theta)$, and locations in the x-y plane $X(x)$ and $Y(y)$ are defined by:

$$A(x, y, \phi, \theta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2\sigma}\left[\sin^2\phi(x\sin\theta - y\cos\theta)^2 + \cos^2\phi\left(x^2+y^2\right)\right]}$$

$$\Phi(x, y, \phi, \theta) = \omega t + \frac{\omega}{c}\sin\phi\left(x\cos\theta + y\sin\theta\right)$$

$$X(x) = H\left[\cos\frac{2\pi x}{d} - 0.9\right]$$

$$Y(y) = H\left[\cos\frac{2\pi y}{d} - 0.9\right]$$

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.6110445055891545e-12
  - *Number of Steps*: 9000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.49.

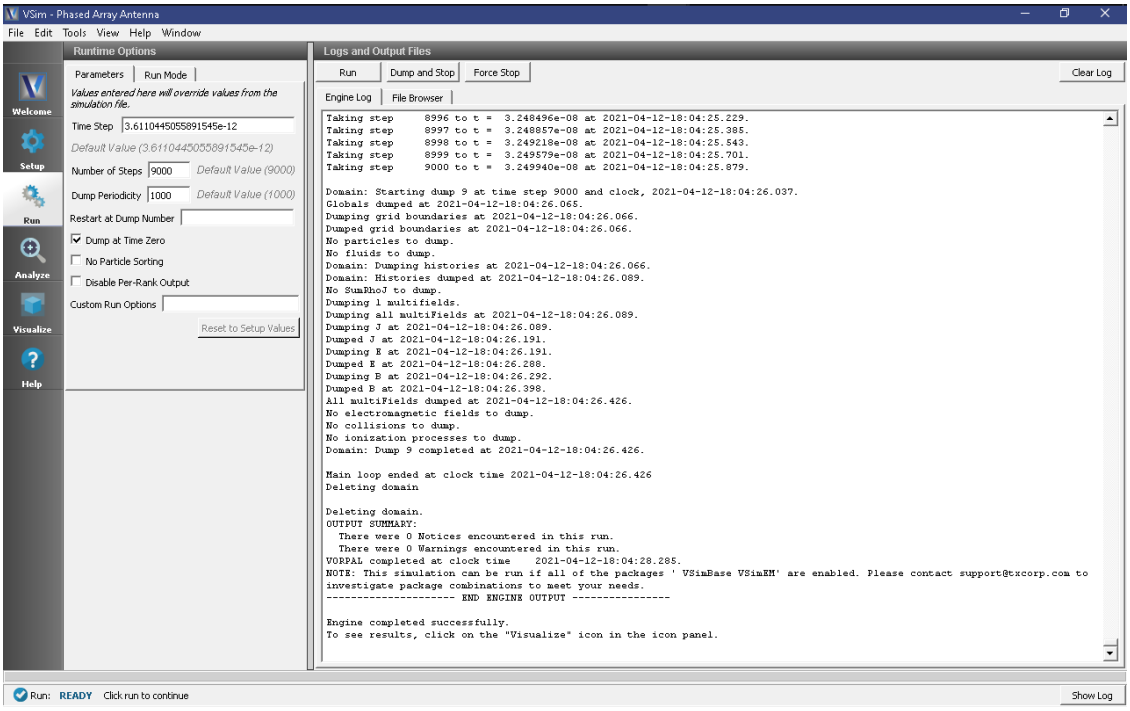


Fig. 3.49: The Run Window at the end of execution.

Analyzing the Results

After performing the above actions continue as follows to compute the far field radiation pattern:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list, select *computeFarFieldFromKirchhoffBox* and press *Open*
- The analyzer fields should be filled as below:
  - *simulationName*: phasedArrayAntenna
  - *fieldLabel*: E
  - *farFieldRadius*: 30.0
  - *numPeriods*: 0.25
  - *numFarFieldTimes*: 2
  - *frequency*: 1.0e9
  - *numTheta*: 16
  - *numPhi*: 32
  - *zeroThetaDirection*: (0,0,1)
  - *zeroPhiDirection*: (1,0,0)
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 30.0
  - principalPlanesOnly - checked

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 3.50.

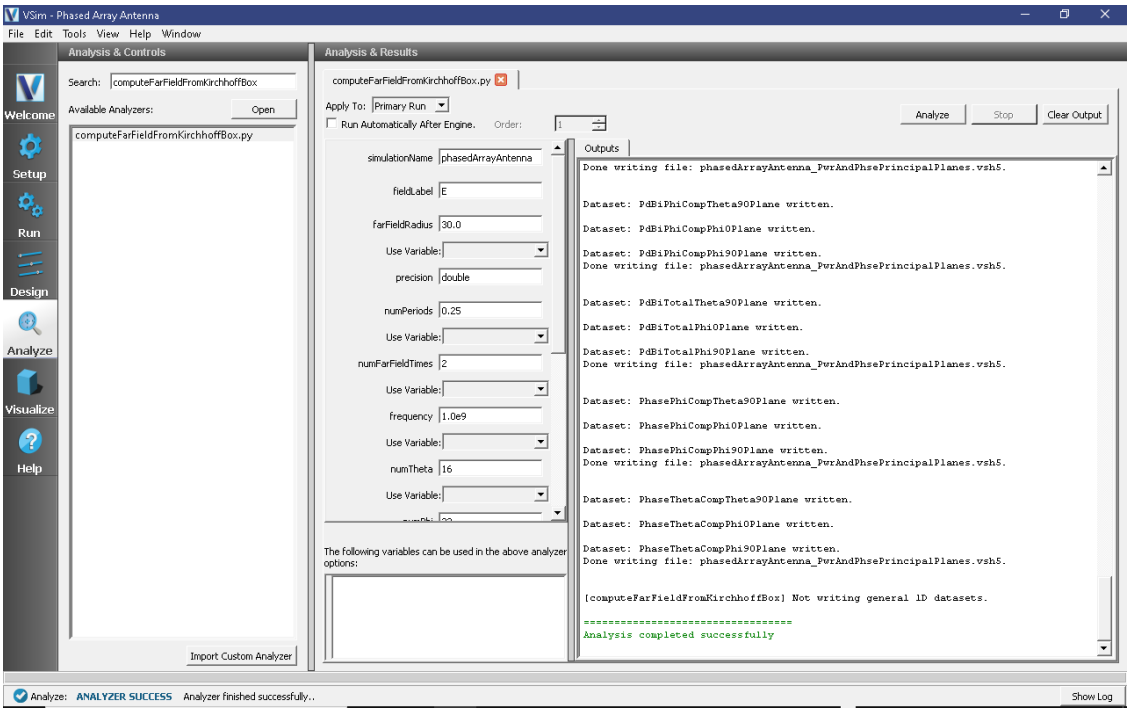


Fig. 3.50: The computeFarFieldFromKirchhoffBox at the end of a successful run.

For more accurate results, use the following input paramters in the analyzer:

- *simulationName*: phasedArrayAntenna
- *fieldLabel*: E
- *farFieldRadius*: 30
- *numPeriods*: 0.25
- *numFarFieldTimes*: 2
- *frequency*: 1e9
- *numTheta*: 60
- *numPhi*: 120
- *zeroThetaDirection*: (0,0,1)
- *zeroPhiDirection*: (1,0,0)
- *varyingRadiusMesh*: 30.0

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Data Overview*.
- Expand *Scalar Data* variables.
- Expand *farE* and check the *farE_Magnitude* box.
- Move the dump slider to see the evolution of the far fields in time.

The resulting visualization is shown in Fig. 3.51.

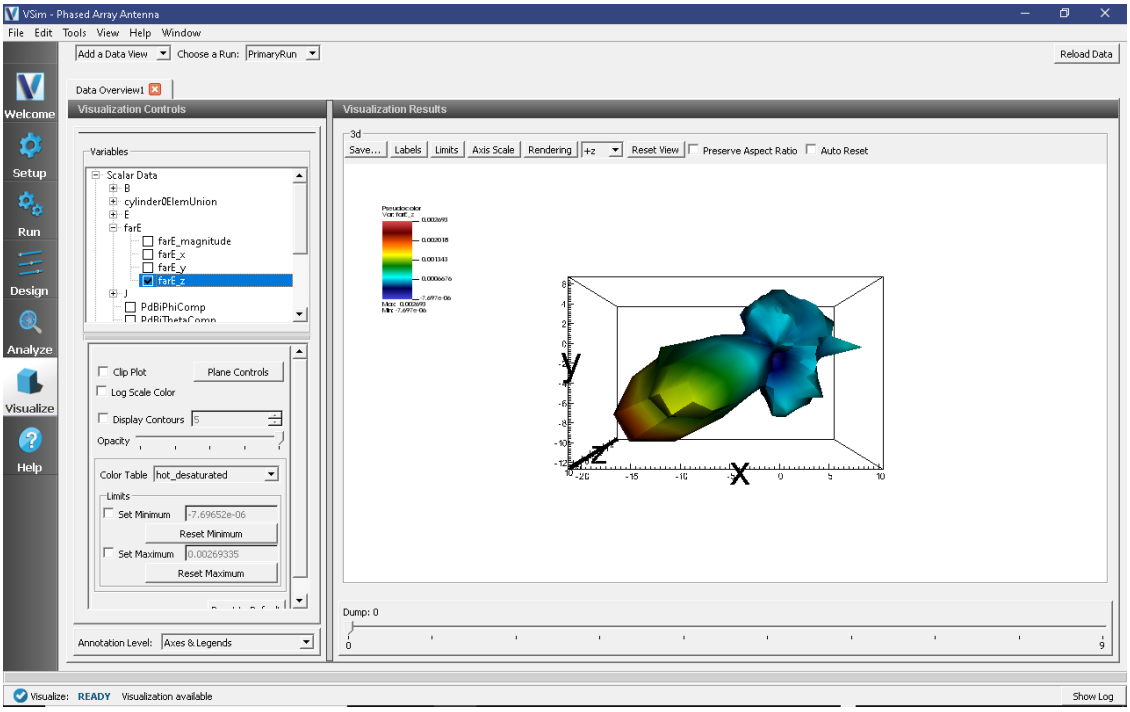


Fig. 3.51: Far field pattern 30 m away from the antenna.

To visualize the 2D far fields proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Field Analysis*
- Under *Field* choose *farE_magnitude*
- Move the dump slider to see the evolution of the 3D far fields as well as the 2D cross-sections in time.

The resulting visualization is shown in Fig. 3.52.

This method of visualizing the far fields can be used for studying properties such as directivity, main and side lobe pattern, radiation strength, etc.

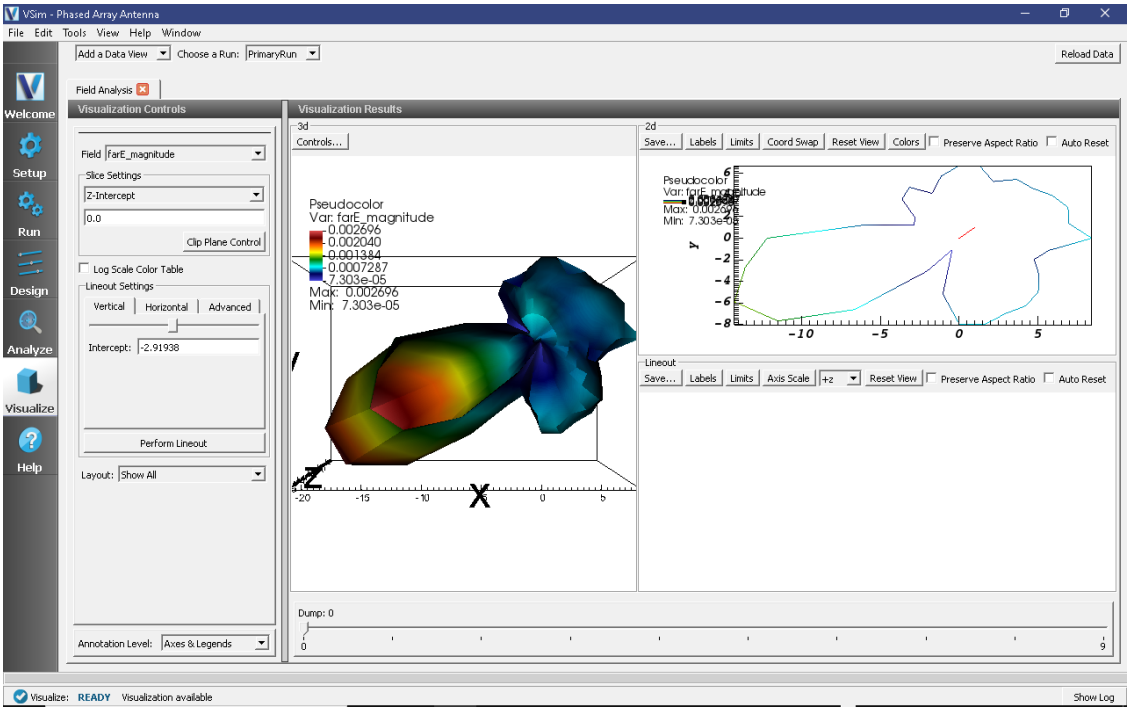


Fig. 3.52: 2D cross-section of the far field patern measured 30 m away from the source.

3.1.12 Antenna on Predator Drone (predatorDrone.sdf)

Keywords:

predatorDrone, far field, radiation

Problem Description

This problem illustrates how to obtain the far field radiation patterns of a current source antenna mounted on a Predator Drone.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Predator Drone example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Antennas* option.
- Select "Antenna on Predator Drone" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with the CAD imported geometry and antenna current distribution accessible to the user. See Fig. 3.53.

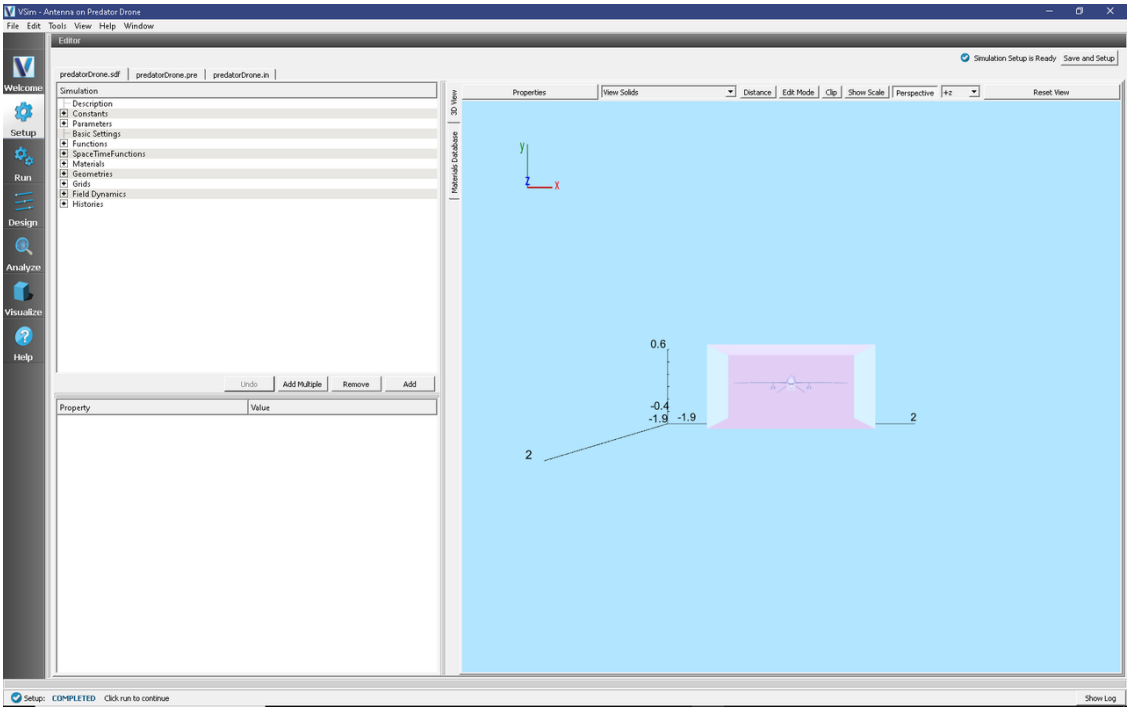


Fig. 3.53: Setup Window for the Predator Drone example.

One can click and unclick the grid, the farFieldBox0 in the histories, the current distribution, and so forth to see where those objects are. One can change locations through changing the values under Constants or, in some cases, the numbers directly in the objects.

Simulation Properties

This file allows the modification of antenna operating frequency, source amplitude, dimensions of the source and the Kirchhoff box by changing the associated variable values under the Constants.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.306815867636764e-12
  - *Number of Steps*: 2500
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.54.

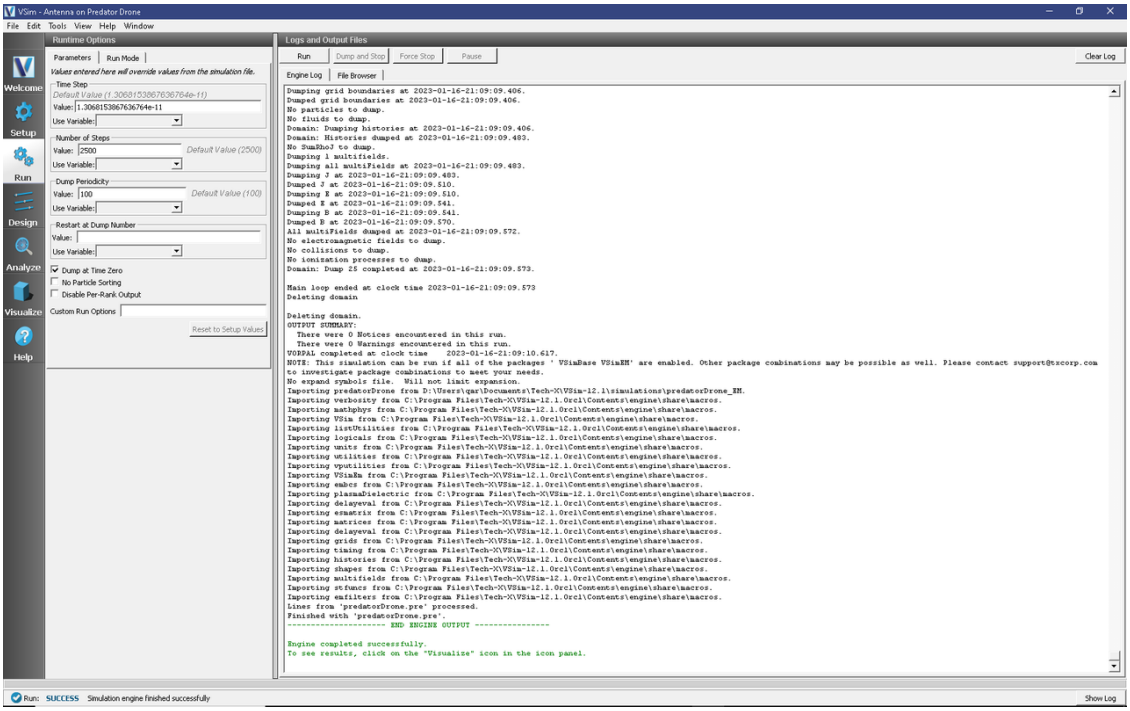


Fig. 3.54: The Run Window at the end of execution.

Analyzing the Results

After the run, one must analyze the Kirchhoff box data to get the far fields. This is done as follows:

- Proceed to the Analysis window by pressing the *Analyze* button in the left column of buttons.
- Click on *computeFarFieldFromKirchhoffBox.py*, then click on the *Open* button.

If you want, you can grab the dividing bar between the list of Analyzers in the *Analysis Controls* window and the *Analysis Results* window, and slide it left to cover up the *Analysis Controls* window, making more room for the *Analysis Results* window.

After performing the above actions continue as follows to compute the far field radiation pattern:

- In the resulting list, select *computeFarFieldFromKirchhoffBox* and press *Open*
- The analyzer fields should be filled as below:
  - *simulationName*: predatorDrone
  - *fieldLabel*: E
  - *farFieldRadius*: 1024.0
  - *numPeriods*: 0.25
  - *numFarFieldTimes*: 2
  - *frequency*: 1.0e9
  - *numTheta*: 45
  - *numPhi*: 60
  - *zeroThetaDirection*: (0,0,1)

  - *zeroPhiDirection*: (1,0,0)
  - incidentWaveAmplitude - blank
  - incidentWaveDirection - (0,0,0)
  - varyingMeshMaxRadius - 1024.0
  - principalPlanesOnly - checked
- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 3.50.

If you want the script to run faster, lower numTheta to 8 and numPhi to 16.

- Press the *Analyze* button in the top left of the window.

At completion, you will see Fig. 3.55. The far field data is written to vsh5 files in the simulation directory.

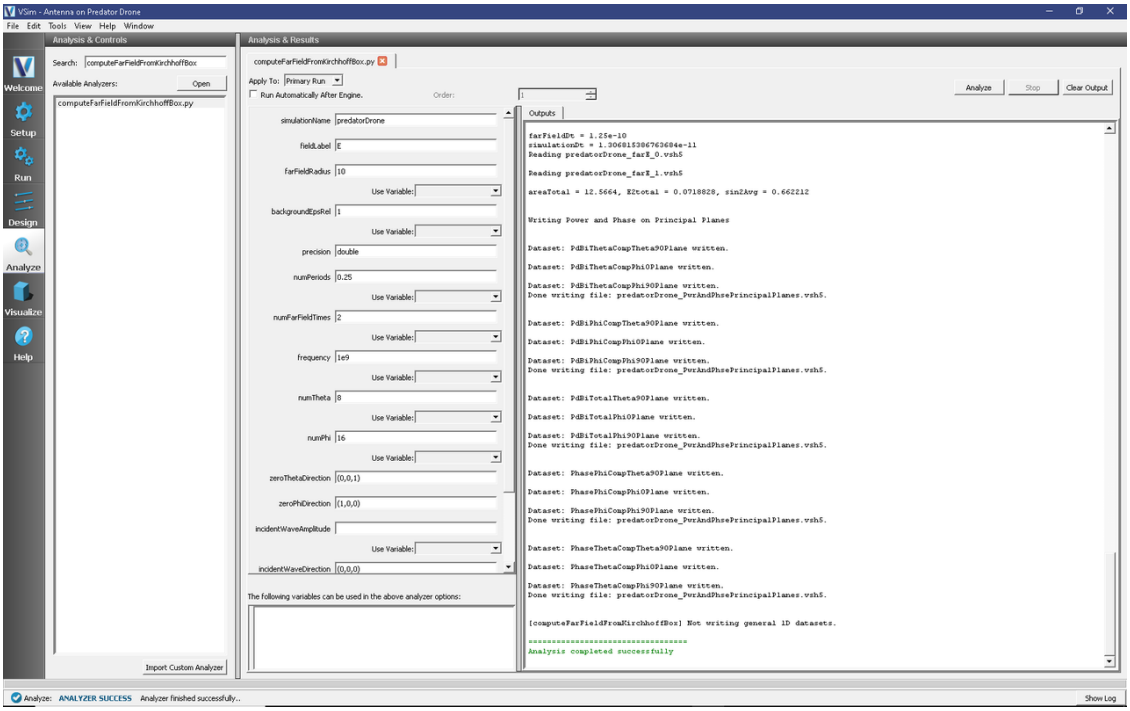


Fig. 3.55: The Analysis window at the end of execution.

Visualizing the Results

Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The radiation pattern in real space can be visualized by doing the following:

- Expand *Scalar Data*
- Expand *E*
- Select one of the scalar fields, such as E_x
- Check *Clip Plot*
- Check *Display Contours* and set the number of contours to 10

- Set minimum to -75 and maximum to 60
- Click on *Plane Controls*, change only Plane3 and set Z to -1.
- Expand Geometries
- Check *poly_surface (predatorGeomSolid)*
- Move the Dump slider to dump 15 to see the same far field as Fig. 3.56.

An odd number of contours will result in a contour at zero field, which often leads to a less attractive plot with the zero contour filling up the space. Thus, in this case, an even number of contours is suggested.

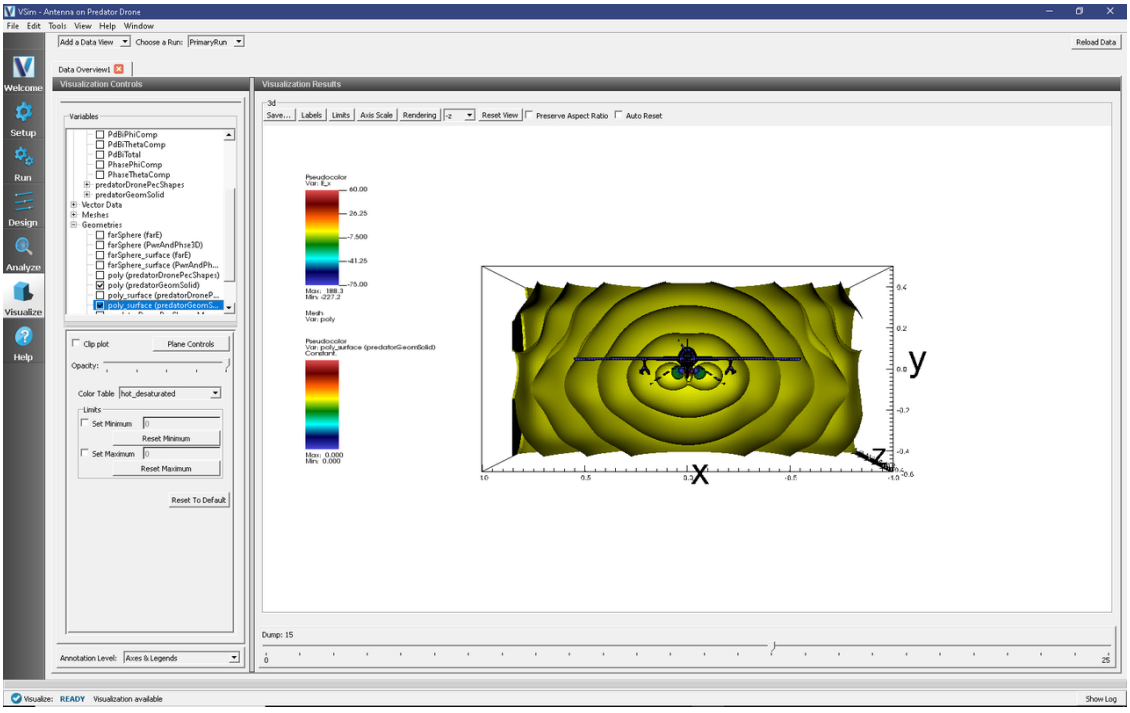


Fig. 3.56: The radiation pattern in real space

The far field radiation pattern, which was computed in the section on *Analyzing the Results* can also be displayed. Remove the previous image. Then check the *PdBi* box under Scalar Data, and move the dump slider to the beginning dump. You will see a 3D radiation surface, representing the Far Field radiation power level at each angle that was processed. Colors and radius are in units of dBi, decibels relative to isotropic. A notable peak in the radiation pattern is evident in the forward, upward, and downward directions, as seen in Fig. 3.57.

Further Experiments

Upon close inspection you will note that the mesh size is slightly too large to fully resolve the thin wing structures of the tail section. You can experiment with smaller cell size to resolve these structures. Beware that more cells will increase the run time.

This example can be extended to meet any antenna placement problem with by addition of parameters to define the current distribution center. The vertical extent of the simulation box could be shrunk to reduce the simulation time, which would then allow greater resolution of the wavelength.

The main driver of simulation accuracy is the number of points per wavelength. Because of this lower frequencies will simulate in less time as they require fewer cells to achieve the same resolution in the wave.

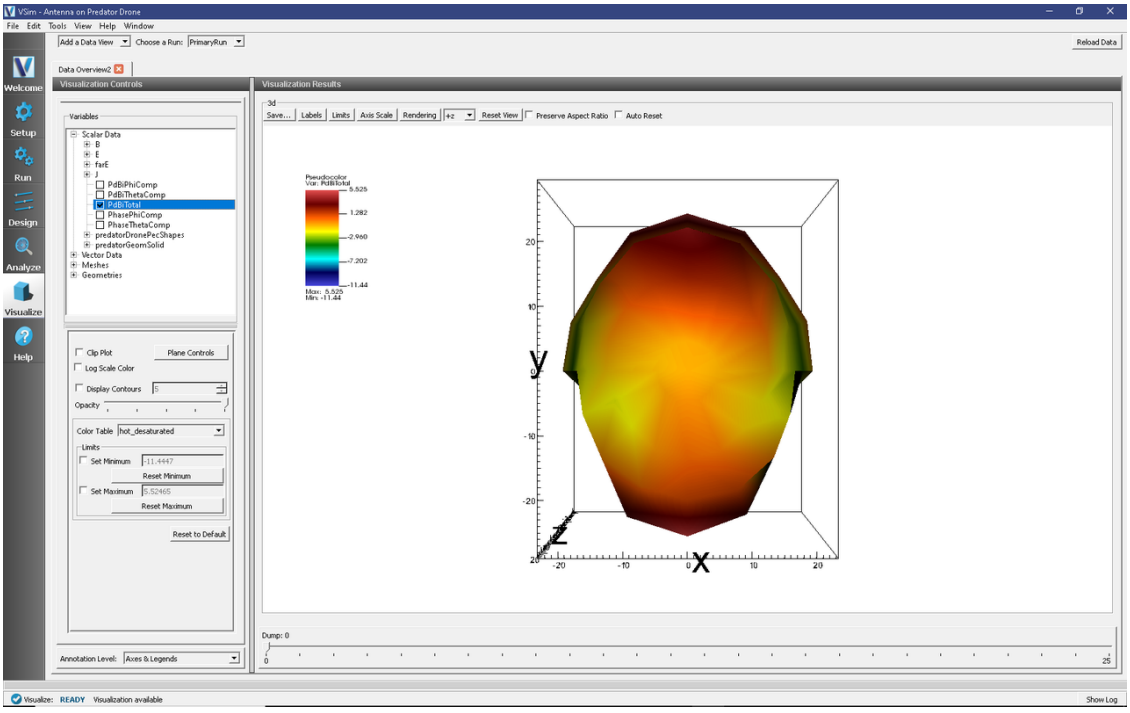


Fig. 3.57: The far field radiation pattern

3.2 Electrostatics

3.2.1 Like-Charge Dipole (esChargedSpheres.sdf)

Keywords:

electrostatics, like-charge dipole

Problem description

This Like-Charge Dipole simulation computes the electrostatic potential and field for a dipole of two spheres with given radius at the same potential.

This simulation can be performed with a VSimEM or VSimPD license, with Composer licensed for Visual Setup.

Opening the Simulation

The Like-Charge Dipole example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Electrostatics* option.
- Select *Like-Charge Dipole* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.58. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

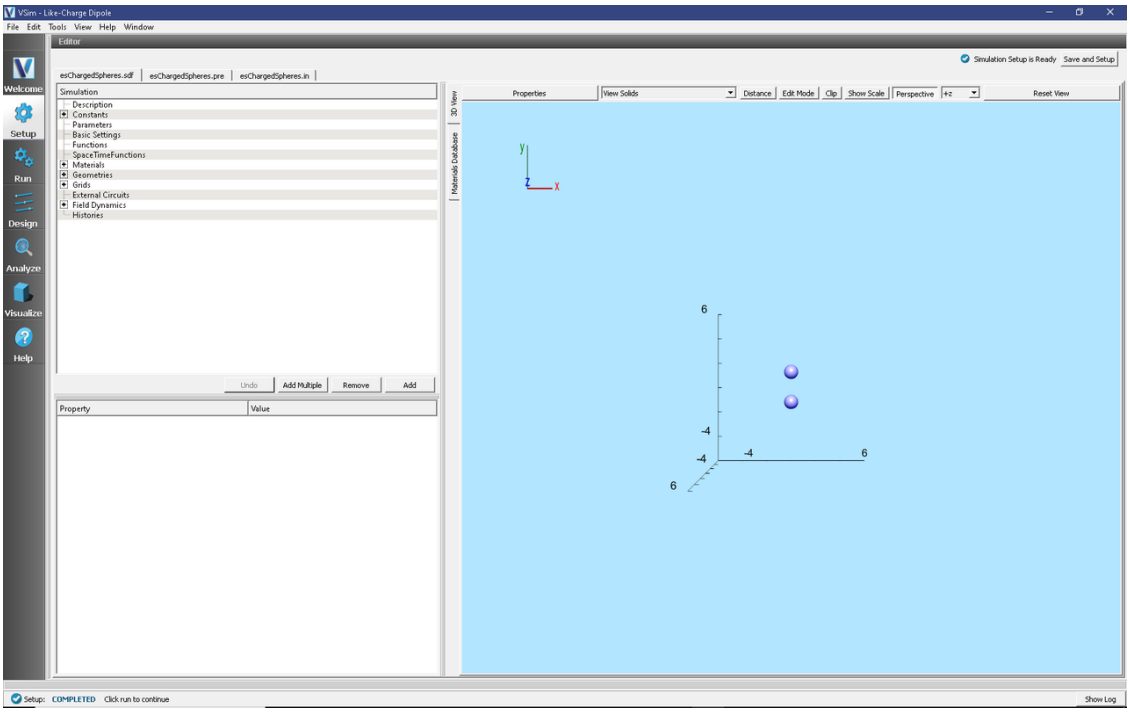


Fig. 3.58: Setup Window for the Like-Charge Dipole example.

Simulation Properties

This simulation uses visual setup to create a simple dipole. To do this we employ a few simple techniques such as Constructive Solid Geometries (CSG), and field Boundary Conditions. The dipole is constructed as two spheres of identical size. A Dirichlet boundary condition with the desired voltage is applied on both spheres.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.59.

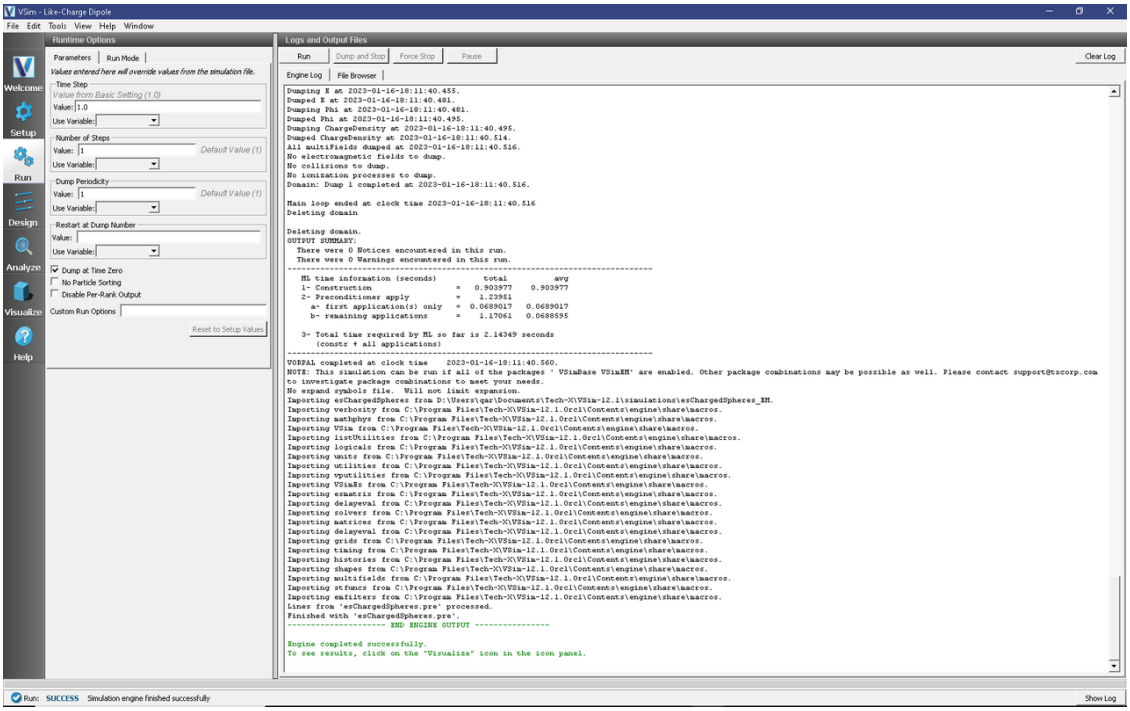


Fig. 3.59: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electrostatic potential of the dipole as seen in Fig. 3.60 do the following:

- Expand *Scalar Data*
- Select *Phi*
- Select *Display Contours*
- Select *Clip Plot*

Further Experiments

Change the distance between spheres and see how the electric field changes.

Change the sphere radius and see how the electric field changes.

Change the sphere's potential to observe a change in the electric field.

Determine how the electric field changes with varying resolution.

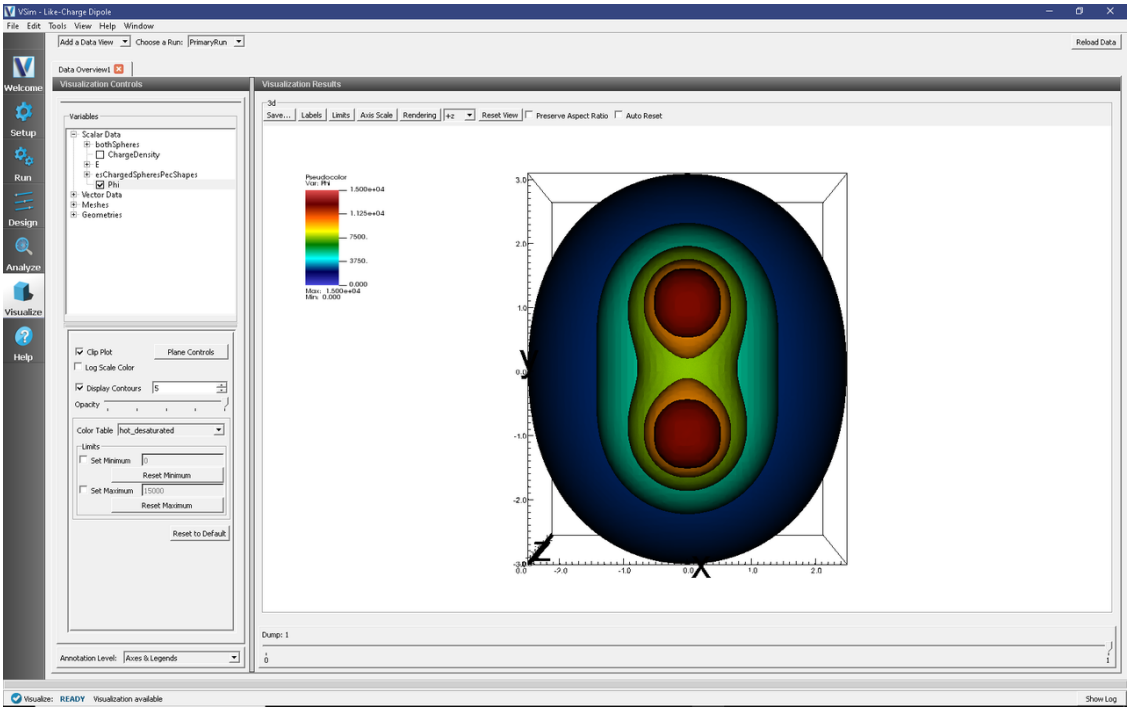


Fig. 3.60: Visualization of Like-Charge Dipole as a pseudocolor plot.

3.2.2 Dielectric in Electromagnetics (dielectricInEM.sdf)

Keywords:

dielectric, electromagnetics, capacitor

Problem Description

This simulation and the *Dielectric in Electrostatics (dielectricInES.sdf)* demonstrate the differences between simulating dielectric materials with electrostatic and electromagnetic solvers. They also demonstrate some of the more general differences between electrostatic and electromagnetic simulations.

Both of these simulations represent the same physical system: a slab of dielectric between two metal plates. The simulation grid is one square meter with a .75m x .25m slab of dielectric centered between the plates.

Unlike in the electrostatics simulation, in this simulation the full, coupled set of Maxwell's equations are considered, so more nuanced and complete physics will be represented in this simulation. The trade-off is that the simulation will take longer to run, and a user has to have a deeper, more fundamental understanding of the physics relevant to the simulation.

For situations when the nuanced and detailed physics is important, an electromagnetic solver is often required. For other cases, the nuances and details are not important and an electrostatic approximation is an appropriate simplification of the system.

A rule of thumb to consider when deciding between electromagnetic and electrostatic solvers is how the wavelength of an EM wave, λ_{EM} compares to the length scale of the simulation domain, L_s. If λ_{EM} is smaller than L_s, an electromagnetic solver will be more appropriate. In other words, if many EM waves of interest fit inside the simulation grid, an electromagnetic solver will be necessary.

This criterion, $\lambda_{EM} < L_s$, is equivalent to a criterion on the period of the EM oscillation T_{EM} and the time it takes light to cross the simulation domain, T_γ. Divide both sides by the speed of light and we get $T_{EM} < T_\gamma$. In this limit, information about changes to fields will not be able to travel across the simulation domain within one timestep, so we must pick a solver that respects relativity.

This simulation can be run with a VSimEM, VSimVE, or VSimPD license.

Opening the Simulation

The Dielectric in Electromagnetics example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Electrostatics* option.
- Select *Dielectric in Electromagnetics* and press the *Choose* button.
- In the resulting dialog box, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 3.61.

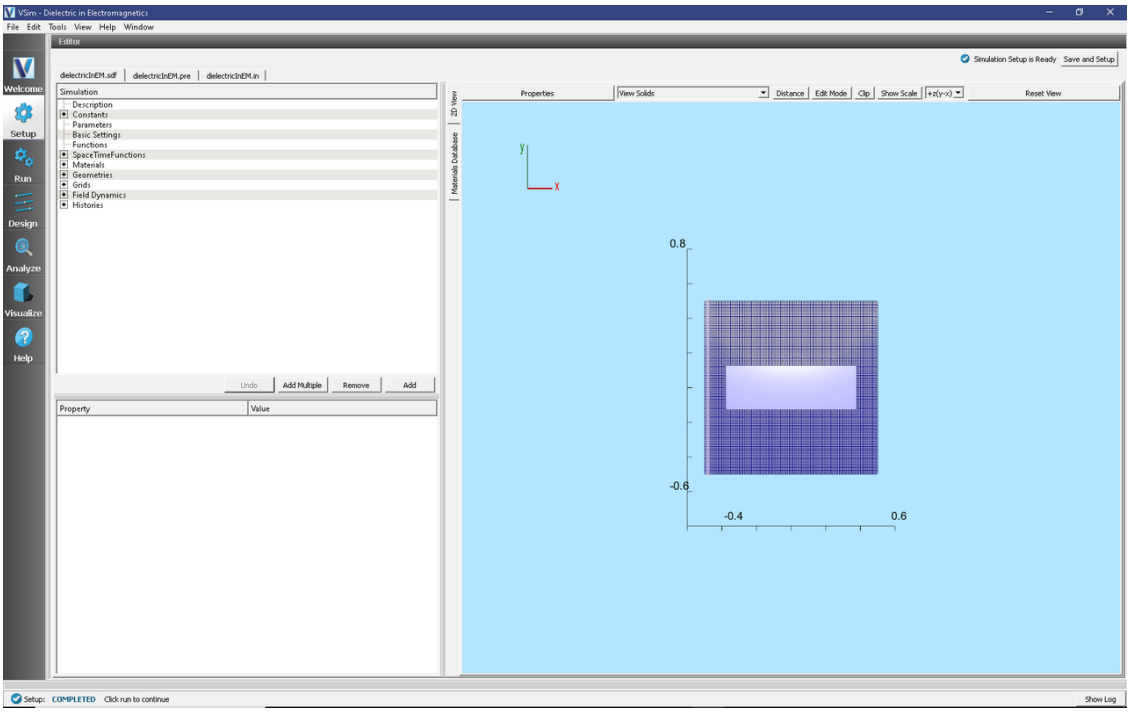


Fig. 3.61: Setup Window for the Dielectric in Electromagnetics example.

Simulation Properties

In full electromagnetics, the electric potential is a quantity that must be derived from line integrals of the electric field since it is not directly calculated (as is the case for electrostatics). This makes setting up potential differences between objects a little more complicated. So, to set a potential difference between the top and bottom plates in this simulation, a Distributed Current is set to run from the bottom of the simulation (lower y) to top (upper y).

The upper and lower y boundaries are set as a "PEC", a perfect electrical conductor, under the Field Boundary Conditions element. The left and right walls (lower and upper x), are set as open boundaries, and so will let EM waves pass through unaffected.

The current effectively moves positive charge from the bottom boundary of the simulation to the top boundary making the top plate positively charged and the bottom plate negatively charged. This will result in an electric field that points down towards the lower y boundary, similar to the *Dielectric in Electrostatics (dielectricInES.sdf)* example.

The functional form of the current is a Gaussian, $I(t) = e^{-(t-t_0)^2/(2*\sigma^2)}$. The constants t_0 and σ are set with the constants DRIVE_PEAK_TIME and DRIVE_SPREAD, respectively. The default values for these constants were chosen somewhat arbitrarily, but so that the simulation results will resemble those from the electrostatic simulation.

The DRIVE_SPREAD (standard deviation of the current Gaussian), will set a time scale for the electromagnetic waves that will propagate through this simulation, so DRIVE_SPREAD was chosen to be much larger than the timestep so that the EM wavelength was much larger than the simulation domain.

Ideally, the PEAK_DRIVE_TIME would be much larger than the DRIVE_SPREAD because whenever a function is used to set a current, the current should be initialized so that $I(0) = \frac{dI}{dt}|_{t=0} = 0$. That is, the current and its derivative are both zero when the simulation begins. This will reduce any "ringing" that may occur by an abrupt turn-on. The default value for PEAK_DRIVE_TIME for this simulation is 0, so at least the derivative of the current is zero. The *Future Experiments* section outlines how to do a higher fidelity simulation, and it will demonstrate the power of the electrostatic approximation. The *Dielectric in Electrostatics (dielectricInES.sdf)* simulation takes only one timestep to run.

To add the dielectric slab to the simulation, first a "Box" primitive shape was added under *Geometries* → *CSG*. Then the `Sapphire` material was added to the simulation and set as the material for the boxDielectic material.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.3502087599863072e-12
  - *Number of Steps*: 2000
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.62.

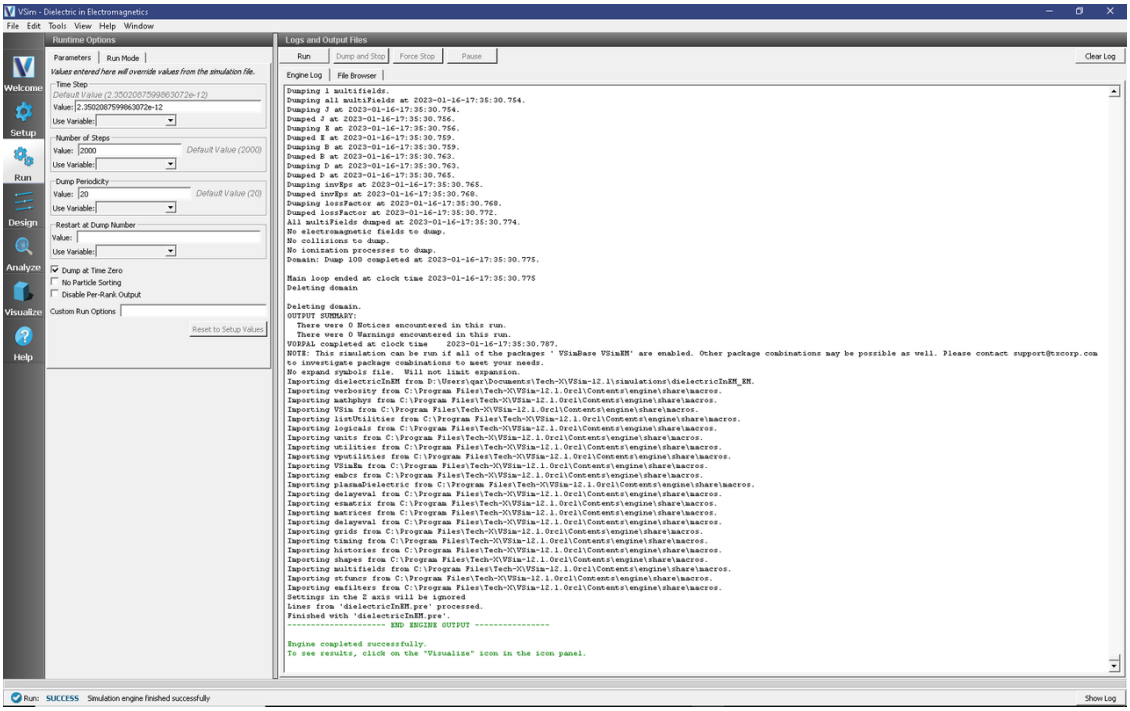


Fig. 3.62: The Run window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

1. Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
2. With the *Data Overview* tab open, expand *Scalar Data* then expand *E*.
3. Check the box for *E_y*. This will plot the y-component of the electric field.
4. Scroll through the dumps to see how the y-component of the electric field changes with time. The last dump is shown in Fig. 3.63.

As you scroll through the dumps, you will notice that a wave front propagates through the simulation from left to right. We see this wave front because electromagnetics respects relativity. Any electromagnetic signal can travel no faster than the speed of light. When the simulation begins, there is no voltage difference between the upper and lower plates. At $t = 0$, the current turns on and then a signal begins traveling (at the speed of light) from the left to the right that a voltage difference has been established.

Additionally, you can see reflections of this wave off the vacuum-dielectric interface, and refracted waves entering dielectric. There is also some "ringing" which appears as ripples in the electric field from the abrupt current turn on.

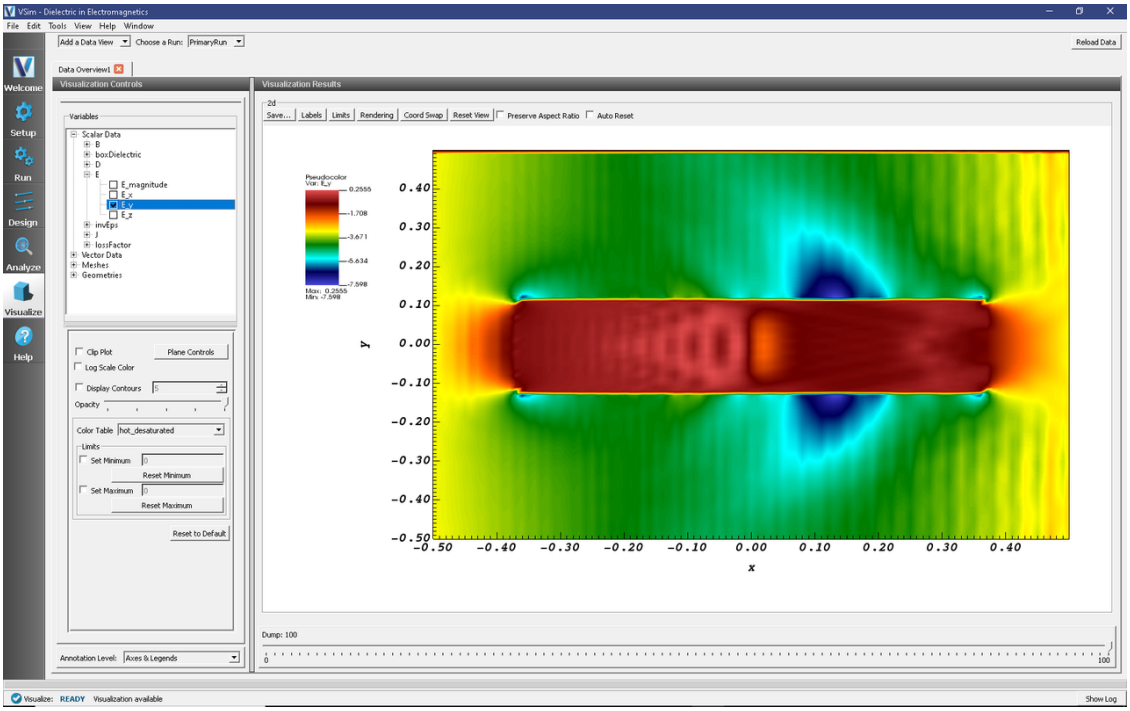


Fig. 3.63: The y-component of the Electric Field.

Further Experiments

1. Experiment with different values of the DRIVE_PEAK_TIME and DRIVE_SPREAD constants that tune the Gaussian current. Try a value of 10^{-7} for the DRIVE_PEAK_TIME while leaving the DRIVE_SPREAD at its default value of 10^{-8}. This will shift peak of the Gaussian far beyond the end of the simulation, so that the smooth, flat, far left tail of the Gaussian, with values close to zero, sets the current. What do you notice about the noisiness of the y-component of the Electric Field? How much longer would you have to run before the current ramps up to its maximum value then drops back down to zero to produce the image below?

2. Then put the DRIVE_PEAK_TIME back to the original, default value of $10^{-}10$ and change the DRIVE_SPREAD to a much smaller value, like $10^{-}10$. Given the discussion about timescales in the *Problem Description* and *Simulation Properties* sections what changes would you expect to see?

3. Normalize the current Gaussian so that you can control the final value of the y-component of the electric field.

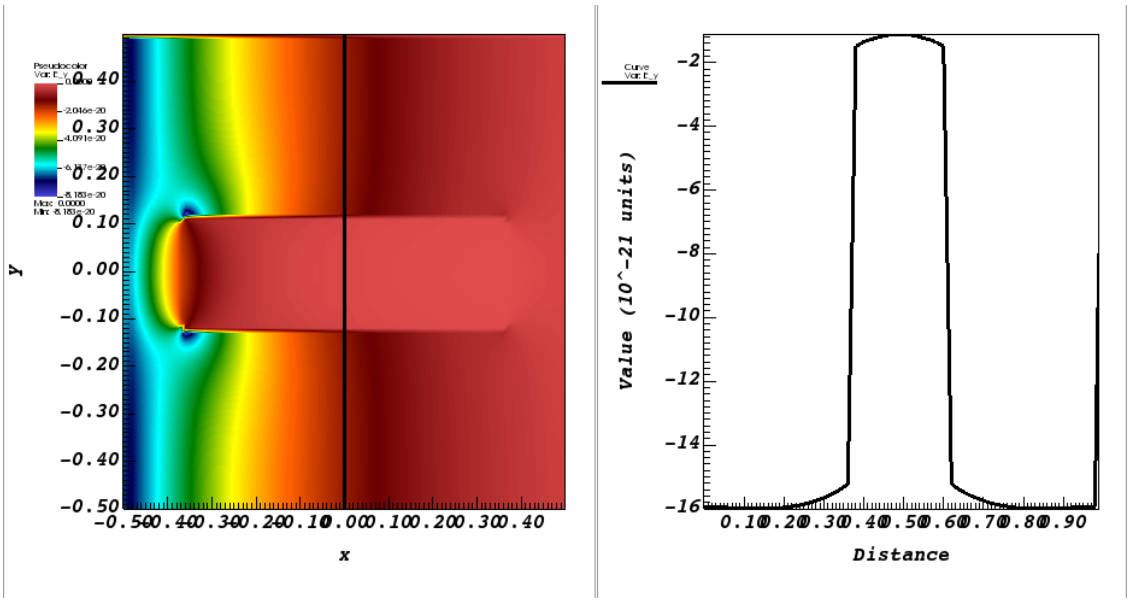


Fig. 3.64: The y-component of the electric field after the current ramped up and then back down to zero.

3.2.3 Dielectric in Electrostatics (dielectricInES.sdf)

Keywords:

dielectric, electrostatics, capacitor

Problem Description

This simulation and the *dielectricInEM* demonstrate the differences between simulating dielectric materials with electrostatic and electromagnetic solvers. They also demonstrate some of the more general differences between electrostatic and electromagnetic simulations.

Both of these simulations represent the same physical system: a slab of dielectric between two metal plates. The simulation grid is one square meter with a .75m x .25m slab of dielectric centered between the plates. The electric potential and electric field are solved over the entire domain.

Electrostatics is an approximation of the full set of Maxwell's equations. According to Faraday's law,

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}.$$

In the electrostatic limit, fields change slowly. More precisely, $\frac{\partial B}{\partial t} \approx 0$, so that any curling electric field is negligible compared to the full electric field. When curling electric fields can be neglected, the electric field is a conservative field and can be written as the gradient of a scalar function. This scalar function is the electric potential, or voltage, and satisfies Poisson's equation

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}.$$

Electrostatics is appropriate if the shortest wavelength of interest, λ_{EM} is much longer than the length scale of the simulation L_s. This criterion, $\lambda_{EM} > L_s$ respects the "fields change slowly" heuristic. Divide both sides of the

expression by the speed of light and we get that the period of an electromagnetic oscillation is longer than the time it takes light to cross the simulation domain. In this limit, any change to a field that occurs within a timestep will have time to propagate throughout the simulation domain within the same timestep.

As can be seen in Poisson's equation, electrostatics does not respect relativity, since any change in ρ will instantaneously change the electric potential everywhere in the simulation. So, it is important to respect the $\lambda_{EM} > L_s$ criterion when doing electrostatics, otherwise, the simulation might neglect some important physical effects.

This simulation can be run with a VSimEM, VSimVE, or VSimPD license.

Opening the Simulation

The Dielectric in Electrostatics example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Electrostatics* option.
- Select *Dielectric in Electrostatics* and press the *Choose* button.
- In the resulting dialog box, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 3.65.

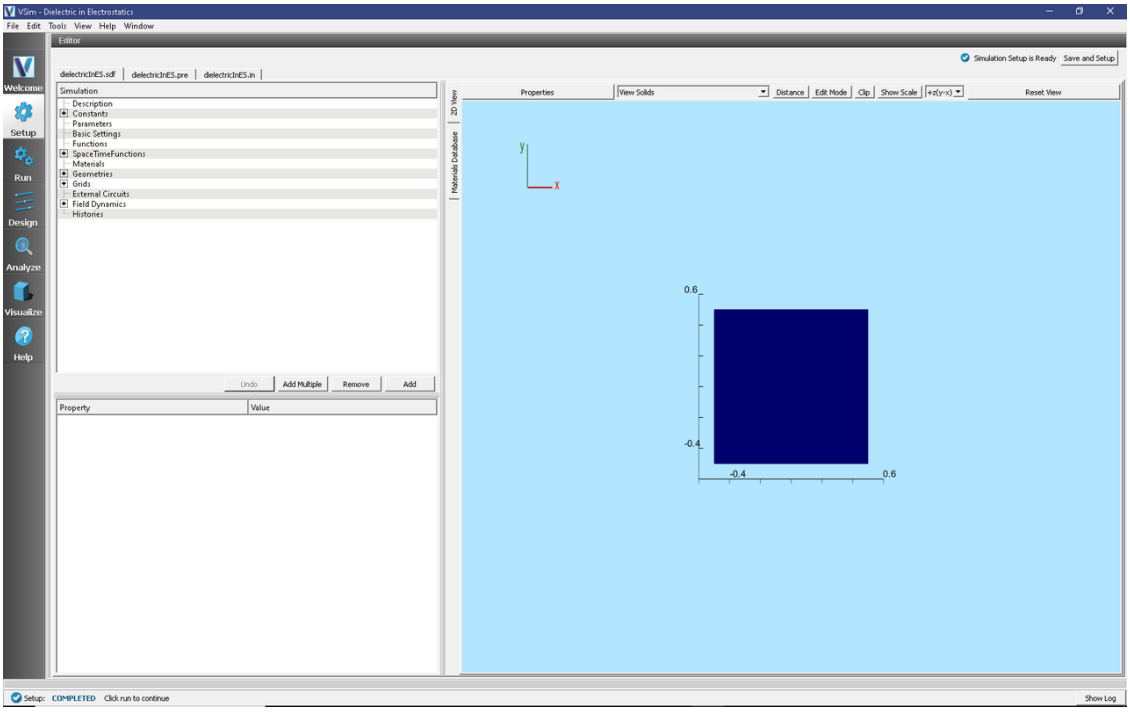


Fig. 3.65: Setup Window for the Dielectric in Electrostatics example.

Simulation Properties

In this simulation, voltages of 10.0 V and 0.0 V are set on the upper and lower boundaries (respectively) with Dirichlet boundary conditions. Neumann boundaries are used on the left and right walls of the simulation domain. In vacuum, this would set up an electric field of 10 V/m pointing down.

A dielectric is introduced to the simulation using a spacetime function `dielectricSapphire`. Sapphire has a relative dielectric constant, $\epsilon_r = \frac{\epsilon_{sapphire}}{\epsilon_0}$, of 9.8. Through the use of Heaviside functions, we set the relative permittivity to be 9.8 in a rectangular region between $x = \pm.375$ meters an $y = \pm.125$ meters and 1 everywhere else.

In the setup tree, the `dielectricSapphire` function is set as the *relative permittivity* under *Field Dynamics* → *PoissonSolver*.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.66.

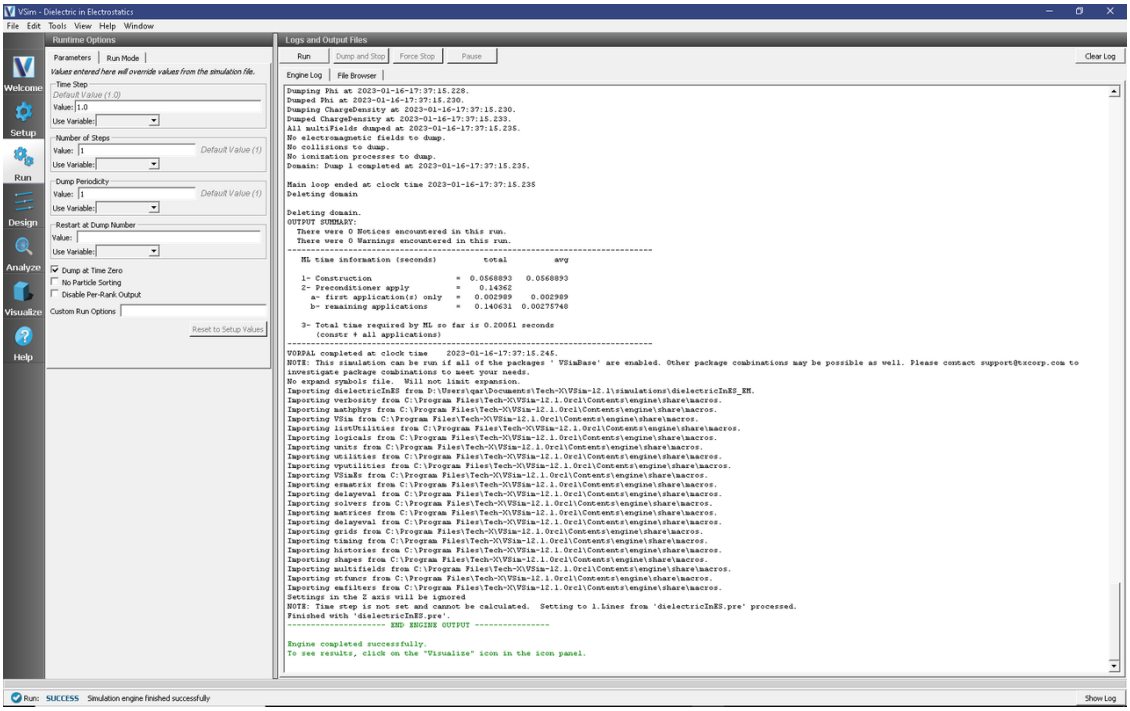


Fig. 3.66: The Run window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

1. Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
2. With the *Data Overview* tab open, expand *Scalar Data* then check the box for *Phi*.

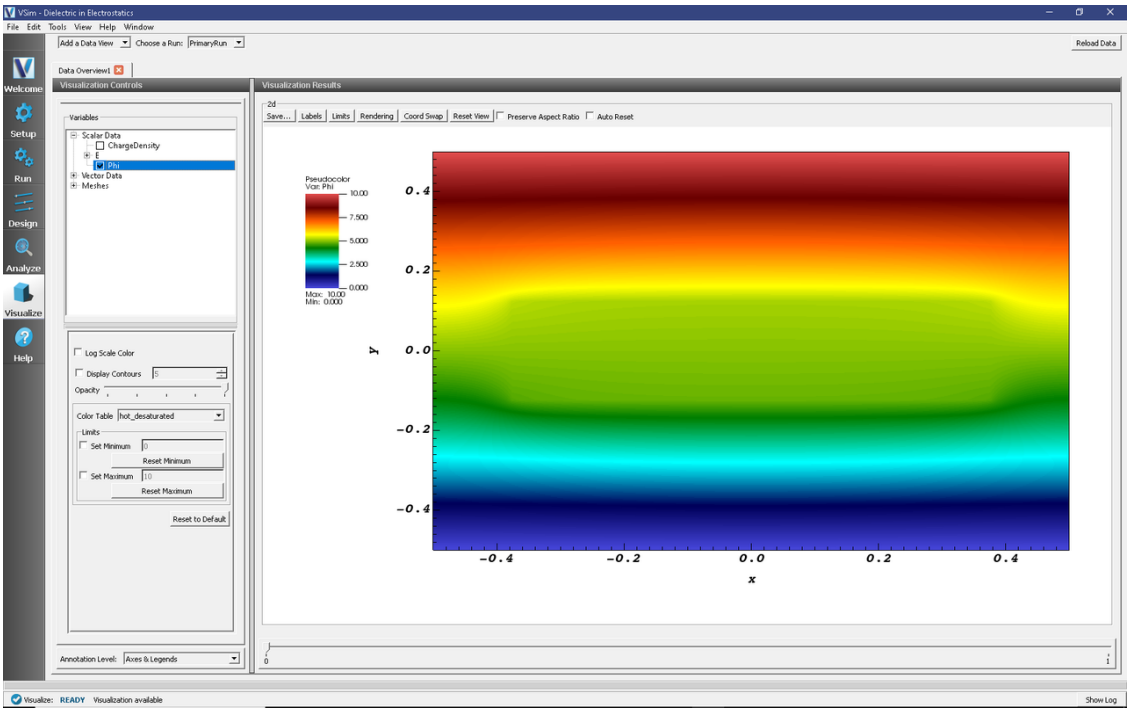


Fig. 3.67: The electric potential between the two parallel plates.

4. For a closer look at the potential, open the *Field Analysis* visualization tab by selecting it from the *Add a Data View* drop down menu at the very top right of the VSim Window.
5. In the new *Field Analysis* tab, from the *Field* drop down menu select “Phi.”
6. The user can switch the location of the line out with the options on the left side of the screen.
7. Shown below is a plot with a horizontal line out at a position $y = .18$ meters. Don’t forget to press the *Perform Lineout* button after adjusting the line out settings!

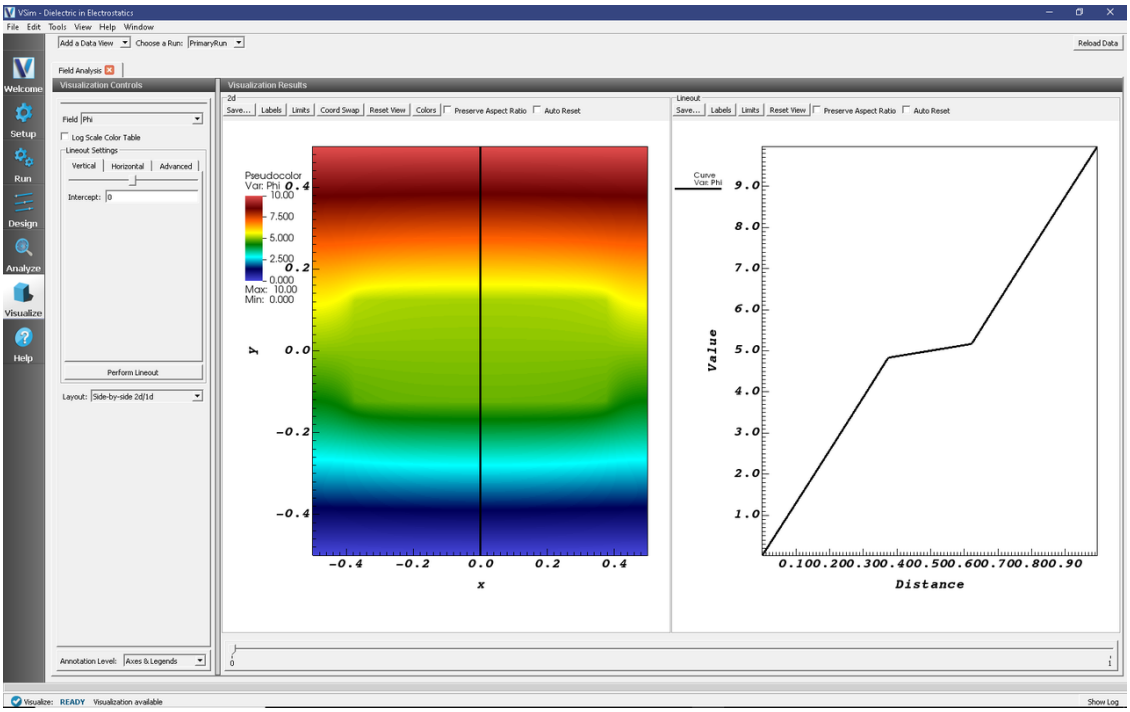


Fig. 3.68: Field Analysis tab showing the electric potential along the black vertical line.

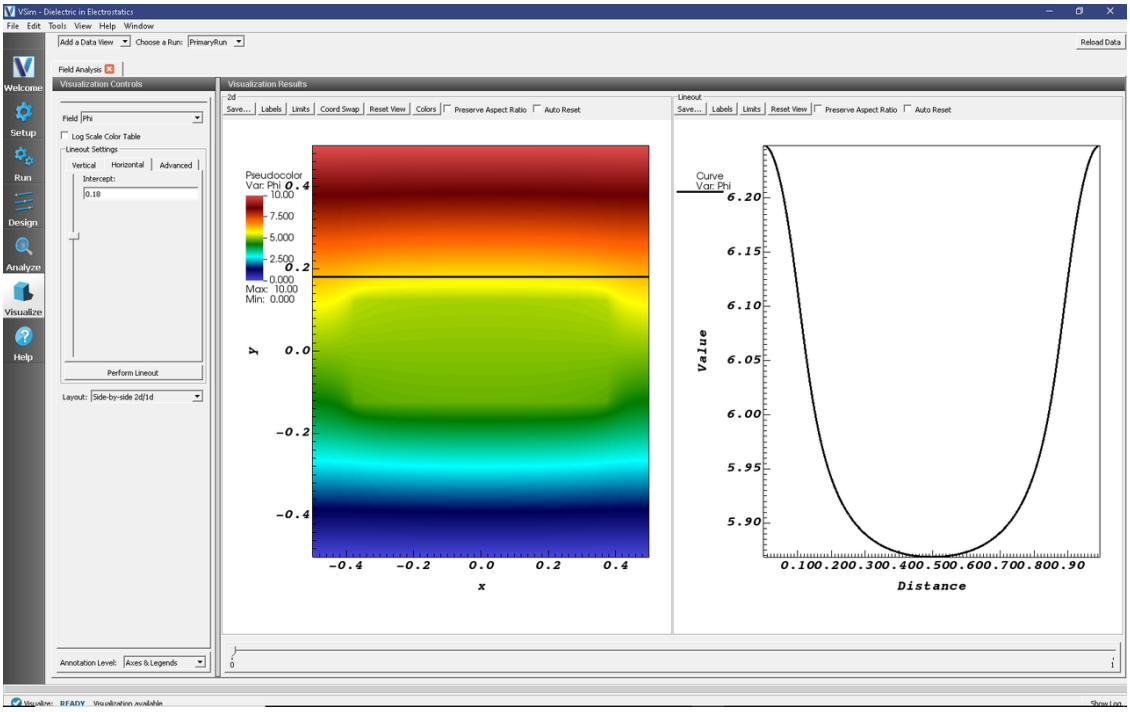


Fig. 3.69: Field Analysis tab showing line out in different position.

Further Experiments

Change the dielectric constant, or change the location and area of the dielectric. Add a sinusoidal voltage on the plates.

3.3 Photonics

3.3.1 Multimode Fiber Mode Calculation (multiModeFiberModeCalc.sdf)

Keywords:

`Mode Extraction, Photonic Waveguide, Guided Mode, Semiconductor`

Problem Description

This example demonstrates the process for extracting the effective index and fields of a guided mode by directly solving an eigenvalue equation. The use of permittivity averaging enables second order accuracy in our solution. The waveguide axis runs parallel to the x-axis, and is surrounded by a background cladding with a lower permittivity. We will run the simulation for 1 step and then use the multiModeFiberModeCalc_invEps_0.h5 file to solve for the guided modes using the computeDielectricModes.py analyzer. This analyzer will find the entire basis set of modes for this fiber and output each into a separate .vsh5 file. These mode files can be used to launch the exact modes into your simulation. This process is shown in the multiModeFiberModeLaunchT example.

Eigenmodes in such a simulation have the form:

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(y, z)e^{i(kx-\omega t)}$$

The effective index of refraction of a waveguide mode is given by $\bar{n} = k/k_0$ where $k_0 = \omega/c$. If the waveguide has index of refraction n_w and the cladding $n_c < n_w$, then a *guided* mode will have a modal index in the range, $n_c < \bar{n} < n_w$.

This simulation can be performed with a VSimEM license.

Opening the Simulation

To open this example open an instance of VSimComposer and follow the steps below:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Multimode Fiber Mode Calculation* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, and press the *Save* button to create a copy of this example.

Simulation Variables

Constants This example contains a number of constants defined to make the simulation easily modifiable.

- WAVELENGTH_VAC: The vacuum wavelength (frequency divided by the speed of light) for the eigenmode of interest. In this example we scale all lengths by 1e6. Therefore, a typical 1.55 micron source is simply 1.55 in this example.
- NA: The numerical aperture of the fiber. This defines the background permittivity relative to the core permittivity.
- PERMITTIVITY_CORE: This is the permittivity of the core material as defined in the *Materials* branch and assigned in the *Geometries* branch.
- RADIUS_CORE: The radius of the fiber core.
- RESOLUTION_YZ: The number of cells per core radius in the transverse (y & z) directions.
- RESOLUTION_X: The number of cells per estimated wavelength in the propagation (x) direction.
- CFL_NUMBER: The time step, DT, will be this value times the limit for numerical stability.

Parameters Many parameters in this simulation are defined to assist with launching the mode in a subsequent example, multiModeFiberModeLaunchT. Some important parameters that are relevant to the mode extraction are given below.

- PERMITTIVITY_BG: The permittivity assigned to the background surrounding the core. This is assigned in the *Basic Settings* branch under *background permittivity*.
- NMODES: The approximate number of modes supported by the fiber. Depends on NA, RADIUS_CORE, & WAVELENGTH_VAC. Includes degenerate modes. More accurate for many modes (>20).
- BGNYZ_SOURCE: The starting position for where we will evaluate the transverse permittivity profile on the analyzer tab. Defined for convenience and clarity. This slice is shown as the "source" geometry in the *3D view*.
- ENDYZ_SOURCE: The ending position for where we will evaluate the transverse permittivity profile on the analyzer tab.

Setting up the Simulation

As delivered, the system is set up to generate the data needed to run the computeDielectricModes.py analyzer. To ensure that your simulation has second order accuracy, expand the *Basic Settings* branch and verify that the *dielectric solver* field is set to *permittivity averaging*. This algorithm is a powerful VSim feature. This setting is shown in Fig. 3.70.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 4.160775453374223e-10
  - *Number of Steps*: 1
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.71.

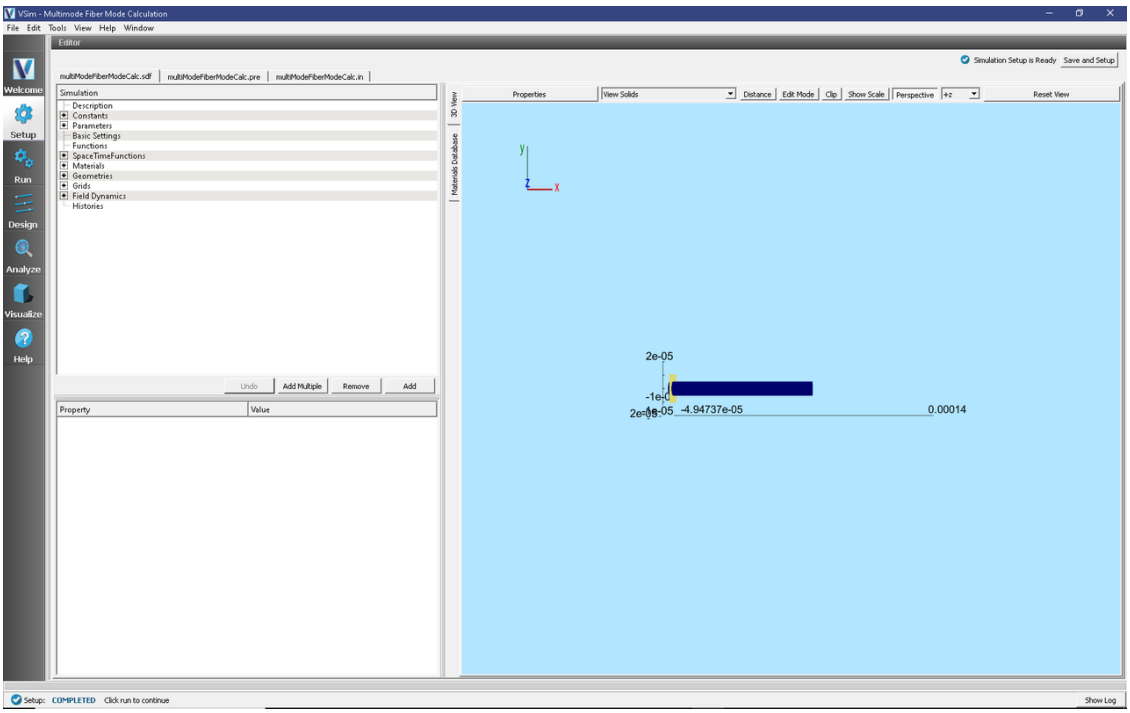


Fig. 3.70: Choosing the second order accurate, *permittivity averaging* for the *dielectric solver* field under *Basic Settings*.

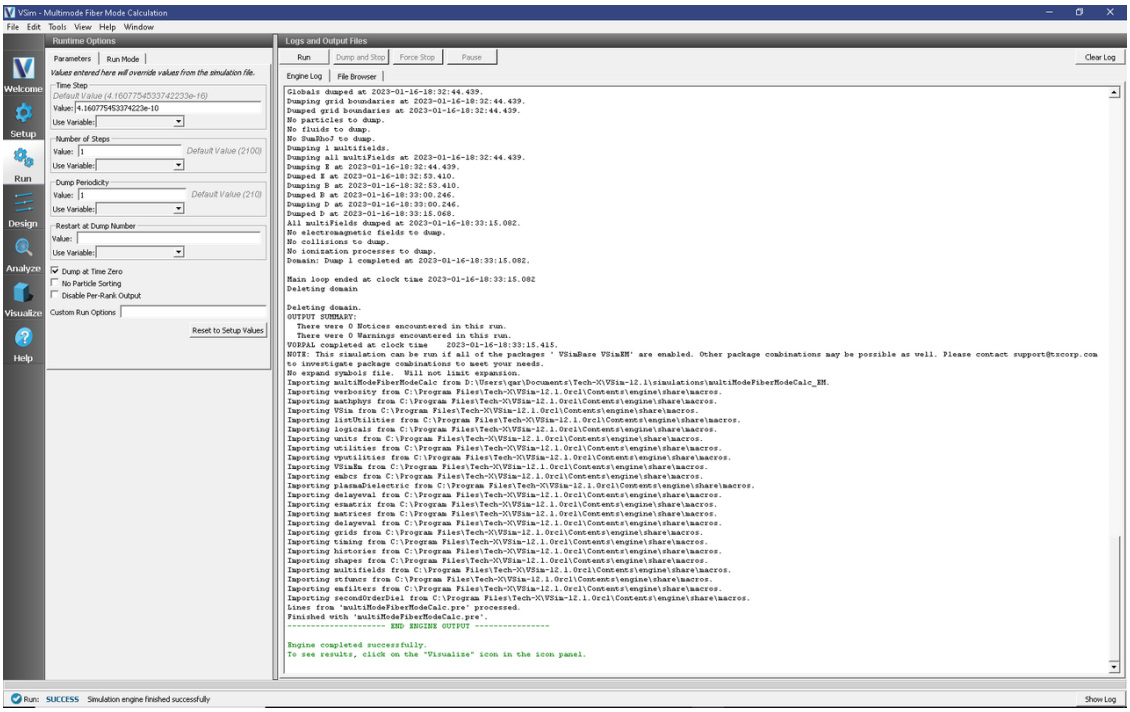


Fig. 3.71: Running the simulation for one step to get the permittivity data for the analyzer. Note that *Dump at Time Zero* is checked.

Solving for the Eigenmodes

After performing the above actions, continue as follows:

- Proceed to the Analyze Window by clicking the *Analyze* button on the left.
- Select *computeWaveguideModes.py* and click *Open* under the list.

Now update the analyzer fields accordingly. Some of these parameters are described above under **Parameters**

- *transverseSliceX*: 0.0
- *transverseSliceLY*: -1.e-5
- *transverseSliceUY*: 1.e-5
- *transverseSliceLZ*: -1.e-5
- *transverseSliceUZ*: 1.e-5
- *vacWavelength*: 1.55e-6
- *nModes*: 25
- *writeFieldProfile*: H,E,D

We set the number of modes (*nModes*) to a value greater than the number of modes we expect. The analyzer will only find guided modes. Also check *Overwrite Existing Files*. Run the analyzer by clicking *Analyze* button in the upper right corner. The analyzer output should resemble Fig. 3.72. We see that the analyzer found 20 modes. They are listed in decreasing order of effective index. After the modes are calculated, the analyzer will dump the solutions to file so they can be visualized - this may take a few minutes.

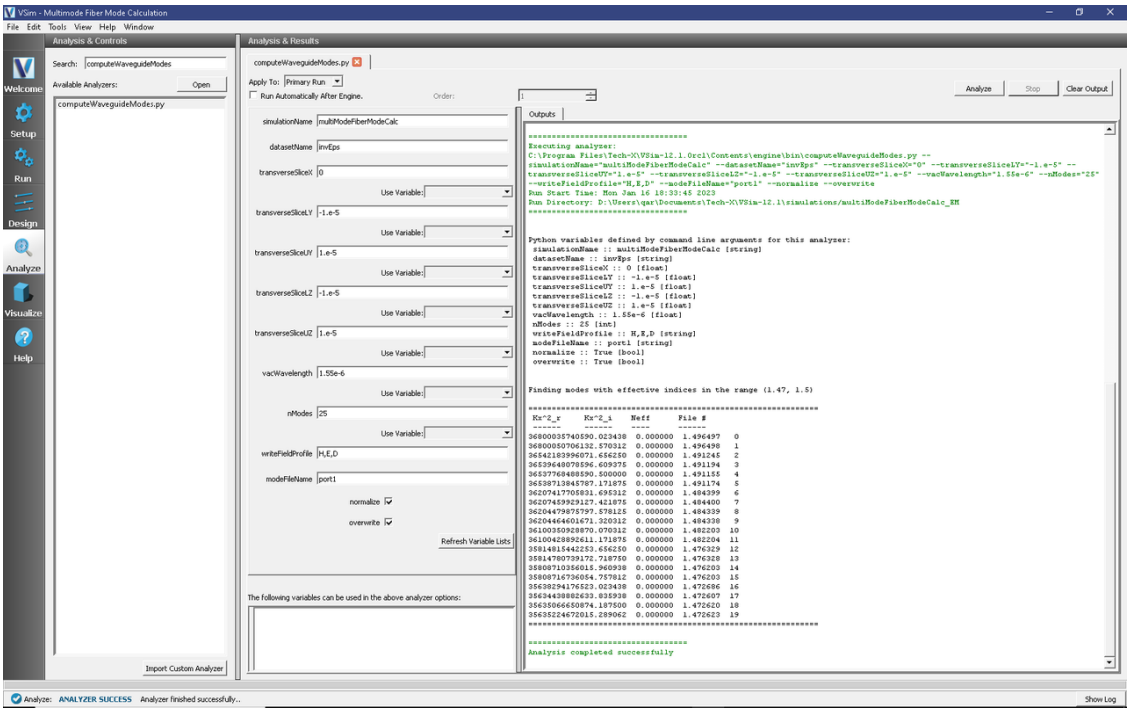


Fig. 3.72: The analyzer window after a successful run of computeDielectricModes.py.

Visualizing the Results

After performing the above actions proceed to the Visualize window by pressing the *Visualize* button in the left column of buttons. You may need to *Reload Data* (bottom left). Visualize an eigenmode by following these steps:

- From the *Data View* dropdown, select *Data Overview*.
- Expand *Scalar Data*, expand *EigenD*, and select *EigenD_z*.
- Below the visualization, the dump slider will allow you to scroll between the modes. Scroll to dump number 13.

The resulting visualization pane should resemble Fig. 3.73.

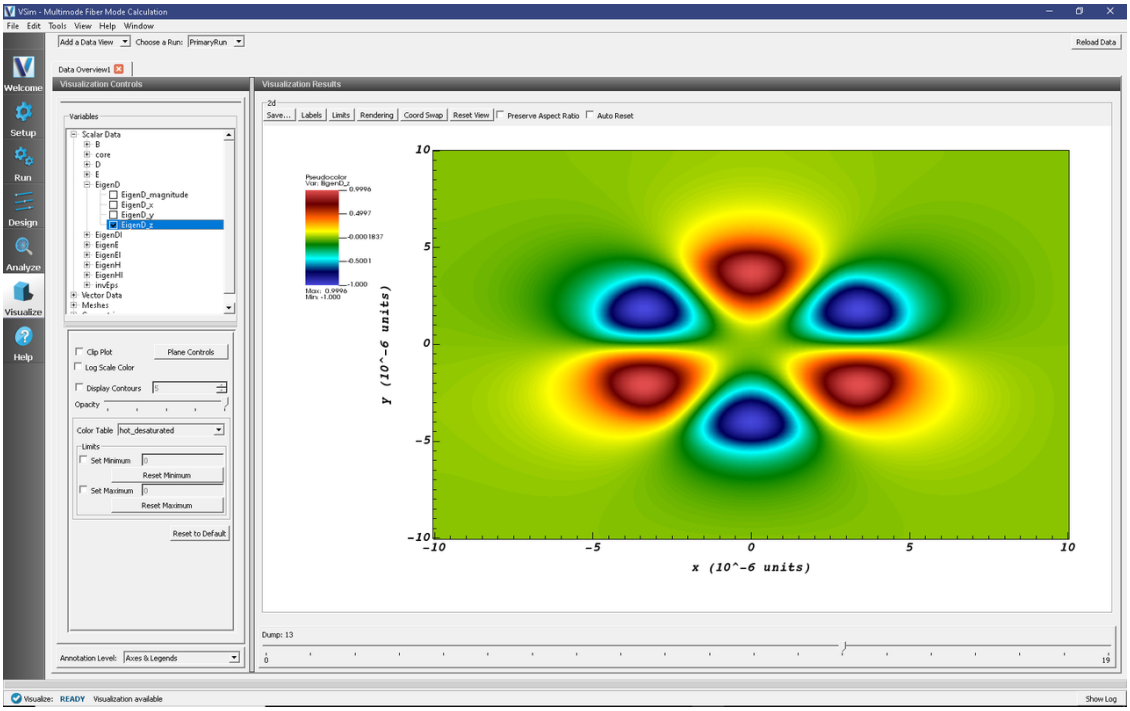


Fig. 3.73: The visualization pane showing the z component of the D field of the M=1, L=3 mode.

One can select other components of the H, E, or D field to see how they vary for the eigenmodes. These eigenmodes are now saved in .vsh5 files in the folder where the simulation was run.

Further Experiments

Increase the radius, decrease the wavelength, or increase the numerical aperture on the Setup window and rerun the simulation and analyzer to see higher order modes.

Once you have your desired mode, launch it down the waveguide using the procedure laid out in the multiModeFiberModeLaunchT example.

One can run a full convergence study of eigenmode effective indices by varying the RESOLUTION_YZ constant in the Setup window and re-running the simulation and mode extraction script. A plot of the effective index as a function of transverse cell area is shown in Fig. 3.74. The linear relationship shows the second order accuracy of our dielectric algorithms.

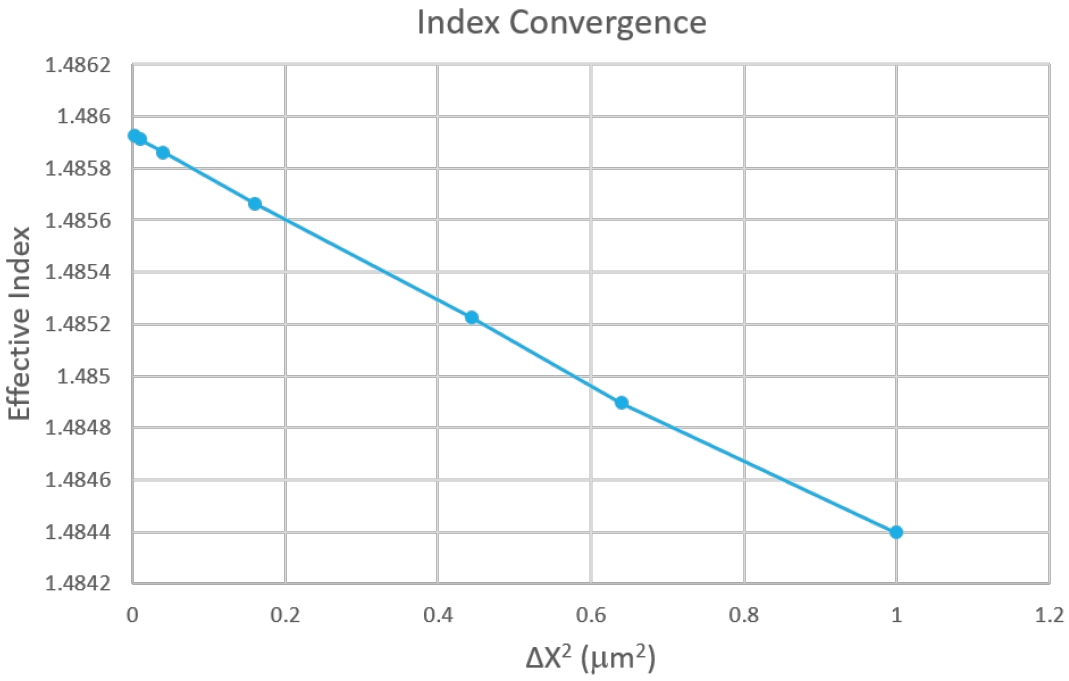


Fig. 3.74: The effective index as a function of transverse cell area for an eigenmode.

3.3.2 Multimode Fiber Mode Extraction (multiModeFiberModeExtract.sdf)

Keywords:

Photonics, dielectric fiber

Problem Description

This example illustrates how to compute the modes of a cylindrical fiber for a given propagation constant, β, which, because the primary direction of propagation in VSim is along the $x - axis$, is also denoted as k_x. The calculation is performed using excitation of a system with only two cells in the $x - dimension$. (The simulation can be performed with one cell in x, but this cannot be easily visualized so two are used instead.) This document will show how to extract the modes and their frequencies, as well as how to get a text-based setup file for further exploration, including solving for the propagation constant as a function of the frequency.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Multimode Fiber Mode Extraction example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Multimode Fiber Mode Extraction* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.75. Expanding the Constants section of the Simulation Tree shows the user-defined constants of this simulation:

LENGTH_UNIT (real):
The length-scale of the simulation. All lengths, such as that of the fiber radius and box size, are divided by this number to make the geometry lengths of order unity as needed by the geometry engine. In this case, LENGTH_UNIT is unity, so it has no effect.

WAVELENGTH_VAC (real):
Wavelength of the signal in vacuum. Determines the excitation frequency.

N_EFF (real):
Estimate of the value of n_{eff} of the expected modes. This determines the wavenumber, $k_x = 2\pi n_{eff}/\lambda_{vac}$, of the modes to be found.

RESOLUTION (real):
The resolution of the simulation grid. The cell size is set to be this number multiplied by the smallest simulation feature, i.e., the fiber radius.

XCELLS (integer):
The number of cells to simulate in the x direction.

CFL_NUMBER (real):
This times the stable time step gives the time step chosen for the simulation.

FREQ_GAP_REL (real):
The gap outside of which the excitation drops off to the suppression level. simulation.

Expanding the Parameters section of the tree shows how the other simulation parameters are computed from the constants. For example, the grid size DX along the $x - axis$ is set to the resolution multiplied by the vacuum wavelength, divided by n_{eff} and scaled by LENGTH_UNIT. The excitation central frequency, frequency, is computed from the vacuum wavelength scaled by the LENGTH_UNIT. The longitudinal wavenumber, KAY, is computed from the desired n_{eff}, and from that the phase shift across cells along the $x - axis$ is calculated.

The range of frequencies to be excited is [FREQ_LOW, FREQ_HIGH]. Outside of this range by FREQ_GAP, the excitation drops off to the suppression value. This requires a successively longer excitation time, TIME_EXCITE and so a successively larger NSTEPS_EXCITE, the number of steps for the excitation.

Absorbing layers have been placed at the y and z limits to damp out modes that would be outgoing for a fiber in infinite space.

In 3D View tab of the right pane of the Setup Window, the fiber and the grid are visible. Right-click and drag to rotate the view. The simulation has been constructed so that the fiber extends beyond the grid in both the positive and negative $x - directions$, with a fiber diameter one-half the perpendicular domain length.

Expanding the Materials section of the Simulation tree shows that the simulation includes FiberMaterial. This was created by importing a material from the Database tab of the right pane of the Setup Window, then changing the name of the material and changing its properties. A material can be changed arbitrarily once it is in the simulation, as shown in Fig. 3.76.

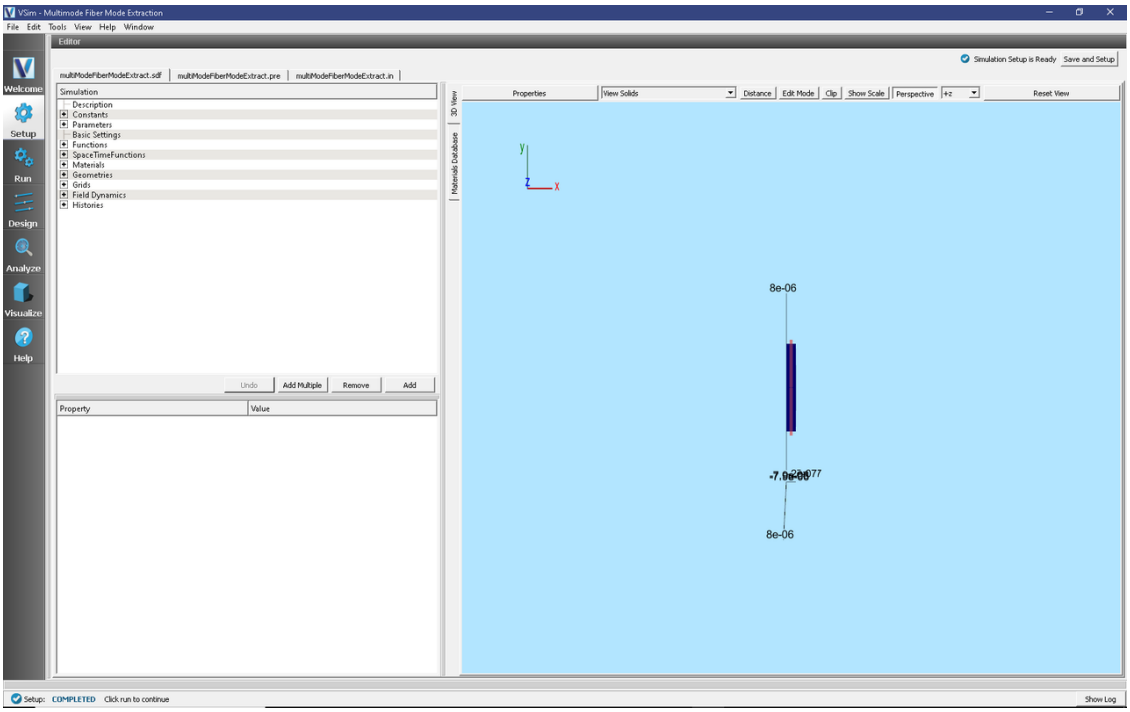


Fig. 3.75: Setup Window for the Multimode Fiber Mode Extraction example.

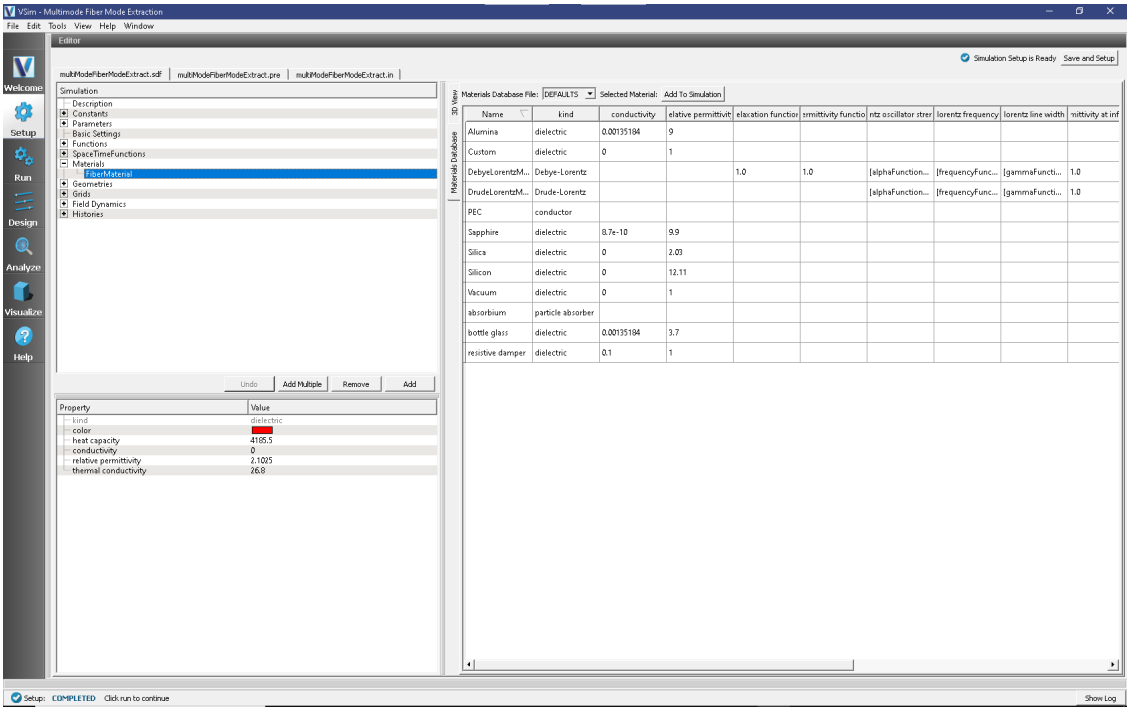


Fig. 3.76: Setup Window for the Multimode Fiber Mode Extraction materials.

Expanding the Geometries of the Elements Tree shows that the simulation includes one geometry, the fiber, and its material is `FiberMaterial`. This is seen in Fig. 3.77.

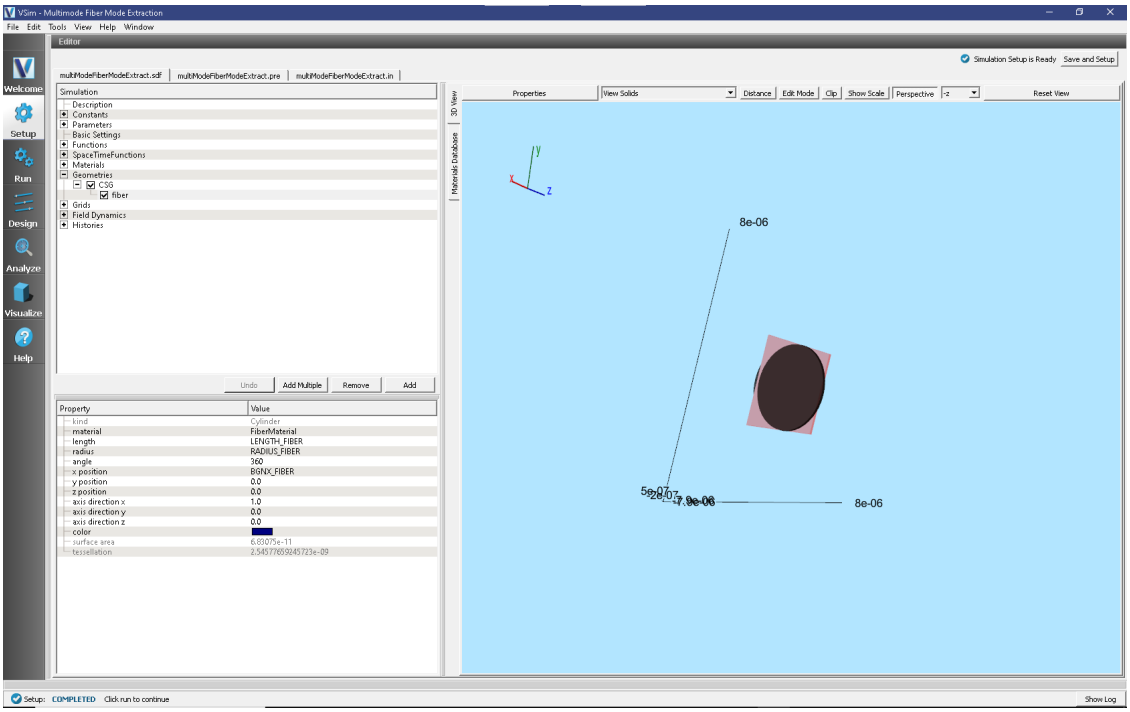


Fig. 3.77: Setup Window for the Multimode Fiber Mode Extraction geometries.

This simulation is excited with the `freqBand` function. This is a function that has a fairly uniform excitation over a band of frequencies, falling off steeply outside of the band. The band has been chosen to be centered near where we expect to find the modes.

A field history has also been implemented in this simulation, so that the Fourier transform of what has been excited can be seen.

As noted above, under the Parameters section of the Tree Elements is defined `NSTEPS_EXCITE` which specifies the number of steps to excite the desired frequency content. Because `FREQ_GAP` also distinguishes the peaks, this excitation time will distinguish the peaks.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.965261272930543e-16
  - *Number of Steps*: 10000
  - *Dump Periodicity*: 2000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

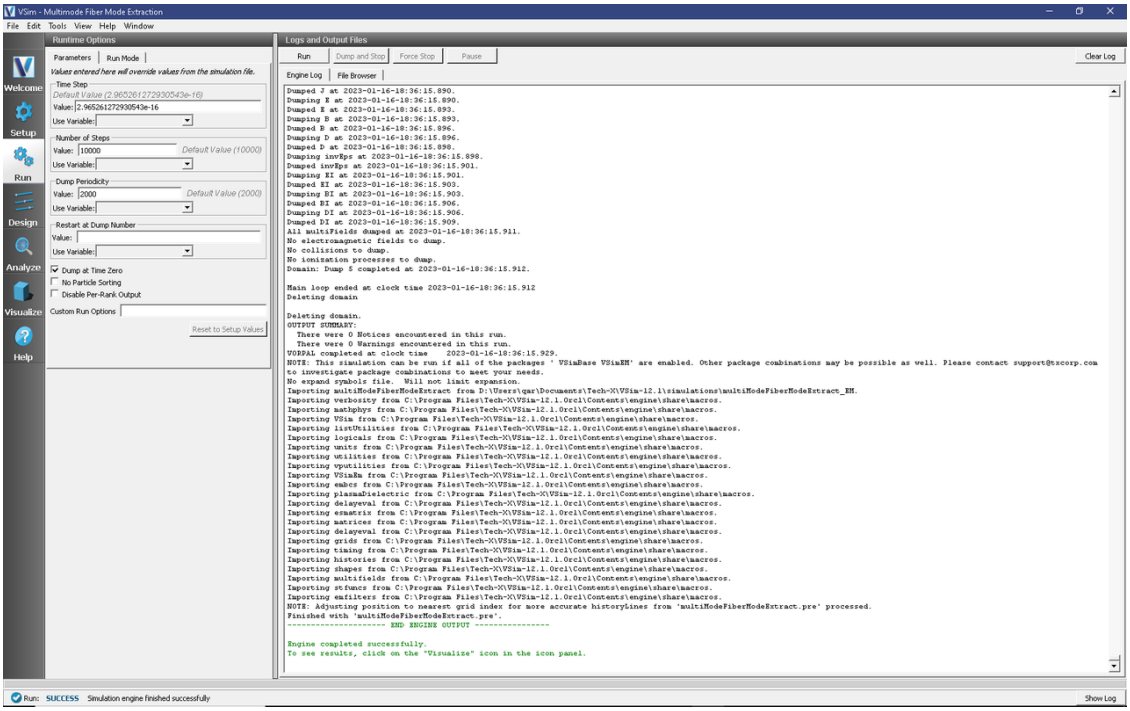


Fig. 3.78: The Run Window at the end of execution.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.78.

This simulation takes approximately 10 seconds on 4 cores of a modern processor.

Visualizing the spectrum

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.
- In the Visualization Controls pane, in the dropdown menu for *Add a Data View* select *History*.
- For graph 1, set the quantity to be plotted to `driveCurrent_2`.
- For graph 2, set the quantity to be plotted to `midUpperRightE_2`.
- In the Visualization Results pane, for each plot, click the *Fourier Amplitudes (dB)* check box.
- Graph 1 shows the square window in frequency space.
- Graph 2 shows several peaks between 200 and 250 THz.
- To see this region in more detail, for each graph press the limits button and set the minimum to 1.7e14 and the maximum to 2.7e14. Peaks in the spectrum are seen at the frequencies, 198 THz, 205THz, 217THz, 233, and several around 250 THz in Fig. 3.79.

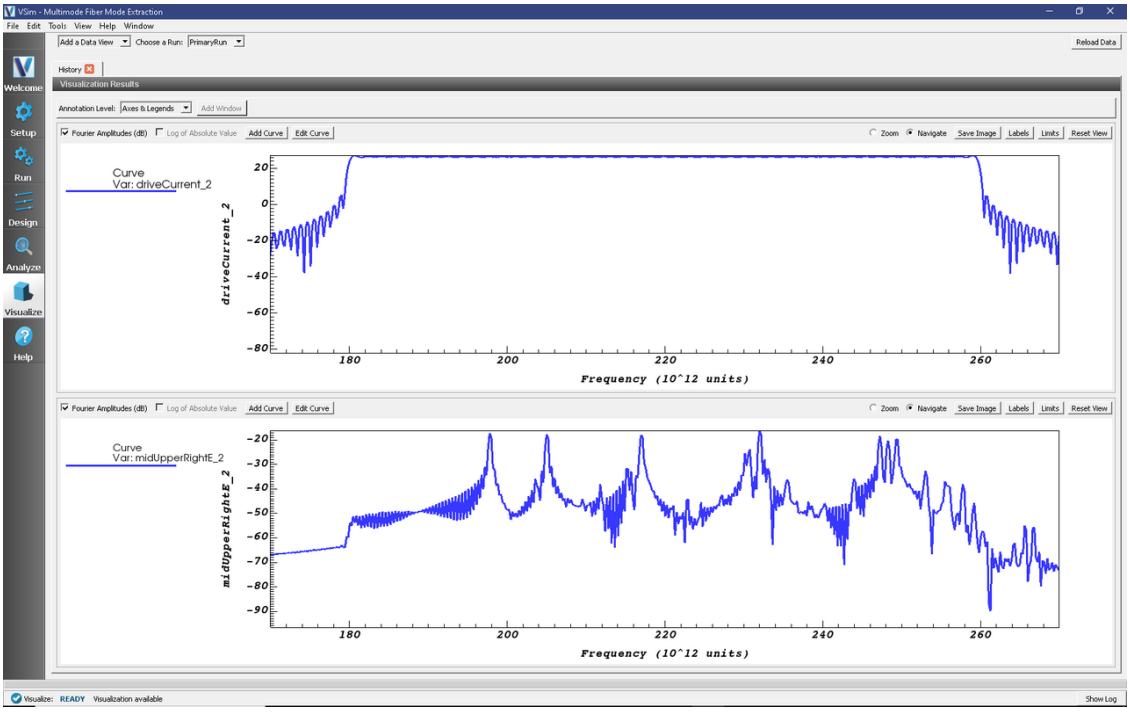


Fig. 3.79: The observed spectrum.

Analyzing the Results

Since 8 modes were seen, we look for 8. This will require 3 dumps per mode, or about 24 additional dumps. The dumps should be spread out over a few oscillations (35 steps each) or so, and it is good to do a few extra. To get these new dumps, return to the Run pane, set *Number of Steps* to 200, *Dump Periodicity* to 5, and *Restart at Dump Number* to 5. This will start a new simulation from where the first stopped. Click the *Run* button in the top left corner of the right pane.

Now go to the Analyze pane, select the *extractModes.py* analyzer, and press the *Open* button. Set the field to E, choose beginDump to be 6, endDump to be 45, nModes to be 8, and 100 of each kind of points. Also check the boxes next to randomSample and construct. Upon hitting the Analyze button of the Analyze pane, we sees the list of detected frequencies, of which the first (mode 0) is the mode of interest, it having frequency of 1.98e14. This is seen in Fig. 3.80.

Note: The sign of the mode may vary on different operating systems. So, the visualization of the Eigen modes could be different from what is seen in Fig. 3.80.

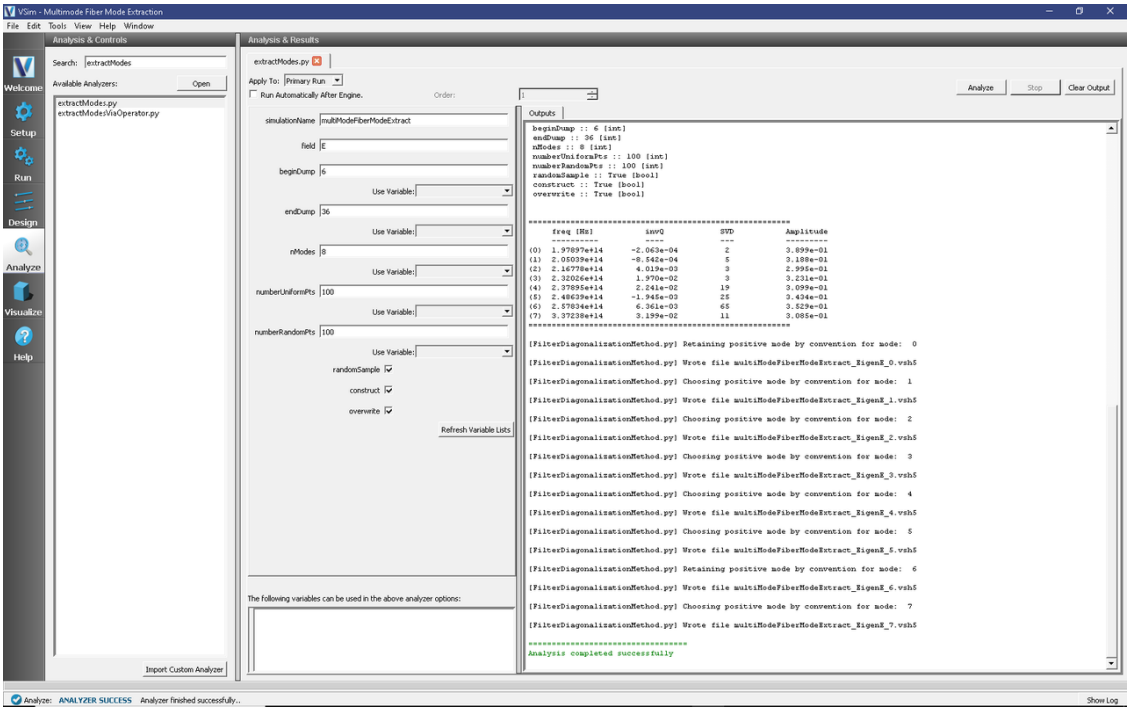


Fig. 3.80: Extraction of the mode frequencies.

Visualizing the eigenmodes

Return to the Visualize Window, reload the data, open Scalar Data -> E, and click on E_z (EigenE). Keep the slider on position 0. With the mouse, turn the image sideways to see the cross section, as shown in Fig. 3.81.

Convergence

This simulation can be repeated for different values of `RESOLUTION` to see how the frequency varies with the meshing. We carried out this experiment with `RESOLUTION` varying over 0.1, 0.05, 0.02, 0.01 and plotted the frequency versus the inverse grid length in Fig. 3.82.

For each value of the resolution do the excitation run followed by the extraction run:

- Excitation run: Press *Reset to Setup Values* to get the correct value for the time step. Then set the number of step in the run panel to what is given by `NSTEPS_EXCITE`, and also modify the number of steps in the second run proportionately. E.g., for `RESOLUTION` = 0.05, `NSTEPS_EXCITE` = 7916, so in the Run panel choose *Number of Steps* = 8000 and *Dump Periodicity* = 2000. Clear the *Restart at Dump Number* box. Press the *Run* button.
- Extraction run: E.g., for `RESOLUTION` = 0.05, set the *Number of Steps* to 400, the *Dump Periodicity* to 10, and *Restart at Dump Number* to be 4.
- Analysis: Same as originally, as all numbers have been scaled.

The linear approach to the axis indicates that this is a first order accurate calculation. In other examples we will show higher-order accuracy. Even so, one can see that the frequency is obtained on the sub-percent level with the finest grid used.

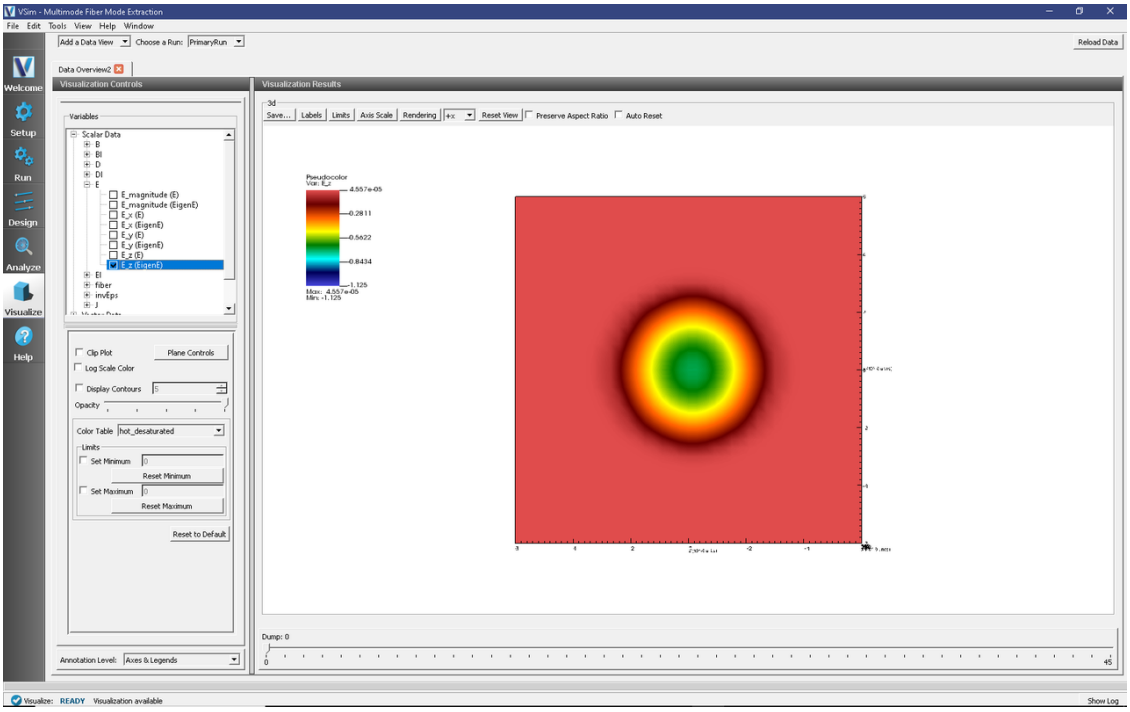


Fig. 3.81: The extracted eigenmode.

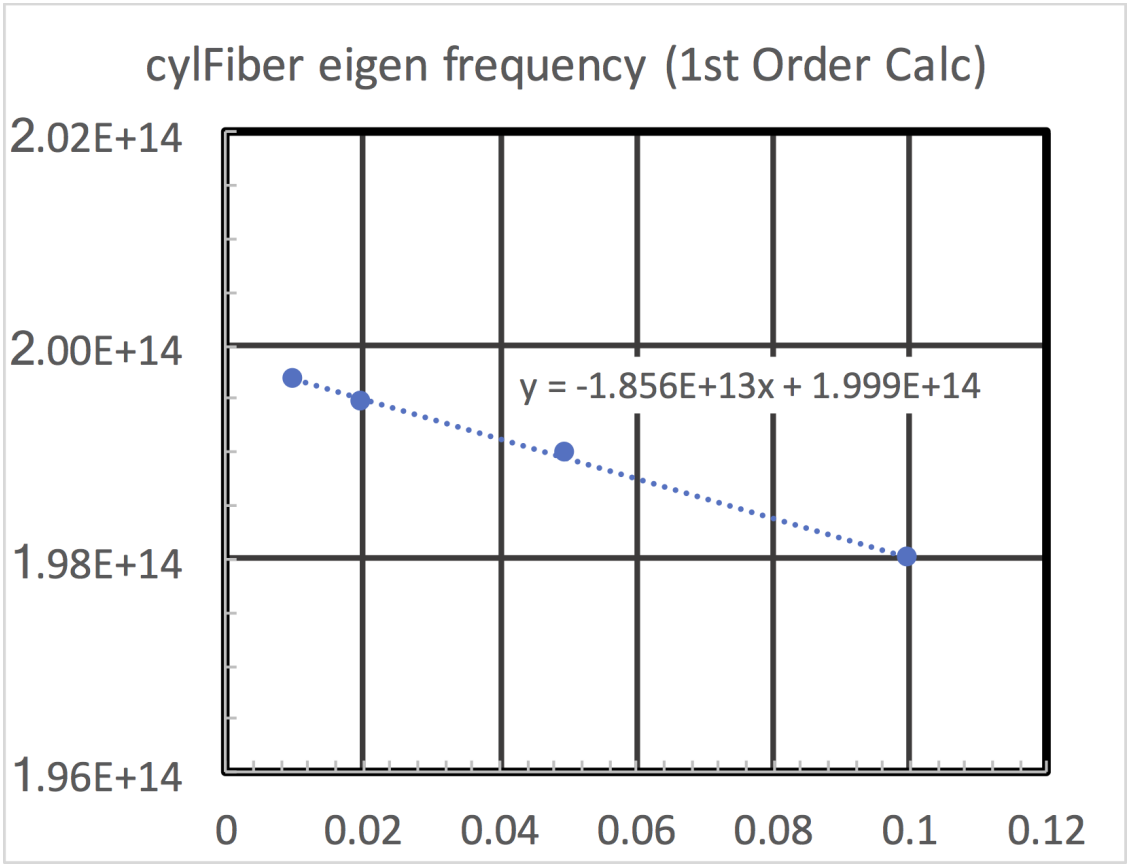


Fig. 3.82: Convergence of the first mode.

Further Experiments

This same process can be used to get the frequency of modes of different wavelengths or of waveguides of different cross sections or made of different dielectrics.

3.3.3 Dielectric Waveguide with Gaussian Launcher (dielectricWaveguideGaussian.sdf)

Keywords:

Photonic Waveguide, Unidirectional Mode Launcher, MAL, Guided Mode, Semiconductor

Problem description

The dielectric waveguide consists of a single, straight silicon waveguide that is parallel to the x-axis and centered at the origin. The waveguide is surrounded by silica. Matched Absorbing Layers (MALs) are used to dampen the E and B fields near the boundary of the simulation to suppress reflected fields.

A space gaussian source with the single frequency is used as a source and propagates in the +x direction.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The dielectric waveguide example can be accessed from within VSimComposer through the following steps:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window, expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Dielectric Waveguide with Gaussian Launcher* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation will now be available in the Setup window as shown in Fig. 3.83. You can expand the tree elements and navigate through the various properties. The right pane shows a 3D view of the geometry, as well as the grid. To show or hide the grid, expand the *Grid* element and select or deselect the box next to *Grid*.

Simulation Properties

This example contains a number of constants defined to make the simulation easily modifiable. Some relevant constants are listed below.

PERMITTVITY_WAVEGUIDE and PERMITTVITY_BACKGROUND: Relative permittivities of silicon and silica. These constants are used in multiple parameters and in the accompanying Python file for solving the waveguide modes.

WAVELENGTH_VAC: Wavelength of the input signal. This wavelength is also used for the calculation of the fundamental guided mode of the device.

NWAVELENGTH_MAL: Approximate number of wavelengths that can fit in a MAL region. The thickness of the MAL regions in this example are measured in wavelengths.

The *Materials* section contains just silicon and silica.

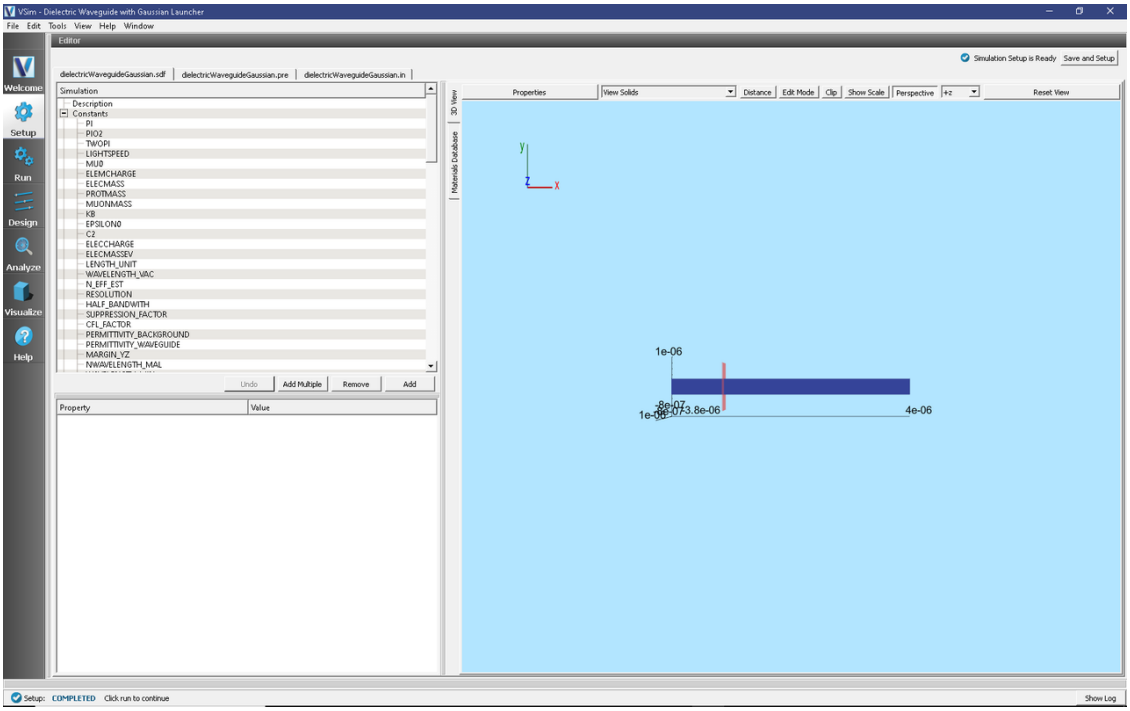


Fig. 3.83: The Setup window for the dielectric waveguide example showing some relevant constants.

The *Geometries* includes the CSG waveguide and its defining parameters.

In *Field Dynamics*, there are *FieldBoundaryConditions* and *CurrentDistributions* to be aware of. In photonics simulations, Matched Absorbing Layers (MALs) are the most stable boundary conditions for preventing reflections. The gaussian approximation is defined under *SpaceTimeFunctions* and is set to drive the y-component of the *currentSource*.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.678655063578495e-17
  - *Number of Steps*: 17290
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.84.

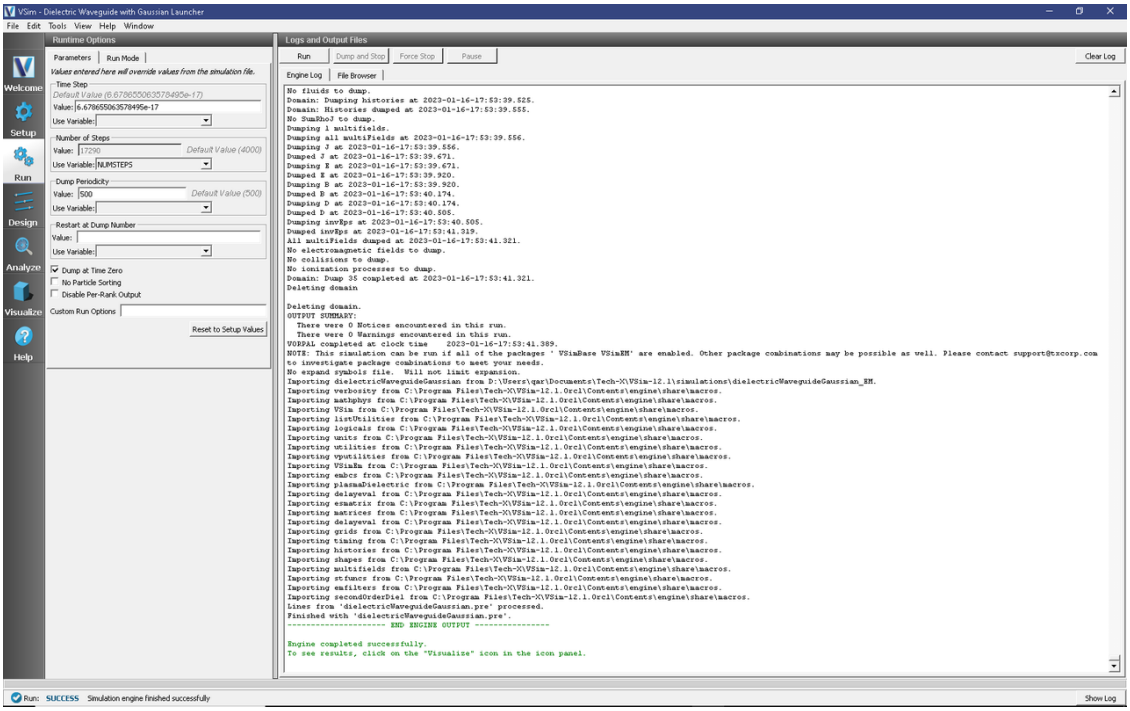


Fig. 3.84: The output after a successful run.

Visualizing the Results

Then proceed to the Visualize window by pressing the *Visualize* button in the left column.

You can verify that the geometry is correct by visualizing the inverse permittivity as follows:

- Near the top left corner of the window, make sure *Data View* is set to *Data Overview*.
- Expand *Scalar Data*, expand *invEps*, and select *invEps_z*
- In the controls below the variables frame, select *Clip All Plots*.

By default, the clipping plane is at z = 0, which is in the middle of dielectric waveguide structure height-wise. As such, this will reveal the dielectric waveguide's 2D layout geometry as seen in Fig. 3.85.

A useful visualization of the dielectric waveguide would be to view the Z component of the B field to qualitatively see the mode propagate down the waveguide.

- Near the top left corner of the window, make sure *Data View* is set to *Data Overview*.
- Expand *Scalar Data*, expand *B*, and select *B_z*
- In the controls below the variables frame, select *Clip All Plots*.

Select the final dump step (dump 8) on the lower right of the screen using the slide bar. Fig. 3.86 shows an example of what one should expect if one has run the simulation for enough cycles.

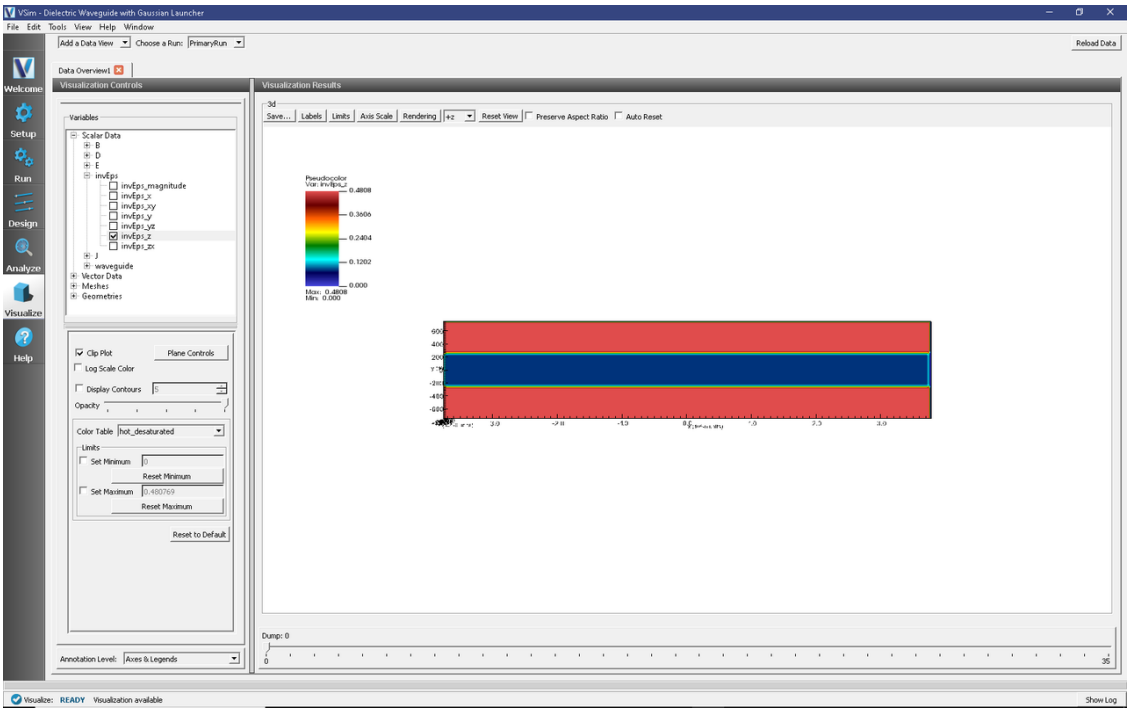


Fig. 3.85: Visualization of inverse epsilon field's Z component

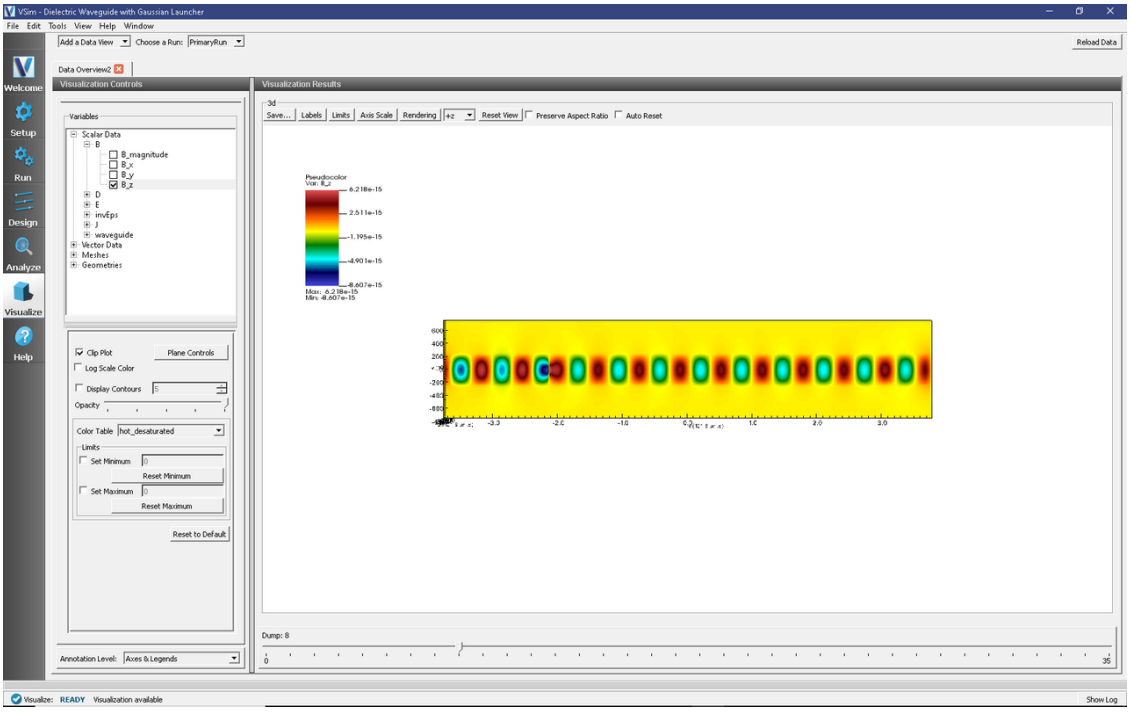


Fig. 3.86: Visualization of the B field's Z component

Further Experiments

One can experiment by changing constants or introducing a different signal to drive the waveguide.

3.3.4 Dielectric Waveguide Mode Calculation (dielectricWaveguideModeCalc.sdf)

Keywords:

`Mode Extraction, Photonic Waveguide, Guided Mode, Semiconductor`

Problem Description

This example demonstrates the process for extracting the effective index and fields of a guided mode by directly solving an eigenvalue equation. The use of permittivity averaging enables second order accuracy in our solution. The waveguide axis runs parallel to the x-axis, and is surrounded by a background cladding with a greater permittivity. We will run the simulation for 1 step and then use the dielectricWaveguideModeCalc_invEps_0.h5 file to solve for the guided modes using the computeDielectricModes.py analyzer. This analyzer will find the entire basis set of modes for this waveguide and output each into a separate .vsh5 file. These mode files can be used to launch the exact modes into your simulation. This process is shown in the multiModeFiberModeLaunchT example.

Eigenmodes in such a simulation have the form:

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(y, z)e^{i(kx-\omega t)}$$

The effective index of refraction of a waveguide mode is given by $\bar{n} = k/k_0$ where $k_0 = \omega/c$. If the waveguide has index of refraction n_w and the cladding $n_c < n_w$, then a *guided* mode will have a modal index in the range, $n_c < \bar{n} < n_w$.

This simulation can be performed with a VSimEM license.

Opening the Simulation

To open this example open an instance of VSimComposer and follow the steps below:

- Select the *New* $\rightarrow$ *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Dielectric Waveguide Mode Calculation* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, and press the *Save* button to create a copy of this example.

Simulation Variables

This example contains a number of variables defined to make the simulation easily modifiable.

- PERMITTVITY_WAVEGUIDE and PERMITTVITY_BACKGROUND: Relative permittivities of silicon and silica. These constants are used in multiple parameters and in the accompanying Python file for solving the waveguide modes.
- WAVELENGTH_VAC: Wavelength of the input signal. This wavelength is also used for the calculation of the fundamental guided mode of the device.
- NWAVELENGTH_MAL: Approximate number of wavelengths that can fit in a Matched Absorbing Layer (MAL) region. The thickness of the MAL regions in this example are measured in wavelengths.

The *Materials* section contains just silicon and silica. The *Geometries* includes the CSG waveguide and its defining parameters. In *Field Dynamics*, there are *FieldBoundaryConditions* and *CurrentDistributions* to be aware of. In photonics simulations, Matched Absorbing Layers (MALs) are the most stable boundary conditions for preventing reflections. The gaussian approximation is defined under *SpaceTimeFunctions* and is set to drive the y-component of the *currentSource*.

Setting up the Simulation

As delivered, the system is set up to generate the data needed to run the computeDielectricModes.py analyzer. To ensure that your simulation has second order accuracy, expand the *Basic Settings* branch and verify that the *dielectric solver* field is set to *permittivity averaging*. This algorithm is a powerful VSim feature. This setting is shown in Fig. 3.87.

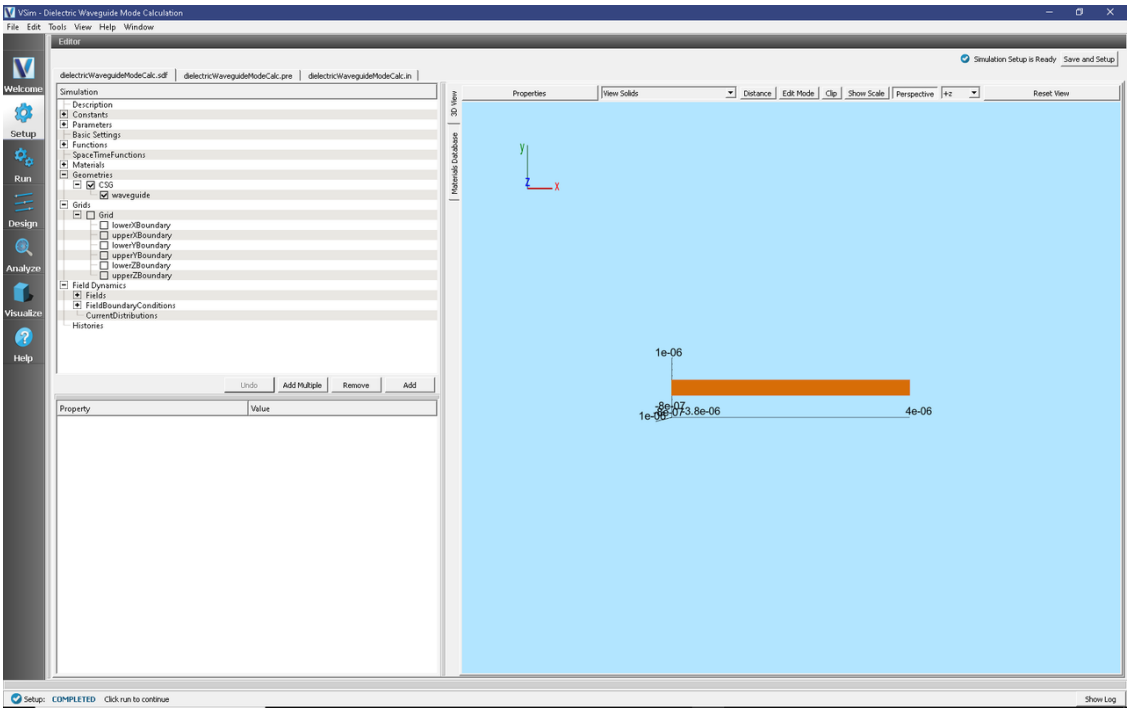


Fig. 3.87: Choosing the second order accurate, *permittivity averaging* for the *dielectric solver* field under *Basic Settings*.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.678655063578495e-17
  - *Number of Steps*: 17290
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.88.

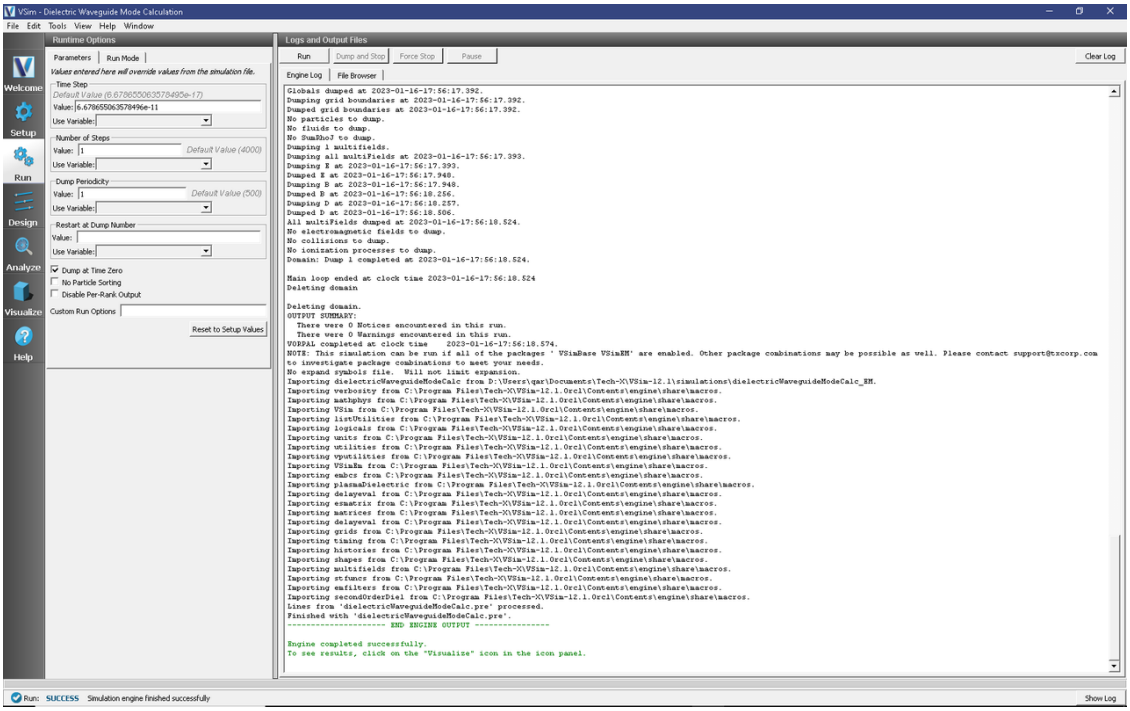


Fig. 3.88: Running the simulation for one step to get the permittivity data for the analyzer. Note that *Dump at Time Zero* is checked.

Solving for the Eigenmodes

After performing the above actions, continue as follows:

- Proceed to the Analyze Window by clicking the *Analyze* button on the left.
- Select *computeWaveguideModes.py* and click *Open* under the list.

Now update the analyzer fields accordingly. Some of these parameters are described above under **Parameters**

- *transverseSliceX* 0.0
- *transverseSliceLY* -0.7e-6
- *transverseSliceUY* 0.7e-6
- *transverseSliceLZ* -0.5e-6
- *transverseSliceUZ* 0.5e-6
- *vacWavelength*: 1.55e-6
- *nModes*: 10
- *writeFieldProfile*: H,E,D

We set the number of modes (*nModes*) to a value greater than the number of modes we expect. The analyzer will only find guided modes. Also check *Overwrite Existing Files*. Run the analyzer by clicking *Analyze* button in the upper right corner. The analyzer output should resemble Fig. 3.89. We see that the analyzer found 3 modes. They are listed in decreasing order of effective index.

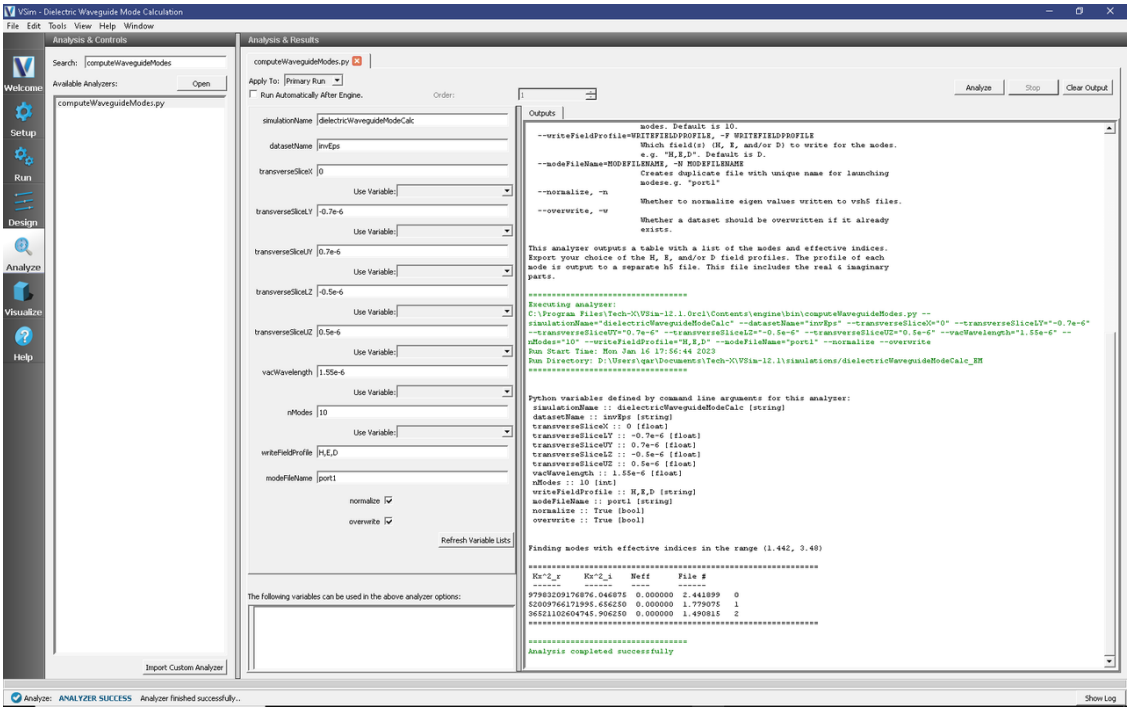


Fig. 3.89: The analyzer window after a successful run of computeWaveguideModes.py.

Visualizing the Results

After performing the above actions proceed to the Visualize window by pressing the *Visualize* button in the left column of buttons. You may need to *Reload Data* (bottom left). Visualize an eigenmode by following these steps:

- From the *Add a Data View* dropdown, select *Data Overview*.
- Expand *Scalar Data*, expand *EigenD*, and select *EigenD_magnitude*.
- Below the visualization, the dump slider will allow you to scroll between the modes.

The resulting visualization pane should resemble Fig. 3.90.

One can select other components of the H, E, or D field to see how they vary for the eigenmodes. These eigenmodes are now saved in .vsh5 files in the folder where the simulation was run.

Further Experiments

Change the geometry on the Setup window and rerun the simulation and analyzer to see the effects on the modes.

Once you have your desired mode, launch it down the waveguide using the procedure laid out in the multiModeFiberModeLaunchT example.

One can run a full convergence study of eigenmode effective indices by varying the RESOLUTION constant in the Setup window and re-running the simulation and mode extraction script. A plot of the effective index as a function of transverse cell area is shown in Fig. 3.91. The linear relationship shows the second order accuracy of our dielectric algorithms.

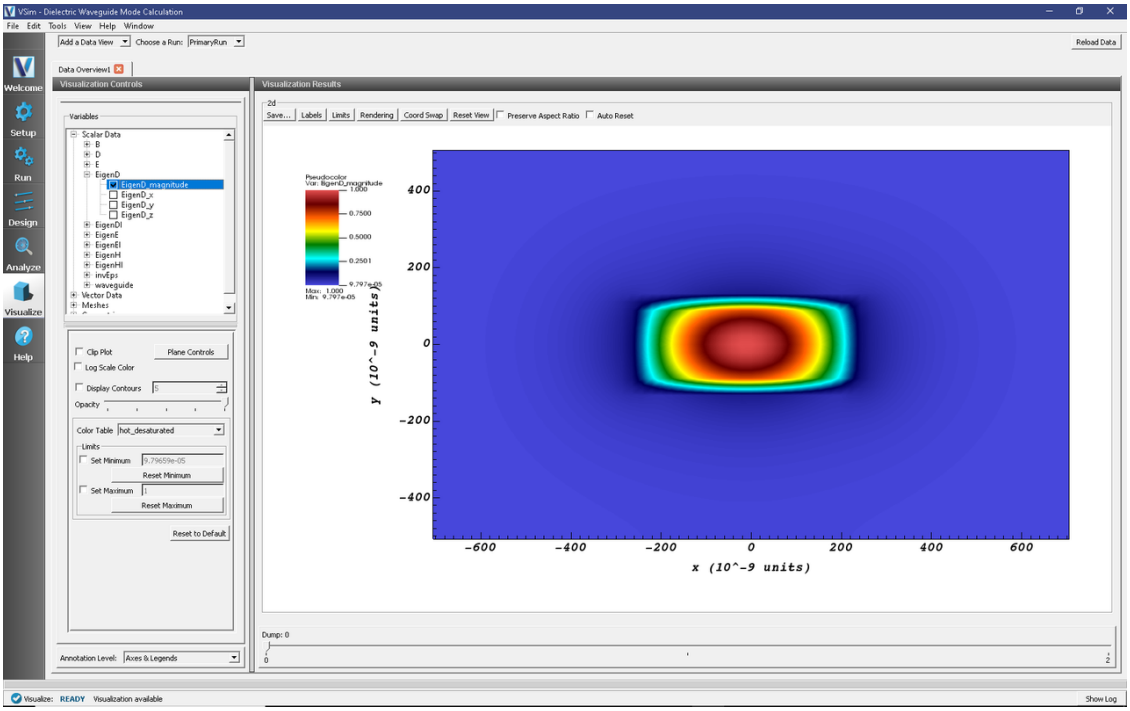


Fig. 3.90: The visualization pane showing the magnitude of the D field of the fundamental mode.

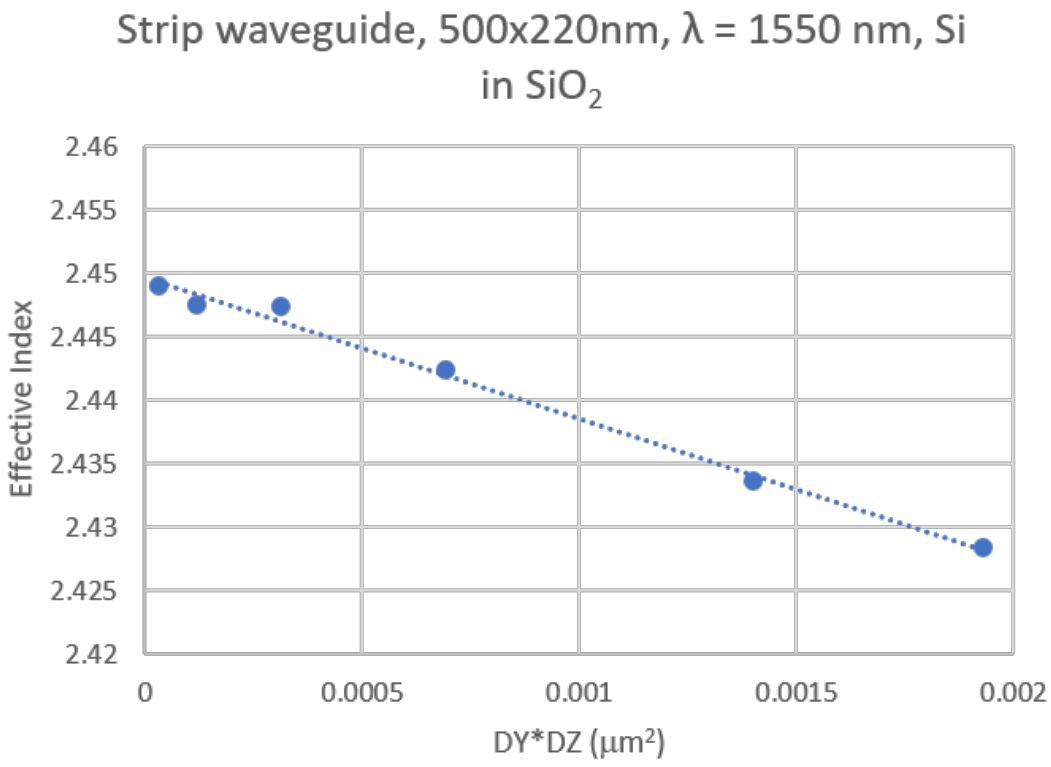


Fig. 3.91: The effective index as a function of transverse cell area for an eigenmode.

3.3.5 Gaussian Laser Beam and Photonic Crystal Cavity (photonicCrystal-GaussSrc.sdf)

Keywords:

Gaussian Beam source, photonic crystal, transmission efficiency

Problem description

This example illustrates how to model a Gaussian beam source that is illuminating a cavity inside a hexagonal photonic crystal lattice. The physical setup is shown in Fig. 3.92.

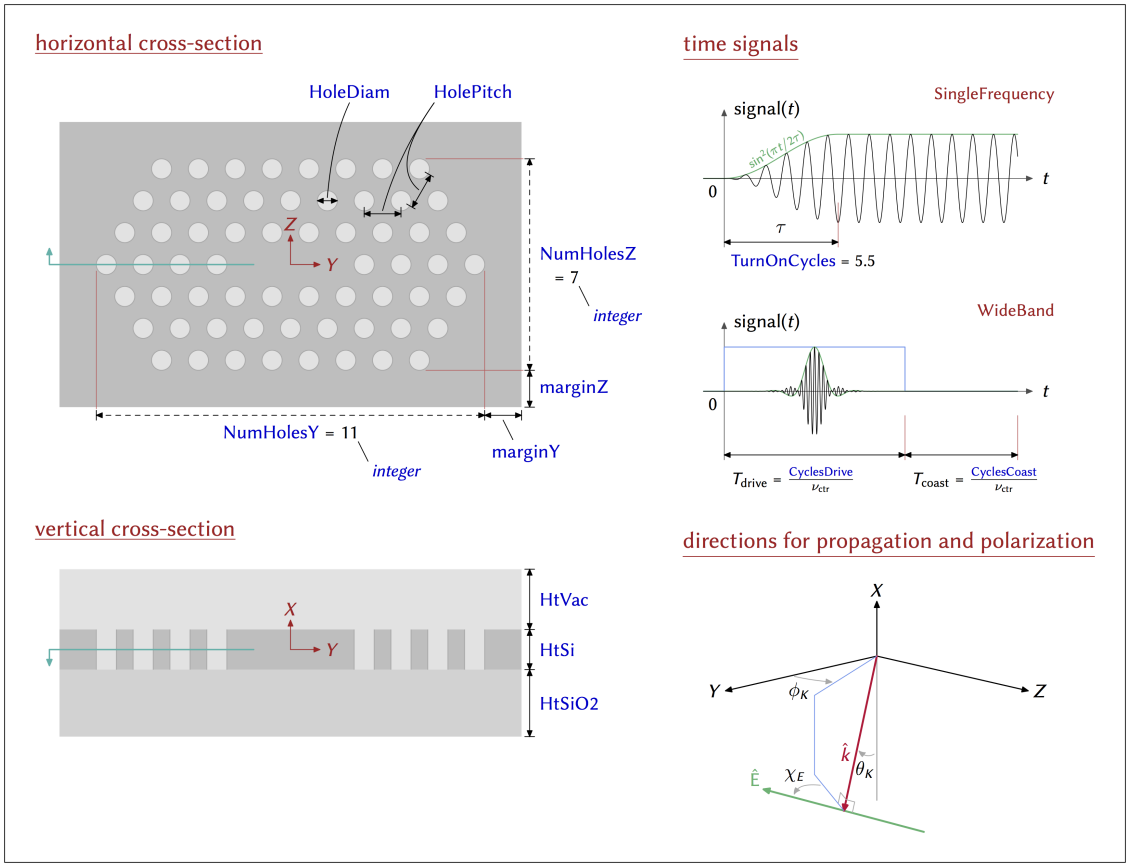


Fig. 3.92: The photonic lattice setup

A Gaussian beam is launched from above into the simulation domain, which comprises three layers: a vacuum region above and a solid dielectric below, which together sandwich a central dielectric layer that contains a lattice of holes. This example includes two possible time signals with which the Gaussian beam will have either WideBand or SingleFrequency.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Photonic Crystal example is accessed from within VSimComposer through the following steps:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window, expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select "Gaussian Laser Beam and Photonic Crystal Cavity" and press the *Choose* button.
- In the resulting dialog, create a new folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the *Setup Window*, as shown in Fig. 3.93. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

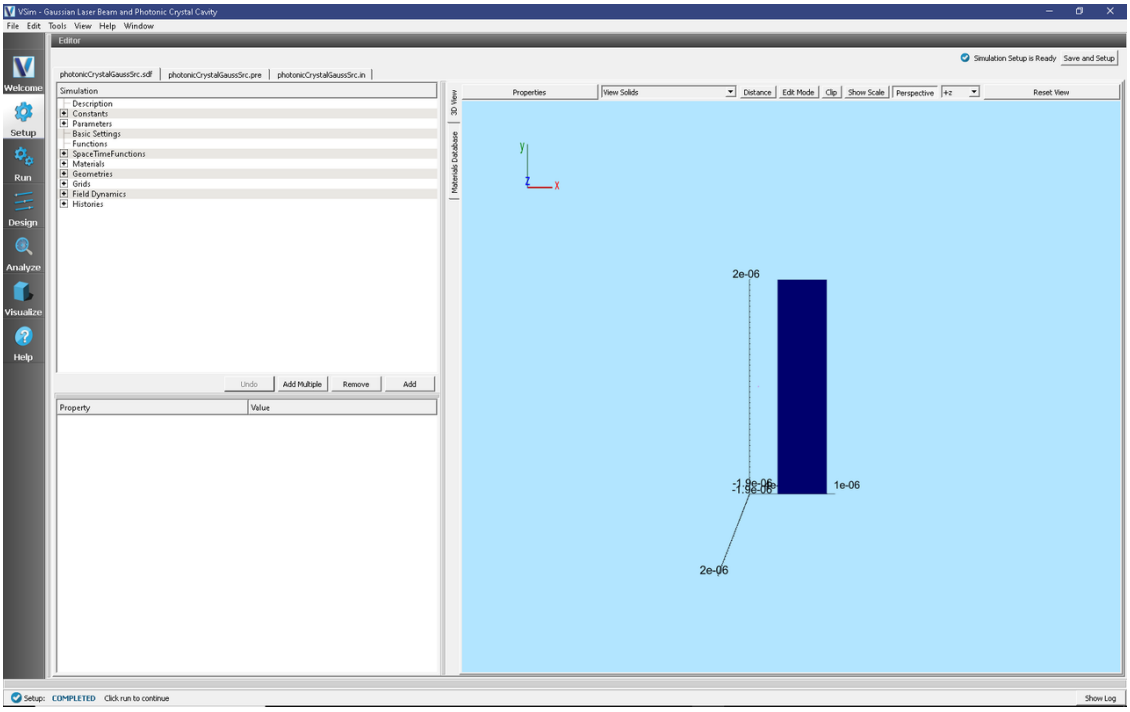


Fig. 3.93: The Setup Window for the Gaussian Laser Beam and Photonic Crystal Cavity example

Simulation Properties

This example contains a number of constants that are defined to make the simulation easily modifiable, as can be seen in Fig. 3.94.

All the following constants should be the only properties you should need to alter in order to specify your simulation domain.

General Simulation Parameters:

- `L{X,Y,Z}` = The length of your simulation domain in the {X,Y,Z} dimension.
- `HT_{VACUUM,SI,SI02}` = The height of the vacuum, SI and SI02 layers of the photonic crystal.

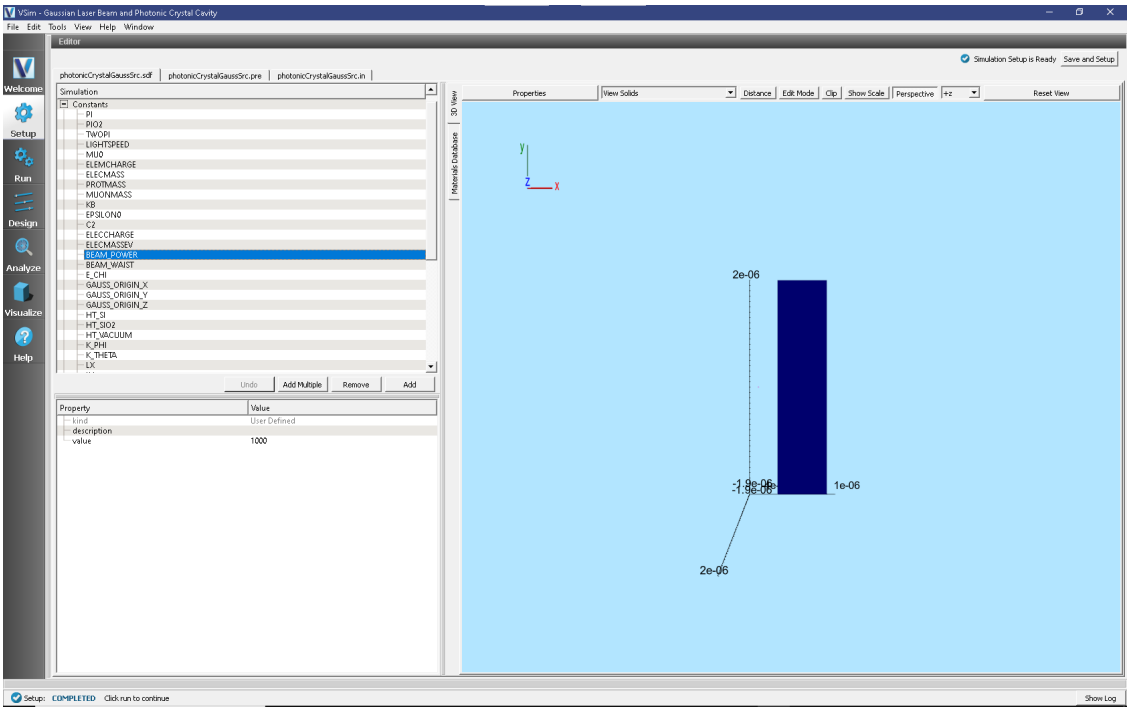


Fig. 3.94: The Setup Window showing the constants

Source Specifications: (located in the *Parameters* section of the *Elements Tree*)

- `{K_THETA,K_PHI,E_CHI}` = The {polar angle, azimuthal, angle of polarization} respectively.
- `WAVEL_CENTER` = The central wavelength of your wideband signal. This is also the frequency used in the single frequency simulation type.
- `WAVEL_BAND` = The wavelength width of your wideband signal, only used in wideBand simType.
- `BEAM_WAIST` = The width at which your beam power falls off like 1/e.
- `BEAM_POWER` = The amplitude of your E/M wave.
- `GAUSS_ORIGIN_{X,Y,Z}` = The point around which your Gaussian profile is centered.
- `TURNONCYCLES` = The number of cycles you want your single frequency to reach full power.
- `SIMCYCLES` = Number of wave cycles you want your simulation to run.
- `CYCLESPERDUMP` = Number of cycles between each dump in the simulation.

The tool used to input the wave into the simulation is a port launcher. It specifies the Electric Displacement Field (D) at a boundary in this case the lower X boundary. The functions defining your D on the boundary are defined in the *SpaceTimeFunctions* element of the *Elements Tree*.

SpaceTimeFunctions:

- `dSingleFreq{Y,Z}` = This is the {x,y,z} component of the single frequency Gaussian beam source, as seen in Fig. 3.94. You put this as a parameter in the current distribution.
- `dWideBand{Y,Z}` = This is the {x,y,z} component of the wideband Gaussian beam source, as seen in Fig. 3.94. You put this as a parameter in the current distribution.

To choose which signal you want to input into this example simulation:

1) Expand the *FieldBoundaryConditions* element.

2) Left click on the *portLauncherLowerX* condition.

At this point, you should see what is shown in Fig. 3.95.

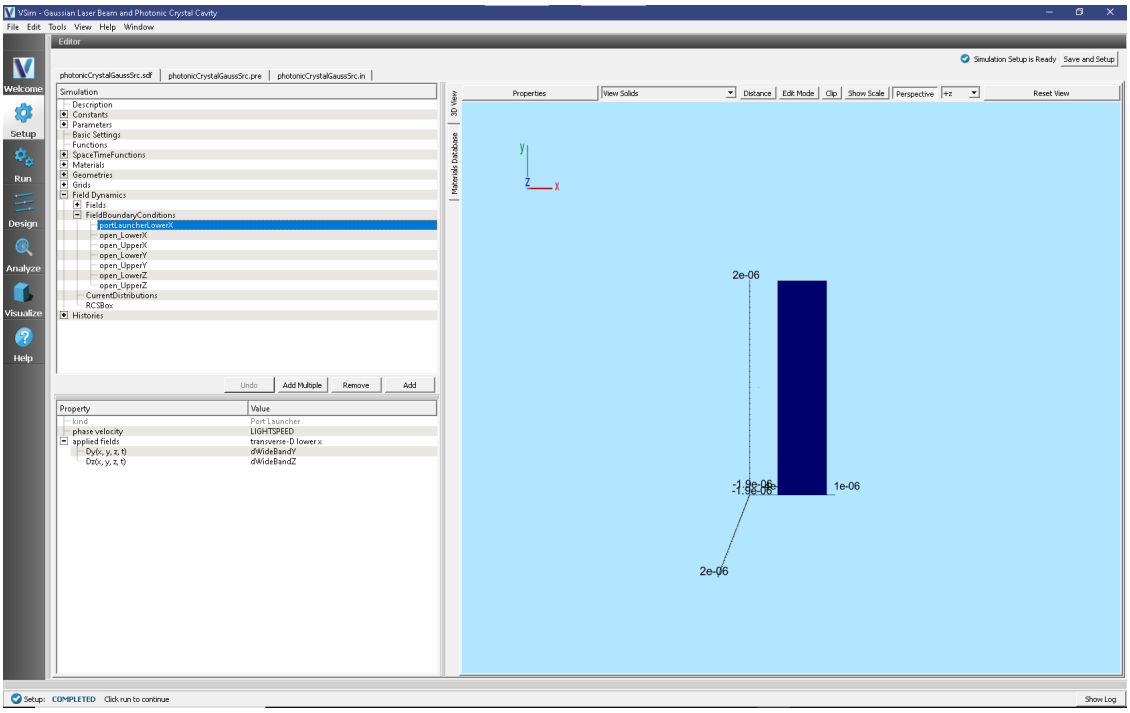


Fig. 3.95: The Setup Window for specifying the signal for the portLauncher

3) To add a signal to the *portLauncherLowerX* just right click on the D{x,y} and select *Assign SpaceTimeFunction*. This will expand another menu that will show you all four defined SpaceTimeFunctions. Select which one you want to input into your simulation. For this documentation, `WideBand{Y,Z}` will be used to demonstrate the functionality of this example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the *Run Window* by pressing the *Run* button in the left column of buttons.
- One can enable MPI options to utilize multi-core systems.
- The default values of `Number of Time Steps` and `Dump Periodicity` are taken from the parameters `STEPSTOTAL` and `STEPSPERDUMP`, which use the constants `SIMCYCLES` and `CYCLESPERDUMP`. The formulae for these variables can be found back in the *Setup Window*. These variables are for convenience to calculate good default values and it is important to know that the override option default values ultimately come directly from the numbers in the *Basic Settings* section.

  Number of Steps and *Dump Periodicity*. Just copy these values into the correct fields in the *Run* menu.

  - *Number of Steps* = `TOTALSTEPS` = 32200
  - *Dump Periodicity* = `STEPSPERDUMP` = 3600
- To run the file, click on the *Run* button in the upper left corner of the Logs and Output Files pane. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully." This is shown in Fig. 3.96.

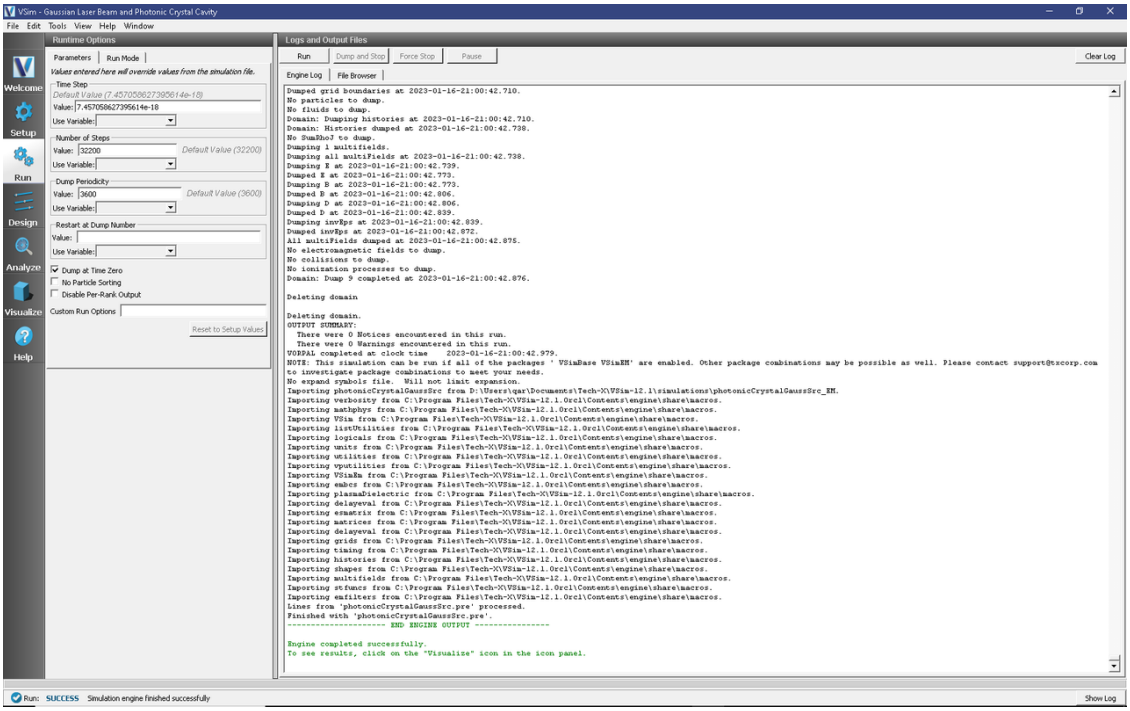


Fig. 3.96: The Run Window for the Gaussian Laser Beam and Photonic Crystal Cavity example

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the *Visualize Window* by pressing the *Visualize* button in the left column of buttons.

In the simulation, there are specific grid points which store field histories. These histories are placed in various positions of the simulation.

- Click the *Add a Data View* dropdown below the menu bar and select *History*.

In Fig. 3.97, one can see there are 4 possible graphs to view at one time in the *Visualize Window*. For each graph, one can select the following fields to analyze: (0 = x, 1 = y, 2 = z).

- {E,B}_AtDet_{0,1,2} is in the middle of (y,z) plane and 60 nm above the surface of the crystal.
- {E,B}_AtSrc_{0,1,2} is aligned with the inCav history in the (y,z) plane and is 60 nm below the Si layer, into the SiO2 layer.
- {E,B}_InCav_{0,1,2} is slightly offset from the middle of one of the cavities in the silicon layer (the layer with the lattice).

In each individual graph, one can choose the *Fourier Amplitudes (dB)* option to view the frequency domain of your field. This can enable the analysis of the frequency response of the photonic crystal cavity.

Fig. 3.97 depicts four graphs of histories. The first two graphs are amplitude vs time, and the second two are Fourier Amplitudes of the first two on a log scale.

The first and third graphs depict the history `AtSrc_2`, while the second and fourth graphs show the `AtDet_2` history.

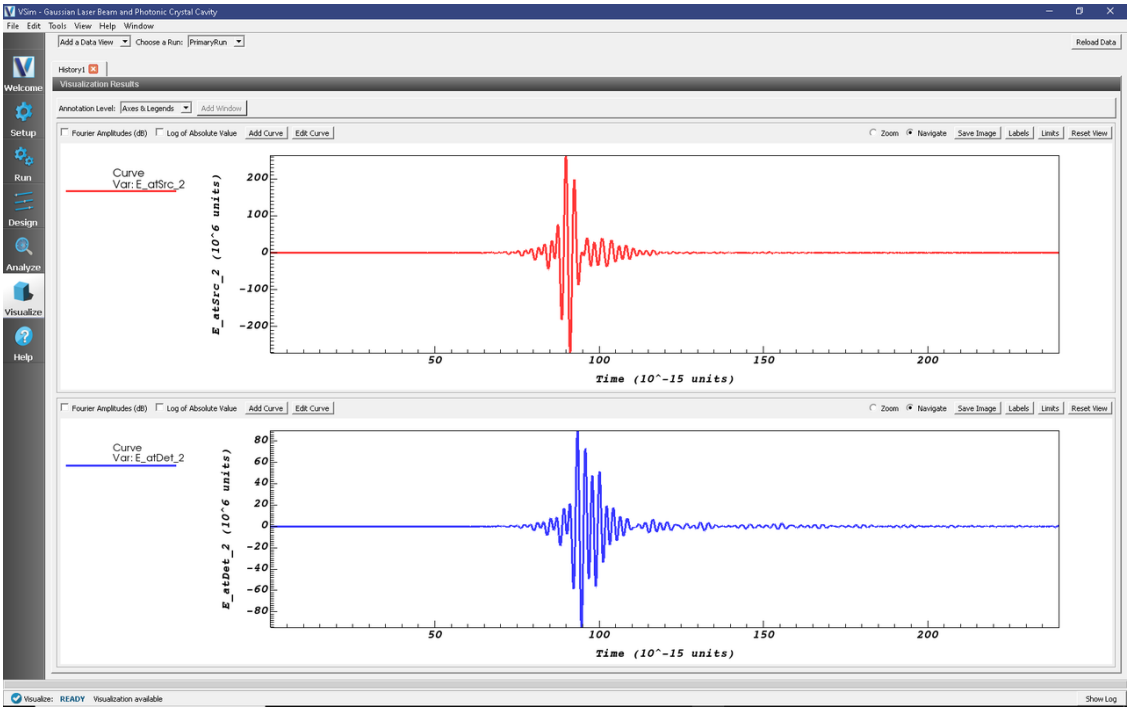


Fig. 3.97: The Visualize Window for the Gaussian Laser Beam and Photonic Crystal Cavity example

Further Experiments

By using the wideband source and examining the field strength detected below the crystal lattice, one may study the frequency response of this photonic crystal as one changes the device geometry, the dielectric constants, and the location and polarizations of the radiation source and detector.

3.3.6 Dipole Source Illuminating a Photonic Crystal Cavity (photonicCrystalDipoleSrc.sdf)

Keywords:

dipole source, photonic crystal, transmission efficiency

Problem description

This example illustrates how to model a dipole source that is illuminating cavities inside a hexagonal photonic crystal lattice. The physical arrangement is shown in Fig. 3.98 and Fig. 3.99.

A point-like dipole lies above the simulation domain, which comprises three layers: a vacuum region above and a solid dielectric below, which together sandwich a central dielectric layer that contains a lattice of holes. This example includes two possible time signals with which to ring the dipole source, as shown in Fig. 3.100.

This simulation can be performed with a VSimEM license.

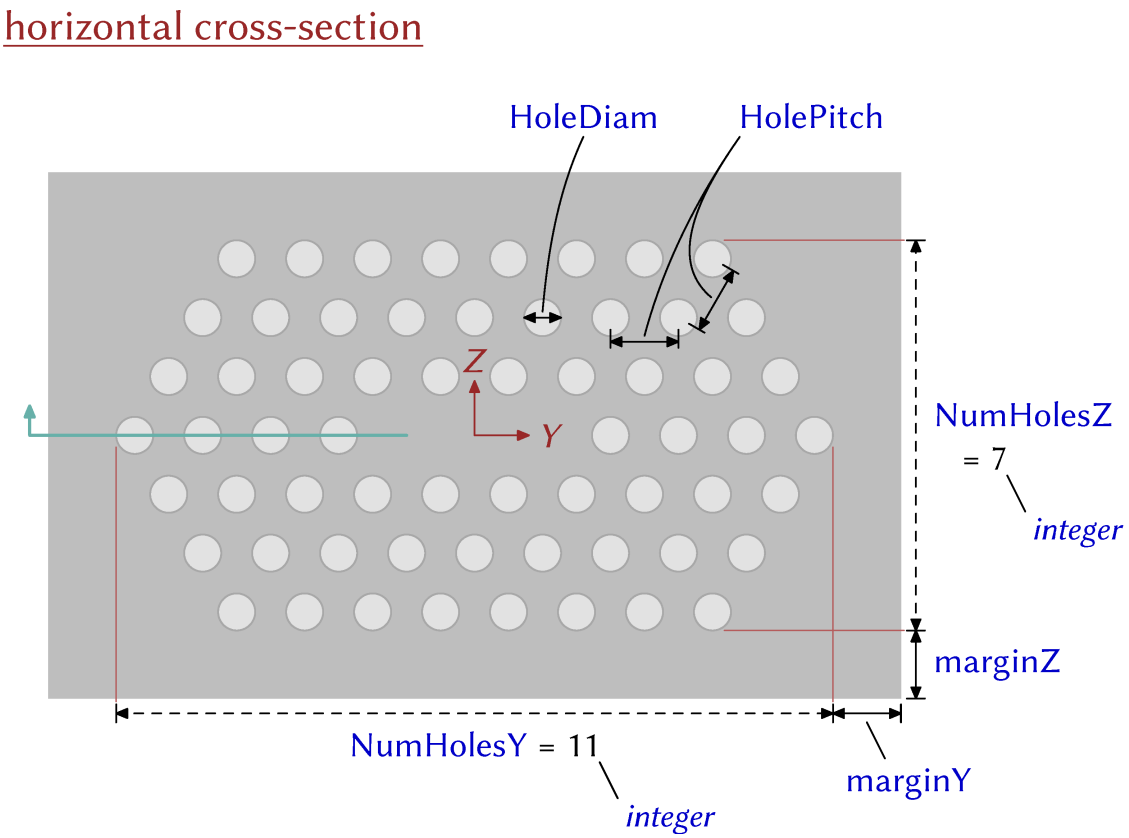


Fig. 3.98: Top view of photonic lattice.

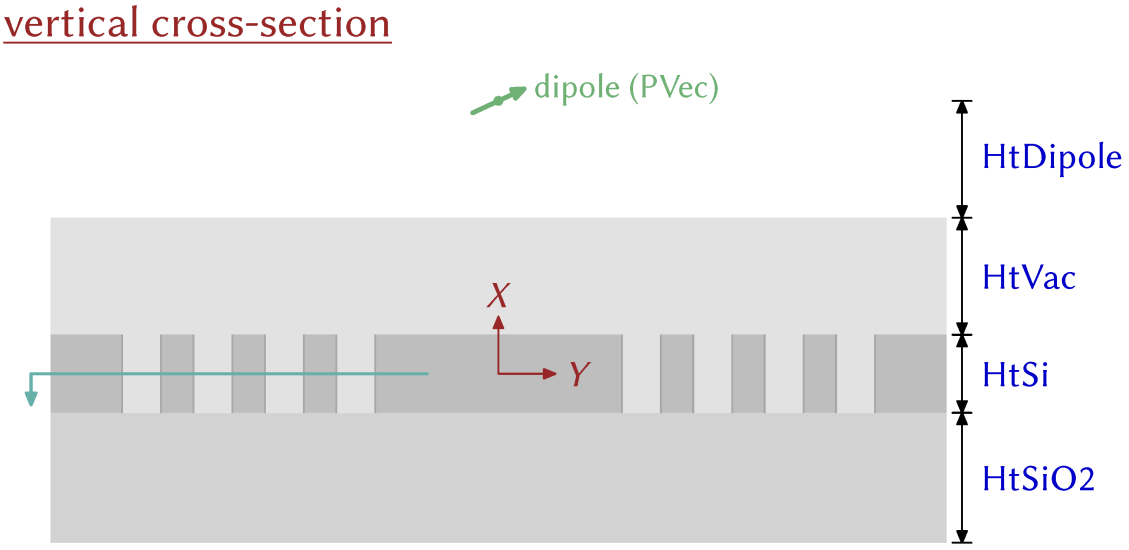


Fig. 3.99: Side view of photonic lattice.

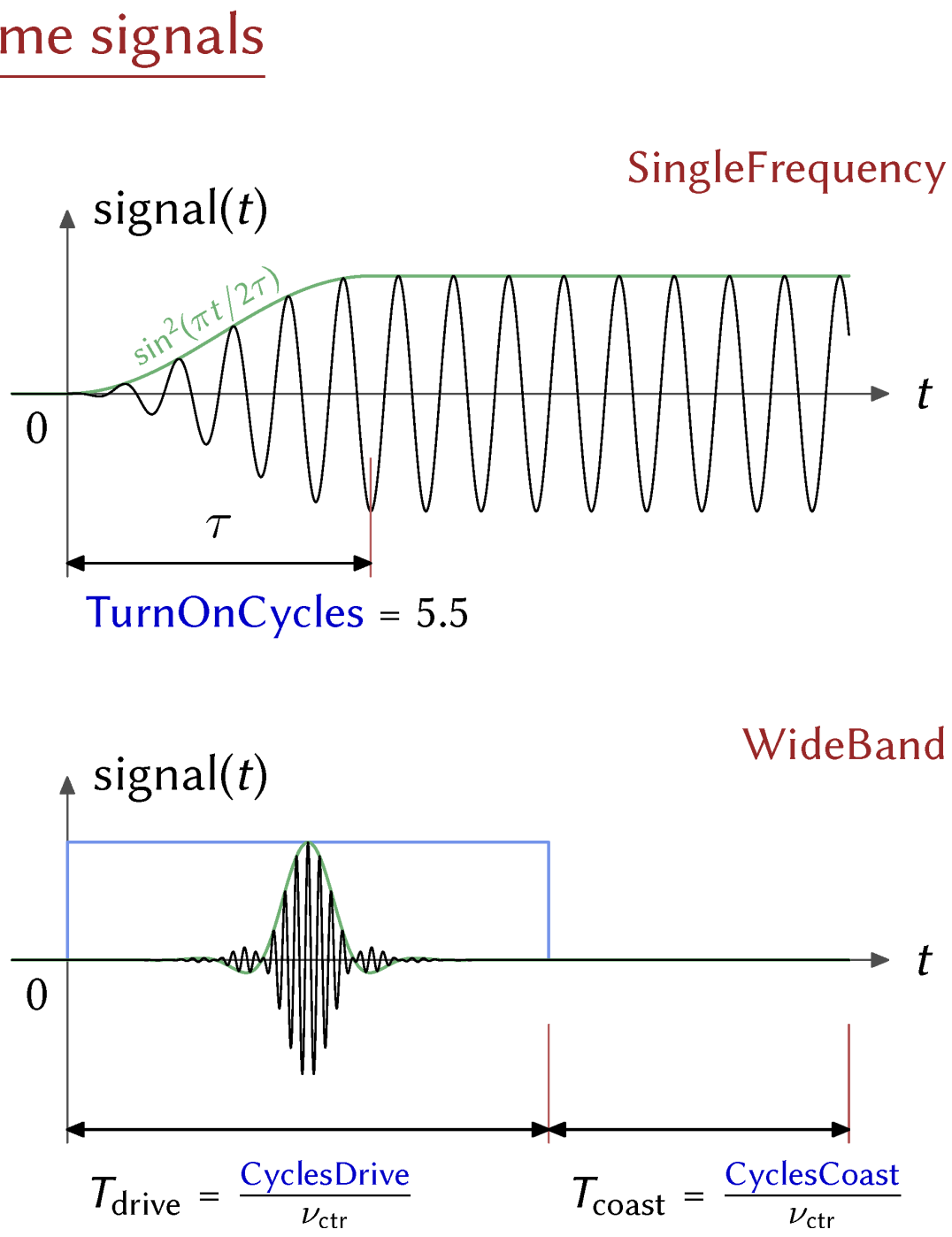


Fig. 3.100: Two possible time signals for ringing the dipole source.

Opening the Simulation

This Photonic Crystal example is accessed from within VSimComposer through the following steps:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window, expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select "Dipole Source Illuminating a Photonic Crystal Cavity" and press the *Choose* button.
- In the resulting dialog, create a new folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the *Setup Window* as shown in Fig. 3.101. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the photonic crystal geometry. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

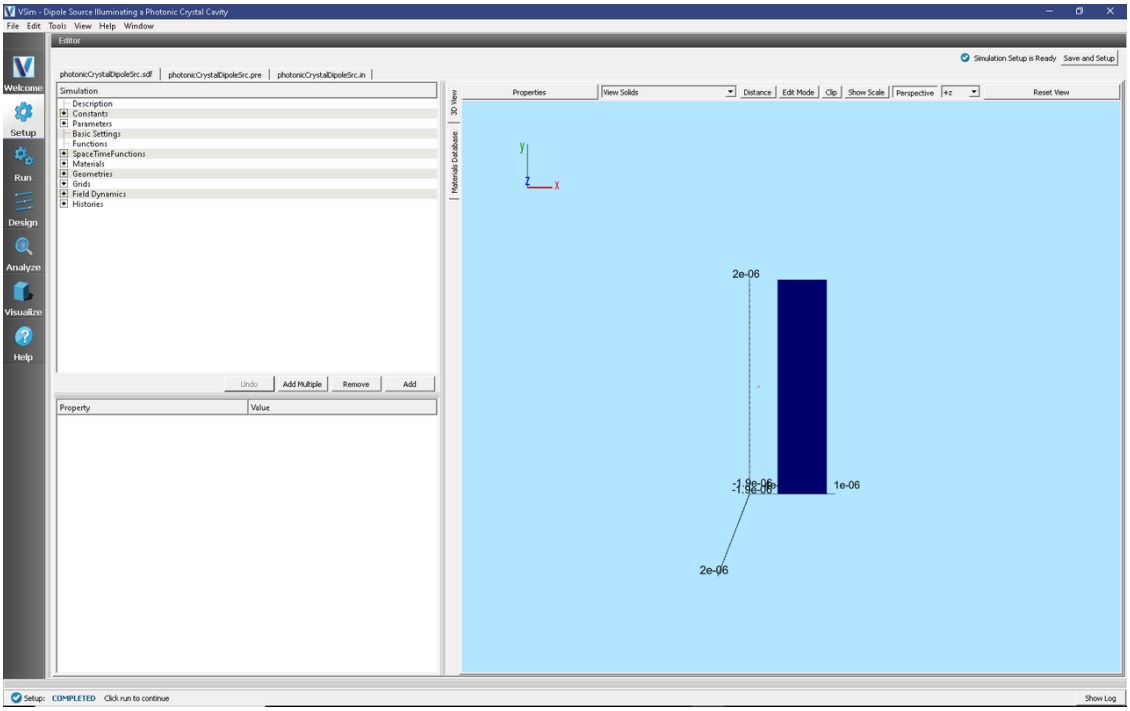


Fig. 3.101: The Setup Window for the Dipole Source Illuminating a Photonic Crystal Cavity example

Simulation Properties

This example contains a number of constants defined to make the simulation easily modifiable, as can be seen in Fig. 3.102.

The following constants should be the only properties you should need to alter in order to specify your simulation domain.

General Simulation Parameters:

- `CYCLES_DRIVE` = How many cycles at which the E/M source is driven.
- `HT_{VACUUM,SI,SI02}` = The height of the vacuum, SI and SI02 layers of the photonic crystal.

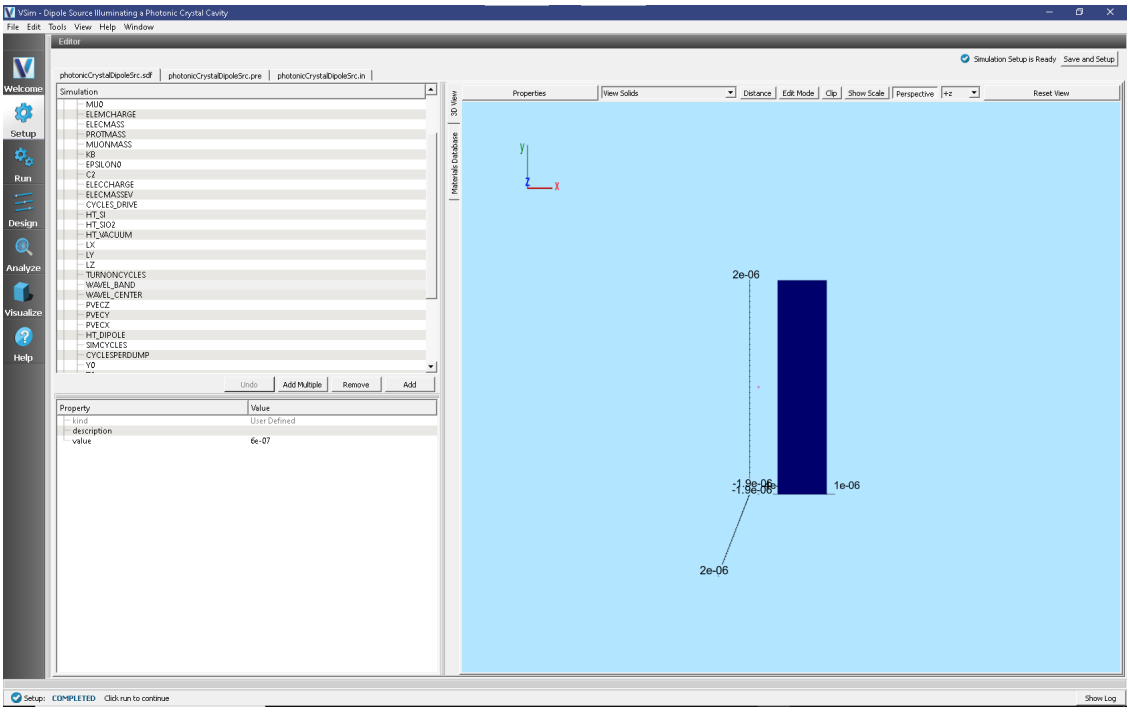


Fig. 3.102: The Setup Window showing the constants

- `L{X,Y,Z}` = The length of your simulation domain in the {X,Y,Z} dimension.

Source Specifications: (located in the *Parameters* section of the *Elements Tree*)

- `TURNONCYCLES` = The number of cycles you want your single frequency to reach full power.
- `WAVEL_BAND` = The wavelength width of your wideband signal, if doing a wideband simulation.
- `WAVEL_CENTER` = The central wavelength of your wideband signal, and is the frequency used in the single frequency simulation type.
- `PVEC{X,Y,Z}` = The {x,y,z} component of your moment vector for your dipole source.
- `HT_DIPOLE` = The height of the dipole from the lowerX boundary.
- `SIMCYCLES` = Number of wave cycles you want your simulation to run.
- `CYCLESPERDUMP` = Number of cycles between each dump in the simulation.

The tool used to input the wave into the simulation is a port launcher. It specifies the Electric Displacement Field (D) at a boundary in this case the lower X boundary. The functions defining the D on the boundary are defined in the *SpaceTimeFunctions* element of the *Elements Tree*.

SpaceTimeFunctions:

- `dSingleFreqDipole{Y,Z}` = This is the {x,y,z} component of the single frequency dipole source; as seen in Fig. 3.103, you put this as a parameter in the PortLauncher.
- `dWideBandDipole{Y,Z}` = This is the {x,y,z} component of the wideband dipole source; as seen in Fig. 3.103, you put this as a parameter in the PortLauncher.

To choose which signal you want to input into this example simulation:

1) Expand the *FieldBoundaryConditions* tab.
2) Left click on the *portLauncherLowerX* condition.

At this point, you should see what is shown in Fig. 3.103:

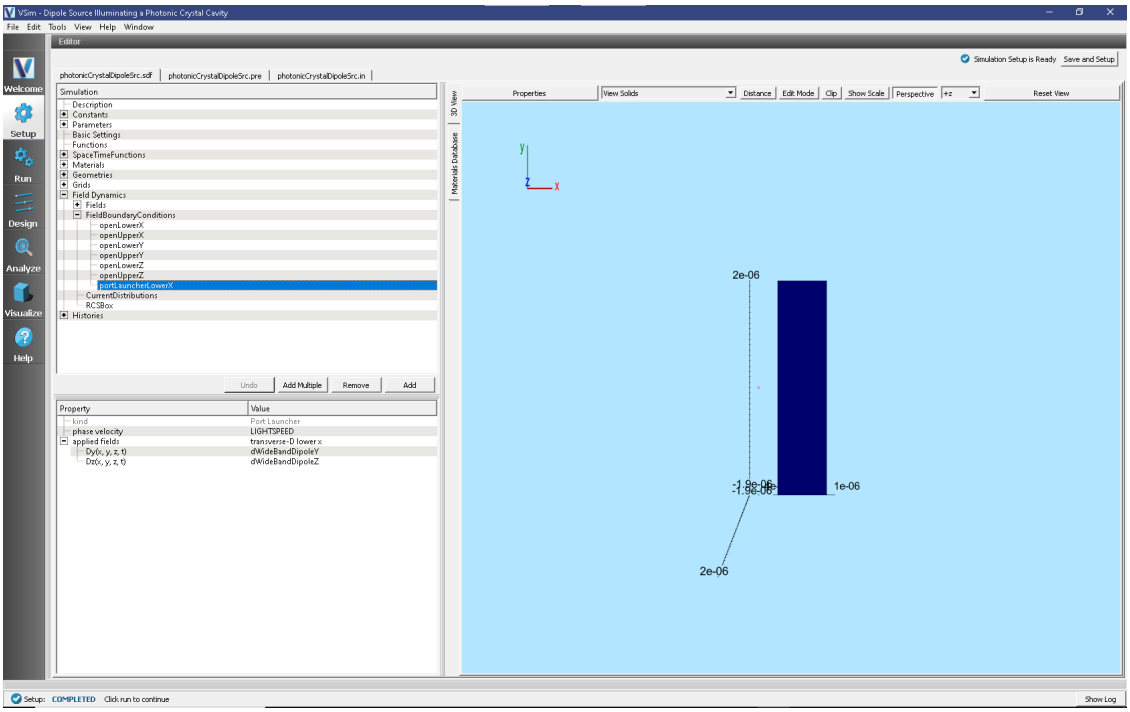


Fig. 3.103: The Setup Window showing where to specifying the applied field signal for the port launcher

3) To change the signal applied to the *portLauncherLowerX*, right click on the Dx(x, y, z, t) or Dy(x, y, z, t) property and select *Assign SpaceTimeFunction*. This will expand another menu that will show you all four defined SpaceTimeFunctions. Select which one you want to input into your simulation. For this documentation, `dWideBandDipole{Y,Z}` is selected by default to demonstrate the functionality of the example.

Running the Simulation

Once finished with the problem setup, continue as follows:

- Proceed to the *Run Window* by pressing the *Run* button in the left column of buttons.
- One can enable MPI options to utilize multi-core systems.
- The default values of `Number of Time Steps` and `Dump Periodicity` are taken from the parameters `STEPSTOTAL` and `STEPSPERDUMP`, which use the constants `SIMCYCLES` and `CYCLESPERDUMP`. The formulae for these variables can be found back in the *Setup Window*. These variables are for convenience to calculate good default values and it is important to know that the override option default values ultimately come directly from the numbers in the *Basic Settings* section.
  - *Number of Steps* = `STEPSTOTAL` = 36250
  - *Dump Periodicity* = `STEPSPERDUMP` = 3600
- To run the file, click on the *Run* button in the upper left corner of the Logs and Output Files pane. You will see the output of the run in that pane. The run has completed when you see the output, "Engine completed successfully." This is shown in Fig. 3.104.

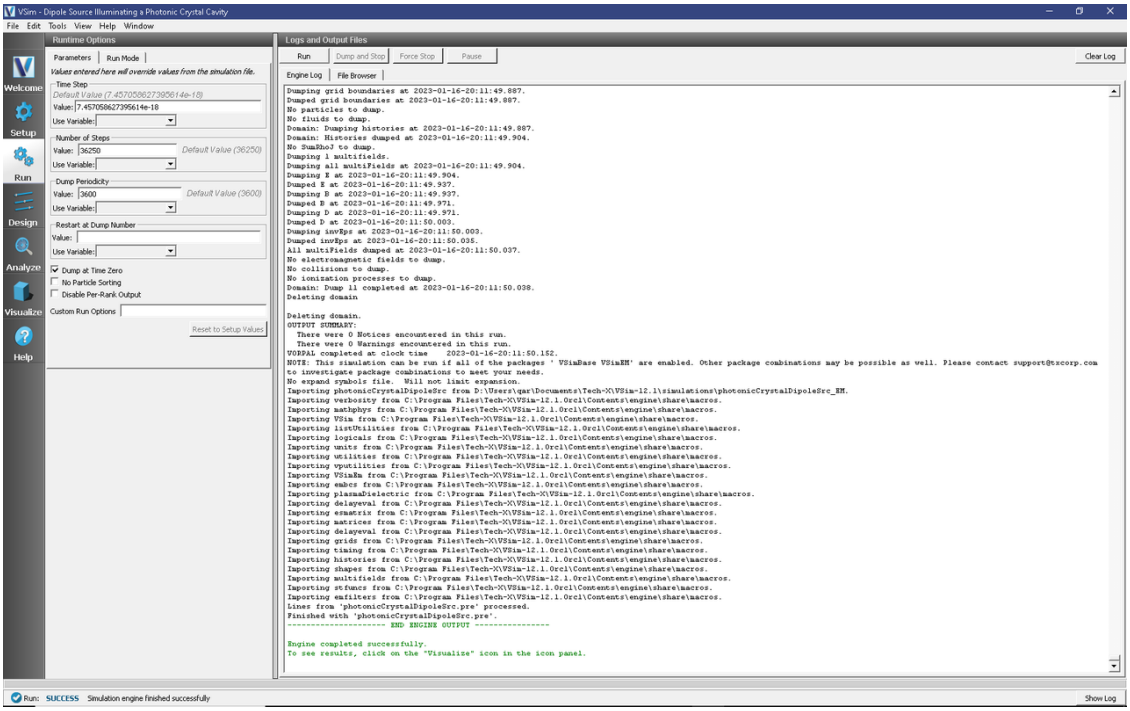


Fig. 3.104: The Run Window for the Dipole Source Illuminating a Photonic Crystal Cavity example

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the *Visualize Window* by pressing the *Visualize* button in the left column of buttons.

In the simulation, there are specific grid points which store field histories. These histories are placed in various positions of the simulation.

- Click the *Add a Data View* dropdown below the menu bar and select *History*.

In Fig. 3.105, one can see there are 4 possible graphs to view at one time in the *Visualize Window*. For each graph, one can select the following fields to analyze: (0 = x, 1 = y, 2 = z).

- {E,B}_AtDet_{0,1,2} = In the middle of (y,z) plane and 60 nm above the surface of the crystal.
- {E,B}_AtSrc_{0,1,2} = Is aligned with the inCav history in the (y,z) plane and is 60 nm below the Si layer, into the SiO2 layer.
- {E,B}_InCav_{0,1,2} = Is slightly offset from the middle of one of the cavities in the Silicon layer (the layer with the lattice).

In each individual graph, one can choose the *Fourier Amplitudes (dB)* option to view the frequency domain of your field. This can enable the analysis of the frequency response of the photonic crystal cavity.

Fig. 3.105 depicts four graphs of histories. The first two graphs are amplitude vs time, and the second two are a Fourier Amplitudes of the first two on a log scale.

The first and third graphs depict the history `AtSrc_2`, while the second and fourth graphs show the *AtDet_2* history.

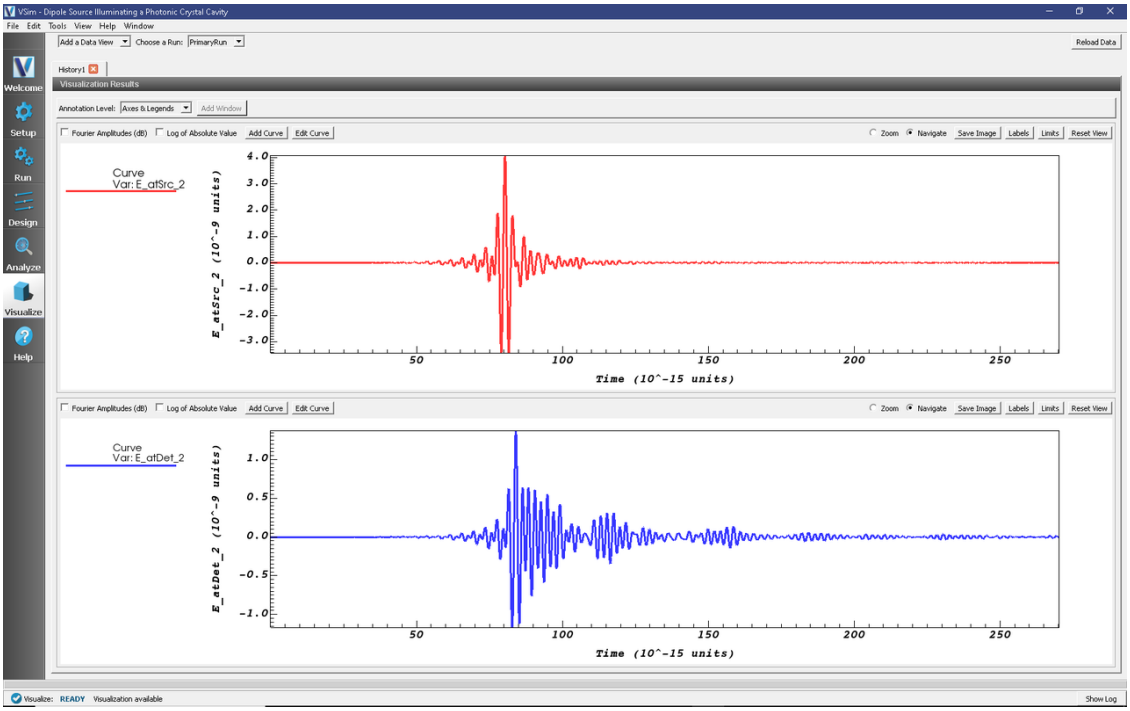
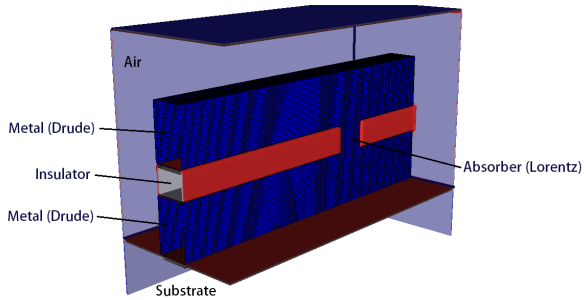


Fig. 3.105: The Visualize Window for the Dipole Source Illuminating a Photonic Crystal Cavity example

Further Experiments

By using the wideband source and examining the field strength detected below the crystal lattice, one may study the frequency response of this photonic crystal as one changes the device geometry, the dielectric constants, and the location and polarizations of the radiation source and detector.

3.3.7 Metal Insulator Metal Waveguide using Drude and Lorentz Materials (drudeLorentzMIM.sdf)



Problem Description

A metal-insulator-metal (MIM) waveguide can propagate optical frequency electromagnetic radiation due to the effective negative index material property of the metal at those frequencies. This negative index material is represented with a time-domain Drude model dielectric, which can support a wide range of frequencies and wide bandwidth.

In addition to the MIM waveguide, a section of the insulator is removed, and replaced with a resonant absorber material, using a time-domain version of the traditional Lorentz material.

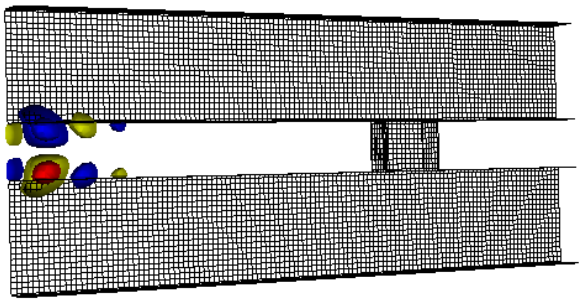


Fig. 3.106: Longitudinal electric field in the MIM waveguide.

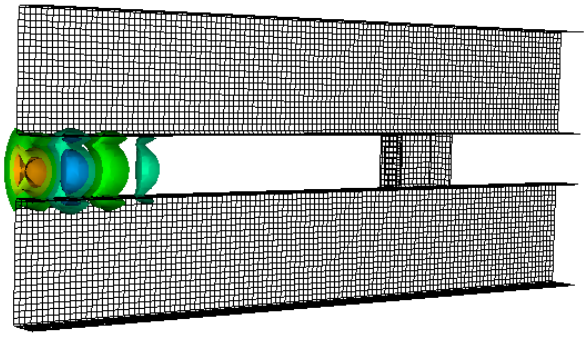


Fig. 3.107: Transverse electric field in the MIM waveguide.

A spatial gaussian waveform is incident on the edge of the MIM waveguide, coupling to it, and propagating down the length of the waveguide until it encounters the Lorentz material inclusion, where the wave is absorbed. For the incident wave to couple effectively to the MIM waveguide, the spatial size of the gaussian waveform must be a good match to the size of the waveguide, or a large portion of the incident wave will scatter off the structure, rather than coupling to it.

Also, the width, strength, and natural oscillation frequency of the Lorentz material inclusion determines whether the wave is reflected, absorbed, or transmitted when it encounters the inclusion. In this example there is only one Lorentz curve, but multiple Lorentz curves can be added to the simulation.

The length of the MIM waveguide, and the direction of wave propagation is in the x-direction. The width of the waveguide is in the z-direction, and the height of the waveguide is in the y-direction. The waveguide sits atop an insulator substrate, and is surrounded by air. The boundaries of the simulation are ports, allowing for incoming and outgoing waves.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The MIM waveguide example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Scattering* option.
- Select "MIM Waveguide" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 3.108.

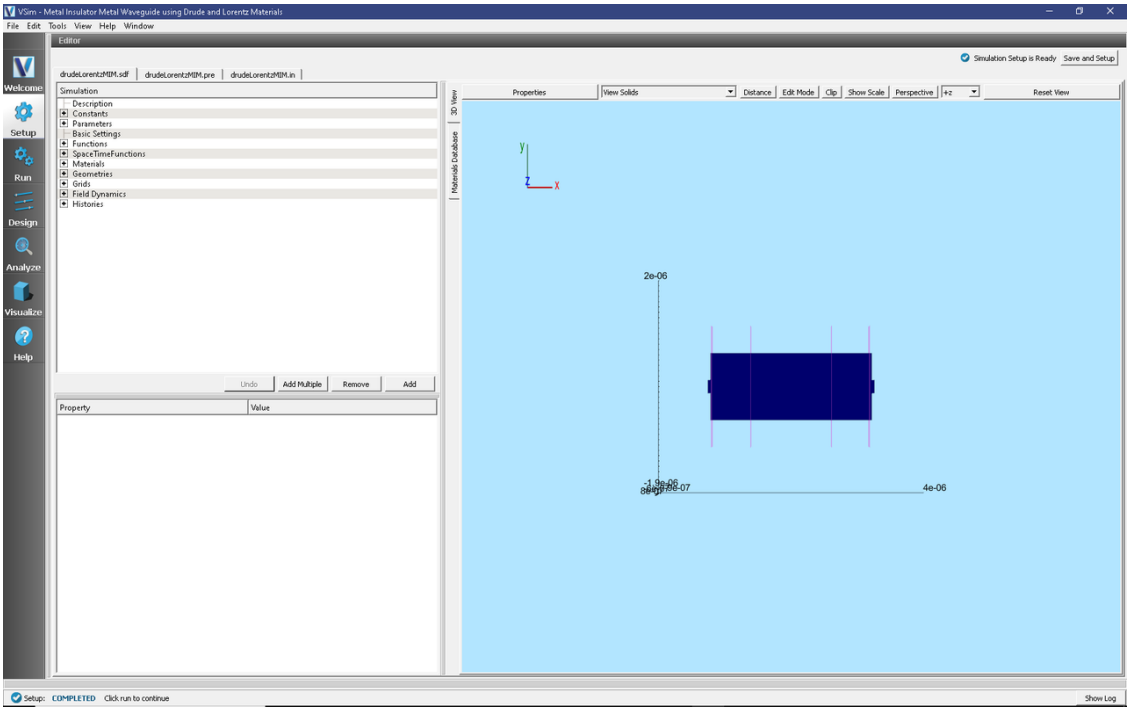


Fig. 3.108: Setup Window for the drudeLorentzMIM example.

Simulation Properties

The geometry of the waveguide is fully parameterized, allowing for easy adjustment to the waveguide.

A port launcher boundary is used at the lower X boundary to launch a Y polarized wave.

The Drude-Lorentz model dielectric allows for full specification of the Drude model collision and conductivity function, as well as a background conductivity. In this example a single Lorentz model is used with the oscillator, frequency and line width. More Lorentz's can be added by adding to the vector of these three properties.

The input file also contains a parameter to adjust the spatial resolution of the mesh.

Default parameters are selected to correspond to violet light, a Drude material corresponding to silver, SiO2 insulator (and substrate), and a Lorentz material corresponding to AlAs. The default variable values can be compared to the well known material properties of these materials to establish the exact correspondence to the well-known mathematical descriptions of the Drude and Lorentz models.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 4.1340777062450576e-17
  - *Number of Steps*: 1001
  - *Dump Periodicity*: 70
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.109.

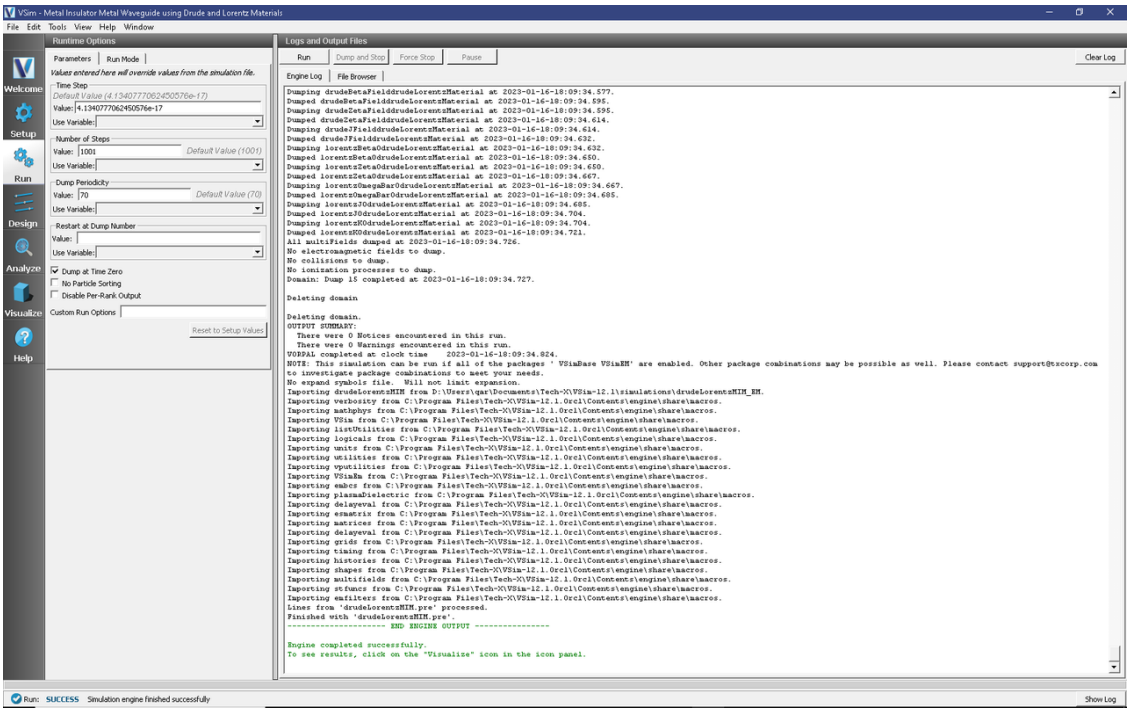


Fig. 3.109: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The results are best viewed by looking at the y component of the electric field. To view the fields, select *Scalar Data* variable and check the *E_y* box. Check the *Clip Plot* checkbox. Set the minimum value to -0.75 and the maximum value to 0.75. The field is shown in Fig. 3.110.

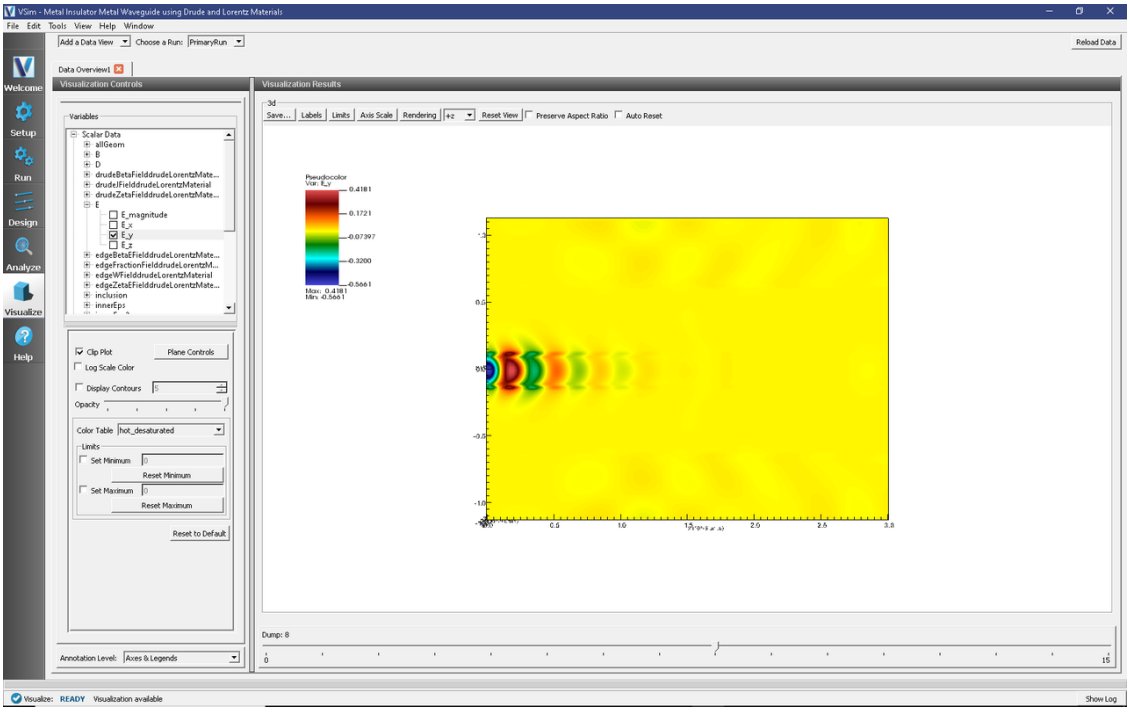


Fig. 3.110: Visualization of the E_y field component.

We can see that fields are well coupled between the two metal layers of the waveguide, with only some small leakage, and transient behavior at the entrance. The fields then diminish abruptly at the inclusion, where the wave is mostly absorbed.

3.3.8 Microring Resonator with Mode Launcher (ringResonatorMode.sdf)

Keywords:

`Ring Resonator, Mode Launcher, MAL, Guided Mode, Photonic Device, Semiconductor`

Problem Description

The Ring Resonator consist of two straight Silicon waveguides and a Silicon waveguide ring that sits between the straight waveguides. All three waveguides rest on top of a Silicon Dioxide slab. The rest of the simulation domain is set to vacuum. Matched Absorbing Layers (MALs) are used to dampen the E, B and D fields near the boundary of the simulation.

The fundamental guided mode profile is launched as a wide band pulse in the input waveguide. This mode is imported from the file save_EigenD_0.vsh5, produced by the computeWaveguideModes.py analyzer. To go through the mode solve process check out the Multimode Fiber Mode Calculation example. We will use the computeSParamsViaOverlapIntegral.py analyzer to determine the transmission coefficients at the thru-port and drop port.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Ring Resonator example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Ring Resonator* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are available in the Setup Window as shown in Fig. 3.111. You can expand the tree elements and navigate through the various properties. The right pane shows a 3D view of the geometry, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to *Grid*.

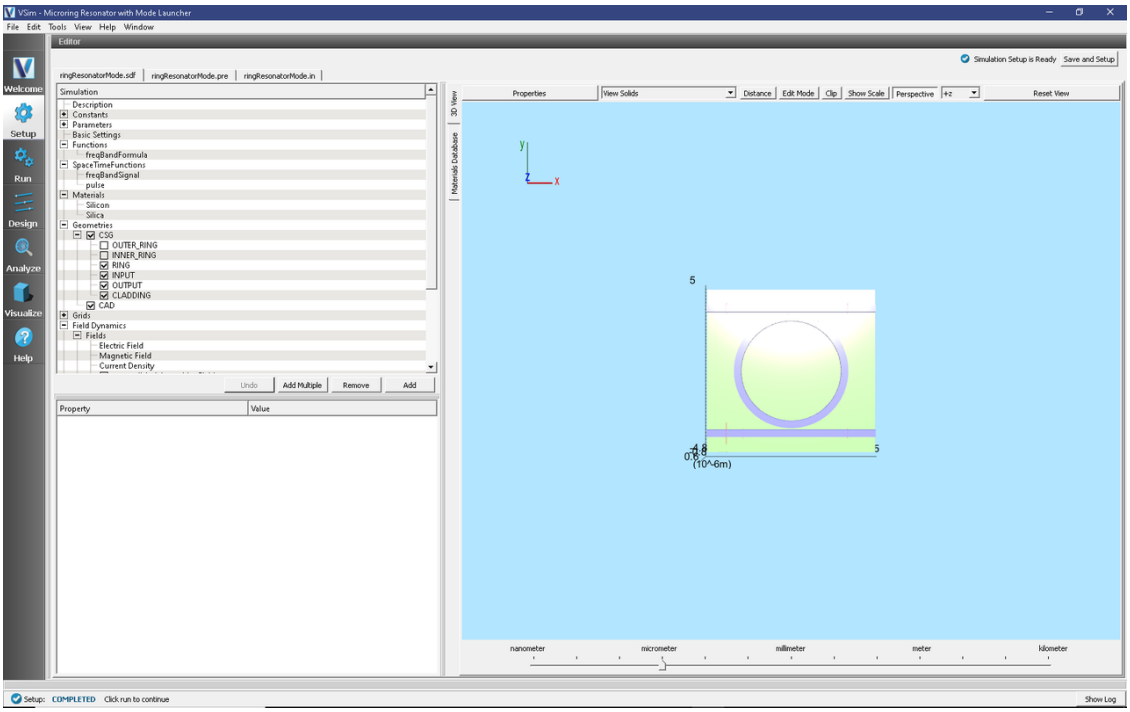


Fig. 3.111: The Setup window for the ring resonator example showing the external mode launching field.

Simulation Properties

This example contains a number of *Constants* defined to make the simulation easily modifiable.

General Simulation Constants:

- RESOLUTION_XY = the inverse of the number of cells per wavelength
- RESOLUTION_Z = the inverse of the number of cells per waveguide height in the z dimension
- WAVELENGTH_CENTER = the central wavelength used in the excitation
- WIDTH_EXCITATION = the width in wavelength space of the wide band signal
- RADIUS_RING = radius of the ring

- WIDTH_WAVEGUIDE = Width of waveguides
- HEIGHT_WAVEGUIDE = Height of waveguides
- WIDTH_GAP = Width of the gap between ring and waveguides

This simulation applies a wide frequency band signal to the fundamental spatial mode profile. The signal is defined under *SpaceTimeFunctions* and then assigned under *Field Dynamics*, *Fields*, *externalModeLaunchingField1* as shown in Fig. 3.111.

The *Materials* section contains just Silicon and Silica. This section is where one can add or edit materials that get attached to CSG objects. These *Materials* contain the relative permittivity.

In *Field Dynamics* there are *FieldBoundaryConditions* which set the boundary conditions of the simulation. In photonics simulations, Matched Absorbing Layers (MALs), are the most stable boundary conditions for preventing reflections.

Under *Basic Settings* you can see that the *dielectric solver* is set to *permittivity averaging*. This feature enables second order accuracy for simulations using dielectrics.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 7.343490630124558e-16
  - *Number of Steps*: 63817
  - *Dump Periodicity*: 6000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.112.

Analyzing the Results

Using post analysis scripts, one can extract the transmission coefficients. This simulation uses 4 "EM Field on Plane" histories (slab0-slab4) and this data is used to calculate S parameters between these 4 locations using the analysis script computeSParamsViaOverlapIntegral.py.

Follow these steps:

- Proceed to the Analyze Window by clicking the *Analyze* button on the left.
- Select *computeSParamsViaOverlapIntegral.py* and click *Open* under the list.

Now update the analyzer fields accordingly.

- *maxWavelength*: 1.7e-6 (or use the corresponding parameter from the setup)
- *minWavelength*: 1.4e-6 (or use the corresponding parameter from the setup)
- *inPlane*: slab0
- *outPlane*: slab1 (or slab3)
- *outputFileSuffix*: S01 (or S03)

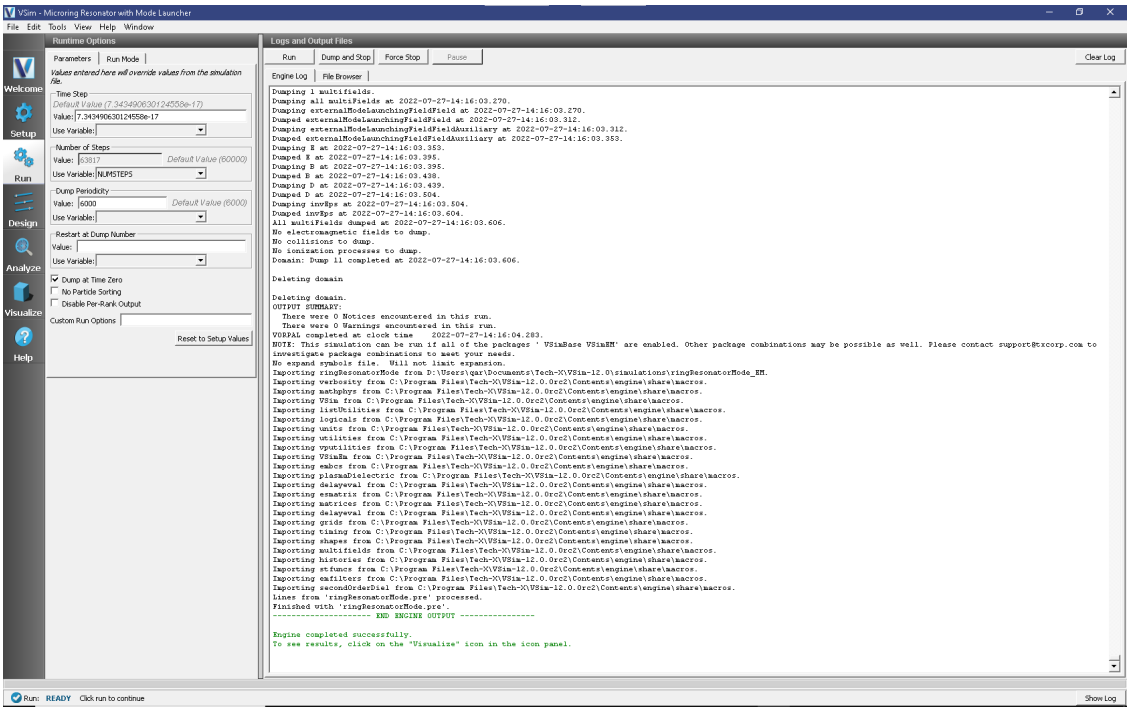


Fig. 3.112: Run window at completion.

The remaining parameter default values will work. Hit the *Analyze* button in the top tight corner. After a successful run the window should resemble Fig. 3.113.

Visualizing the results

After performing the above actions proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

One can visualize the magnetic field by performing the following:

- Near the top left corner of the window, select *Data Overview* from the *Add a Data View* drop-down.
- Expand *Scalar Data*, then *B*, then select *B_magnitude*
- In the bottom left, select *Clip All Plots*, and set z=0 in *Plane Controls*
- Finally, move the dump slider on the bottom of the window to watch the light propagate

The results are shown in Fig. 3.114.

One can visualize the transmission coefficients by performing the following:

- Near the top left corner of the window, select *1-D Fields* from the *Add a Data View* drop-down.
- In the Plot Control panel select the Slab1 and Slab3 SParams data for Graphs 1 and 2, respectively.
- Set the other Graphs to *None*

The results are shown in Fig. 3.115. As expected, we see coupling of resonant wavelengths with the ring.

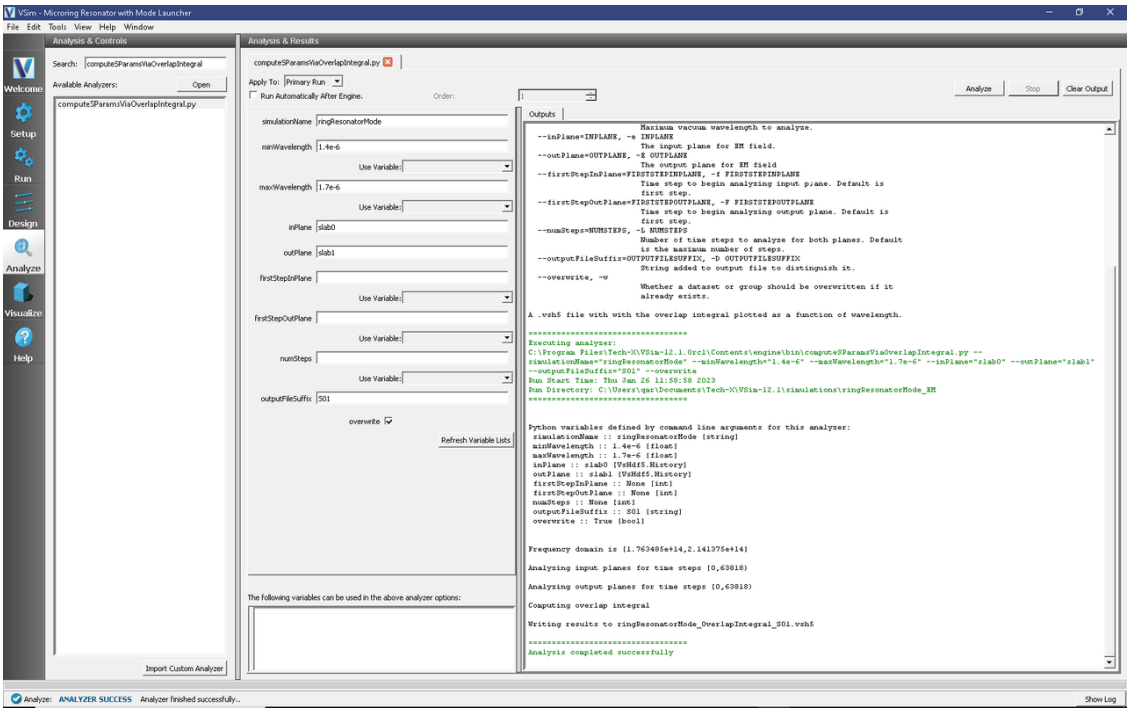


Fig. 3.113: Analyze window with output from computeSParamsViaOverlapIntegral.py.

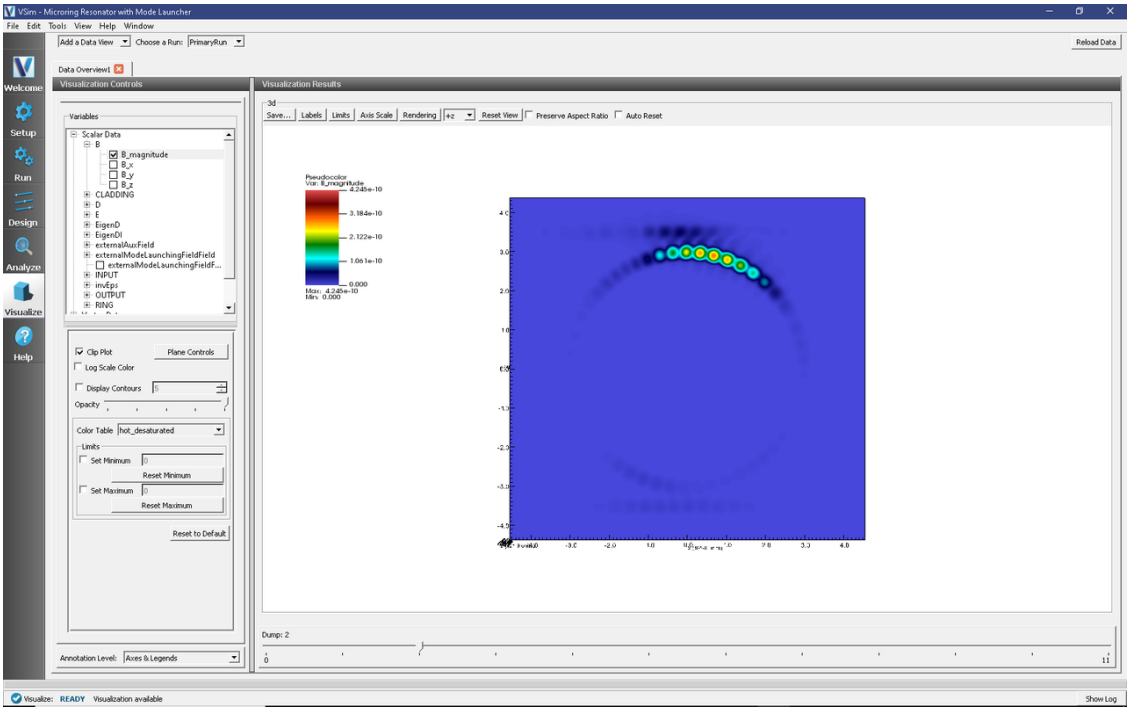


Fig. 3.114: Visualization of magnetic field.

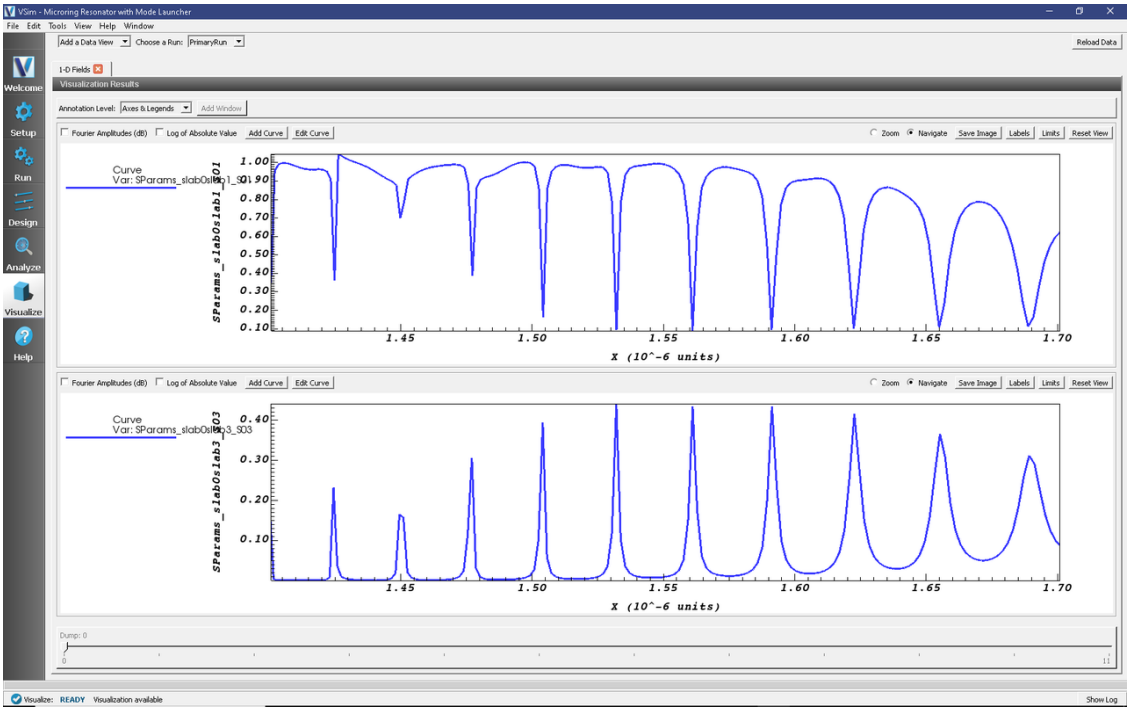


Fig. 3.115: Visualization of the s-parameters.

3.3.9 Microring Resonator with Gaussian Launcher (ringResonatorGaussianMode.sdf)

Keywords:

`Ring Resonator, Mode Launcher, MAL, Guided Mode, Photonic Device, Semiconductor`

Problem Description

The Ring Resonator consist of two straight Silicon waveguides and a Silicon waveguide ring that sits between the straight waveguides. All three waveguides rest on top of a Silicon Dioxide slab. The rest of the simulation domain is set to vacuum. Matched Absorbing Layers (MALs) are used to dampen the E, B and D fields near the boundary of the simulation.

The approximate fundamental guided mode profile is launched as a wide band pulse in the input waveguide. This mode is a simple 2D Gaussian distribution centered at the center of the waveguide. This approximate mode is accurate enough for this simulation. The exact mode can be calculated using the computeWaveguideModes analyzer. To go through the mode solve process check out the Multimode Fiber Mode Calculation example. We will use the computeSParamsViaOverlapIntegral.py analyzer to determine the transmission coefficients at the thru-port and drop port.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Ring Resonator example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Ring Resonator* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are available in the Setup Window as shown in Fig. 3.116. You can expand the tree elements and navigate through the various properties. The right pane shows a 3D view of the geometry, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to *Grid*.

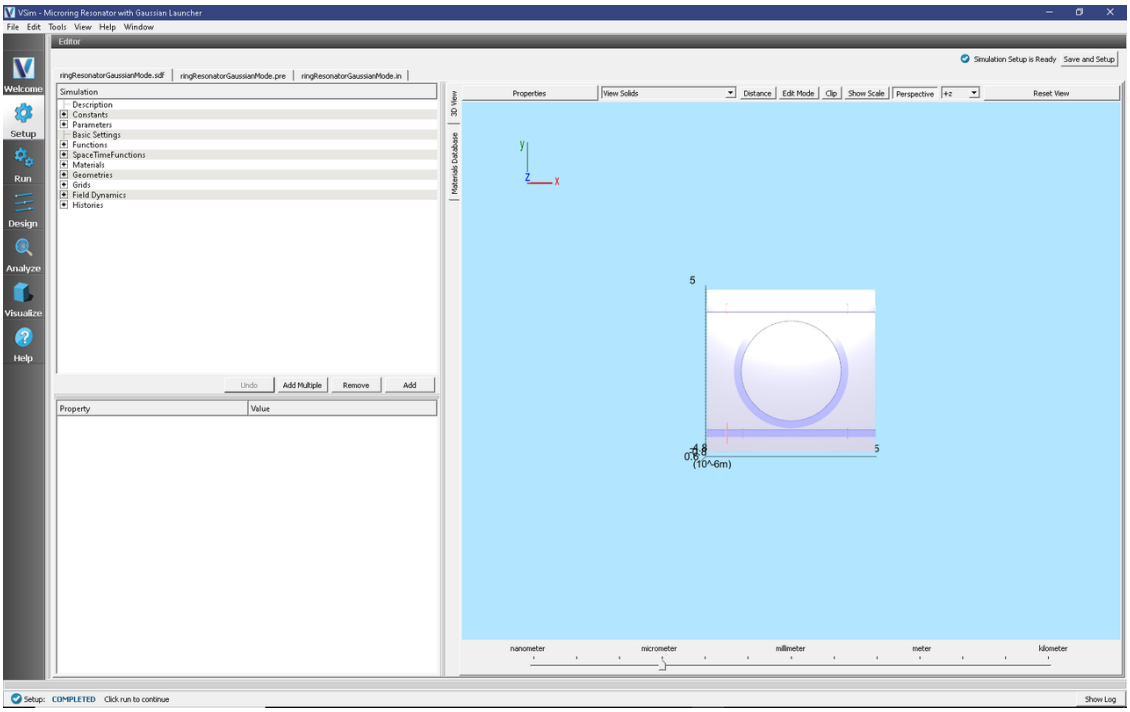


Fig. 3.116: The Setup window for the ring resonator example showing the external mode launching field.

Simulation Properties

This example contains a number of *Constants* defined to make the simulation easily modifiable.

General Simulation Constants:

- RESOLUTION_XY = the inverse of the number of cells per wavelength
- RESOLUTION_Z = the inverse of the number of cells per waveguide height in the z dimension
- WAVELENGTH_CENTER = the central wavelength used in the excitation
- WIDTH_EXCITATION = the width in wavelength space of the wide band signal
- RADIUS_RING = radius of the ring

- WIDTH_WAVEGUIDE = Width of waveguides
- HEIGHT_WAVEGUIDE = Height of waveguides
- WIDTH_GAP = Width of the gap between ring and waveguides

This simulation applies a wide frequency band signal to the approximate fundamental spatial mode profile. The signal is defined under *SpaceTimeFunctions* and then assigned under *Field Dynamics*, *CurrentDistributions*, *generalDistributedCurrent* as shown in Fig. 3.116.

The *Materials* section contains just Silicon and Silica. This section is where one can add or edit materials that get attached to CSG objects. These *Materials* contain the relative permittivity.

In *Field Dynamics* there are *FieldBoundaryConditions* which set the boundary conditions of the simulation. In photonics simulations, Matched Absorbing Layers (MALs), are the most stable boundary conditions for preventing reflections.

Under *Basic Settings* you can see that the *dielectric solver* is set to *permittivity averaging*. This feature enables second order accuracy for simulations using dielectrics.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: DT: 7.34349e-17
  - *Number of Steps*: NUMSTEPS: 63817
  - *Dump Periodicity*: 6000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.117.

Analyzing the Results

Using post analysis scripts, one can extract the transmission coefficients. This simulation uses 4 "EM Field on Plane" histories (slab0-slab4) and this data is used to calculate S parameters between these 4 locations using the analysis script computeSParamsViaOverlapIntegral.py.

Follow these steps:

- Proceed to the Analyze Window by clicking the *Analyze* button on the left.
- Select *computeSParamsViaOverlapIntegral.py* and click *Open* under the list.

Now update the analyzer fields accordingly.

- *maxWavelength*: 1.7e-6 (or use the corresponding parameter from the setup)
- *minWavelength*: 1.4e-6 (or use the corresponding parameter from the setup)
- *inPlane*: slab0
- *outPlane*: slab1 (or slab3)
- *outSLabB*: slab1 (or slab3)
- *outputFileSuffix*: S01 (or S03)

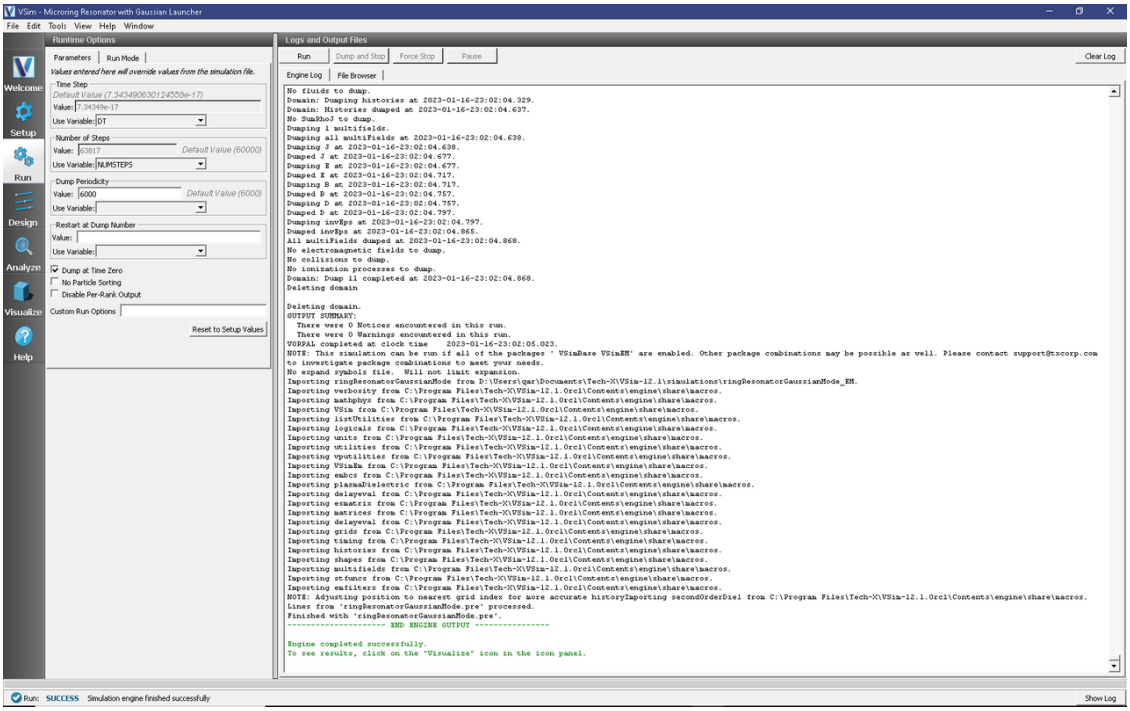


Fig. 3.117: Run window at completion.

The remaining parameter default values will work. Hit the *Analyze* button in the top right corner. After a successful run the window should resemble Fig. 3.118. Continue by analyzing the drop-port. To do this change the *outSlabE* and *outSlabB* fields to slab3_E and slab3_B, respectively.

Visualizing the results

After performing the above actions proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

One can visualize the magnetic field by performing the following:

- Near the top left corner of the window, select *Data Overview* from the *Add a Data View* drop-down.
- Expand *Scalar Data*, then *B*, then select *B_magnitude*
- In the bottom left, select *Clip Plot*, and set z=0 in *Plane Controls*
- Finally, move the dump slider on the bottom of the window to watch the light propagate

The results are shown in Fig. 3.119.

One can visualize the transmission coefficients by performing the following:

- Near the top left corner of the window, select *1-D Fields* from the *Add a Data View* drop-down.
- In the Plot Control panel select the Slab1 and Slab3 SParams data for Graphs 1 and 2, respectively.
- Set the other Graphs to *None*

The results are shown in Fig. 3.120. As expected, we see coupling of resonant wavelengths with the ring.

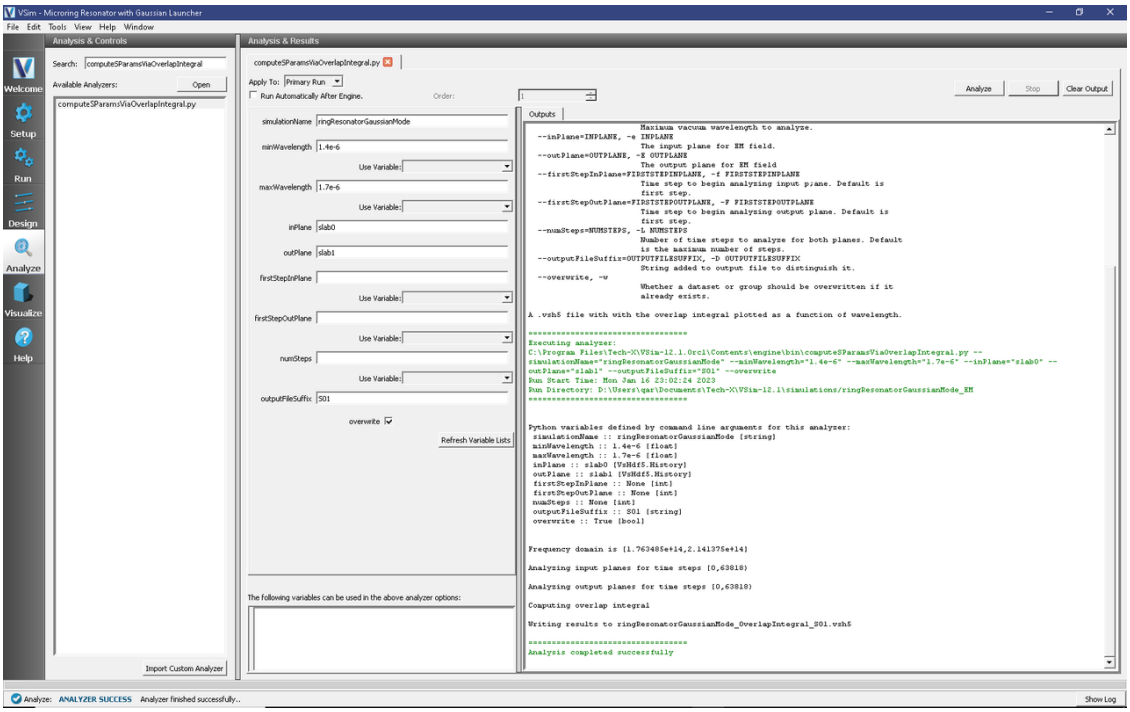


Fig. 3.118: Analyze window with output from computeSParamsViaOverlapIntegral.py.

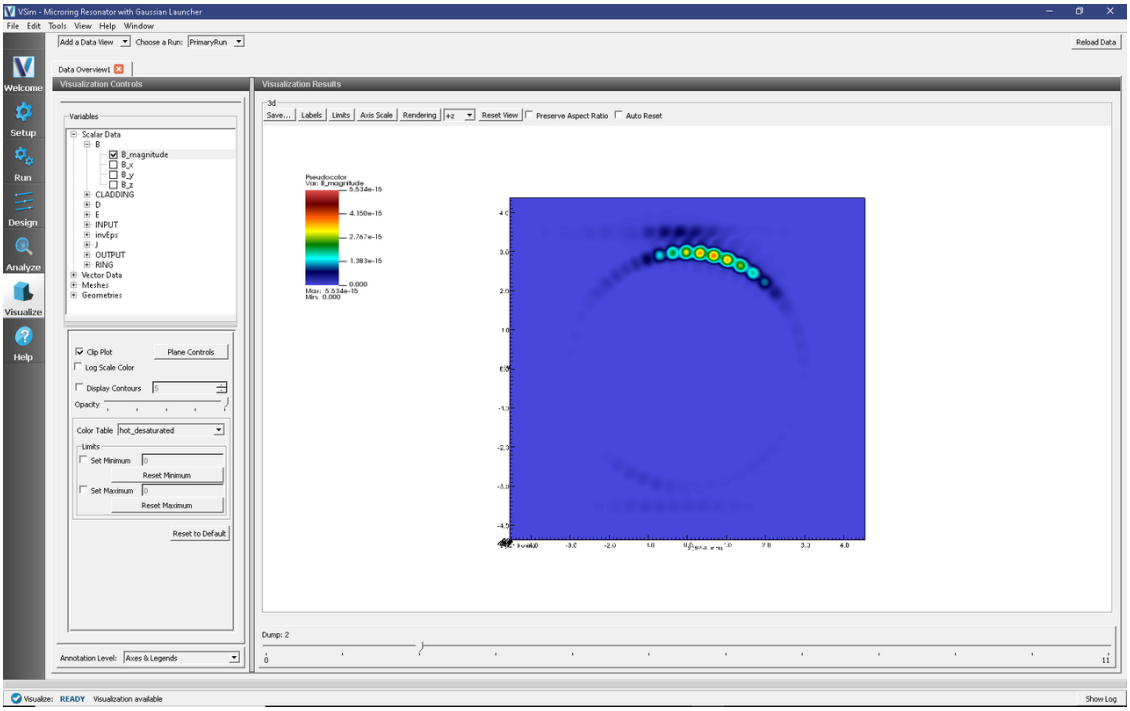


Fig. 3.119: Visualization of magnetic field.

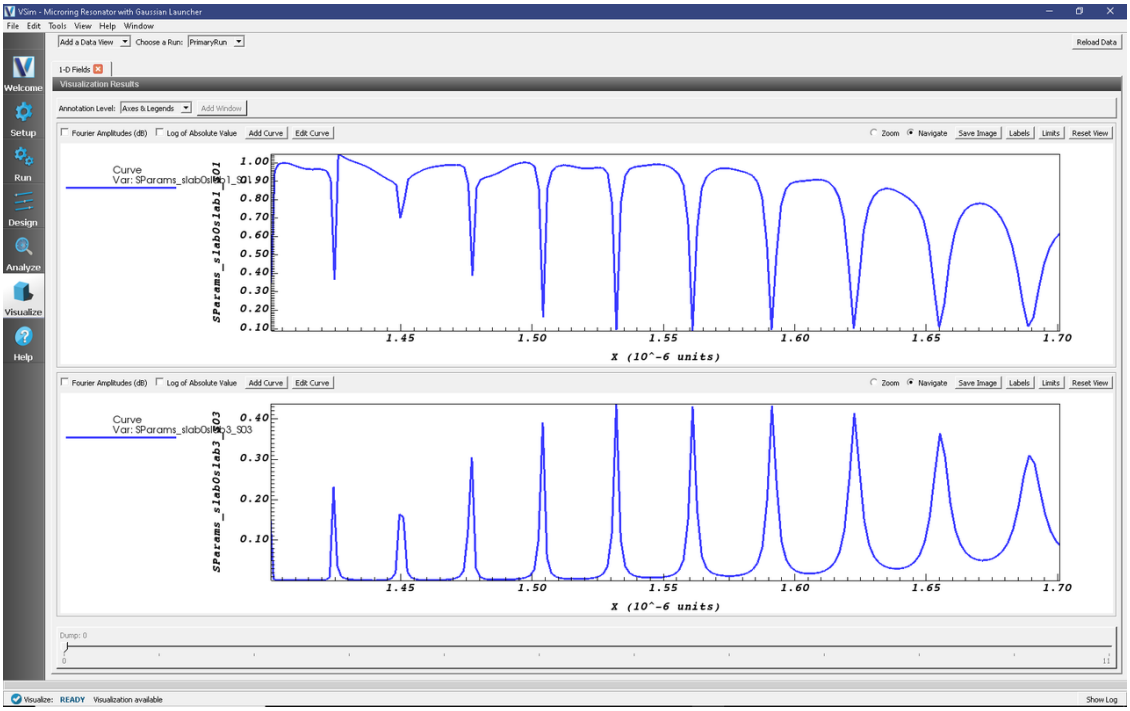


Fig. 3.120: Visualization of the s-parameters.

3.3.10 Y Splitter (ySplitter.sdf)

Keywords:

S Parameter, Mode Launcher, MAL, Guided Mode, Photonic Device, Semiconductor

Problem Description

The Y Splitter makes use of a gds file of a passive photonic device, intended to split the power of a single incoming wave into two separate branches.

The device itself is silicon, surrounded by silicon dioxide.

This examples makes use of a "Photonics simulation template" intended to allow for rapid setup of any passive photonic device, provided the ports are aligned with the X-Axis. Matched Absorbing Layers (MALs) are used to dampen the E, B and D fields near the boundary of the simulation.

The fundamental guided mode profile is launched as a wide band pulse in the input waveguide. This mode is imported from the file port1LowRes_EigenD_0.vsh5, produced by the computeWaveguideModes.py analyzer. We will use the computeSParamsViaOverlapIntegral.py analyzer to determine the transmission coefficients at the two exit ports of the device.

This simulation out of the box is set to a minimal resolution, allowing for a faster simulation time, with 8 cells per wavelength (in Silicon) used. For typical use cases a value of 12-18 cells per wavelength is recommended.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Y Splitter example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Photonics* option.
- Select *Y Splitter* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are available in the Setup Window as shown in Fig. 3.121. You can expand the tree elements and navigate through the various properties. The right pane shows a 3D view of the geometry, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to *Grid*.

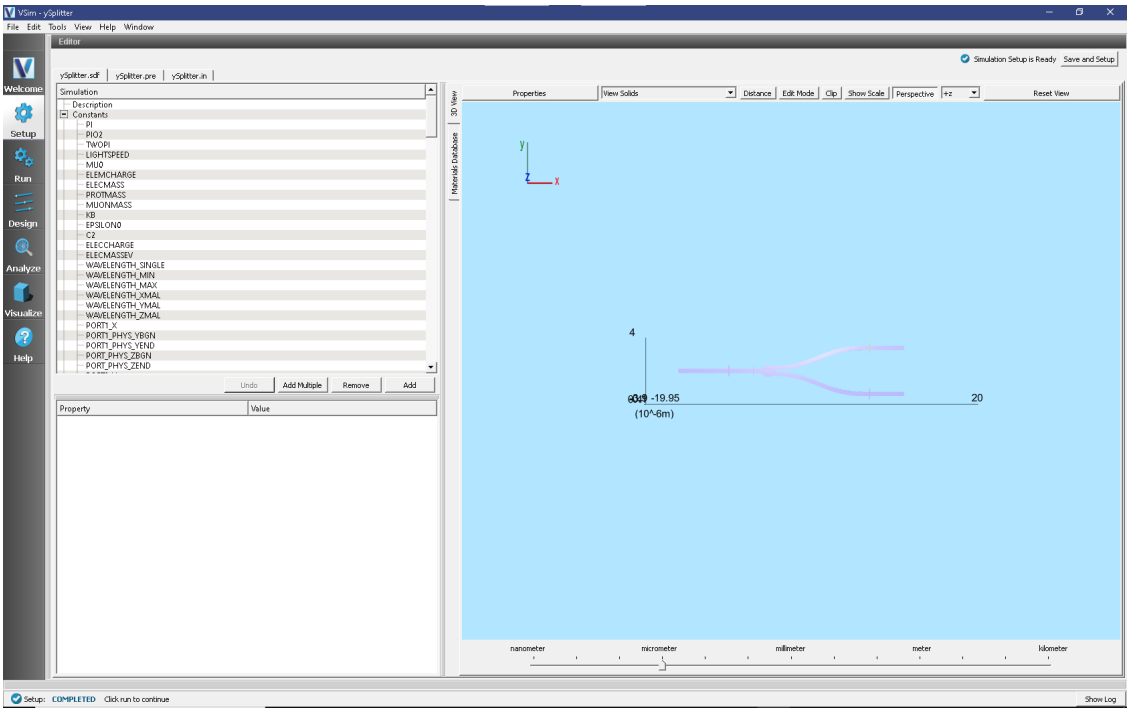


Fig. 3.121: The Setup window for the y splitter example showing the imported gds file.

Simulation Properties

This example contains a number of *Constants* defined to make the simulation easily modifiable. These are also intended to be reset for a different gds file and will redefine the simulation size and parameters

General Simulation Constants:

- WAVELENGTH_SINGLE = Used for a single wavelength simulation and calculation of simulation information based on wavelength.
- WAVELENGTH_MIN = Minimum wavelength for a multi-wavelength simulation.
- WAVELENGTH_MAX = Maximum wavelength for a multi-wavelength simulation.

- WAVELENGTH_XMAL = Number of wavelengths of MAL in the X-direction.
- WAVELENGTH_YMAL = Number of wavelengths of MAL in the Y-direction.
- WAVELENGTH_ZMAL = Number of wavelengths of MAL in the Z-direction.
- PORT1_X = Location of port 1 (excitation port) on the X-axis.
- PORT1_PHYS_YBGN = Beginning of Port 1 on the Y-axis.
- PORT1_PHYS_YEND = End of Port 1 on the Y-axis.
- PORT_PHYS_ZBGN = Beginning of all ports on the Z-axis
- PORT_PHYS_ZEND = End of all ports on the Z-axis
- PORT2_X = Location of port 2 on the X-axis.
- PORT2_PHYS_YBGN = Beginning of Port 2 on the Y-axis.
- PORT2_PHYS_YEND = End of Port 2 on the Y-axis.
- PORT3_X = Location of port 3 on the X-axis.
- PORT3_PHYS_YBGN = Beginning of Port 3 on the Y-axis.
- PORT3_PHYS_YEND = End of Port 3 on the Y-axis.
- PORT4_X = Location of port 4 on the X-axis.
- PORT4_PHYS_YBGN = Beginning of Port 4 on the Y-axis.
- PORT4_PHYS_YEND = End of Port 4 on the Y-axis.
- PORT5_X = Location of port 5 on the X-axis.
- PORT5_PHYS_YBGN = Beginning of Port 5 on the Y-axis.
- PORT5_PHYS_YEND = End of Port 5 on the Y-axis.
- PORT1_LEFT_SIDE = Set to 1 if on the left side of the simulation, -1 if on the right.
- PORT2_LEFT_SIDE = Set to 1 if on the left side of the simulation, -1 if on the right.
- PORT3_LEFT_SIDE = Set to 1 if on the left side of the simulation, -1 if on the right.
- PORT4_LEFT_SIDE = Set to 1 if on the left side of the simulation, -1 if on the right.
- PORT5_LEFT_SIDE = Set to 1 if on the left side of the simulation, -1 if on the right.
- MIN_Y_COORDINATE = Minimum Y coordinate of the component, used if less than any of the ports.
- MAX_Y_COORDINATE = Maximum Y coordinate of the component, used if greater than any of the ports.
- CELLS_PER_WAVELENGTH_AXIAL = Number of cells per wavelength (in Silicon) along the X axis.
- CELLS_PER_WAVELENGTH_CROSSSECTION = Number of cells per wavelength (in Silicon) along the Y and Z axis.

This simulation applies a wide frequency band signal to the fundamental spatial mode profile. The signal is defined under *SpaceTimeFunctions* and then assigned under *Field Dynamics*, *Fields*, *port1*

The *Materials* section contains just Silicon and Silica. This section is where one can add or edit materials that get attached to CSG objects. These *Materials* contain the relative permittivity.

In *Field Dynamics* there are *FieldBoundaryConditions* which set the boundary conditions of the simulation. In photonics simulations, Matched Absorbing Layers (MALs), are the most stable boundary conditions for preventing reflections.

Under *Basic Settings* you can see that the *dielectric solver* is set to *permittivity averaging*. This feature enables second order accuracy for simulations using dielectrics.

GDSII File Import

The GDS File has already been imported, however this example serves as a good demonstration of how to do so

It may be imported like any other CAD file, however a second dialog box will appear, shown below.

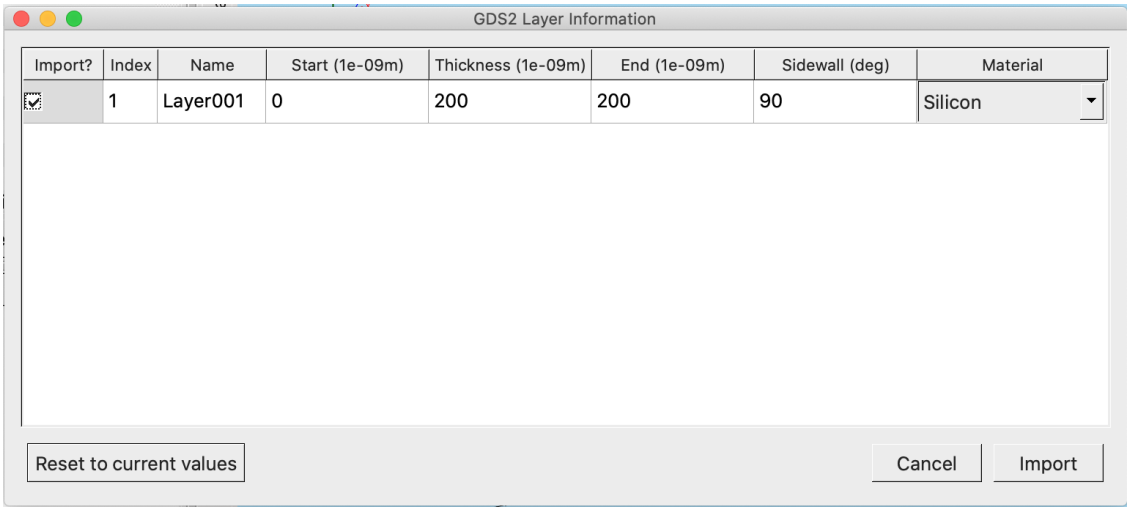


Fig. 3.122: GDS layer selection.

This allows for selection if the layer should be imported, it's starting position on the Z axis, and thickness. Sidewall angles can also be set however this is a feature that is still under active development at this time and is recommended to be kept at 90 degrees.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.512416904445238e-16
  - *Number of Steps*: 2600
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.123.

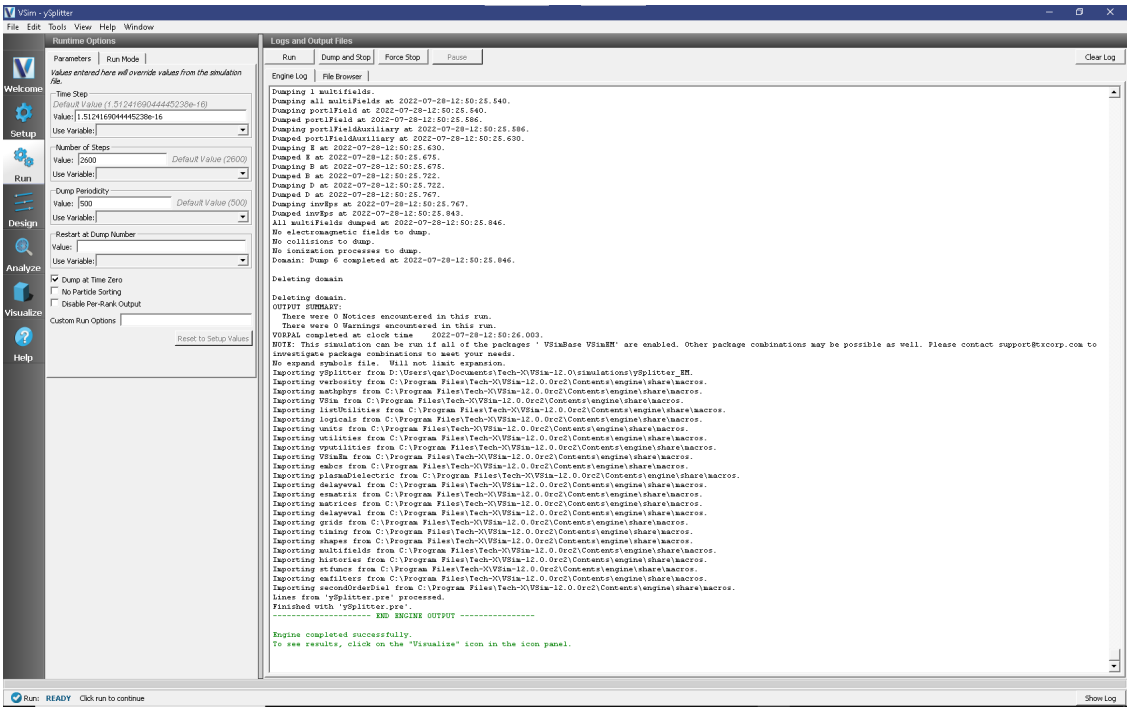


Fig. 3.123: Run window at completion.

Analyzing the Results

Using post analysis scripts, one can extract the transmission coefficients. This simulation uses 4 “EM Field on Plane” histories (Port1, Port2, Port3, Port1Enter) and this data is used to calculate S parameters between these 4 locations using the analysis script computeSParamsViaOverlapIntegral.py.

Port1Enter is described in Further Experiments.

Follow these steps:

- Proceed to the Analyze Window by clicking the *Analyze* button on the left.
- Select *computeSParamsViaOverlapIntegral.py* and click *Open* under the list.

Now update the analyzer fields accordingly.

- *maxWavelength*: 1.7e-6 (or use the corresponding parameter from the setup)
- *minWavelength*: 1.4e-6 (or use the corresponding parameter from the setup)
- *inPlane*: Port1_History (or Port1Enter_History)
- *outPlane*: Port2_History (or Port3_History)

The remaining parameter default values will work. Hit the *Analyze* button in the top tight corner. After a successful run the window should resemble Fig. 3.124.

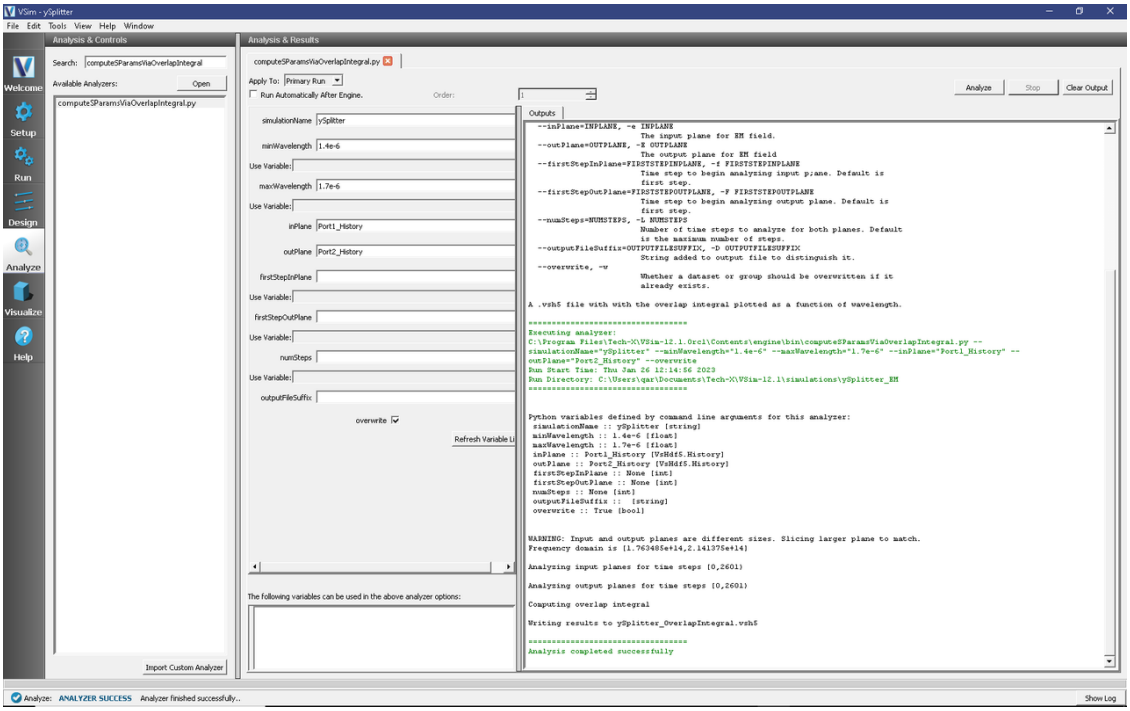


Fig. 3.124: Analyze window with output from computeSParamsViaOverlapIntegral.py.

Visualizing the results

After performing the above actions proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

- Near the top left corner of the window, select *1-D Fields* from the *Add a Data View* drop-down.
- In the Plot Control panel select the Port2 and Port3 SParams data for graph 1.
- Set the other Graphs to *None*

The results are shown in Fig. 3.125. As expected, we see equivalent power split between the two ports across the wavelength range

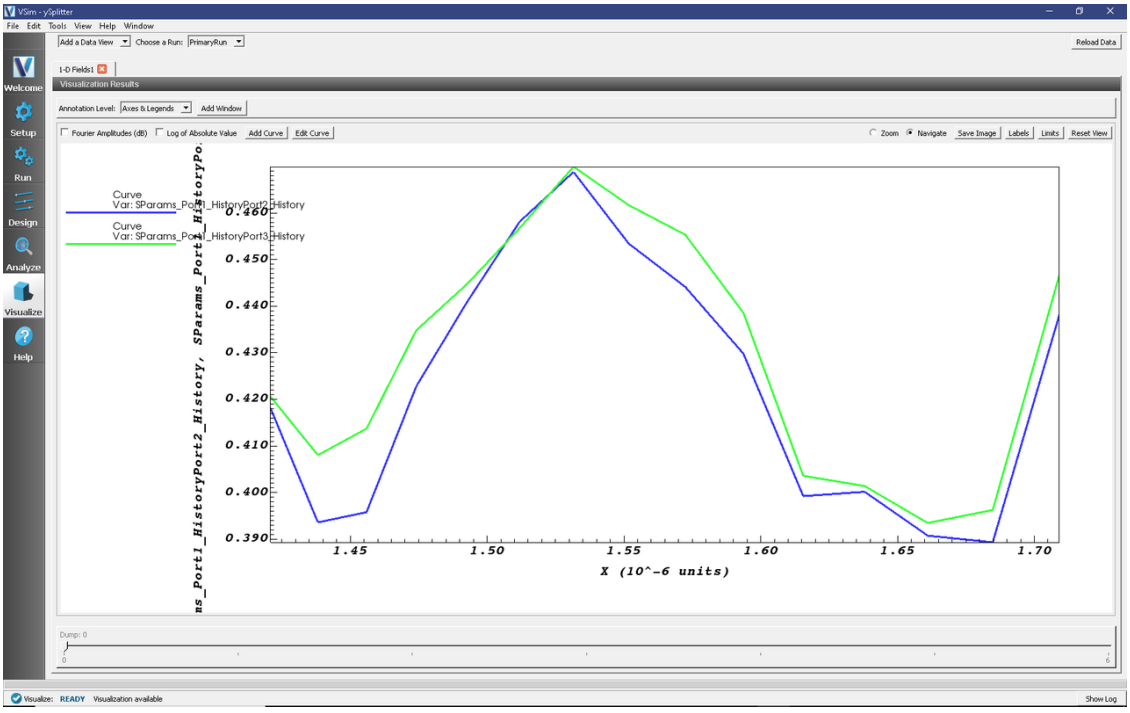


Fig. 3.125: Visualization of the s-parameters.

Further Experiments

This example comes with a second port "Port1Enter" Calculating the modes from this port to ports 2/3 will show a slightly higher transmission coefficient. This is because the mode solve is somewhat inaccurate at a low resolution so some loss occurs in the first few wavelengths. Try increasing the resolution, recalculating the mode and these two values should grow closer in agreement.

This example can be easily adapted for different GDS files.

3.4 Photonics (text-based setup)

3.4.1 Multimode Fiber with Mode Launcher (multiModeFiberModeLaunchT.pre)

Keywords:

`Mode Loading, Photonic Waveguide, Unidirectional Mode Launcher, MAL, Guided Mode, Semiconductor`

Problem Description

This example consists of a single, straight cylindrical fiber waveguide that is parallel to the x-axis and centered at the origin. The waveguide is surrounded by a background material with a greater permittivity. Matched Absorbing Layers (MALs) are used to dampen the E and B fields near the boundary of the simulation. This is a way to dampen reflected fields from the simulation boundaries.

The fundamental guided mode is launched in the waveguide. The fundamental mode was extracted in the "Multimode Fiber Mode Calculation" example using the computeDielectricModes.py analyzer. A sample mode comes with this example saved in the file save4Launch_EigenD_0.vsh5, but this can be replaced another mode from the mode calculation example if the user desires. We take the field profile from the save4Launch_EigenD_0.vsh5 file and then apply time dependence via a SpaceTimeFunction, timeCompSingleFrequency. By launching the true eigenmode into the waveguide we should minimize losses and see a constant field profile.

This simulation can be performed with a VSimEM license.

Opening the Simulation

This example can be accessed from within VSimComposer through the following steps:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window, expand the *VSim for Electromagnetics* option.
- Expand the *Photonics (text-based setup)* option.
- Select *Multimode Fiber with Mode Launcher (text-based setup)* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, and press the *Save* button to create a copy of this example.

Some relevant parameters should now be visible as seen in Fig. 3.126.

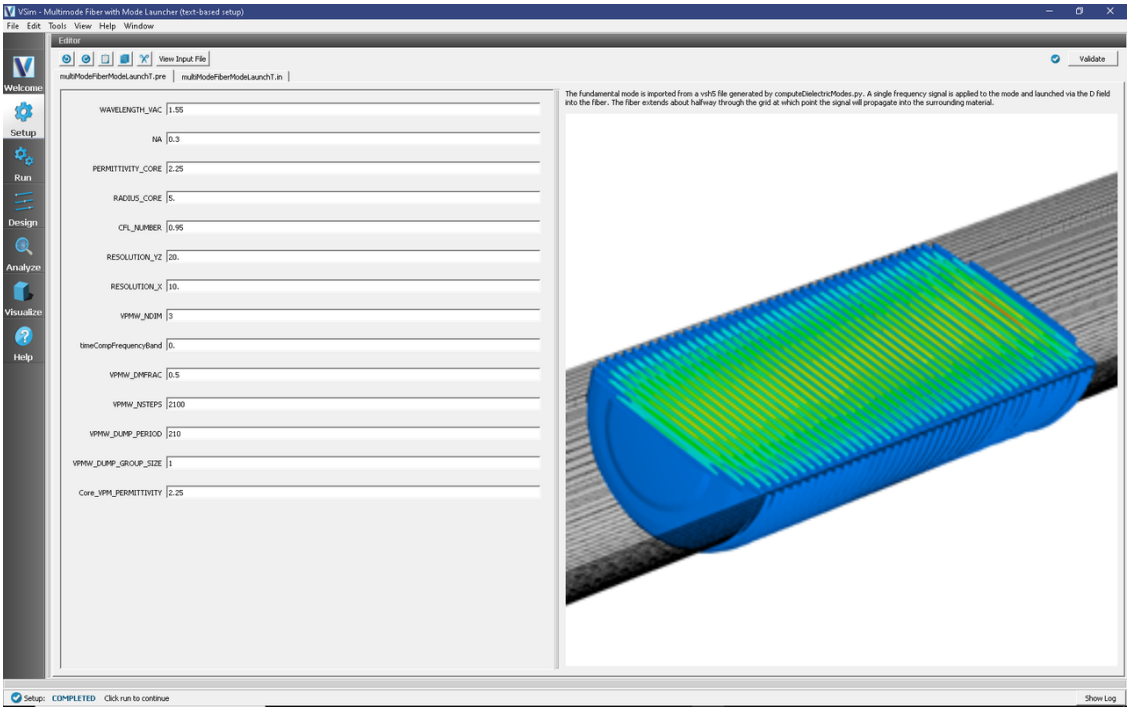


Fig. 3.126: The Setup window for the showing some relevant parameters.

Simulation Properties

This example contains a number of constants defined in the Multimode Fiber Mode Calculation example. These constants should not be modified if you wish to launch a true eigenmode. Some relevant constants that could be modified are listed below.

RESOLUTION_X: The number of cells per estimated wavelength in the propagation (x) direction.

CFL_NUMBER: The time step, DT, will be this value times the limit for numerical stability.

To expose more variables and see the geometries, boundary conditions, and fields, select *View Input File*. From here you can see the modifications made to import the eigenmode from the .vsh5 file. The modifications are clearly set apart with rows of equal signs as seen in Fig. 3.127.

The variables NBGNX_SOURCE, NENDX_SOURCE, NBGNYZ_SOURCE, and NENDYZ_SOURCE define where the source is located in integer grid cells. This should likely correspond to the location you specified when running the computeDielectricModes.py analyzer. To ensure the source is aligned with the fiber, we recommend using the same grid for mode extraction and mode launching and then defining the aforementioned variables as is seen in the input file.

The D field in the specified source location depends spatially on the imported mode and temporally on the expression timeCompSingleFrequency, which drives the mode at its respective frequency for a length of time, TIME_EXCITE. In photonics simulations, Matched Absorbing Layers (MALs) are the most stable boundary conditions for limiting reflections.

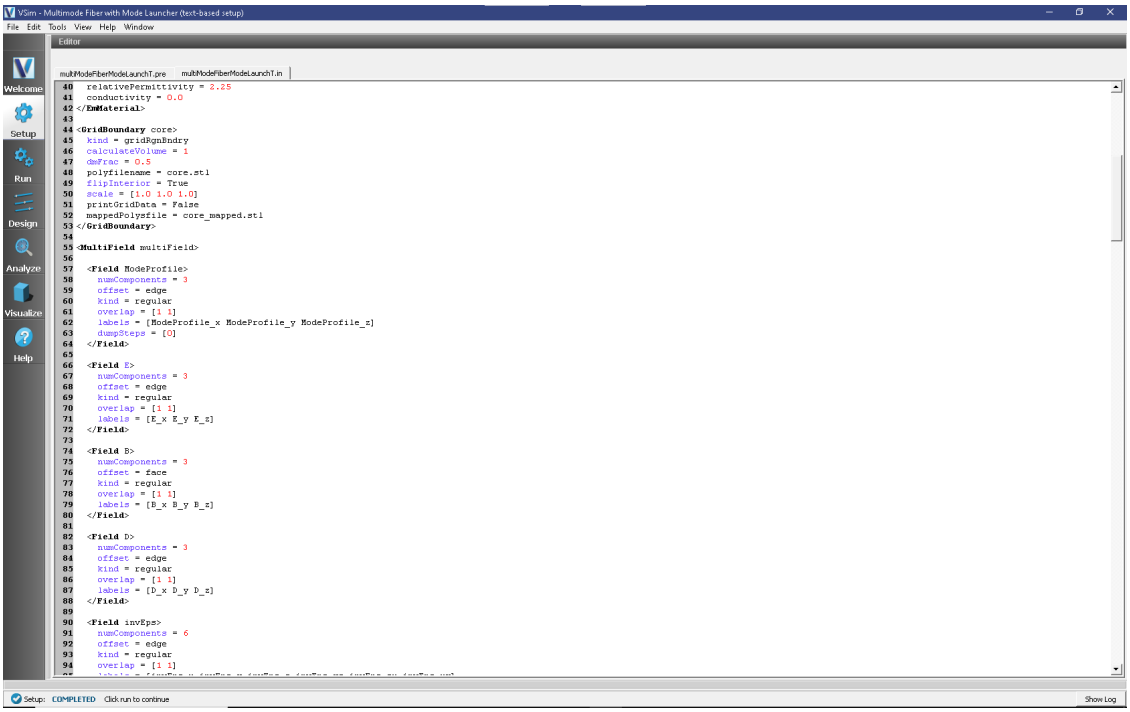


Fig. 3.127: The input multiModeFiberModeLaunchT.pre file showing the newly defined field.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 4.160775453374223e-10
  - *Number of Steps*: 2100
  - *Dump Periodicity*: 210
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.128.

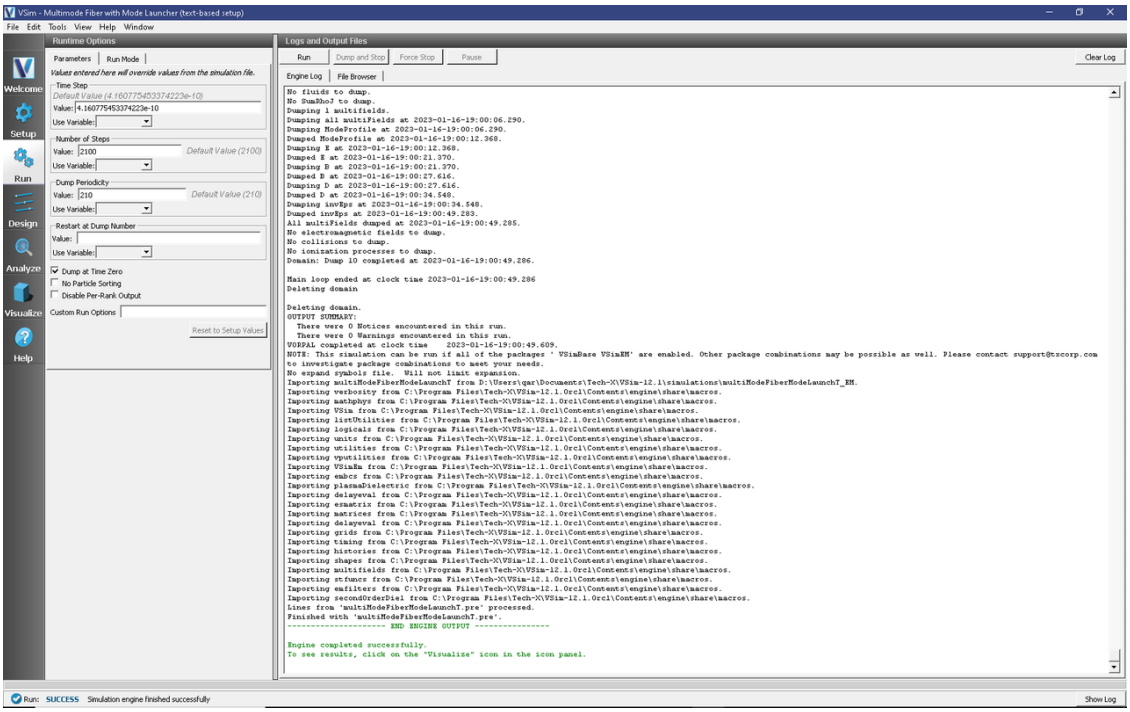


Fig. 3.128: The output after a successful run.

Visualizing the Results

Then proceed to the Visualize window by pressing the *Visualize* button in the left column.

A useful visualization of the dielectric waveguide would be to view the magnitude of the D field to qualitatively see the mode propagate down the waveguide.

- Near the top left corner of the window, make sure *Data View* is set to *Data Overview*.
- Expand *Scalar Data*, expand *D*, and select *D_magnitude*
- Check the *Clip Plot* checkbox.

- Expand *Geometries* and select *poly* to show how far the waveguide extends.
- Once again, check the *Clip Plot* checkbox.
- Slide the Dump Slider (beneath the Visualization Results) to Dump 3

Your screen should resemble Fig. 3.129. Indeed, the mode launch is quite clean! To see what happens at the end of the fiber slide the dump slider further.

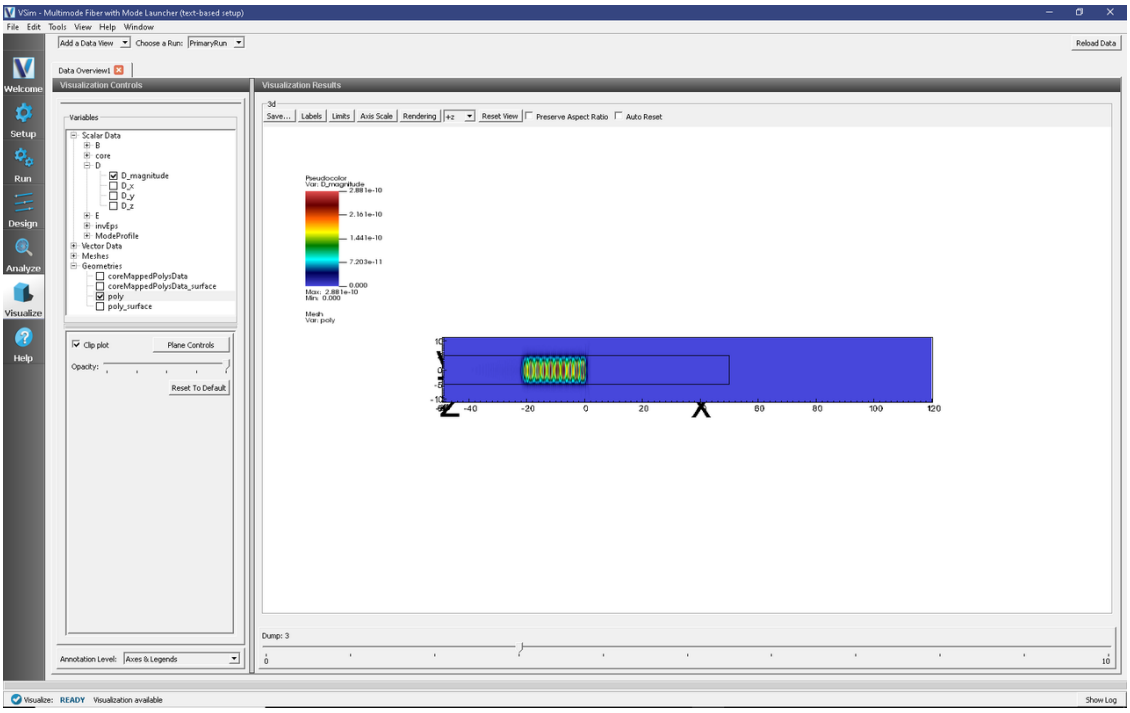


Fig. 3.129: Visualization of the D field.

Further Experiments

One can experiment by changing constants or introducing a different signal to drive the waveguide and note the effects on loss or propagation.

One could also choose a different mode generated by the Multimode Fiber Mode Calculation example and launch that.

3.5 Scattering

3.5.1 Scattering off Multiple Objects (dielecPlusMetalObjs.sdf)

Keywords:

`electromagnetics, pulse, dielectric`

Problem Description

The Scattering off Multiple Objects simulation illustrates the ability to define different materials with different dielectric properties (perfect electric conductor, sapphire, alumina) and have an electromagnetic pulse reflect off of both a complex metal surface and dielectric medium. It also illustrates a wave launcher to be used with different dielectric materials. This example can also be modified to calculate Radar Cross Sections.

This simulation can be performed with a VSimEM, VSimVE or VSimPD license.

Opening the Simulation

The Scattering off Multiple Objects example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Scattering* option.
- Select "Scattering off Multiple Objects" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.130. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

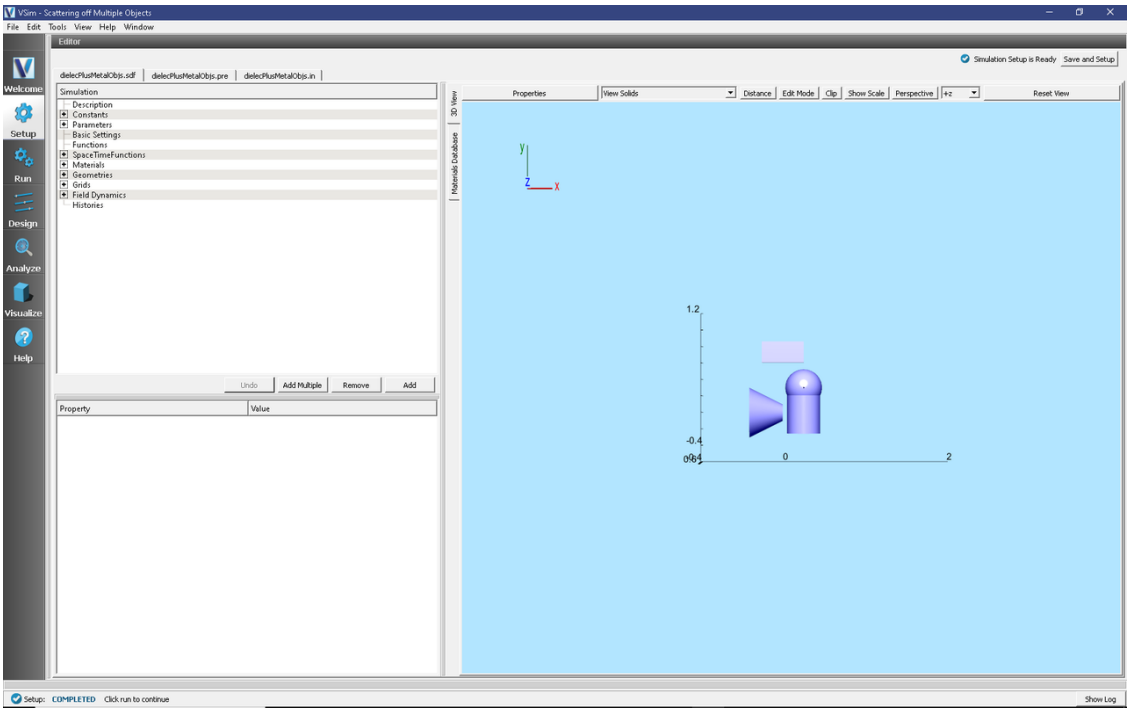


Fig. 3.130: Setup Window for the Scattering off Multiple Objects example.

Simulation Properties

This simulation includes just one user defined constant, WAVELENGTH, and just two user defined parameters, FREQUENCY and OMEGA. These three terms will define the incoming wave which is defined in the SpaceTimeFunctions element.

CSG shapes are used to define the geometries of the simulation. A sphere is unioned with a cylinder and given a material of sapphire. The box is an alumina structure and the truncated cone serves as a perfect electric conductor.

Placing all of these shapes and various materials in the same simulation shows how the electromagnetic wave can scatter off of different materials.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.473991708760349e-11
  - *Number of Steps*: 200
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.131.

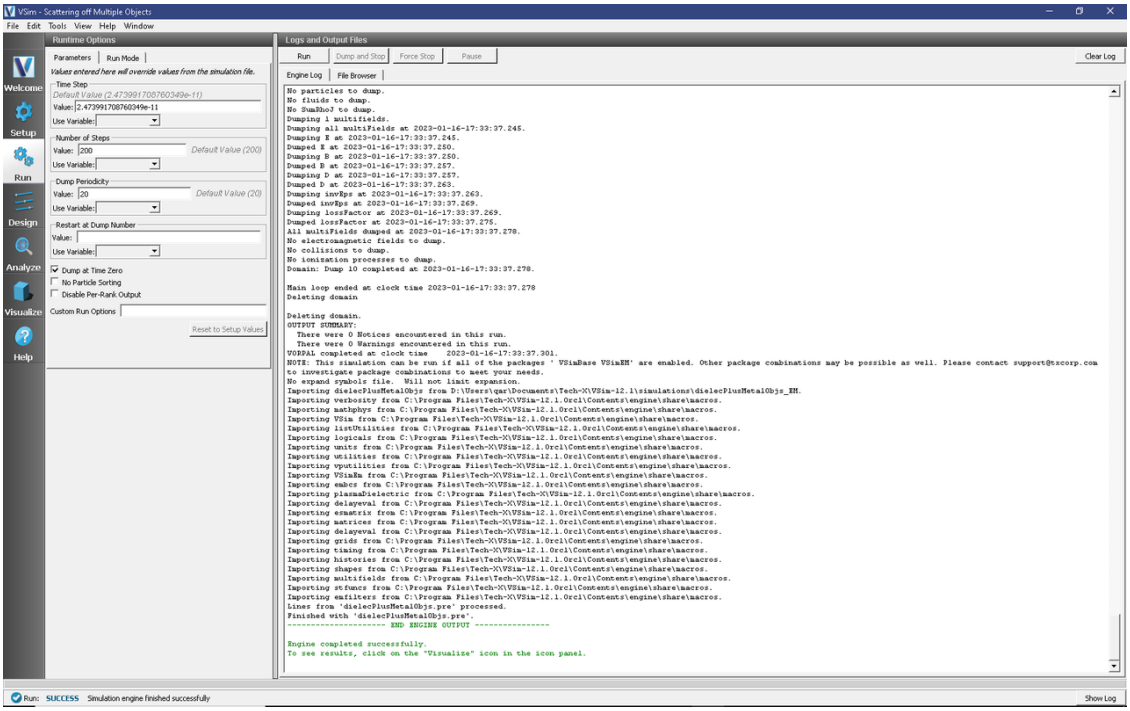


Fig. 3.131: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric field, as well as the geometries as shown in Fig. 3.132, do the following:

- Expand *Scalar Data*
- Expand *E*
- Select *E_z*
- Check *Clip Plot*
- Set the color limits to -2 and 2
- Expand *Geometries*
- Select *poly (AluminaObjectMappedPolyData)*, *poly (PECObject)*, *poly (sapphireObject)* and check *Clip Plot* for each

Initially, no field will be seen, as one is looking at Dump 1 when no fields are yet in the simulation. Move the slider at the bottom of the right pane to see the electric field at different times.

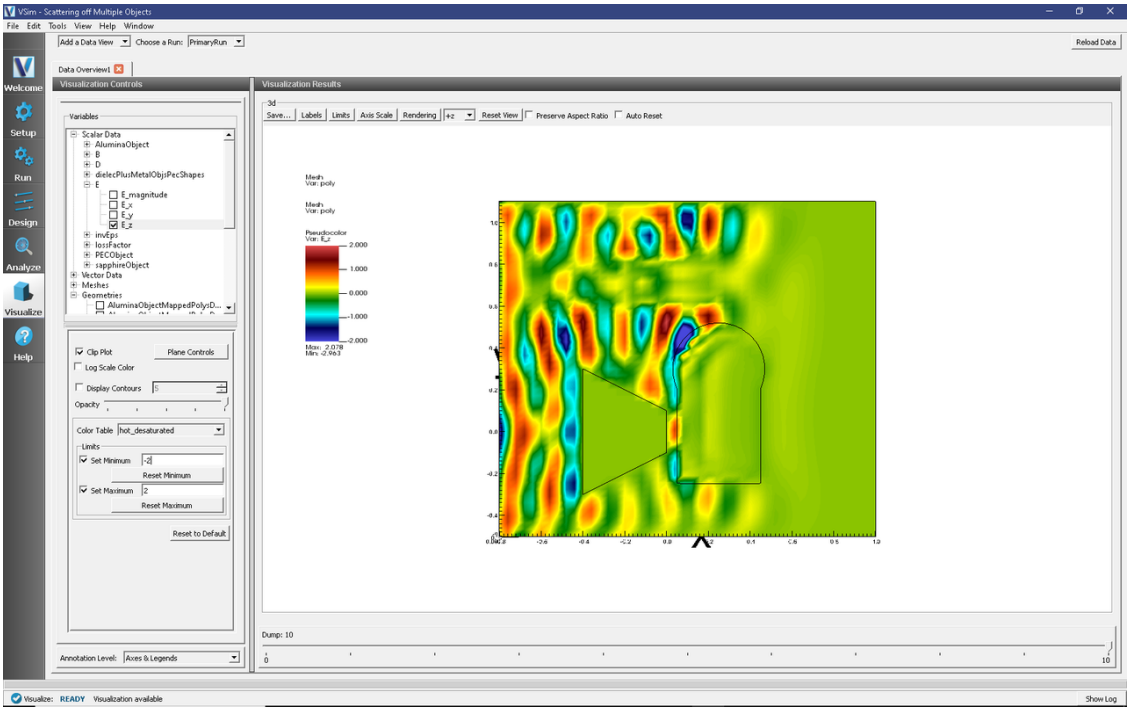


Fig. 3.132: Visualization of the wave as it hits the objects.

Further Experiments

One idea is to include radar cross section histories at setup time to be able to visualize the far fields.

This example is easily modifiable to include a different geometry and wave form.

Try changing the materials to see how it affects the wave.

3.5.2 Scattering off a Metal Sphere (metalSphere.sdf)

Keywords:

`Mie Scattering Off Metal Sphere`

Problem description

The example describes the scattering of electromagnetic waves off a metal sphere. This phenomenon is often referred to as Mie scattering, where the radius of the sphere is comparable to the wavelength of the incident radiation.

An incident plane wave is launched toward the sphere. VSim computes the resulting fields in the vicinity of the sphere, within a computational domain by applying the proper boundary conditions around the surface of the sphere. The waves that exit the computational domain are absorbed into MAL layers.

The fields for points far away from the sphere, and beyond the computational domain are computed with the help of an analyzer that is part of the VSim distribution. The histories of the electric and magnetic fields are recorded along a closed surface known as a Kirchhoff box that lies within the MAL layers. This field information is then used to compute fields far away from the sphere center by applying the Kirchhoff integral theorem.

In this example, the radius of the metal sphere is set to equal 0.3367 times the wavelength of the incident radiation, which is 1m in length.

The wave is launched from the positive z direction, and the incident wave electric field is polarized along the x direction.

This example is set up as a cube, entirely parameterized off the NUM_WAVELENGTHS, WAVELENGTH and CELLS_PER_WAVELENGTH Constant. It is designed so that it may be easily adapted to take the radar cross section of any geometry, at any wavelength.

Two wavelengths on all sides are devoted to the MAL absorbing boundary conditions. The resolution of the grid corresponds to 16 cells per wavelength, near the middle of the typically used 10-20 cells. The time step (Parameter DT) is chosen to be very close to the Courant condition limit, calculated using the DX, CFL_NUM and DMFRAC Parameters.

The recording time for the Kirchhoff box is calculated using the parameters TBGNKBOX and TENDKBOX. TBGNKBOX is set by adding the turn on time of the excitation source, and 2* the time it would take to cross the diagonal of the RCS Box. TENDKBOX is set by taking TBGNKBOX, and then adding the amount of time to cross the entire RCS box, +2.5 periods. This allows for the collection of 2.5 periods of data.

The number of timesteps (Parameter NUM_STEPS) for the simulation corresponds to TENDKBOX/DT. Note that the number of steps in the simulation must be set by hand in **Basic Settings**, and verify that the value used in the Run Panel corresponds to this parameter.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Mie Scattering, Metal Sphere example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Scattering* option.
- Select "Mie Scattering - Metal Sphere" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.133. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of any geometry, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

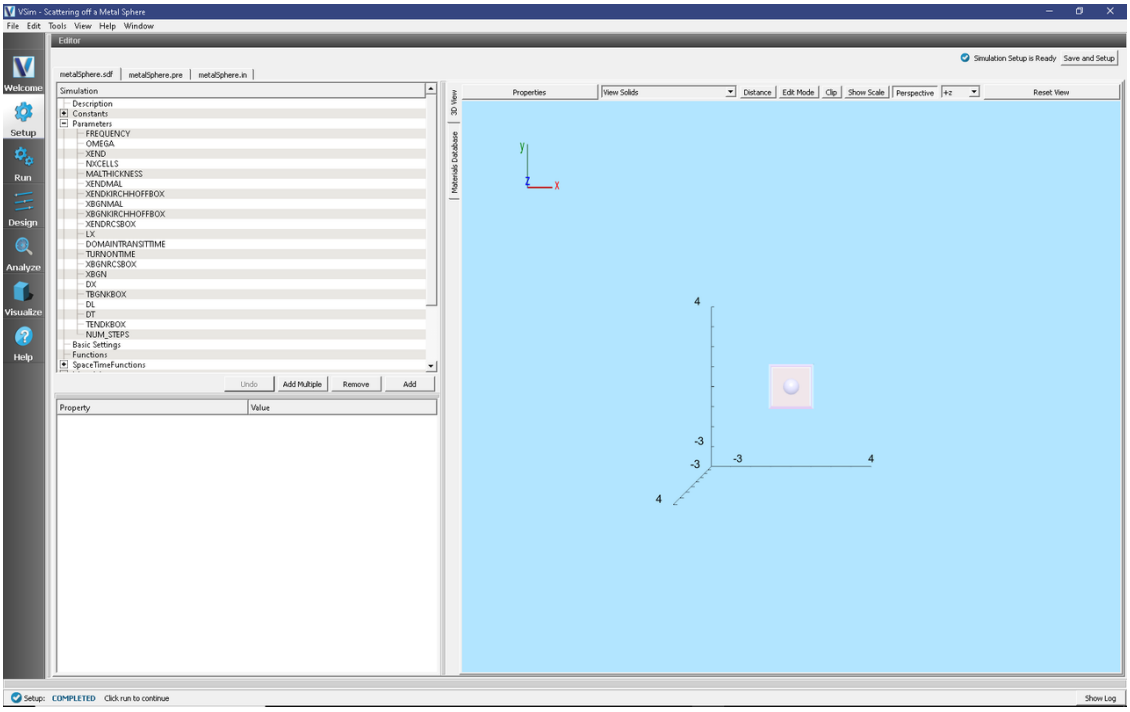


Fig. 3.133: Setup Window for the Mie Scattering example.

The Setup Window shows the Kirchhoff box, with the metal sphere at the center. To see the grid, click on the drop down menu of "Grids" on the left side panel. Check the box beside "Grid". In order to view or change the wave frequency, click on the drop down menu "Parameters" and then click on "Frequency". To view or change the direction of the incident wave or polarization, you can click on the drop down menu "Field Dynamics", then the drop down menu "RCSBox". Following this, check the box beside "rcsBox0". The lower left panel displays a table with the wave property and its corresponding value.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.71337236814229e-11
  - *Number of Steps*: 2015
  - *Dump Periodicity*: 300
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.134.

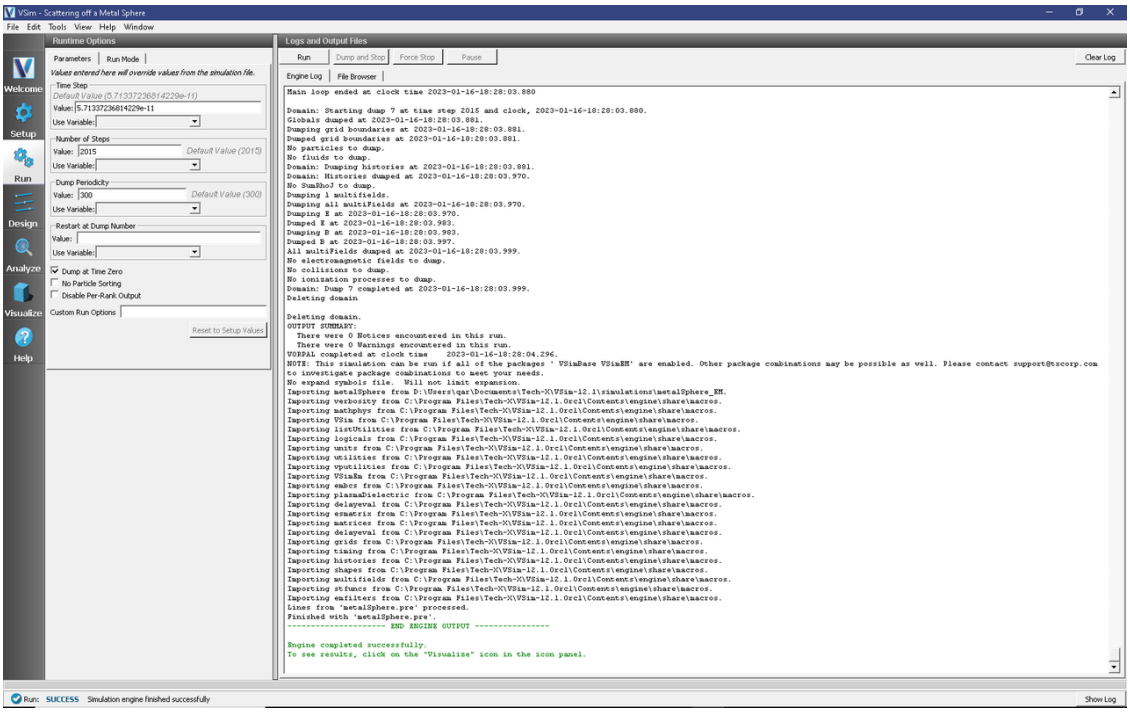


Fig. 3.134: The Run Window at the end of simulation.

Running in 3D, this simulation uses 2000 time steps. The run takes about 5 minutes on a 4-core 2.3 GHz processor.

Running the Analyzer

- Proceed to the Analysis window by pressing the Analyze button in the left column of buttons.
- Select the Default *computeFarFieldFromKirchhoffBox.py* Analyzer
- Input values for the variables given on the left hand side of the screen. Check that these have the following values:
  - simulationName - metalSphere
  - fieldLabel - E
  - farFieldRadius - 1024.0
  - numPeriods - 0.25
  - numFarFieldTimes - 2
  - frequency - 0.3e9
  - numTheta - 45 (number of points in the theta direction)
  - numPhi - 90 (number of points in the phi direction)
  - zeroThetaDirection - (0,0,1)
  - zeroPhiDirection - (1,0,0)
  - incidentWaveAmplitude - 1.0
  - incidentWaveDirection - (0,0,1)
  - varyingMeshMaxRadius - 1.0
  - principalPlanesOnly - checked
- Click the *Analyze* button near the top right of the window.

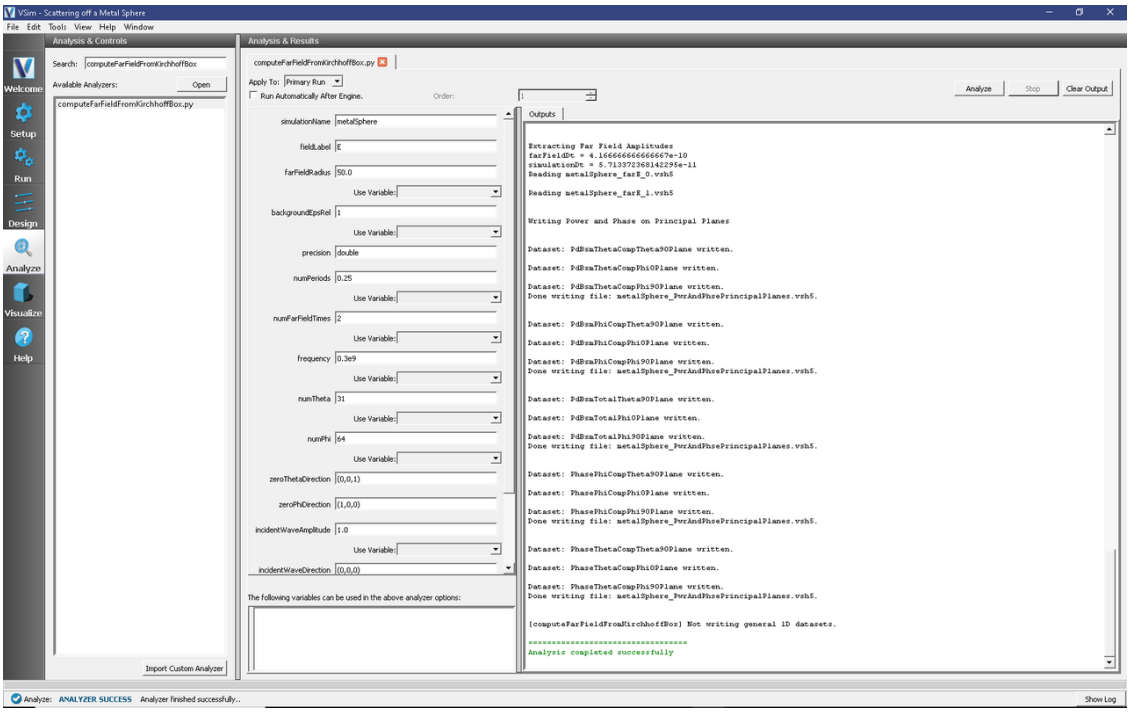


Fig. 3.135: The Analyze Window at the end of analyzer execution.

Visualizing the results

After performing the above actions, click on *Visualize* in the column of buttons at the left. The program will load the data and provide you with certain options.

One of the quantities that is of interest in such scattering phenomena is radar cross section (RCS) measured in dBsm. The RCS, sometimes designated as σ, having units of m^2, is given as

$$RCS = 4\pi R_s^2 \frac{P_r}{P_i}$$

where R_s is the radial distance from scatterer, P_r is the power flux received at the point of interest, and P_i is the incident power flux. In MKS units the power flux is measured in W/m^2. RCS in dBsm is given as

$$10 \log_{10}(RCS)$$

To obtain plots of this quantity, click on the drop down menu, *Add a Data View*. In this menu, choose 1-D Fields. There is a large list of options to choose from. Figure Fig. 3.136.

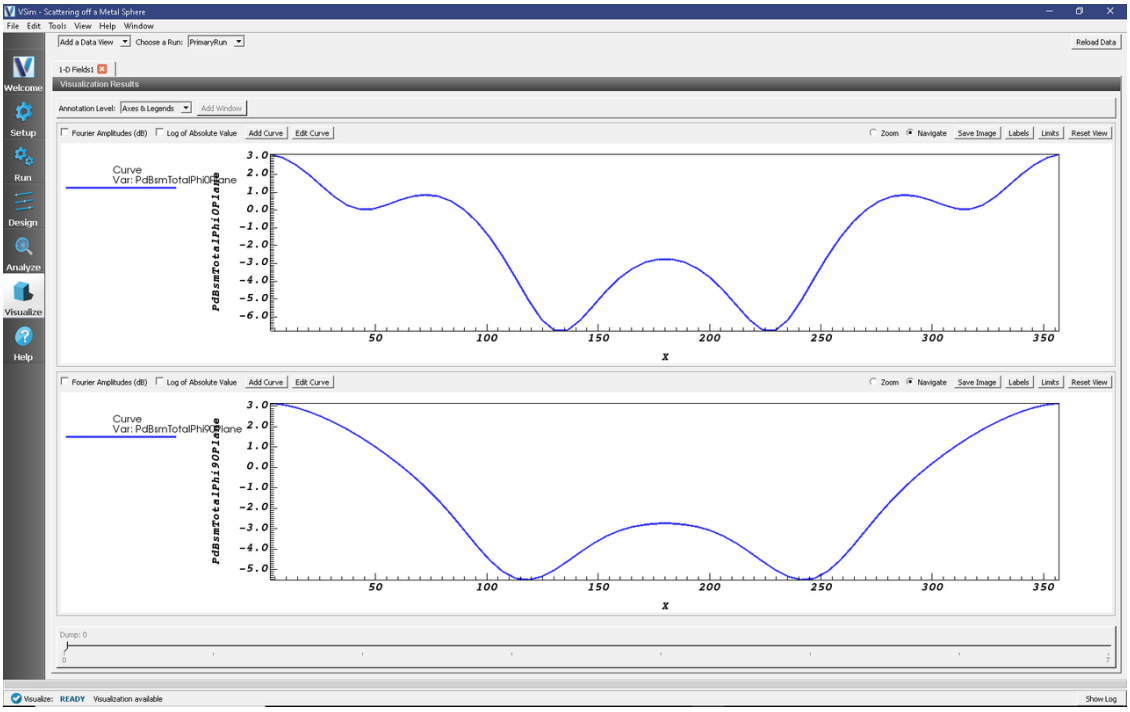


Fig. 3.136: The Visualize Window at the end of execution.

Further Experiments

You may try the example that includes a dielectric coating over the same metal sphere to compare the effects of such a coating over the RCS.

3.5.3 Scattering off a Metal Sphere with a Dielectric Coating (dielecCoatedMetalSphere.sdf)

Keywords:

`Mie Scattering Dielectric Coated Metal Sphere`

Problem description

The example describes the scattering of electromagnetic waves off a metal sphere with a dielectric coating, which is a modification of the previous example that described scattering off a pure metal sphere.

An incident plane wave is launched toward the sphere. VSim computes the resulting fields in the vicinity of the sphere, within a computational domain by applying the proper boundary conditions around the surface of the sphere. The waves that exit the computational domain are absorbed into MAL layers.

The fields for points far away from the sphere, beyond the computational domain, are computed with the help of an analyzer that is part of the VSim distribution. The histories of the electric and magnetic fields are recorded along a closed surface known as a Kirchhoff box that lies within the MAL layers. This field information is then used to compute fields far away from the sphere center by applying the Kirchhoff integral theorem.

In this example, the radius of the metal sphere is set to equal 0.3367 times the wavelength of the incident radiation, which is 1m in length. The thickness of the coating is 0.1 times the wavelength. The computational domain extent is set to three times the wavelength in all directions along the three coordinate axes. The thickness of the MAL layer is twice the wavelength. The resolution of the grid corresponds to 24 cells per wavelength. This parameter is chosen such that the thickness of the dielectric layer is resolved. The time step is chosen to be very close to the Courant condition limit. The wave is launched from the positive z direction, and the incident wave electric field is polarized along the x direction. Care needs to be taken so that the simulation is performed for a sufficient number of time steps, so that the wave reaches the surface of the Kirchhoff box where the histories are recorded. Thus, changing the frequency or the resolution of the grid would alter the time step, and the number of steps required to complete the run will need to be changed accordingly.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Mie Scattering, Dielectric Coated Metal Sphere example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Scattering* option.
- Select "Scattering off a Metal Sphere with a Dielectric Coating" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 3.137. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`. While the setup is similar to the previous example of a pure metal sphere, the additional components in this example may be found as follows: Expand the Menu under `Material` to see the element `COATING`. As showed in Fig. 3.137, clicking on `COATING` shown the properties of the dielectric material. In addition, expand the menu under `Geometries`, followed by the menu under `CSG` to see the additional geometry element, `coating`.

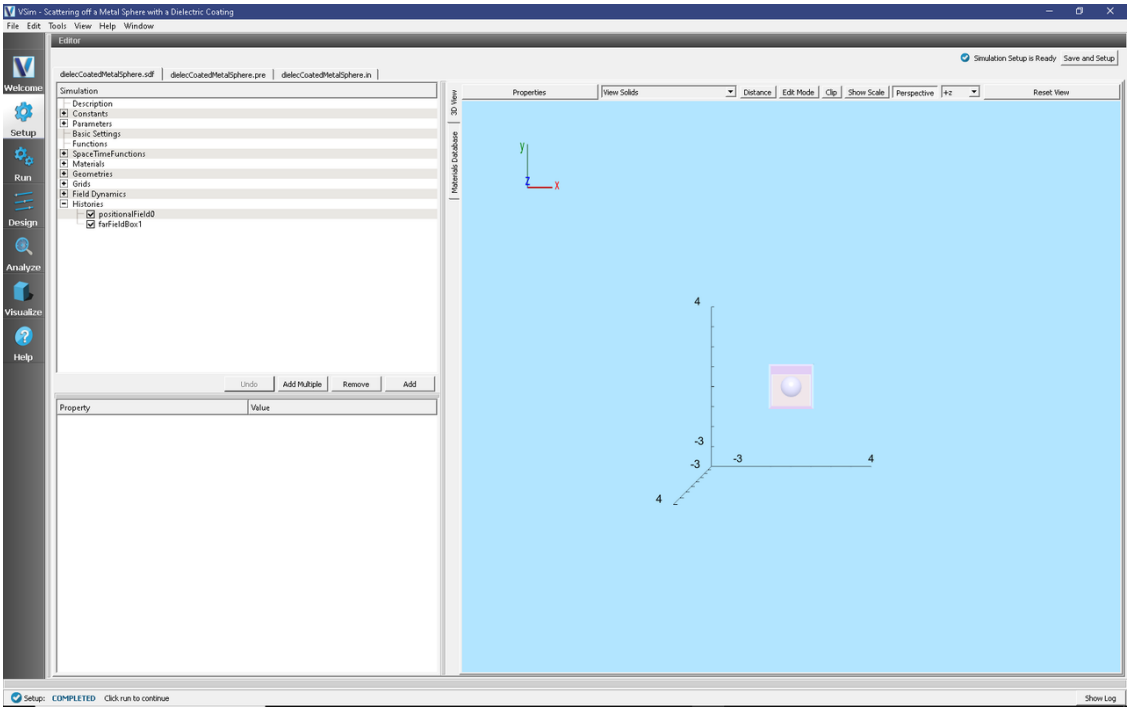


Fig. 3.137: Setup Window for the Mie Scattering example.

The Setup Window shows the Kirchhoff box, with the metal sphere at the center. To see the grid, click on the drop down menu of "Grids" on the left side panel. Check the box beside "Grid". In order to view or change the wave frequency, click on the drop down menu "Parameters" and then click on "Frequency". To view or change the direction of the incident wave or polarization, you can click on the drop down menu "Field Dynamics", then the drop down menu "RCSBox". Following this, check the box beside "rcsBox0". The lower left panel displays a table with the wave property and its corresponding value.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.8115448780608225e-11
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 400
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.138.

Running in 3D, this simulation uses around 4000 time steps. The run takes about 15 minutes on a 4-core 2.3 GHz processor.

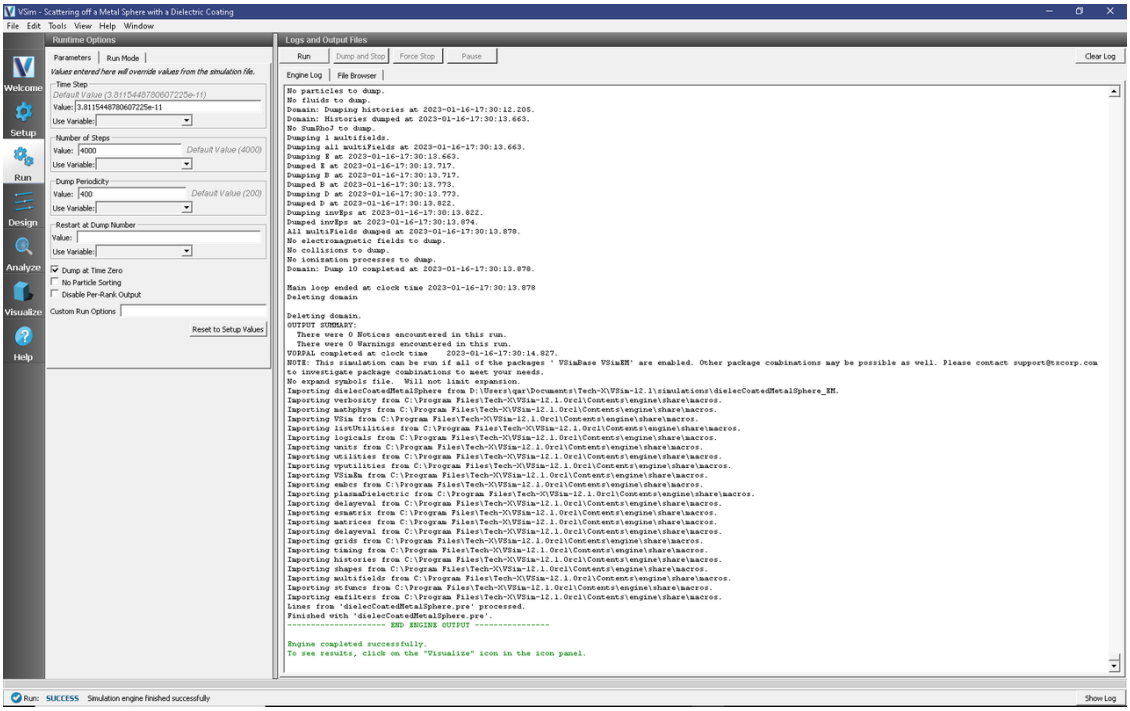


Fig. 3.138: The Run Window at the end of simulation.

Running the Analyzer

After completing the run, one can run the analyzer to compute field values at far away points. To bring up the analyser script, Click on the Analyze icon. The panel that appears will be named computeFarFieldFromKirchhoffBox.py, along with a set of text boxes in which the necessary parameters need to be filled. For the default settings of the file you may use the following:

- *simulationName* : dielectricCoatedMetalSphere
- *fieldLabel* : E
- *farFieldRadius* : 50.0
- *numPeriods* : 0.25
- *numFarFieldTimes* : 2
- *frequency* : 0.3e9
- *numTheta* : 31
- *numPhi* : 64
- *zeroThetaDirection* : (0,0,1)
- *zeroPhiDirection* : (1,0,0)
- *incidentWaveAmplitude* : 1.0
- *incidentWaveDirection* : (0,0,1)
- *varyingMeshMaxRadius* : 1
- *principalPlanesOnly* : checked

After entering the above parameters, also shown in Fig. 3.139, press the "Analyze" button that appears on the upper right side.

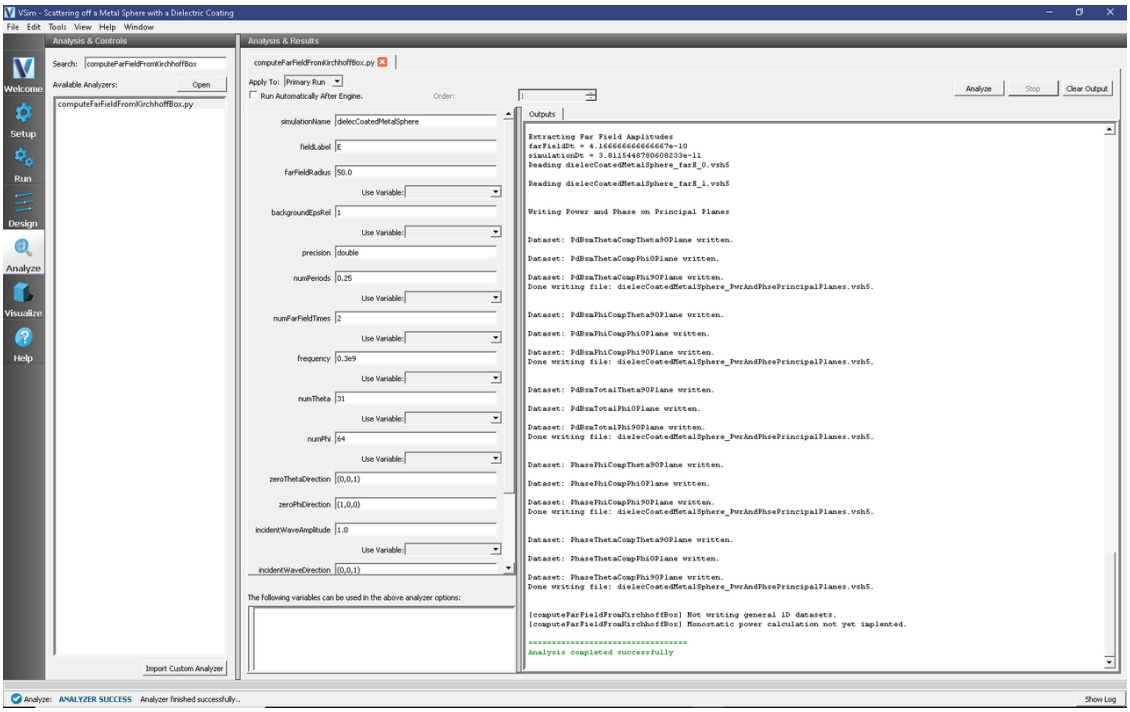


Fig. 3.139: The Analyze Window at the end of analyzer execution.

Visualizing the results

After performing the above actions, click on *Visualize* in the column of buttons at the left. The program will load the data and provide you with certain options.

One of the quantities that is of interest in such scattering phenomena is radar cross section (RCS) measured in dBsm. The RCS, sometimes designated as σ, having units of m^2, is given as

$$RCS = 4\pi R_s^2 \frac{P_r}{P_i}$$

where R_s is the radial distance from scatterer, P_r is the power flux received at the point of interest, and P_i is the incident power flux. In MKS units the power flux is measure in W/m^2. RCS in dBsm is given as

$$10log_{10}(RCS)$$

To obtain plots of this quantity, click on the drop down menu, *Add a Data View*. In this menu, choose 1-D Fields. There is a large list of options to choose from. Figure Fig. 3.140.

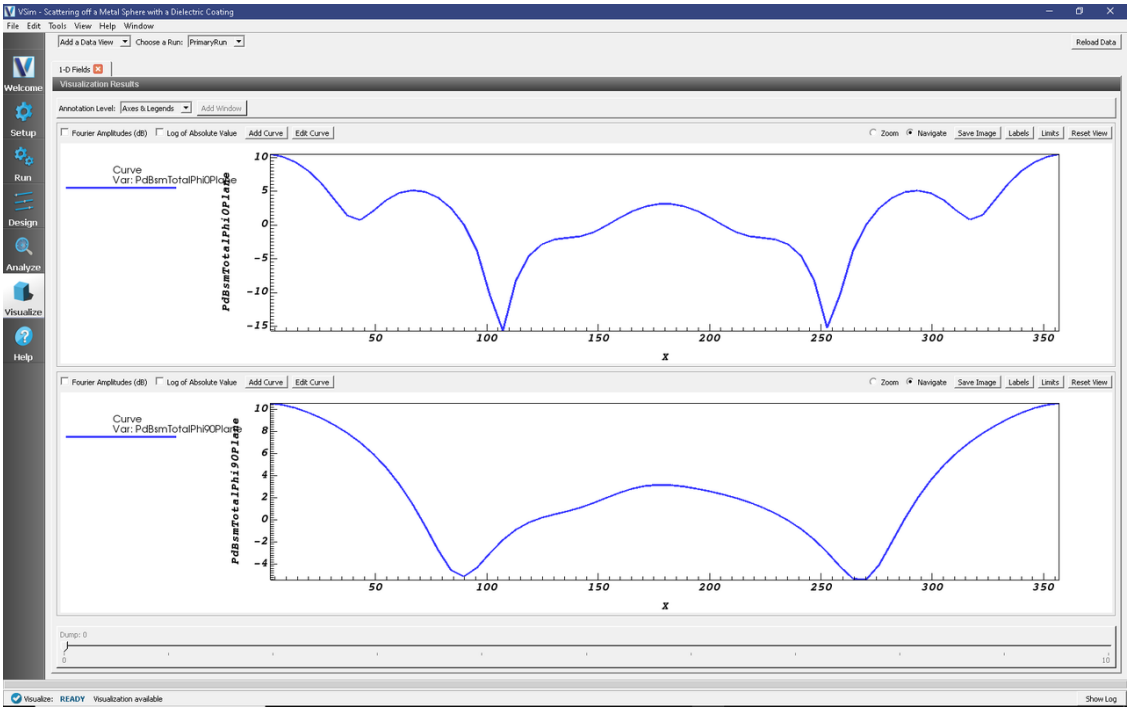


Fig. 3.140: The Visualize Window at the end of execution.

Further Experiments

Alter the thickness or the dielectric constant of the coating to see its effect on the computed RCS.

3.6 Scattering (text-based setup)

3.6.1 Ground Penetrating Radar (groundPenetratingRadarT.pre)

Keywords:

GPR, ground penetrating radar, lossy dielectric

Problem description

This simulation launches a plane wave, polarized in the Z-direction into a lossy dielectric. Embedded within the lossy dielectric is a mine, modelled as a pure electric conductor. The return wave at the surface can be monitored with histories. The simulation is 2D, but with minor effort can be expanded to 3 dimensions.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Ground Penetrating Radar example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Scattering (text-based setup)* option.
- Select "Ground Penetrating Radar (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The key parameters of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 3.141.

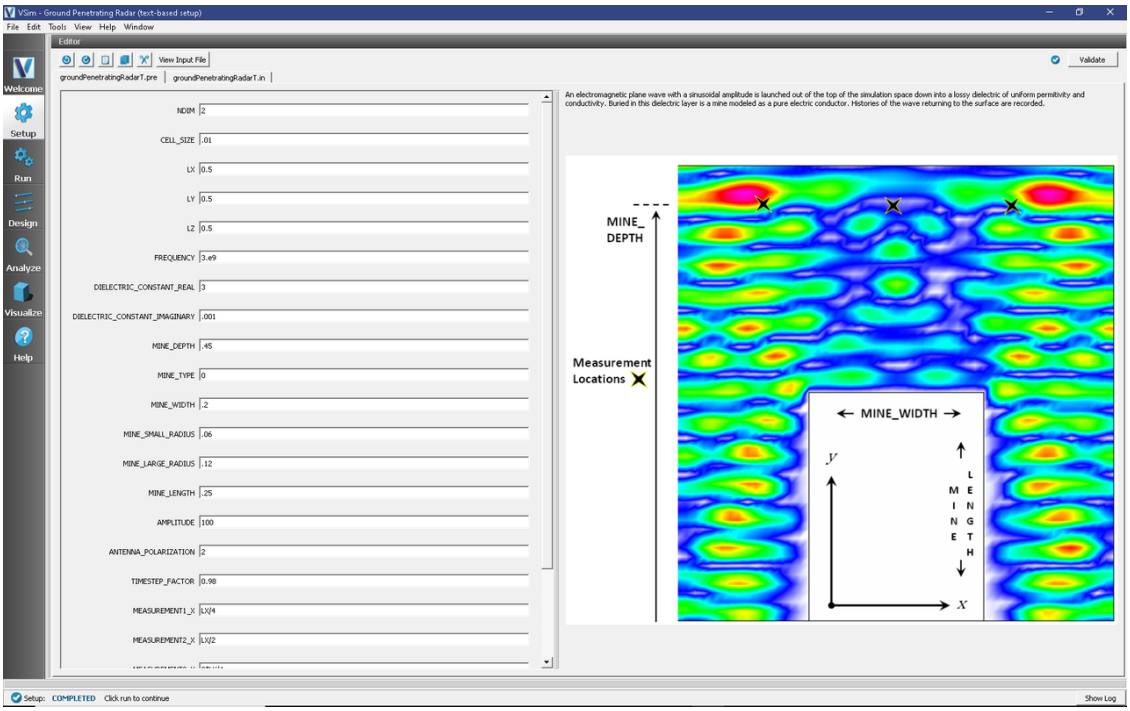


Fig. 3.141: Setup Window for the Ground Penetrating Radar example.

Input File Features

This file allows for the modification of plane wave operating frequency, simulation domain size, resolution, dielectric permittivity, size and conductivity, mine size and location as well as history location.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.7336109375110176e-11
  - *Number of Steps*: 1000
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.142.

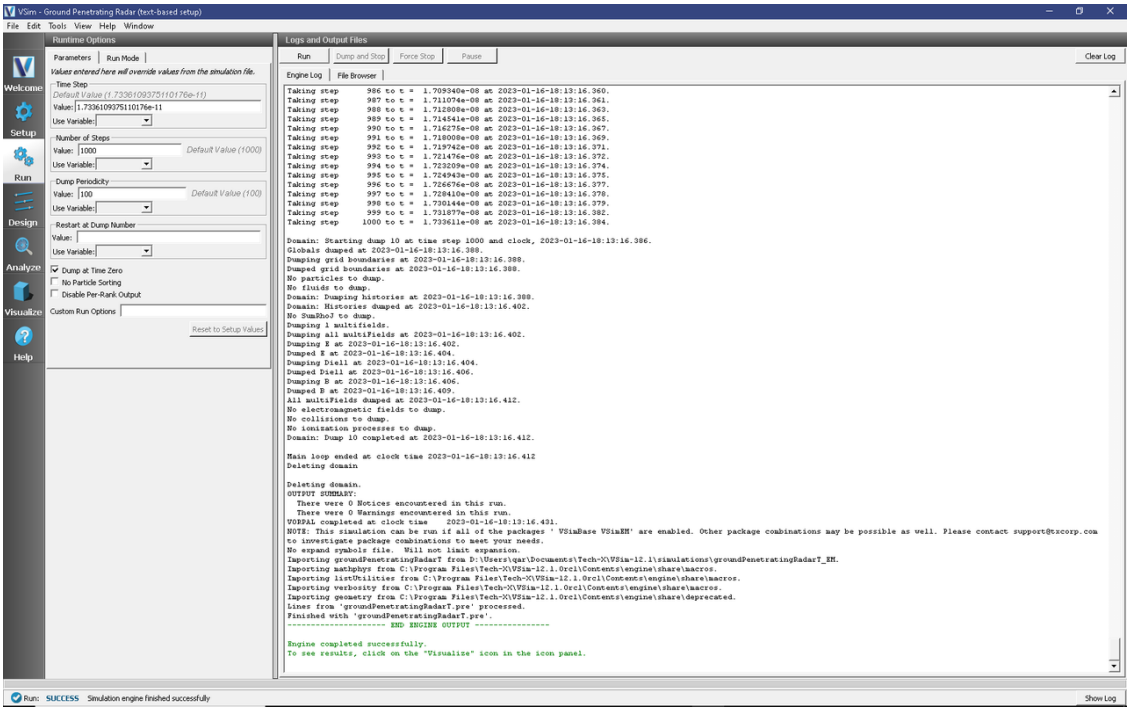


Fig. 3.142: The Run Window at the end of execution.

Visualizing the Results

After the simulation has completed running, click on the Visualize Window.

The electric field can be viewed by:

- Expand *Scalar Data*
- Expand *E*
- Select *E_z*
- Expand *Geometries*
- Select *poly*
- Move the dump slider forward in time

The wave reflection measured at the three surface locations can be viewed under the *Histories* Data View

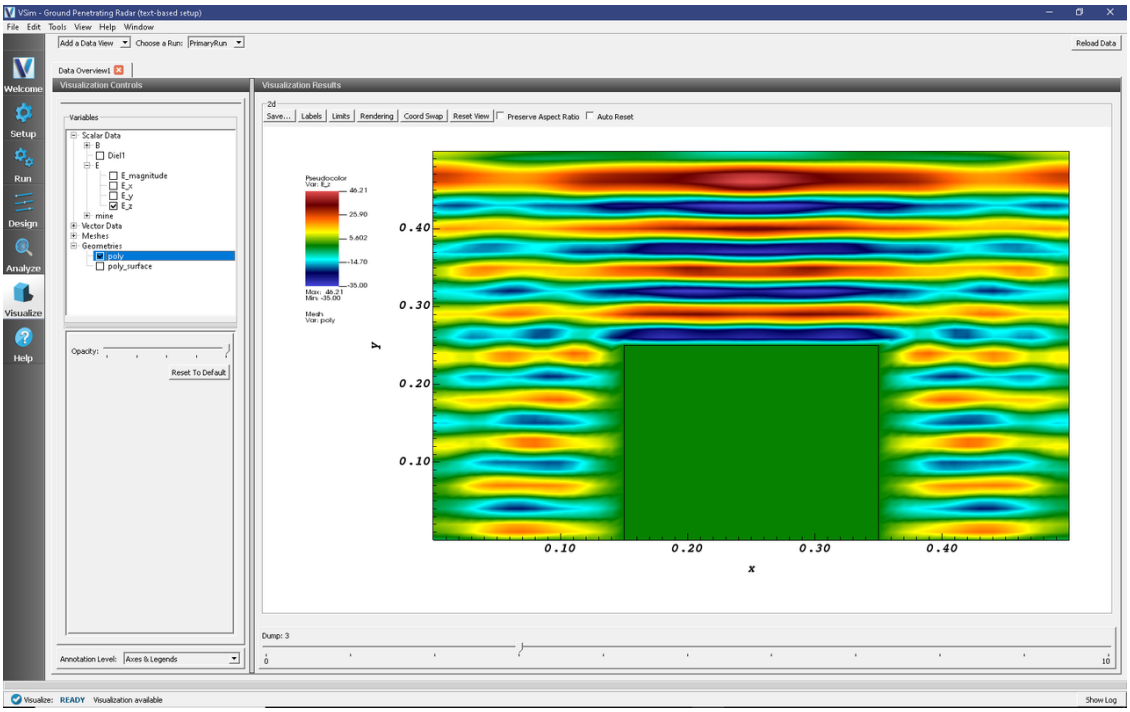


Fig. 3.143: The electric field in the simulation space. Seen here: the cylindrical cone mine-shape.

Further Experiments

The parameters of the dielectric can be easily modified. It would also be possible to modify the sources to be horn antennas instead of point sources; this would more accurately model a real world ground penetrating radar situation.

3.7 Other EM

3.7.1 Spherical Lens (sphericalLens.sdf)

Keywords:

refraction, focusing, dielectrics

Problem Description

The Spherical Lens is a full wave solution to a simple, thin lens with spherical surfaces. Focusing occurs because light rays farther from the center hit the surface at a more oblique angle, resulting in more bending, according to Snell's law. The focusing length of a spherical lens is given by $f = R/(2 - 2/\epsilon_r^{1/2})$, where ϵ_r is the relative permittivity of the material making up the lens.

This simulation can be performed with a VSimEM license.

Opening the Simulation

The Spherical Lens example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Other EM* option.
- Select "Spherical Lens" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the setup window as shown in Fig. 3.144. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

Simulation Properties

The spherical lens is constructed in CSG using the intersection of two spheres. You can pull the spheres apart to get a taller lens, and you can change the radius of the spheres to have a lens with more curvature. The grid is set so that it will capture the focus at the right for the initial setup.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 8.151822279267447e-12
  - *Number of Steps*: 600
  - *Dump Periodicity*: 50
  - *Dump at Time Zero*: Checked

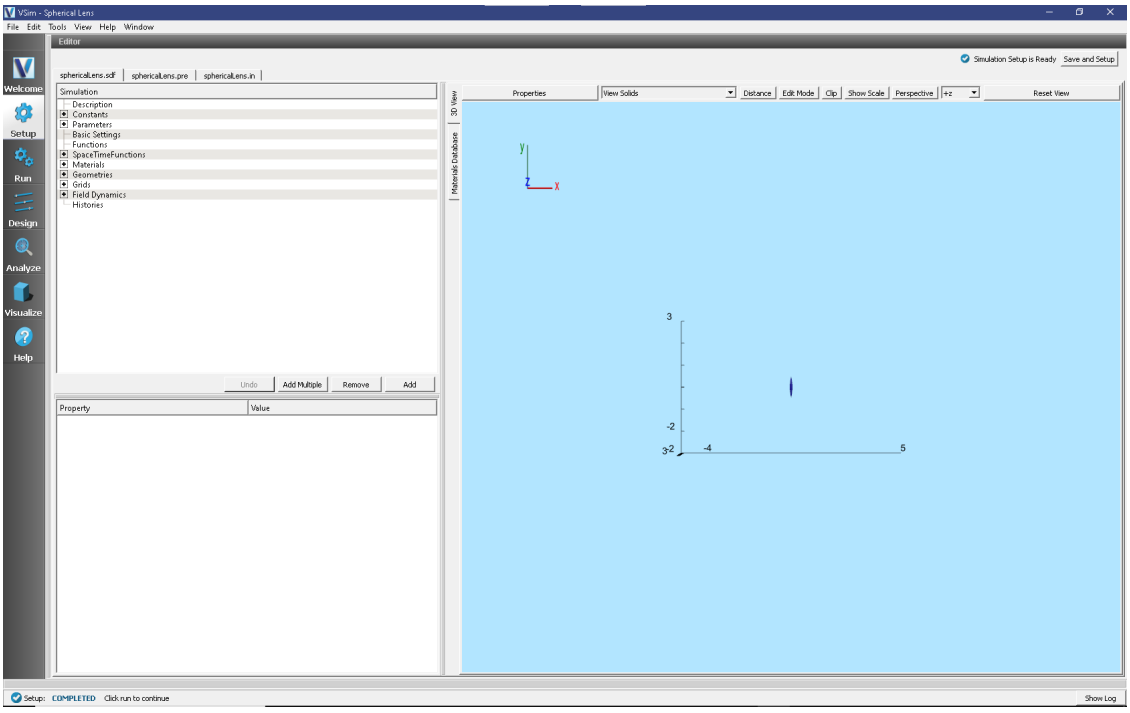


Fig. 3.144: Setup window for the Spherical Lens example.

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.145.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window by pressing the Visualize button in the left column of buttons.

To see the field focus after the lens as shown in Fig. 3.146, do the following:

- Expand *Scalar Data*, expand *E*
- Select *E_z* and check the box *Clip Plot*
- For the limits set the *Fix Minimum* to -10 and the *Fix Maximum* to 10.
- Expand *Geometries*
- Select *poly* and check the box *Clip Plot*
- Move the dump slide to the right to see the wave come in, focus after the lens, and then diverge again after approximately x=0.4. One can see interference of the incoming wave with the reflection off the face of the lens. One can also see interference patterns within the lens.

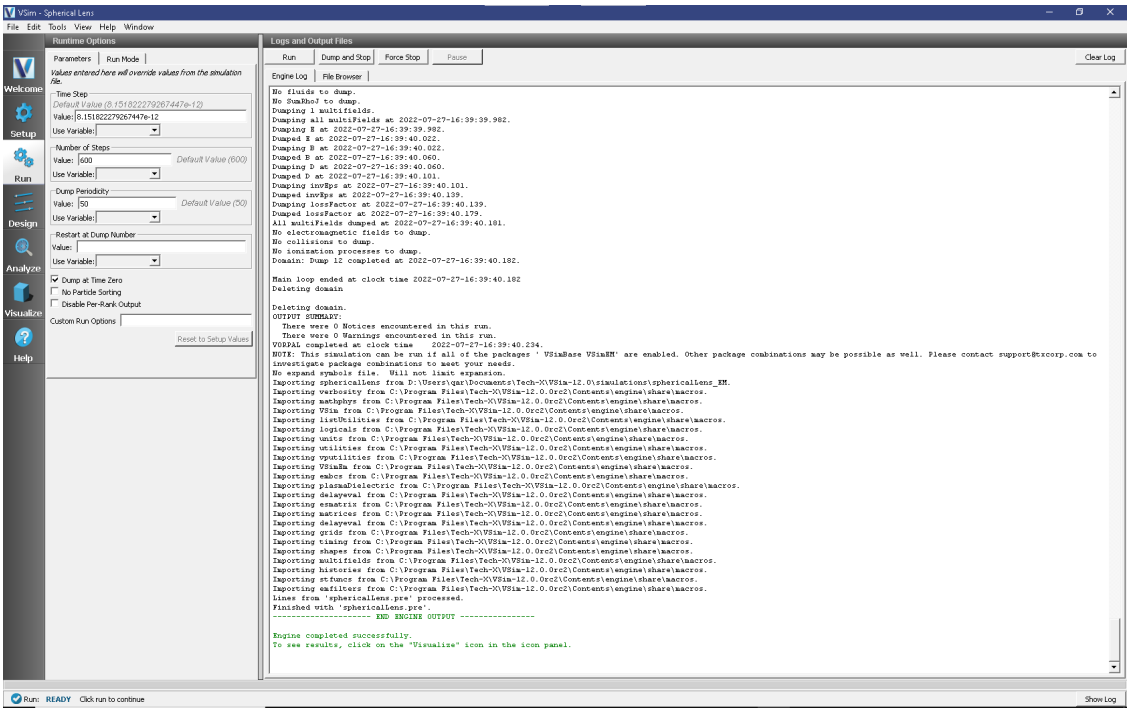


Fig. 3.145: The Run window at the end of execution.

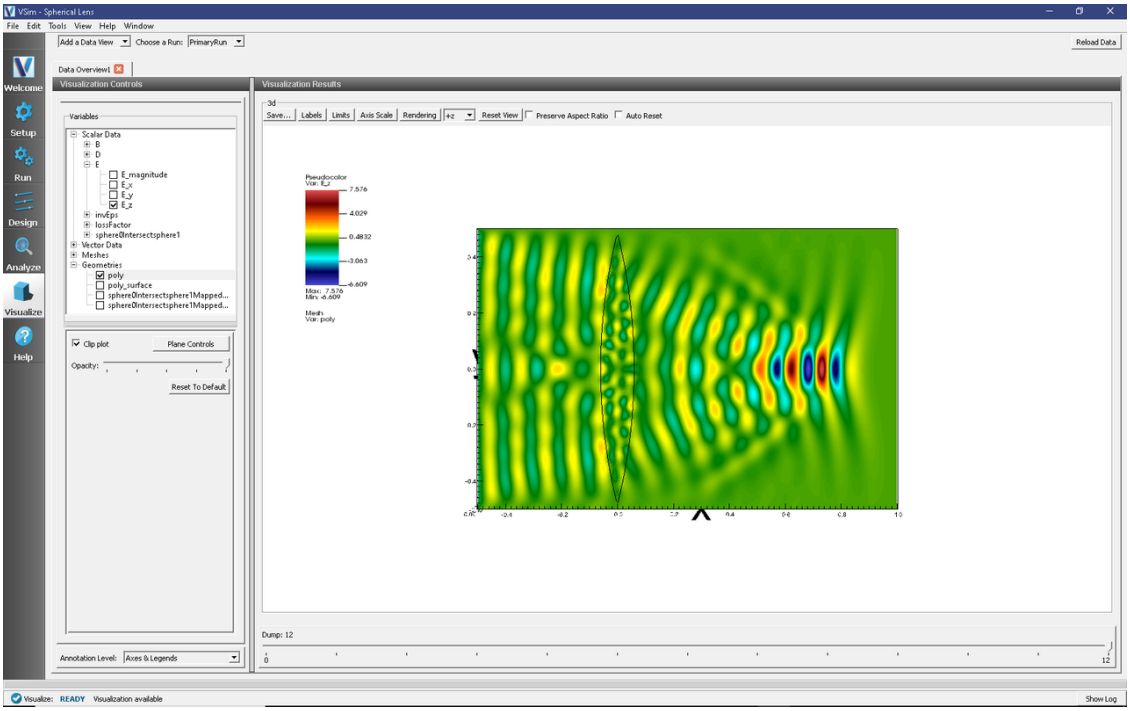


Fig. 3.146: Visualization of the lens focusing

Further Experiments

Use a material of larger dielectric constant to see more focusing.

Reduce the sphere radii to have more focusing.

3.8 Other EM (text-based setup)

3.8.1 Specific Absorption Rate (humanHeadT.pre)

Keywords:

dielectrics, power calculations, stl files

Problem Description

The Specific Absorption Rate simulation computes the power absorption in a human head where the brain tissue is approximated using a salt water model. A dipole source is included to imitate a simple antenna source from a cell phone. This example can serve as the basis for a true specific absorption rate calculation for a human head with a source coming from a cell phone antenna.

This simulation can only be performed with a VSimEM, VSimVE or VSimPD license.

Opening the Simulation

The Human Head example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Other EM (text-based setup)* option.
- Select "Specific Absorption Rate (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the right pane of the "Setup" window, as shown in Fig. 3.147.

Input File Features

The input file allows one to select the frequency of the dipole source as well as the number of grid points to include per wavelength for the wave in a vacuum. One can also set the dielectric value and conductivity value in the human head. We have also included the ability to select the position of the dipole source approximating the cell phone antenna. A voxel representation of the human head can also be used for more specific tissue values via a voxel dat file with python.

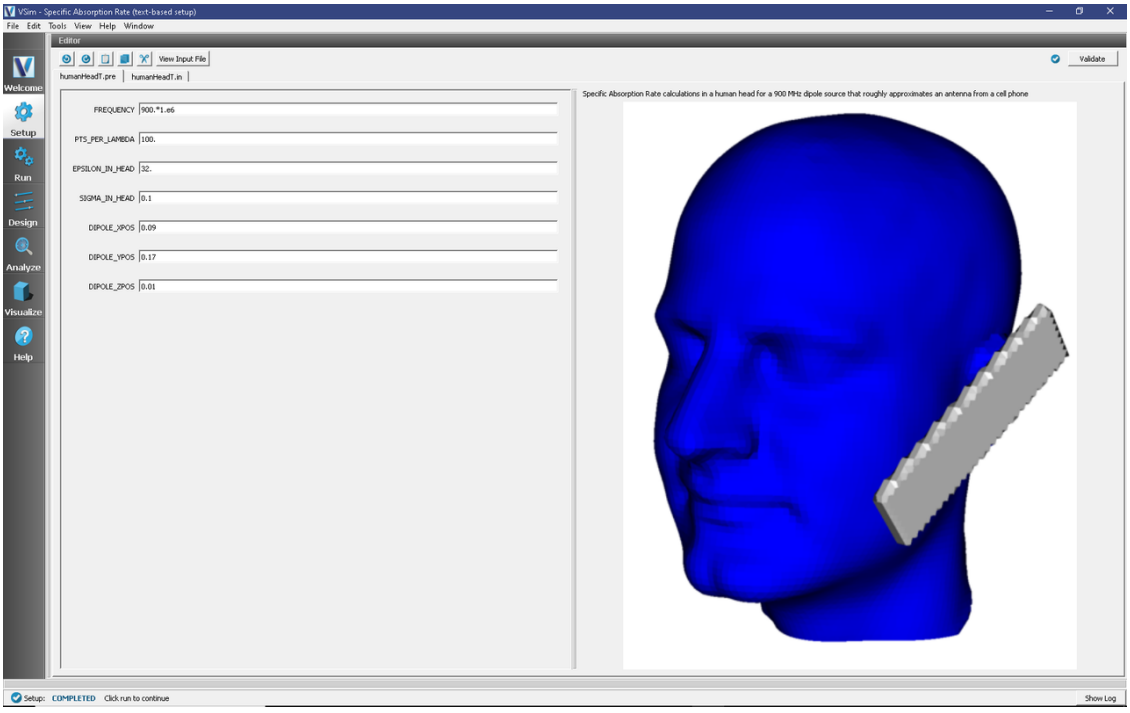


Fig. 3.147: Setup window for the Human Head example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.111758109234897e-17
  - *Number of Steps*: 100
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.148.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize window by pressing the Visualize button in the left column of buttons.

To create the image shown in Fig. 3.149:

- Expand *Scalar Data*
- Select *E* and *ESquared*
- Select *Log Scale Color*

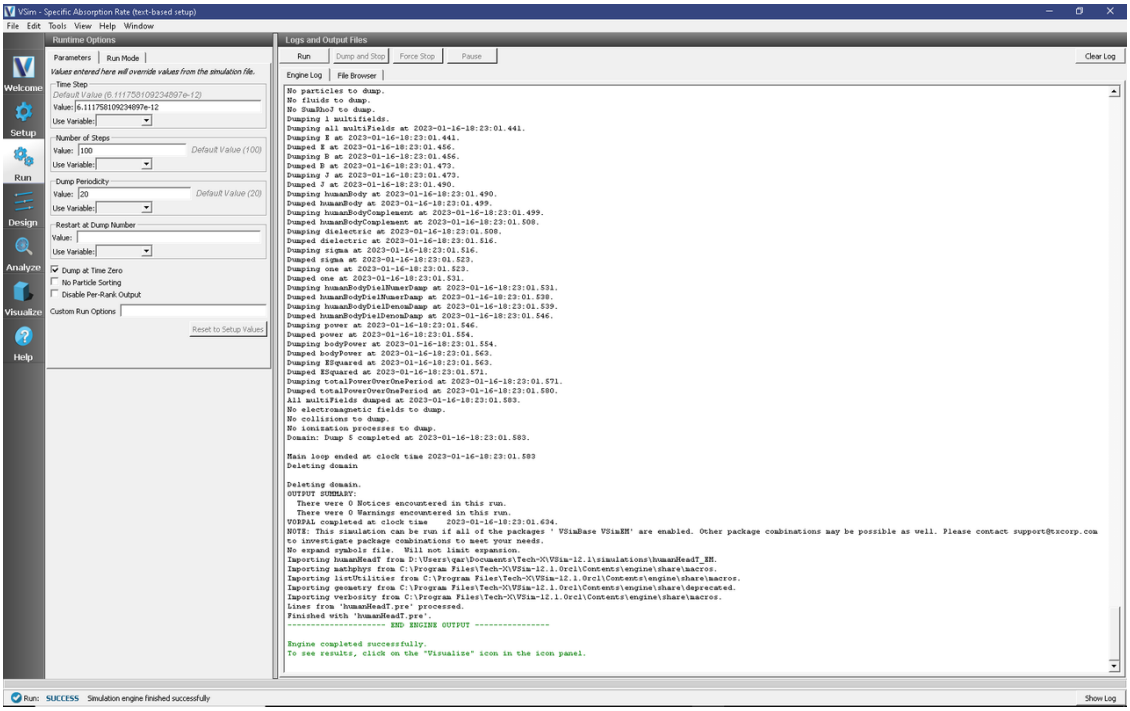


Fig. 3.148: The Run window at the end of execution.

- Select *Display Contours* and set the # of contours to 7
- Select *Clip Plot* and in the *Plane Controls* set the *Clip Plane Normal* to X and set the *Origin Of Normal Vector* to X = 0.1, Y = 0, Z = 0
- Expand *Geometries*
- Select *poly*
- Move the dump slider forward in time
- Click and drag with the mouse to rotate the image

Further Experiments

We suggest the user change the frequency of the dipole source to imitate different cell phone models at different frequencies.

We also suggest the user change the position of the dipole implying a change in location of the cell phone antenna.

It would also be interesting to change the dielectric and conductivity value to model a dipole source in a vacuum.

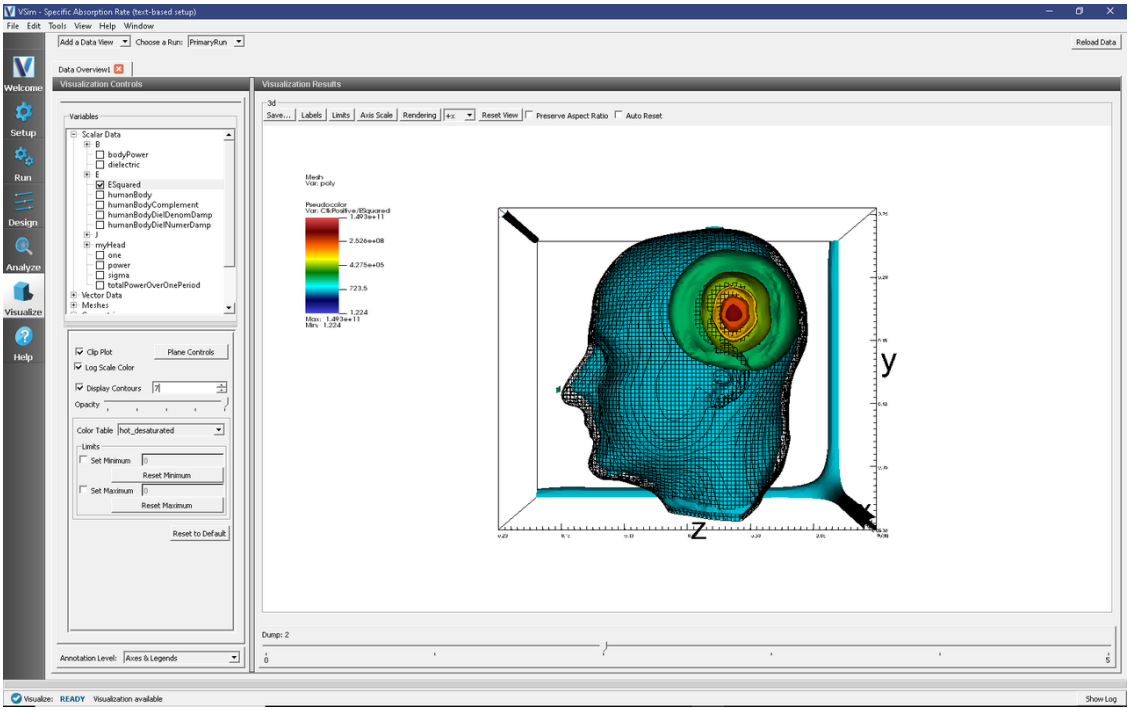


Fig. 3.149: Visualization of the absorption of power by a human head via a clip.

3.8.2 Photonic Crystal in Metal Cavity (phcInMetalCavityT.pre)

Problem Description

A photonic crystal (PhC) is capable of confining electromagnetic fields in waveguides and cavities using a periodic geometry. This simulation features a dielectric photonic crystal cavity—a triangular lattice of dielectric rods, with one rod removed—inside a metal cavity. The cavity axis, and the dielectric rods, are in the z direction.

The photonic crystal structure is similar to that described in [BWC08], truncated after two layers of the lattice structure. The metal cavity resembles an elliptical (or rounded pillbox) cavity, with short beam tubes.

Modeling dielectric and metal can be difficult: at dielectric corners or triple points (where dielectric, metal, and vacuum meet), the electromagnetic fields generally must diverge (to infinity) to preserve continuity dictated by Maxwell's equations [Had02]. However, when the interface between dielectric and vacuum is always perpendicular to the metal surface, as in this simulation, the fields remain finite.

This simulation demonstrates a method for combining dielectric and metal, as long as the metal surface is perpendicular to x, y, or z whenever it intersects dielectric (and the vacuum/dielectric interface remains perpendicular to the metal surface at those points).

When the PhC cavity mode is excited, the fields are trapped radially mainly by the dielectric rods.

This simulation can be performed with a VSimEM, VSimVE or VSimPA license.

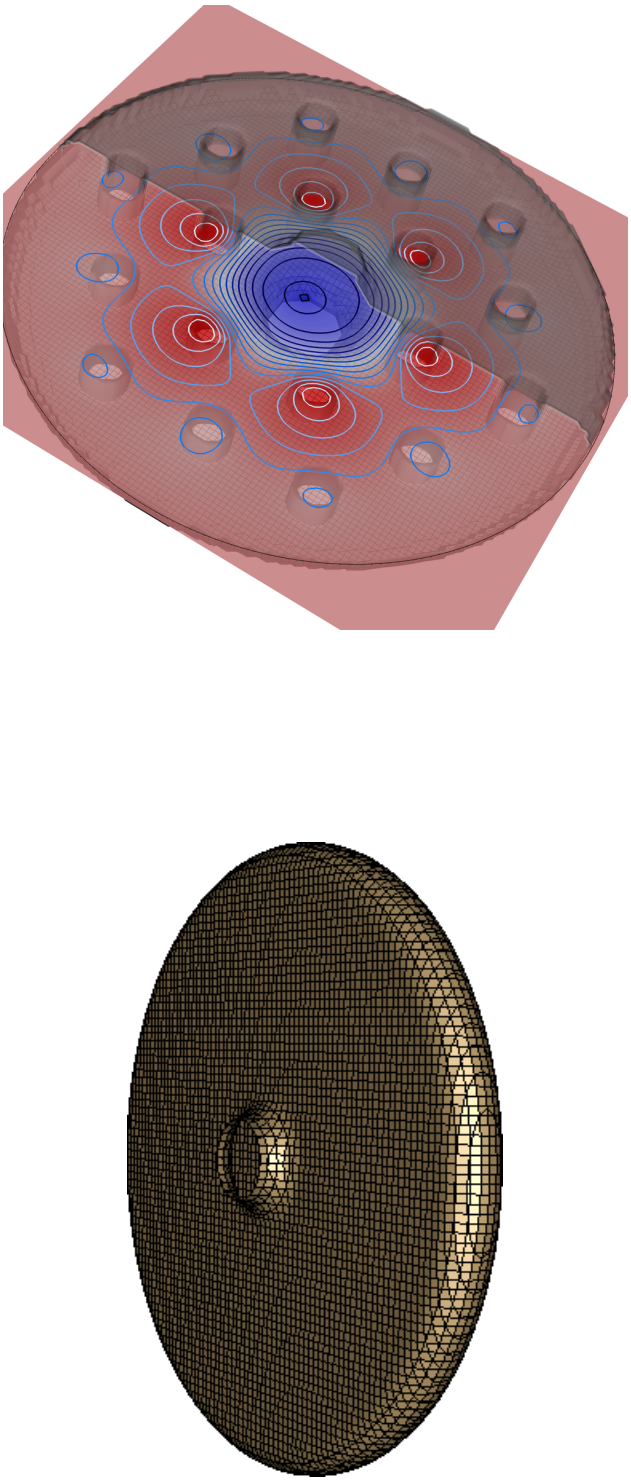


Fig. 3.150: The metal cavity surrounding the PhC structure.

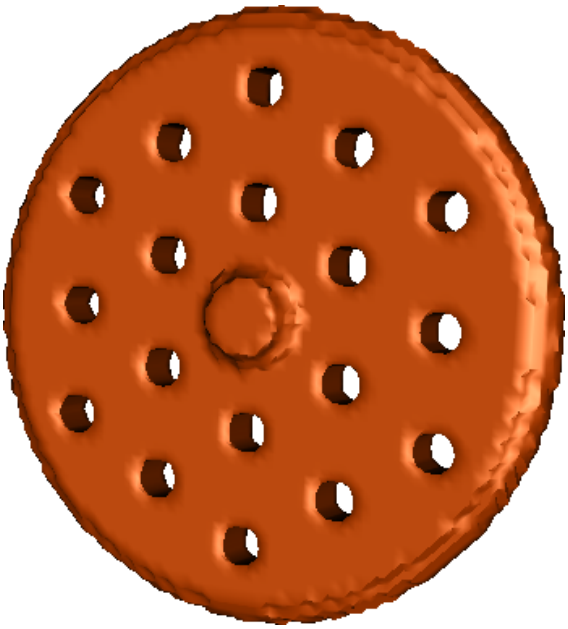


Fig. 3.151: The vacuum region (inside the metal cavity, outside the dielectric rods).

Opening the Simulation

The PhC in Metal Cavity example is accessed from within VSimComposer by the following actions

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Electromagnetics* option.
- Expand the *Other EM (text-based setup)* option.
- Select "Photonic Crystal in Metal Cavity (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a new folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem will now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 3.152.

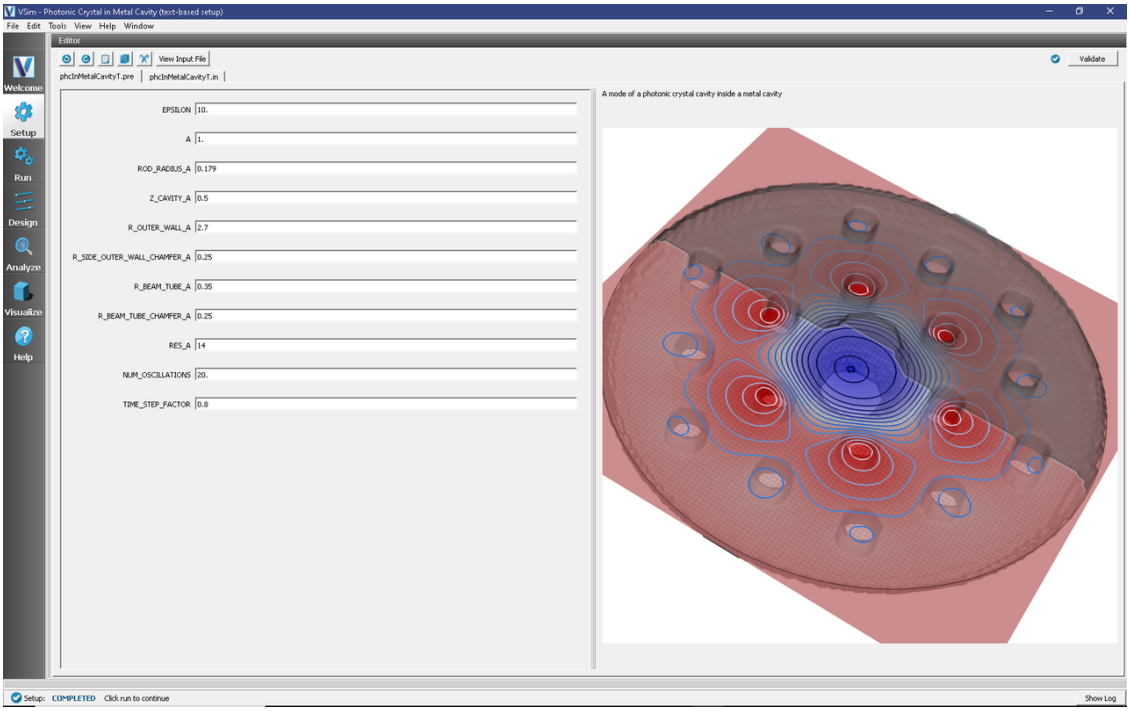


Fig. 3.152: Setup Window for the phcInMetalCavityT example.

Input File Features

The input file allows the user to choose the dielectric contrast and radius of the rods, the shapes and sizes of the cavity and beam tubes (to some extent), the grid resolution, and the number of oscillations to simulate after excitation. The entire simulation is scaled to the lattice constant, which is set to 1 by default.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.1004761151694115e-10
  - *Number of Steps*: 6070
  - *Dump Periodicity*: 1214
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 3.153.

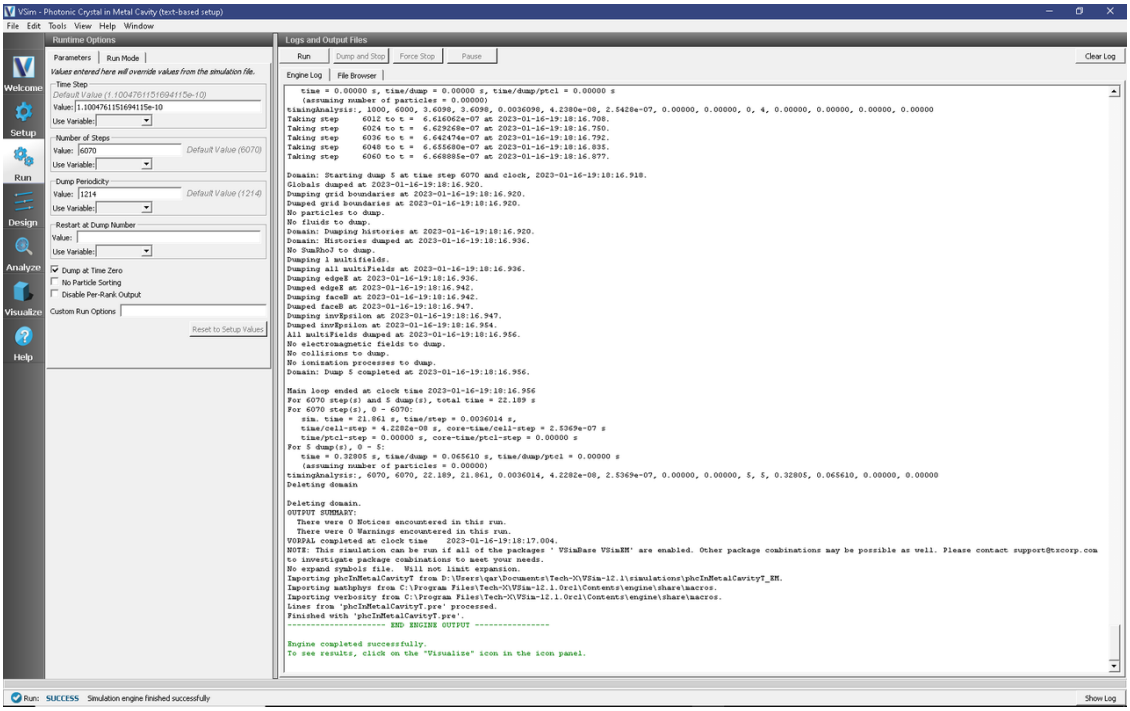


Fig. 3.153: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

Due to the symmetry of this system, the results are best viewed by looking at the z component of the electric field as follows:

- Expand *Scalar Data*
- Expand *edgeE*
- Select *edgeE_z* and check the box next to *Clip Plot*
- Expand *Geometries*
- Select *poly* and check the box next to *Clip Plot* again

The field at dump 2 is shown in Fig. 3.154.

We can see that fields are trapped by the two layers of dielectric rods, and to a lesser (but final) extent by the surrounding metal cavity.

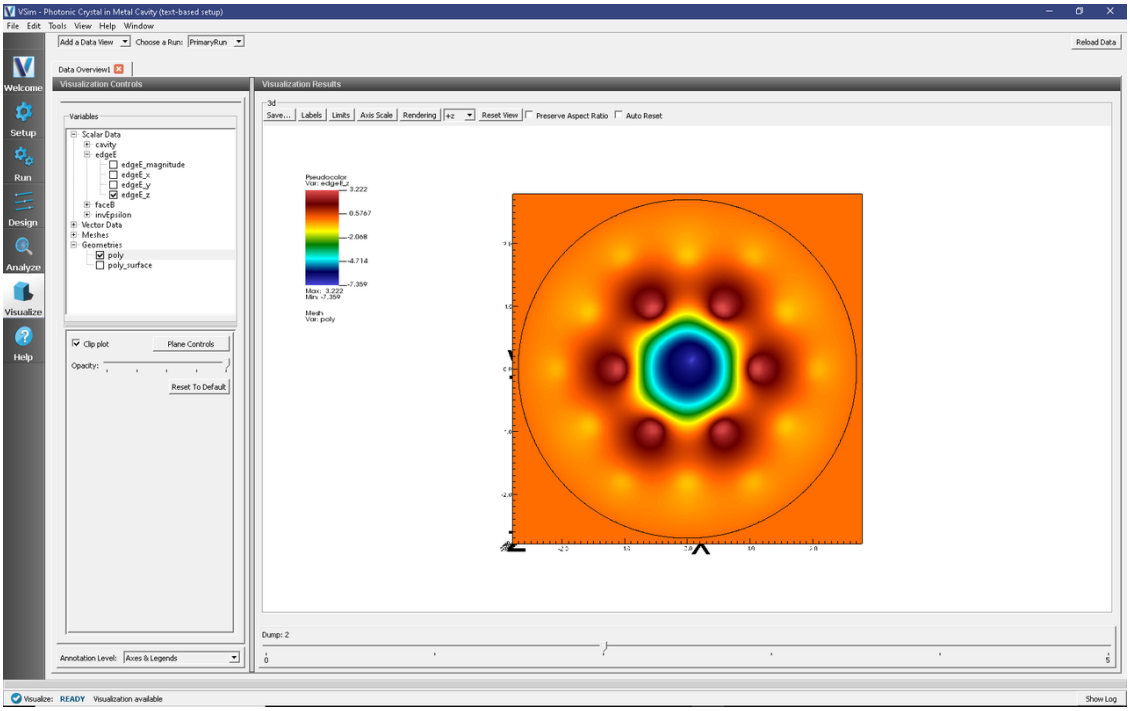


Fig. 3.154: Visualization of the E_z field component.

CHAPTER

FOUR

VSIM FOR VACUUM ELECTRONICS EXAMPLES

These examples illustrate how to solve complex problems in vacuum electronics.

These examples can be run with a VSimVE license.

4.1 Cavities and Waveguides

4.1.1 Circular Metal Waveguide Dispersion (circMetalWaveguideDisp.sdf)

Keywords:

`Waveguide, Dispersion Relation, Fourier Transform, Phase Shifting Boundary Conditions`

Problem description

This XSimEM example demonstrates several unique capabilities of XSim that can be used to efficiently model waveguides. One unique capability is the use of phase shifting periodic boundary conditions. These work by adding a phase to a wave at a boundary to mimic a much longer physical dimension. We also demonstrate how to use an analyzer called extractModesViaOperator.py to accurately compute the excited modes in the waveguide, even if some of the modes are much weaker than the dominant mode. In this example, we use extractModesViaOperator.py to compute the dispersion relation (ω vs k) and compare the numerically determined dispersion relation with the theoretical dispersion relation using standard waveguide theory.

This example involves five steps. In the first step, the waveguide is "pinged" with a short pulse in the current density that excites a range of modes. The Fourier transform then shows the range of frequencies of the modes. In the second step, the waveguide is excited using a sinc pulse function multiplied by a Gaussian envelope to excite a flat band of frequencies with sharp cutoffs at either end. The excitation current density is in the transverse directions (z and y) which excites an electric field primarily in the transverse direction. In the third step, the data is restarted from the end of the second run and saved at shorter time intervals in order to resolve the frequencies of interest. The output from the third step is used by the extractModesViaOperator.py analyzer to compute the eigenmodes in step 4. Finally, in step 5, the dispersion relation is computed by varying the wavelength which is resolved in the simulation.

Opening the Simulation

The circular metal waveguide dispersion example is accessed from within XSimComposer by the following actions:

- Go to *File* → *New* → *From Example…*
- In the resulting *Examples* window expand the *XSim for Electromagnetics* option.
- Expand the *Cavities and Waveguides* option.
- Select "Circular Metal Waveguide Dispersion" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The properties and values that create the simulation are accessible in the left pane when the Setup Window is selected as shown in Fig. 4.1. The right pane shows a 3D view of the selected geometry components, grids and current distributions.

The geometry can be visualized by expanding "Geometries" in the left pane. The hollow circular waveguide can be seen more clearly by de-selecting the "Grid" option. The length in the direction of propagation (x) is a small fraction of either transverse direction. This is possible because we are using "phase shifting periodic" boundary conditions in the x -direction. The phase shifting BCs are selected under "Basic Settings".

A sinc hat function is used to excite the waveguide.

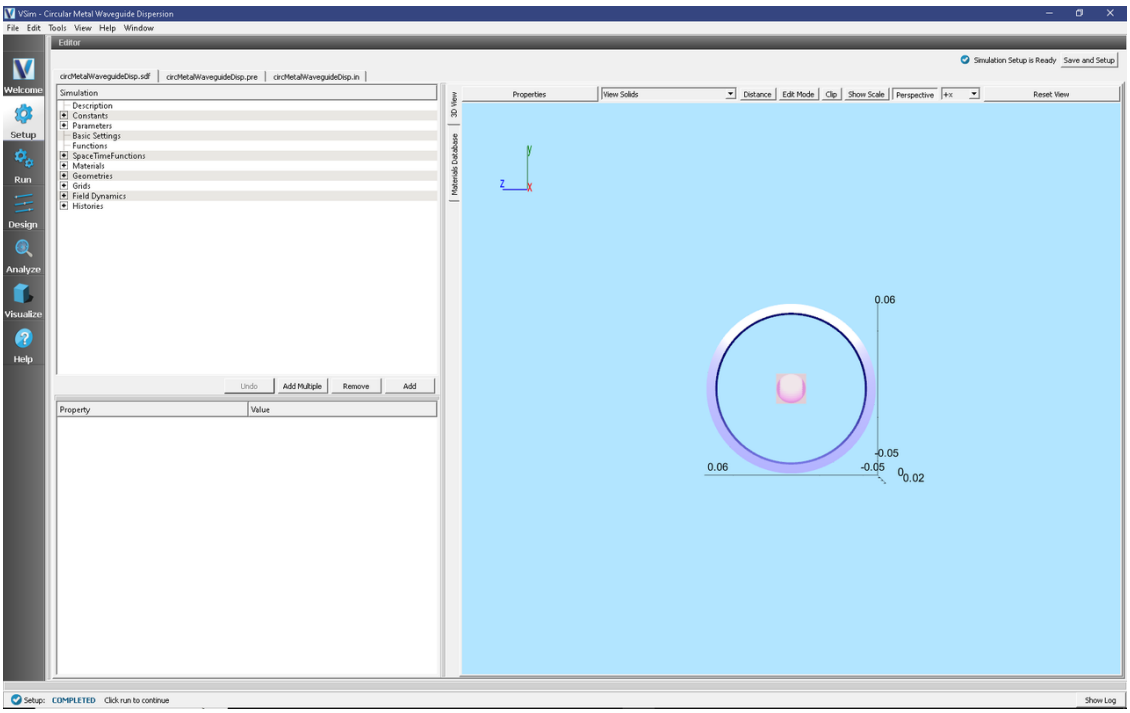


Fig. 4.1: Initial Setup Window for the Waveguide Dispersion example. The block in the middle is the region in which the current density is driven.

Phase Shifting Boundary Conditions and Phase Shift

Before discussing phase-shifting periodic boundary conditions, we first review ordinary periodic BCs. In this discussion, periodic BC's are applied in the *x*-direction. With normal periodic BC's, there are two criteria in resolving a wave (or mode) of interest. (1) There must be enough grid points along the wavelength to resolve the spatial profile. Typically we sample at least 20 cells along a wavelength (λ_x), or $DX = \lambda_x/20$, and (2) The length of the simulation domain, represented by L_x, must be one wavelength long, $L_x = \lambda_x$. Periodic BC's in the *x*-direction means that $F(0) = F(L_x)$, where F is any field quantity. Now introduce a grid that extends from 0,1,...,nx and let $x = 0$ at grid point 0 and $x = L_x$ at grid point *nx*. Periodicity on the grid implies $F(0) = F(nx)$. Finally, let's assume that $F(x) \sim \sin(k_x x)$. Then, applying the condition for periodicity, $\sin(0) = \sin(k_x L_x)$, which is exactly met if $L_x = \lambda_x$.

With phase-shifting periodic BC's, we are no longer required to meet the second criteria discussed in the preceding paragraph. To see this, let's suppose that $L_x < \lambda_x$. Then the periodicity condition can still be met by setting $k_x L_x - \phi_0 = 0$, where ϕ_0 is the phase shift equal to $k_x L_x$, which is the exact phase shift we have chosen to apply in XSim for this example. The numerical implementation is more challenging than the conceptual picture we just discussed. To implement phase-shifting periodic BC's, we need to treat the fields as complex numbers and set $F(L_x) = \exp(i\phi_0)F(0)$. For the grid, we pick 2 cells such that $L_x = 2DX$.

By using phase-shifting periodic BC's, we can simulate different physical lengths without changing the simulation length L_x through the phase shift $\phi_0 = k_x L_x$. Because $k_x = 2\pi/L_x$, we can solve for $\omega(k_x)$ without requiring a simulation of length L_x.

Running the Simulation and Analyzing Results

We now walk through the five steps discussed in the Introduction. In the first step, we test to determine the minimum frequency that will propagate through the waveguide. For the circular waveguide in this example, we know the analytical result which is the lowest cutoff frequency. However, we still do this step to demonstrate how to determine the lowest frequency that will propagate for cases that are not analytic. In the second step, the current density "rings up" to a maximum value, then rings down to 0. Because we are exciting modes at resonant frequencies of the cavity, the *E*- and *B*-fields continue to oscillate after the excitation is turned off. We wish to determine the resonant modes using Eigen mode analysis using data saved in Step 3 when the externally driven source is turned off and the cavity is "ringing" at its natural frequencies. In step 4, extractModesViaOperator.py is used to compute the excitation frequencies in the cavity at a given mode. Finally, in step 5, you will change the value of "mode", which is defined under "Constants" to compute the dominant frequencies which are excited in the cavity at a given wavelength. We assume the maximum wavelength which can be resolved in a traditional periodic simulation is 0.2 m and denote this as *lambdaMax*. We then define the parameter $k_x = \frac{mode}{12}\frac{2\pi}{lambdaMax}$ and run 25 simulations with *mode* =0,1,2,...,24. Finally, we set the phase shift to $k_x \times L_x$ to ensure the correct phase shift is applied for the phase shifting periodic BC's. In this way, we are able to compare the simulation with waveguide theory without explicitly changing the length of the simulation domain in the *x* -direction.

Step 1: Determining the lowest cutoff frequency - The "Ping" Run

The Ping run is used to determine the lowest propagation frequency in the waveguide. In this simulation, we can analytically compute the lowest propagation frequency at a given *k* based on the allowable modes in a circular wave guide. We can then compare the computed lowest propagation frequency with theory. However, for arbitrarily-shaped waveguides, this step is necessary since no theory is available to compute the lowest propagation frequency. We have defined a PINGON constant (with values of 0 or 1) in order to easily transition from the "Ping" run to the "Excitation" run in Step 2. The default is PINGON=1 to do the "Ping" run first. For Step 1, perform the following steps

- Click on the Run Window.
- This simulation may be accelerated by changing the Run Mode to Parallel
- Click the *Run* button on the upper left corner of the *Logs and Output Files* pane

The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.2.

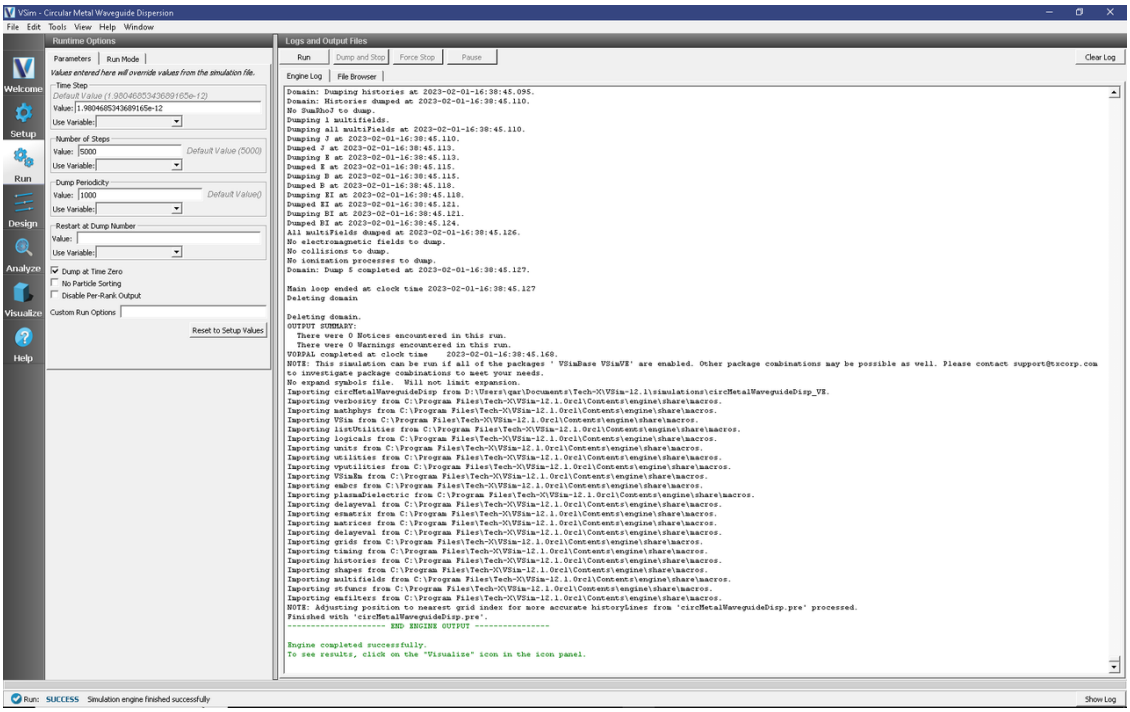


Fig. 4.2: The Run window at the end of a Step 1.

After the run has completed, click on the *Visualize* tab on the left side of the visualization window. After the data has loaded, click on *Add a Data View* and then select *History*. Perform the following steps to analyze the history:

- Graph 1 select *jMid_1*
- Graph 2 select *eMid_1*

In Graph 1, to see the data, click on the "Limits" option above the plot. Set the X-axis upper limit to 2e-10. You should see a step function in the current density beginning at t=0 and ending abruptly after about 20 time steps. This is the "ping" that we impose on the simulation. To determine the lowest frequency mode that we excite, click the "Fourier Amplitudes (dB)" box in Graph 2. Again, click on the "Limits" button above and to the right of the graph. Set the X-axis upper limit to 4e9. You will see that the first peak occurs at a frequency of about 1.75×10^9 Hz, which is the lowest cutoff frequency in the simulation and is what we find analytically using waveguide theory. Therefore, we have confirmed that XSim reproduces linear theory. You can confidently use XSim to numerically determine the lowest cutoff frequency for non-analytically solvable shapes. The visualization window after the above steps have been performed is shown in Fig. 4.3

Step 2: Excitation

From Step 1, we know that the lowest propagation frequency is $\sim 1.75 \times 10^9$ Hz. We can now check that the lowest cutoff frequency (*frequency low* in **SincHat**) is correct. The parameter *FREQ_MIN* is passed into *frequency low* in the **SincHat** function and is indeed $\sim 1.75 \times 10^9$ Hz. We can now proceed to excite the waveguide with confidence knowing that lowest excitation frequency is correct. To excite the waveguide, perform the following steps:

- Go to the Setup Window and expand the *Constants* option
- Set *PINGON* to 0

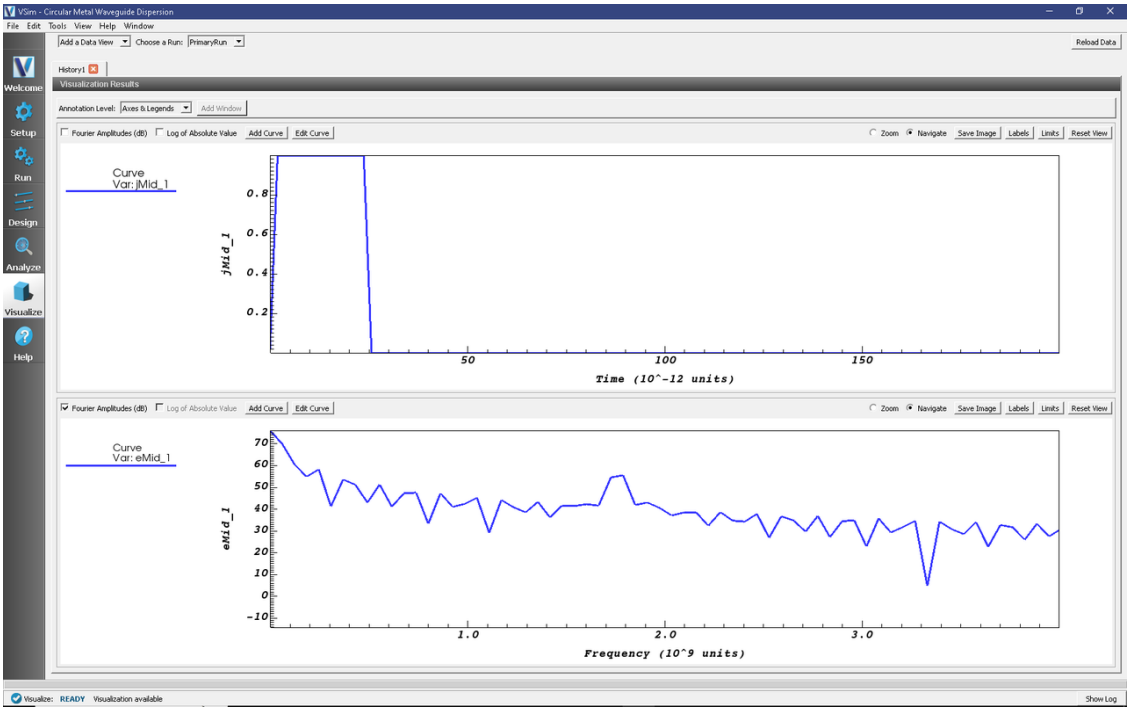


Fig. 4.3: History plots showing the lowest cutoff frequency at 1.75×10^9 Hz as the result of pinging the waveguide with an abruptly applied current density.

- This will change the applied current to the **SincHat** function.
- Click on *Save and Setup* in the upper right corner of the visualization window
- Go to the Run Window by pressing the Run button in the left column of buttons.
- Set Number of Steps to 21000. This ensures that the simulation runs long enough for the current density to "ring up" then "ring down" to 0.
- Leave the "Dump Periodity" at 1000.
- This simulation may be accelerated by running on multiple MPI ranks. The parallel options are in the *Run Mode* tab
- To run the file, click on the *Run* button in the upper left corner of the *Logs and Output Files* pane. You will see the output of the run in this pane. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.4.

Step 3: Evolving the excited cavity

The purpose of Step 3 is to continue the simulation with only the *E*- and *B*- fields excited due to the externally imposed current density from Step 2. We will also save more data which we can analyze using Eigenmode analysis for Step 4.

- Go to the Setup Window and expand the Basic Settings option.
- Change "number of steps" to "10000".
- Change "steps between dumps" to "100".
- Change "dump in groups of" to "3".
- Click on *Save and Setup* in the upper right corner of the visualization window.

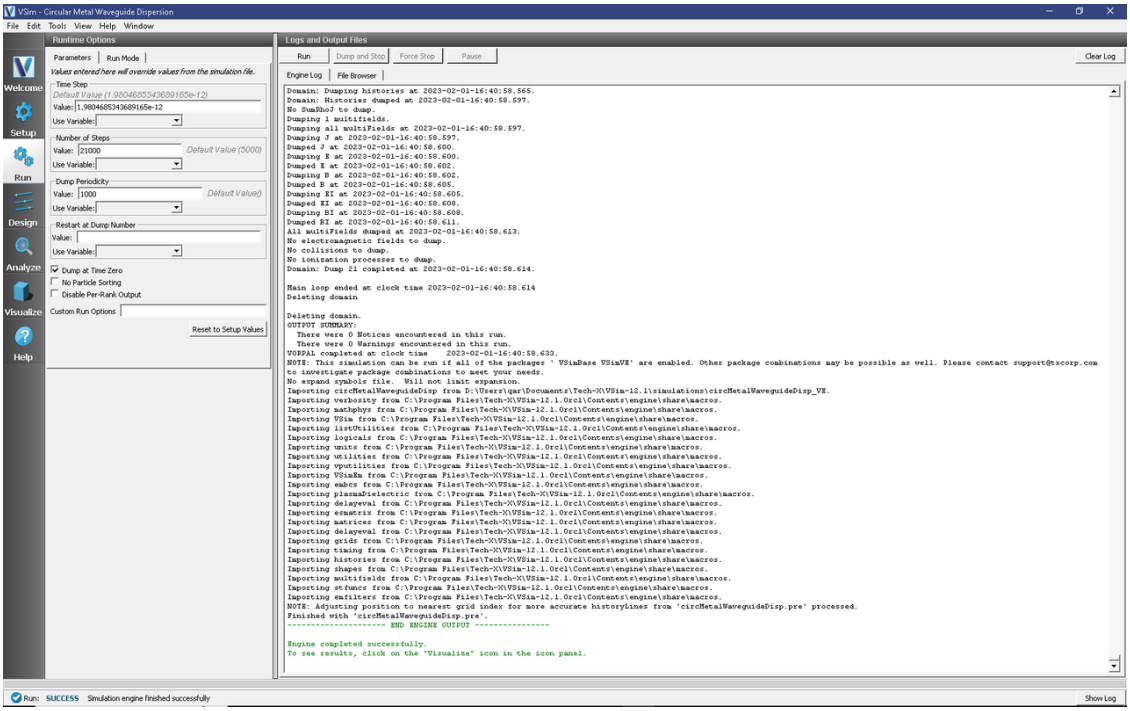


Fig. 4.4: The Run window at the end of a Step 2.

- Go to the Run Window and click the "Reset to Setup Values" button in the lower right corner of the "Run Options" section.
- In the *Run Options* section, uncheck the *Dump at Time Zero* box and set the *Restart at Dump Number* to 21.
- NOTE: the "Dump Periodicity" must be blank for the "dump in groups of 3" setting to work. In this case, the simulation will revert to the values defined in "Basic Settings" which are to dump every 100 time steps in groups of 3 (21000,21001,21002, …, 21100,21101,21102,…, etc). If you fill in an integer into Dump Periodicity, the default gets overwritten and the data are not dumped in groups of 3, which is required for the extractModesViaOperator.py analyzer. So, there should be 300 new dumps making a total of 321 dumps.
- Click run. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.5. When this run is finished, the last step should be step 31000.

Step 4: Computing the eigenmodes

- Go to the analyzer window by selecting *Analyze* in the left column.
- Select *extractModesViaOperator.py* from the list of available analyzers. Then click "Open" on the top right of the *Analysis Controls* pane.
- Compute the electric field eigenfunctions. After the analyzer loads, ensure the following parameters are entered:
  - **`simulationName:`** "circMetalWaveguideDisp"
  - **`outputsimName:`** leave blank
  - **`realFields:`** "E"
  - **`imagFields:`** leave blank
  - **`secondFieldFactor:`** leave blank

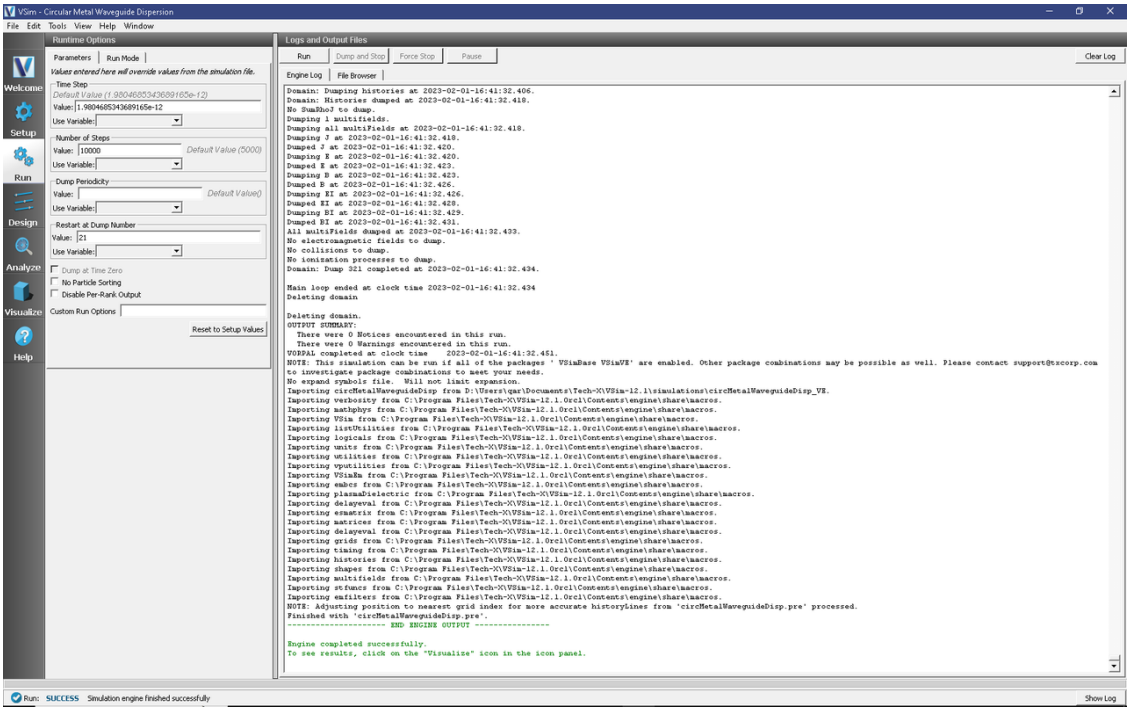


Fig. 4.5: The Run window at the end of Step 3.

- **operator:** "d2dt2"
- **dumpRange:** "21:321"
- **cellSamples:** ":,5:55:5,5:55:5"
- **cutoff:** "1e-12"
- **maxNumModes:** "-1"
- **initialModeNumber:** "0"
- **normalizeModes:** checked
- **testing:** leave blank
- **compMajorC:** leave blank
- **overwrite:** checked

The dump range runs only over the data saved in step 3 and we are only sampling every 5 cells in the z- and y- directions which is adequate to compute the eigen modes. Double-check your entries against what is shown in Fig. 4.6. After you run the analyzer, you will need to scroll up to find the computed frequencies. The screenshot shown in Fig. 4.6 is from a visualization window that is scrolled up so that the computed frequencies can be compared with what you ran. Figure Fig. 4.6 shows that there are 6 unique modes. One indication that you are using extractModesViaOperator.py correctly is that the imaginary part of the frequency (which represents attenuation of the wave) is nearly 0 or at least much smaller than the real part. The lowest excited mode is $\sim 1.76 \times 10^9$ Hz, which is discussed further below in the context of standard waveguide theory.

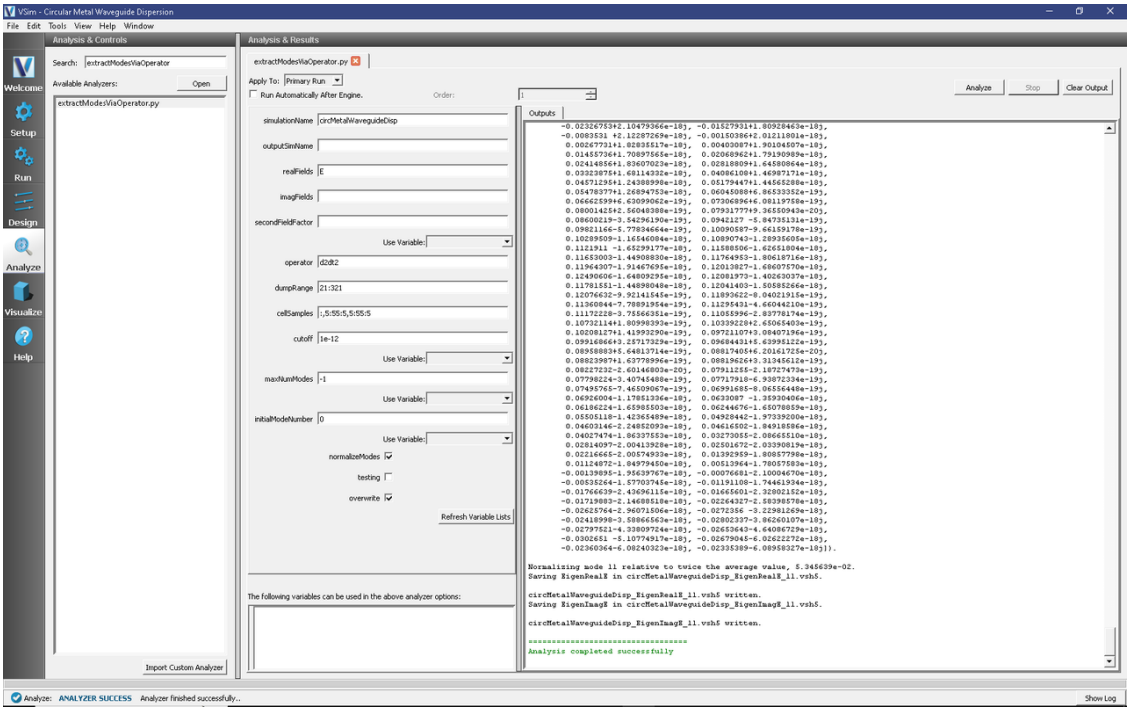


Fig. 4.6: Computing the electric field eigenfunctions and frequencies using the extractModesViaOperator.py analyzer.

Step 5: Computing the Dispersion Relation

Once the Eigenmode analysis is complete in Step 4, it is necessary to record the three lowest-order modes. The preloaded value of *mode* is 1, which means we are simulating $k_x = \frac{1}{24}\frac{2\pi}{\lambda}$, where $\lambda = 0.2$ m. Also, the waveguide dispersion relation is given by $\omega^2 = k_x^2 c^2 + \omega_{mn}^2$, where $\omega_{mn}^2 = \frac{c^2}{R^2}(x'_{mn})^2$, where m and n are integers and x'_{mn} is the nth root of $J'_m(x) = 0$ (the derivative of the cylindrical Bessel function of the first kind). The first three allowable modes are $x'_{11} \approx 1.841, x'_{21} \approx 3.054$ and $x'_{01} \approx 3.832$. Furthermore, the frequency range that is excited lies between $f_l = 1.75 \times 10^9$ Hz (which is the lowest allowable propagation frequency) and $f_h = 5.2 \times 10^9$ Hz. Given these parameters, we expect from waveguide theory for the three lowest modes to be $\sim 1.76 \times 10^9, 2.92 \times 10^9, 3.66 \times 10^9$ Hz, which is what is found from extractModesViaOperator.py. Repeating these steps for modes 1 to 24 yields the dispersion relation shown in Fig. 4.7. The overlap between the simulation results and theoretical values is evident in Fig. 4.7.

Convergence Study

To demonstrate that the simulation results converge to the theoretical value, we have performed a series of simulations in which $DX = DY = DZ$ are varied. The values chosen are *DX* = 0.25, 0.33, 0.5 and 0.733 cm. We then computed the lowest propagation frequency using *extractModesViaOperator.py* and plotted this frequency versus DX^2. Using Richardson extrapolation, we then compute the lowest propagation frequency for $DX^2 = 0$, which provides a better comparison with the theoretical frequency than a simulation with finite DX^2. The field calculation error scales approximately with DX^2 so a plot of frequency versus DX^2 should be a line. The linear correlation between frequency and DX^2 is shown in Fig. 4.8. The extrapolated frequency at $DX^2 = 0$ is $\sim 1.75686 \times 10^9$ Hz. The theoretical value is $\sim 1.75681 \times 10^9$. Therefore, we see from Fig. 4.8 that the computation of the lowest propagation frequency for the DC mode converges with order DX^2, which is expected since the field solve is 2nd order accurate. Furthermore, using Richardson extrapolation, we see that the difference between theory and simulation, with $DX^2 = 0$, is 0.003 %.

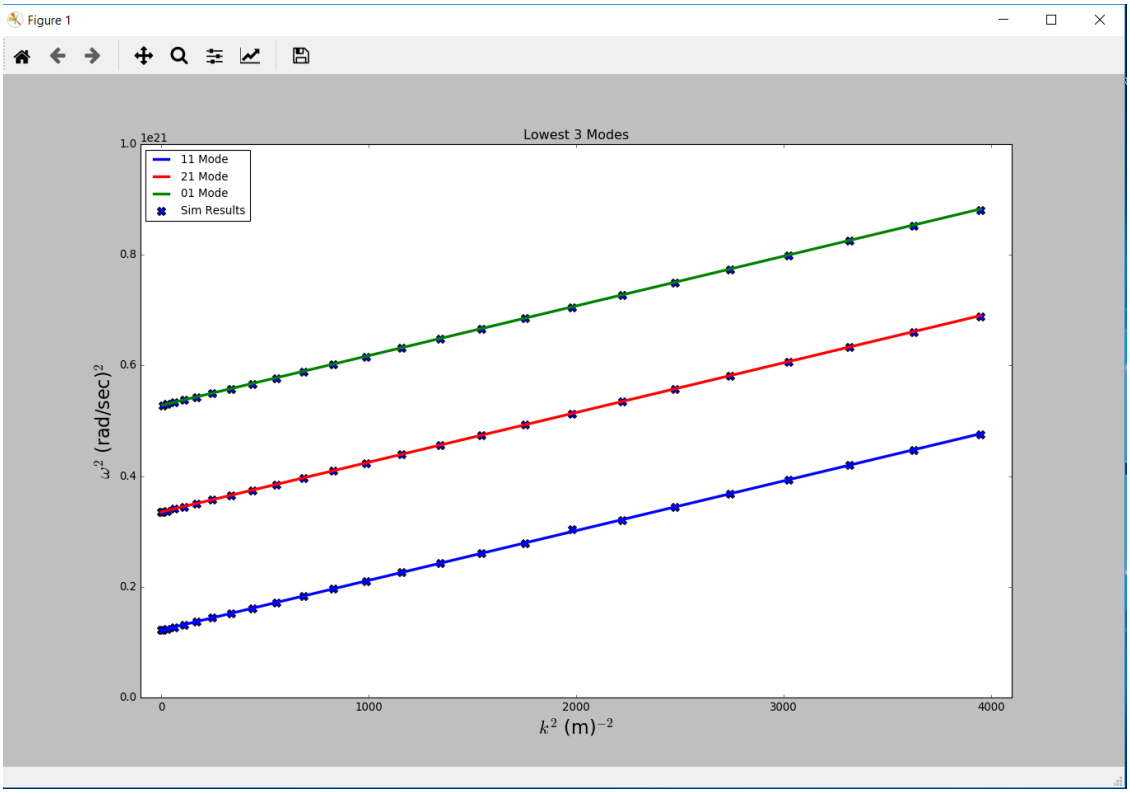


Fig. 4.7: Dispersion relation found by changing *mode* in XSim. The solid line is theoretical dispersion relation $\omega^2 = k_x^2 c^2 + \omega_{mn}^2$. The 'X's represent data from the simulation results.

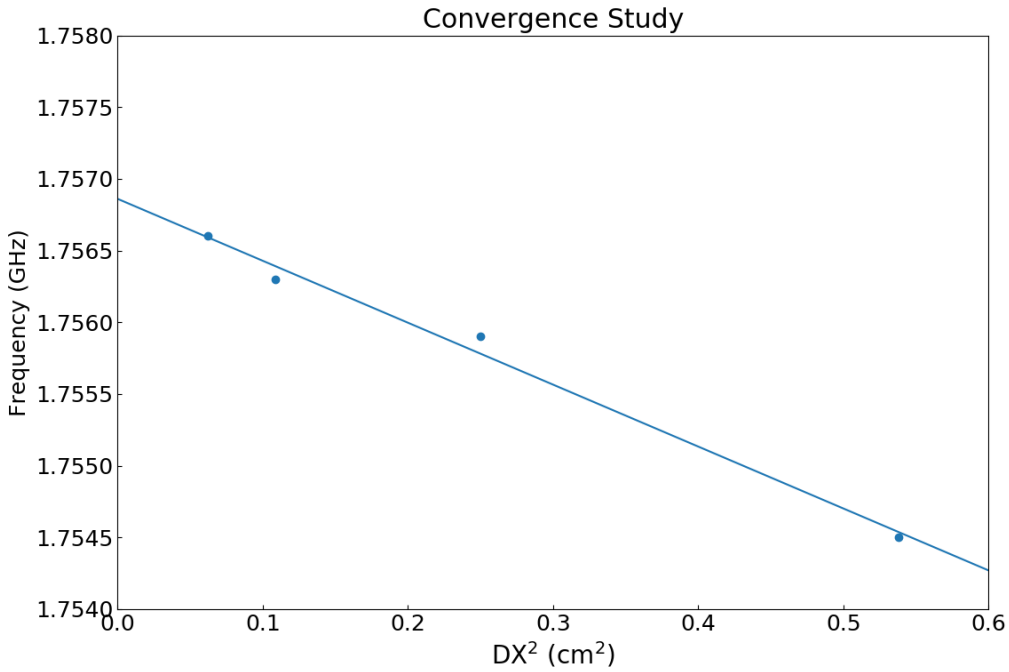


Fig. 4.8: Plot demonstrating convergence of frequency calculation.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.
- Click on *Reload Data*

The first step will be to ensure that we are driving the current density as expected and that the *E*- and *B*- fields are "ringing" as a result of driving the current density. Follow these steps to perform this check:

- Click on the *Add a Data View* pull-down menu at the top of the visualization window
- Click on *History*. This will open a new tab.
- Under Graph 1 plot *jMid_1*. This is the *y*- component of the current density
- Under Graph 2 plot *eMid_1*.

Your plots should be similar to Fig. 4.9. The current density is driven for a short time period. However, because we are driving resonant modes, the current density excites the transverse electric field and parallel magnetic field. You can also plot *eMid_0*, *bMid_1*, and *bMid_2* to compare with Fig. 4.9. Since *eMid_0* is ~ 0, we are driving a TE waveguide.

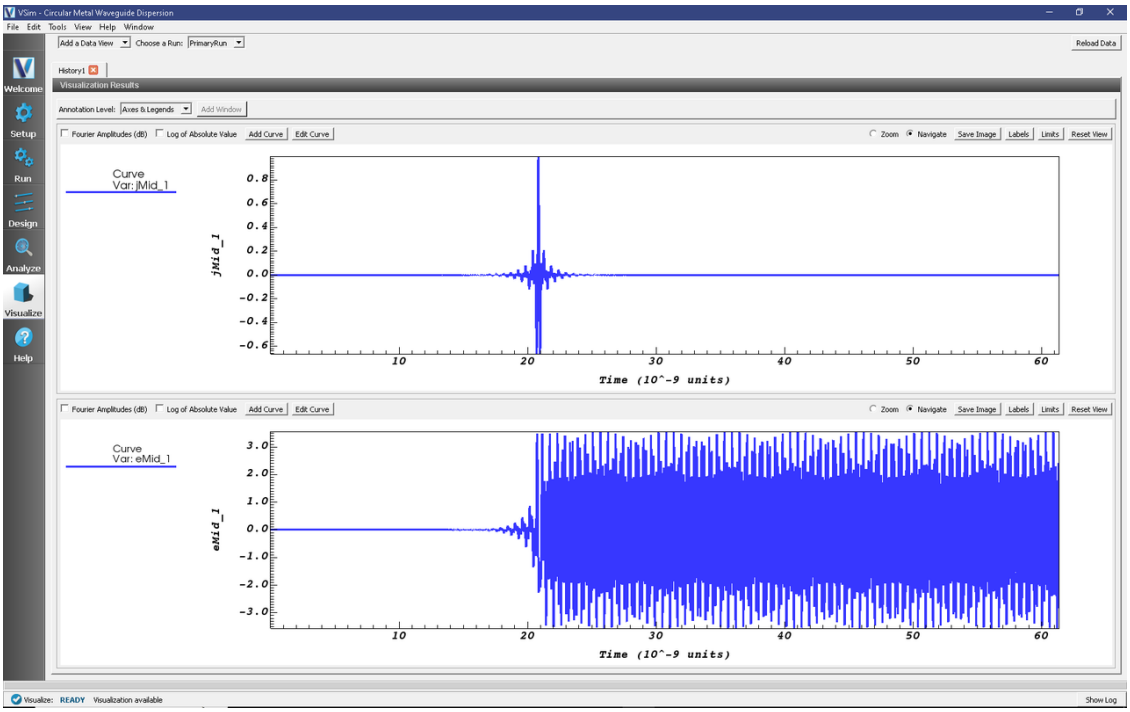


Fig. 4.9: History plots showing the modes driven in this simulation

We next wish to examine the spectral characteristics of the current density, which is driven between *FREQ_MIN* and *FREQ_MAX*. Therefore, the Fourier Transform of J_y or J_z should be greatest in this frequency range. Returning to the History visualization window, under Graphs 2, 3, and 4, change the plotted quantity to *none*, so that only Graph 1 shows a plot. Now check the "Fourier Amplitudes (dB)" box in the upper left corner. Finally, check the "Zoom" box on the right side of the visualization window and highlight from 0 to 10^{10} Hz which will expand the lower frequency part of the plot. After you have zoomed in on the plot, re-check the "Navigate" box. The result of these steps should lead to a plot that looks similar to Fig. 4.10. The driving frequencies lie between *FREQ_MIN* and *FREQ_MAX* as expected. The rate at which the Fourier signal dampens below *FREQ_MIN* and above *FREQ_MAX* depends on the Gaussian envelope and the parameter called *OMEGA_SIGMA*.

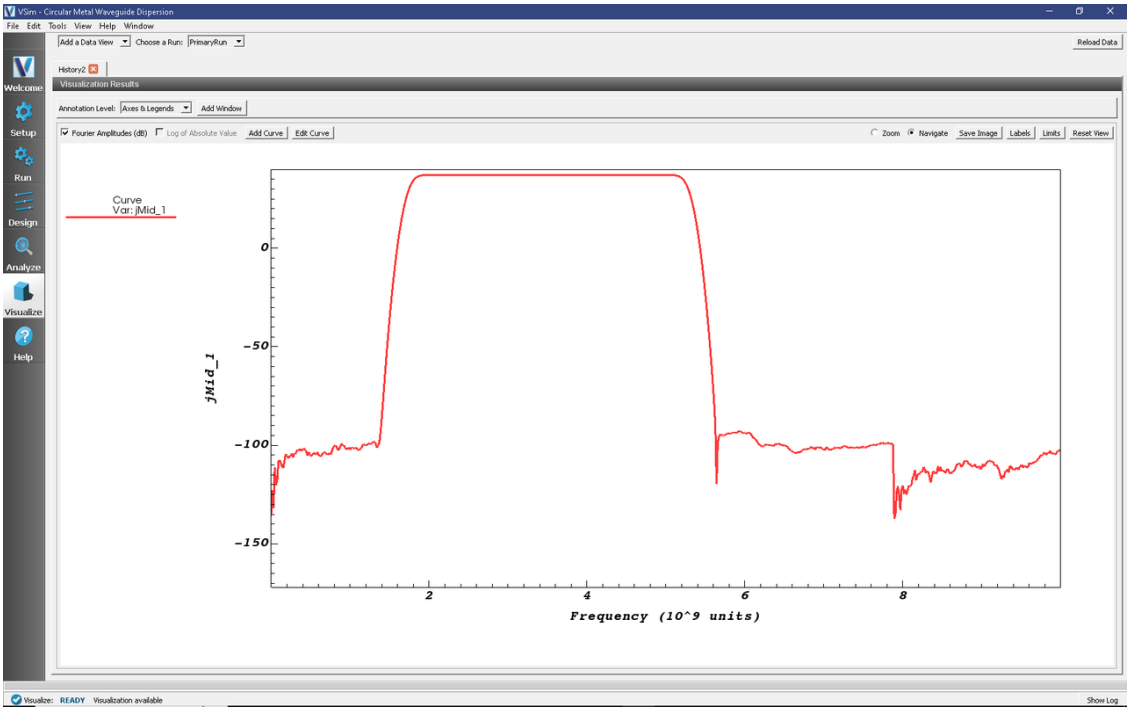


Fig. 4.10: Fourier Transform of the current density showing that the current density is mainly driven between *FREQ_MIN* and *FREQ_MAX* as expected.

Further Experiments

The result of varying *mode* from 0 to 24 is shown in Fig. 4.7. One experiment you can perform is to reproduce Fig. 4.7 by running 25 simulations with *mode* varying from 0 to 24. Each simulation takes just a few minutes so the 25 simulations takes about one hour. For each simulation record the three lowest frequencies that are excited using extractModesViaOperator.py.

Another experiment would be to change the dimensions of the waveguide. The constant *InnerRadius* is used to determine the lowest frequency that will propagate in the waveguide. Therefore, changing *InnerRadius* will automatically compute *FREQ_CUTOFF_TE*. You will then need to change *BGNY*, *ENDY*, *BGNZ*, and *ENDZ* so that the primitive fits within the simulation domain. The primitive geometry called "pipe0" scales with the constant *InnerRadius*.

A third experiment would be to modify *FREQ_MIN* and *FREQ_MAX* and compute the dispersion curve for these new values. No mode will propagate below *FREQ_CUTOFF_TE* so do not set *FREQ_MIN* below *FREQ_CUTOFF_TE*.

Lastly, you can try to propagate a TM mode instead of a TE mode.

4.1.2 Coaxial Cylinder (coax.sdf)

Keywords:

coax, coaxial geometry, cylinder, current pulse, rlc circuit, step potential

Problem description

This example probes the electromagnetic properties of a semi-infinite coaxial cylinder. One end of the cylinder lies in the simulation space. The length of the cable is large compared to its diameter. The outer radius is 8 cm, the inner radius is 2 cm, and the section considered is 20 cm long. The inner cylinder is shorter than the outer cylinder and there is an electron absorbing cap on the end of the outer cylinder. When the simulation initiates, a single EM pulse is launched into the open, continuous end of the geometry and propagates to the capped tip. Electrons are ejected from the tip of the inner cylinder when the pulse reaches it.

This computational model is equivalent to applying a step-potential to one end of a coaxial cable. The step-potential propagates at the speed of light until it reaches the tip of the inner cylinder. The RLC nature of the coax cable causes overshoot and ringing of the potential. At the inner tip, an attenuating series of oscillations occurs accompanied by electron emissions. Gradually the tip potential stabilizes at the applied potential.

This simulation can be performed with a VSimVE license.

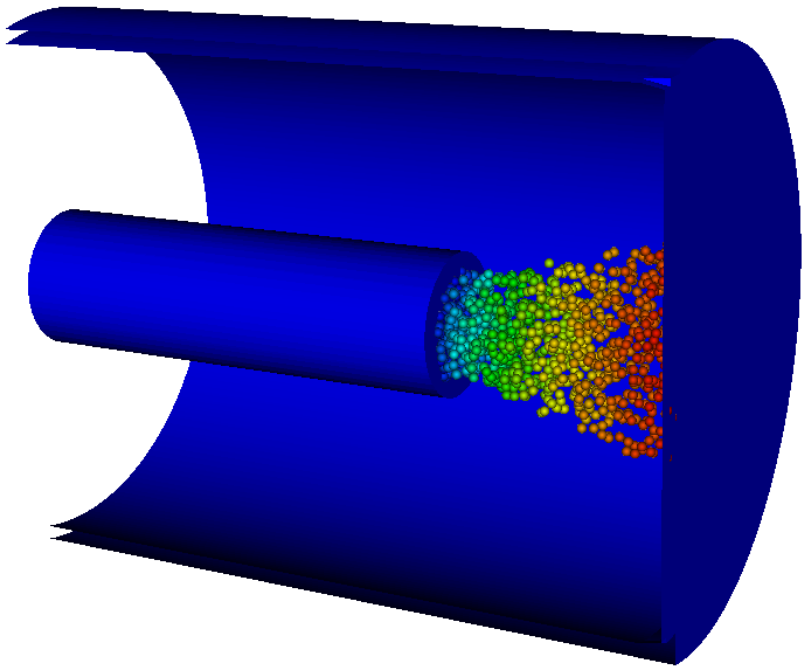


Fig. 4.11: The electrons are emitted from the tip of the inner cylinder after the pulse reaches it.

Opening the simulation

The coax example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Cavities and Waveguides* option.
- Select *Coaxial Cylinder* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.12. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

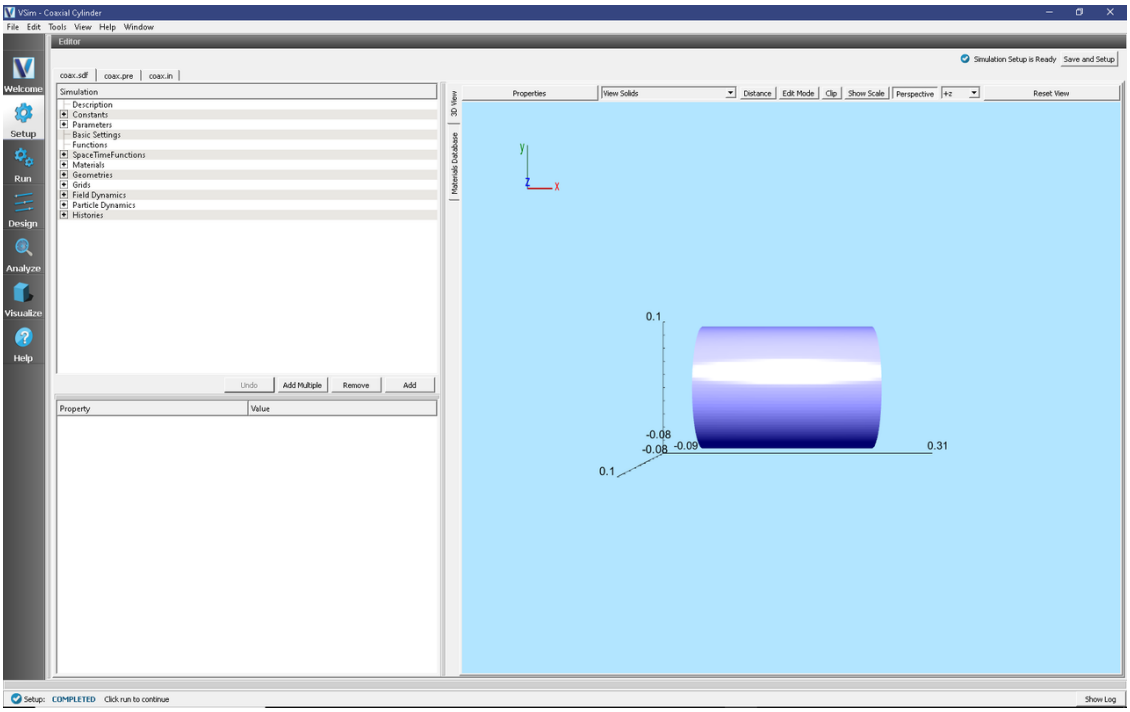


Fig. 4.12: Setup Window for the Coaxial Cylinder example.

Simulation properties

The coax example includes several Constants for easy adjustment of simulation properties. Those include:

- TFACTOR: A ramping factor of the applied field
- EFACTOR: The amplitude of the applied field
- EMITTED_CURRENT: The current emitted from the tip of the inner cylinder

There are also several SpaceTimeFunctions defined for easy application to wave launchers and particle emitters. Those include:

- edgeDy: The applied field in the y-direction
- edgeDz: The applied field in the z-direction
- nomask: This allows emission from the entire geometry of the flux emitter

Other Properties of the simulation include CSG defined geometries, a wave launcher on the lower x boundary, and a settable flux emitter on the tip of the inner cylinder.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.2900756453477 41e-12
  - *Number of Steps*: 1523
  - *Dump Periodicity*: 60
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.13.

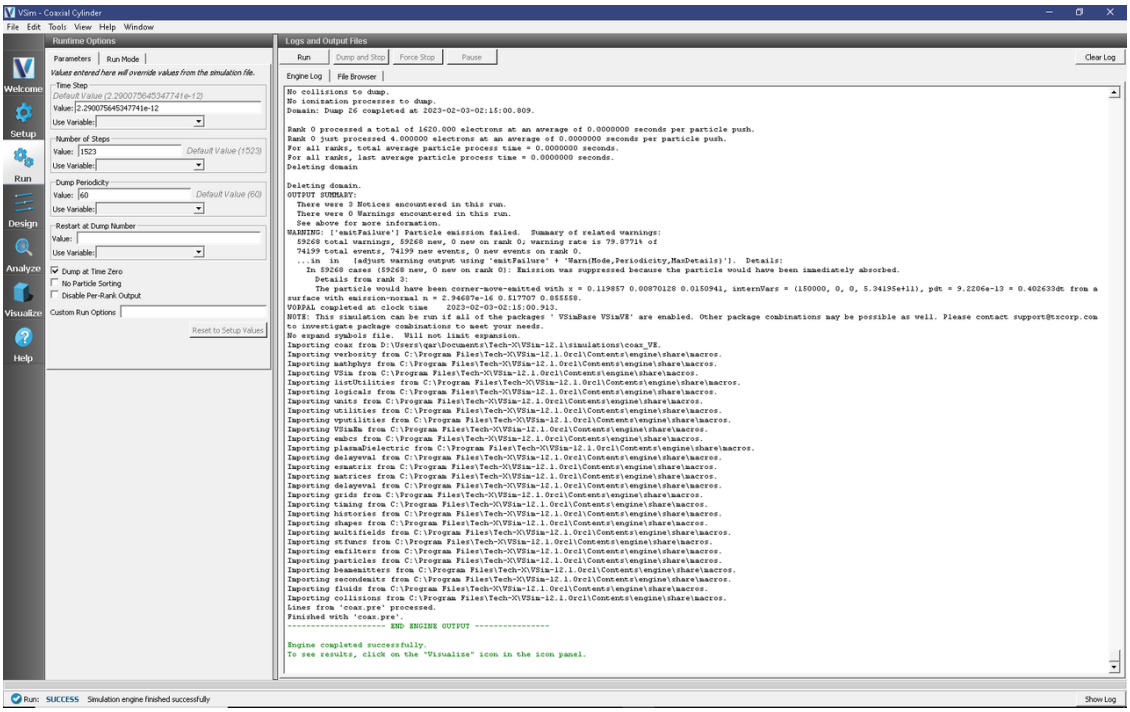


Fig. 4.13: The Run Window at the end of a successful execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by clicking the *Visualize* button in the left column.

To create the image seen in Fig. 4.14, proceed as follows:

- In the variables tree expand *Scalar Data*
- Expand *E*
- Select *E_y*

- Click the *Clip Plot* checkbox
- Click the *Display Contours* and set the # of contours to 10
- Expand *Geometries*
- Select *poly (coaxGeom)*
- Click the *Clip Plot* checkbox
- In the variables tree expand *Particle Data*
- Expand *electrons*
- Select *electrons_ux*
- Set the size to 6
- Now in the right pane move the dump slider forward in time
- The axis and legends can be hidden using the dropdown menu in the lower left corner of the window

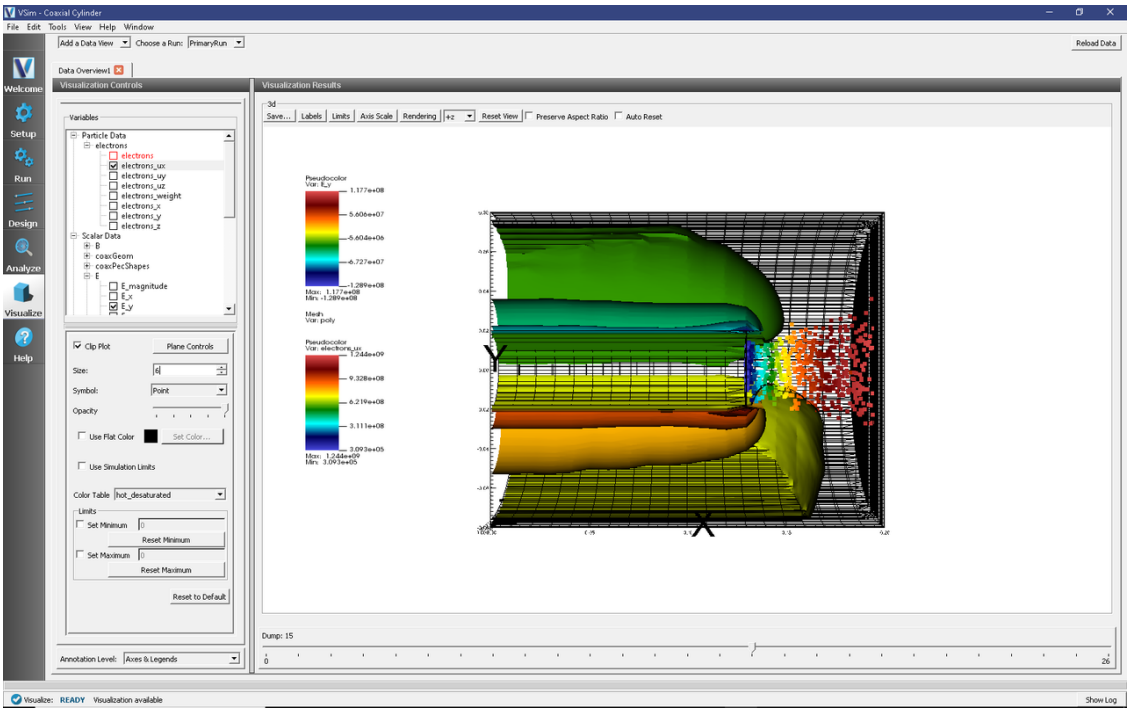


Fig. 4.14: Visualization of the coaxial cylinder as a color contour plot.

To obtain a clearer picture of what is happening at the cylinder tip, switch the Data View (in the left pane) to *History*. One dimensional plots of the number of electrons (called numMacroPtcls), the electric potential (phi), and the emitted and absorbed current should come up automatically.

You can set the location of Graph 2 to Window 1 as in Fig. 4.15.

The potential is measured between the interior of the inner cylinder and the capped end of the outer cylinder. The plot of the potential is noisy due to the emission of electrons from the tip. It may be insightful to run the simulation once without electrons so you can see the ringing on the waveform of phi. A similar signal is obtained by hooking up an oscilloscope to a coaxial cable. Electrons can be suppressed by setting the EMITTED_CURRENT parameter to 0 during setup.

The coaxial cylinder behaves like an RLC circuit: the cylinders provide a series resistance along their length, they are coupled capacitively, and generate self-inductance due to the current. By default, the rise-time of the pulse is near the

resonance of the circuit, resulting in an acceptable rise time, low overshoot, and quick damping. This makes it a good driver of the circuit.

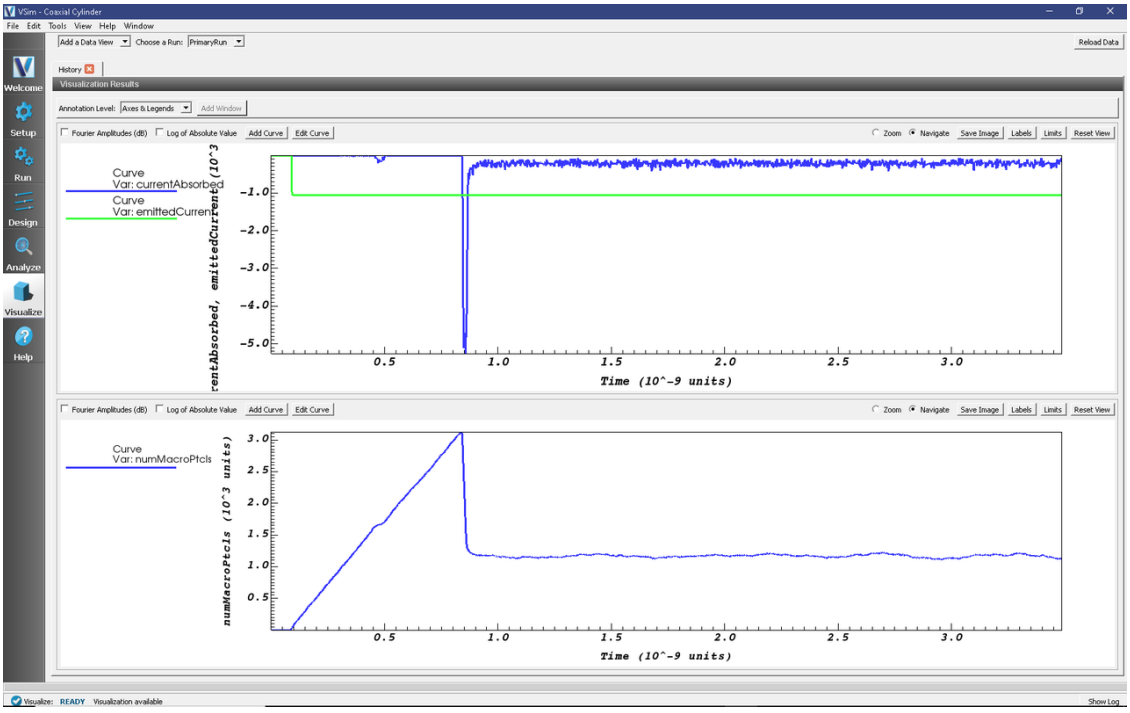


Fig. 4.15: The History visualization window with the electrons.

Further Experiments

Try experimenting with different dimensions of coax. In particular, note how the radii and pulse profile affect the potential response on the phi History plot.

4.1.3 Cylindrical Waveguide (cylindricalWaveguide.sdf)

Keywords:

`electromagnetics, waveguide, dispersion`

Problem Description

This VSimVE example illustrates how to find the modes of a cylindrical waveguide.

This simulation can be performed with a VSimVE license.

Simulation Properties

A section of cylindrical waveguide is simulated with the goal of extracting its propagating mode frequencies. The simulation is only two cells wide in X, but through the use of a phase-shifting periodic boundary condition, a much longer waveguide is simulated. The modes are extracted for longitudinal k-vectors, $\frac{2\pi n}{L_x}$. The maximum current is $I_0 = I(\tau/2)$. The waveguide is first excited with a transverse current that is off axis so as to excite modes of any symmetry. The temporal excitation is chosen to excite only a range of frequencies, from somewhat below the lowest cutoff up to the modes corresponding to $n = 1$. The Fourier transform of a history recording the electric field shows a clean output with a modest number of modes. Precise values for those frequencies can be obtained using the extractModes analyzer.

Opening the Simulation

The Cylindrical Waveguide example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Cavities and Waveguides* option.
- Select *Cylindrical Waveguide* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.16. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. (To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.) For the current view, the setup has been rotated to be able to see down the waveguide, and the view of the grid has been turned off. The box inside the waveguide is the location of the current source that will drive the waveguide.

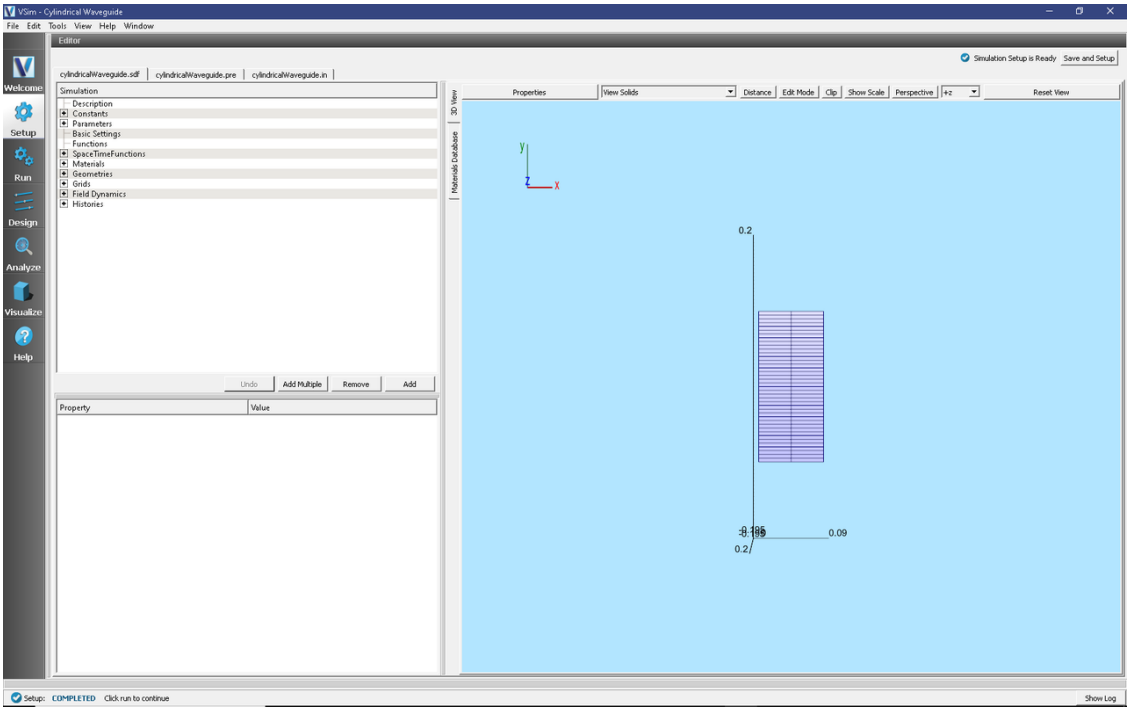


Fig. 4.16: Initial Setup Window for the Cylindrical Waveguide example.

The sinc hat function is used to excite this example. This function has a Fourier spectrum that is fairly flat for $f_l < f < f_h$ and falls off rapidly over a frequency width of δ_f, so that it is nearly zero for $f < f_l - \delta_f$ or $f < f_h + \delta_f$. δ_f is automatically calculated by the sinc hat function based on the suppression factor and frequency gap factor. This excitation gives a range of modes to be analyzed.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.168041416871939e-12
  - *Number of Steps*: 20000
  - *Dump Periodicity*: 2000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.17.

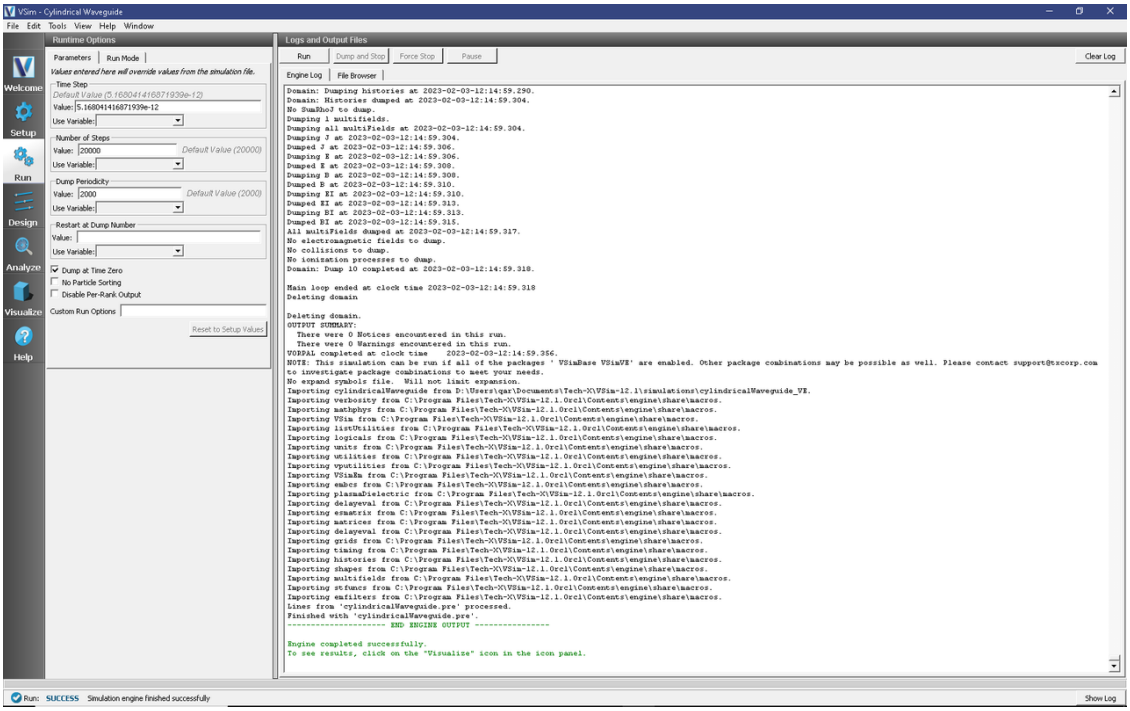


Fig. 4.17: Run Window for the Cylindrical Waveguide example after the initial run.

Visualizing the Spectrum

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize icon in the left panel.
- Select History under Data View. The first History tab will have eMid_0 and eMid_1 plotted. Open a second History tab in order to plot eMid_2 as well.
- Then for each plot select the Fourier Amplitude (dB) checkbox
- In the upper right corner of each plot, select Limits and set X-Axis max to 2e9.
- The result should be that shown in Fig. 4.18.

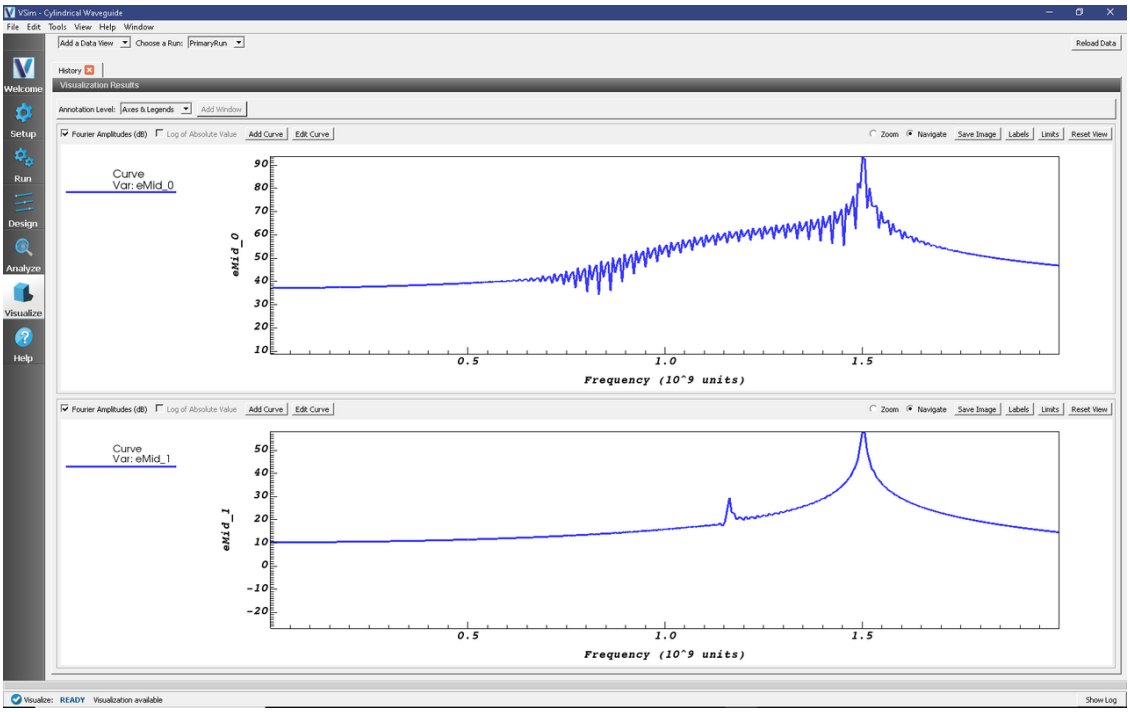


Fig. 4.18: Spectrum for the Cylindrical Waveguide example after the initial run.

One can see the TM mode in this spectrum. One can measure the mode frequency by projecting the spectrum down on the axis. With this simulation of 20,000 steps, for a total time of 103 ns, one expects the peak to have a width of roughly 1/103 ns or 0.01 GHz. This gives the error in the frequency from this method.

Computing More Accurate Modes

We can obtain more accurate frequencies using the Filter Diagonalization Method. To do this, we need to take a bit more data. We need to have the number of dumps equal to three times the number of modes, so we run again, restarting from dump 10 for another 300 steps, dumping every 50 time steps. This will give us an additional 6 dumps. The Run Window for this part of the simulation is shown in Fig. 4.19.

We now move to the Analyze Window, open extractModes, and set the field to be E. Then set the number of modes to be 2, and the begin and end dumps to be 10 and 16, respectively. Also set sampleType to 1. Upon hitting the `Analyze` button in the upper right, one sees the analysis output as shown in Fig. 4.20.

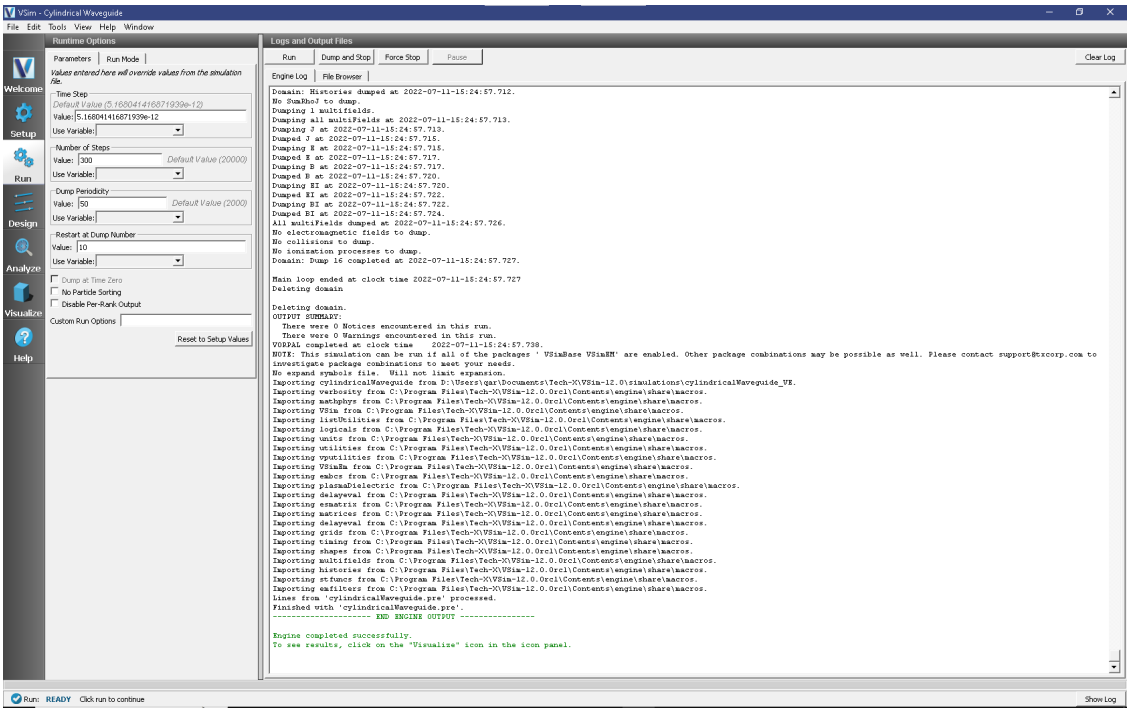


Fig. 4.19: Run Window for the Cylindrical Waveguide example for the second run.

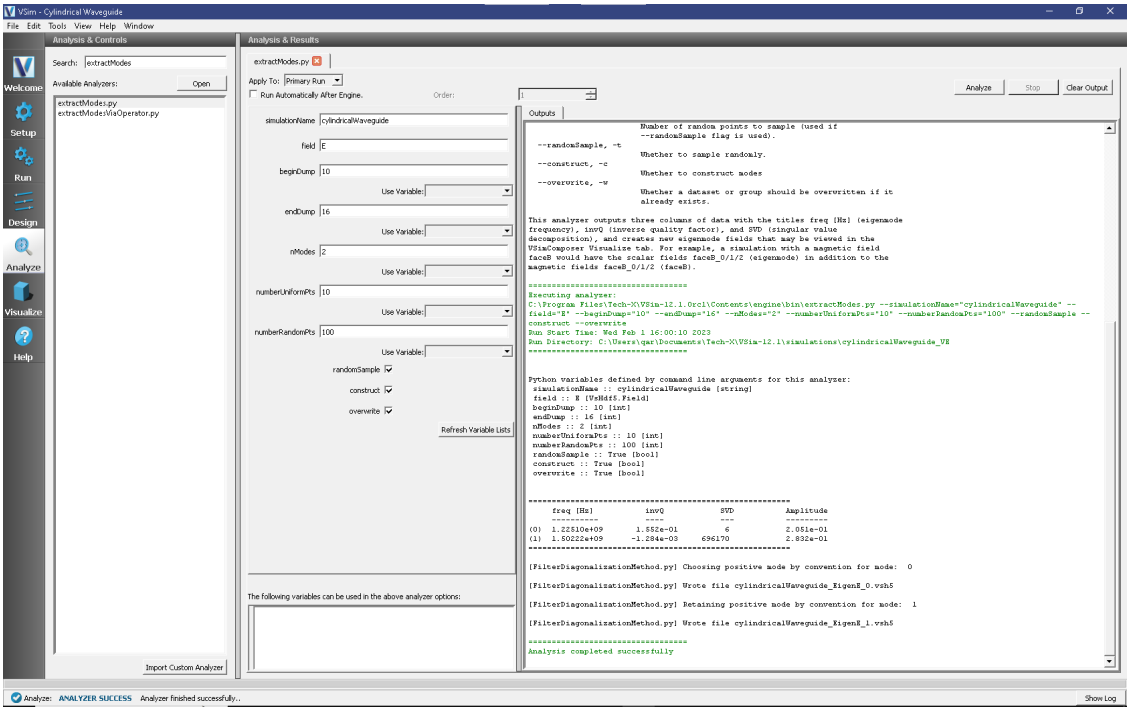


Fig. 4.20: Analysis window for the Cylindrical Waveguide example for mode extraction.

The computed mode frequencies are shown along with the inverse-Q values. Since this system is not lossy, the values of invQ, when significant, indicate that the mode calculations are dubious. However, we see that the 2nd mode has been well obtained.

These modes will now show up in the visualize panel, where one can reload the data, and modes will show up as seen in Fig. 4.21. The well obtained mode occupies dumps 1-16.

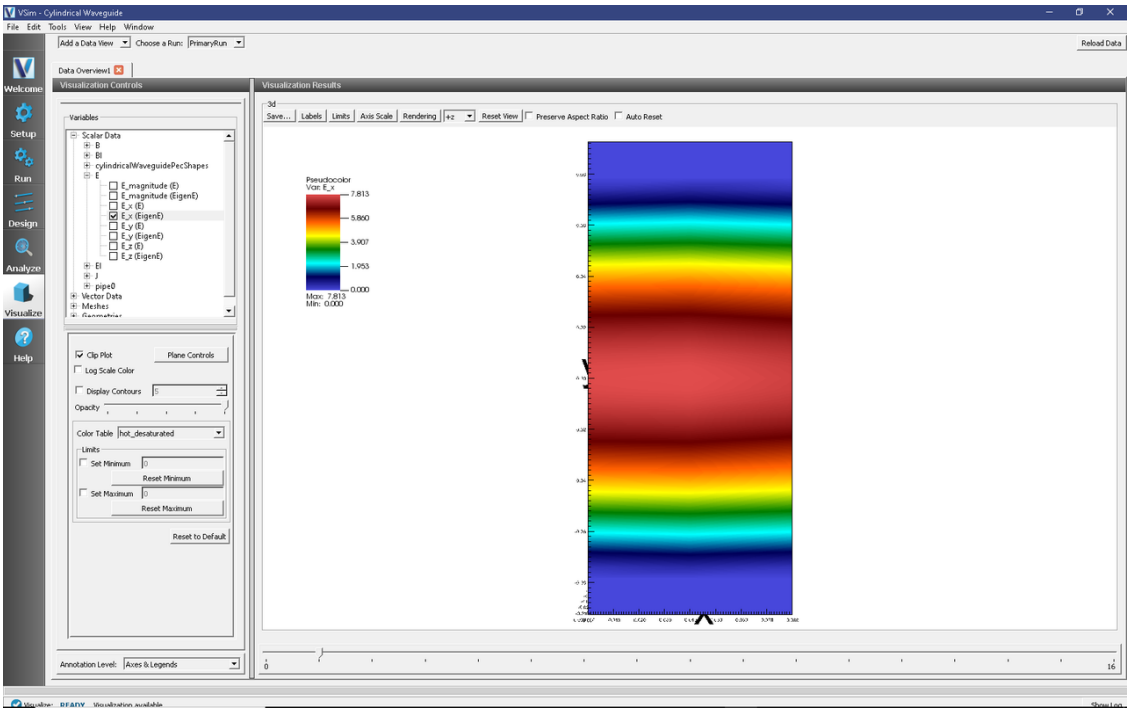


Fig. 4.21: Analysis window for the Cylindrical Waveguide example for mode extraction.

4.1.4 Pillbox Cavity (pillboxCavity.sdf)

Keywords:

`Pillbox cavity, Figures of merit, Transit time factor, Geometry factor`

Problem description

This VSimVE example demonstrates the usage of VSim in computing the eigenmodes and figures of merit of two simple cavities. One may select either the closed pillbox cavity for which the analytic solution is well known, or a cavity based on the closed pillbox, but having outlets leading to the periodic domain boundaries. Like other examples utilizing the extractModes.py analyzer, the simulation run is done in two steps. In the first step, the cavity is excited by a sinc pulse current source and output is dumped only at the end of this excitation run. Then in the second step, output is dumped at intervals which are sufficiently short compared to the frequencies of interest. The output from the second run is used by the extractModes.py analyzer to compute the eigenmodes. Then, the computeTransitTimeFactor.py and computeCavityG analyzers are used to compute the transit time factors and geometry factors of the eigenmodes.

This simulation can be performed with a VSimVE or VSimEM license.

Opening the Simulation

The pillbox cavity example is accessed from within VSimComposer by the following actions:

- Go to *File* → *New* → *From Example…*
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Cavities and Waveguides* option.
- Select "Pillbox Cavity" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The properties and values that create the simulation are accessible in the left pane when the Setup Window is selected. The right pane shows a 3D view of the selected geometry components, grids and current distributions.

The geometry of the closed pillbox cavity is called *pillboxCavityAnalytical* and the geometry of the periodic cavity with outlets on either end is called *pillboxCavityWithTube*. These can be visualized individually by expanding *Geometries*, de-selecting and then expanding *CSG*, and then selecting either *pillboxCavityAnalytical* or *pillboxCavityWithTube*.

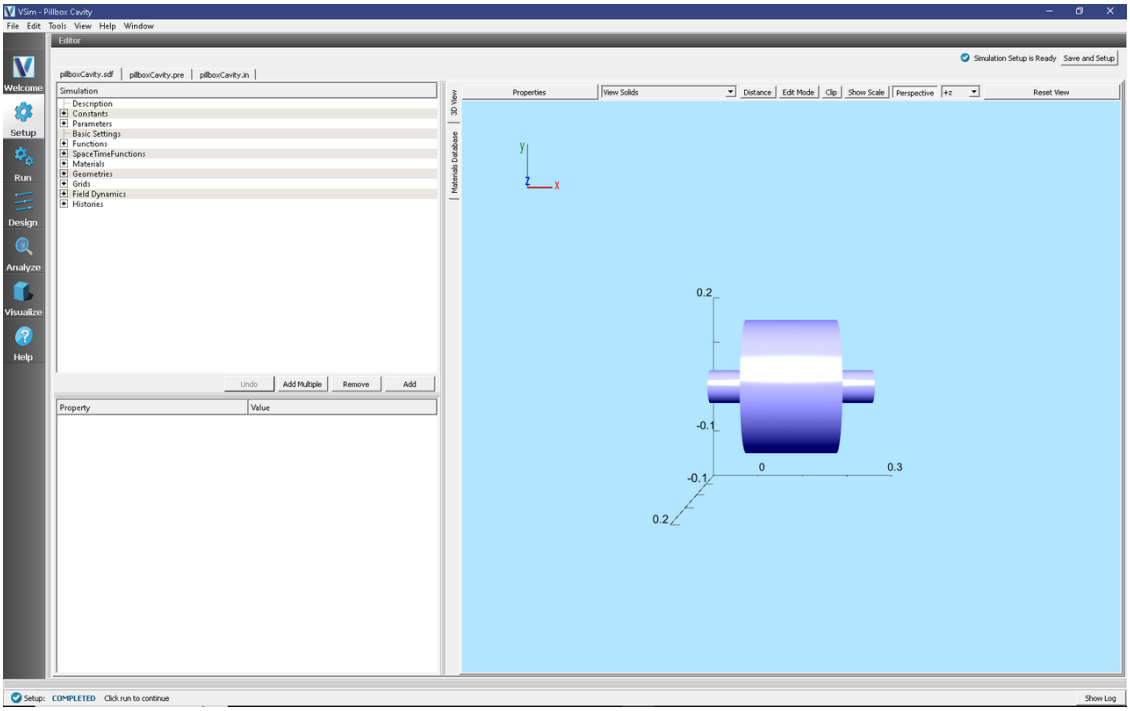


Fig. 4.22: Visualizing the periodic cavity geometry in the Setup Window.

Running the Simulation and Analyzing Results

Step 1: Cavity selection

- If you want to model the closed cavity, skip **Step 1** and go to **Step 2**. The closed cavity is set by default.
- To model the periodic cavity, go to the Setup Window.
- Go to *Geometries* → *CSG*.
- Click on *pillboxCavityAnalytical* under *CSG*.

- The bottom left pane will show properties of the selected geometry. At this time, the material should be set to *PEC* (perfect electric conductor). Double click on *PEC* and select the blank line.
- Now click on *pillboxCavityWithTube* under *CSG*.
- Select *PEC* as the material for *pillboxCavityWithTube*.

Step 2: Excitation

- Go to the Run Window by pressing the Run button in the left column of buttons.
- This simulation may be accelerated by running on multiple MPI ranks. The parallel options are in the *Run Mode* tab
- To run the file, click on the *Run* button in the upper left corner of the *Logs and Output Files* pane. You will see the output of the run in this pane. The simulation will run for 30000 time steps and dump output once at the end. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.23.

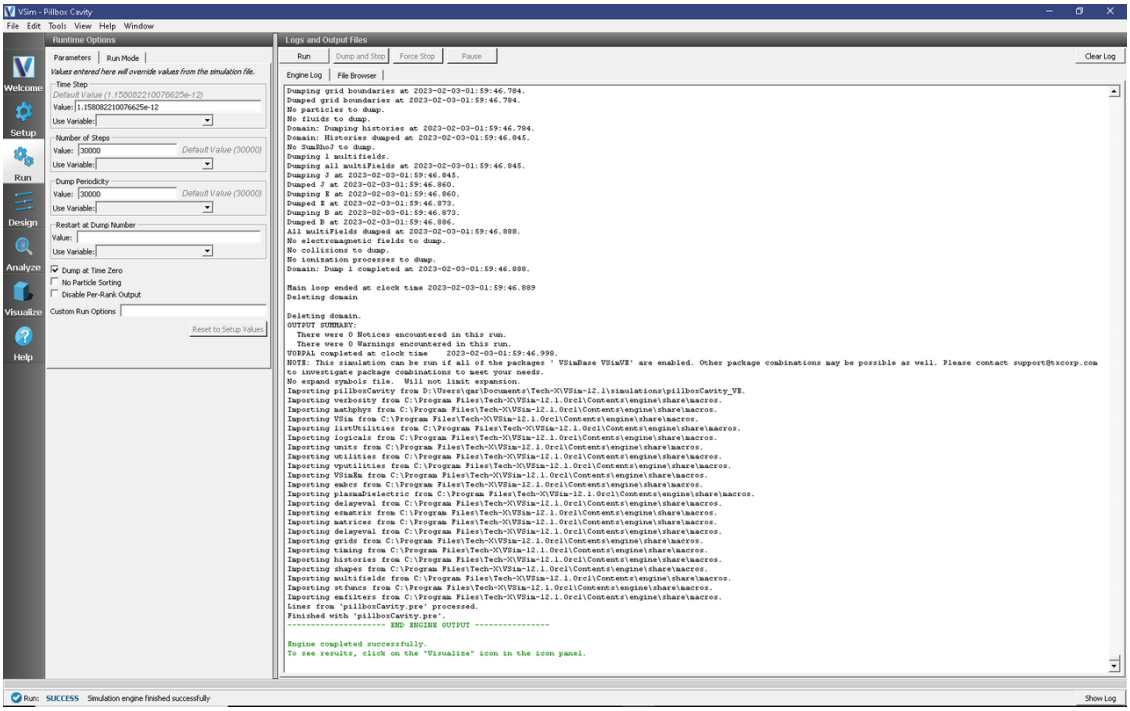


Fig. 4.23: The Run window at the end of a successful execution.

Step 3: Evolving the excited cavity

- After the first step is complete, change *Number of Steps* to 2000, change *Dump Periodicity* to 100.
- In the *Additional Run Options* Box, make sure that the *Dump at Time Zero* box is unchecked and that *Restart at Dump Number* is set to 1.
- Click run. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.24. When this run is finished, the last step should be step 32000.

Note: The simulation must be run in two steps because there must be no driving currents flowing in the simulation while dumping data used to extract the eigenmodes. So, while the drive is ringing the cavity, there is no need to dump data. We switch the dump periodicity after the driving current has shut off in order to resolve the frequency of the eignemodes of interest.

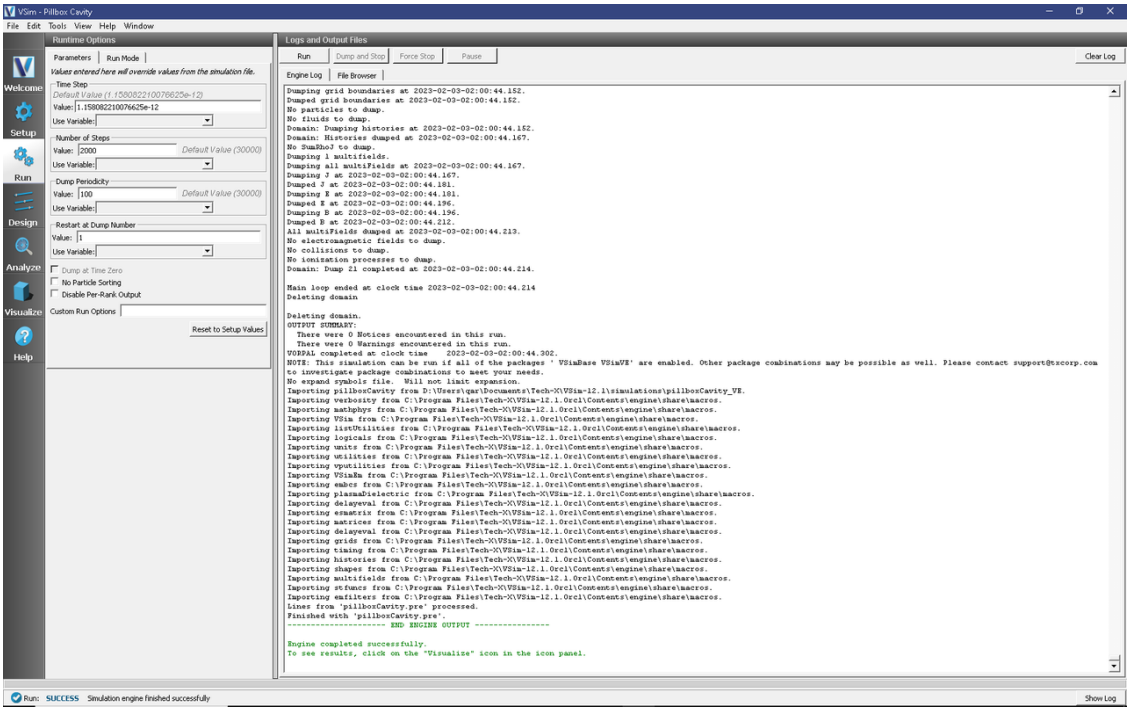


Fig. 4.24: The Run window at the end of a successful execution.

Step 4: Computing the eigenmodes

- Go to the analyzer window by selecting *Analyze* in the left column.
- Select *extractModes.py* from the list of available analyzers. Then click "Open" on the top right of the *Analysis Controls* pane.
- Compute the electric field eigenfunctions. After the analyzer loads, ensure the following parameters are entered:
  - **simulationName:** "pillboxCavity"
  - **field:** "E"
  - **beginDump:** "2"
  - **endDump:** "21"
  - **nModes:** "5"
  - **sampleType:** "0"
  - **numberUniformPoints:** "20"
  - **numberRandomPoints:** "100"
  - **construct:** "checked"

Also, check the "Overwrite Existing Files" box. Double-check your entries against what is shown in Fig. 4.25.

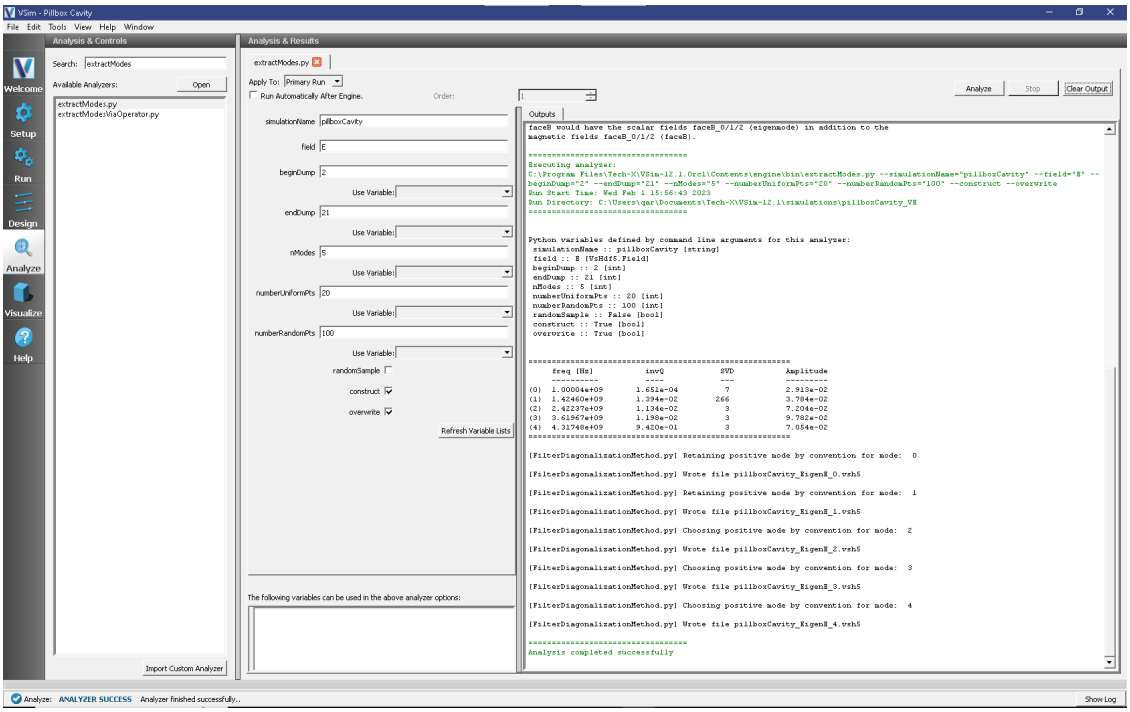


Fig. 4.25: Computing the electric field eigenfunctions and frequencies using the extractModes.py analyzer.

- Press the *Analyze* button which is located in the upper right corner.
- Compute the magnetic field eigenfunctions with the following parameters.
  - **simulationName:** "pillboxCavity"
  - **field:** "B"
  - **beginDump:** "2"
  - **endDump:** "21"
  - **nModes:** "5"
  - **sampleType:** "0"
  - **numberUniformPoints:** "20"
  - **numberRandomPoints:** "100"
  - **construct:** "1"

  After the analysis is finished, and scrolling down in the *Outputs* log pane you should see what is shown in Fig. 4.26.
- Note that *extractModes.py* outputs the frequencies of the computed modes in the *Run Output* pane. The first mode, mode 0, should have a frequency of approximately 1 GHz.

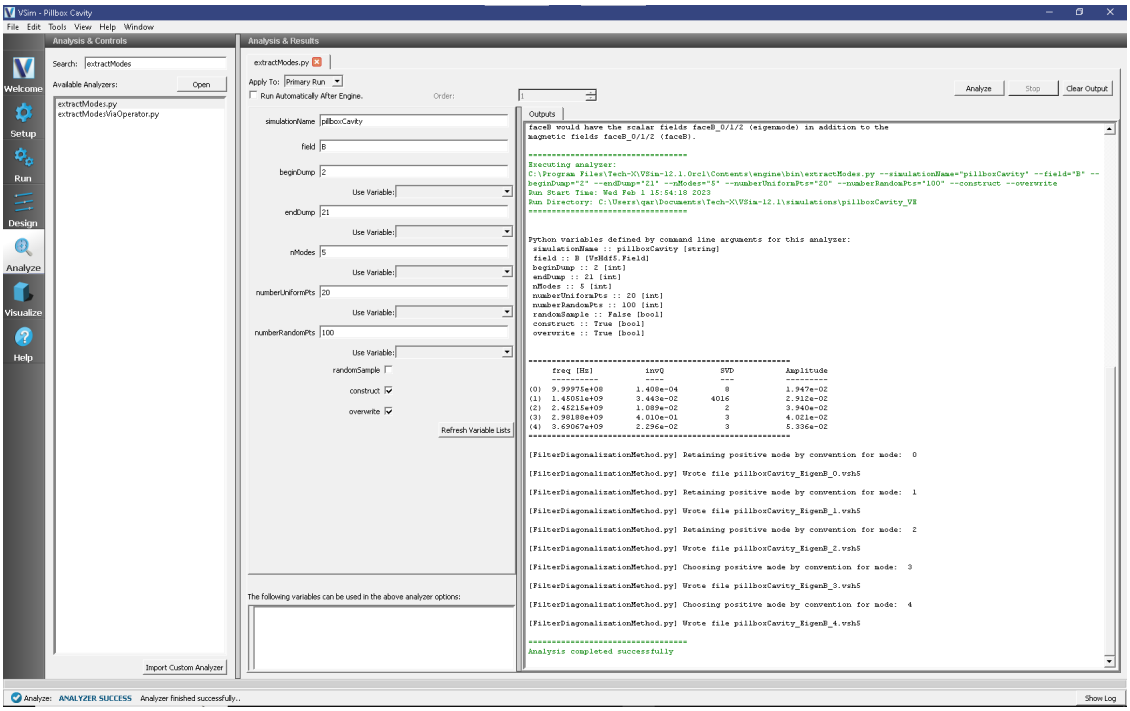


Fig. 4.26: The *Outputs* pane after Analyzing to determine the eigenmodes of the magnetic field.

Step 5: Computing the transit time factor

- Select *computeTransitTimeFactor.py* from the available analyzers and press "Open" on the top right of the *Analysis Controls* pane.
- After the analyzer loads, ensure the following parameters are entered:
  - **`simulationName:`** "pillboxCavity"
  - **`beginDump:`** "0"
  - **`endDump:`** "0"
  - **`beta:`** "1"
  - **`axis:`** "0"
  - **`offsetx0:`** "0"
  - **`offsetx1:`** "0"

  And compare against what is shown in Fig. 4.27
- Press *Analyze*.
- If you have selected the closed cavity, the transit time factor (the value following "Transit time factor, T=Vacc/V0 =") should be very close the analytic value of $2/\pi$.

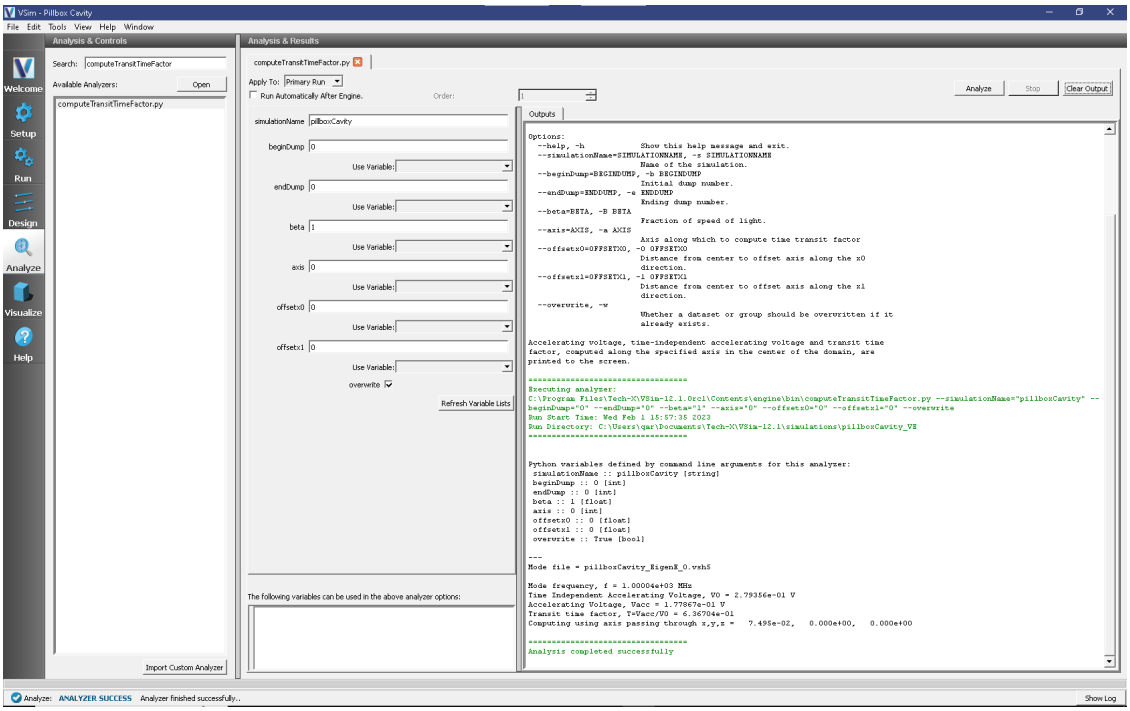


Fig. 4.27: Computing the transit time factor for the eigenmode of interest.

Step 6: Computing the geometry factor

- Select *computeCavityG.py* and click "Open".
- If you have selected the closed cavity, then enter "pillboxCavityAnalytical" for cavityGeometryName. Otherwise, enter "pillboxCavityWithTube" for cavityGeometryName.
- Select begin dump to 0 and end dump to 2.
- If you have selected the closed cavity, the geometry factor at the mode frequency of 999.97 MHz should be very close the analytic value of 257.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To see the projection of the magnetic field of the fundamental mode onto the cavity walls, do the following:

- Expand *Scalar Data*
- Expand *Bsurf*
- Check *Bsurf_magnitude*
- Click the *Plane Controls* button at the bottom of the *Visualization Controls* pane on the left of the Composer window.
- Select *X* as the "Clip Plane Normal" and ".05" as the "Origin of Normal Vector" for "X". Leave the "Origin of Normal Vector" for "Y" and "Z" as 0.
- Rotate the visualization by left clicking and dragging with your mouse.

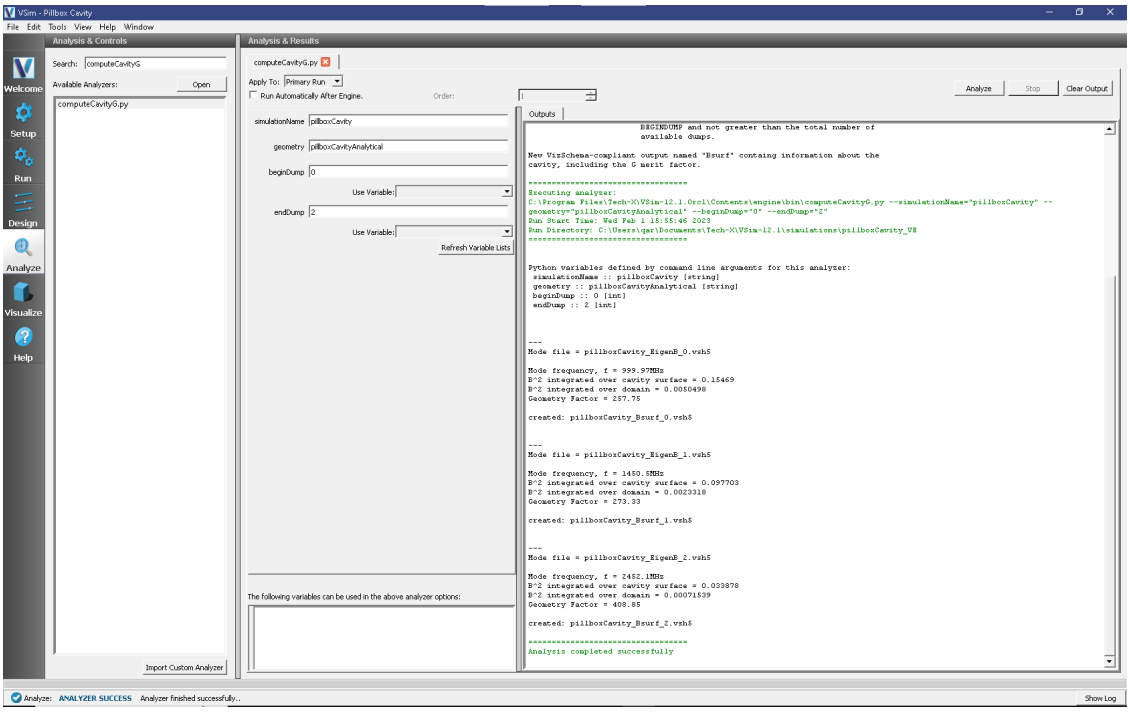


Fig. 4.28: Computing the geometry factor for the eigenmode of interest.

- You should see a visualization of the magnitude of the magnetic field of the fundamental mode projected onto the wall of the cavity as in Fig. 4.29

To see a more quantitative visualization of the eigenmode fields, as shown in Fig. 4.30, do the following:

- Add a *Field Analysis Data View*
- Select the *E_x (EigenE)* as a field
- Under the *Layout* drop-down menu, select *Side-by-side 2d/1d*

The Bessel function dependence of the x-component of the electric field will be clearly plotted on the right.

4.1.5 Rectangular Waveguide (rectangularWaveguide.sdf)

Keywords:

`Field Boundary Condition, rectangularWaveguide, Rectangular Waveguide`

Problem description

This example illustrates how to create a rectangular waveguide using the Rectangular Waveguide Field Boundary Condition and Constructive Solid Geometry.

Three waveguides are demonstrated in this example .

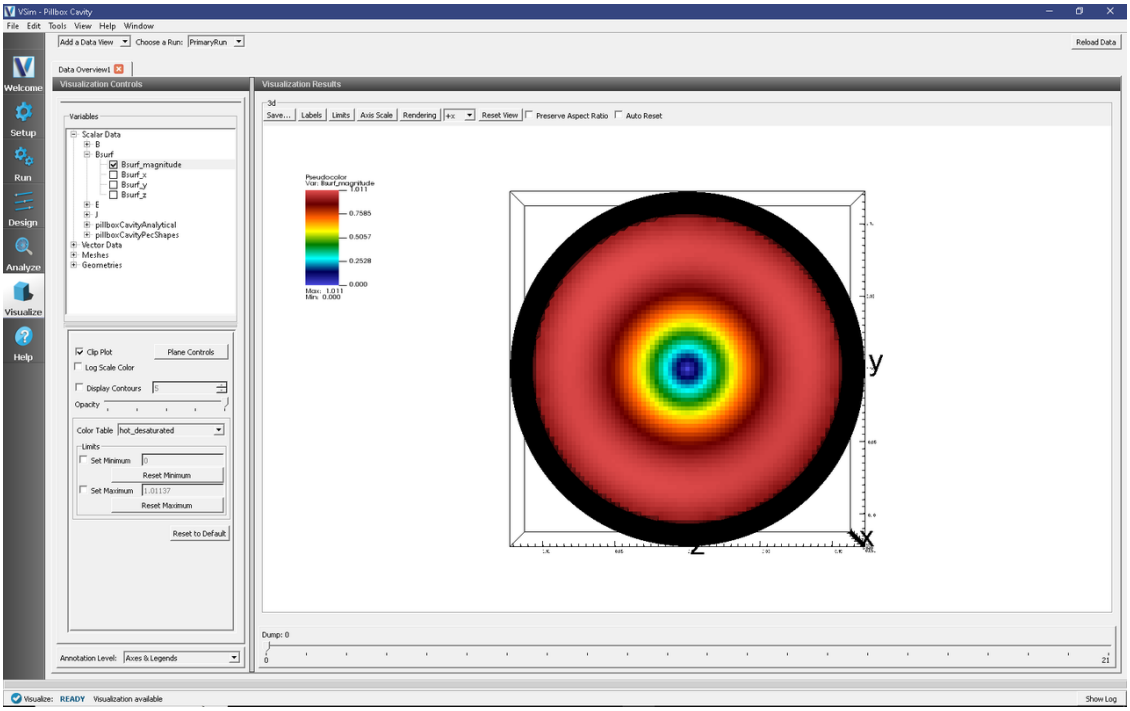


Fig. 4.29: The magnitude of the magnetic field on the wall of the cavity

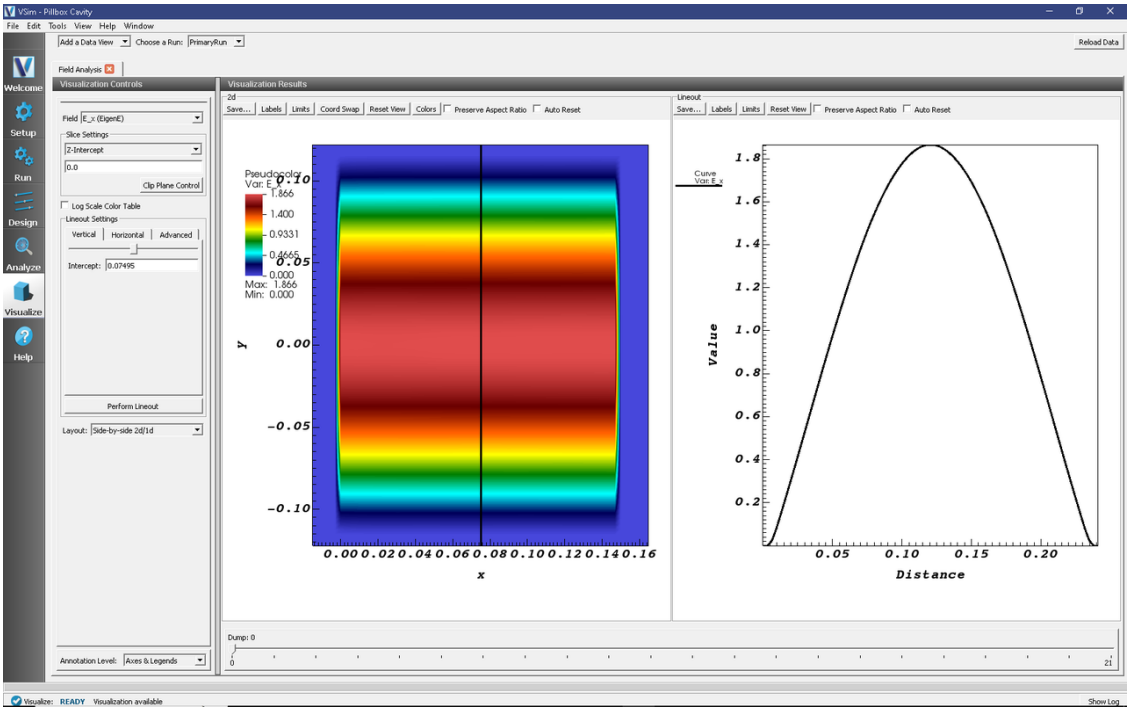


Fig. 4.30: Axial component of the electric field in the $z = 0$ plane (left) and plot of the axial electric field along $z = 0, x = 0.07495$ (right).

Opening the Simulation

The Rectangular Waveguide example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Eletronics* option.
- Expand the *Cavities and Waveguides* option.
- Select *Rectangular Waveguide* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The Setup Window is shown in Fig. 4.31.

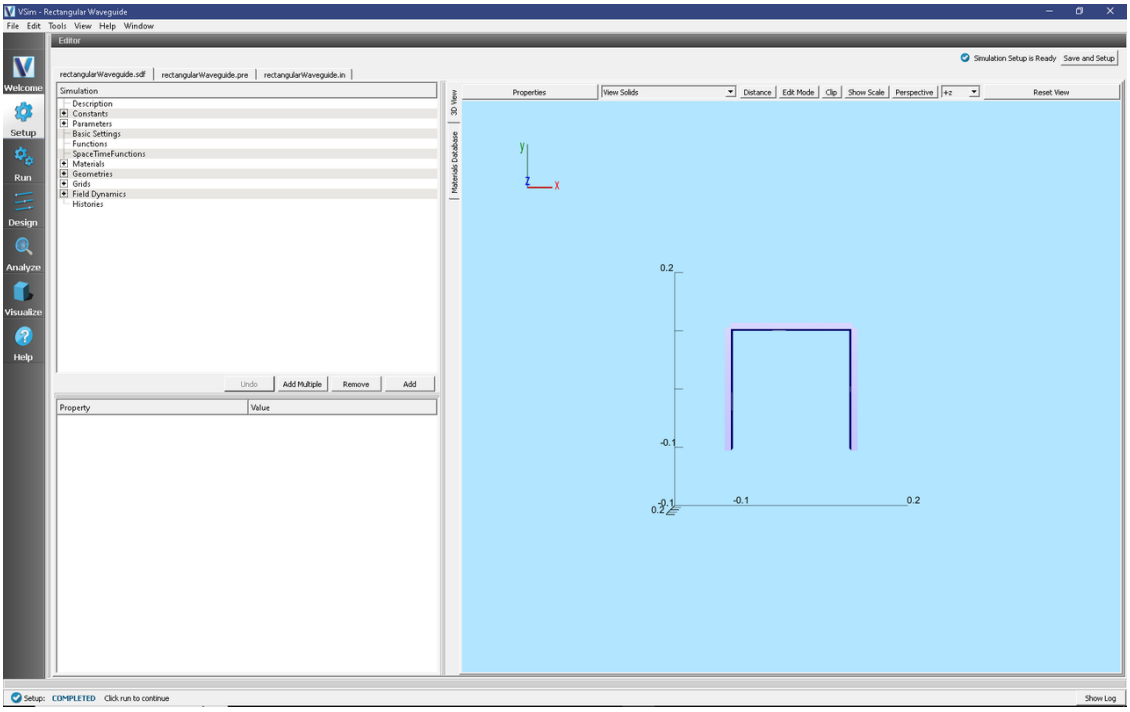


Fig. 4.31: Setup Window for the Rectangular Waveguide example.

Simulation Properties

This simulation demonstrates how to create a rectangular waveguide. There are three rectangular waveguides in this simulation. Each has been constructed by creating a physical waveguide on the simulation boundary, and defining the wave that is carried into the simulation. First a metal plate from a box primitive has been placed on the simulation boundary. It is important that this plate extends from at least one cell outside of the simulation boundary to at least one cell inside of the simulation. Next a box primitive corresponding to the size and orientation of the actual waveguide has been created. This is then subtracted from the previously created metal plate. It is important to note here that the polarization parameter will always be parallel to the width. The wave carried in this waveguide is then created by adding a FieldBoundaryCondtion of Rectangular Waveguide. The waveguide surface must be specified to match the intended simulation boundary and on the right location to match the physically constructed waveguide.

Several standard waveguide sizes are available, or User-Defined may be selected to specify a custom size. If no "Turn On Time" is specified, it will be set to a time of 2.5 periods of the carried signal, and a warning will be provided after running the simulation.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.8295415414691 47e-12
  - *Number of Steps*: 400
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.32.

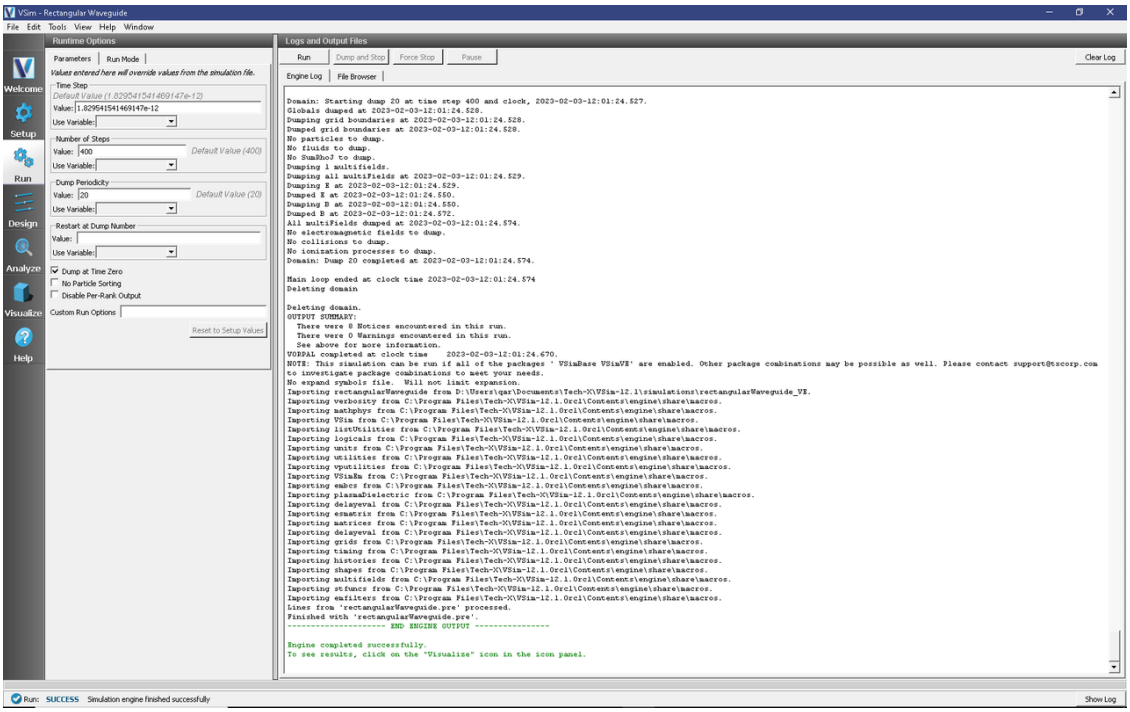


Fig. 4.32: The Run Window at the end of execution.

Visualizing the Results

After a successful run, go to the Visualize Window by pressing *Visualize* in the left column.

Expand *Scalar Data*, *E*, and select E_y. To slice inside the field, check the *Clip Plot* box. Now step through time using the Dump slider on the bottom of the right pane. This is shown below.

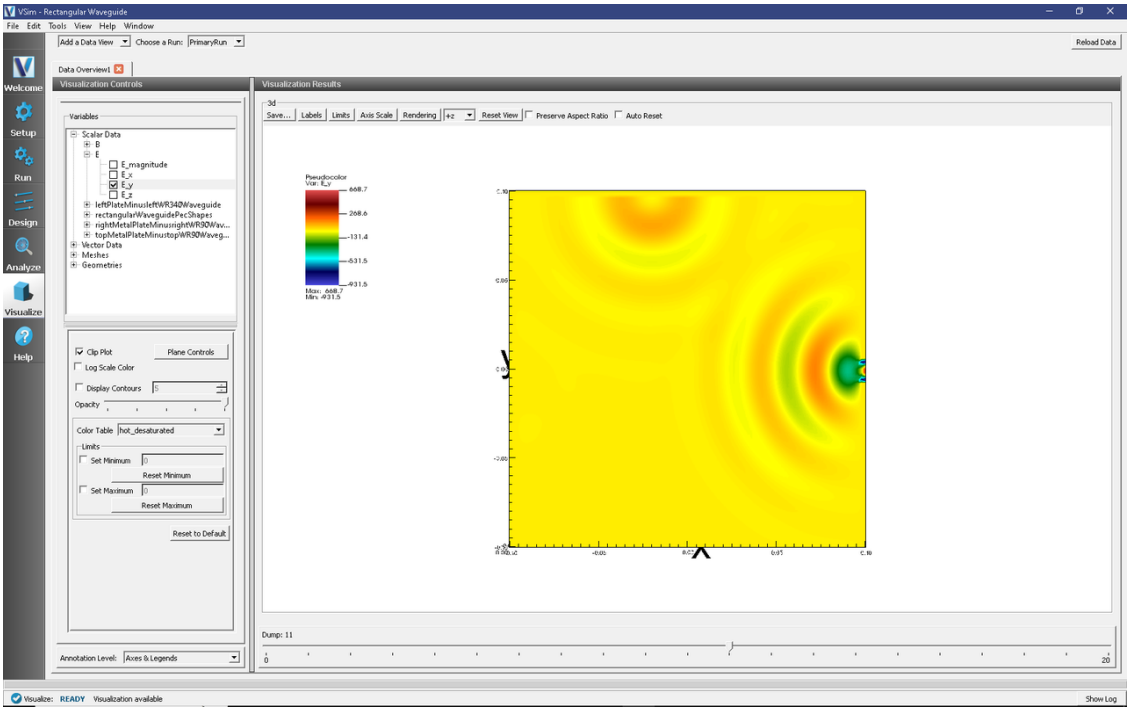


Fig. 4.33: The E_y field propagating out of the two waveguides centered on the z axis.
The effects of the third waveguide can be viewed by adjusting the "Origin of Normal Vector" parameter under the Plane Controls button.

Further Experiments

Waveguides can be added or subtracted to this simulation.

4.1.6 Rectangular Metal Waveguide Dispersion (rectMetalWaveguideDisp.sdf)

Keywords:

`Waveguide, Dispersion Relation, Fourier Transform, Phase Shifting Boundary Conditions`

Problem description

This VSimVE example demonstrates several unique capabilities of VSim that can be used to efficiently model waveguides. One unique capability is the use of phase shifting periodic boundary conditions. These work by adding a phase to a wave at a boundary to mimic a much longer physical dimension. We also demonstrate how to use an analyzer called extractModesViaOperator.py to accurately compute the excited modes in the waveguide, even if some of the modes are much weaker than the dominant mode. In this example, we use extractModesViaOperator.py to compute the dispersion relation (ω vs k) and compare the numerically determined dispersion relation with the theoretical dispersion relation using standard waveguide theory.

This example involves five steps. In the first step, the waveguide is "pinged" with a short pulse in the current density that excites a range of modes. The Fourier transform then shows the range of frequencies of the modes. In the second step, the waveguide is excited using a sinc pulse function multiplied by a Gaussian envelope to excite a flat band of frequencies with sharp cutoffs at either end. The excitation current density is in the transverse directions (z and y) which excites an electric field primarily in the transverse direction. In the third step, the data is restarted from the end of the second run and saved at shorter time intervals in order to resolve the frequencies of interest. The output from the

third step is used by the extractModesViaOperator.py analyzer to compute the eigenmodes in step 4. Finally, in step 5, the dispersion relation is computed by varying the wavelength which is resolved in the simulation.

Opening the Simulation

The rectMetalWaveguideDisp example is accessed from within VSimComposer by the following actions:

- Go to *File* → *New* → *From Example…*
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Cavities and Waveguides* option.
- Select "Rectangular Metal Waveguide Dispersion" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The properties and values that create the simulation are accessible in the left pane when the Setup Window is selected as shown in Fig. 4.34. The right pane shows a 3D view of the selected geometry components, grids and current distributions.

The geometry can be visualized by expanding "Geometries" in the left pane. The hollow rectangular waveguide can be seen more clearly by de-selecting the "Grid" option. The length in the direction of propagation (x) is a small fraction of either transverse direction. This is possible because we are using "phase shifting periodic" boundary conditions in the *x* -direction. The phase shifting BCs are selected under "Basic Settings".

The simulation is excited with a *sinc hat* function, which has a formula of

$$(t, f_l, f_h, \delta_f, t_{off}) = H(t_{off} - t)\exp(-0.5\delta_f^2(t - 0.5t_{off})^2)\times \frac{\sin(2\pi f_h(t - 0.5t_{off})) - \sin(2\pi f_l(t - 0.5t_{off}))}{(2\pi f_h - 2\pi f_l)(t - 0.5t_{off})}$$

δ_f is calculated according to. frequencyGap = (frequency high - frequency low)*frequency gap factor

numSigma = sqrt(-2.0*log(suppression factor))

sigmaT = (TWOPI*frequencyGap)/numSigma

As mentioned in the introduction, this function has a Fourier spectrum that is fairly flat over the desired range, $f_l < f < f_h$, of frequencies and falls off rapidly over a frequency width of δ_f, so that it is nearly zero for $f < f_l - \delta_f$ or $f > f_h + \delta_f$.

Phase Shifting Boundary Conditions and Phase Shift

Before discussing phase-shifting periodic boundary conditions, we first review ordinary periodic BCs. In this discussion, periodic BC's are applied in the *x*-direction. With normal periodic BC's, there are two criteria in resolving a wave (or mode) of interest. (1) There must be enough grid points along the wavelength to resolve the spatial profile. Typically we sample at least 20 cells along a wavelength (λ_x), or $DX = \lambda_x/20$, and (2) The length of the simulation domain, represented by L_x, must be one wavelength long, $L_x = \lambda_x$. Periodic BC's in the x-direction means that $F(0) = F(L_x)$, where F is any field quantity. Now introduce a grid that extends from 0,1,…,nx and let $x = 0$ at grid point 0 and $x = L_x$ at grid point *nx*. Periodicity on the grid implies $F(0) = F(nx)$. Finally, let's assume that $F(x) \sim \sin(k_x x)$. Then, applying the condition for periodicity, $\sin(0) = \sin(k_x L_x)$, which is exactly met if $L_x = \lambda_x$.

With phase-shifting periodic BC's, we are no longer required to meet the second criteria discussed in the preceding paragraph. To see this, assume $L_x < \lambda_x$. Then the periodicity condition can still be met by setting $k_x L_x - \phi_0 = 0$, where ϕ_0 is the phase shift equal to $k_x L_x$, which is the exact phase shift we have chosen to apply in VSim for this example. The numerical implementation is more challenging than the conceptual picture we just discussed. To implement phase-shifting periodic BC's, we need to treat the fields as complex numbers and set $F(L_x) = \exp(i\phi_0)F(0)$. For the grid, we pick 2 cells such that $L_x = 2DX$.

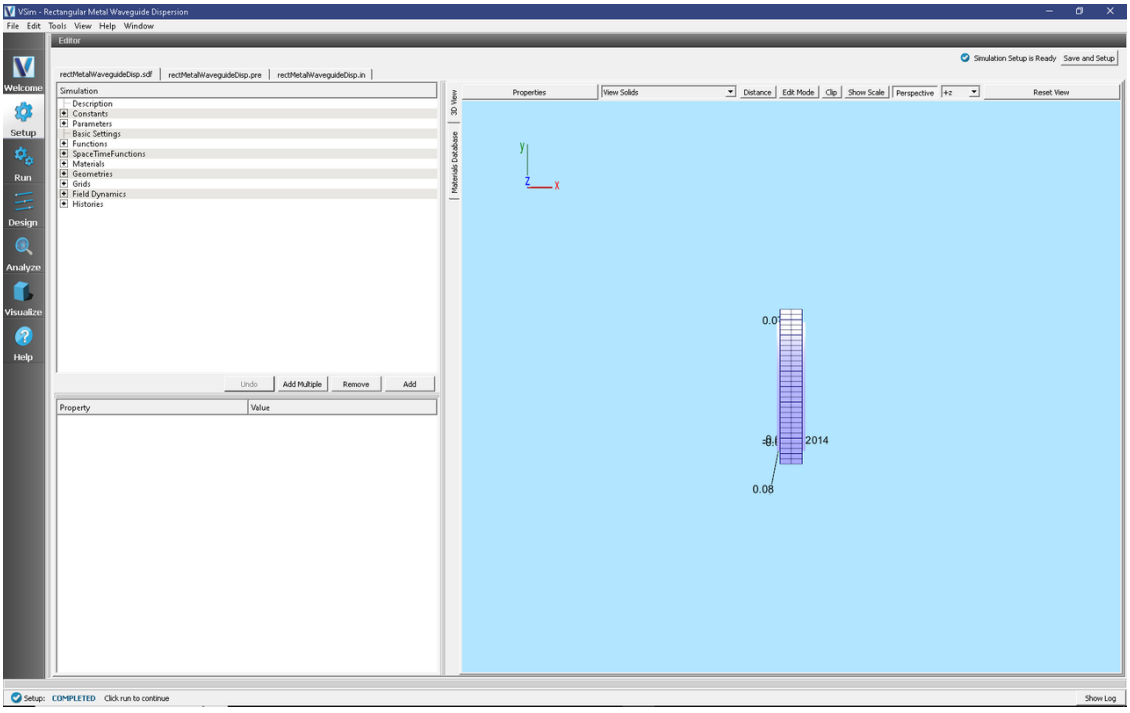


Fig. 4.34: Initial Setup Window for the Waveguide Dispersion example. The block in the middle is the region in which the current density is driven.

By using phase-shifting periodic BC's, we can simulate different physical lengths without changing the simulation length L_x through the phase shift $\phi_0 = k_x L_x$. Because $k_x = 2\pi/L_x$, we can solve for $\omega(k_x)$ without requiring a simulation of length L_x.

Running the Simulation and Analyzing Results

We now walk through the five steps discussed in the Introduction. In the first step, we test to determine the minimum frequency that will propagate through the waveguide. For the rectangular waveguide in this example, we know the analytical result which is the lowest cutoff frequency. However, we still do this step to demonstrate how to determine the lowest frequency that will propagate for cases that are not analytic. In the second step, the current density "rings up" to a maximum value, then rings down to 0. Because we are exciting modes at resonant frequencies of the cavity, the *E*- and *B*-fields continue to oscillate after the excitation is turned off. We wish to determine the resonant modes using Eigen mode analysis using data saved in Step 3 when the externally driven source is turned off and the cavity is "ringing" at its natural frequencies. In step 4, extractModesViaOperator.py is used to compute the excitation frequencies in the cavity at a given mode. Finally, in step 5, you will change the value of "mode", which is defined under "Constants" to compute the dominant frequencies which are excited in the cavity at a given wavelength. We assume the maximum wavelength which can be resolved in a traditional periodic simulation is 0.2 m and denote this as *lambdaMax*. We then define the parameter $k_x = \frac{mode}{12}\frac{2\pi}{lambdaMax}$ and run 25 simulations with *mode* =0,1,2,...,24. Finally, we set the phase shift to $k_x \times L_x$ to ensure the correct phase shift is applied for the phase shifting periodic BC's. In this way, we are able to compare the simulation with waveguide theory without explicitly changing the length of the simulation domain in the x -direction.

Step 1: Determining the lowest propagation frequency - The "Ping" Run

The Ping run is used to determine the lowest propagation frequency in the waveguide. In this simulation, we can analytically compute the lowest propagation frequency at a given k based on the allowable modes in a square wave guide. We can then compare the computed lowest propagation frequency with theory. However, for arbitrarily-shaped waveguides, this step is necessary since no theory is available to compute the lowest propagation frequency. We have defined a PINGON constant (with values of 0 or 1) in order to easily transition from the "Ping" run to the "Excitation" run in Step 2. The default is PINGON=1 to do the "Ping" run first. For Step 1, perform the following steps

- Click on the Run Window.
- This simulation may be accelerated by changing the Run Mode to Parallel.
- Click the *Run* button on the upper left corner of the *Logs and Output Files* pane

The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.35.

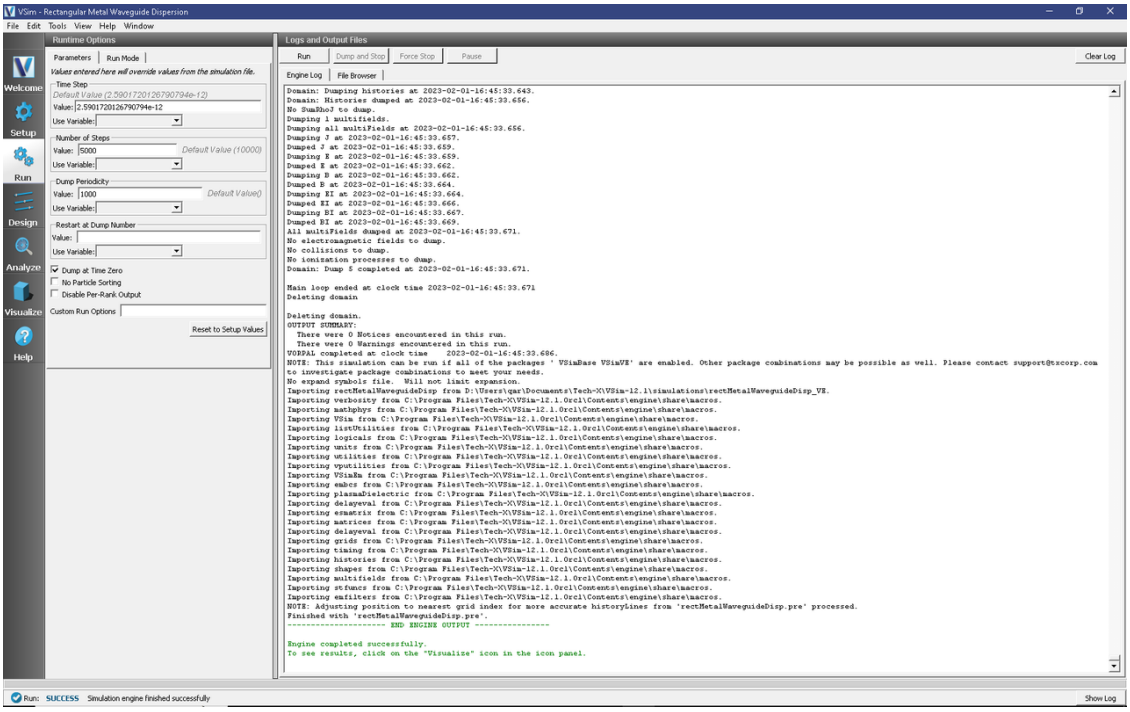


Fig. 4.35: The Run window at the end of a Step 1.

After the run has completed, click on the *Visualize* tab on the left side of the visualization window. After the data has loaded, click on *Add a Data View* and then select *History*. Perform the following steps to analyze the history:

- Graph 1 select *jMid_1*
- Graph 2 select *eMid_1*

In Graph 1, to see the data, click on the "Zoom" option above the plot. Left click with your mouse on the upper left corner of the graph and drag the "zoom" box to about 0.2×10^{-9} s (hold the left mouse button when you drag). You should see a step function in the current density beginning at t=0 and ending abruptly after about 20 time steps. This is the "ping" that we impose on the simulation. To determine the lowest frequency mode that we excite, click the "Fourier Amplitudes (dB)" box in Graph 2. Again, zoom in on the left most portion of the plot. You will see that the first peak occurs at a frequency of about 1.5×10^{9} Hz, which is the lowest cutoff frequency in the simulation and is what we find analytically using waveguide theory. Therefore, we have confirmed that VSim reproduces linear theory. You can

confidently use VSim to numerically determine the lowest cutoff frequency for non-analytically solvable shapes. The visualization window after the above steps have been performed is shown in Fig. 4.36

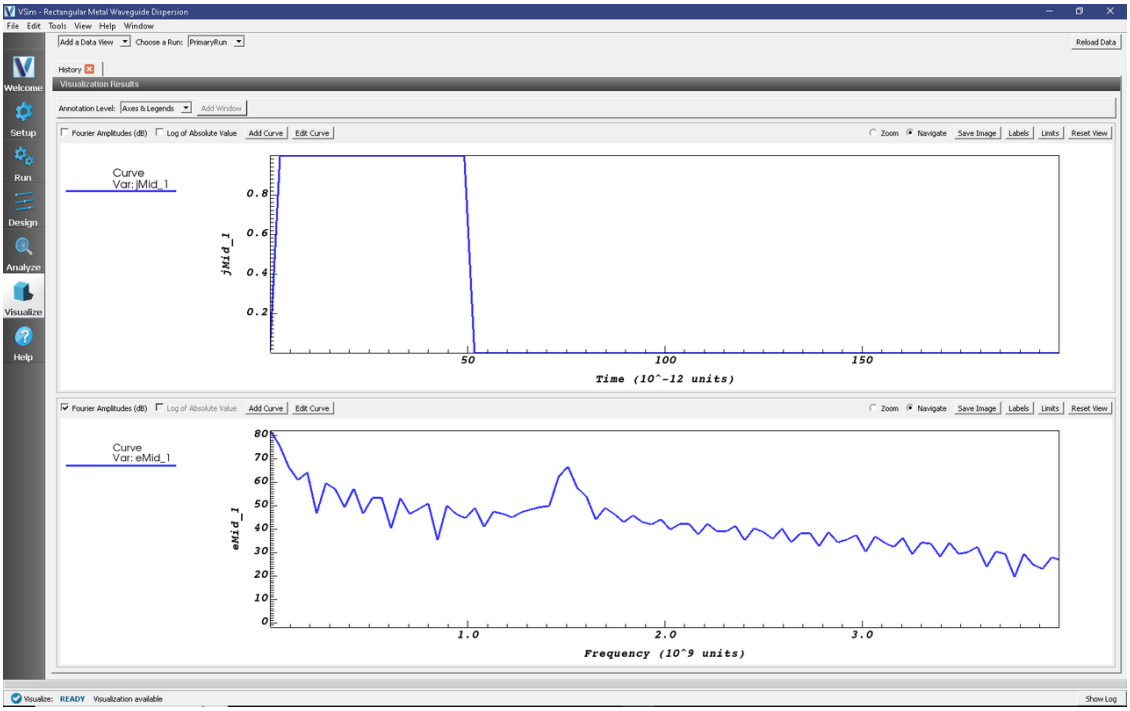


Fig. 4.36: History plots showing the lowest cutoff frequency at 1.5×10^9 Hz as the result of pinging the waveguide with an abruptly applied current density.

Step 2: Excitation

From Step 1, we know that the lowest propagation frequency is $\sim 1.5 \times 10^9$ Hz. We can now check that the lowest cutoff frequency (*frequency low* in *SincHat*) is correct. The parameter *FREQ_MIN* is passed in to *frequency low* and is indeed $\sim 1.5 \times 10^9$ Hz. We can now proceed to excite the waveguide with confidence knowing that lowest excitation frequency is correct. To excite the waveguide, perform the following steps:

- Go to the Setup Window and expand the *Constants* option
- Set *PINGON* to 0
- Click on *Save and Setup* in the upper right corner of the visualization window
- Go to the Run Window by pressing the Run button in the left column of buttons.
- Set Number of Steps to 21000. This ensures that the simulation runs long enough for the current density to "ring up" then "ring down" to 0.
- Leave the "Dump Periodity" at 1000.
- This simulation may be accelerated by running on multiple MPI ranks. The parallel options are in the *Run Mode* tab
- To run the file, click on the *Run* button in the upper left corner of the *Logs and Output Files* pane. You will see the output of the run in this pane. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.37.

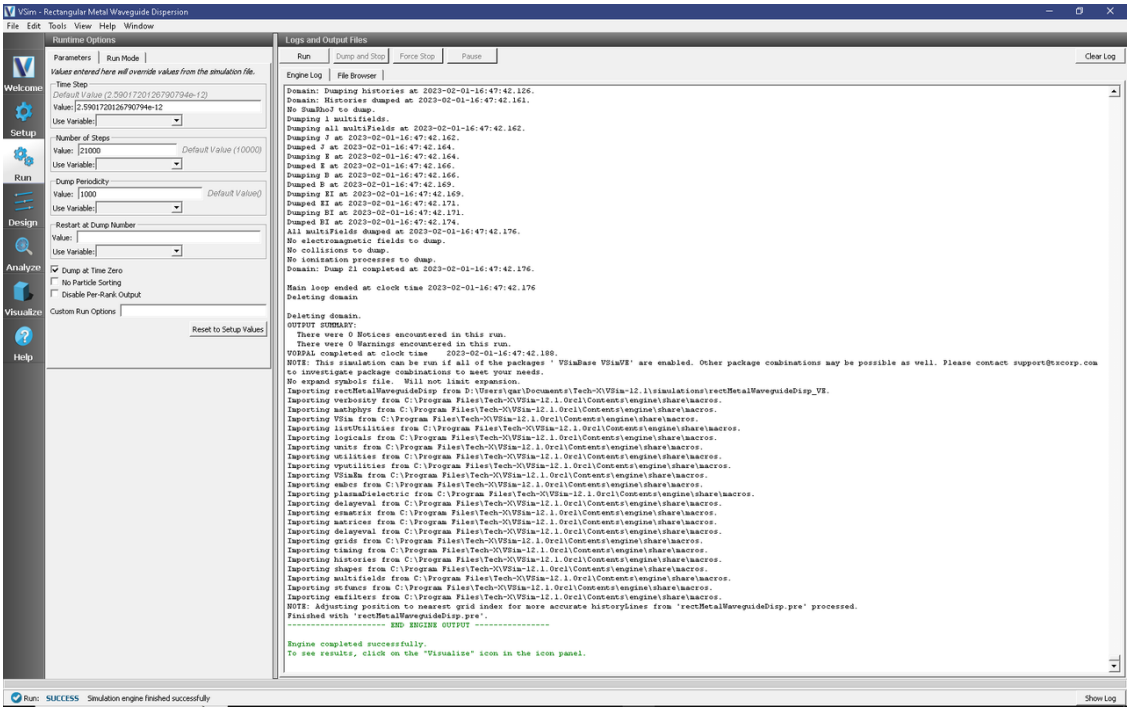


Fig. 4.37: The Run window at the end of a Step 2.

Step 3: Evolving the excited cavity

The purpose of Step 3 is to continue the simulation with only the *E*- and *B*- fields excited due to the externally imposed current density from Step 2. We will also save more data which we can analyze using Eigenmode analysis for Step 4.

- Go to the Setup Window and expand the *Basic Settings* option.
- Change "number of steps" to "10000".
- Change "steps between dumps" to "100".
- Change "dump in groups of" to "3".
- Click on *Save and Setup* in the upper right corner of the visualization window.
- Go to the Run Window and click the "Reset to Setup Values" button in the lower right corner of the "Run Options" section.
- In the *Run Options* section, uncheck the *Dump at Time Zero* box and set the *Restart at Dump Number* to 21.
- NOTE: the "Dump Periodicity" must be blank for the "dump in groups of 3" setting to work. In this case, the simulation will revert to the values defined in "Basic Settings" which are to dump every 100 time steps in groups of 3 (21000,21001,21002, …, 21100,21101,21102,…, etc). If you fill in an integer into Dump Periodicity, the default gets overwritten and the data are not dumped in groups of 3, which is required for the extractModesVia-Operator.py analyzer. So, there should be 300 new dumps making a total of 321 dumps.
- Click run. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run completion is shown in Fig. 4.38. When this run is finished, the last step should be step 31000.

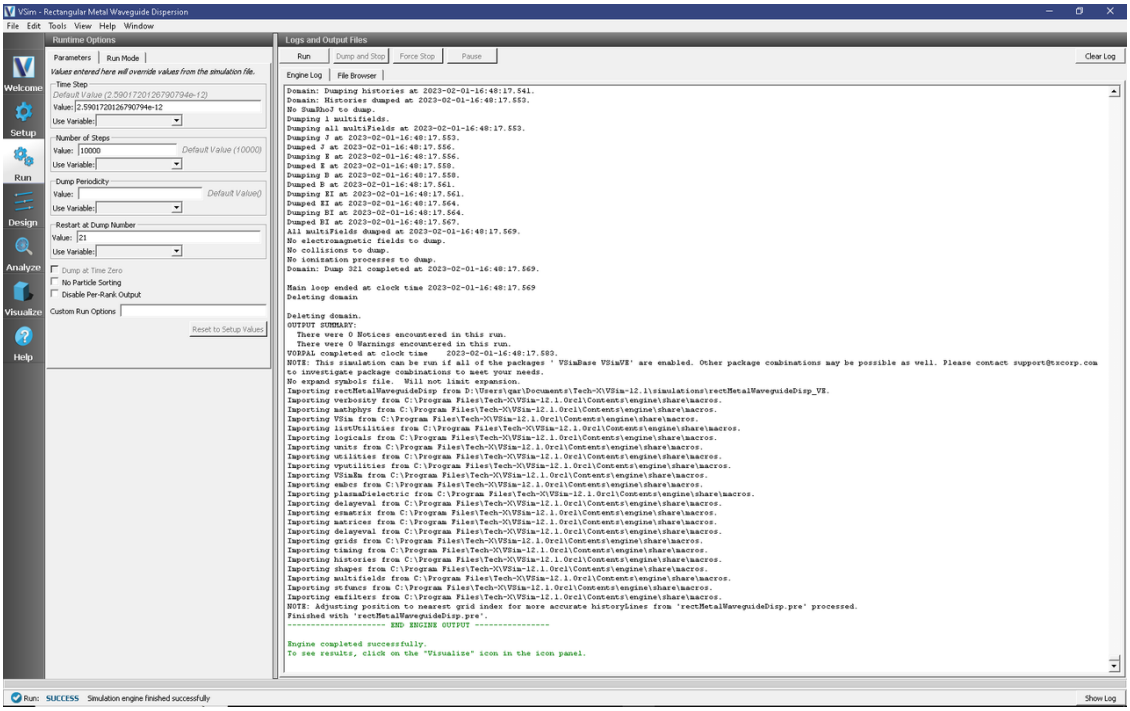


Fig. 4.38: The Run window at the end of Step 3.

Step 4: Computing the eigenmodes

- Go to the analyzer window by selecting *Analyze* in the left column.
- Select *extractModesViaOperator.py* from the list of available analyzers. Then click "Open" on the top right of the *Analysis Controls* pane.
- Compute the electric field eigenfunctions. After the analyzer loads, ensure the following parameters are entered:
  - **simulationName:** "rectMetalWaveguideDisp"
  - **outputsimName:** leave blank
  - **realFields:** "E"
  - **imagFields:** leave blank
  - **secondFieldFactor:** leave blank
  - **operator:** "d2dt2"
  - **dumpRange:** "21:321"
  - **cellSamples:** ":,5:25:5,5:45:5"
  - **cutoff:** "1e-12"
  - **maxNumModes:** "-1"
  - **initialModeNumber:** "0"
  - **normalizeModes:** checked
  - **testing:** leave blank
  - **overwrite:** checked

Also, check the "Overwrite Existing Files" box. The dump range runs only over the data saved in step 3 and we are only sampling every 5 cells in the z- and y- directions which is adequate to compute the eigen modes. Double-check your entries against what is shown in Fig. 4.39. After you run the analyzer, you will need to scroll up to find the computed frequencies. The screenshot shown in Fig. 4.39 is from a visualization window that is scrolled up so that the computed frequencies can be compared with what you ran. Figure Fig. 4.39 shows that there are 6 modes, but two are degenerate resulting in 5 unique modes. One indication that you are using extractModesViaOperator.py correctly is that the imaginary part of the frequency (which represents attenuation of the wave) is nearly 0 or at least much smaller than the real part. The lowest excited mode is $\sim 1.5 \times 10^9$ Hz, which is discussed further below in the context of standard waveguide theory.

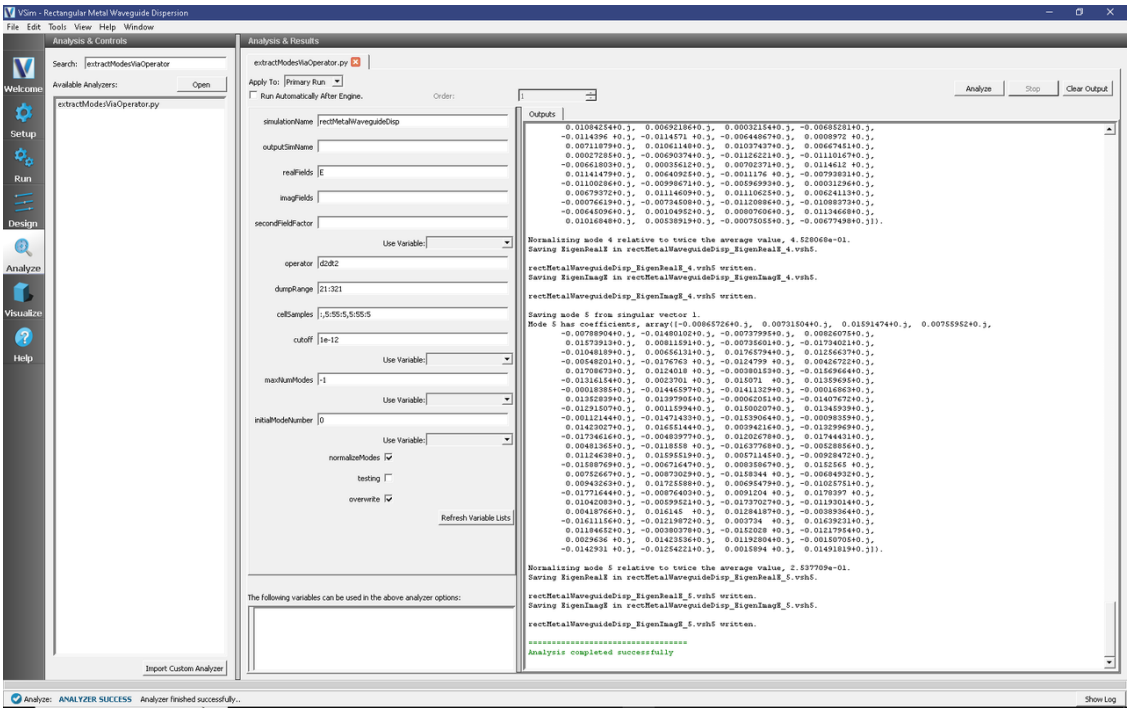


Fig. 4.39: Computing the electric field eigenfunctions and frequencies using the extractModesViaOperator.py analyzer.

Step 5: Computing the Dispersion Relation

Once the Eigenmode analysis is complete in Step 4, it is necessary to record the three lowest-order modes. The pre-loaded value of *mode* is 0, which means we are simulating $k_x = 0$. The waveguide dispersion relation is given by $\omega^2 = k_x^2 c^2 + \omega_{mn}^2$, where $\omega_{mn}^2 = c^2\pi^2\left((m/a)^2 + (n/b)^2\right)$, and where a and b are the y and z dimensions, respectively and m and n are integers. In this simulation, we analyzed the (m, n) = (1,0),(0,1) and (1,1) modes. Furthermore, the frequency range that is excited lies between $f_l = 1.5 \times 10^9$ Hz (which is the lowest allowable propagation frequency) and $f_h = 4.5 \times 10^9$ Hz. Given these parameters, we expect from waveguide theory for the three lowest cutoffs to be $\sim 1.5 \times 10^9, 3 \times 10^9, 3.35 \times 10^9$ Hz, which is what is found from extractModesViaOperator.py. Repeating these steps for modes 1 to 24 yields the dispersion relation shown in Fig. 4.40. The overlap between the simulation results and theoretical values is evident in Fig. 4.40.

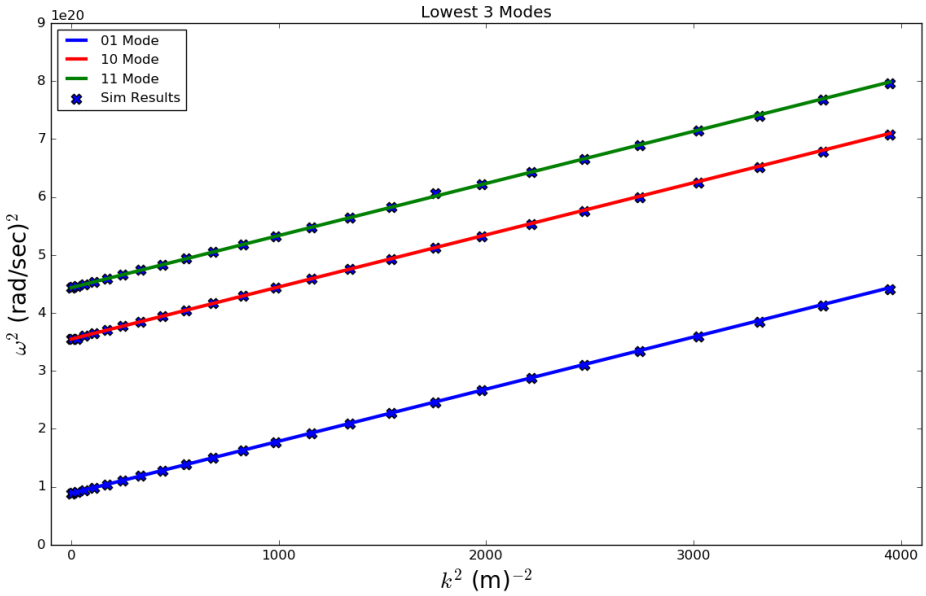


Fig. 4.40: Dispersion relation found by changing *mode* in VSim. The solid line is the theoretical dispersion relation $\omega^2 = k_x^2 c^2 + \omega_{mn}^2$. The 'X's represent data from the simulation results.

Convergence Study

To demonstrate that the simulation results converge to the theoretical value, we have performed a series of simulations in which $DX = DY = DZ$ are varied. The values chosen are *DX* = 0.205, 0.41, 0.50 and 0.615 cm. We then computed the lowest propagation frequency using *extractModesViaOperator.py* and plotted this frequency versus DX^2. Using Richardson extrapolation, we then compute the lowest propagation frequency for $DX^2 = 0$, which provides a better comparison with the theoretical frequency than a simulation with finite DX^2. The field calculation error scales approximately with DX^2 so a plot of frequency versus DX^2 should be a line. The linear correlation between frequency and DX^2 is shown in Fig. 4.41. The extrapolated frequency at $DX^2 = 0$ is $\sim 1.4992 \times 10^9$ Hz. The theoretical value is $\sim 1.4990 \times 10^9$. We see from Fig. 4.41 that the computation of the lowest propagation frequency for the DC mode converges with order DX^2, which is expected since the field solve is 2nd order accurate. Furthermore, using Richardson extrapolation, we see that the difference between theory and simulation, with $DX^2 = 0$, is 0.02 %.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The first step will be to ensure that we are driving the current density as expected and that the *E*- and *B*- fields are "ringing" as a result of driving the current density. Follow these steps to perform this check:

- Click on the *Add a Data View* pull-down menu at the top of the visualization window
- Click on *History*. This will open a new tab.
- Click on *Reload Data*.
- Under Graph 1 plot *jMid_1*. This is the *y*- component of the current density
- Under Graph 2 plot *eMid_1*.

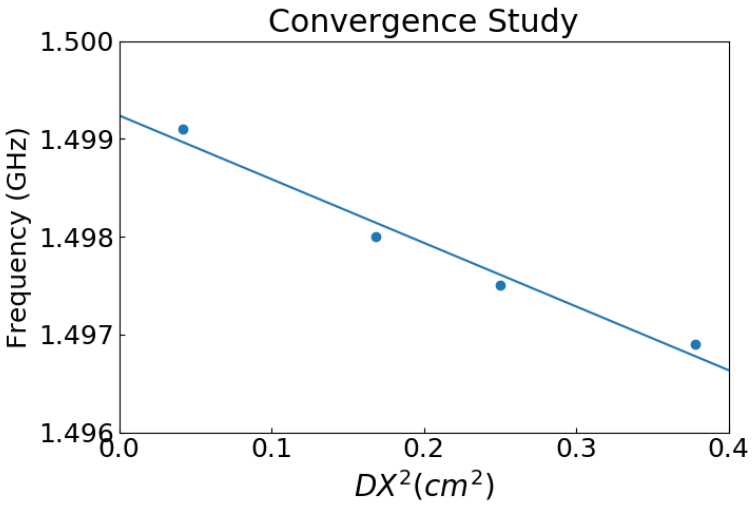


Fig. 4.41: Plot demonstrating convergence of frequency calculation.

- Under Graph 2 click the reset button to put the axis scaling back from the first plots make in Step 1 above.

Your plots should be similar to Fig. 4.42. The current density is driven for a short time period. However, because we are driving resonant modes, the current density excites the transverse electric field and parallel magnetic field. You can also plot *eMid_0*, *bMid_1*, and *bMid_2* to compare with Fig. 4.42. We have driven a TE mode since *eMid_0* is nearly 0.

We next wish to examine the spectral characteristics of the current density, which is driven between *FREQ_MIN* and *FREQ_MAX*. Therefore, the Fourier Transform of J_y or J_z should be greatest in this frequency range. Returning to the History visualization window, under Graphs 2, 3, and 4, change the plotted quantity to *none*, so that only Graph 1 shows a plot. Now check the "Fourier Amplitudes (dB)" box in the upper left corner. Finally, check the "Zoom" box on the right side of the visualization window and highlight from 0 to 10^{10} which will expand the lower frequency part of the plot. After you have zoomed in on the plot, re-check the "Navigate" box. The result of these steps should lead to a plot that looks similar to Fig. 4.43. The driving frequencies lie between *FREQ_MIN* and *FREQ_MAX* as expected. The rate at which the Fourier signal dampens below *FREQ_MIN* and above *FREQ_MAX* depends on the Gaussian envelope and the parameter called *OMEGA_SIGMA*.

Further Experiments

The result of varying *mode* from 0 to 24 is shown in Fig. 4.40. One experiment you can perform is to reproduce Fig. 4.40 by running 25 simulations with *mode* varying from 0 to 24. Each simulation takes just a few minutes so the 25 simulations take about one hour. For each simulation record the three lowest frequencies that are excited using extractModesViaOperator.py.

Another experiment would be to change the dimensions of the waveguide. The Constants *a* and *b* are used to determine the lowest frequency that will propagate in the waveguide. Therefore, changing *a* and *b* will automatically compute *FREQ_CUTOFF_TE*. You will then need to change *BGNY*, *ENDY*, *BGNZ*, and *ENDZ* accordingly. Finally, you will need to modify the dimensions and position of the primitives constructed under *Geometries* which are used to construct the waveguide.

A third experiment would be to modify *FREQ_MIN* and *FREQ_MAX* and compute the dispersion curve for these new values. No mode will propagate below *FREQ_CUTOFF_TE* so do not set *FREQ_MIN* below *FREQ_CUTOFF_TE*.

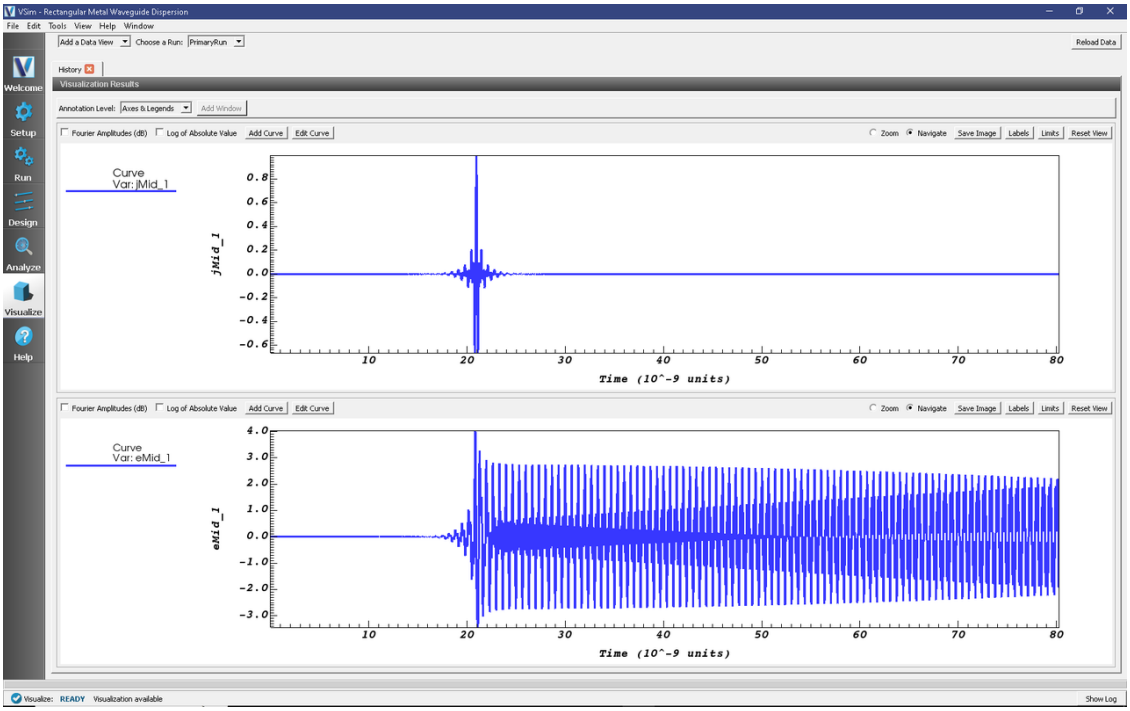


Fig. 4.42: History plots showing the modes driven in this simulation

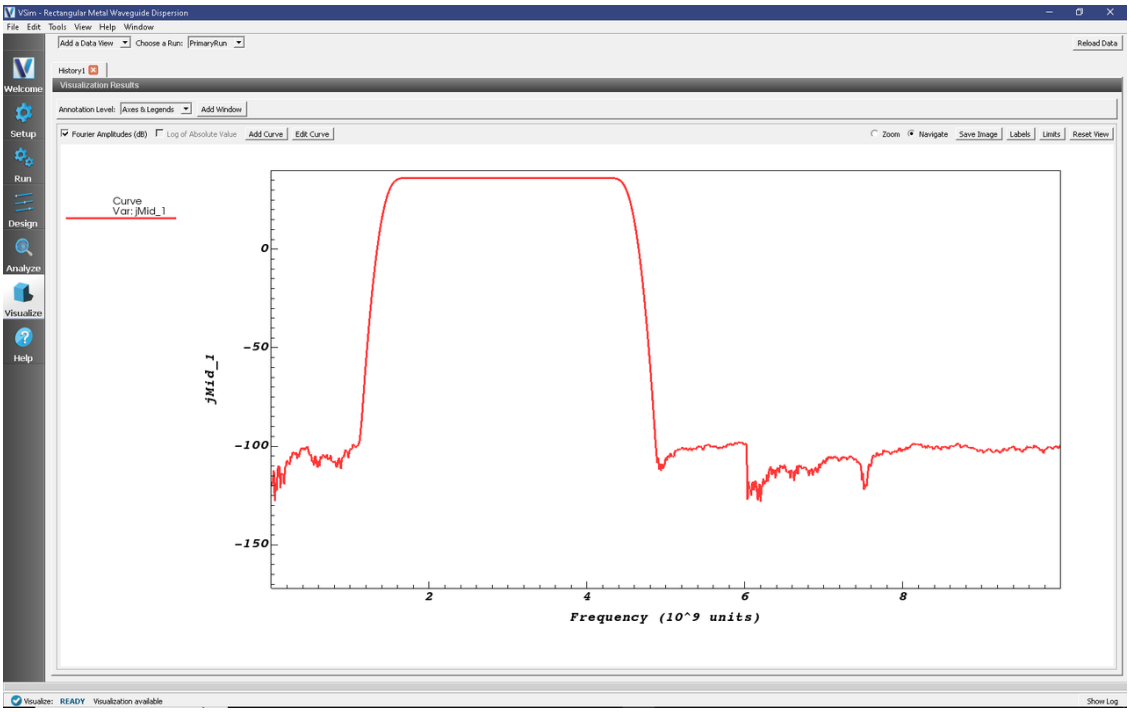


Fig. 4.43: Fourier Transform of the current density showing that the current density is mainly driven between *FREQ_MIN* and *FREQ_MAX* as expected.

Lastly, you can try to excite a TM mode instead of a TE mode.

4.1.7 S-Matrix of Box Cavity (sMatrix.sdf)

Keywords:

electromagnetics, sMatrix

Problem description

A common measurement made on a 2-port RF device is reflection and transmission of an RF signal, for either a single frequency, or for a range of frequencies. This measurement results in the Scattering-Matrix, or S-Matrix, whose elements S11 and S21 are the reflected and transmitted signal for unit input at Port 1. VSim provides the capability to simulate these S-Matrix parameters for arbitrarily complex devices connected to waveguides propagating TE, TM, and TEM modes. To demonstrate this capability, we show in this example how to measure S11 and S21 in a dual-mode cavity filter, connected to a WR-90 waveguide, with the narrow-band band-pass tuned to pass frequencies between 9.95 and 10.05 GHz.

The Dual Mode Cavity Filter operates by coupling the TE01 waveguide mode into the two nearly degenerate TE102 and TE201 modes of the cavity, since the length of the cavity is very close to its width. The differences in these values, along with the symmetry breaking along the waveguide axis, determine the frequency separation of the two modes. This separation is what gives the filter finite-bandwidth since frequencies between these modes are passed, and frequencies above or below the modes are rejected. A pole in the transmitted signal just below the band contributes to sharpness of the band's lower edge, but this pole moves easily to the upper frequency edge with small adjustments to the cavity dimension parameters, and the user is encouraged to experiment in finding optimal placement of this pole. Some relevant parameters are shown in Fig. 4.44.

Opening the Simulation

The Scattering Matrix example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Cavities and Waveguides* option.
- Select "S-Matrix of Box Cavity" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with the waveguide in the *3D View*. Fig. 4.45.

Simulation Properties

The simulation geometry consists of a standard WR-90 rectangular waveguide with the filter cavity (also referred to as the Device-Under-Test (DUT) in this writeup) in the center. A planar antenna in the waveguide, near the DUT, launches the incident wave while allowing reflected signals to pass through into the waveguide behind it. The antenna is constructed of two planar current sources with each current source one cell thick in the x-direction and directly adjacent to each other along x. The amplitudes and phases of the current sources are tuned so that the electric and magnetic fields which launch in the -x direction cancel whereas in the +x direction, the fields add to a non-trivial value. The waveguide ends are terminated in gradual absorbing layers with negligible reflection, and the reflected and transmitted signals are measured just in front of these absorbers.

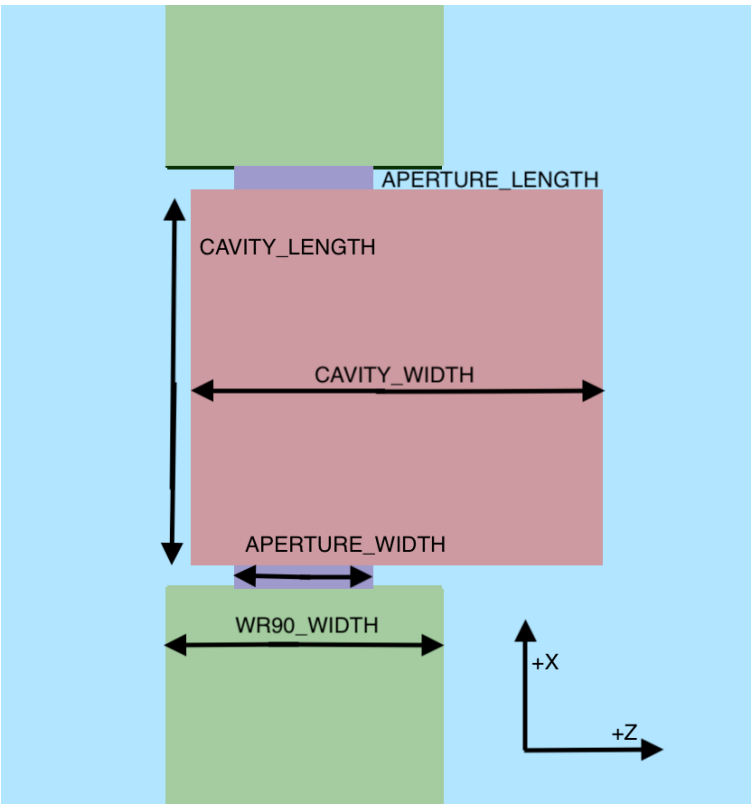


Fig. 4.44: Some relevant parameters for the S-Matrix Box Cavity example.

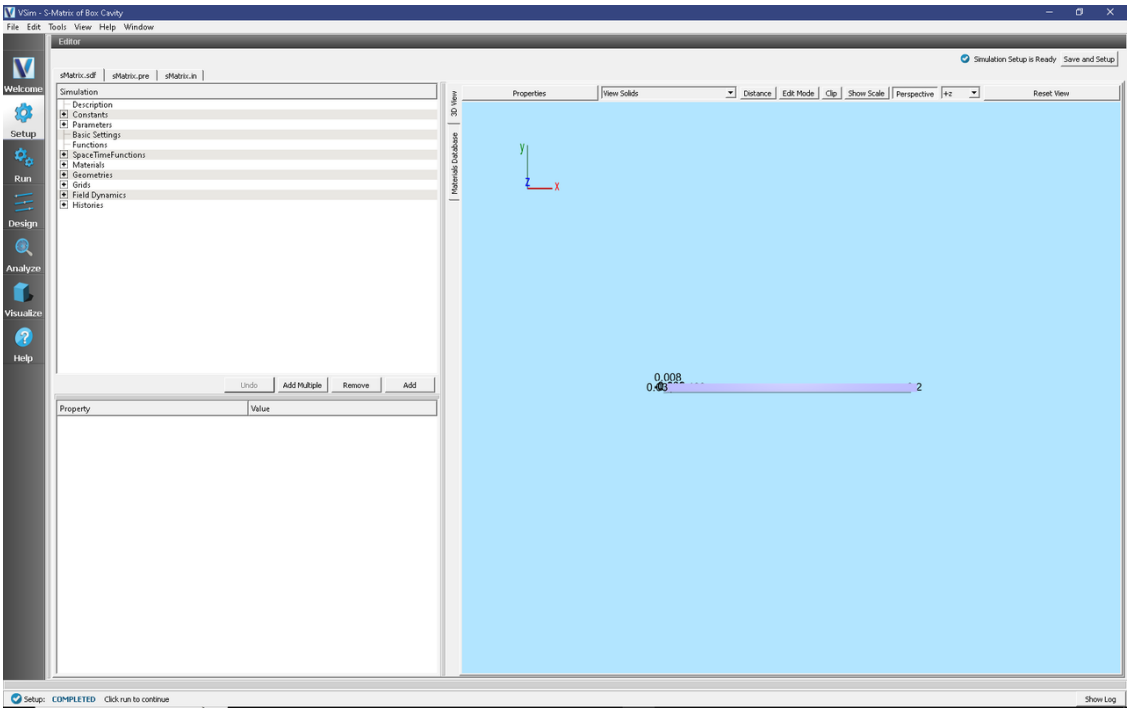


Fig. 4.45: Setup Window for the Scattering Matrix example.

This example is parameterized in the waveguide and DUT geometry specification, allowing for easy modification to either. Thus this example is effectively a template for an S-Matrix simulation of any device. The time histories of voltage signals used to measure S11 and S21 are also built in and automated for easy substitution. Furthermore, these signals are easily turned into S11 and S21 frequency variation curves using the standard "Fourier Amplitudes" capabilities in VSimComposer, or if single frequency, then the S11 and S21 values are just the amplitudes of the signals.

The x axis is the axial direction of the waveguide, with the parameters WAVEGUIDE_LENGTH, APERTURE_LENGTH, and CAVITY_LENGTH controlling the lengths of each component. These parameters are also used to control the position of each component, allowing a change to one of them to properly adjust the component positions.

The height (Y axis) of each component is standardized to the parameter WR90_HEIGHT, and centered around the Y axis.

The waveguide and aperture widths are centered around the Z axis, while the cavity is not.

The excited mode is the standard lowest mode, TE01, and in particular note that for this mode, the Ez component of the field is zero. The spatial profile of the current source is consistent with the TE01 mode. Since we are launching a TE01 mode, the perpendicular component of the electric field is 0 at the boundaries. Because the larger waveguide dimension is along z the lowest order mode coincides with the y-component of the electric field being excited. Therefore the function "waveguideEyProfile" is the spatial function used in the current source in order to launch the desired waveguide mode.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.2250750302237241e-12
  - *Number of Steps*: 17899
  - *Dump Periodicity*: 182
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.46.

This example is more sophisticated than some of the others, in that successful determination of S-Matrix parameters is not the result of a single run, but rather a result of a procedure involving several runs. This includes at least one Calibration Run, and at least one Data Run to determine S11 and S21. Below we discuss in detail some of the features of this example.

Frequency Band vs. Single Frequency

The user may choose whether to compute a single-frequency value of the S-Matrix parameters, or to compute the variation of the parameters as a function of frequency across a user specified frequency band. The constant, FREQCENTER, specifies either the single frequency or the center frequency of the band. The constant, FREQBANDWIDTH, provides the bandwidth or is set to 0 if a single-frequency simulation is desired.

With a single frequency simulation, the constant, NUMBEROFCYCLESTODRIVE, should be large enough to ensure that the S11 and S21 histories reach a steady amplitude. The *History* data view can be used to obtain the S-Matrix value, which is just the amplitude of the signal.

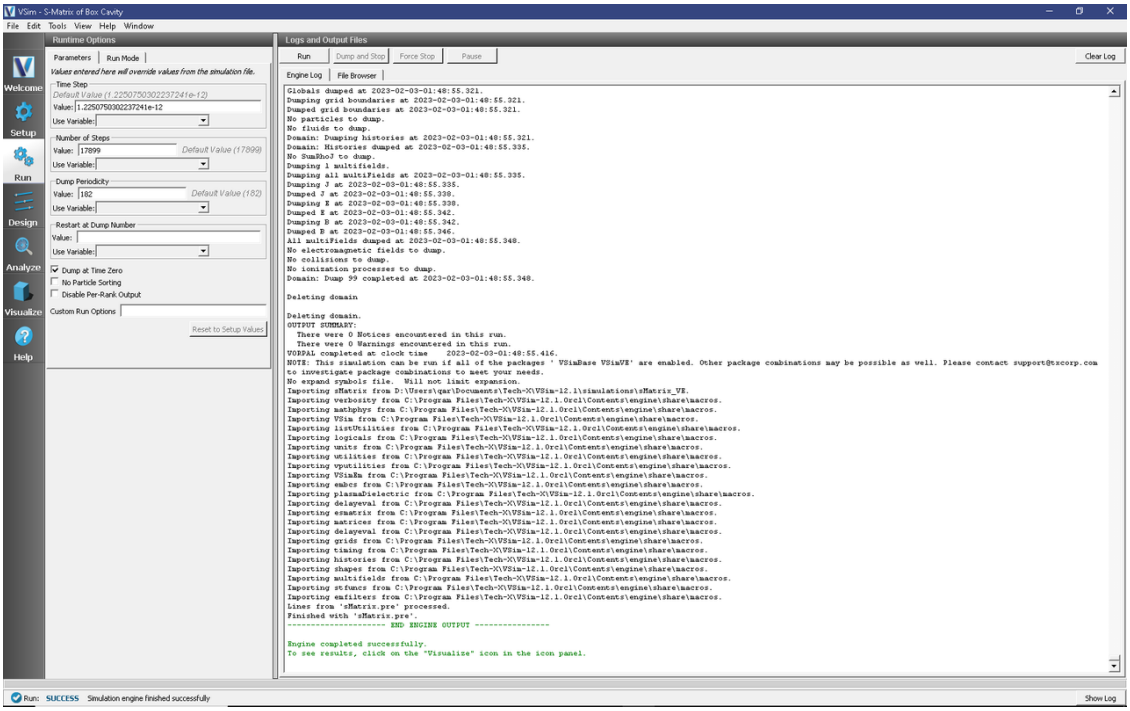


Fig. 4.46: The Run Window at the end of execution.

With a finite frequency band, the same constant, NUMBEROFCYCLESTODRIVE, can be adjusted upward to increase the detail and sharpness of the S-Matrix variation with frequency. In particular, increasing NUMBEROFCYCLESTODRIVE causes the FFT of the S11 and S21 histories to attain a sharper cutoff at FREQHI and FREQLO. The constant, NUMBEROFCYCLESTOCOAST, may also need to be adjusted upward if the DUT contains internal mode oscillation of large Q (quality) factor. This variable needs to be large enough so that the signal histories have decreased to a negligible value (10^{-4}, relative to maximum) by the end of the simulation. The *FFT* button in the *History* data view is then used to give the S-Matrix variation with frequency, with the plot's Y-axis units being dB. Be aware that it is usually necessary to zoom in significantly on this plot in order to see the frequency band of interest.

Finally, in both these cases, only the amplitude of the complex-valued S-Matrix parameters can be obtained with VSimComposer. More sophisticated post-processing (not covered in this example) is needed in order to get the phase information.

Calibration Run

The Calibration Run is done first, and the user must ensure that in the geometries, only the material of the object *myCalibrationWaveguide* is set to PEC, i.e., ensuring the material of the object *myWaveguideAndDUT* is set to empty. In the Calibration Run, the DUT is automatically omitted and replaced with a continuation of the waveguide, so that this is a near trivial simulation of a straight length of waveguide that should have effectively 100% transmission. The calibration run serves two very important purposes:

To ensure that there is negligible (below 1% amplitude, -40 dB) reflected voltage (S11). If the reflection is too high it indicates that either the absorbing boundaries (MAL's) are not working well enough, or that the waveguide's "modeProfile" description is not accurate enough, and/or that there is not enough grid resolution. To decrease reflections at the MAL boundaries, you can decrease the "damping factor" in the MAL boundary condition. If you do this, you may need to increase the length of the MAL. Another potential issue is the value of TRISE, which is the length of time over which the current source is turned in the single frequency runs. Increasing TRISE could lead to a better measure of S11 and S21.

To adjust the DRIVENORMALIZATION constant, which runs in proportion to observed transmitted voltage (S21), so that the next time the calibration run is done, the transmitted voltage (S21) will be exactly unit amplitude (single frequency) or zero dB (across frequency band). For example, if the first Calibration Run shows an amplitude of 0.667 for S21, change DRIVENORMALIZATION to 1.5 times its present value for the next Calibration Run, since 1/0.667 = 1.5.

Changing center frequency, or any waveguide parameter, or even the nominal cell size, will require re-calibration. If not sure, always recalibrate, when changing a parameter.

Data Run

Once the Calibration Run is successful at achieving unit transmission with negligible reflection, the Data Run is then done. The user should ensure that only the material of the object *myWaveguideAndDUT* is set to PEC, i.e., ensuring the material of the object *metalMinuscalibrationWaveguide* is set to empty.

Visualizing the results

After performing the above actions, continue as follows:

Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The S-Matrix results are shown by adding a *History* data view. Once the history graphs are displayed check *Fourier Amplitudes* to get an FFT of the data. To look at the results from 8 to 12 GHz, click *Limits* in the upper right corner of each graph and set the X-axis lower limit to 6e9, and upper limit to 14e9.

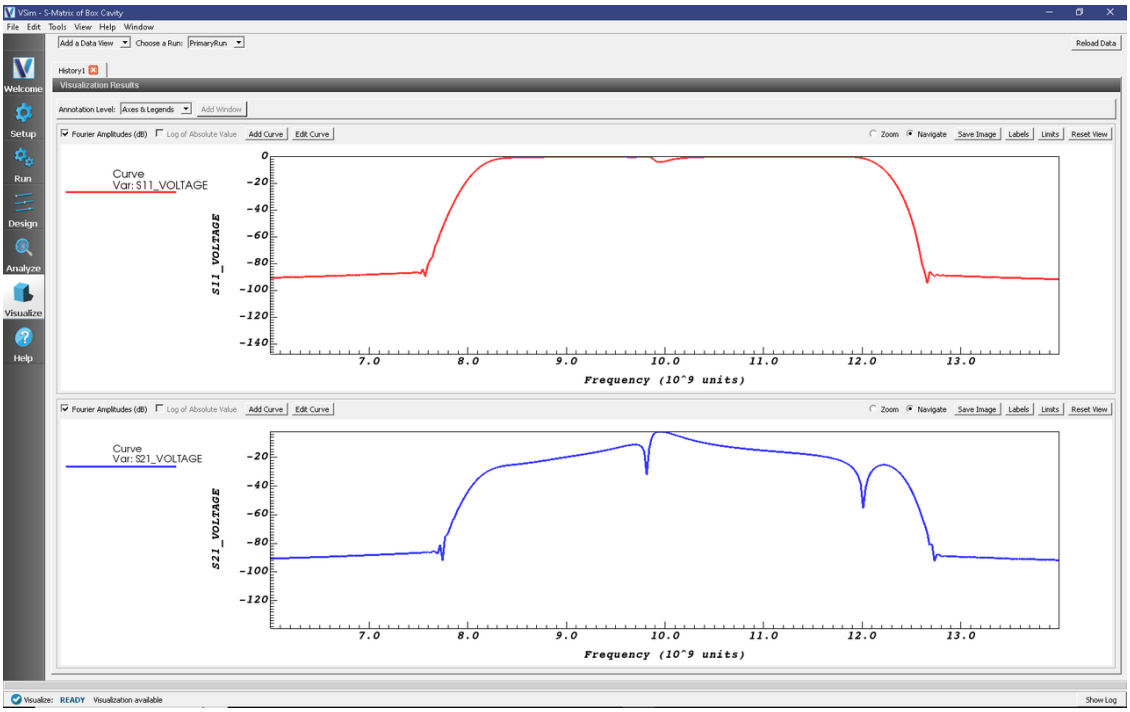


Fig. 4.47: Fourier transforms of the histories S11_Voltage and S21_Voltage as a function of frequency (in GHz).

Further Experiments

Experiment with finding optimal placement of the pole in the transmitted signal.

4.2 Cavities and Waveguides (text-based setup)

4.2.1 A15 Crab Cavity (crabCavityT.pre)

Keywords:

electromagnetic cavities, accelerators, mode frequencies

Problem Description

The Crab Cavity simulation illustrates how to extract the modes and frequencies of an accelerator cavity in a given frequency range. The range of interest here is 3.9 to 4.1 GHz. The simulation is performed by exciting the cavity with a broadly filtered pulse that excites modes in a given range. The excitation occurs through a temporally and spatially specified current source that excites the frequencies of interest. The simulation features a variable sampling frequency, allowing the cavity to first be rung up without generating excessive memory dumps. After the simulation has been rung up, sampling frequency increases, and when combined with post-processing find the modes and frequencies. The algorithm is detailed in [1].

This simulation can be performed with a VSimEM, VSimVE or VSimPD license.

Opening the Simulation

The Crab Cavity example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Cavities and Waveguides (text-based setup)* option.
- Select "A15 Crab Cavity (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 4.48.

Input File Features

The input file allows the user to control a number of features of the Crab Cavity simulation. The FREQ_LO_GHZ and FREQ_HI_GHZ defines the range of frequencies that we are interested in extracting whereas the DELTA_FREQ_GHZ specifies the separation in frequency between the range of interest and the next nearest mode (at 4.3 GHz).

The input file is written to run for a long time, sufficient to ring up the cavity, then dump periodically during the free oscillation period. The modes and frequencies will be extracted from those dumps. This can be seen in crabCavityT.in.

The remaining key parameter values correspond to the geometry and discretization of the cells. The focus of the Crab Cavity simulation is on a four cell cavity with end holes that were originally used for measurement purposes. See [2]. The final ZSQUASH parameter is used to squeeze each cell of the cavity to eliminate the degeneracy due to cylindrical symmetry.

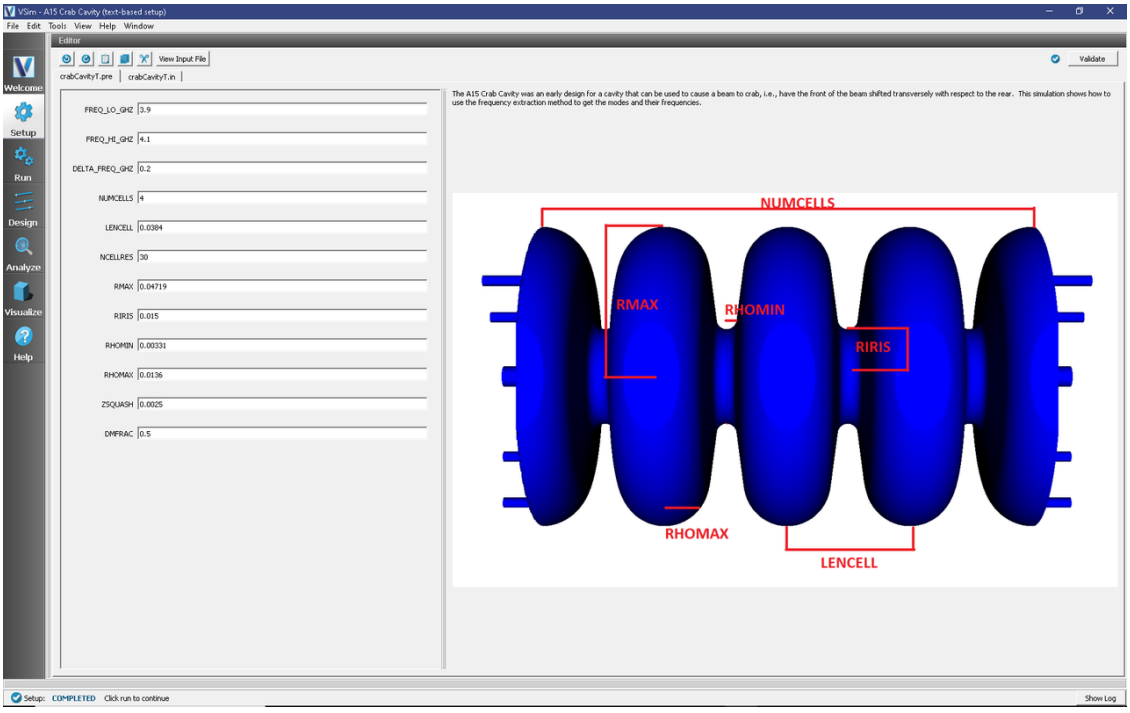


Fig. 4.48: Setup Window for the Crab Cavity example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.3722635090482095e-12
  - *Number of Steps*: 39026
  - *Dump Periodicity*: blank
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.49.

Analyzing the Results

It is possible to extract the modes of the A15 crab cavity via post processing using the Extract Modes Analysis Script* as follows:

- Press the Analyze button in the left column of buttons.
- From the list of Available Analyzers, select *extractModes.py* and press *Open*.
- Enter the following parameters in the appropriate fields. the default simulation values are used:
  - simulationName = crabCavityT

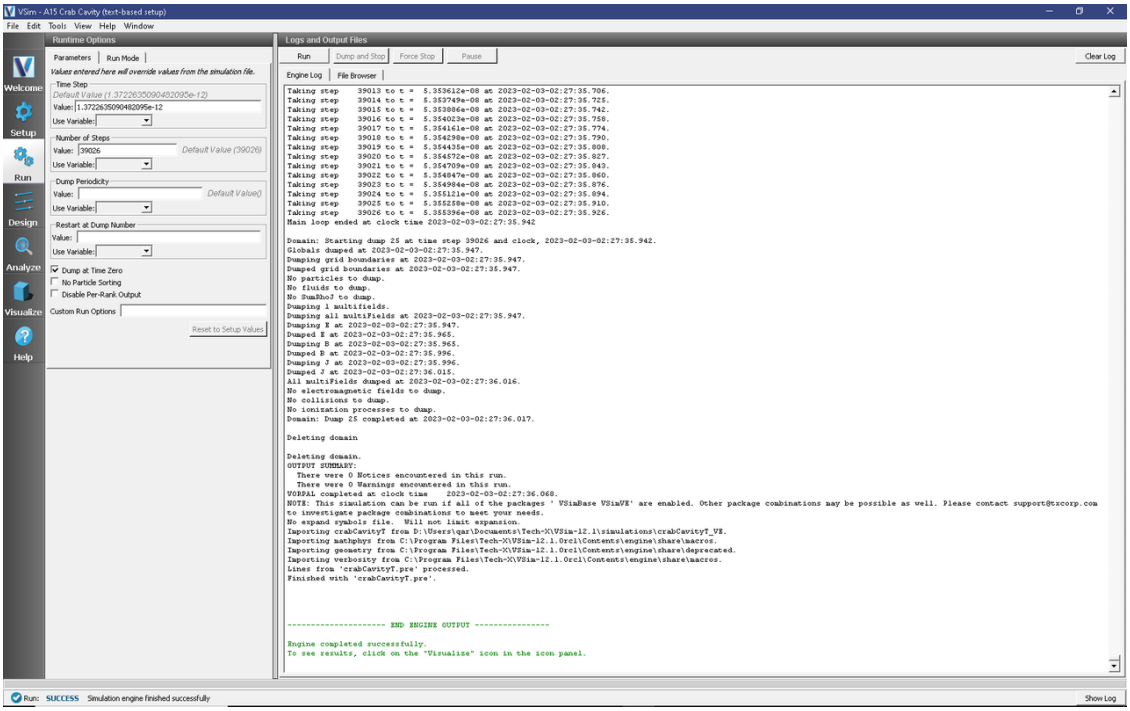


Fig. 4.49: The Run Window at the end of execution.

  - field = B
  - beginDump = 2
  - endDump = 22
  - nModes = 5
  - numberUniformPts = 20
  - numberRandomPts = 20
- Uncheck the *randomSample* box, and check the *construct* box.
- Click the *Analyze* button in the upper right corner of the window.

As shown in Fig. 4.50 below, three columns of data with the titles “freq [Hz]” (eigenmode frequency), “invQ” (inverse quality factor), and “SVD” (singular value decomposition) will be output in the right pane. The analysis has completed when you see the output “Analysis completed successfully.” One can see 5 modes, but the first one is not real as one can see from its unrealistic value of invQ, which should in fact be zero for this ideal (non-lossy) cavity, and the fact that it has zero frequency.

The magnetic fields at each of the eigenmode frequencies will be available to view in the Visualize Window under the *B* Field.

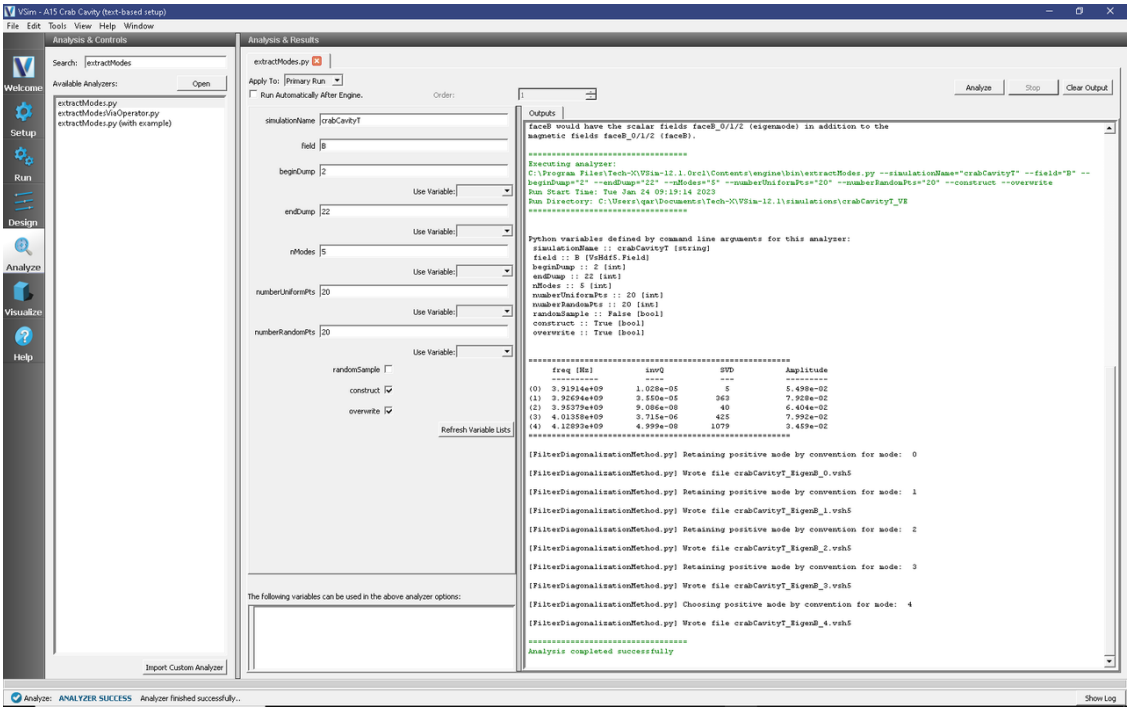


Fig. 4.50: The Analysis window at the end of execution of the extractModes.py script.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric field:

- Expand *Scalar Data*
- Expand *E*
- Select *E_z*
- Check the *Clip Plot* box
- Expand *Geometries*
- Select *poly*
- Check the *Clip Plot* box
- Move the slider at the bottom of the right pane to see the electric field at different times.

One can instead view the eigenmodes, which are so labeled under *B*. E.g., Unclick *E_z* click *B_y (Eigenmode)*. For these plots you may want to individually control the field colors. This is done by while you have *B_y (Eigenmode)* selected.

*Check the *Set Minimum* box and set the value to -0.005 *Check the *Set Maximum* box and set the value to 0.005

This will give a sharper contrast of the eigenmode The slider can be moved to see the eigenmodes, as it is used for the mode number rather than periods in time. Slider positions past the last eigenmode will display only the last eigenmode.

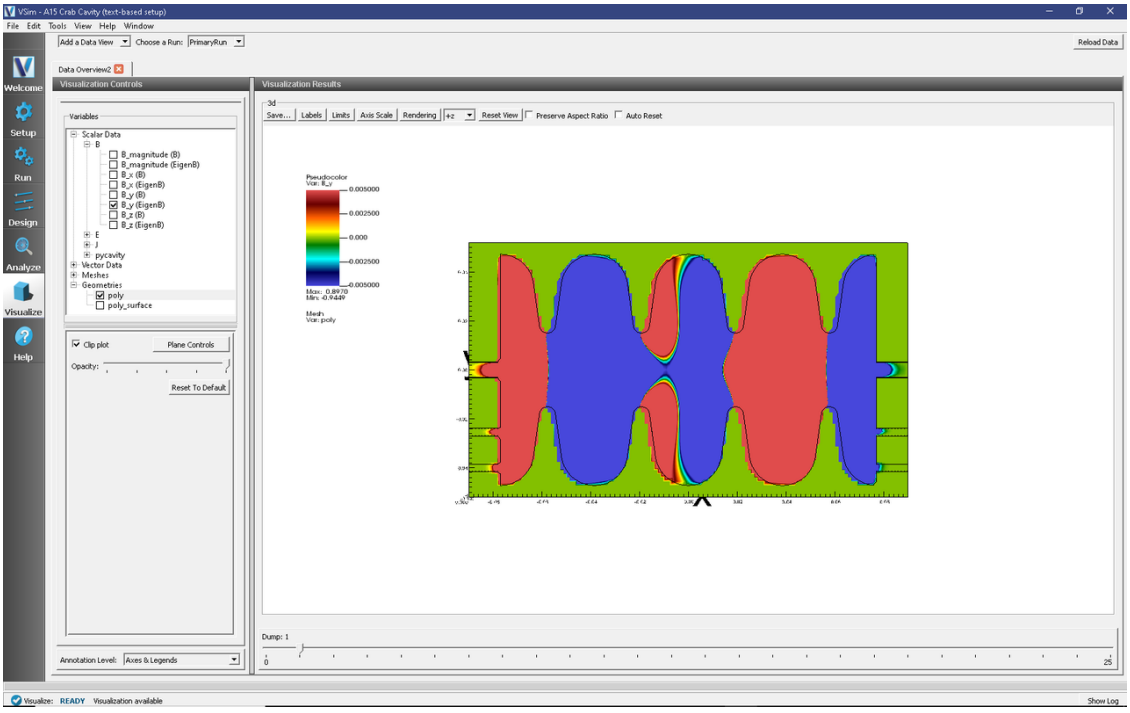


Fig. 4.51: Visualization showing an eigenmode

Further Experiments

Additional experiments worth investigating are:

- Use Histories to record the power flow, to compute the coupling efficiency.
- Simulate one period of the waveguide with periodic boundary conditions and a user-defined phase shift, and use the frequency extraction feature to compute the waveguide modes and dispersion curves.

References

[1] G. R. Werner and J.R. Cary, "Extracting modes and frequencies from time-domain simulations with filter-diagonalization", J. Comp. Phys., 227 (10), 5200-5214, 2008.

[2] T. M. Austin et al., "Validation of frequency extraction calculations from time-domain simulations of accelerator cavities", Comput. Sci. Disc., 4, 015004, 2011.

4.2.2 Stairstep Cavity in coordinateGrid (emCavityCoordProdT.pre)

Keywords:

`stairstep boundary, coordinateGrid, Klystron cavity`

Problem description

This example demonstrates how to set up a complex geometry structure in VSim that uses the *coordinateGrid* system for a varying mesh size. There are two benefits of constructing a grid of kind `coordProdGrid` via `coordinateGrid` blocks. The first is a flexible choice of either Cartesian (x, y, z) or cylindrical (z, r, ϕ) coordinate systems to construct the grid. The second is that it enables one to vary the cell size along each axis of the grid. For example, a fine grid resolution can be used in a region of the domain consisting of complicated geometry, while a coarse resolution can be used in a different region of the domain where the geometry is simple. This method reduces the memory requirement for large multiscale simulations. The `gridBoundary` block (implemented in this example through the `geometry` macro) is used by VSim to represent complex geometrical surfaces with boundary conditions.

This example simulates a klystron cavity using a non-uniform Cartesian mesh generated by VSim's *coordinateGrid* system. Klystron cavities have wide applications as RF power sources by amplifying an RF input with electron beams. The simulated cavity is defined by a set of VSim geometry macros. Grid cell size is varied in the longitudinal direction so that a fine mesh exists at the round nose surface connecting the center drifting tube and outer ring cavity. Larger cell sizes are used at both ends of the drifting tube. The fundamental transverse magnetic (TM) mode is excited by a Gaussian current pulse.

This simulation can be performed with either a VSimEM, VSimVE, or VSimPD license.

Opening the Simulation

The emCavityCoordProdT example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Cavities and Waveguides (text-based setup)* option.
- Select "Stairstep Cavity in Coordinate Grid (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the Setup Window, as shown in Fig. 4.52.

Input File Features

- At the top of the Editor pane, click *View Input File*.

The first important feature of this input file is the setup of the non-uniform simulation grid. Scroll to the `Grid` block on line `262` (Fig. 4.53). The variable spacing in x in the non-uniform grid is specified in the definitions of `sectionBreaks` and `deltaAtBreaks` in the `coordinateGrid dir0` block. The `deltaAtBreaks` field specifies the grid cell spacing at each of the `sectionBreaks` positions, and the grid is generated such that the cell spacing transitions gradually between these positions. In this specific example, on lines `266` and `267`, from $x =$ `XBGN` to $x =$ `CAV_START` the cell spacing transitions from $\Delta x =$ `DX` to $\Delta x =$ `DX/3.0`, then from $x =$ `CAV_START` to $x =$ `CAV_END` the cell spacing stays at a constant value of $\Delta x =$ `DX/3.0`, and finally from $x =$ `CAV_END` to $x =$ `XEND` the cell spacing transitions from $\Delta x =$ `DX/3.0` back to $\Delta x =$ `DX`.

The second important feature of this input file is the electromagnetic solver for this type of grid. Both the Faraday and Ampere updaters are set to kind `curlUpdaterCoordProd`. By setting `interiorness = cellcenter` in both updaters, the curl operation is performed with a stair-stepped `gridBoundary`.

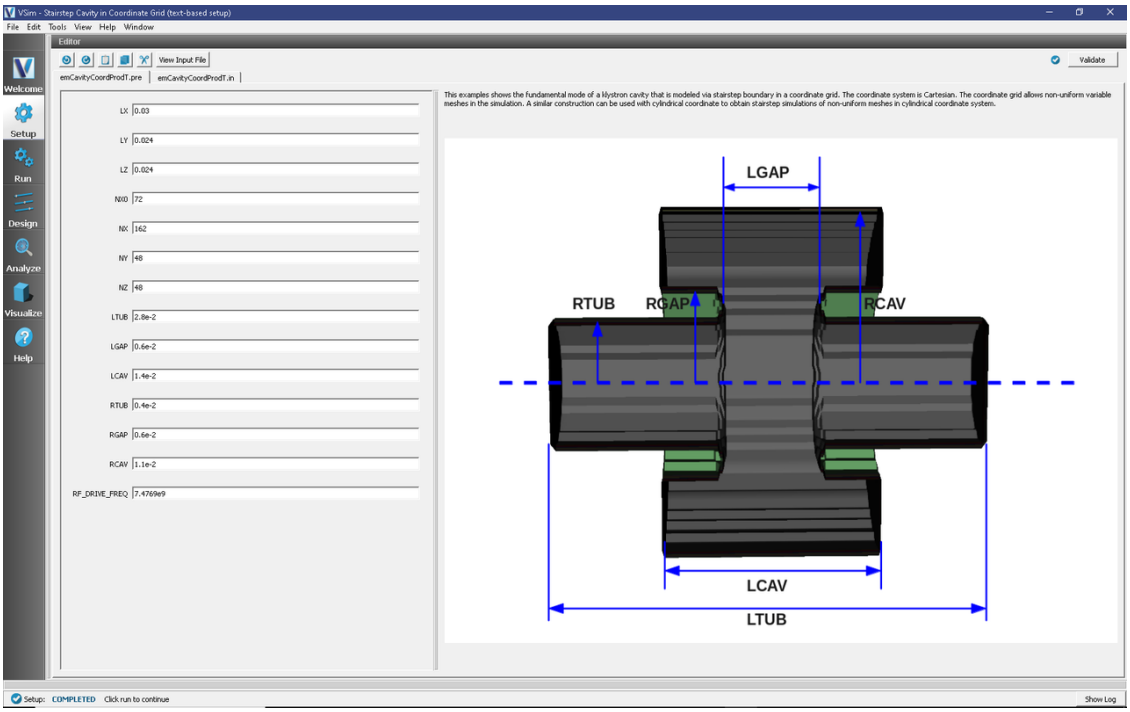


Fig. 4.52: Setup Window for the emCavityCoordProdT example.

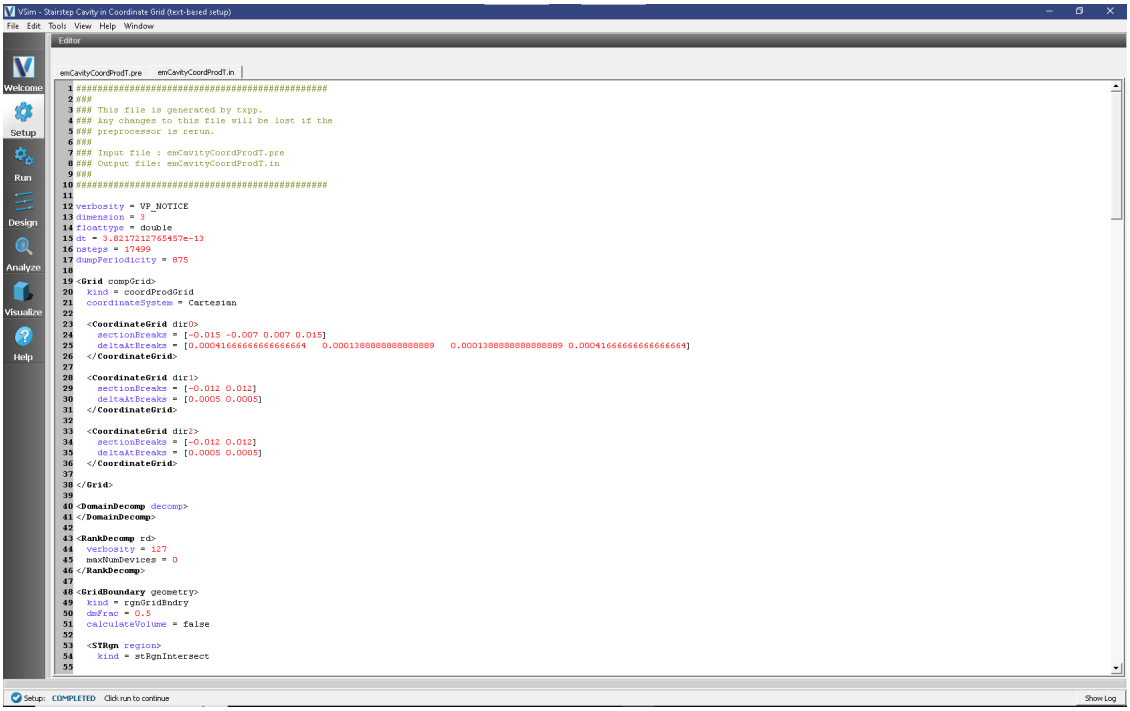


Fig. 4.53: Input file for the emCavityCoordProdT example, showing the setup of the *coordinateGrid* system.

Running the simulation

Because the cells are not uniformly spaced, the number of cells in the simulation is unknown until calculated by VSim's Vorpal engine. However, the number of cells in each dimension is required for VSim to preprocess the input file. To correctly set the number of cells `NX` in the input file, take the following steps:

- Set the parameter `NX0` (the default is 72). This specifies the grid spacing (`DX`) at the ends of the simulation domain as `NX0/LX`.
- Run the simulation for one time-step by clicking the **Run** button in the left column of buttons, and entering "1" in both the *Number of Steps* and *Dump Periodicity* fields.
- After the simulation completes, scroll through the log file to find the value of `numPhys` in the first row of `Global grid`, as circled in Fig. 4.54.
- Go back to the Setup Window by clicking **Setup** in the left column of buttons, and enter this value into the field for `NX`. For the default values of this example, this number should be 162.

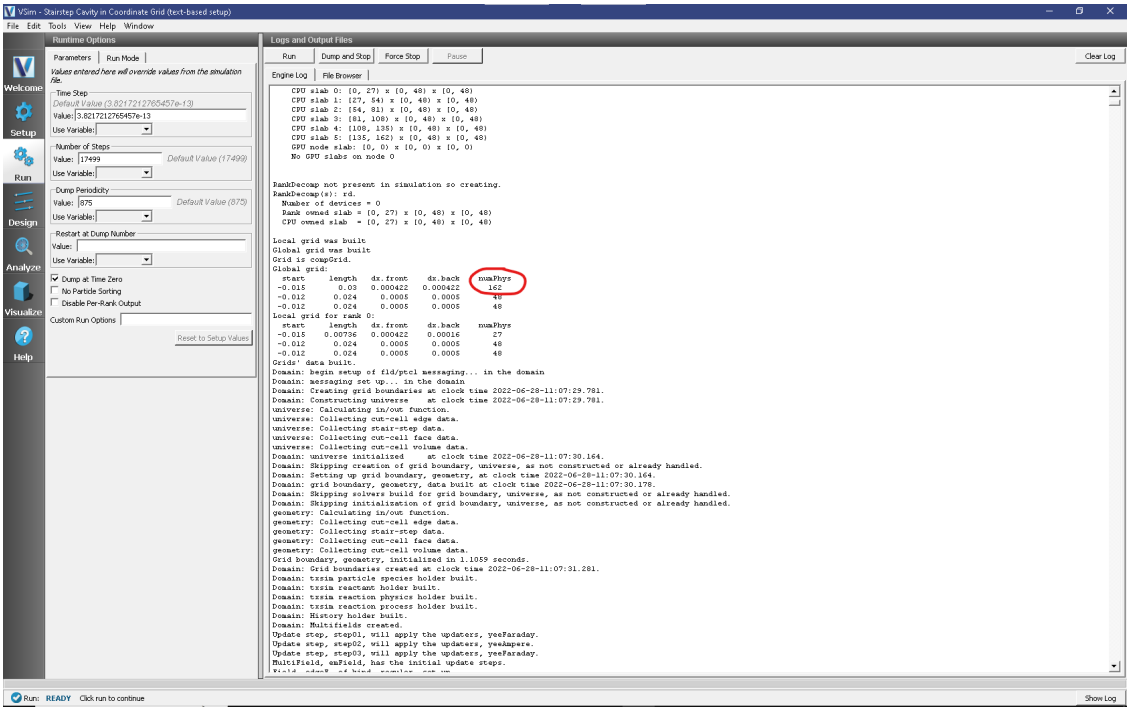


Fig. 4.54: Location of the `numPhys` output to be entered into the `NX` field by the user.

The simulation is now ready to run. Return to the Run Window, enter the desired values for *Number of Steps* and *Dump Periodicity* and click *Run* once again. The run has completed when you see the output, "Engine completed successfully" as shown in Fig. 4.55. This will require approximately two hours of computation time when run in parallel on four processors on a modern CPU.

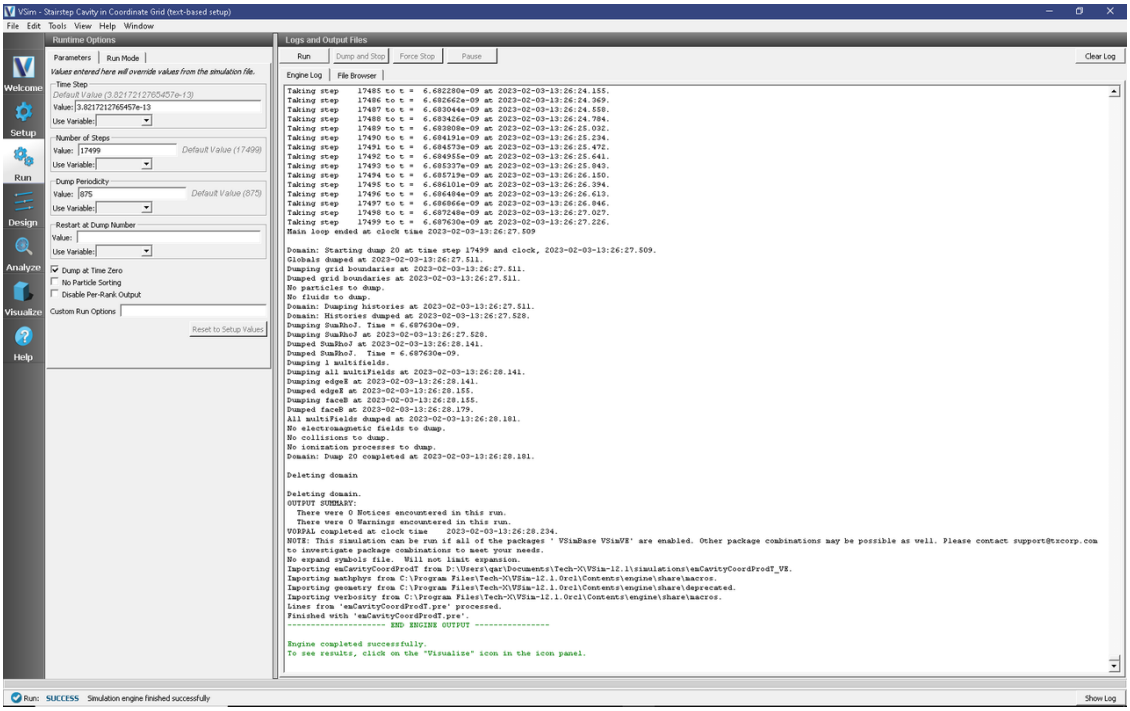


Fig. 4.55: The Run Window during the execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by clicking **Visualize** in the left column of buttons.

To create the plot as shown in Fig. 4.56:

- In the Variables section of the Visualization Controls pane, Expand *Geometries*
- Select *poly_surface*
- Check the *Clip Plot* box
- Expand *Meshes*
- Expand *compGridGlobal*
- Select any of the grid choices, for they are all identical for this simulation
- Check the *Clip Plot* box
- Expand *Scalar Data*
- Expand *edgeE*
- Select *edgeE_x*
- Check the *Clip Plot* box
- Decrease the Opacity by moving the Opacity slider the left to better see the fields through the grid
- At the bottom of the Visualization Results pane, move dump slider forward in time

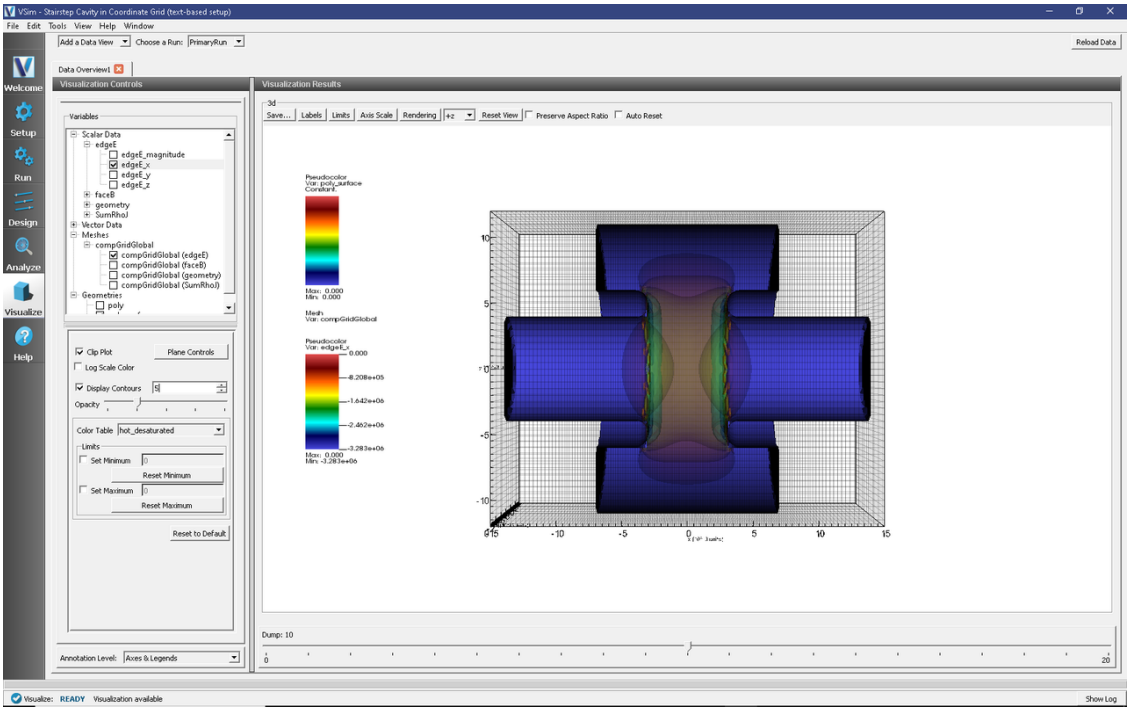


Fig. 4.56: Visualization of the x-component of the electric field in the simulation of a klystron cavity with a non-uniform mesh.

Further Experiments

The *coordinateGrid* system is also capable of creating non-uniform grids in cylindrical coordinates, by setting `coordinateSystem = Cylindrical` in the `Grid` block. The `curlUpdaterCoordProd` updater also works with the same settings in cylindrical coordinates.

4.3 Radiation Generation

4.3.1 Smith-Purcell Radiation (SmithPurcellRadiation.sdf)

Keywords:

`diffraction grating, radiation generation, coherent mode, Smith-Purcell`

Warning: This example used more than 8GB of RAM as configured, so if your machine does not have a lot of memory, then you can reduce the number of cells in the Grid (say by a factor of 2 to the size 950x800x2) to avoid running out of memory.

Problem Description

This VSim for Vacuum Electronics example illustrates how to setup a device that emits coherent Smith-Purcell Radiation (SPR). This phenomenon occurs when charged particles pass over a periodically graded surface in very close proximity resulting in the emission of a form of Cherenkov radiation. In recent years, engineers have been building SPR-emitting devices that can generate frequencies in the terahertz range, otherwise difficult to obtain via other methods. This example demonstrates how the design of an SPR-emitting device can be optimized with simulations.

This simulation can be run with a VSimVE license.

Opening the Simulation

The Smith-Purcell Radiation example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select *Smith-Purcell Radiation* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.
- The resulting Setup Window is shown Fig. 4.57.

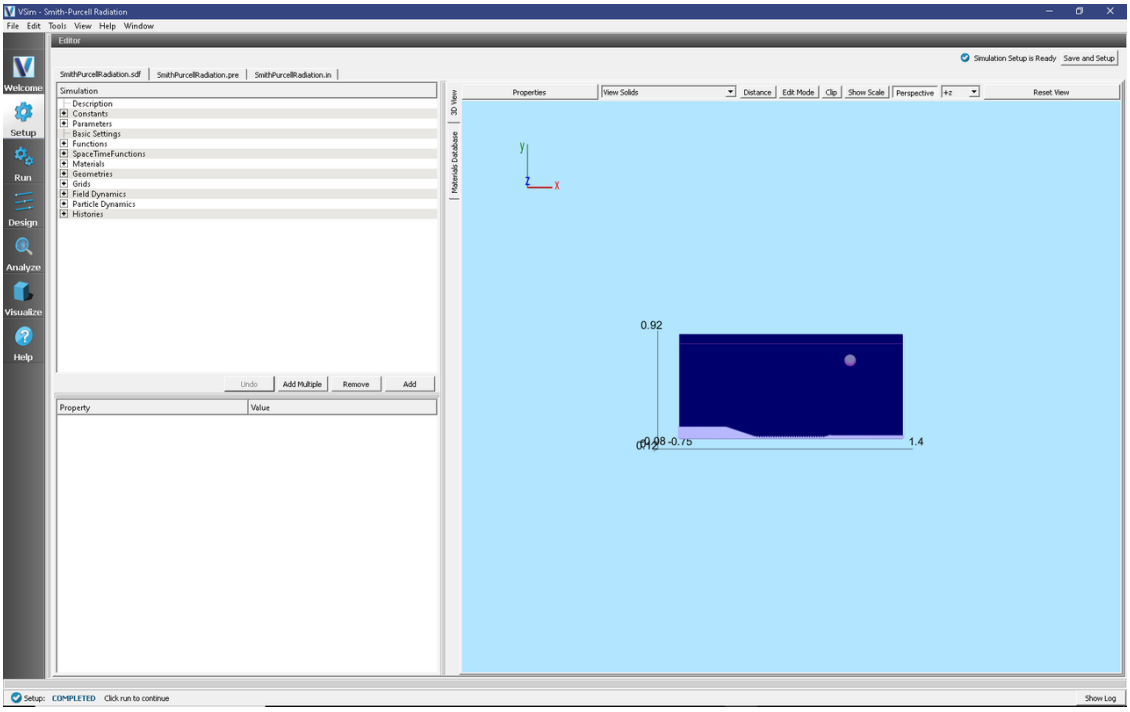


Fig. 4.57: Setup Window for the Smith-Purcell Radiation example.

Simulation Properties

The simulation setup was based on Donohue & Gardelle 2005 [DG05] who used 2D simulations for their study: a grating structure that is perfectly conducting, a cathode from which the electron beam is emitted, and a vacuum enclosure in which radiation propagates. The walls of the vacuum box are matched absorbing layers (MALs) which absorb the electromagnetic fields and eliminate any reflection. This is a quasi-3D simulation: the thickness to the gating structure is 2cm and the simulation is periodic in z (the direction normal to the grating). The grid resolution was set high enough to resolve the small structures of the grating: 1890, 1600, and 2 cells in the x, y, and z directions, respectively. The 5 mm electron beam was generated with a 125 A/m current. The incident electron energy is 100 keV. There is an external magnetic field of 2 T in the x-direction for beam confinement.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 7.653323230160254e-13
  - *Number of Steps*: 48000
  - *Dump Periodicity*: 2000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.58.

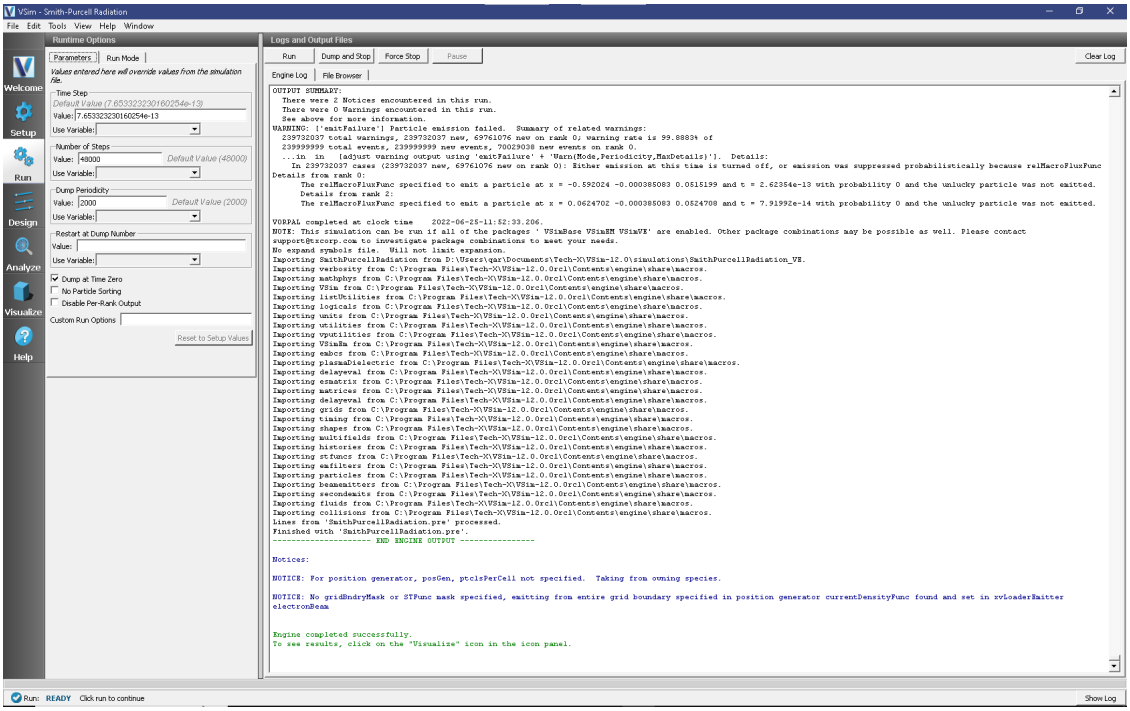


Fig. 4.58: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Data Overview*.
- In the variables tree, expand *Scalar Data*.
- Expand *B*.
- Select *B_z*.
- Check Set Minimum and Set Maximum and set to -1e-5 and 1e-5, respectively
- In the bottom of the right pane, mode the dump slide forward in time.
- The resulting visualization is shown in Fig. 4.59.

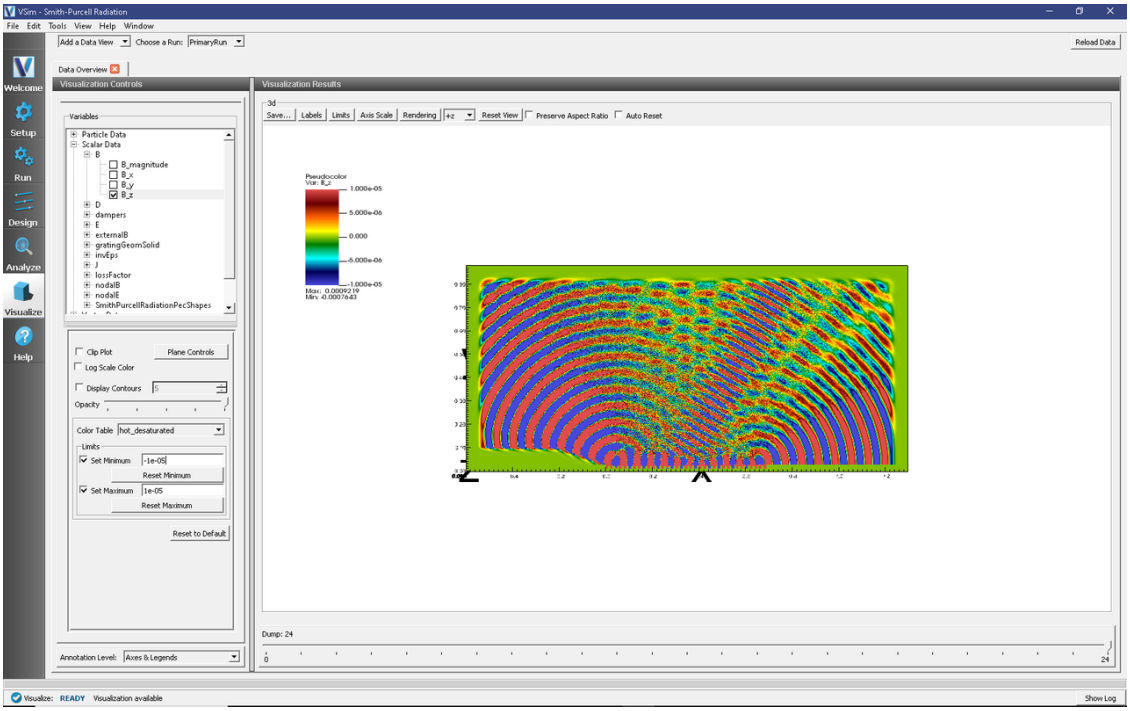


Fig. 4.59: Bz at the end at 25 ns (at dump 24).

The magnetic field in the z direction (Bz) plotted in Fig. 4.59 shows that at 85 cm and 64 degrees from the center of the grading the SPR emission was the strongest (this is known as the SPR propagating mode). This is consisted with the results found by Donohoe and Gardelle. The strong emission seen on the left side is known as the evanescent mode, but this is considered non-SPR emission.

To measure the frequencies of these modes proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *History*.
- Select *Bz64deg_2* from the drop-down menu in Graph 1.
- Select *None* for Graphs 2,3, and 4.
- In the top left corner of the right pane, check the *Fourier Amplitude (dB)* option.

- In the upper right corner of each plot, select Limits and set X-Axis max to 1.2e10 and click *OK*.
- The resulting visualization is shown in Fig. 4.60.

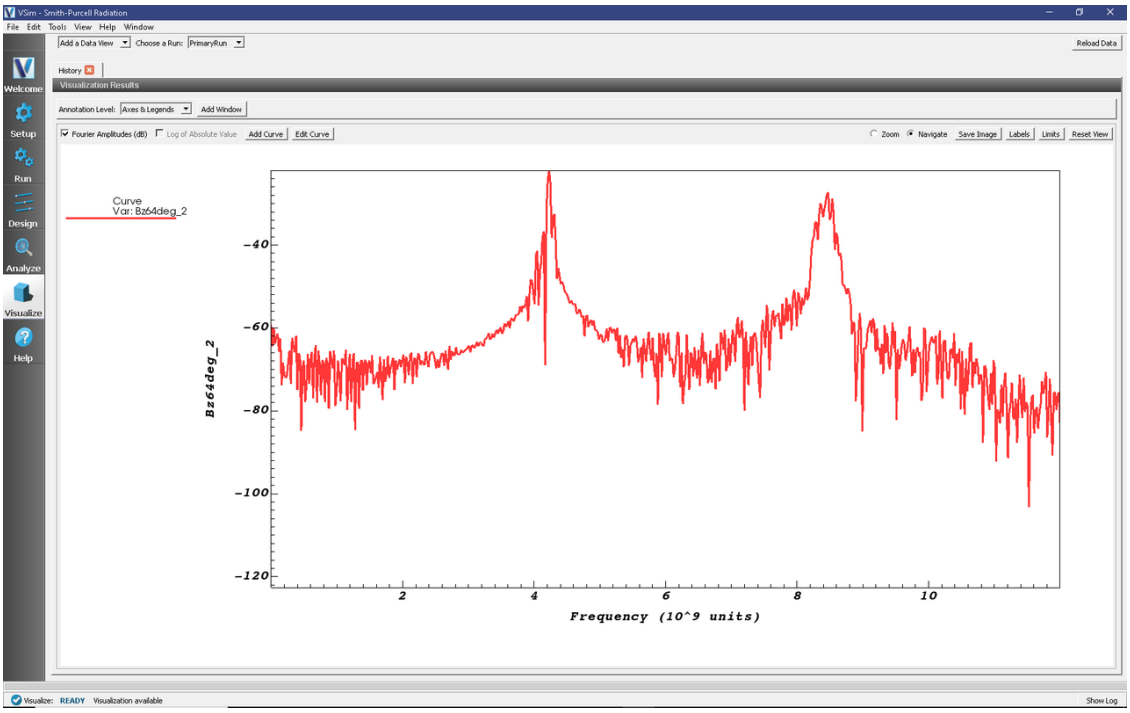


Fig. 4.60: FFT of the Bz measured at 85 cm and 64 degrees from the center of the grading where the SPR emission was the strongest. The frequencies of the evanescent and the propagating modes can be seen at around 4.5 and 9 GHz.

The FFT of this signal is shown in Fig. 4.60 where the frequencies corresponding to the evanescent mode and the propagating mode can be seen at around 4.5 and 9 GHz. The evanescent mode becomes dominant over the propagating mode when the dampers are not present. Note: it is expected for the propagating mode frequency to be an integer multiple of the evanescent mode (see Donohue and Gardelle 2005 [DG05] for more details).

Another signature of SPR emission is electron bunching inside the particle beam. To visualize the electron bunching, proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Phase Space*.
- For the *X-axis*, select *electrons_x*.
- For the *Y-axis*, select *electrons_ux*.
- Click *Draw*.
- Move the dump slider further in time.
- The resulting visualization is shown in Fig. 4.61.

Fig. 4.61 shows a phase-space of the electron speed in the propagation direction vs. their position. The very strong bunching effect can be observed and this effect becomes more defined and increases with time.

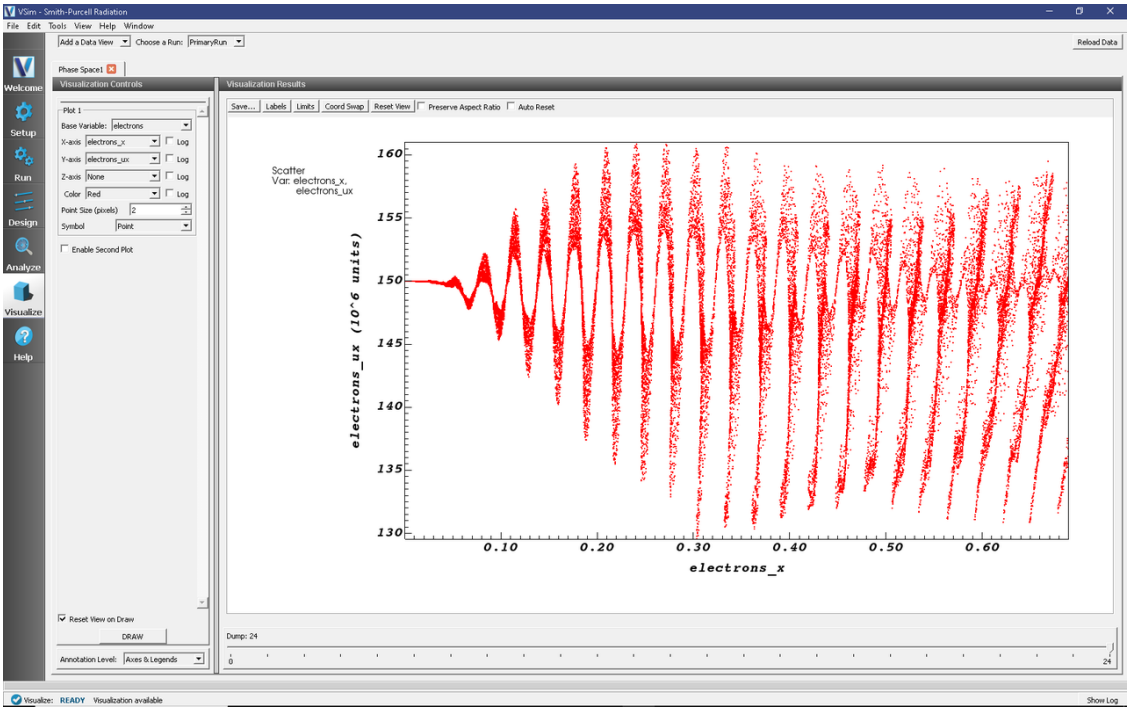


Fig. 4.61: The phase-space visualization for the Smith-Purcell Radiation example.

Further Experiments

When running the simulation without the dampers, the evanescent mode is dominant and strong fields can be seen at the beginning and end of the electron beam. Adding wedge-like dielectric structures can help damp the strong non-SPR beam. Further extension of the cathode damper and adjusting the dielectric constant makes the SPR beam became dominant as show in this simulation. The dielectric dampers are critical in obtaining a strong SPR emission.

Using this basic setup, one can develop a simulation for special SPR emission which is generally obtained by narrowing the grooves inside the grating.

4.3.2 A6 Magnetron 1: Modes (a6Magnetron1Modes.sdf)

Keywords:

magnetron, cavity modes, A6

Problem Description

This VSimVE example simulates MIT's cylindrical A6 magnetron cavity with no outlets in three dimensions. The structure is generated using shape primitives within the VSim composer. The cavity is excited by a sinc pulse ping using a distributed current source within one of the resonant cavities. The spectrum of the cavity is used to find the modes, and FDM is used to extract the exact mode profile of the cold cavity.

This simulation can be performed with a VSimVE license.

Opening the Simulation

The A6 Magnetron example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Radiation Generation* option.
- Select "A6 Magnetron 1:Modes" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the setup window as shown in Fig. 4.62. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

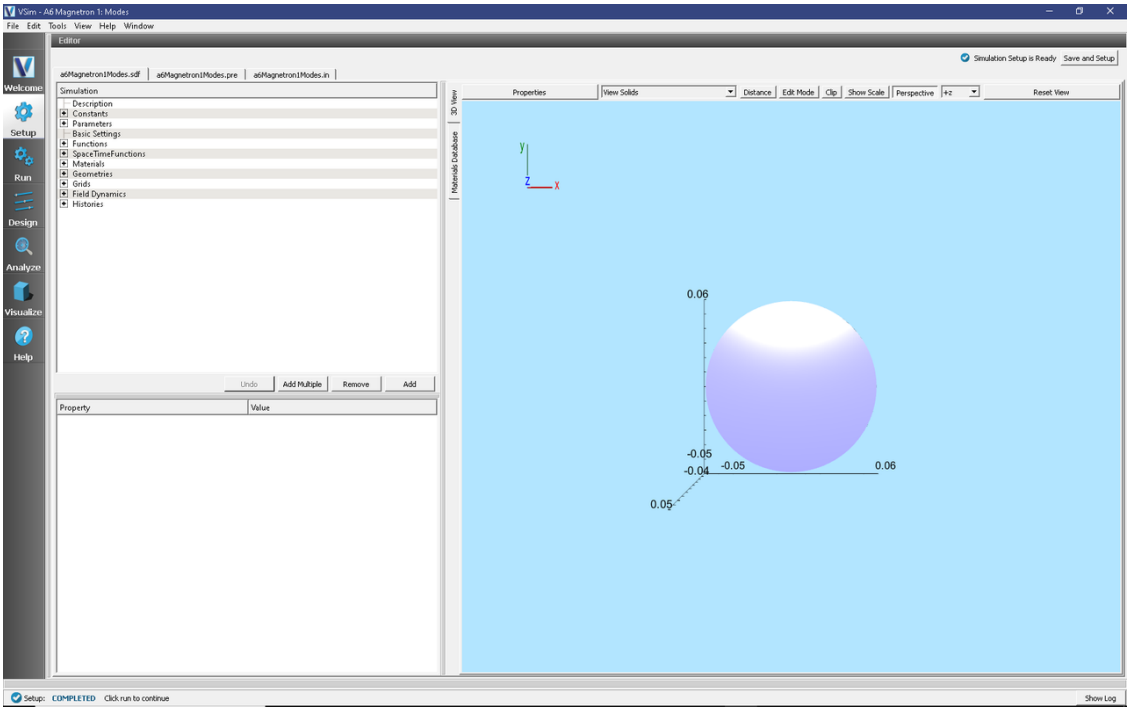


Fig. 4.62: Setup window for the A6 Magnetron example showing cathode and anode vanes only.

Simulation Properties

The A6 Magnetron example includes several constants for easy adjustment of simulation properties. User changeable parameters include:

- **RADIUS_ANODE** → Inner radius of anode.
- **RADIUS_ANODE_OUTER** → Outer radius of anode.
- **ANGLE_CAVITY** → Angle of resonant cavity openings, in degrees.
- **THICKNESS_WALL_OUTER** → Thickness of all walls.
- **WIDTH_VANES** → Total width of anode vanes in z-direction.

- **RADIUS_CATHODE** → Radius of the emitting section of the cathode.
- **RADIUS_CATHODE_INNER** → Radius of the inner section of the cathode.
- **WIDTH_CATHODE** → Width (in z-direction) of the emitting section of the cathode.
- **FREQ_LOW** → Lower frequency of excitation source range.
- **FREQ_HIGH** → Upper frequency of excitation source range.
- **(X,Y,Z)POS_CURR** → Position of excitation distributed current source.
- **(XY,Z)SIZE_CURR** → Size of excitation distributed current source region.
- **(X,Y,Z)POS_HIST** → Position of electric field history.

The axis of the cavity coincides with the z-axis and the center is at z = 0. The emitting cathode region is 4.0 cm long. All surfaces are perfect electric conductors. Histories of the electric and magnetic fields are taken at the inside of one of the cavities to find the modes. The FFT of the history shows the mode frequencies, and the exact value and profile is found using *extractModes.py - Extract Modes Analysis Scripts*.

The excitation frequency range can be set using the constants FREQ_LOW and FREQ_HIGH. The total excitation time is calculated in TIME_EXCITE. The simulation should be run for longer than TIME_EXCITE to allow the excitation source to complete.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 8.779733459572495e-13
  - *Number of Steps*: 10000
  - *Dump Periodicity*: 10000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.63.

The simulation is best run in two steps: The first with course dump periodicity to excite the modes, and the second with fine dump periodicity to observe the modes.

- Initially, the simulation is run for 10,000 time steps, writing one dump file at the end, to allow the current source excitation to finish.
- After the initial run, change the Number of Time Steps to 2,000, the Dump Periodicity to 50, and enter 1 into Restart at Dump Number. This will record details of the excited field after the source has finished.

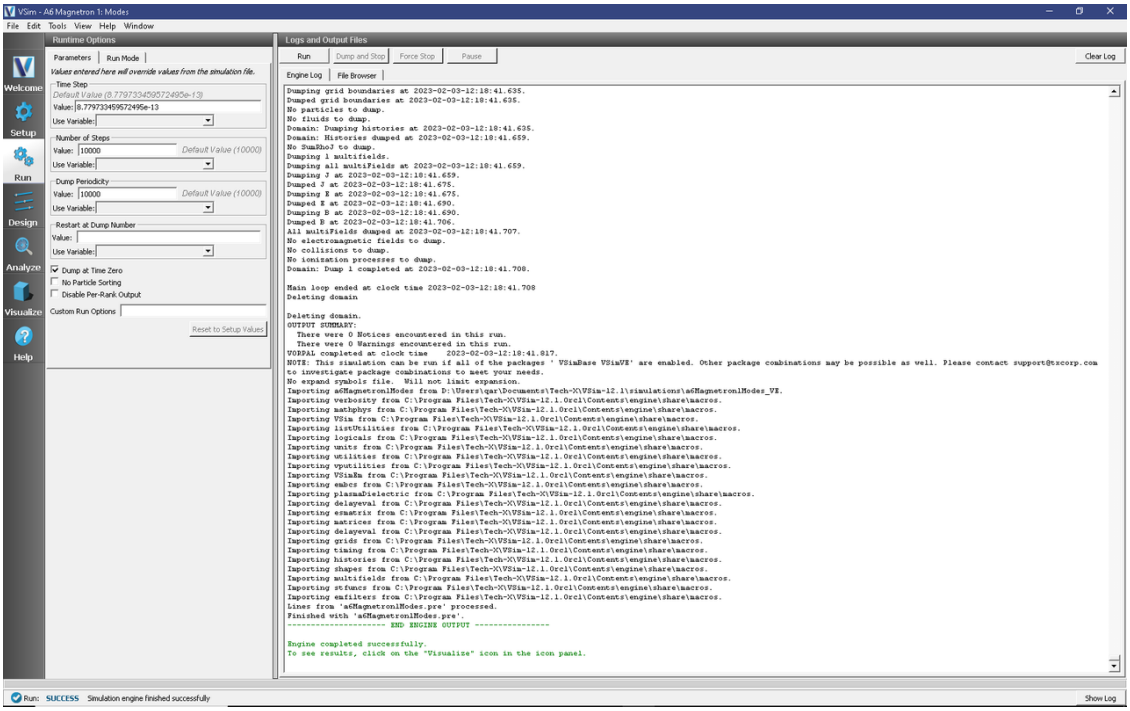


Fig. 4.63: Run window for the A6 Magnetron mode extraction example after the initial run..

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window by pressing the Visualize button in the left column of buttons.

To visualize a run to determine the resonant frequency, select *History* from the *Data View* pull-down menu. Select outE_0 for *Graph 1* and *Graph 2*, and click *Fourier Amplitudes (dB)* to the left of one of the outE_0 plot in the *Visualization Results* pane. .

- Proceed to the Visualize window by pressing the Visualize icon in the left panel.
- Select History under Data View.
- Then for Graph 2 select the *Fourier Amplitudes (dB)* checkbox * In the upper right corner of the same plot, select Limits and set X-Axis max to 1e10.
- The result should be that shown in Fig. 4.64.

Note that running the simulation longer will more sharply resolve the mode frequencies in the FFT.

Analyzing the Results

It is possible to extract the modes of the A6 magnetron cavity via post processing using the *extractModes.py - Extract Modes Analysis Script* as follows:

- Press the Analyze button in the left column of buttons.
- Select *extractModes.py(default)*.
- Enter the following parameters in the appropriate fields:
  - simulationName = a6Magnetron1Modes

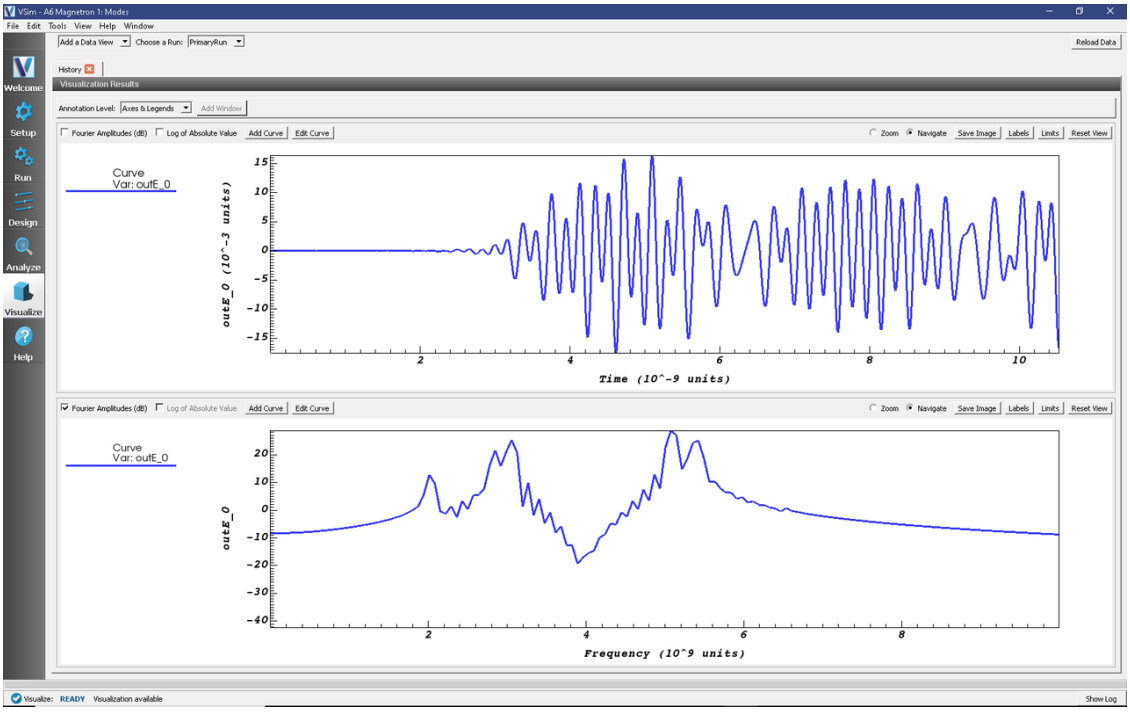


Fig. 4.64: Fourier transform of outE_0 versus time (in Hertz).

  - field = B
  - beginDump = 2
  - endDump = 41
  - nModes = 7
  - numberUniformPts = 20
  - numberRandomPts = 100
  - randomSample = unchecked
  - construct = checked
- Click the *Analyze* button in the upper right corner of the window.

Three columns of data with the titles "freq [Hz]" (Eigenmode frequency), "invQ" (inverse quality factor), and "SVD" (singular value decomposition) will be output in the right pane. The analysis has completed when you see the output "Analysis completed successfully." One can see 7 modes in Fig. 4.65.

- Proceed to the Visualize window by pressing the Visualize icon in the left panel.
- Click the 'Reload Data' button in the top-right corner.
- Select *Data Overview* under *Data View*.
- Expand *Scalar Data*
- Expand *B*
- Select *B_z (EigenB)*.
- Select the *Clip Plot* checkbox.
- Move the dump slider first to dump 2 and then to dump 5.

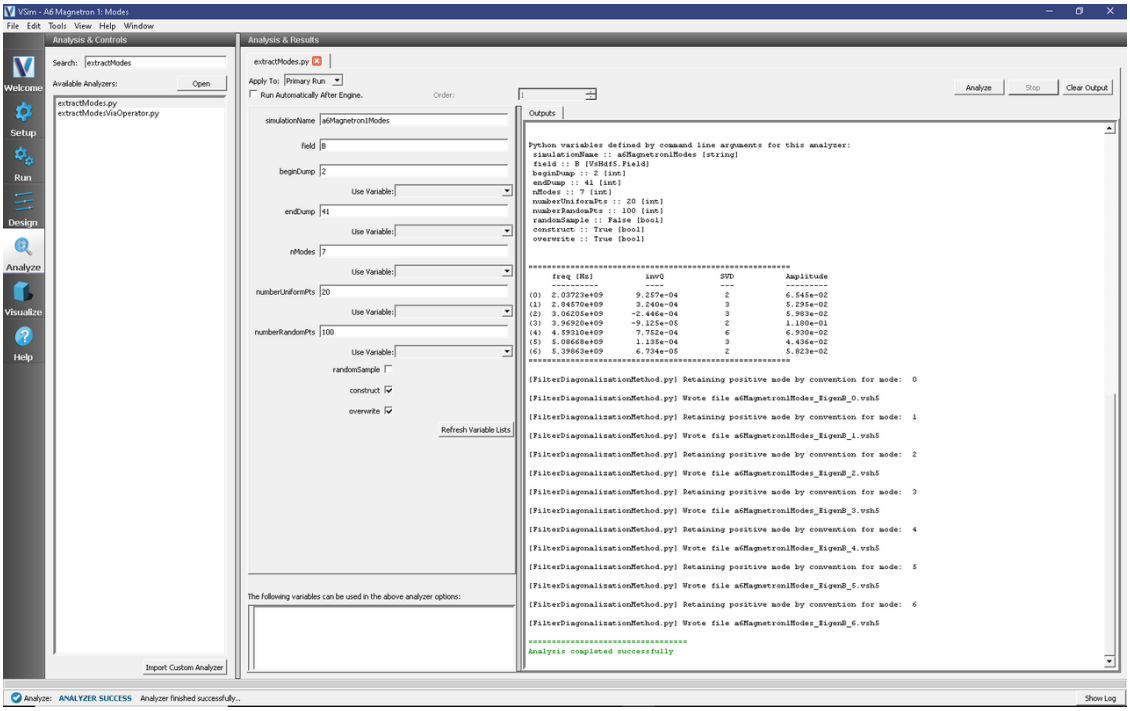


Fig. 4.65: The Analysis Window, showing 7 modes.

The axial magnetic field inside the cavity during the π and 2π mode operations are shown in Fig. 4.66 and Fig. 4.67, respectively:

Further Experiments

The values of FREQ_LOW and FREQ_HIGH can be adjusted to find additional modes, or to focus in on a specific mode. Narrowing the excitation range to fewer modes will produce a mode-accurate frequency and Q-factor extraction for the mode.

4.3.3 A6 Magnetron 2: Power (a6Magnetron2Power.sdf)

Keywords:

magnetron, bunching, space charge, A6

Warning: Due to the randomness of the particle generation, the results of this example will differ slightly with MPI ranks. To reproduce the images exactly described in this documentation, we recommend using an MPI setting of 4 cores.

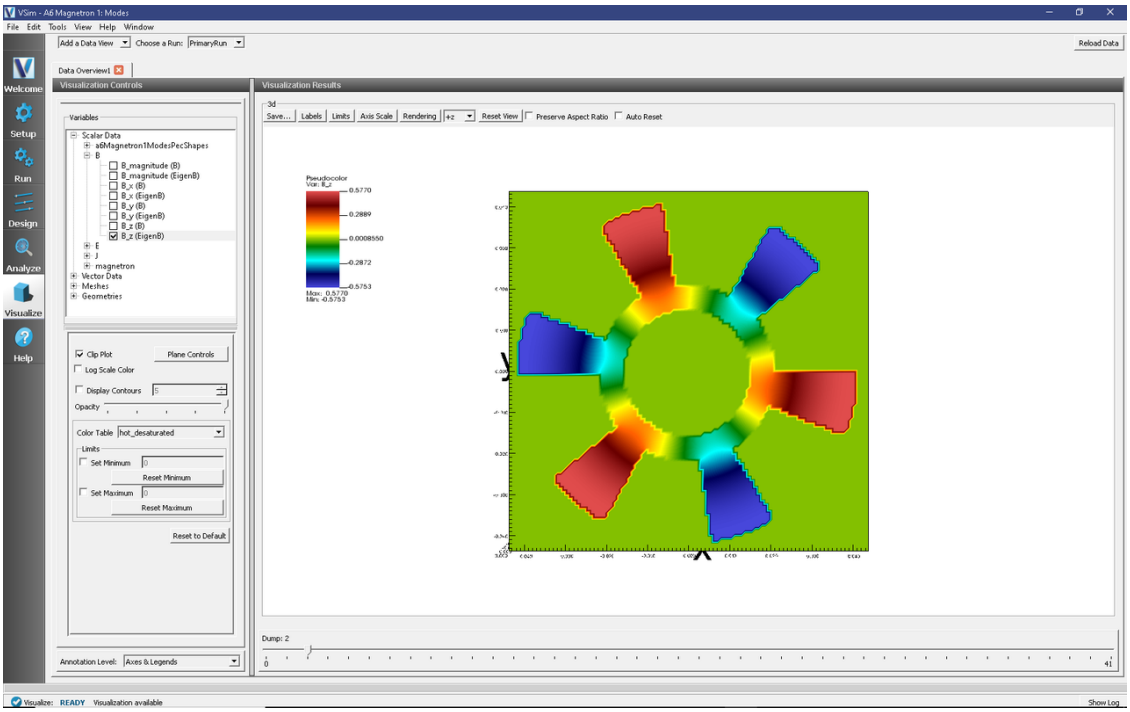


Fig. 4.66: Visualization of the axial B-field in the π Eigenmode.

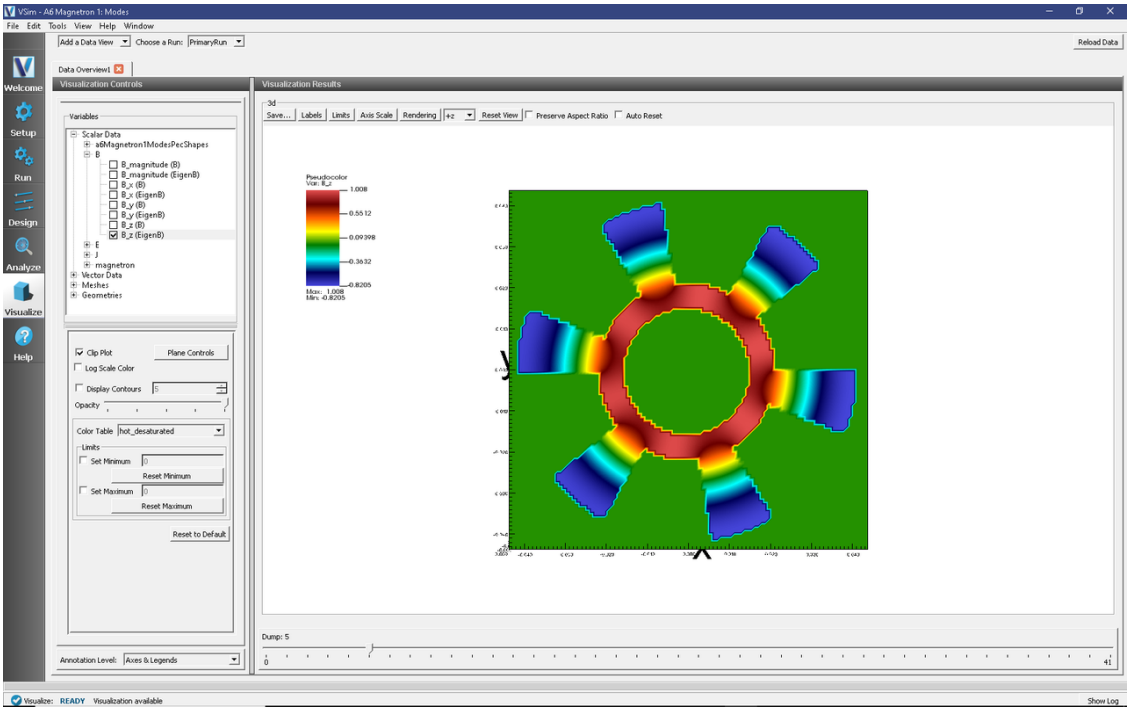


Fig. 4.67: Visualization of the axial B-field in the 2π Eigenmode.

Problem Description

This VSimVE example simulates MIT's cylindrical A6 magnetron cavity with a slot outlet in three dimensions. The geometry was defined by using VSimComposer's constructive solid geometry (CSG) capabilities. The cathode-anode voltage is ramped up from zero to around 360 kV by a current distribution source. Electrons are emitted from the emitter section of the cathode, and undergo $E \times B$ drift. Bunching of the space-charge distribution occurs and kinetic energy from the electrons is transferred to the electromagnetic modes of the cavity. If the simulation is run long enough, it will be seen that the 2π mode dominates.

This simulation can be performed with a VSimVE license.

Opening the Simulation

The A6 Magnetron example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select *A6 Magnetron 2: Power* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.68. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or de-select the box next to `Grid`.

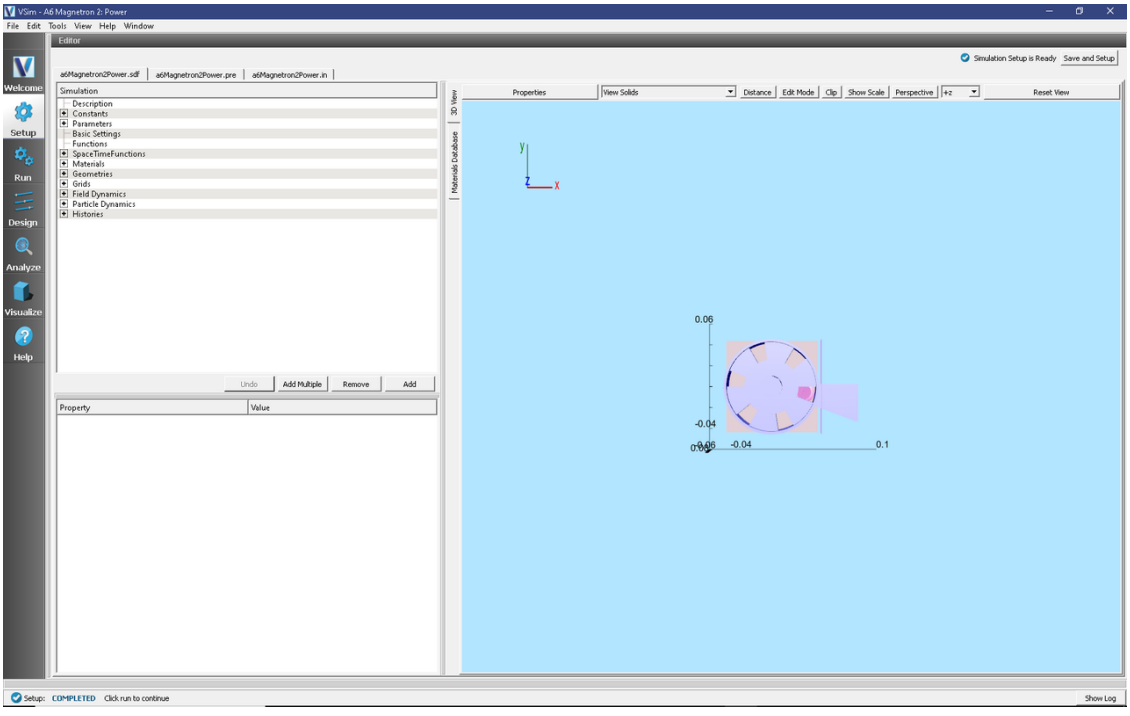


Fig. 4.68: Setup Window for the A6 Magnetron example.

Simulation Properties

The A6 Magnetron example includes several constants for easy adjustment of simulation properties. User changeable parameters include:

- **RADIUS_ANODE** → Inner radius of anode.
- **RADIUS_ANODE_OUTER** → Outer radius of anode.
- **ANGLE_CAVITY** → Angle of resonant cavity openings, in degrees.
- **THICKNESS_WALL_OUTER** → Thickness of all walls.
- **WIDTH_MAGNETRON** → Total width of magnetron in z-direction.
- **RADIUS_OUTLET** → Radius of outlet horn in x-direction.
- **WIDTH_IRIS** → Width of outlet slit opening.
- **WIDTH_VANES** → Total width of anode vanes in z-direction.
- **RADIUS_CATHODE** → Radius of the emitting section of the cathode.
- **RADIUS_CATHODE_INNER** → Radius of the inner section of the cathode.
- **WIDTH_CATHODE** → Width (in z-direction) of the emitting section of the cathode.
- **(X,Y,Z)POS_HIST** → Position of electric field history.

The axial magnetic field is uniform with a constant value of $B_z = 0.6$ T. There is an opening at the back of one of the cavities that allows microwave energy to leave the magnetron through a horn antenna and into a matched absorbing layer (MAL) boundary. A Poynting Flux history records the power output through the antenna. The emitting region of the cathode has a slightly larger radius than the rest of the cathode. There are also end caps, on either side of the vanes, in electrical contact with the cathode.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 4.876598843722272e-13
  - *Number of Steps*: 200000
  - *Dump Periodicity*: 5000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully".

This simulation is setup so that the cathode emission current and anode-cathode (AK) voltage ramp up relatively slowly (over many RF periods). Once the AK voltage is high enough, the bunching of the electrons will occur. If the simulation is run for long enough, around 100000 time steps, the 2π mode will eventually dominate as has been seen experimentally for this magnetron.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

After the simulation has been run for a sufficient amount of time, spokes will form in the electron distribution (bunching). Since the A6 is a six-cavity magnetron, operation in the 2π mode will correspond to six spokes. To visualize the spokes:

- Select *Phase Space* from the *Data View* pull-down menu
- Select *electrons_x* for the *X-axis*
- Select *electrons_y* for the *Y-axis*
- Use the *Dump* bar at the bottom of the screen to advance through the solution and visualize each dump file

Eventually, a steady state will be reached in which the electron distribution has six spokes similar to Fig. 4.69 taken at Dump 35.

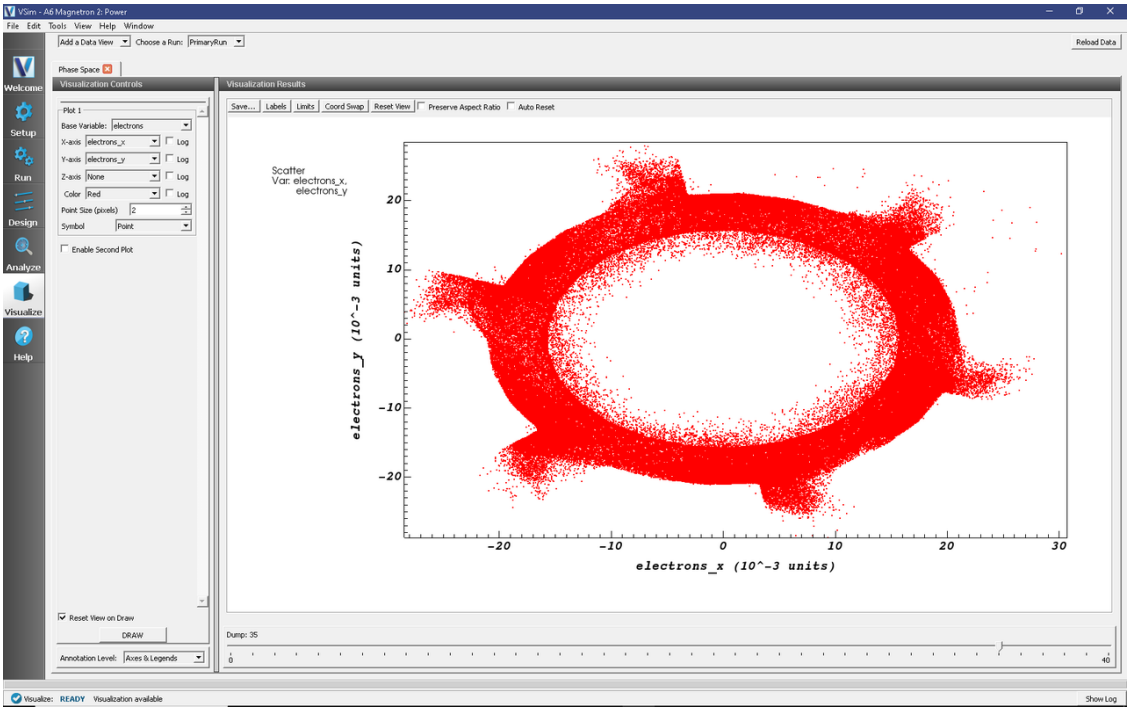


Fig. 4.69: Phase-space plot of the electron distribution showing the formation of six spokes corresponding to operation in the 2π mode.

To visualize the axial magnetic field during the 2π mode operation, proceed as follows:

- Select *Data Overview* from the *Data View* pull-down menu
- Expand *B*
- Select *B_z*
- Select the *Clip Plot* checkbox
- Check the *Set Minimum* box and set the value to -0.06
- Check the *Set Maximum* box and set the value to 0.06

- Expand *Geometries*
- Select *poly (a6Magnetron2PowerPecShapes)*
- Select the *Clip Plot* checkbox
- Move the dump slider forward in time to see the evolution.

Image Fig. 4.70 was taken at Dump 35.

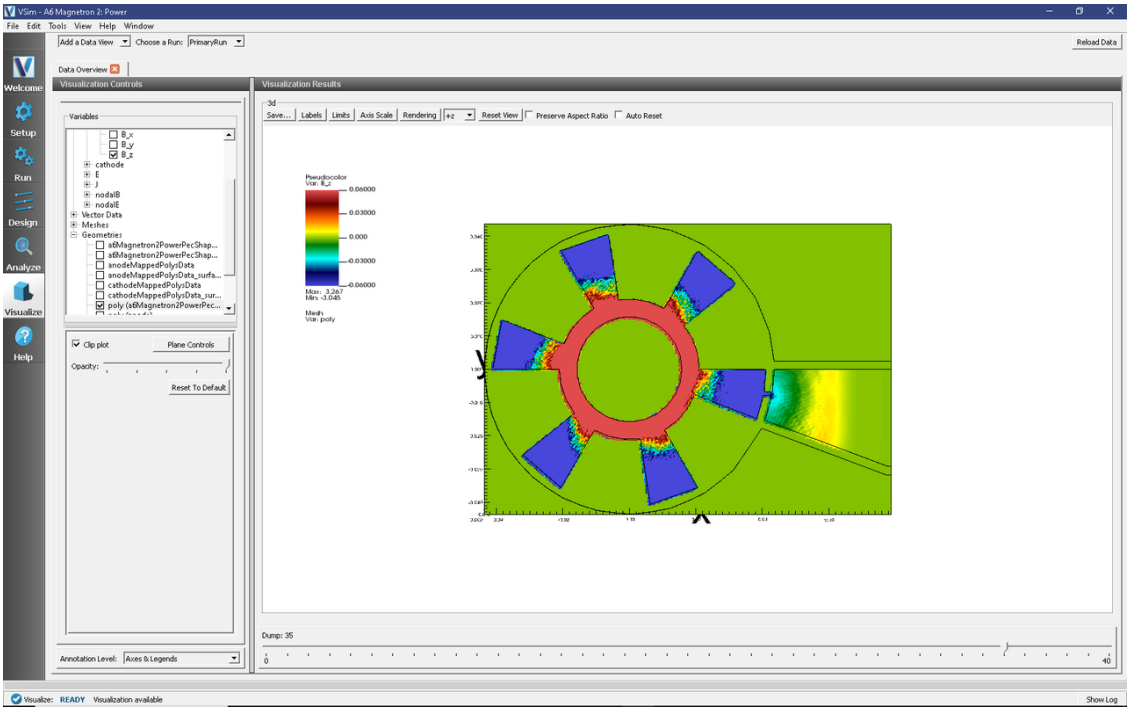


Fig. 4.70: Axial magnetic field of the magnetron operating in the 2π mode.

To determine the operating frequency:

- Select *History* from the *Data View* pull-down menu
- Select *outB_2* for *Graph 1* and *Graph 2*
- Click *Fourier Amplitudes (dB)* to the left of one of the plots in the *Visualization Results* pane
- Zoom in on the maximum of this plot to determine the approximate resonance mode frequencies

The resulting plot will resemble Fig. 4.71. If the simulation has been run for long enough, the peak at 4.6 GHz, which corresponds to the 2π mode, should be the most prominent.

Further Experiments

The power output and operating mode is affected by the E/B ratio and the geometry. The user could try adjusting the strength of the magnetic field and the geometry of the cathode, including the radius of the emitting region and the configuration of the end-caps, to see how this affects magnetron operation.

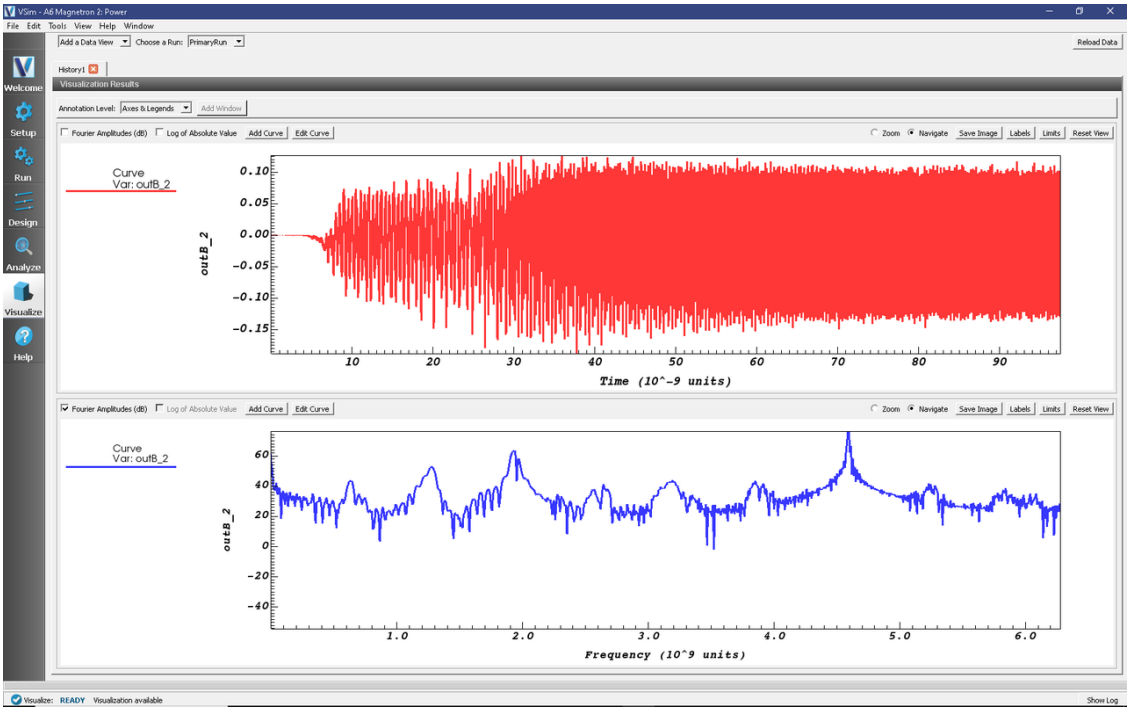


Fig. 4.71: Plot of outB_2 vs. time and vs. frequency (Fourier transform).

4.3.4 Field Emitter Array (fieldEmitterArray.sdf)

Keywords:

field-induced emission, particle beam, FEA, emitter array, Fouler-Nordheim, space charge

Problem Description

Obtaining high currents and high current densities via electron emission from cold cathodes is a high demand for scientists and engineers. Field emitter arrays (FEAs) operate via field-induced particle emission from very thin cathodes and are highly efficient. For this reason, they have been widely studied via experimental methods.

This VSim for Vacuum Electronics example illustrates how to setup a 3x3 FEA. VSim uses a cut-cell field emitter following a space-charge corrected Fowler-Nordheim emission model [1]. VSim has the capability of managing geometry structures at the micron and even nanometer range, effectively meshing single emitters and emitter arrays. In addition, VSim also models dielectric to second-order accuracy, making it possible to include dielectrics in the FEA design.

This simulation can be run with a VSimVE license.

Opening the Simulation

The Field Emitter Array example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select *Field Emitter Array* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.
- The resulting Setup Window is shown Fig. 4.72.

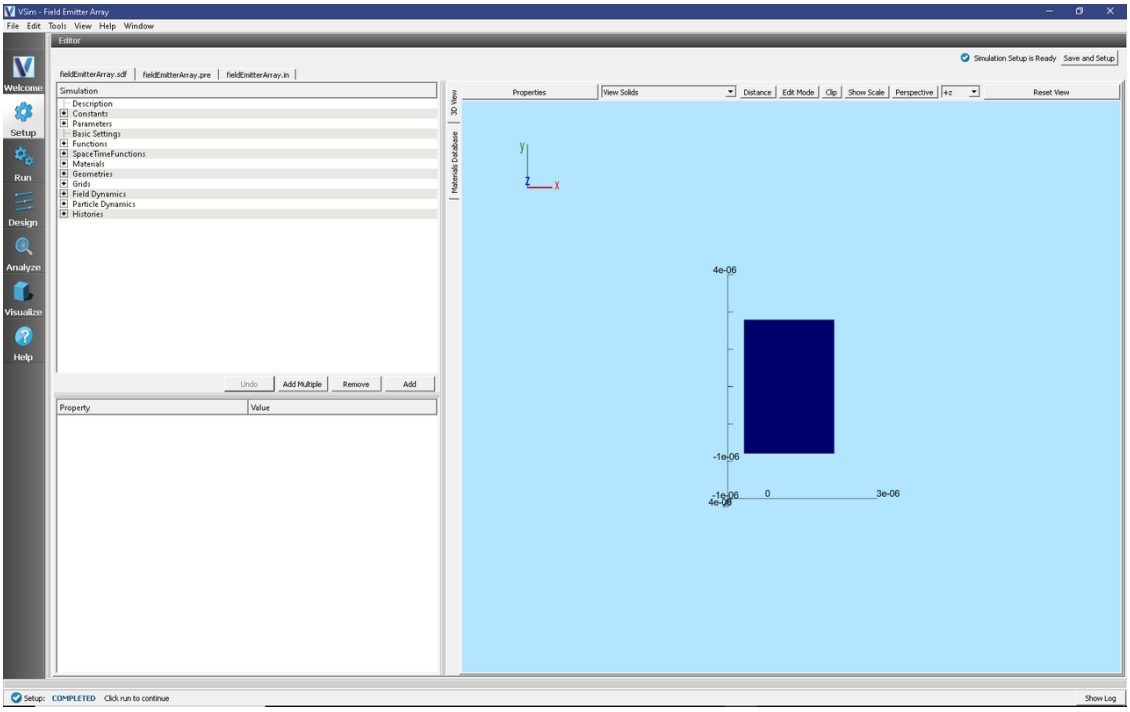


Fig. 4.72: Setup Window for the Field Emitter Array example.

Simulation Properties

The simulated device is a 3x3 field emission array with a dielectric substrate. In order to simplify the setup of the geometry, each emitter tip was set up as a thin cylinder of length of 0.55 microns and a radius of 0.05 microns. The emitter tips are 0.05 microns deep in inside the gate openings which are 0.15 microns in radius. The metal gate thickness is 0.1 microns. The distance between the emitter and the cavity wall is 1.15 microns. The distance between the centers of adjacent emitters is 1.00 microns. The metal gate was topped with a dielectric layer with a thickness of 0.1 microns. Alumina was set for the dielectric material. The voltage between the cathode and the gate was set to 100 V, while the gate to anode voltage was set to 4000 V. These voltages were set through a feedback algorithm.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.6444034218591645e-17
  - *Number of Steps*: 20000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.73.

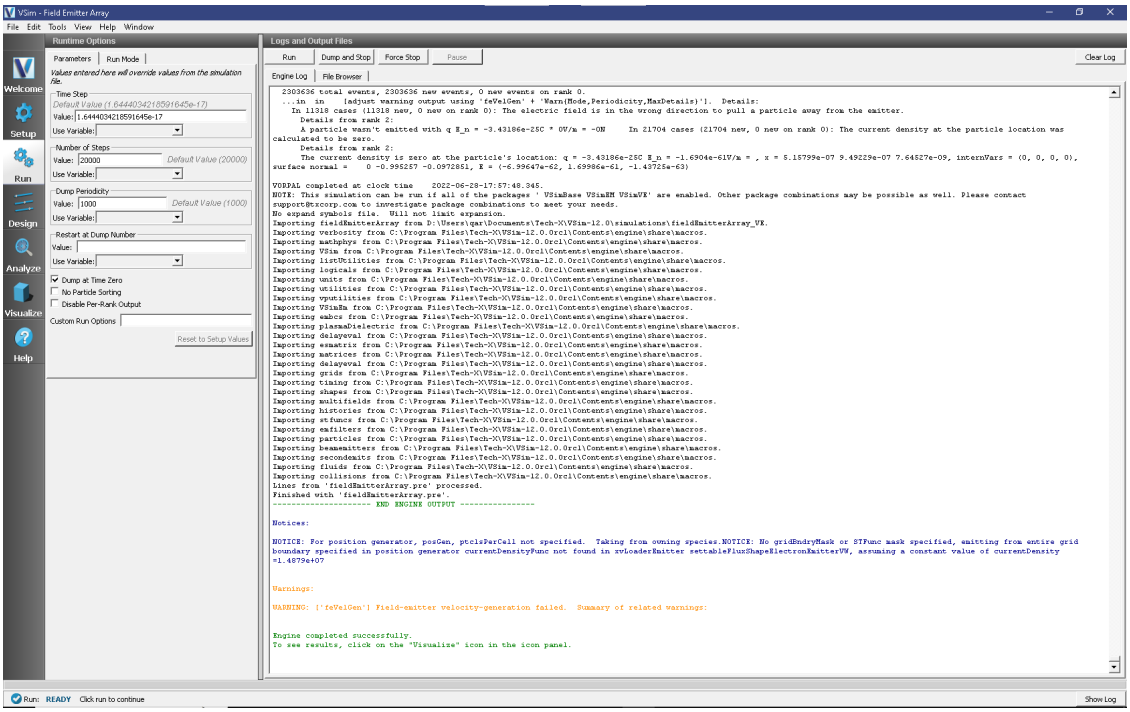


Fig. 4.73: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Data Overview*.
- In the variables tree, expand *Particle Data*.
- Select *electrons*.
- In the variables tree, expand *Geometries*.

- Select *poly_surface (fieldEmitterArrayPecShapes)*.
- Check the *Clip plot* box and select the *Plane Controls* button.
- Under *Clip Plane Normal* select *X (plane normal to x-axis)*.
- Under *Origin of Normal Vector* type *1.7e-6* and click *Ok*.
- Select *poly_surface (substrateGeomSolid)*.
- Check the *Clip plot* box and select the *Plane Controls* button.
- Under *Clip Plane Normal* select *X (plane normal to x-axis)*.
- Under *Origin of Normal Vector* type *1.7e-6* and click *Ok*.
- In the bottom of the right pane, move the dump slide forward in time.
- The resulting visualization is shown in Fig. 4.74.

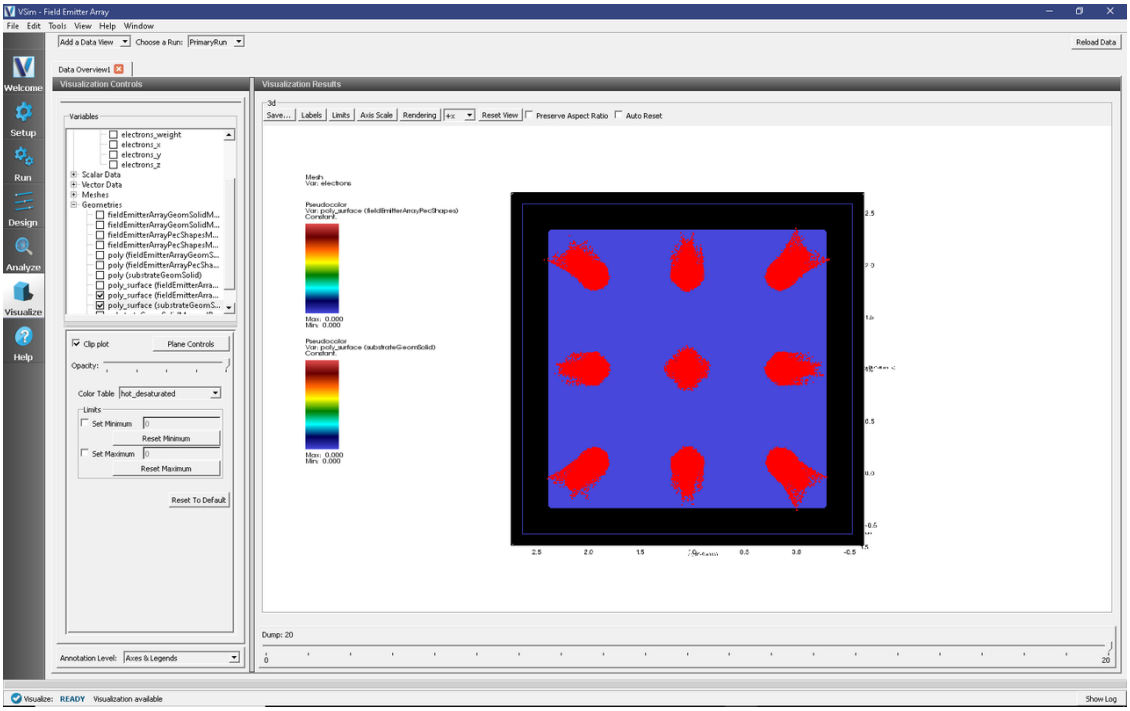


Fig. 4.74: Electron beams originating from the emitter tips behind the dielectric substrate.

To perform an analysis of the axial electric field, proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Field Analysis*.
- Under *Field* select *E_x* from the drop-down menu.
- Select *Log Scale Color Table*.
- Under *Intercept* input *6.5e-7*.
- Under *Layout* select *Side-by-side 2d/1d*.
- Click *Perform Lineout*
- Select *Controls* on the 2D plot and select *Colors*. Click *Fix Maximum* with the value *1e+10*.

- In the bottom of the right pane, move the dump slide forward in time.
- The resulting visualization is shown in Fig. 4.75.

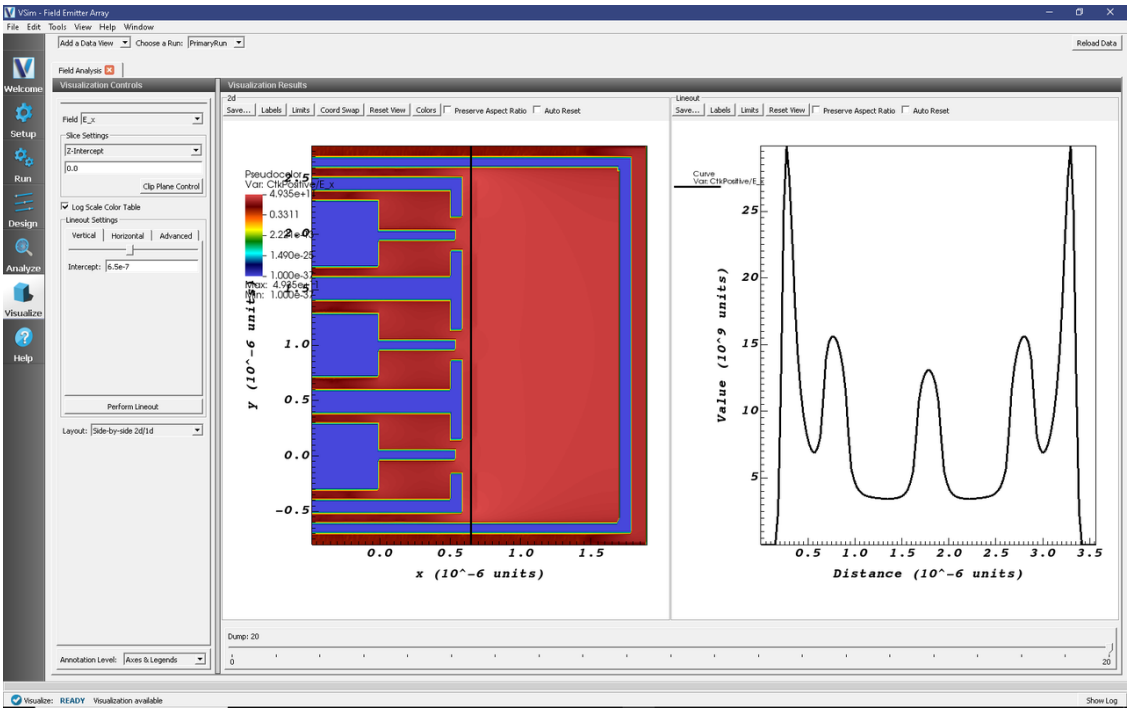


Fig. 4.75: 2D and 1D studies of the electric field which is highly space-charge dominated. The 1D lineout was performed along the dielectric substrate.

To visualize the electron energy and current histories, proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *History*.
- The resulting visualization is shown in Fig. 4.76.

To visualize the electron Px-x phase space, proceed as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- From the *Data View* dropdown menu, select *Phase Space*.
- For the *X-axis*, select *electrons_x*.
- For the *Y-axis*, select *electrons_ux*.
- Click *Draw*.
- Move the dump slider further in time.
- The resulting visualization is shown in Fig. 4.77.

Fig. 4.74 shows the first results: narrow strong beams of particles emitted from the tips of the 9 emitters. In addition, Fig. 4.75 shows the axial component of the electric field which is highly space-charge dominated. A lineout measurement is performed at the location of the dielectric substrate (right-hand image). The histories of the emitted and absorbed particle currents and the electron energy are shown in Fig. 4.76. Lastly, the distribution of field-emitted electron on the Px-x phase space is shown in Fig. 4.77.

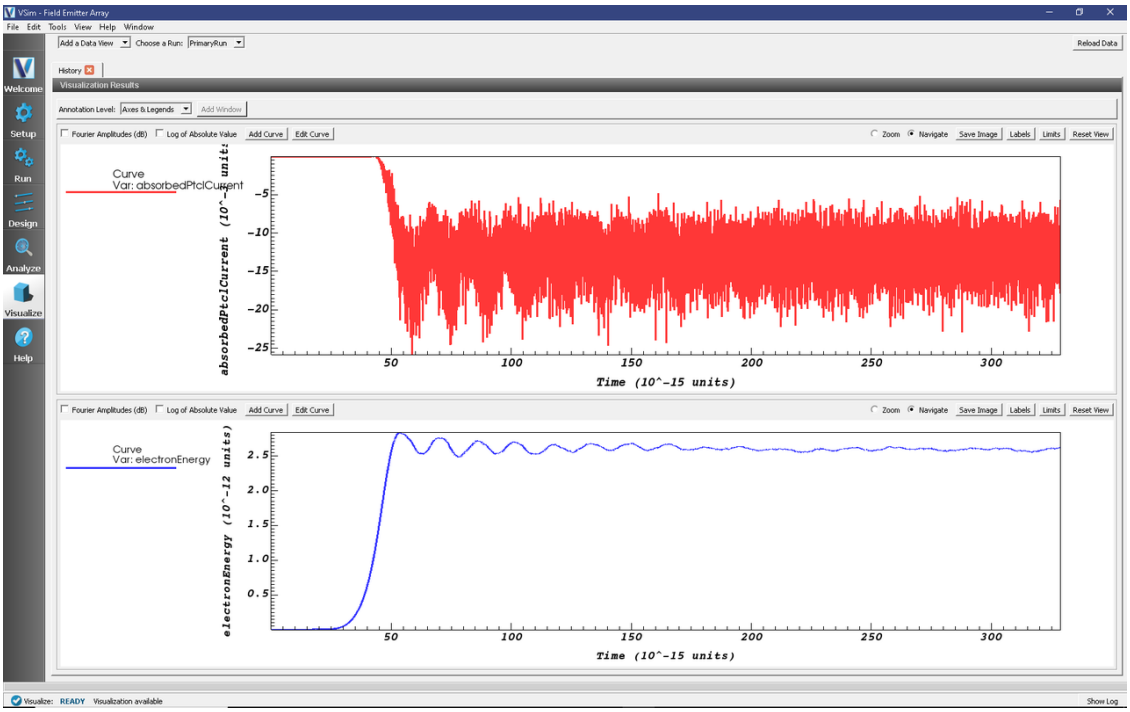


Fig. 4.76: The histories of the emitted and absorbed particle current, and the electron beam energies.

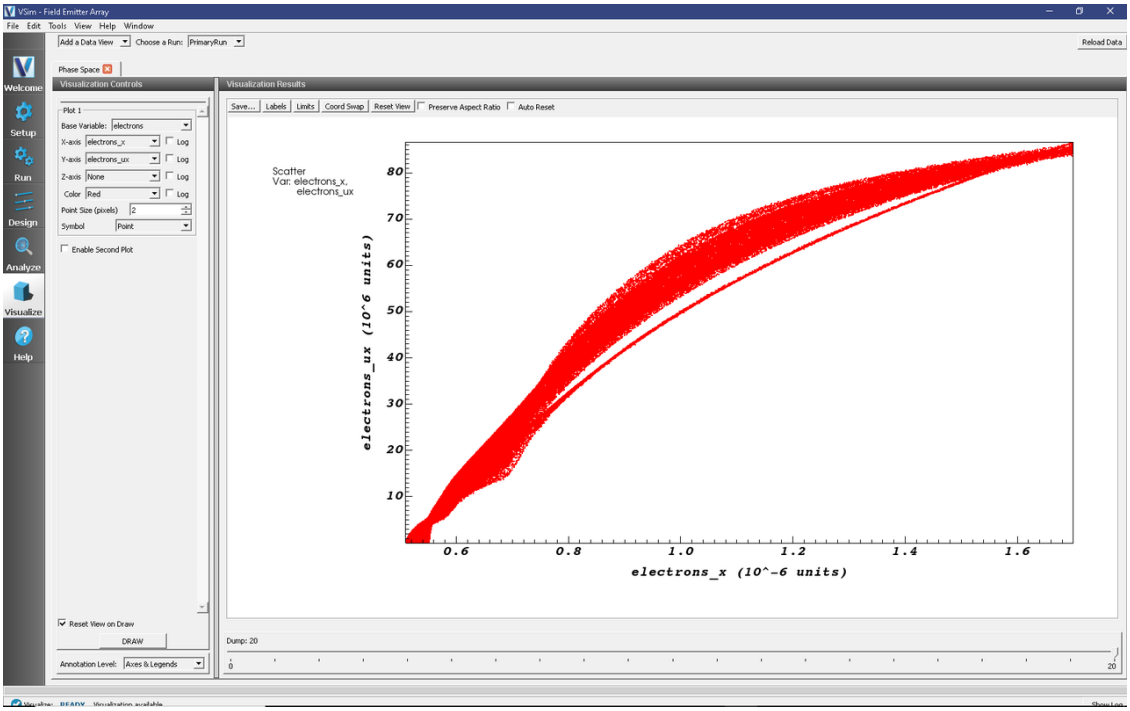


Fig. 4.77: The distribution of field-emitted electrons on the Px-x phase space.

Further Experiments

One of the first tests that can be performed easily using this simulation is to investigave how the electron emission behaves when changing the anode and cathode voltages. These voltages are defined in the setup element tree under ANODE_VOLTAGE and DC_BIAS, respectively.

Another study can be performed by changing the properties of the dielectric substrate and investigating the resulting effects. The user can edit the dielectric material properties directly in the setup window under "Materials" by selecting the material and then manually changing the property values (conductivity, permittivity, etc.) in the pane below.

4.3.5 Gyrotron Mode (gyrotronMode.sdf)

Keywords:

`gyrotron`

Problem description

This VSimVE example illustrates a very high order mode, TE-22-6, propagating in a cylindrical waveguide, very near to the cutoff frequency, which is a common situation in a gyrotron. The example is intended to allow investigation of the axial phase and group velocity of such a mode, as a function of frequency, and to highlight the intricacies of simulating a mode that is propagating within a percent or two of its cutoff frequency.

This simulation can be performed with a VSimVE license.

Opening the Simulation

The Gyrotron Mode example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select "Gyrotron Mode" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 4.78.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 4.78.

Simulation Properties

There are only two geometrical input parameters; the waveguide radius and length. The user may also control the excitation frequency, the duration of the simulation, and the nature of the excitation, specifically whether it is pulsed or continuous-wave. Additional exposed parameters include the grid sizes, and the tuning of the exiting wave boundary condition, which allows for more in-depth study with this example.

The excitation may be pulsed or continuous-wave, depending on the current input values in the element tree under *Field Dynamics* → *Current Distributions* → *distributedCurrent0*. The default *J_y* and *J_z* values are *driveOffEy* and *driveOffEz*, respectively, for a pulsed driver. The user can change these values to *driveOnEy* and *driveOnEz* for a continuous driver. The two methods of driving the cavity are described in the following.

Pulsed Simulation (driveOffE)

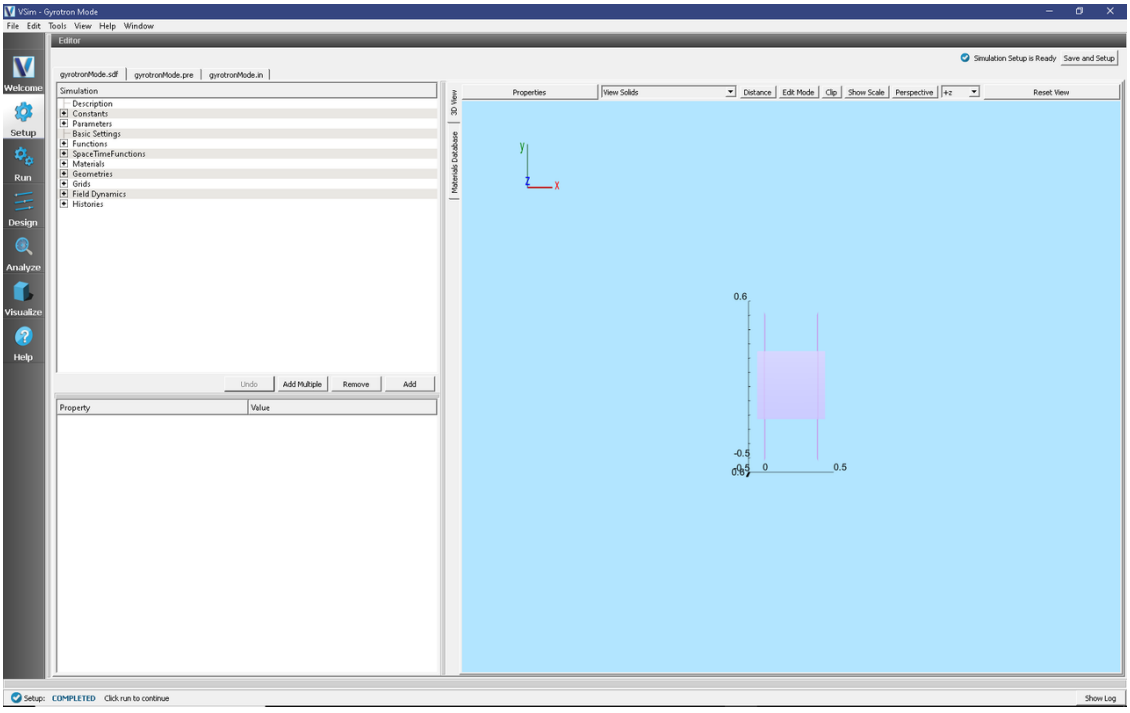


Fig. 4.78: Setup Window for the Gyrotron Mode example.

In this case, the wave is driven for half of the simulation duration, with a smooth turn-on / turn-off time window. Then, for the remaining half of the periods, the excitation propagates freely. The axial profile of the pulse will be very short, typically just one or two axial wavelengths. It will propagate slowly down the waveguide, as expected from the group velocity which is very small near cutoff. In the center of the pulse the TE-22-6 mode is preserved, but because this is a pulse, nearby modes in frequency are also present. One can observe a rich set of other mode patterns just a few grid planes away from the center of the pulse.

Continuous-Wave Simulation (driveOnE)

The drive may be kept on, instead of having it turn off halfway through the simulation. After an initial transient, this sets up a single TE-22-6 traveling wave mode pattern throughout the waveguide. This allows for accurate measurement of the axial wavenumber, beta, for the mode.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 4.433803316484881e-12
  - *Number of Steps*: 4201
  - *Dump Periodicity*: 210
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, “Engine completed successfully”. This result is shown in Fig. 4.79.

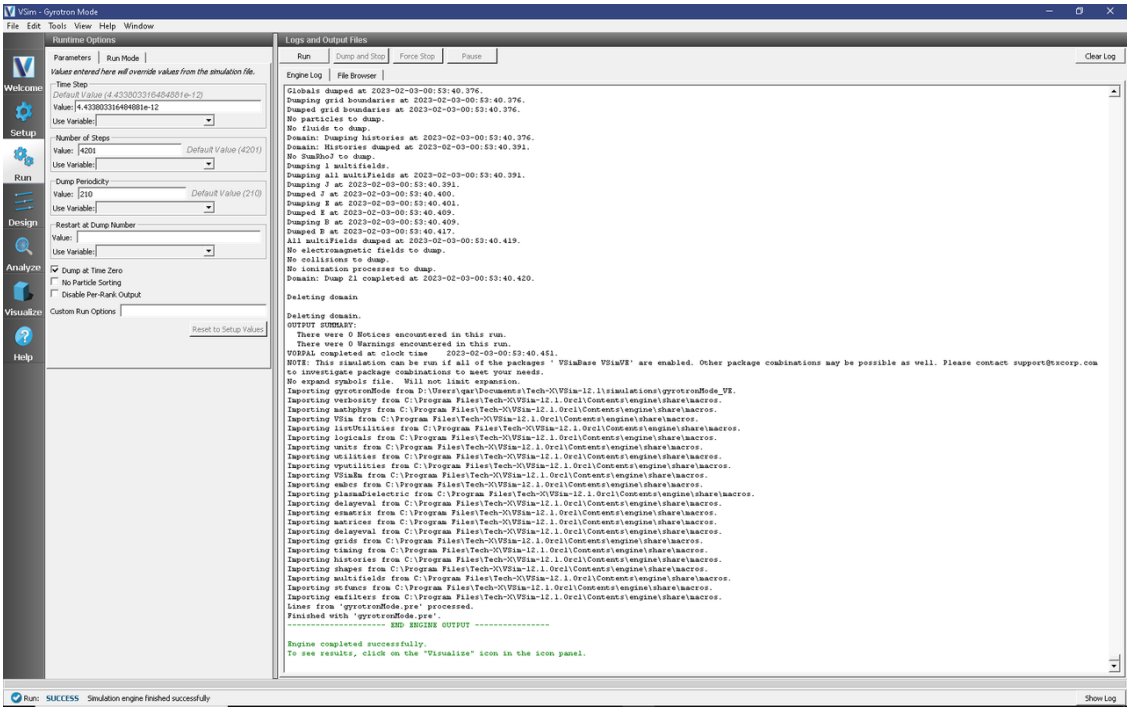


Fig. 4.79: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The B_x field is the best component for looking at in this simulation, as shown in Fig. 4.80.

- Expand *Scalar Data*.
- Expand *B*
- Select *B_x*
- Using the cursor, grab the image and rotate it from right to left by 90 degrees.
- Move the dump slider to dump 11.

The initial parameters are selected so that the excitation frequency is just barely above cutoff. While the axial phase velocity is high in this case, the group velocity is quite low, and the simulation shows a narrow wavepacket slowly moving down the length of the tube, while remarkably still maintaining the very high order TE-22-6 pattern. Contamination of the pattern increases as the duration of the excitation is reduced, since more frequencies are brought into the transient. The user is encouraged to look at the mode pattern and contamination properties as frequency and duration are varied.

The TE-22-6 mode's cutoff frequency, for the suggested initial radius of 20 cm, is known analytically to be 10.8845 GHz, which derives from the value of the 6th root of the J_{22} bessel function, which is 45.624312. However, the user will note that the suggested initial drive frequency is below this, at 10.74 GHz, and yet the wave appears to propagate! This illustrates an important property of finite-difference dispersion, that in fact the speed of light is ever-so-slightly slower in the finite-difference-time-domain simulation than in reality. In most cases, this is hardly noticed, however, when operating this close to the cutoff frequency of a waveguide, this difference can be readily seen, as this example illustrates. The discrepancy between the discrete FDTD cutoff frequency and the analytic cutoff frequency, depends on the grid resolution of the wave, and in general decreases as δx^2, where δx is the grid size.

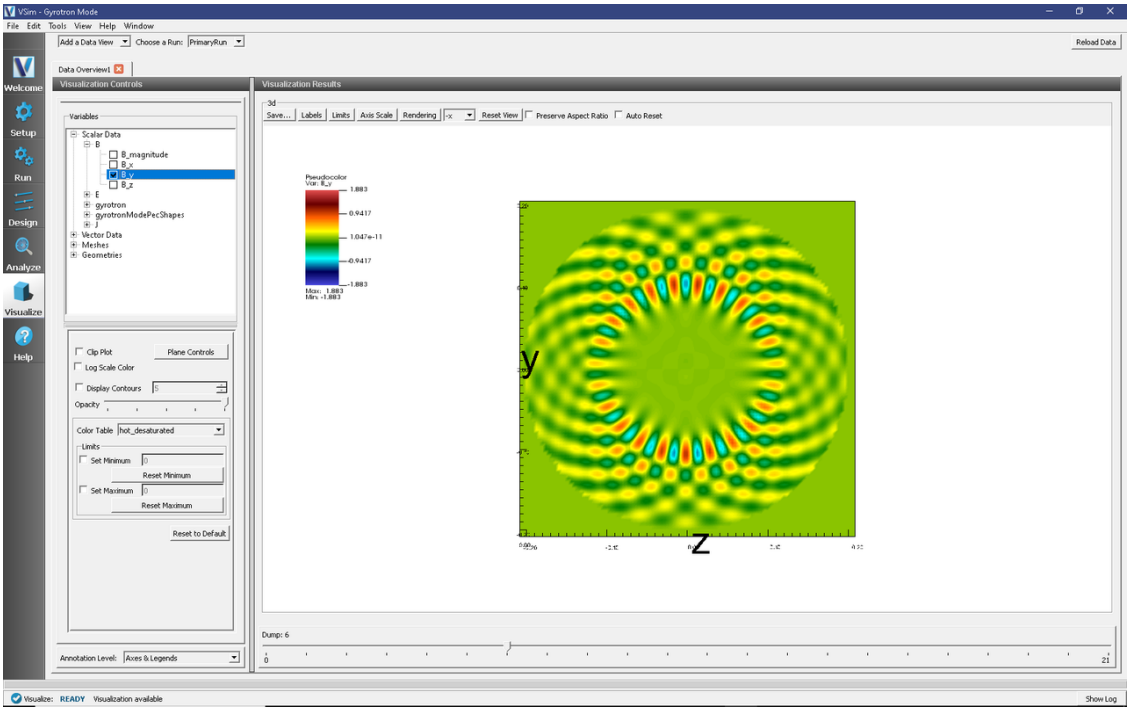


Fig. 4.80: Illustration of the mode pattern, and propagation of the mode down the length of the tube.

A very useful piece of information is the FDTD cutoff frequency. This may be found with a series of simulations, each at different drive frequencies, ω. The KEEP_DRIVE_ON parameter should be set to 1, so that the axial wavelength, β, can be measured from the field plots. A plot of ω^2 vs. β^2 should be essentially linear, with the intercept on the ω^2 axis being the FDTD cutoff frequency, ω_{cutoff}^2 ($\omega^2 = \omega_{cutoff}^2 + c^2\beta^2$), and with slope being the FDTD speed-of-light-squared. A spreadsheet showing this exercise for the suggested initial values of the example is shown below. The result of this study is that the FDTD cutoff frequency is actually 10.675 GHz, or 2% below the known analytical result, for the initial suggested grid resolution.

Further Experiments

The user is encouraged to repeat the simulations discussed in the previous section with a finer resolution, to see how the FDTD cutoff frequency approaches the analytic result as resolution improves.

The detailed TE-22-6 mode pattern is very carefully crafted using polynomial fitting functions, and is introduced into the axial magnetic field, B_x, at the left side of the simulation. There is no direct option to use a different mode, although the user may attempt to edit the detail of the input to do so.

Finally, a boundary condition tuning parameter, VPHASE_PORT, is offered to allow the user to experiment with tuning of the outgoing wave boundary condition in this near cutoff scenario. In this circumstance, the optimal phase velocity may be 5 to 10 times the speed of light.

An additional exposed user parameter, FREQ_CUTOFF, is offered, and may be used to store the value derived from the simulations discussed in the previous section. By default, this parameter is not used. However the user may look into the detail of input file, and notice a comment line that indicates how this parameter might be used to set the value of VPHASE_PORT more accurately.

Frequency	Wavelength		beta^2	omega^2
10.54	*cutoff*			4385.721
10.64	*very long*			4469.336
10.74	0.20		986.9604	4553.741
10.84	0.14		2014.205	4638.935
10.94	0.11		3262.679	4724.919
11.04	0.09		4873.879	4811.693
Cutoff Frequency		<==		**intercept**
10.675				4498.7

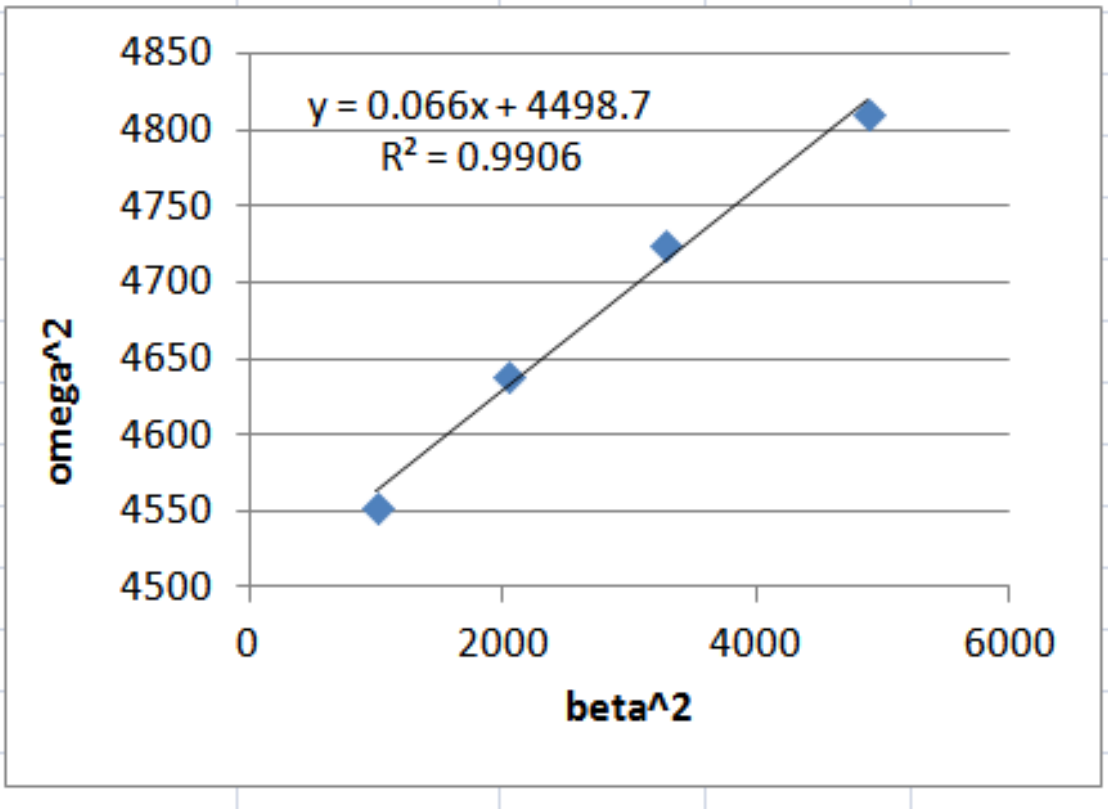


Fig. 4.81: Computing the FDTD cutoff frequency of the TE-22-6 mode.

4.3.6 Helix Traveling Wave Tube 1: Dispersion (helixTwt1Dispersion.sdf)

Keywords:

`Helix TWT Dispersion Analysis Run`

Problem description

This VSimVE example is one of a set of simulations showing different calculations to aid the design of a helix traveling wave tube (TWT) in three dimensions. The 100-turn helix with end feeds is imported from a CAD file, but all other geometrical parts are created with the Constructive Solid Geometry (CSG) capabilities within VSimComposer. The dependence of the geometries on the constants and parameters will be discussed in *Helix Traveling Wave Tube 2: Impedance and Attenuation (helixTwt2ImpedAtten.sdf)*.

This simulation addresses the dispersion analysis of the tube and as such runs with a grid covering a reduced number of helix turns. An impulse signal is excited between the helix and the body tube (which would be the vacuum interface in a real device) and periodic boundary conditions are enforced at the two ends. The tube is allowed to run for sufficiently long to observe the behavior at relatively low frequencies. We are able to recover the phase velocity of the wave on the helix (and so the structure/RF curve on an omega beta diagram) from this simulation. It differs from the other simulations of helix TWT in that the simulated region contains no coaxial coupler. As well the attenuator is outside the simulated region. For other studies of the TWT, see

- *Helix Traveling Wave Tube 2: Impedance and Attenuation (helixTwt2ImpedAtten.sdf)*
- *Helix Traveling Wave Tube 3: Power Run (helixTwt3PowerRun.sdf)*

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The Helix TWT example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select "Helix Traveling Wave Tube 1: Dispersion" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.82. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

The geometry of the helix can be made more visible by unselecting the tube and emitter disk parts under Geometries/CSG in the tree (e.g. driftTubeSolid, tubeSolid, driftTubeVoid, tubeVoid, tube, and emitterDisk) or by changing their color property and selecting a low alpha on Windows or Linux (or opacity on Mac). See color property setting in the User Guide.

setting is made available by clicking on the "Properties" button.

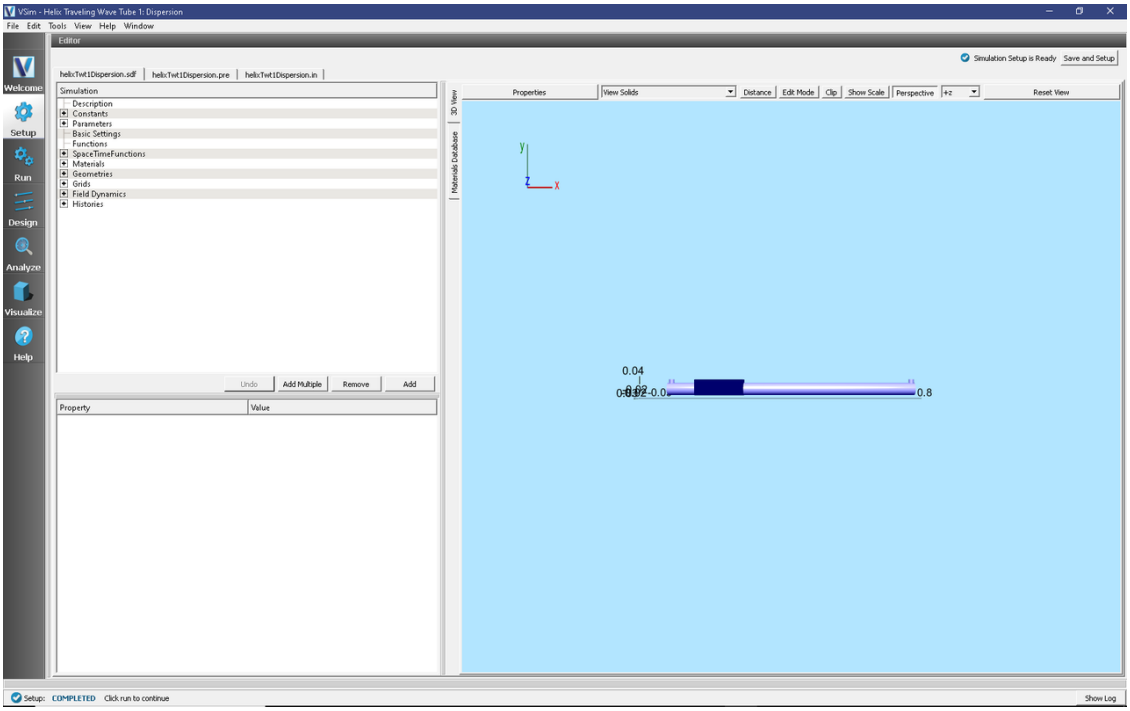


Fig. 4.82: Setup Window for the Helix TWT example.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.969479871884134e-13
  - *Number of Steps*: 300000
  - *Dump Periodicity*: 30000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.83.

The simulation allows a frequency domain analysis to be performed. In order to resolve low frequency signals, a large number of steps is required. Increasing the number of steps further may help to improve the frequency domain resolution, especially at the low frequency end of the spectrum. The Dump Periodicity may be increased to reduce the number of data dumps and save space at the expense of being able to view up to date simulation data while it runs.

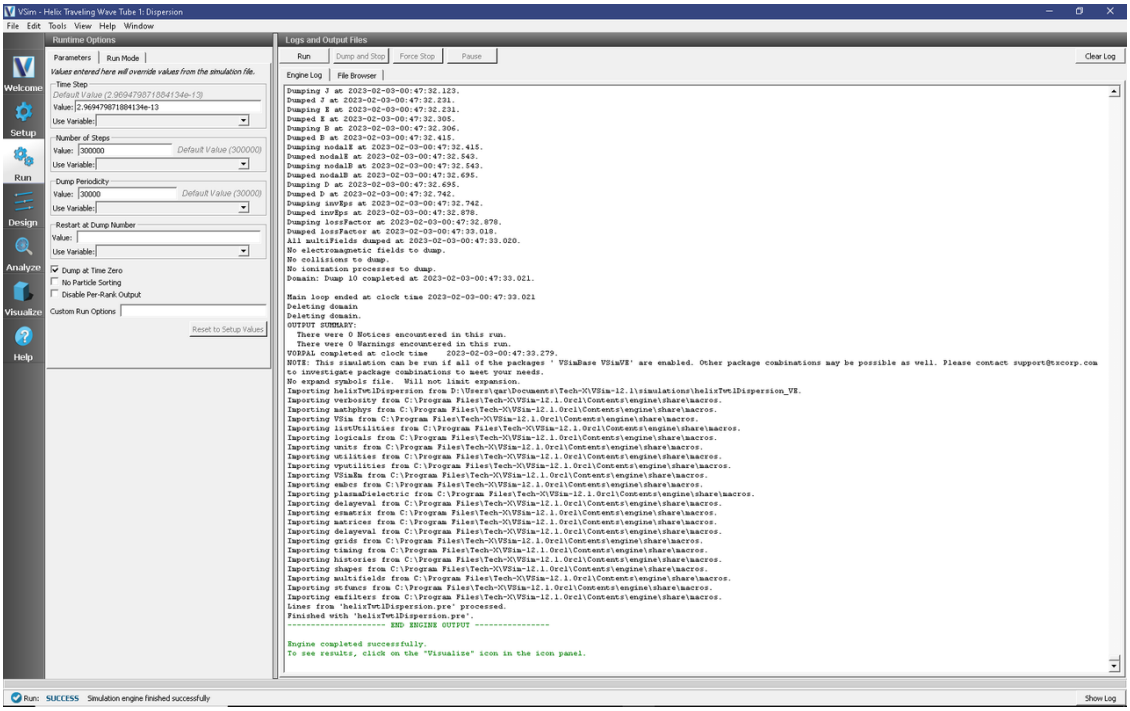


Fig. 4.83: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To see the fields inside the tube as shown in Fig. 4.84, do the following:

- Expand *Scalar Data*
- Expand *E*
- Select *E_x*
- Select the *Clip Plot* checkbox
- Select the *Set Minimum* checkbox and set to -0.05
- Select the *Set Maximum* checkbox and set to 0.05
- Select the *Display Contours* checkbox and set # of contours to 4.
- Expand *Geometries*
- Select *poly (helixTwtWithFeedsGeomSolid)*
- Click the *Clip Plot* checkbox
- Move the dump slider forward in time to see the evolution
- Click and drag to rotate the image

The wave travels along the helix, and the strongest fields occur between turns. The individual modes are not separated out in this case.

The *History* records can be used to calculate the dispersion curve:

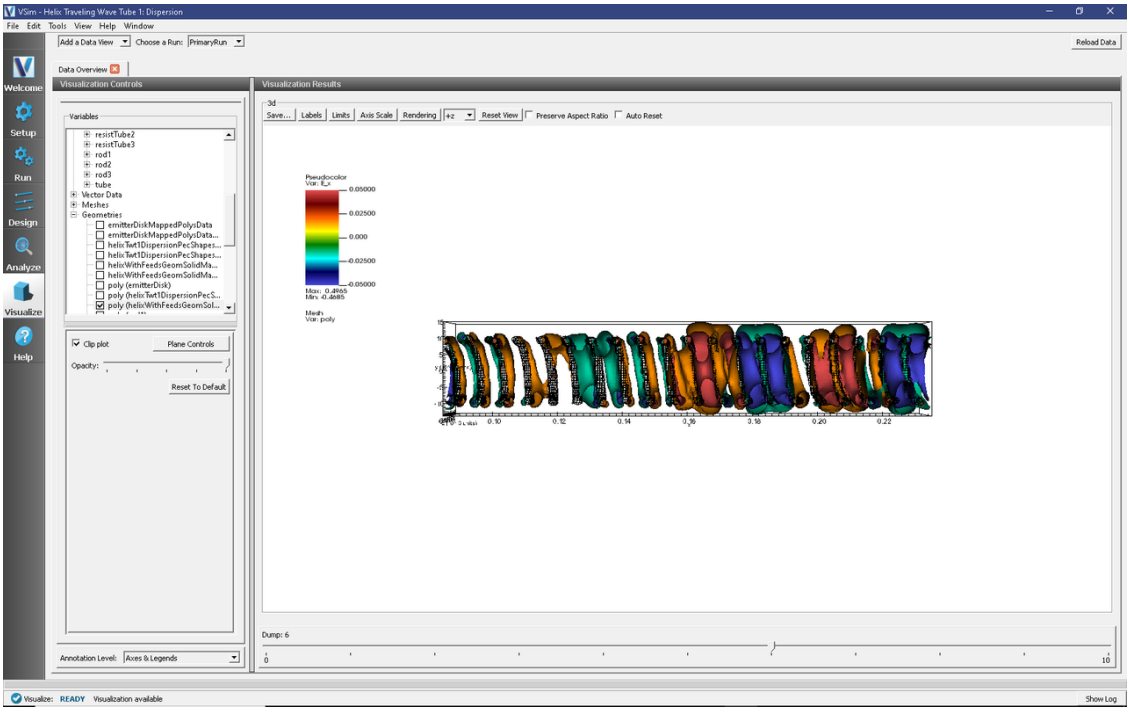


Fig. 4.84: Longitudinal field, E_x, for the dispersion run at time step 120,000.

- Select the *Add A Data View* dropdown menu and click *History*
- Set EonAxisA_0 under Graph 1
- Set EonAxisA_1 under Graph 2
- Under Graph 3 and Graph 4 change the dataset to <*None*>
- Check "Fourier Amplitudes (dB)" button at top left of plot
- Select Zoom radio button
- Using the *Limits* button above the plot set both to have limits of 0 to 2e9.

The result is shown in Fig. 4.85 (to which we have added vertical measuring lines using an external image editing software). A series of peaks can be seen. The mode frequencies correspond to the maxima of this plot. Having more than one history is important as due to mode variation in space, one history may pick up modes another misses and vice-versa.

Record the frequencies at which these peaks occur, e.g. in a spreadsheet. With the view mode switched from *Zoom* to *Navigate*, a wheel mouse can be scrolled up and down to zoom in and out. This may expedite the process of collecting the data. Or, as we have done, one can add vertical measuring lines after opening the image in some external software.

The first seven frequencies from the 300000 step simulation are listed in the table below. To determine the phase velocity v_n for each mode frequency, first note that the wave number for the n-th mode is given by

$$k_n = \frac{2\pi}{L} n$$

where L is the length of the helix TWT. The phase velocity for the n-th mode is then

$$\frac{v_n}{c} = \frac{2\pi f_n}{c k_n} = \frac{L f_n}{c n}$$

where f_n is the frequency of the n-th mode and c is the speed of light. The first 10 mode phase velocities are listed in the table below for L = 15 cm. For large frequencies, we should expect the phase velocity to approach the ratio of the helix pitch (0.75 cm) to the circumference (6.28 cm), or 0.119.

n	frequency (GHz)	phase velocity (c)
1	0.285	0.1425
2	0.555	0.1387
3	0.810	0.1350
4	1.048	0.1310
5	1.285	0.1285
6	1.520	0.1267
7	1.770	0.1264

Higher resolution and longer duration simulation could be used to better measure the frequencies and, hence, determine the phase velocity. Even more precise frequencies could be obtained by the Filter Diagonalization Method.

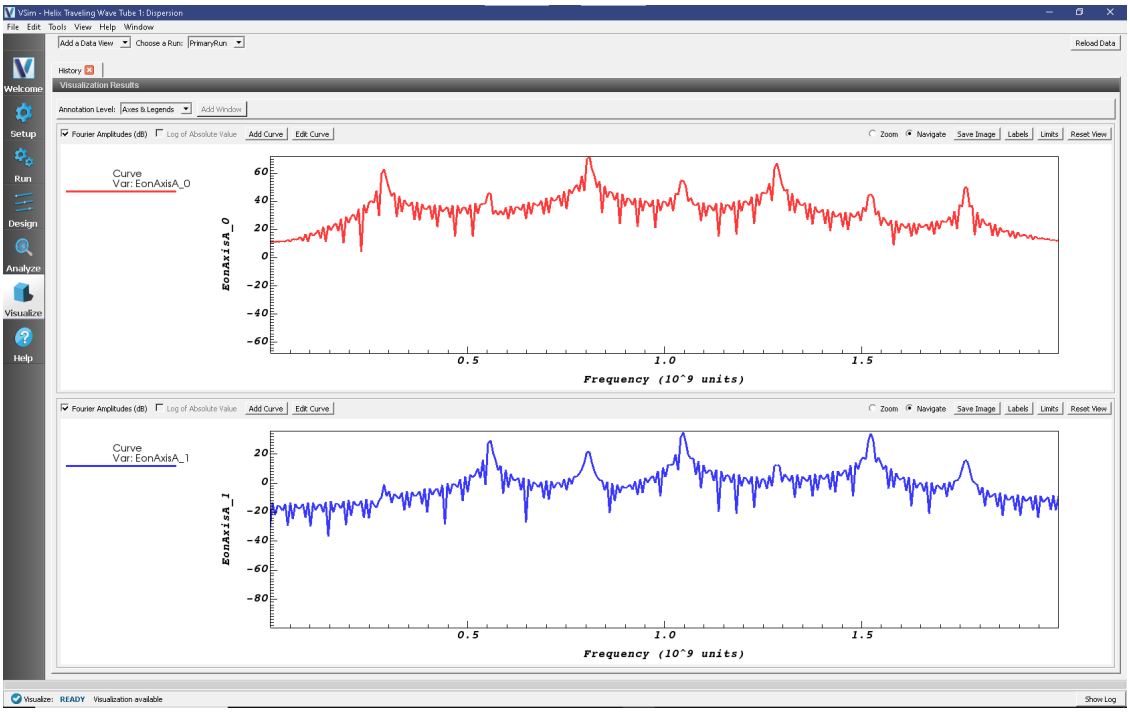


Fig. 4.85: Fourier transform of various histories after 300000 timesteps.

Further tests

The axial phase velocity is chosen to be synchronous with the beam. Adjust the helix parameters (in an external CAD editor) and observe the changes to the phase velocity.

Restarting after the default 300000 steps allows more accurate definition of the frequencies.

Use the Filter Diagonalization Method to get the frequencies more precisely.

4.3.7 Helix Traveling Wave Tube 2: Impedance and Attenuation (helixTwt2ImpedAtten.sdf)

Keywords:

Helix TWT Impedance and Attenuation Run

Problem description

This VSimVE example is one of a set of simulations showing different calculations to aid the design of a helix traveling wave tube (TWT) in three dimensions. The 100-turn helix with end feeds is imported from a CAD file, but all other geometrical parts are created with the Constructive Solid Geometry (CSG) capabilities within VSimComposer.

An input signal is sent into a short section of coaxial input waveguide and a similar section of coaxial waveguide at the opposite end of the tube provides an output power port. The geometry includes three dielectric support rods, each clad by a section of resistive tubing for attenuation. The Impedance and Attenuation simulation enables the user to calculate the transverse impedance and Pierce interaction impedance of the helix TWT. The transverse impedance is relevant for impedance matching at the input and output coaxial ports, and the Pierce interaction impedance is related to the interaction of the particles with the signal, and thus the signal gain.

The user may wish to run this simulation type multiple times, varying parameters such as the coax radius and dielectric permittivity, in order to result in a design with the correct impedance parameters.

Related simulations:

- *Helix Traveling Wave Tube 1: Dispersion (helixTwt1Dispersion.sdf)*
- *Helix Traveling Wave Tube 3: Power Run (helixTwt3PowerRun.sdf)*

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The Helix TWT Impedance and Attenuation example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select "Helix Traveling Wave Tube 2: Impedance and Attenuation" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are available in the Setup Window as shown in Fig. 4.86, with the *Elements Tree* in the upper center, and the *Property Editor* in the lower center. The right pane shows a 3D view of the geometry as well as the grid, if its visibility has been activated (which it was not when this image was captured).

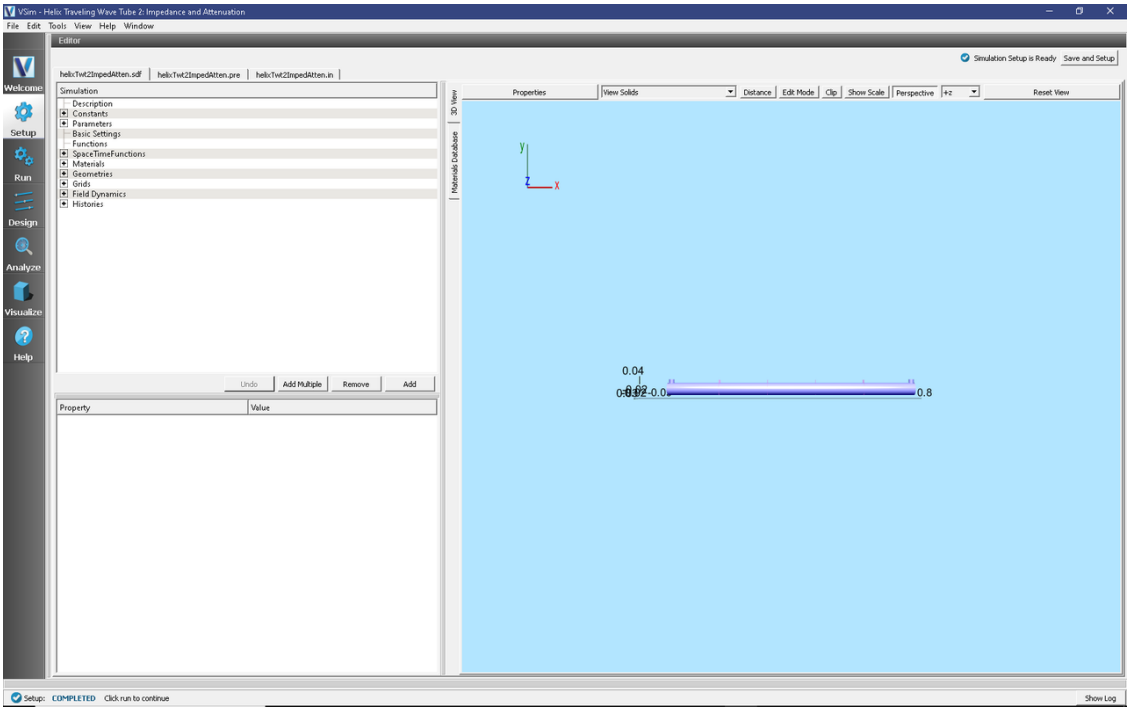


Fig. 4.86: Setup Window for the Helix TWT impedance and attenuation example.

Geometry details

The various geometrical objects can all be seen in the tree by pulling down the bar separating the Elements Tree from the Property Editor and then expanding *Geometries*, *CSG*, and *Grids*. Make sure *tube* and *Grid* are unclicked, *helixWithFeedsGeom* is clicked, and that the *Toggle Axes* button is set to remove the axes from the view. This allows one to see the interior geometrical objects, including the incoming feed, the dielectric support rods, the resistive tubes in the center, the particle emission disk at the left, and various planes where measurements are taken.

Constants and Parameters

Pulling the separator bar between the Elements Tree and the Property Editor and opening the Constants part of the tree gives the view shown in Fig. 4.88.

There are three types of constants. The first set of constants, from `PI` through `ELECMASSEV` are not changeable by the user. These are the various mathematical and physical constants that the simulation will use. The second set of constants are those with `HELIX` in the name. These must correspond to the helix geometry, the beginning, mid-radius, wire radius, pitch, and number of turns of the helix. These cannot be set arbitrarily, as the helix was imported as an STL file. Instead they must be set to match the imported helix parameters. The remaining constants define fundamental geometry quantities, such as where the tube begins and its radius, other physical simulation parameters, such as the wave frequency, and numerical parameters, such as the number of cells in each direction.

Moving the scroll bar and opening the Parameters part of the tree shows the Parameters, values that come from arithmetically combining constants and other parameters. This is shown in Fig. 4.89.

As an example, `LENGTH_HELIX` is shown. The expression shows that this is the number of helix turns times the helix pitch. It also shows the value. Of course, the expression is editable, while the value is not.

Both constants and parameters have a *description* field that allows the user to document the quantity.

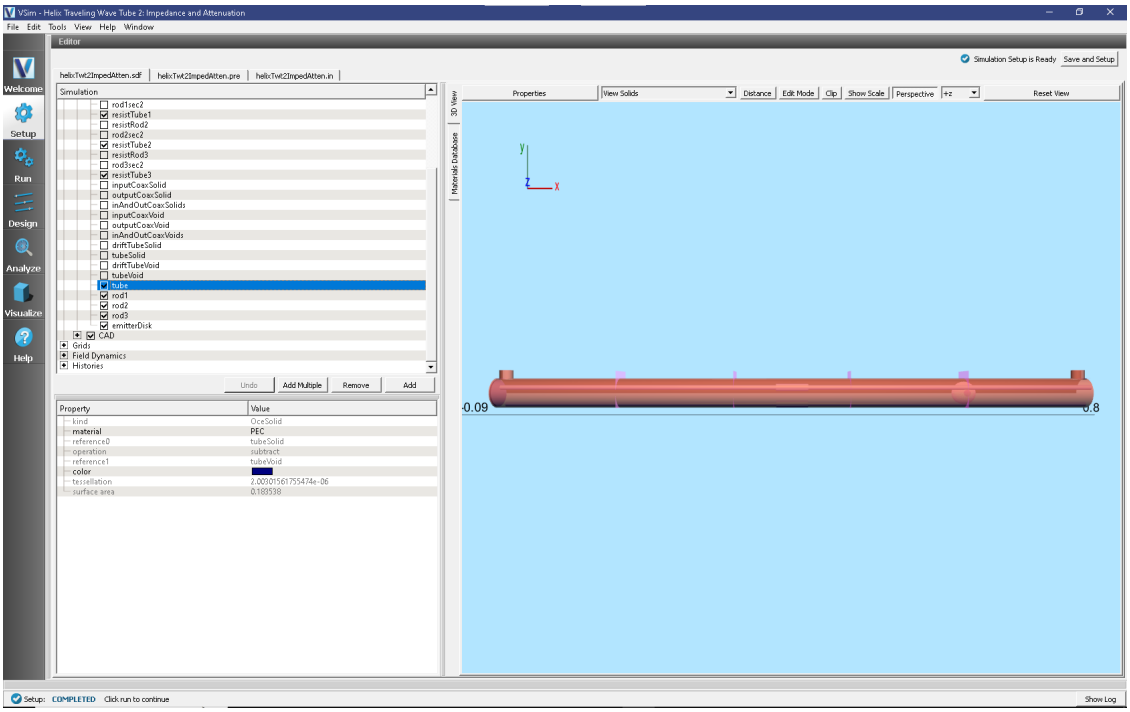


Fig. 4.87: Interior geometry for the Helix TWT impedance and attenuation example.

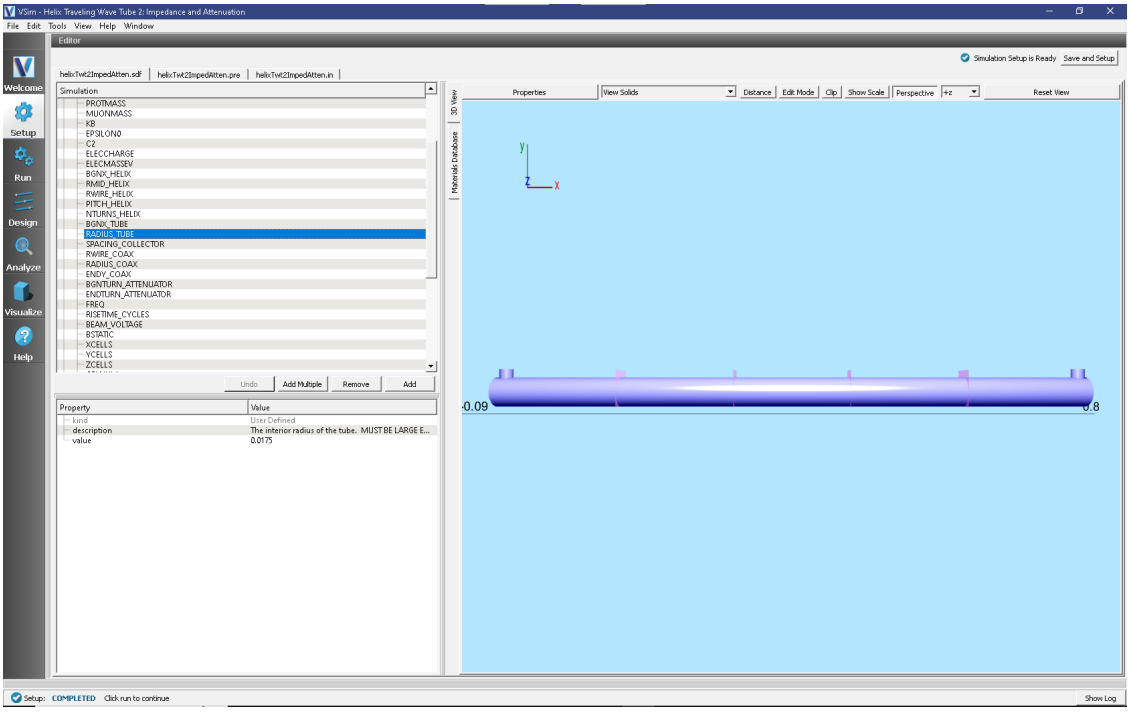


Fig. 4.88: Constants for the Helix TWT impedance and attenuation example.

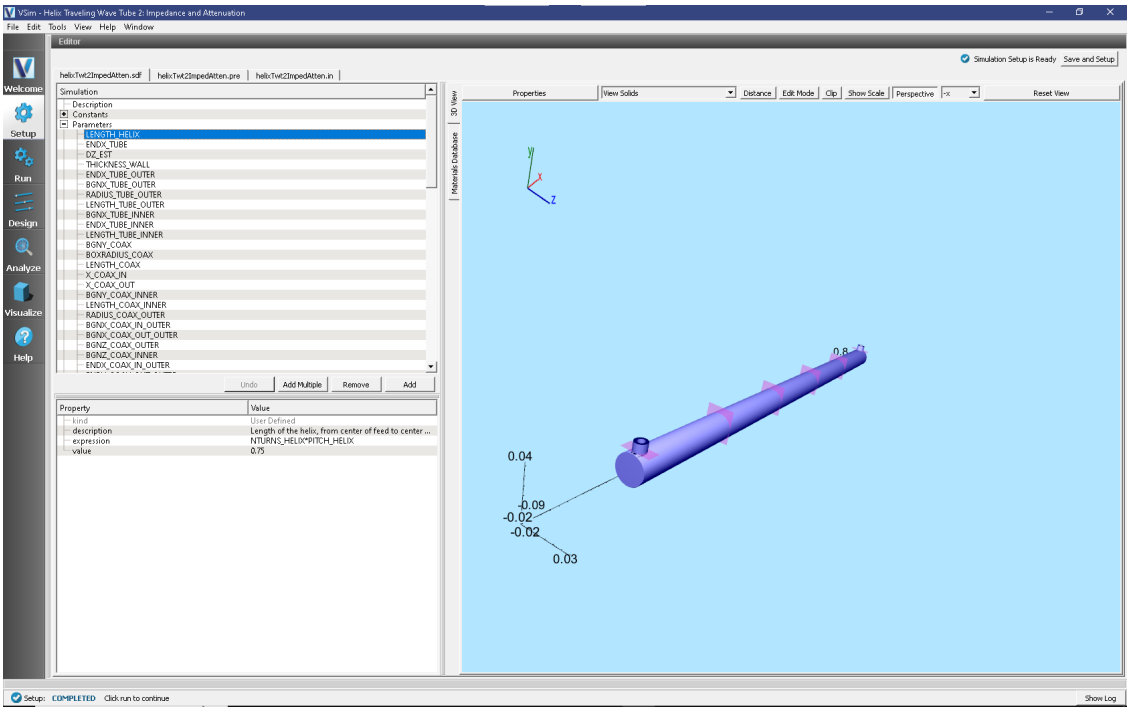


Fig. 4.89: Parameters for the Helix TWT impedance and attenuation example.

Materials

To bring materials in the simulation, in the right pane, select the *Database* tab, select one or more materials (with ctrl-click) and hit the button *Add To Simulation*. The materials will then appear under *Materials* in the tree view. At this point one can change the properties of the materials including the name. In this example we imported *resistive damper*, changed its name to *LossyMaterial*, and changed its value of conductivity to *0.55*. This is shown in Fig. 4.90.

Once one has materials in the simulation, one can set the materials of any of the geometries. Click on the geometry, then in the Property Editor pane, double click on the material value. A context menu will allow you to set the material of the geometry to any material in the simulation.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.969479871884134e-13
  - *Number of Steps*: 100000
  - *Dump Periodicity*: 2000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, “Engine completed successfully”. This result is shown in Fig. 4.91.

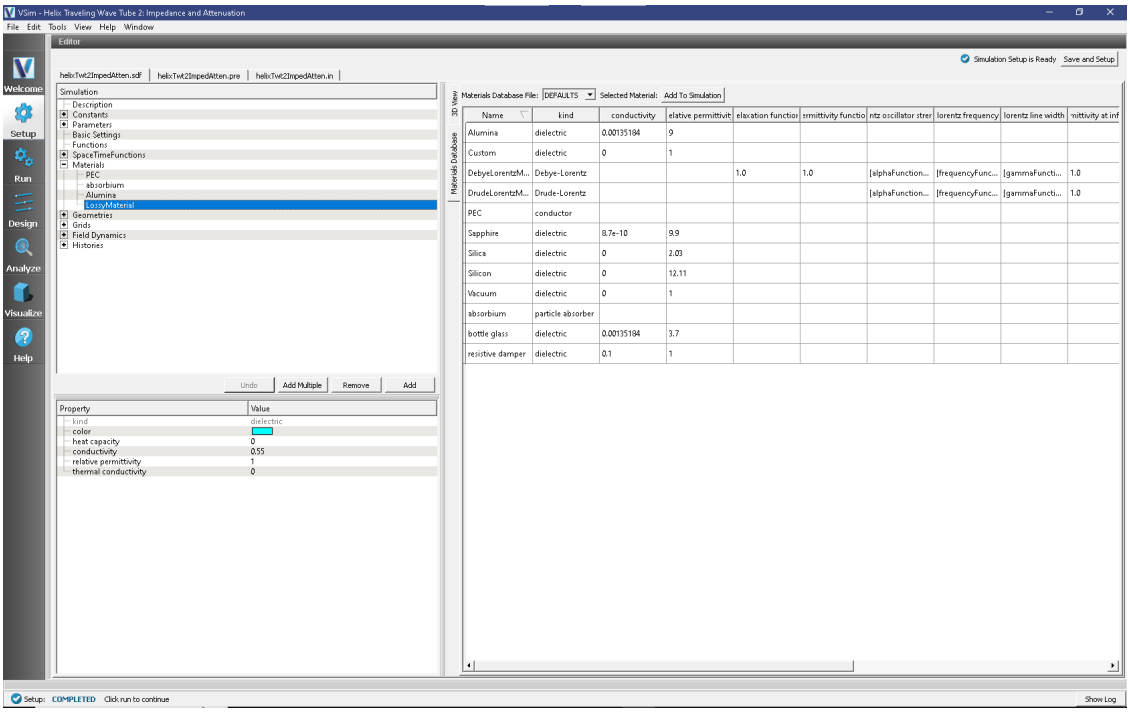


Fig. 4.90: Materials for the Helix TWT impedance and attenuation example.

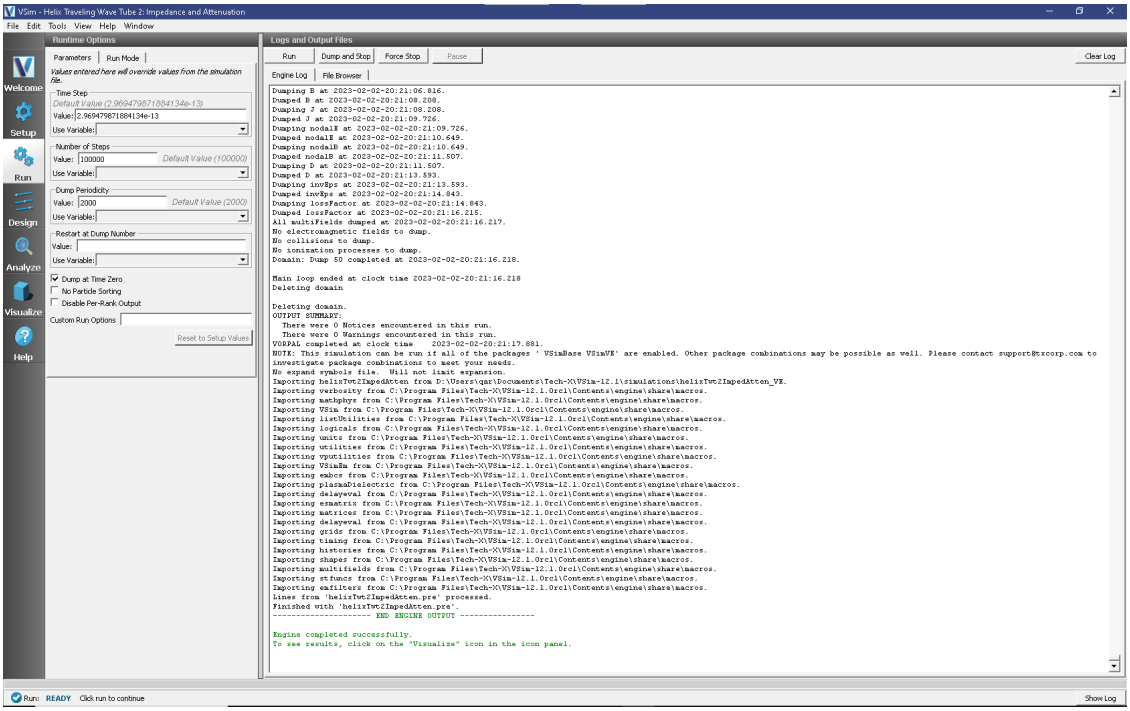


Fig. 4.91: The Run Window at the end of execution.

The simulation to determine the impedance should run long for any mismatch at the outgoing boundary to stabilize. That is, the simulation must be run long enough for the electromagnetic wave to reach the far end of the tube and for any reflections to return some distance to the last history in the tube. This will take about 100,000 steps. On a 4-core machine, we have observed 0.23s/step, so this simulation will take about 7 hours. This simulation parallelizes well up to 16 cores, so with a sufficient license and workstation or cluster, one can bring this simulation time down to about 2 hours.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To see the fields inside the tube as shown in Fig. 4.92, continue as follows:

- Select Data View: *Data Overview*
- Expand *Scalar Data* then *D*, then select field *D_y*.
- Check the *Clip Plot* box, which cuts through the data at the $z = 0$ plane.
- Check *Set Minimum* and set it to -400, then check *Set Maximum*, set it to 400.
- Expand *Geometries* then select *poly (rod1)*.
- Check the *Clip Plot* box
- Move the dump slider forward in time to see the evolution.

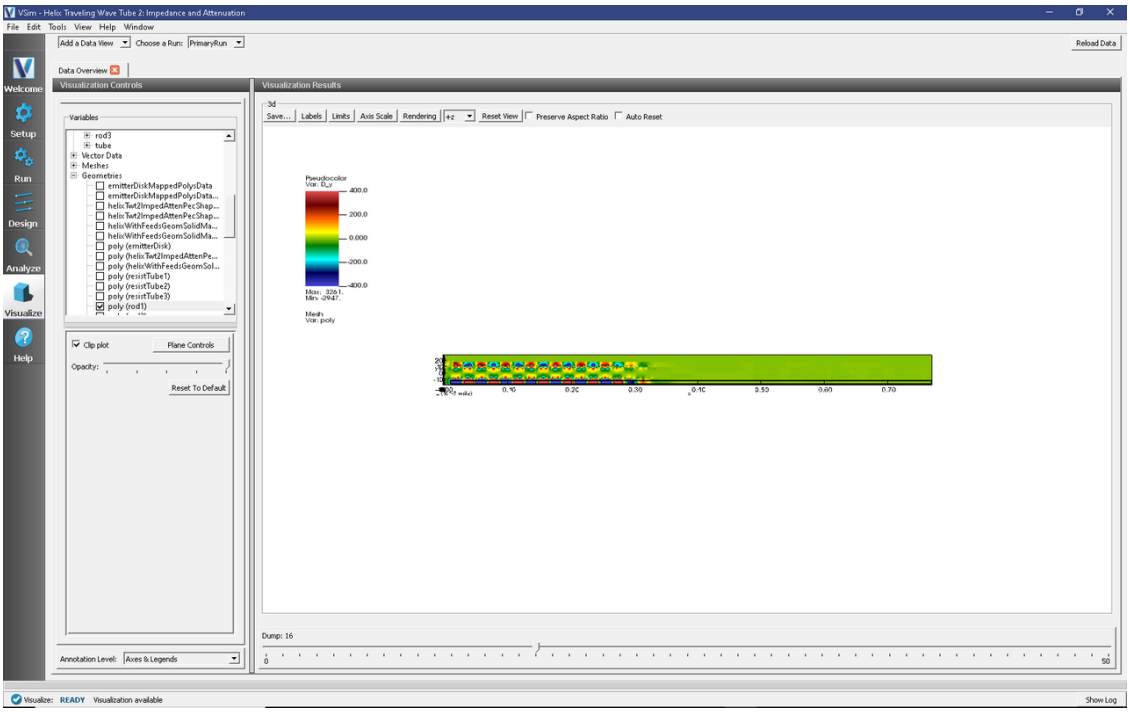


Fig. 4.92: The transverse displacement field, Dy, on the central x-y plane at dump 31.

This plot shows the transverse displacement field. Once can see that it is confined inside the tube (sanity check), and that it is most intense inside the dielectric rod at the bottom. The field is larger at the left, as it is just entering and propagating down the tube.

At any time one can leave this visualization pane to move back to the run pane to see how the simulation is progressing.

The longitudinal field inside the tube is shown in Fig. 4.93, which can be obtained by the steps:

- Select Data View: *Field Analysis*
- Select Field *E_x*.
- Select *Horizontal* under *Lineout Settings*, set the Intercept to `0`, and click *Perform Lineout*.
- Under *Layout* select *Stacked 2d/1d*
- Move the dump slider forward in time to see the evolution.

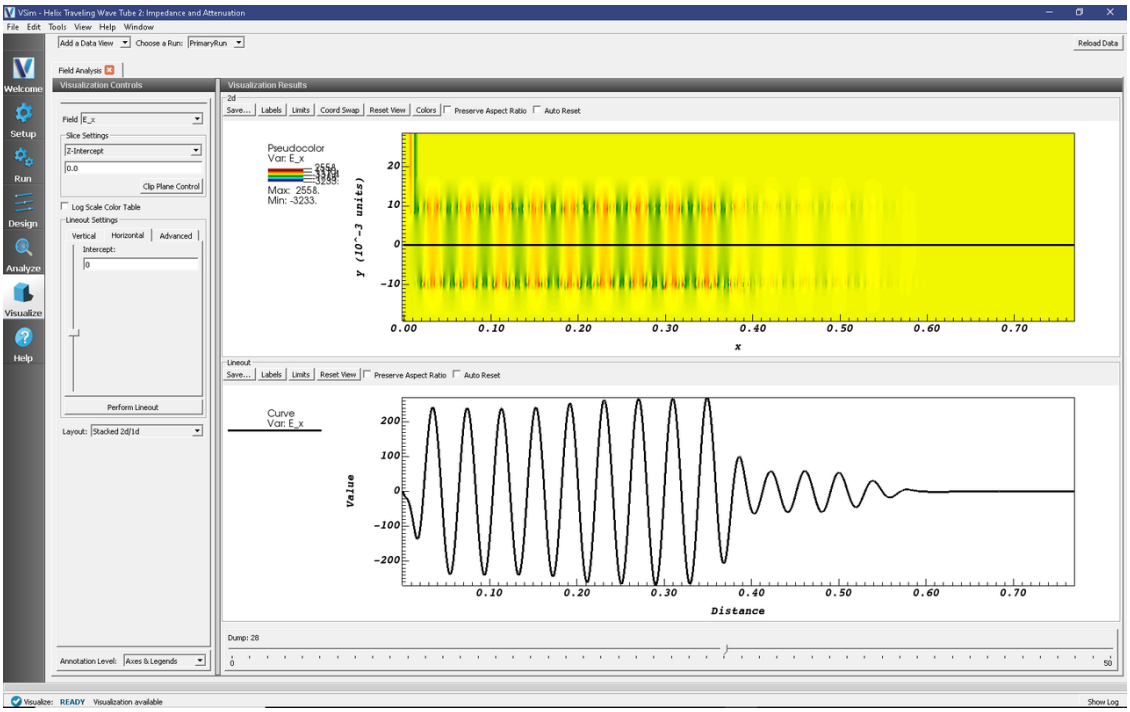


Fig. 4.93: The longitudinal field, Ex, on axis at dump 28, which is time step 56,000.

As seen in Fig. 4.93, the longitudinal field has dropped from about `240 V/m` to about `68 V/m` in the center of the simulation where the resistive tubes are. This corresponds to about `14 dB` of attenuation. The purpose of this attenuation is to have sufficient damping so that reflections coming back from the end to the beginning and then reflection again do not grow, as that would change the device into an oscillator, with energy growth that could destroy the system. If the *Helix Traveling Wave Tube 3: Power Run (helixTwt3PowerRun.sdf)* shows that this is happening, one can return to this run and increase the conductivity of the LossyMaterial or the length of the resistive tube (through `BGNTURN_ATTENUATOR` and `ENDTURN_ATTENUATOR`) to provide more attenuation.

Histories contain the time evolution of quantities defined in the input file. These can be seen by selecting the *Data View*, *History*. To determine various impedances we want particular histories obtained by the process:

- Select Data View: *History*
- Under Graph 1 select *poyntingA*
- Under Graph 2 select *transverseVoltageA*
- Under Graph 3 select *EonAxisA_0*
- Under Graph 4 select *<None>*

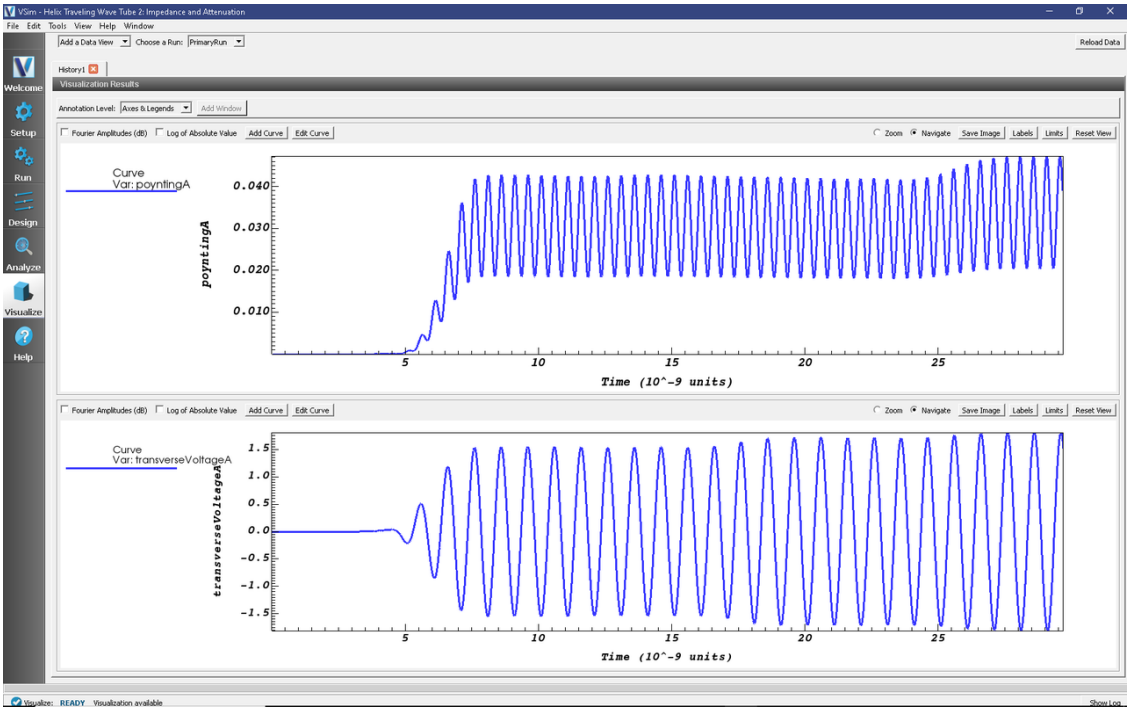


Fig. 4.94: Poynting power (W), transverse voltage (V), and electric field (V/m), at Plane A, along the helix TWT as a function of time (s).

The result is shown in Fig. 4.94. The power through the plane was defined such that incoming is negative.

Impedance parameters of interest are the transverse impedance

$$Z_t = \frac{V_t^2}{2P}$$

and the Pierce interaction impedance

$$Z_p = \frac{E_x^2 \lambda^2}{8\pi^2 P}$$

where P is the poynting power (recorded in the history poyntingA), V_t is the transverse Voltage amplitude (recorded in the histories transverseVoltage), E_x is the electric field amplitude (recorded in the history EonAxis), and λ is the wavelength of the field along the helix TWT axis.

The histories show the graphs of these quantities. To get precise values for any of these, one can press the *Limits* button, which will pop up a window with the precise values. First, the *X-Axis* limits show that the units are ns. Secondly, one needs to choose a consistent time period, where all amplitudes are roughly constants. The period $28ns < t < 32ns$ is chosen. One can now adjust the limits until the peaks line up with the limits. We want average poynting power. We find $P_{min} = 18.\ mW$ and $P_{max} = 44.\ mW$. Hence, $P_{av} = 31.\ mW$. During that same time interval we find $V_t = 2.4\ V$ and $E_x = 240\ V/m$.

Fig. 4.93 can be used to obtain the wavelength. One can see four wavelengths between $0.20m$ and $0.357m$. Therefore the wavelength is $(.357m - .20m)/4 = 0.039m$

We now compute

$$Z_t = \frac{2.4 * 2.4}{2 * .031} = 92.9\ \Omega$$

and the Pierce interaction impedance is

$$Z_p = \frac{240^2 \cdot 0.039^2}{8\pi 0.031} = 35.8\ \Omega.$$

Further Experiments

As noted above, one can change the attenuation by varying the conductivity of the resistive tubs or their length. For any given length, there is a maximum attainable attenuation, as there is no attenuation at zero conductivity (infinite resistance, i.e., vacuum) and none as well at infinite conductivity (metallic shielding). So if more than 14 dB attenuation is needed one can vary the conductivity, but a maximum will be observed, and if that is insufficient one will have to vary the rod length.

With additional computing resources, one could increase the grid resolution so that the resistive tube could be made thinner. As it is made thinner, one can go to greater conductivity without having the skin depth less than the resistive tube thickness.

The coupling is determined by the transverse impedance of the structure, which in turn depends on the capacitance provided by the rods. Varying the relative permittivity changes the transverse impedance.

4.3.8 Helix Traveling Wave Tube 3: Power Run (helixTwt3PowerRun.sdf)

Keywords:

`Helix TWT Power Run`

Problem description

This VSimVE example is the last of a set of simulations showing different calculations to aid the design of a helix traveling wave tube (TWT) in three dimensions. The 100-turn helix with end feeds is imported from a CAD file, but all other geometrical parts are created with the Constructive Solid Geometry (CSG) capabilities within VSimComposer.

An input signal is sent into a short section of coaxial input waveguide and a similar section of coaxial waveguide provides an output power port. The geometries in and constant parameters of this simulation are described in more detail in *Helix Traveling Wave Tube 2: Impedance and Attenuation (helixTwt2ImpedAtten.sdf)*. Electrons are injected at the left end of the tube. Gain can be computed from the ratio of voltages in the input and output waveguides.

The user may wish to run this simulation type multiple times, varying parameters such as the input signal power and the electron energy, in order to result in a design with maximum output power.

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The Helix TWT Power Run example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Radiation Generation* option.
- Select "Helix Traveling Wave Tube 3: Power Run" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.95. You can expand the tree elements and navigate through the various properties. Some of these changes will affect the geometry, and so one should review the look of the geometry in the right pane as one changed geometrical variables. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`. One can, e.g., hide the tube to see inside it.

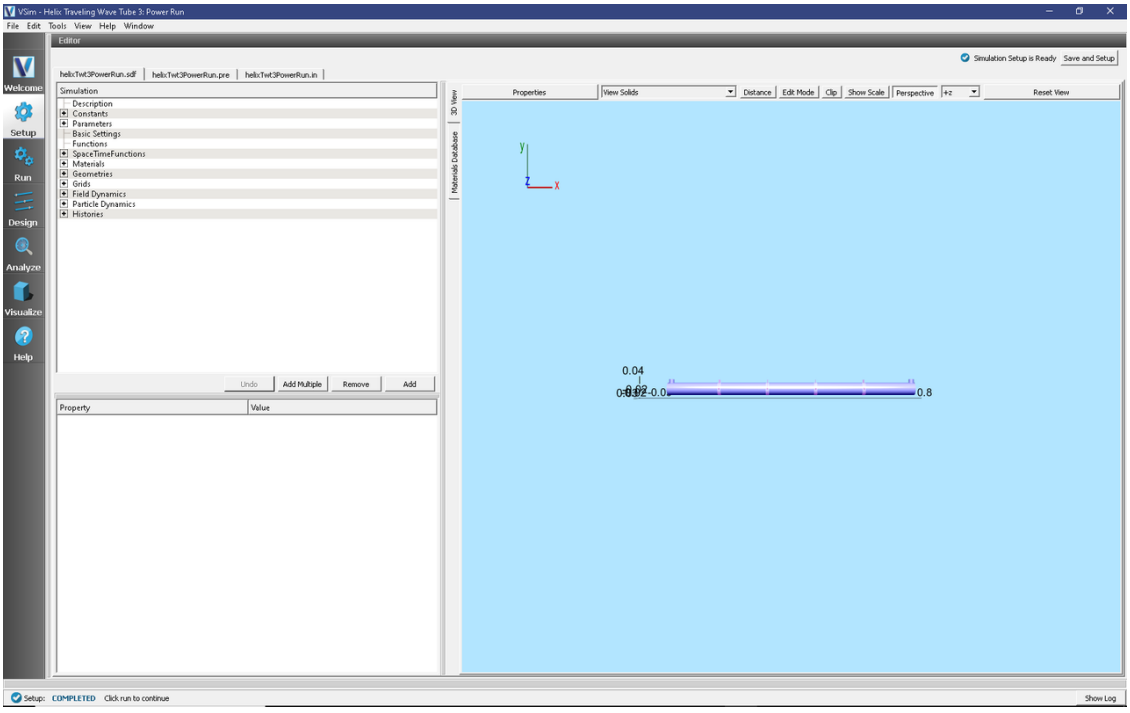


Fig. 4.95: Setup Window for the Helix TWT example.

The geometry of the helix can be made more visible by unselecting the tube and emitter disk parts under Geometries/CSG in the tree (e.g. driftTubeSolid, tubeSolid, driftTubeVoid, tubeVoid, tube, and emitterDisk) or by changing their color property and selecting a low alpha on Windows or Linux (or opacity on Mac). See color property setting in the User Guide.

Additional detail of the geometry is shown in figure Fig. 4.96. Fig. 4.95 shows the dielectric rods and Fig. 4.96 shows how the coaxial waveguide connects to the helical wire.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.969479871884134e-13
  - *Number of Steps*: 100000
  - *Dump Periodicity*: 2000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, “Engine completed successfully”. This result is shown in Fig. 4.97.

The default number of time steps will run the simulation long enough to verify that the electron beam is traveling down the tube, that the input signal has entering the simulation and propagated down the tube, that the amplified signal is leaving the system, and that the amplification has reached a steady state. However, the simulation has not been run

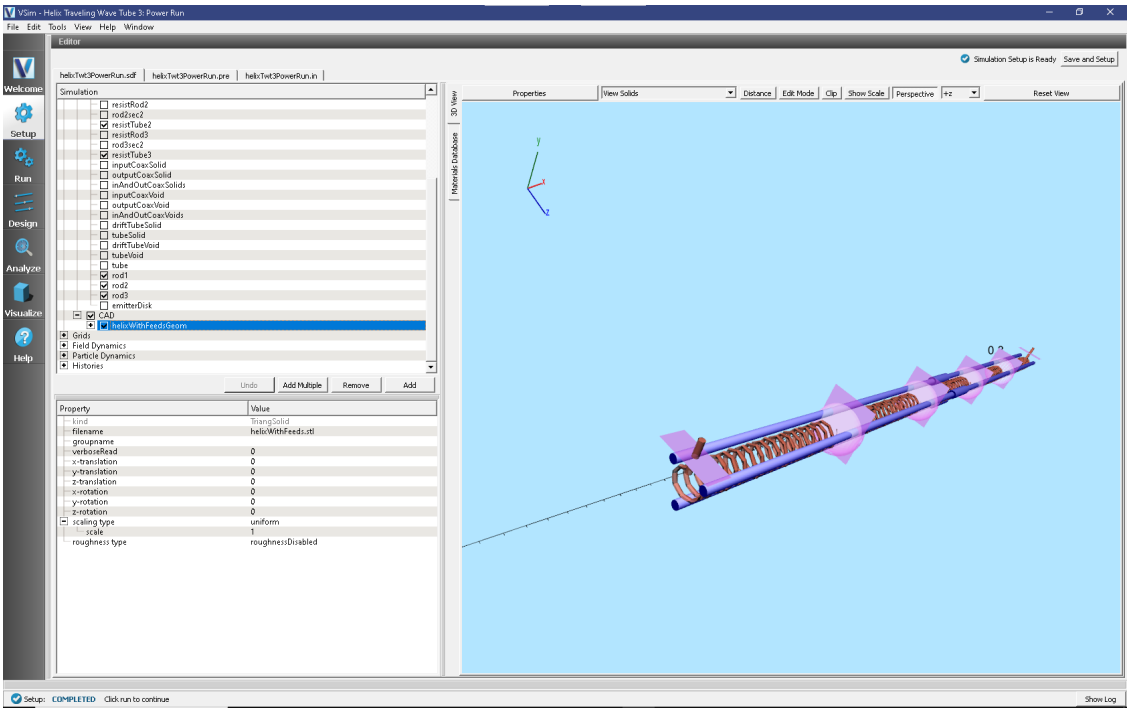


Fig. 4.96: A view in through the input coax.

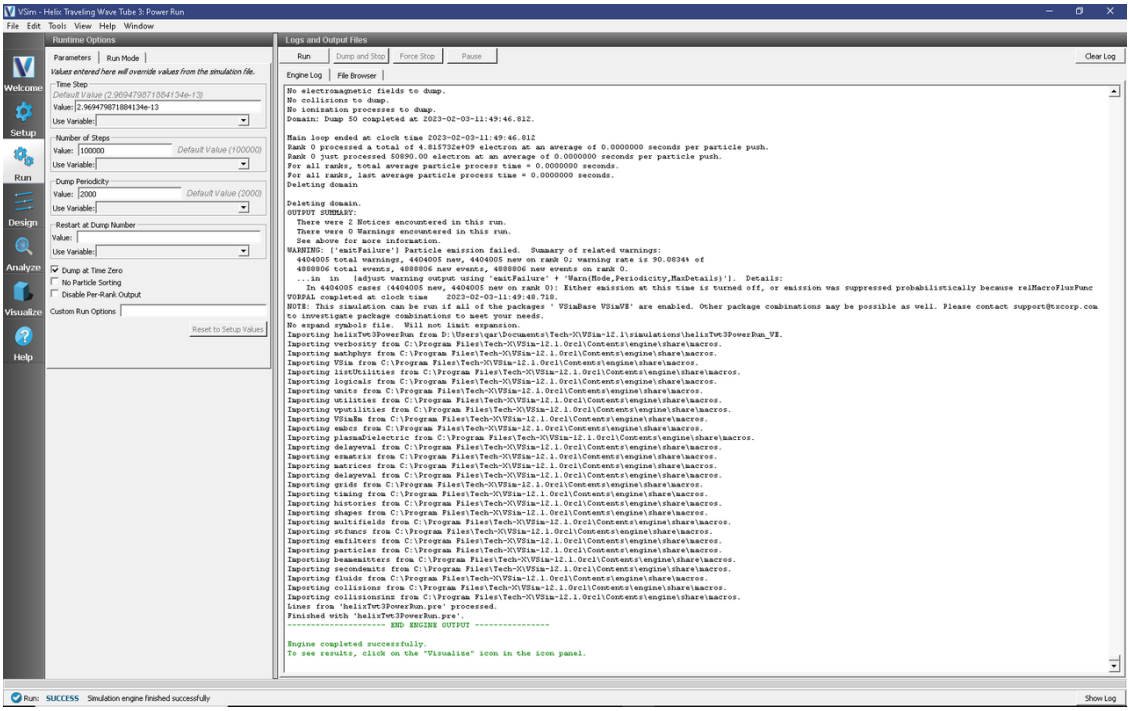


Fig. 4.97: The Run Window at the end of execution.

long enough to ensure that there are no deleterious, backward wave oscillations. To determine that, one should run the simulation twice as long (ensuring a backward and forward traversal) or more, depending on the growth rate of the oscillation.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

The particle phase space, Fig. 4.98, shows how the energy is being extracted from electron beam. To generate this image:

- For *Data View* select *Phase Space*.
- Set *X-axis* to electron_x.
- Set *Y-axis* to electron_ux.
- Press *Draw*.
- Move the dump slider forward in time to see the evolution
- The image is at dump 37.

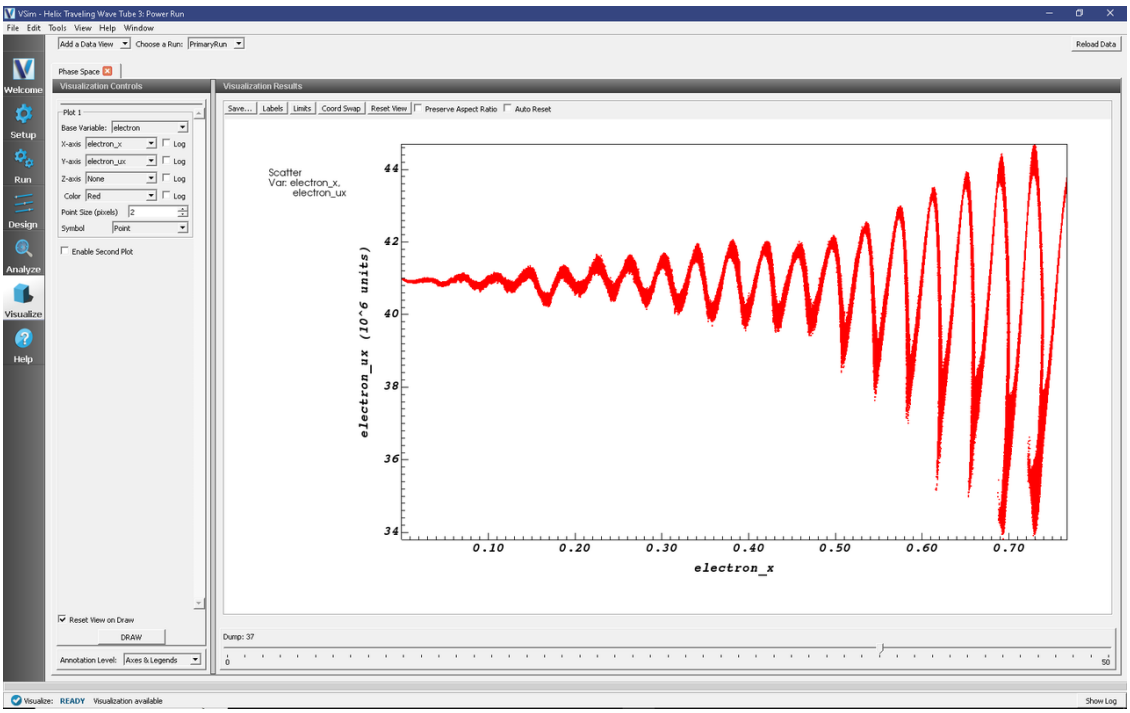


Fig. 4.98: Longitudinal phase space of the electron beam.

One can see in Fig. 4.98 that the beam has been overdriven, such that trapping is beginning to occur. Hence, one must either reduce the input power or one must reduce the gain. In the middle of the tube one can see that the beam oscillation for one cycle decays a bit before taking off again. This is where the attenuator is located.

The effect of overdriving the tube can also be seen in the longitudinal field, Fig. 4.99. This image is obtained by

- For *Data View* select *Field Analysis*.
- Set *Field* to E_x.

- For *Lineout Settings*, choose *Horizontal* with Intercept of 0.
- For *Layout* select Stacked 2d/1d.
- Press *Perform Lineout*.
- Click the *Colors* button and set the limits to Minimum = -2e3 and Maximum = 2e3.
- Move the dump slider forward in time to see the evolution.
- The image is at dump 37.

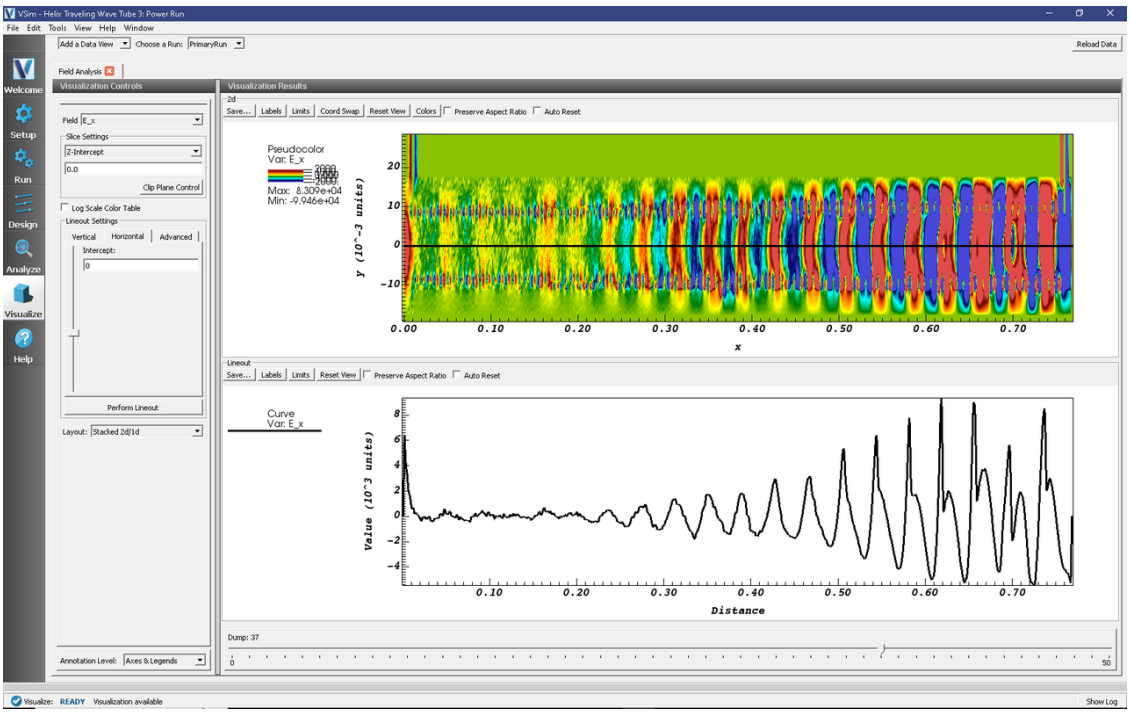


Fig. 4.99: Longitudinal electric field in the center of the tube.

As expected, the longitudinal field is largely confined within the helix. Again, at around x=0.4, one sees the field being damped out by the attenuator. Because the tube has been overdriven, harmonics are appearing in the field at the right. This image shows that the harmonics occur at about 1/5 of the current output power, indicating the amount by which one should decrease the input power or the gain to obtain linear operation.

The gain can be seen in the History records, which are available under the *History* Data View. A sample of these is shown in Fig. 4.100.

To obtain this history image:

- For *Data View* select *History*.
- For *Graph 1* select inputVoltage.
- For *Graph 2* select outputVoltage.
- For *Graph 3* and *Graph 4* select <None>

This image shows that the voltage gains is about a factor of 10 or 20 dB. The voltage history also shows the harmonics in the output that come from overdriving the tube.

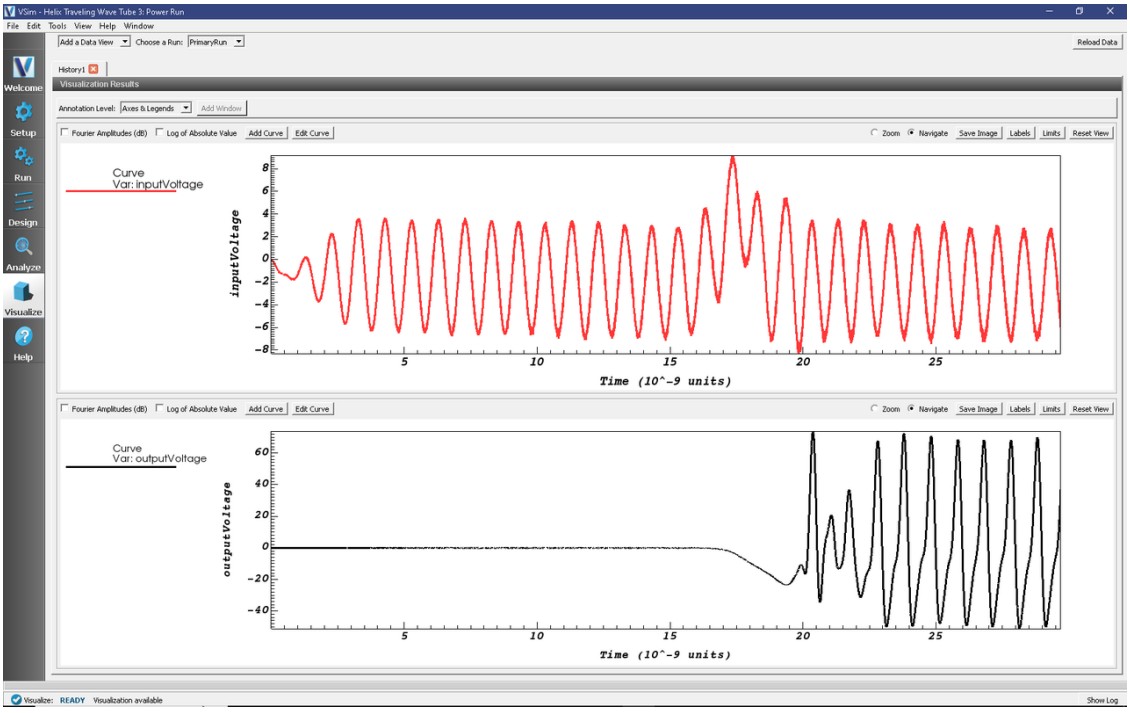


Fig. 4.100: Input and output voltage histories.

Further Experiments

As noted at the beginning, this run could be run for many more time steps to determine whether backward oscillations are present. Additionally, one can experiment with the beam energy to determine what energy gives the most gain. Varying the input power can determine the maximum output power, which happens when the beam begins trapping at the end of the tube, or the input power at which one obtains large gain while remaining in the linear regime.

4.3.9 Klystron (klystron.sdf)

Keywords:

klystron

Problem description

This VSimVE example simulates a two cavity klystron in three dimensions. The first cavity is driven at its lowest resonant frequency. The resultant cavity voltage creates a velocity modulation in the electron beam which translates to charge modulation as the beam travels in the tube between cavities. The charge modulation then drives the second cavity. The cavities are loaded to give them finite Q.

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The Klystron example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Radiation Generation* option.
- Select *Klystron* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the setup window as shown in Fig. 4.101. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to *Grid*.

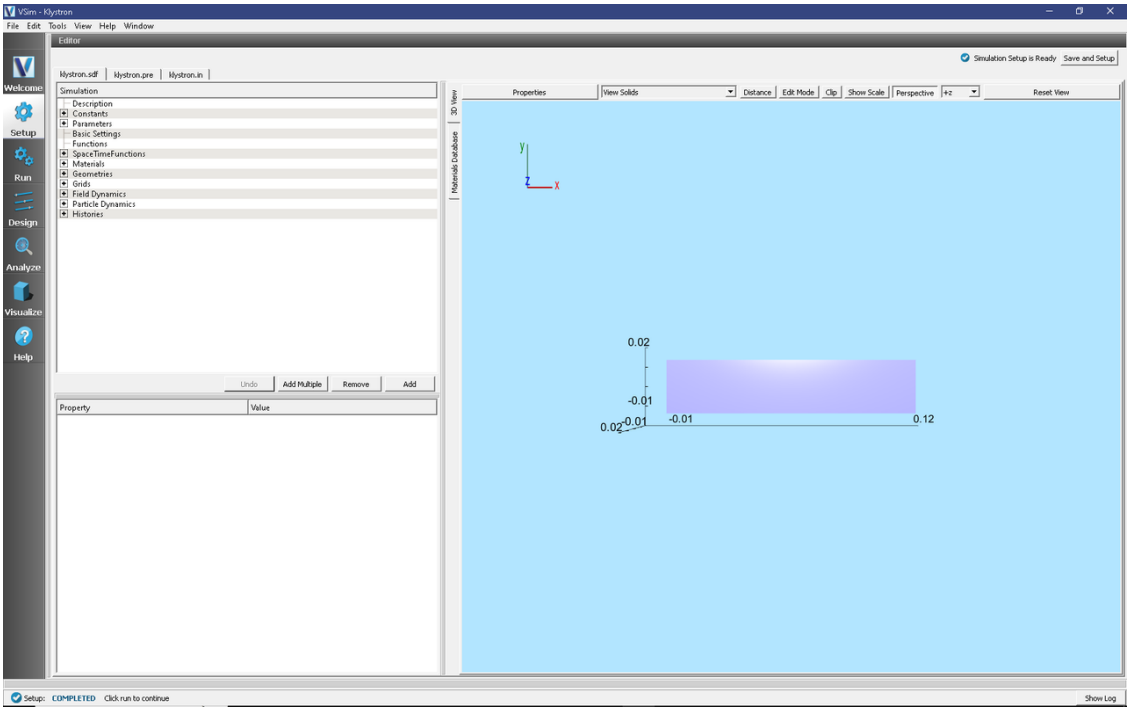


Fig. 4.101: Setup Window for the Klystron example.

This example illustrates two methods for generating geometries. Under *Geometries* in the elements tree there are two paths, *CSG* and *load1Geom*. The CSG components are constructed from primitives within VSim. The *load1Geom* was imported as an STL file. Highlighting any geometry under the CSG group shows how it was created, either as a primitive with parameters or by operations on other shapes.

Simulation Properties

This simulation is set up to do a Power Run with full capabilities. After completing the Power Run and visualizing the results, you may wish to refine the performance of the klystron by adjusting the setup. Some useful tuning procedures are described in the **Further Experiments** section. These include the **Resonant Frequency Run** and the **Attenuation Calibration Run**.

Some constants that you may wish to modify include:

FREQUENCY:The frequency (in Hz) at which the signal across cavity is driven. This can be tuned to the resonant frequency once determined.

BEAMRADIUS: The radius of the emitted beam of electrons into the klystron.

BEAMCURRENT: The current of the electron beam.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.8238168632444674e-13
  - *Number of Steps*: 10000
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.102.

Visualizing the Results

After the simulation run has completed successfully, you may proceed to the Visualize Window by pressing the *Visualize* button in the left column. To reproduce Fig. 4.103 follow these steps:

- Select *Data Overview* from the *Data View* pull-down menu.
- Expand *Particle Data*
- Expand *electrons0*
- Select *electrons0_ux*
- Expand *Geometries*
- Select *poly (klystronPecShapes)*
- Select the *Clip Plot* checkbox
- Step through time using the dump slider on the bottom of the right pane.

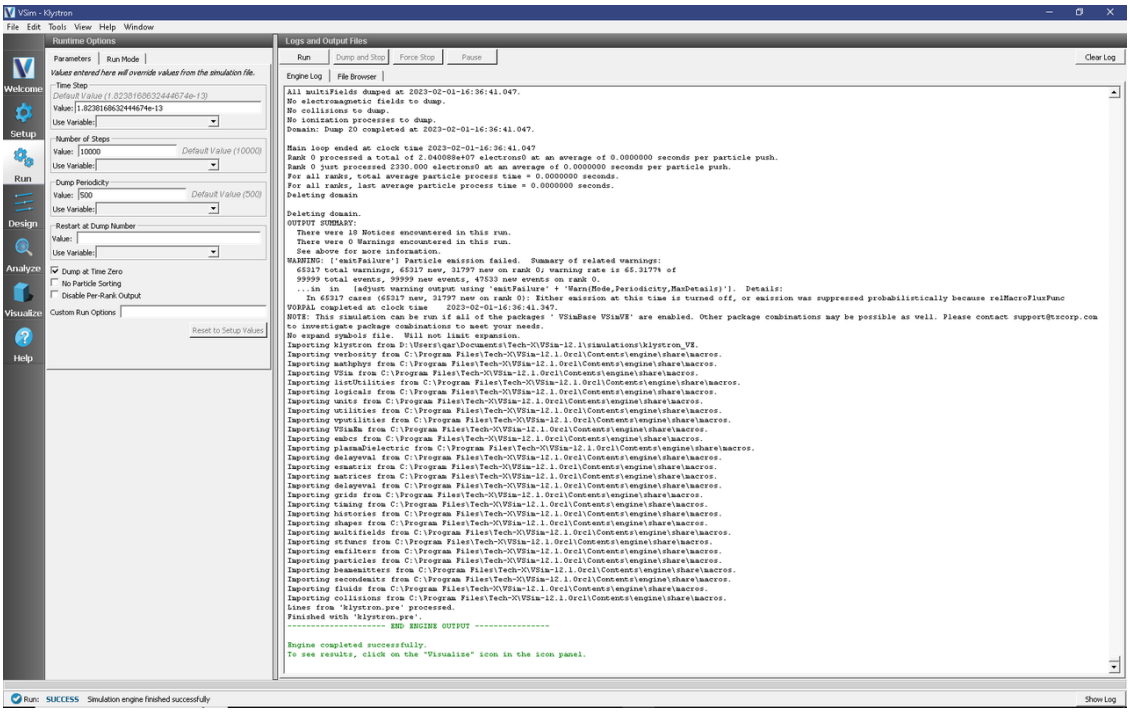


Fig. 4.102: The Run Window at the end of execution.

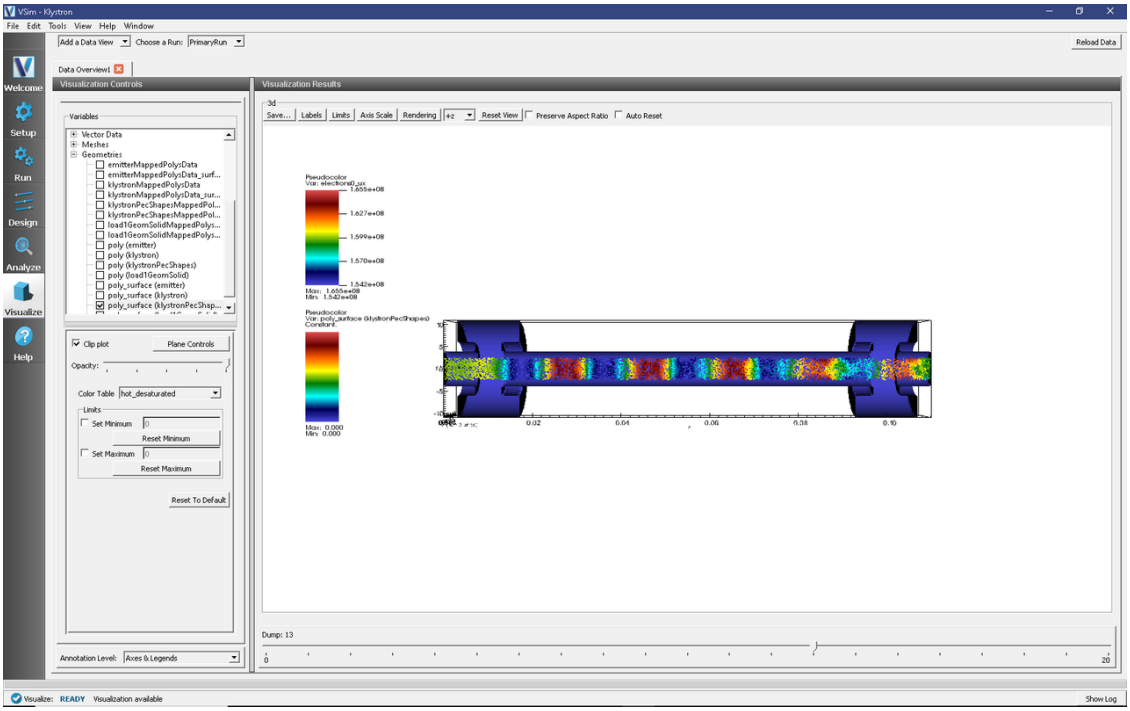


Fig. 4.103: A power run with an electron beam.

Further Experiments

The **Attenuation Calibration Run** and **Resonant Frequency Run** are outlined below. These experiments will allow you to tune the klystron. You may want to iterate through these experiments to get the desired performance. Once the cavity performance is satisfactory you can repeat the Power Run to see the effects on the electrons. To see the full behavior of the device, increase the number of steps to (5 x Default). This will allow you to see the saturation of the second cavity.

Resonant Frequency Run

To determine the resonant frequency of the first cavity we will analyze the fourier transform of its voltage. In the Setup window, under *Basic Settings*, set *particles* to *no particles*. Then, under *SpaceTimeFunctions*, in *ring1J* change the turn on function to from "standard" to "up and down". This will ping Cavity 1 and allow us to observe the ringing signal. Run the simulation with this setup.

To determine the resonant frequency proceed to the Visualize window. Select *History* from the *Data View* pull-down menu. Click FFT to the left of the Cavity1Voltage plot in the *Visualization Results* pane. The resulting plot will resemble Fig. 4.104. Zoom in on the maximum of this plot to determine the resonant frequency. You can now update the FREQUENCY under *Constants* in the Setup window with this new value and use it to drive future simulations.

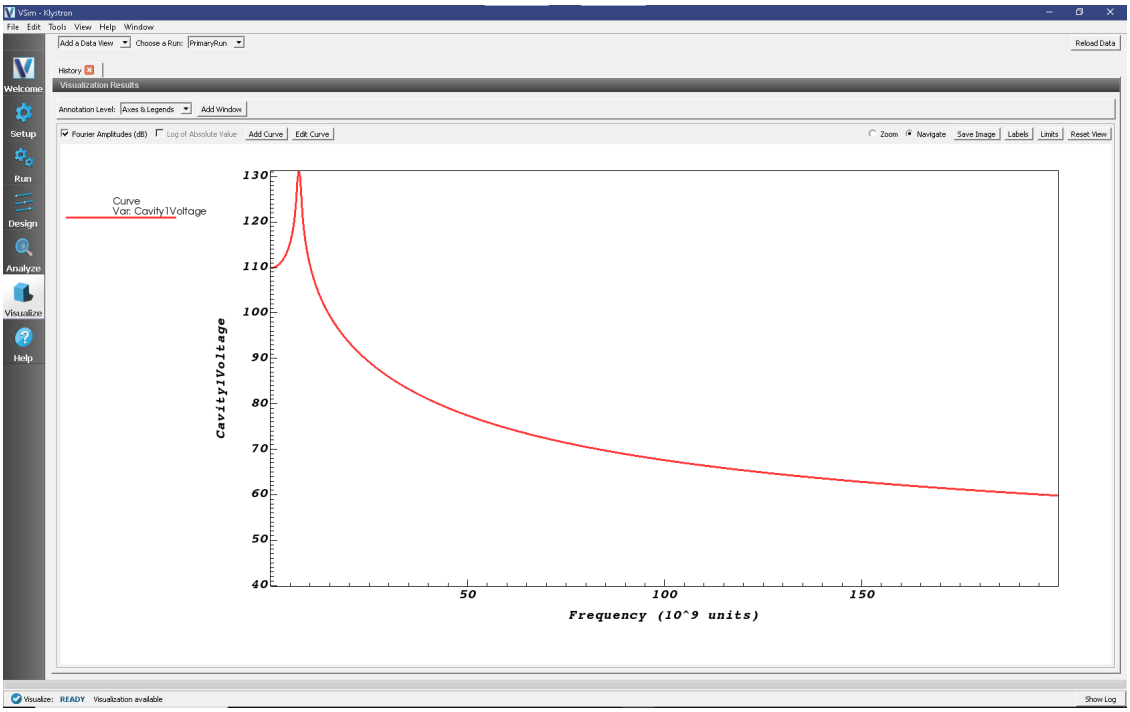


Fig. 4.104: Fourier transform of Cavity1_Voltage versus time (0-2 GHz).

Attenuation Calibration Run

The user can integrate this run type in order to calibrate the observed attenuation to the desired loss. The attenuation can be tuned by modifying the *conductivity* of the material, *resistive damper*. The Q of the cavity can be computed using a feature of the Analysis Tab, as described below.

For the **Attenuation Calibration Run**, use the same Setup as the **Resonant Frequency Run**. After running the simulation, the quality factors, Q_1 and Q_2, for cavities 1 and 2 can be calculated using the *computeInverseQ.py* script in the Analyze window.

- Press the Analyze button in the left column of buttons.
- Select the *computeInverseQ.py* analyzer, then *Open*.

- Enter Cavity1Voltage or Cavity2Voltage in the *historyName* field to designate the history to analyze.
- Enter the value of the FREQUENCY constant as defined in the Setup window in the *frequency* field to designate the frequency at which the history will be analyzed.
- Update the *outputFileName* field if desired
- Click the *Analyze* button in the top right corner of the window. As shown in Fig. 4.105 below. Two columns of data with the titles "Time (s)" and "Inverse Q" will be output in the right pane. The analysis has completed when you see the output "Analysis completed successfully."

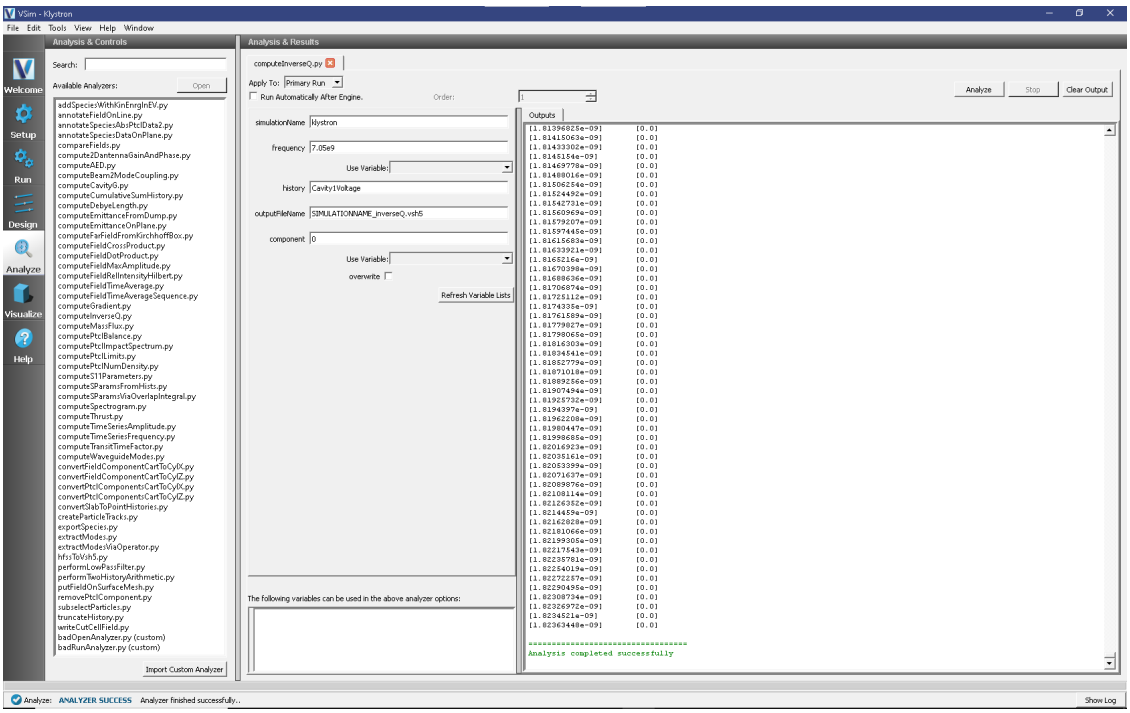


Fig. 4.105: The Analysis window at the end of execution of the computeInverseQ.py script.

Scrolling through or plotting the output data in the Visualize window enables the user to understand the Klystron's performance. The user may iterate this run type to achieve the desired attenuation.

4.3.10 2D Magnetron (magnetron2D.sdf)

Keywords:

`magnetron`

Problem description

This VSimVE example simulates a rising sun magnetron in two dimensions. A load is added to one cavity, representing a coupler to the magnetron through the quality factor, Q. Upon configuring an electrostatic voltage across the anode and cathode, particles are introduced to the simulation, exhibiting a five spoke pi-mode.

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The 2D Magnetron example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Radiation Generation* option.
- Select "2D Magnetron" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries. See Fig. 4.106.

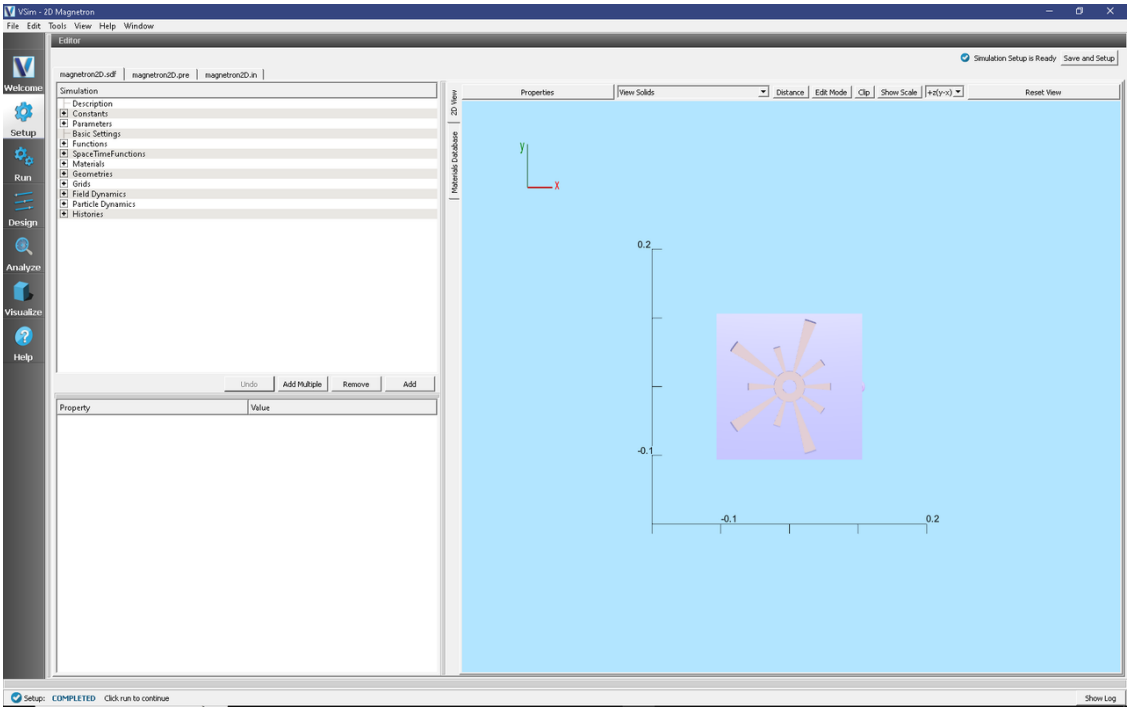


Fig. 4.106: Setup Window for the 2D Magnetron example.

Simulation Properties

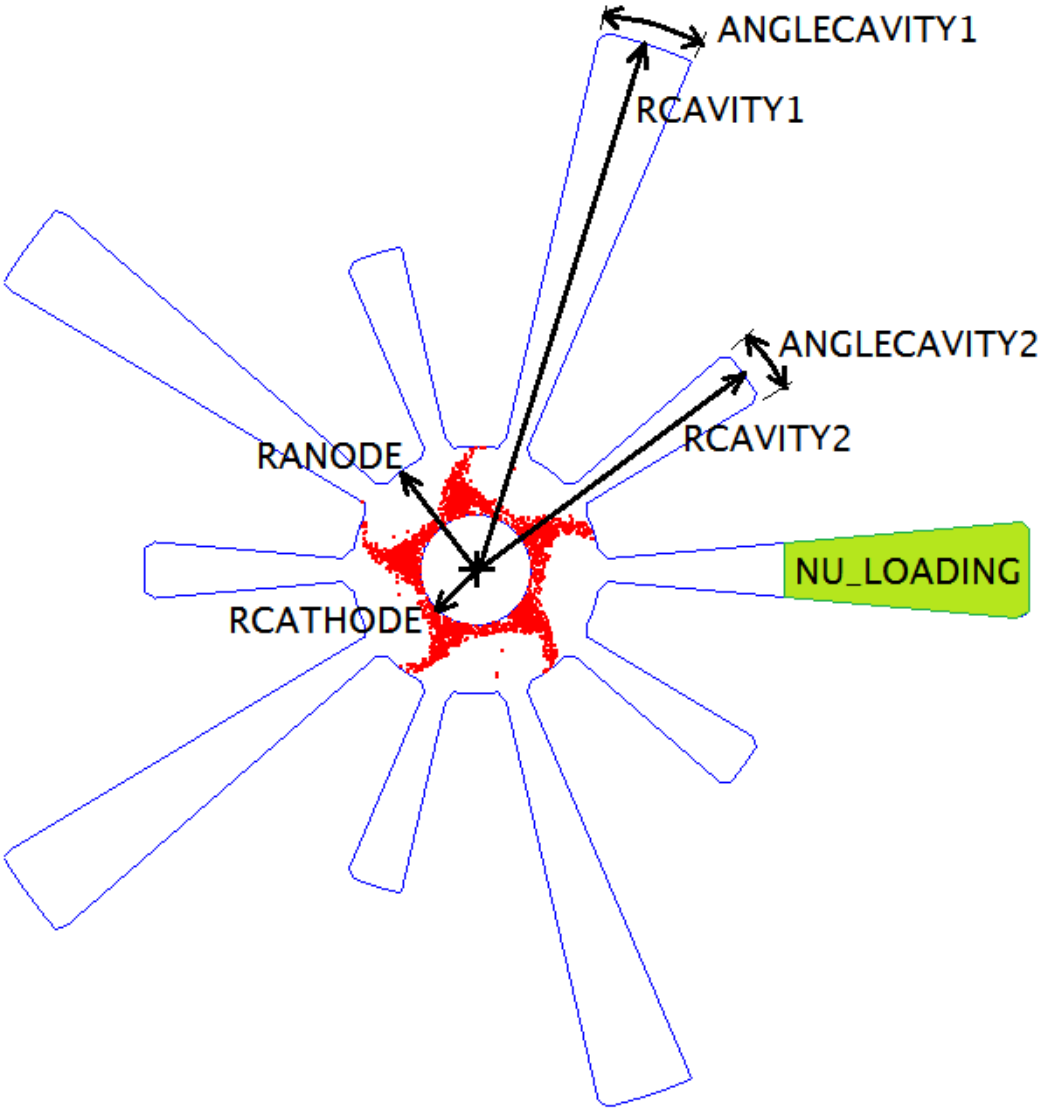


Fig. 4.107: Some exposed variables of the 2D Magnetron example.

As seen in Fig. 4.107 of the rising sun magnetron, the radius of the cathode is RCATHODE and the radius of the anode is RANODE. Long cavities have radius RCAVITY1 and opening angle ANGLECAVITY1. Short cavities have radius RCAVITY2 and opening angle ANGLECAVITY2. These dimensions control the spectrum and thus the operating frequency, which for the default parameters is approximately 960 MHz.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.3114812500146902e-12
  - *Number of Steps*: 259573
  - *Dump Periodicity*: 5191
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.108.

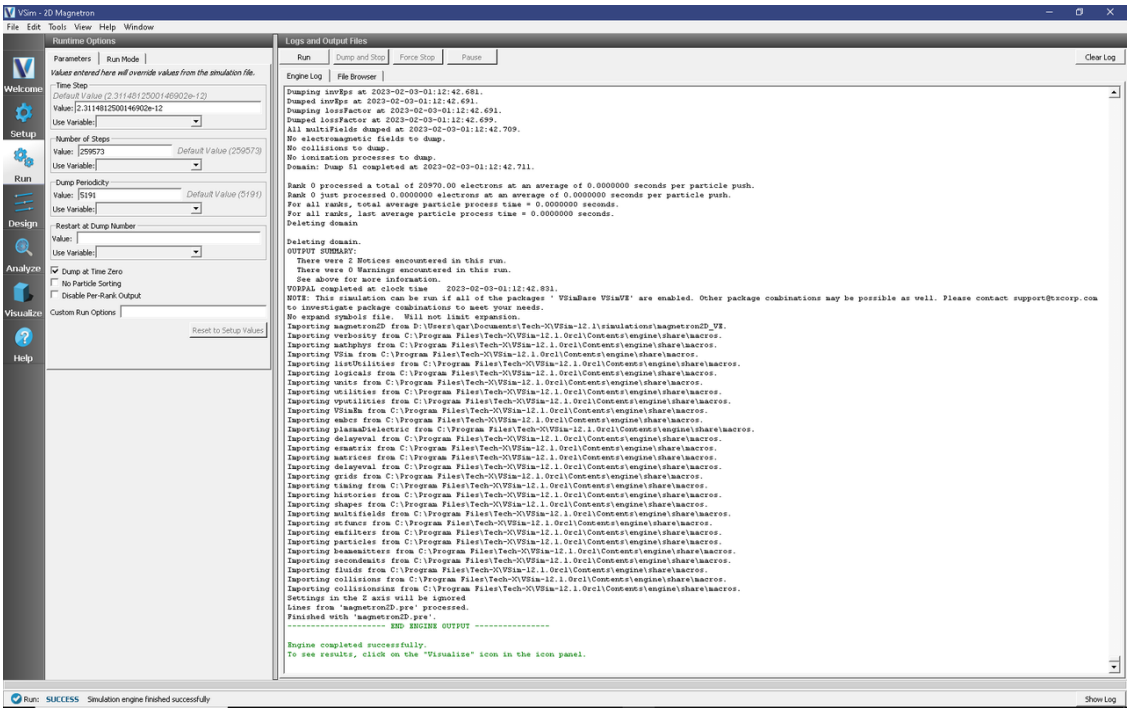


Fig. 4.108: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column.
- Expand *Particle Data*
- Expand *electrons*
- Select *electrons*
- Expand *Geometries*

- Select *poly (magnetron2DGeomSolid)*

The electron modes can be viewed in the right pane. Use the dump slider on the bottom of the right pane to step through time. When electrons are emitted from the cathode, the four spoke 650 MHz pattern is present during start-up. At approximately 250 ns, the five spoke begins to dominate and eventually appears as seen in Fig. 4.109.

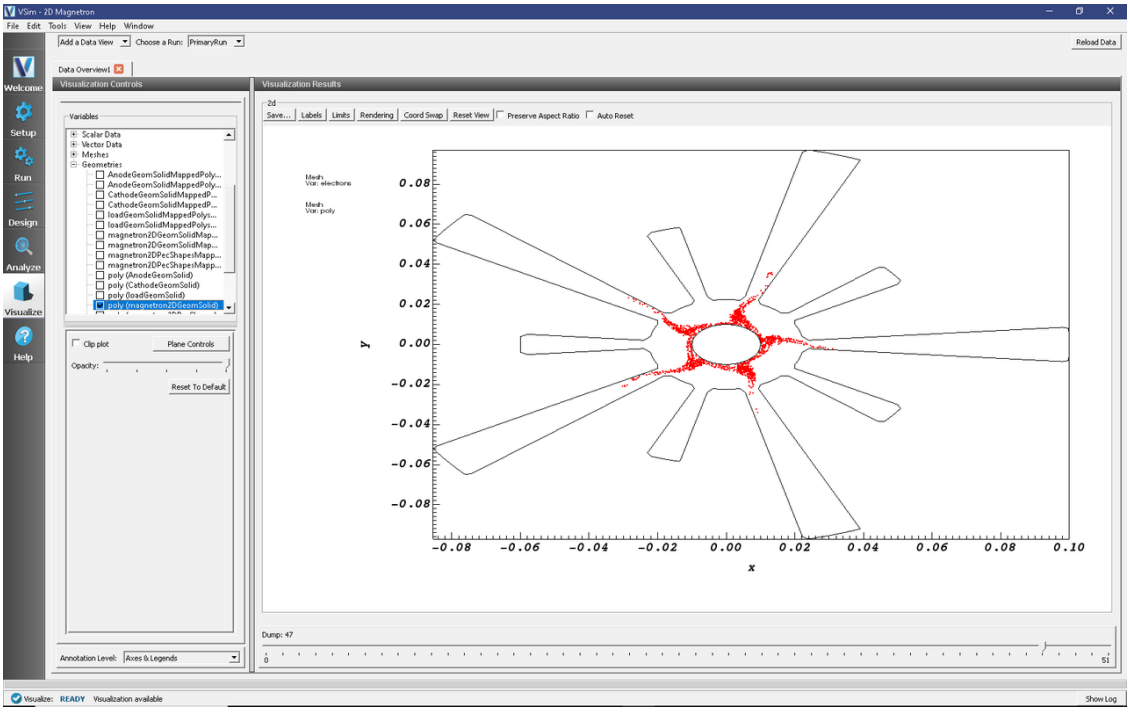


Fig. 4.109: The five spoke pi-mode at 600 ns.

4.4 Multipacting

4.4.1 Multipacting Growth in Waveguide (multipactingGrowth.sdf)

Keywords:

`multipacting`

Problem description

Multipacting, which is the resonant buildup of secondary electrons, is often a concern in microwave devices. Anytime there is an oscillating electromagnetic field across a gap between two surfaces there exists the possibility that for the right voltage across the gap a resonance condition will exist allowing the exponential buildup of secondary electrons. A coaxial waveguide is such a type of structure where these conditions can exist.

This simulation can be performed with the VSimVE or VSimPD license.

Opening the Simulation

The Multipacting Growth example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Multipacting* option.
- Select "Multipacting Growth in Waveguide" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.110. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

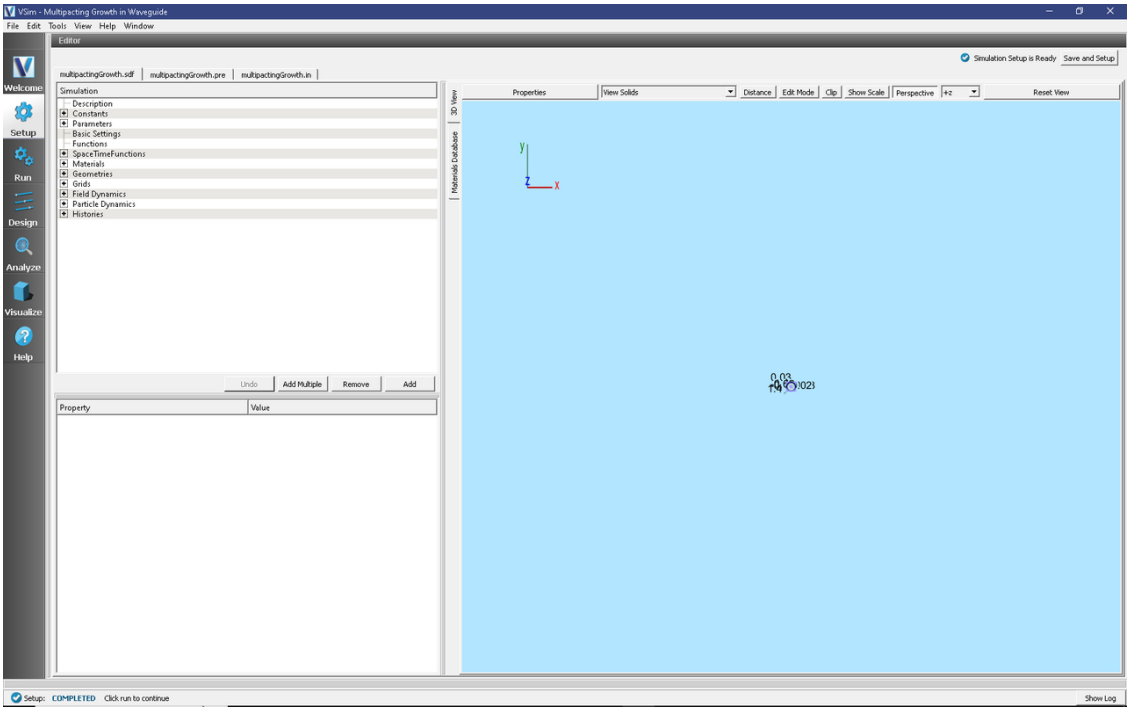


Fig. 4.110: Setup Window for the Multipacting Growth example.

Simulation Properties

This example contains a number of *Parameters* to allow for easy manipulation of the device. Those include:

- R_O: The outer coax radius
- R_I: The inner coax radius
- FREQUENCY: The wave launcher frequency

SpaceTimeFunctions are used to create expressions defining the drive frequency and amplitude of the applied field.

CSG is used to create the coax structure by combining cylinders and cubes.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.703189536968598e-13
  - *Number of Steps*: 25600
  - *Dump Periodicity*: 6400
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.111

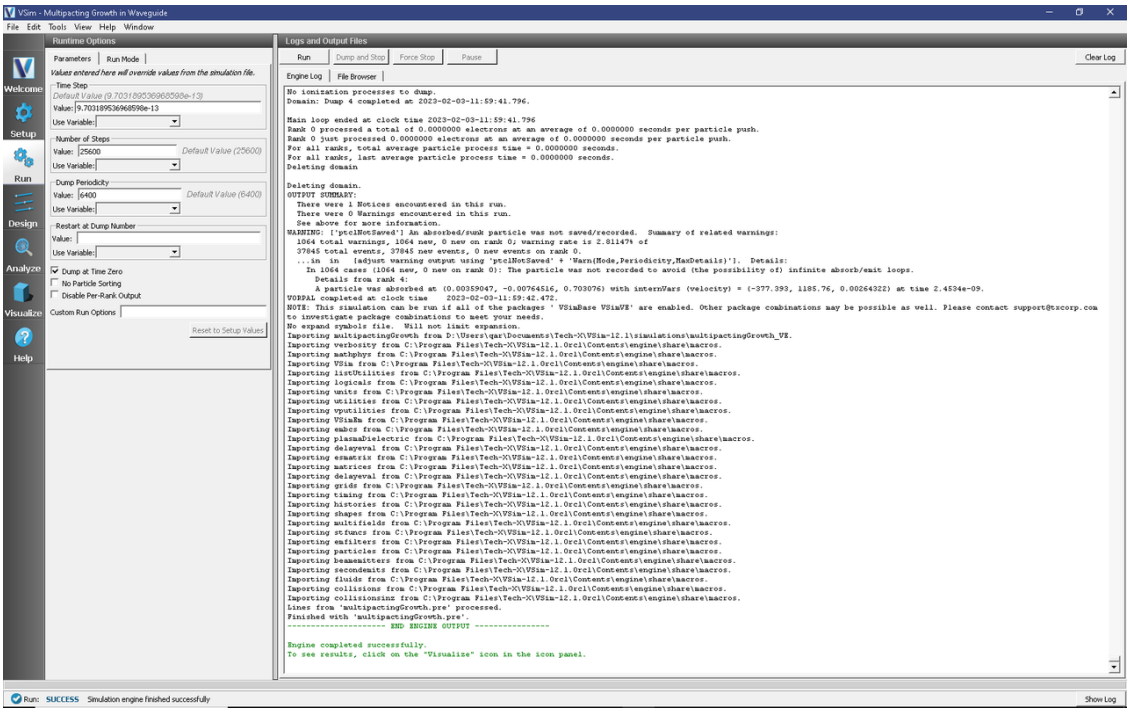


Fig. 4.111: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view growth in the number of electrons, as shown in Fig. 4.112, do the following:

- Select *History* from the *Data View* pull down menu
- Set Graphs 1&2 to "None"
- Graph 3 should already be set to *numElectrons* (if not, set it)

The overall trend in the number of electrons is an exponential growth with an oscillatory signal that corresponds to the frequency of the traveling wave.

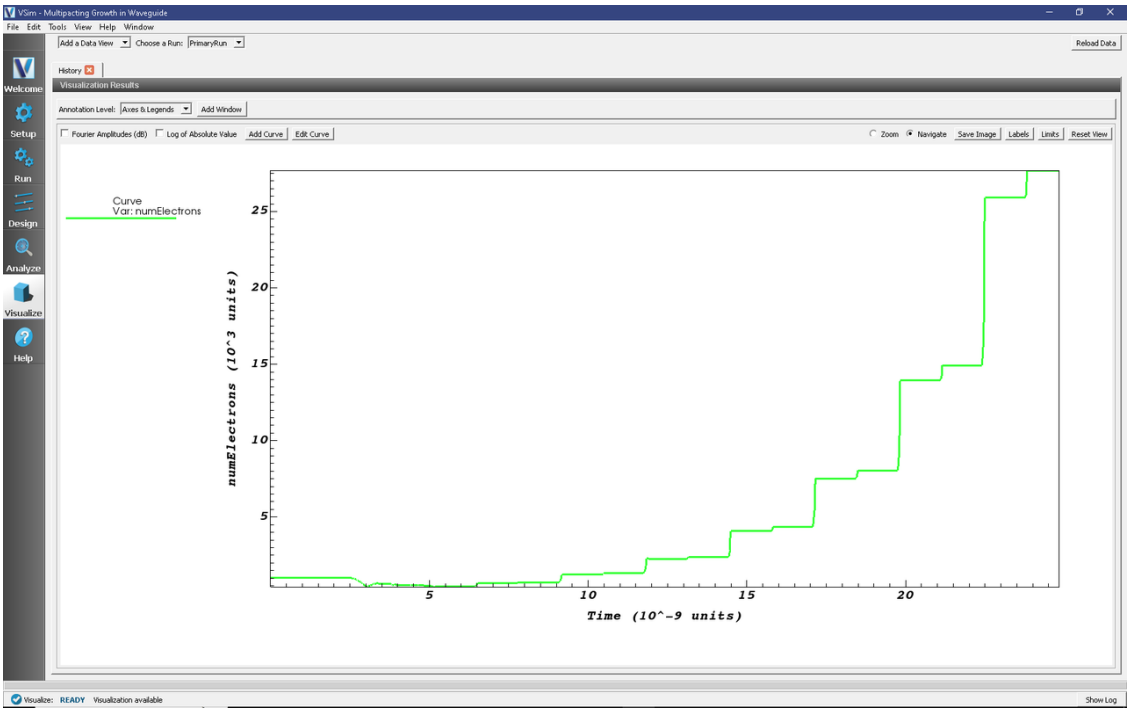


Fig. 4.112: Visualization of the exponential growth of the electrons due to multipacting.

Further Experiments

Try changing the gap voltage or the frequency of the wave to see if one can take the simulation in and out of resonance.

4.4.2 Multipacting Resonances in Waveguide (multipactingResonances.sdf)

Keywords:

multipacting , multipactingResonances

Problem description

Multipacting, which is the resonant buildup of secondary electrons, is often a concern in microwave devices. Anytime there is an oscillating electromagnetic field across a gap between two surfaces there exists the possibility that for the right voltage across the gap a resonance condition will exist allowing the exponential buildup of secondary electrons. A coaxial waveguide is such a structure where these conditions can exist.

This simulation can be performed with the VSimVE license.

Opening the Simulation

The Multipacting Resonances example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Multipacting* option.
- Select "Multipacting Resonances in Waveguide" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 4.113.

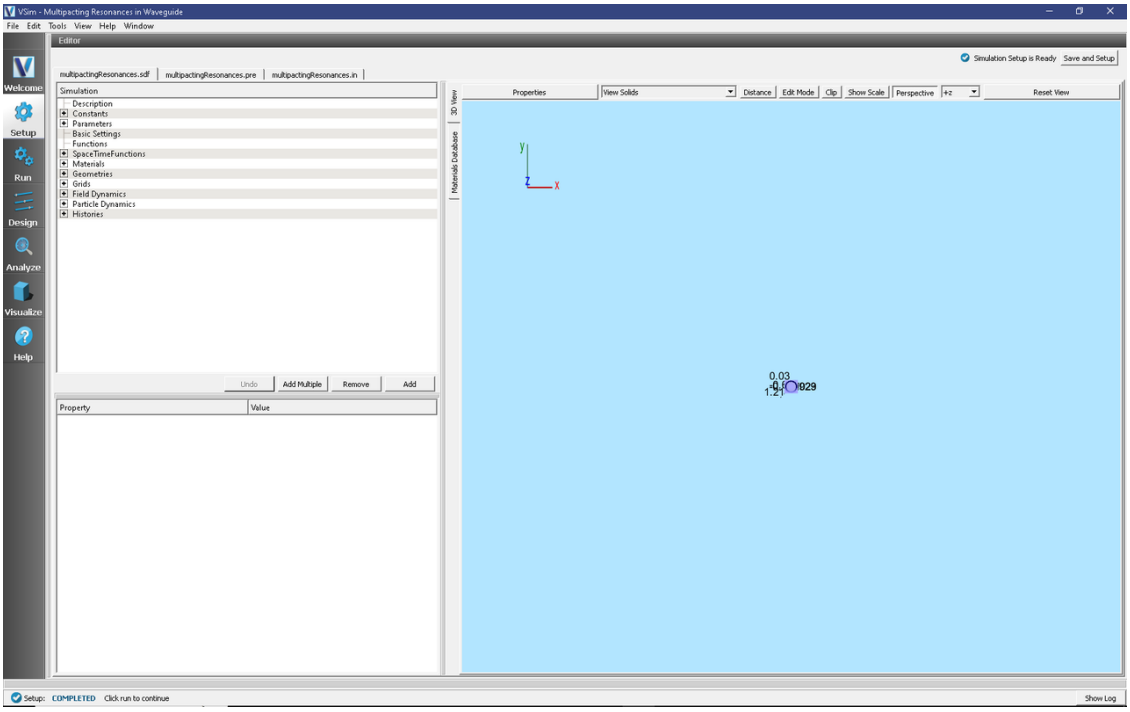


Fig. 4.113: Setup Window for the Multipacting Resonances example.

Simulation Properties

The input file sets the number of cells along the propagation (x) direction to resolve the wavelength. The electrons are seeded in the middle of the waveguide once the wave has passed. A special electron species is used that allows scans over power to be done in a single simulation. The time step is chosen to be at 90% of the CFL (stability) limit.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.4420382121606601e-12
  - *Number of Steps*: 17660
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.114.

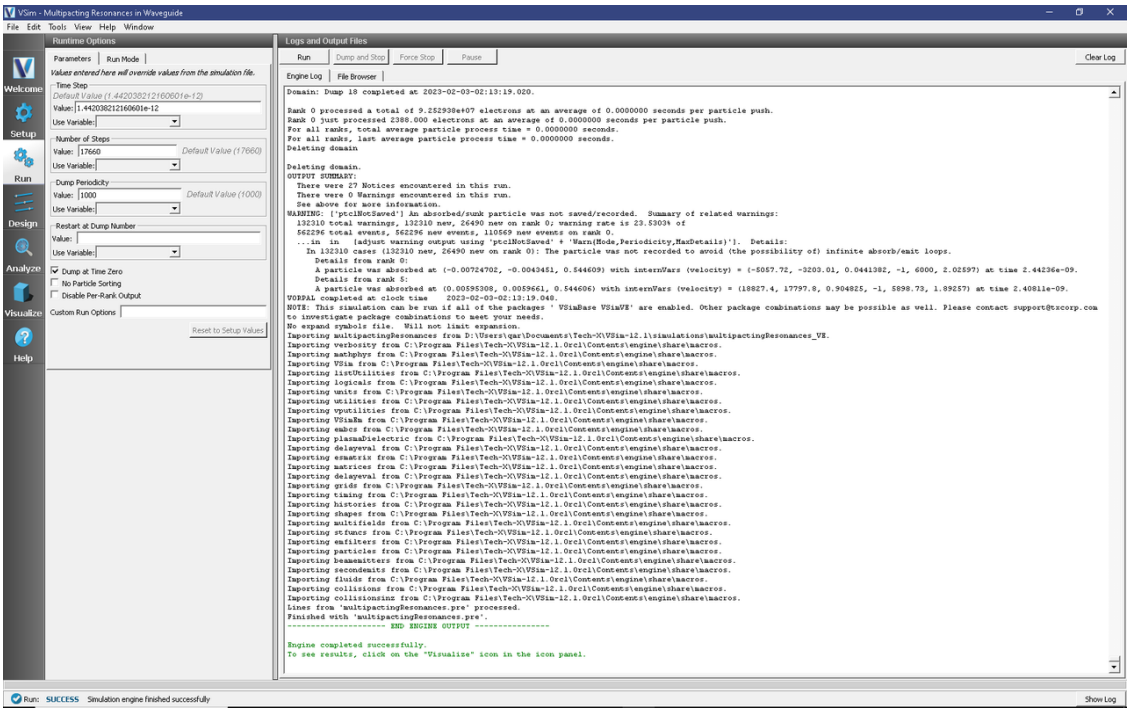


Fig. 4.114: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To track the electrons and their field scaled parameters as shown in Fig. 4.115, proceed as follows:

- Select *Phase Space* from the *Add a Data View* pull down menu
- Select *electrons_x* for the *X-axis*
- Select *electrons_y* for the *Y-axis*.
- Select *electrons_fieldScaleParam* for the *Color*.
- Click on *Draw*.
- Move the *Dump* slider to *Dump: 11*.

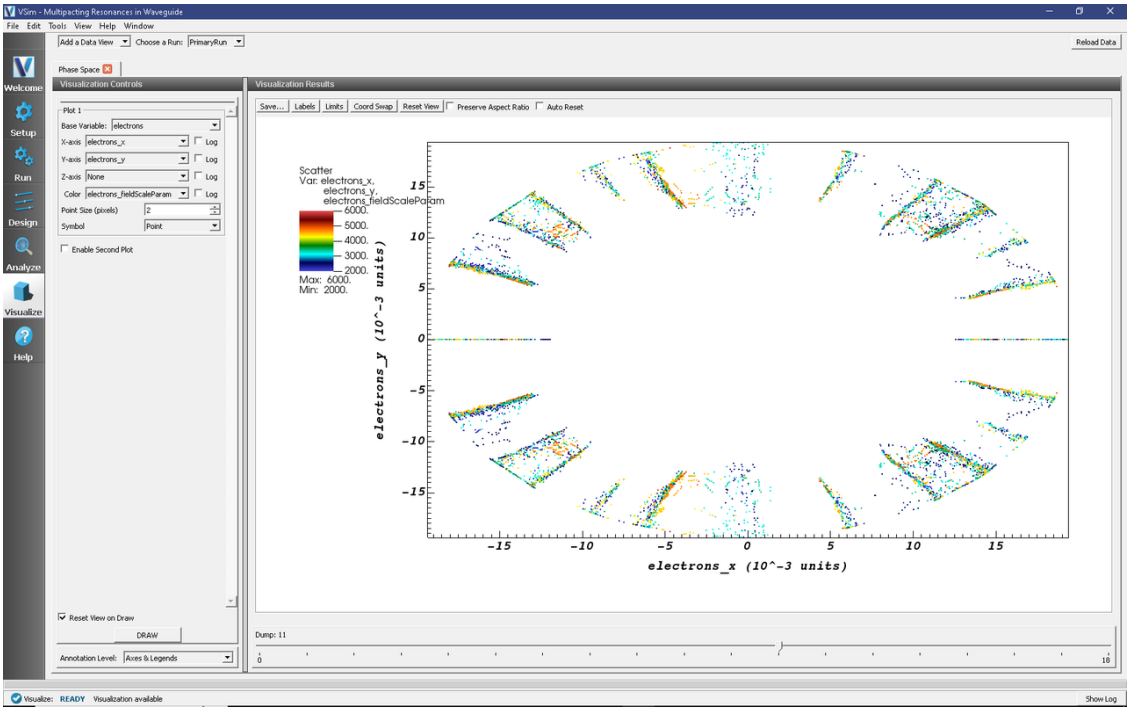


Fig. 4.115: Location of electrons and their field scaled parameters.

To view growth in the number of electrons, proceed as follows:

- Select *Binning* from the *Add a Data View* pull down menu
- Select *electrons_fieldScaleParam* for the *Dimension 1*
- Set the *bins* value to 80, the number of scale factors in the simulation
- Select *Count* for the *Operator*.
- Click on *Draw*.
- Move the *Dump* slider to the far right.

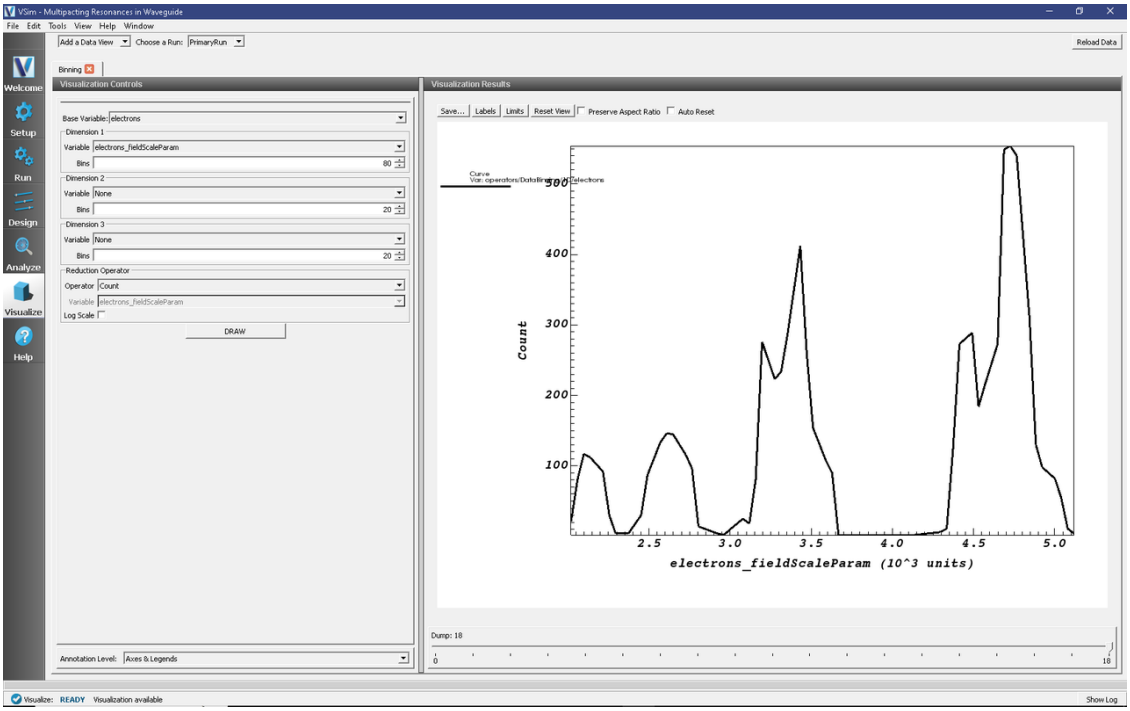


Fig. 4.116: Visualization of the resonance bands.

Further Experiments

Try seeing how changing the gap voltage or the frequency of the wave changes the multipacting resonances.

4.4.3 Multipacting Growth Using Prescribed Fields (multipactingGrowthPrescribedFields.sdf)

Keywords:

`multipacting`

Problem description

Multipacting, which is the resonant buildup of secondary electrons, is often a concern in microwave devices. Anytime there is an oscillating electromagnetic field across a gap between two surfaces there exists the possibility that for the right voltage across the gap a resonance condition will exist allowing the exponential buildup of secondary electrons. This example simulates multipacting growth in a spherical PEC cavity. The fundamental mode profile for the spherical PEC cavity is imported onto the VSim grid, then advanced in time by a single frequency time signal.

This simulation can be performed with the VSimVE or VSimPD license.

Opening the Simulation

The Multipacting Growth Prescribed Fields example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Multipacting* option.
- Select "Multipacting Growth Using Prescribed Fields" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 4.117. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

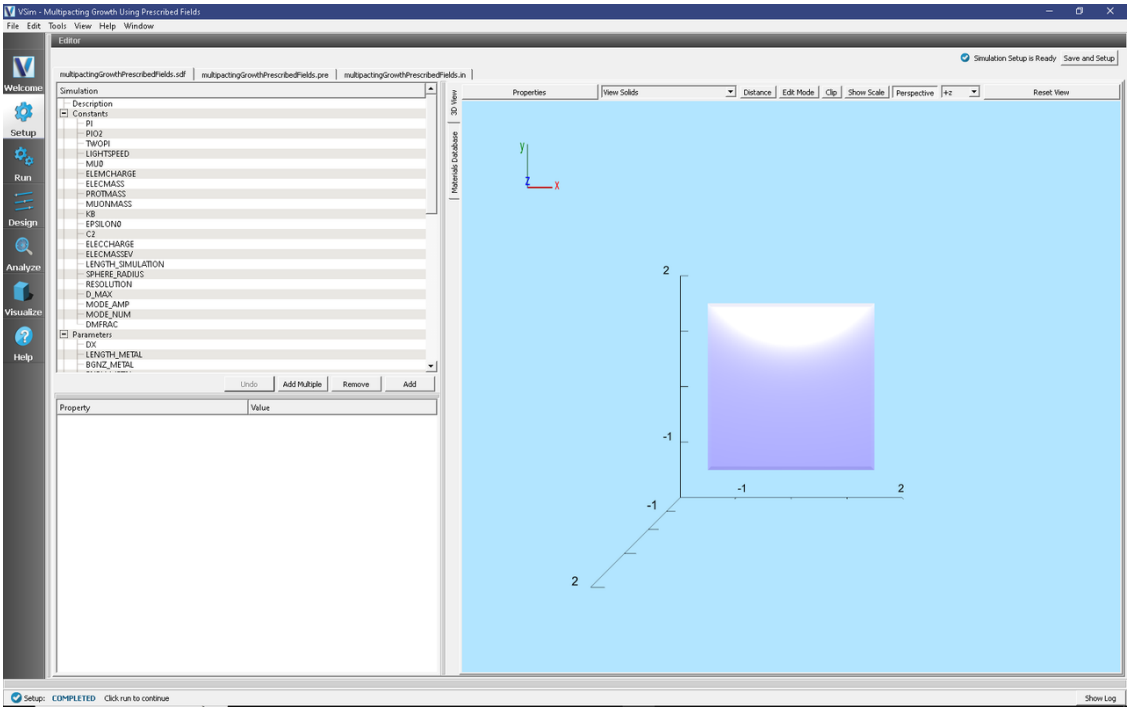


Fig. 4.117: Setup Window for the Multipacting Growth example.

Simulation Properties

This example contains a number of *Constants* to allow for easy manipulation of the device. Those include:

- **`SPHERE_RADIUS`**: radius of spherical cavity
- **`LENGTH_METAL`**: Length of metal box in each dimension (must be larger than 2*SPHERE_RADIUS)
- **`RESOLUTION`**: The number of cells per wavelength in each dimension
- **`MODE_NUM`**: The mode number determining the frequency of field oscillation

SpaceTimeFunctions are used to create expressions defining the drive frequency and amplitude of the applied field.

The amplitude and frequency of this driving function is defined in *Parameters*:

- **MODE_FREQ**: frequency at which the mode profile oscillates.
- **MODE_AMP**: amplitude that is applied to the mode profile each time step.

CSG is used to create the spherical PEC cavity by subtracting sphere from a cube.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.367922350136669e-11
  - *Number of Steps*: 20000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.118

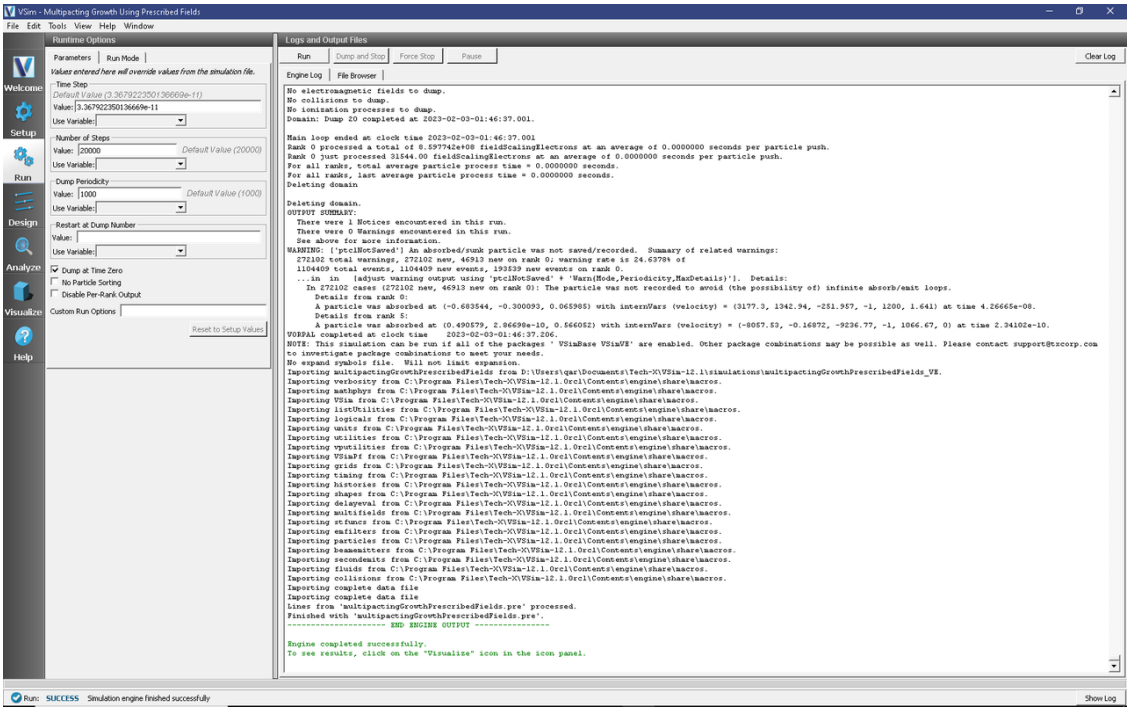


Fig. 4.118: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.
- Select *Binning* from the *Data View* pull down menu.
- Select *Auto Reset* at the top of the *Visualization Window*.

To view the field-scaling values at which multipacting occurs, as shown in Fig. 4.119, use the following settings in *Visualization Controls*:

- Set *Dimension 1* → *Variable* to *fieldScalingElectrons_fieldScaledParam*.
- Set *Dimension 1* → *Bins* to 100 (Note: always set the number of bins to be greater or equal than the number of scaling factors used in the particle setup).
- Under *Reduction Operator* set *Operator* to *Sum* and set *Variable* to *fieldScalingElectrons_weight*.
- Click *DRAW*.
- Move the dump cursor all the way to the right.

The overall trend in the number of electrons is that of an exponential growth with time at the correct field strengths that are controlled by the user's power settings during the design of the device.

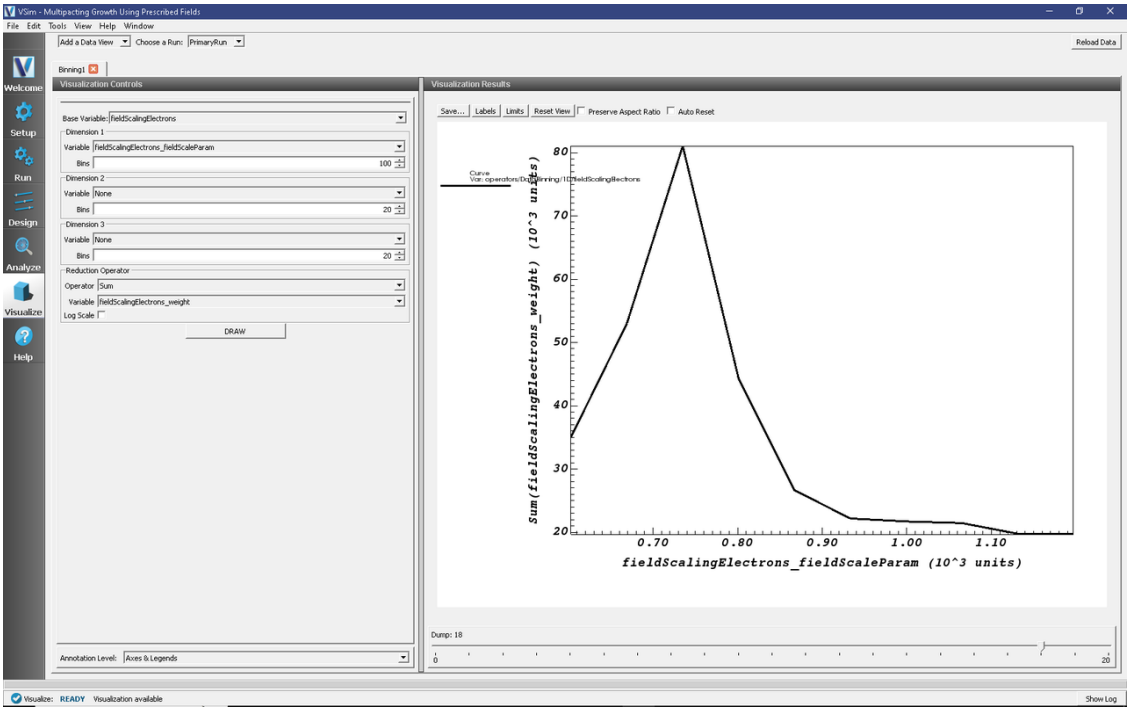


Fig. 4.119: Visualization of the exponential growth of the electrons due to multipacting.

Further Experiments

Multipacting behavior is sensitive to a number of factors, including the surface material properties, the field strength, and the oscillation frequency. One unmodeled parameter that can greatly affect multipacting is surface roughness. Varying the surface meshing tolerance, set by the **DM_FRAC** constant in this simulation, can be used as an analogue to tweak the multipacting strength. Try changing the parameters **DM_FRAC**, **MODE_AMP** and **MODE_NUM** to see if one can take the simulation in and out of resonance.

4.5 EmissionT (text-based setup)

4.5.1 Vaughan Secondary Emission (VaughanSecondaryElecT.pre)

Keywords:

VaughanSecondaryElecT

Problem description

Sometimes secondary emission processes are not adequately explained by the Furman-Pivi model, and sometimes we deliberately wish to compare how simulation results would be affected by different result files. In this example we show how to set up a user defined secondary emission model

Opening the Simulation

The Vaughan Secondary Emission example is accessed from within VSimComposer by the following actions:

- Select the *New From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Emission (text-based setup)* option.
- Select "Vaughan Secondary Emission (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 4.120.

Input File Features

The Vaughan Secondary Emission example has the following input parameters:

- NDIM allows adjusting of the number of dimensions
- NX, NY and NZ allow the setting of the number of cells in x, y and z respectively.
- LX, LY and LZ allow the setting of the size of the physical domain to be modeled respectively.
- E_BEAM_ENERGY specifies the energy of the incident electron beam in eV
- E_BEAM_CURRENT specifies the incident beam current
- E_BEAM_ANGLE chooses the angle at which the electrons are incident on a plane surface. We modify the angle of the geometry in this simulation, rather than moving the beam around.

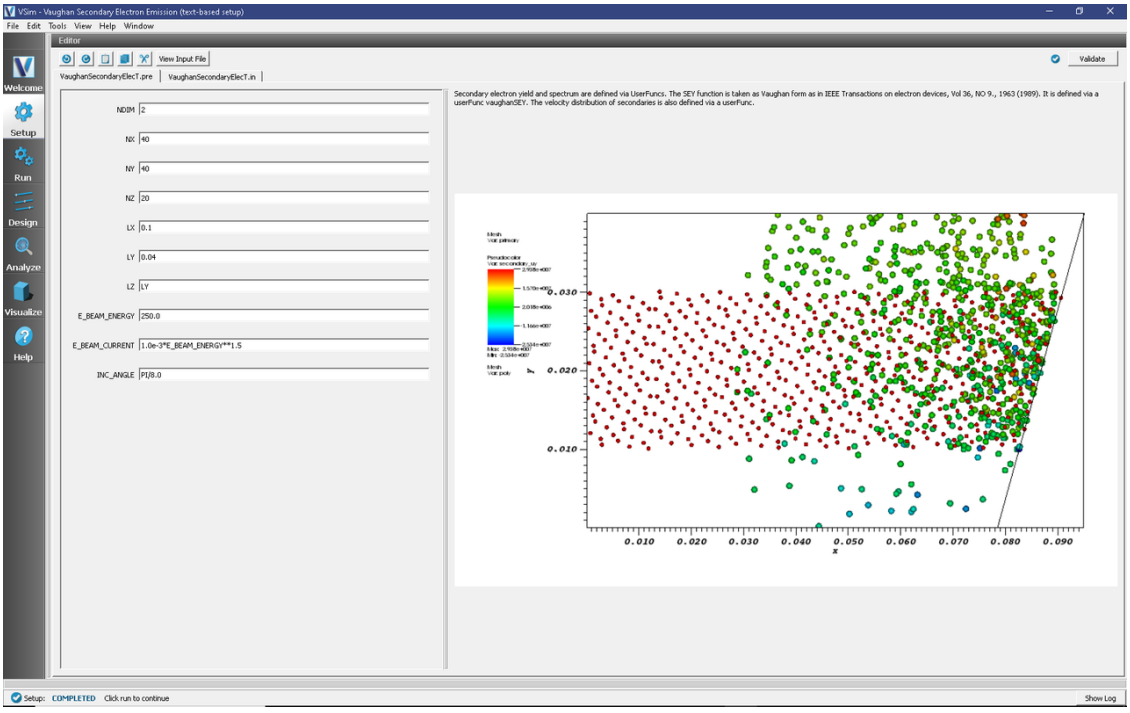


Fig. 4.120: Setup Window for the Vaughan Secondary Emission example.

Many of the interesting features in this file require us to click on *View Input File*.

The `userFunc` vaughanSEY around line 100 pairs up with

```
<UserFunc vaughanSEY>
  kind = expression
  inputOrder = [engInc alpha]
```

in the secondaryEmitter definition. By looking after lines 100 we see how the vaughanSEY arguments are read into this userFunc. We determine the type of data these arguments should contain then build up functions that depend on these arguments. Various terms are built up and then combined in the expression statement

```
expression= sigmaMax * funcF((engInc - Eth) / (EMax - Eth))
```

at the end. The second userFunc defines a cosine squared direction distribution, and the third the outgoing energy spectrum.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.0e-11
  - *Number of Steps*: 240
  - *Dump Periodicity*: 20

  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.121.

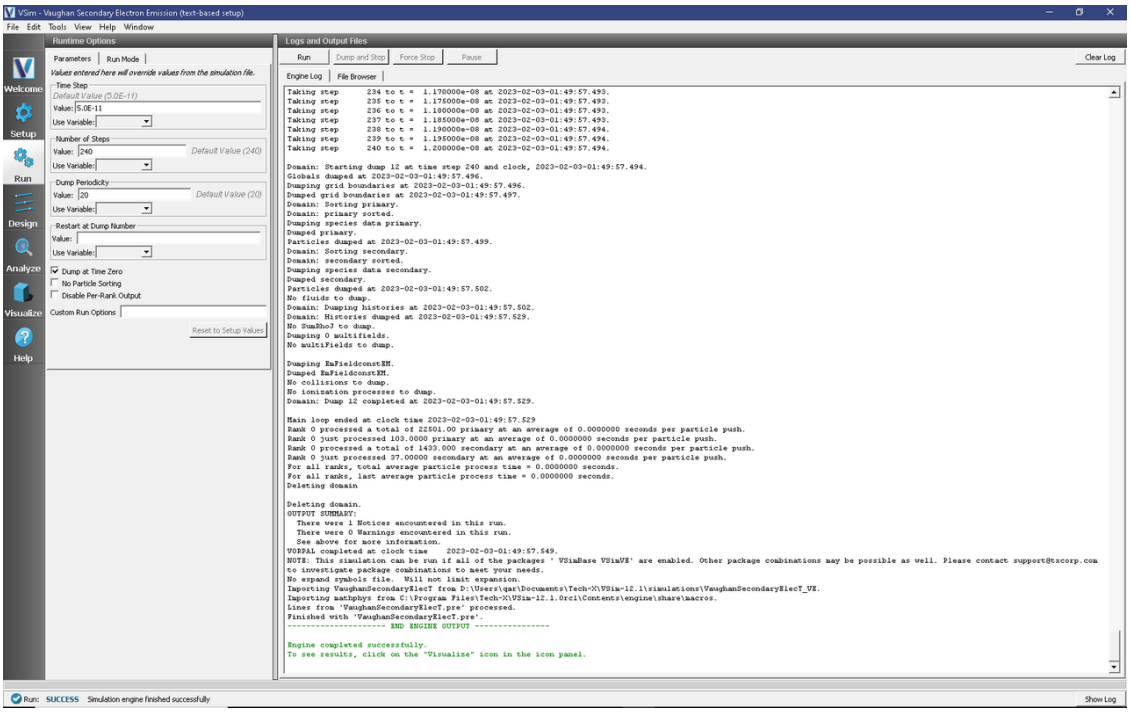


Fig. 4.121: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electrons as in Fig. 4.122:

- Select *Particle Data->primaries* and *Particle Data->secondaries* in the data tree
- If you have a high res monitor you may wish to increase the particle display size in the *Size* option under *Particle Style*.
- If you have run the analyzer since visualizing, you will want to click *Reload Data* before continuing.
- Select *Geometries->poly* to view the wall with which the particles are colliding.
- Move the dump slider to higher dump numbers to see the particles bouncing off the wall and more secondaries be created.

It is also possible to gain information about the effective secondary emission yield, the number of particles out given the particles going in, by comparing the number of primaries and secondaries in the simulation, and the rate at which they are created and lost at steady state.

In this simulation we just start by including histories for the total number of particles of each species, which may be viewed by selecting *Histories* under *Data View* in the top left.

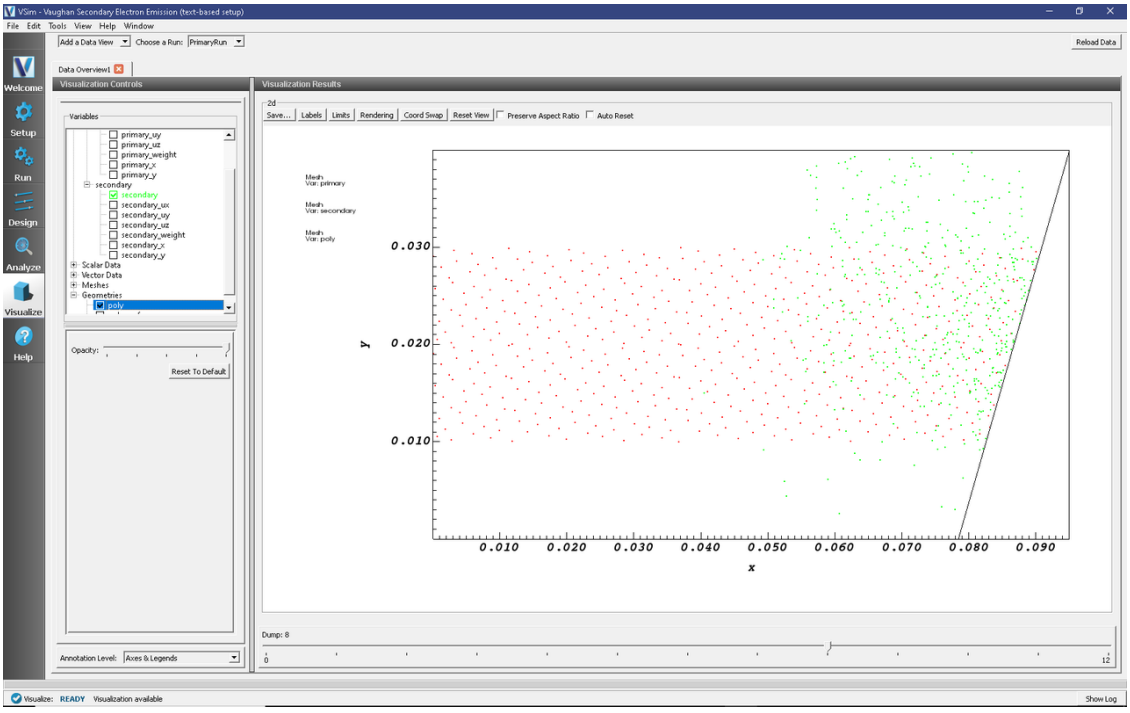


Fig. 4.122: Visualization of particles hitting the wall in Vaughan Secondary Electron Emission example.

Further Experiments

Extra histories have been included to measure the primary electron current absorbed on the wall, and a particle emission history to measure the rate at which the secondaries are coming away. For example with:

```
<History primCur>
  kind=speciesCurrAbs
  species= [primary]
  ptclAbsorbers = [plateAbsorber]
</History>
<History secCur>
  kind = speciesCurrEmit
  species = [ secondary ]
  ptclSource = secondary.secondaryEmitter
  sourceType = 0
</History>
```

One can then plot the histories as shown in Fig. 4.123. To add a history plot, click on *Add a Data View*, then click on *History*. You will notice a new visualization tab has been added next to "Data Overview". To change the font on any of the plots, click on "Tools", then click on "Settings", and finally click on "Visualization Options".

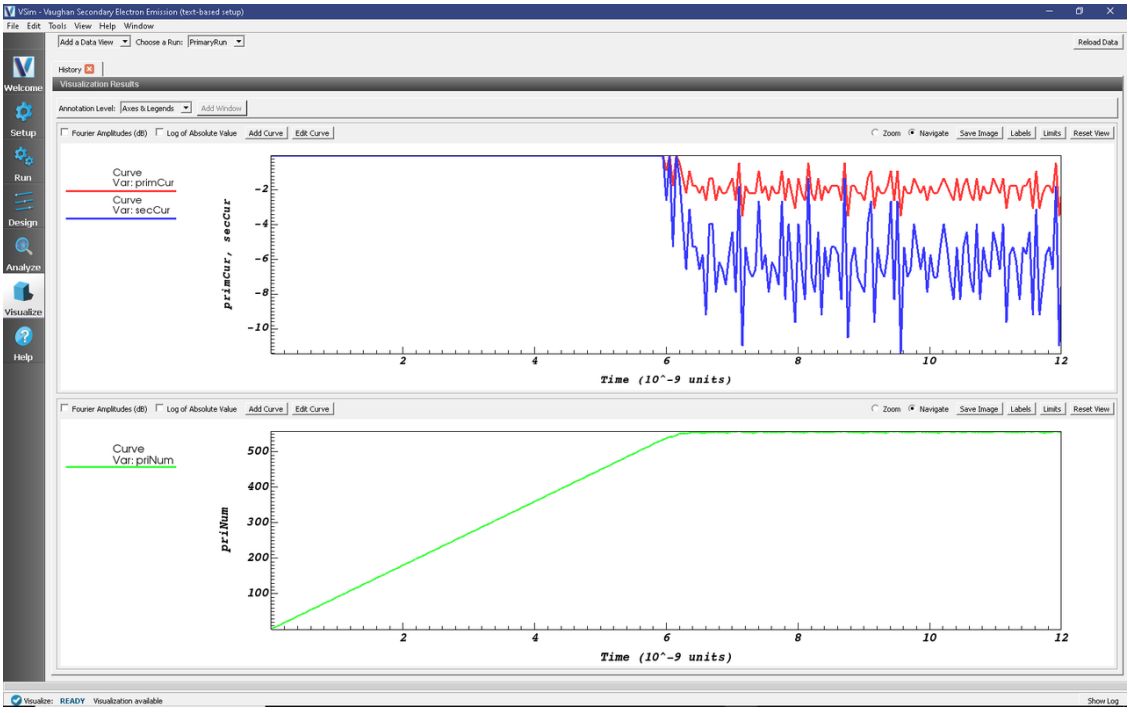


Fig. 4.123: Visualisation of ratio of primary and secondary particles in Vaughan Secondary Electron Emission example.

4.5.2 2D Laminar Brillouin Flow (laminarBrillouinFlowT.pre)

Keywords:

laminarBrillouinFlowT

Problem description

Many VSimVE applications require a smooth beam to achieve good performance. Simulating such devices can be computationally complex, and commonly we choose to work in 2D instead to save time. In this simulation, we demonstrate how to set up a beam that may be used in the interaction region of any vacuum electronic device you might simulate in 2D, with the interaction structure removed for simplicity.

This simulation can be performed with a VSimVE license.

Opening the Simulation

The Brillouin Flow example is accessed from within VSimComposer by the following actions:

- Select the *New From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Microwave Devices* option.
- Expand the *Emission (text-based setup)* option.
- Select "Laminar Brillouin Flow (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 4.124.

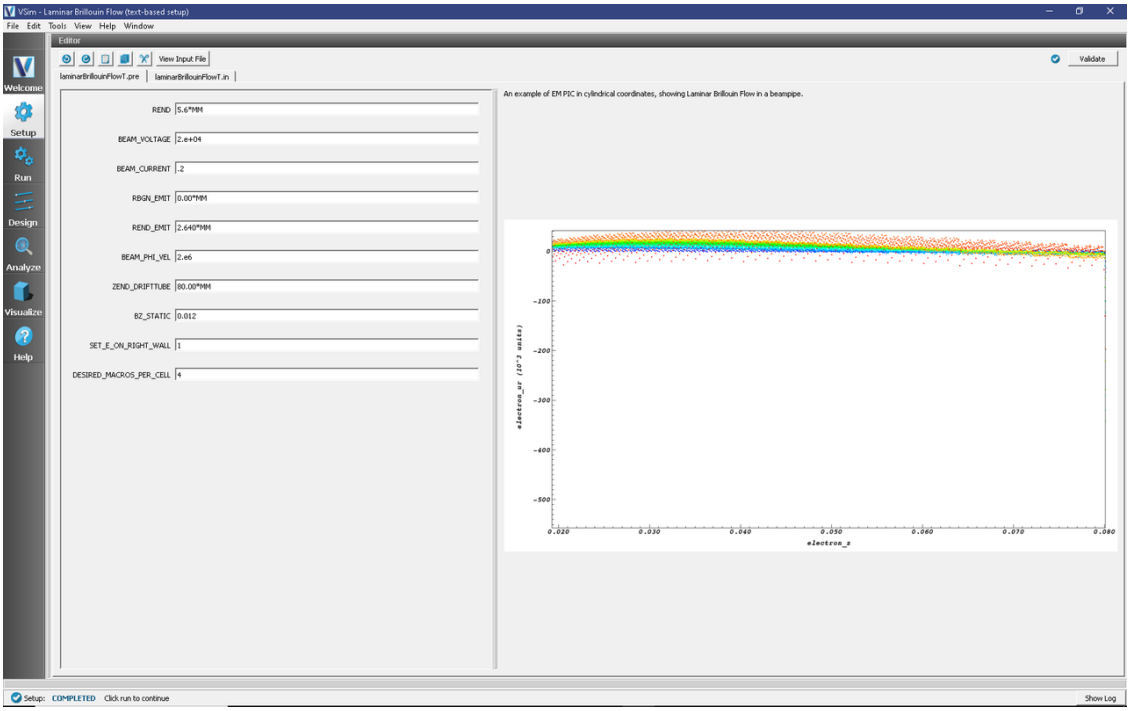


Fig. 4.124: Setup Window for the Brillouin Flow example.

Input File Features

The Laminar Brillouin Flow example has the following input parameters:

- REND is the radial extent of the problem.
- BEAM_VOLTAGE specifies the starting voltage for the electron beam.
- BEAM_CURRENT specifies the beam current.
- RBGN_EMIT and REND_EMIT specify the inner and outer radius respectively of the beam source on the left side of the simulation domain.
- BEAM_PHI_VEL sets the rotational velocity of particles at the outside of the beam. Those inside will be given azimuthal velocity proportional to radius.
- ZEND_DRIFTUBE determines the amount of beam pipe to simulate.
- BZ_STATIC sets the magnetic field (in Tesla)
- SET_E_ON_RIGHT_WALL allows for hard-coding a function for the field distribution on the right wall. When set to 1, and the other parameters have default values, the simulation behaves as if the right side of the simulation domain is open. Set to 0, a wall bounds the right side.
- DESIRED_MACROS_PER_CELL sets the particle discretization.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.66802682599226e-14
  - *Number of Steps*: 59987
  - *Dump Periodicity*: 1499
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.125.

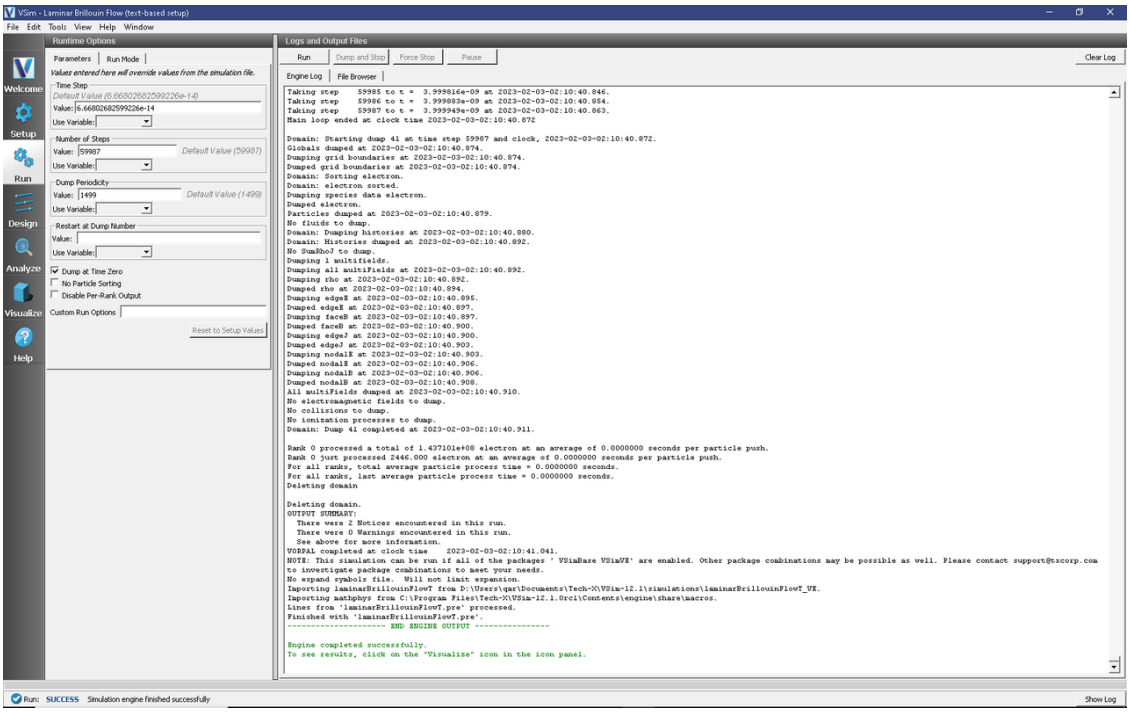


Fig. 4.125: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the exponential increase in electrons as in Fig. 4.126:

- Select *Field Analysis* under the *Data View* drop down
- Set the field to *edgeE_r*
- Pull the slider bar to Dump:40

- Set the layout to stacked 2d/1d

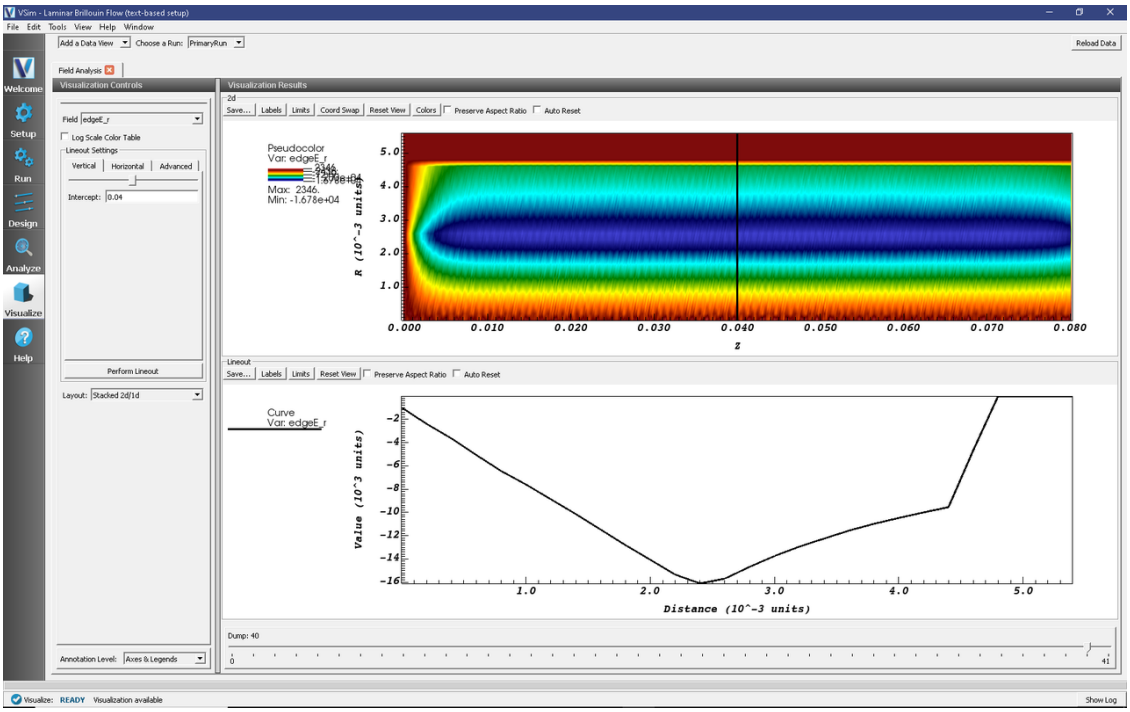


Fig. 4.126: One can see the transverse field profile.

The transverse field increases with radial distance inside the beam, follows a 1/r distribution outside the beam and rapidly drops to zero at the metal interface.

To view the velocity of the particles in the beam, such as that seen in Fig. 4.127:

- Select *Phase Space* under the *Data View* drop down
- Set the X-axis to *electron_z*
- Set the Y-axis to *electrons_uz*
- Set the Color to *electrons_r*
- Press *Draw*.
- Move the slide to the right to see how the beam stabilizes.

Switch to beam longitudinal velocity (Y-axis to *electrons_uz*), and note the orders of magnitude of difference.

Further Experiments

Try varying the starting and ending voltages, and see if the function used to set the right wall needs to be varied, and by how much.

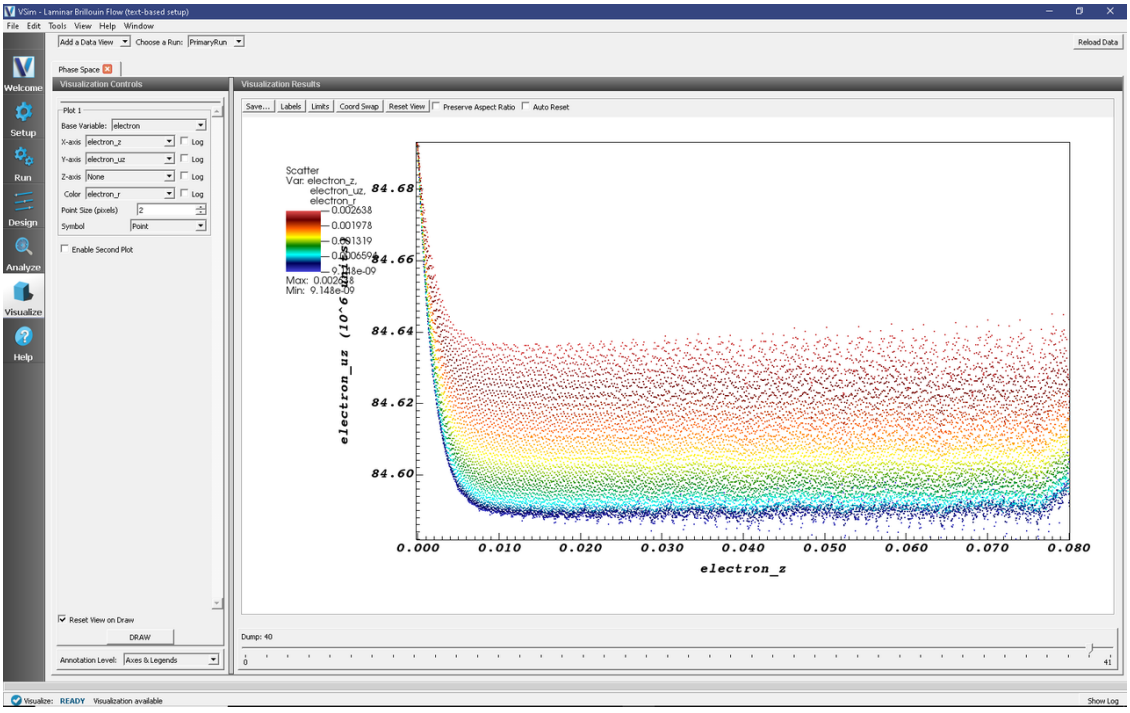


Fig. 4.127: The beam stabilizes fairly quickly and becomes close to monoenergetic with small transverse velocity.

4.6 Other

4.6.1 Electron Gun (electronGun.sdf)

Keywords:

`electron, gun, beam, collimate`

Problem description

Electron guns are devices that are often found in vacuum electronics as well as in more advanced technologies such as klystrons, electron microscopes, and particle accelerators. They produce narrow, collimated beams of electrons with precisely tuned kinetic energies. They were often found in cathode ray tubes at the heart of television sets prior to the digital revolution. Electron guns are composed of a cathode, an anode, and repulsive rings. A DC or RF signal is applied to the cathode to produce electrons via thermionic emission. The electrodes produce electric fields that focus the electron beam. Often an additional anode is placed between the cathode and the main anode to act as a repulsive ring that focuses the beam into a small hole in the main anode. The small hole in the main anode acts to collimate the beam.

This example is a specialized electron gun for klystrons and TWTs. It is characterized by high power, a consequence of which is that electrons not successfully collimated can damage the device. To minimize this effect, the gun includes a focusing anode cone, the angle of which is conducive to laminar flow of the electron beam.

Opening the Simulation

The Electron Gun example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Other VE* option.
- Select "Electron Gun" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 4.128.

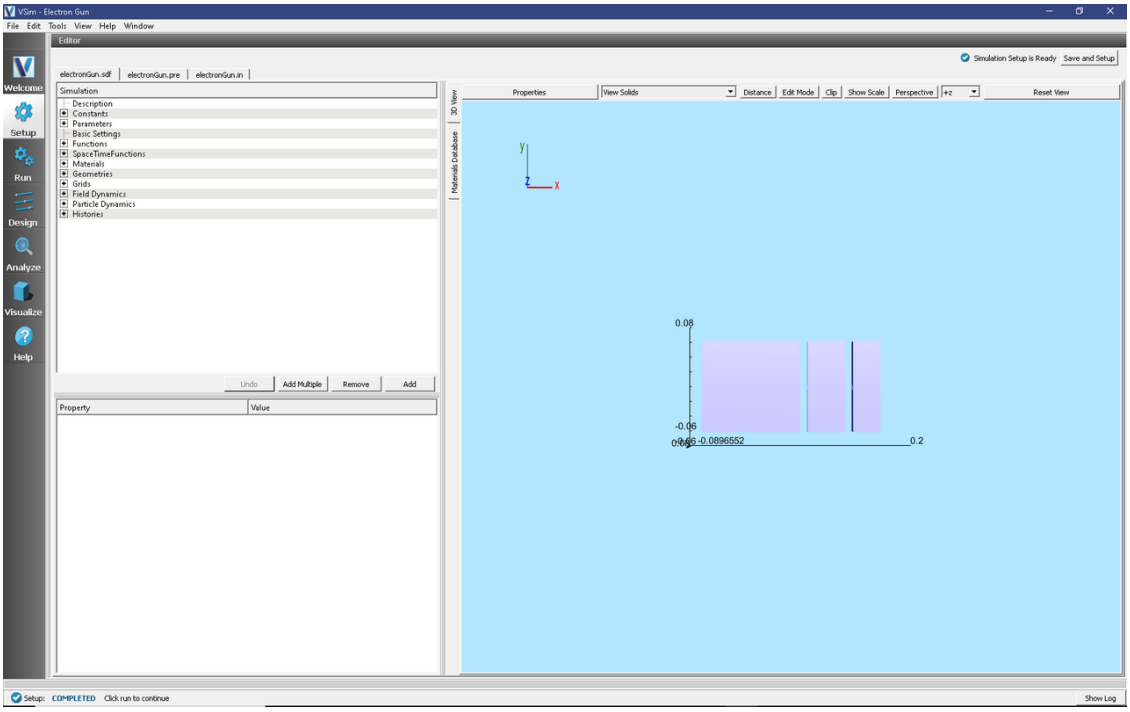


Fig. 4.128: Setup Window for the Electron Gun example.

Simulation Properties

The input parameters give you total flexibility in defining the geometry of the example. Along with these one can define the nominal cell size, the driving voltages, the strength of the magnetic field, and the beam current.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 8.787778096277544e-13
  - *Number of Steps*: 13690
  - *Dump Periodicity*: 684
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.129.

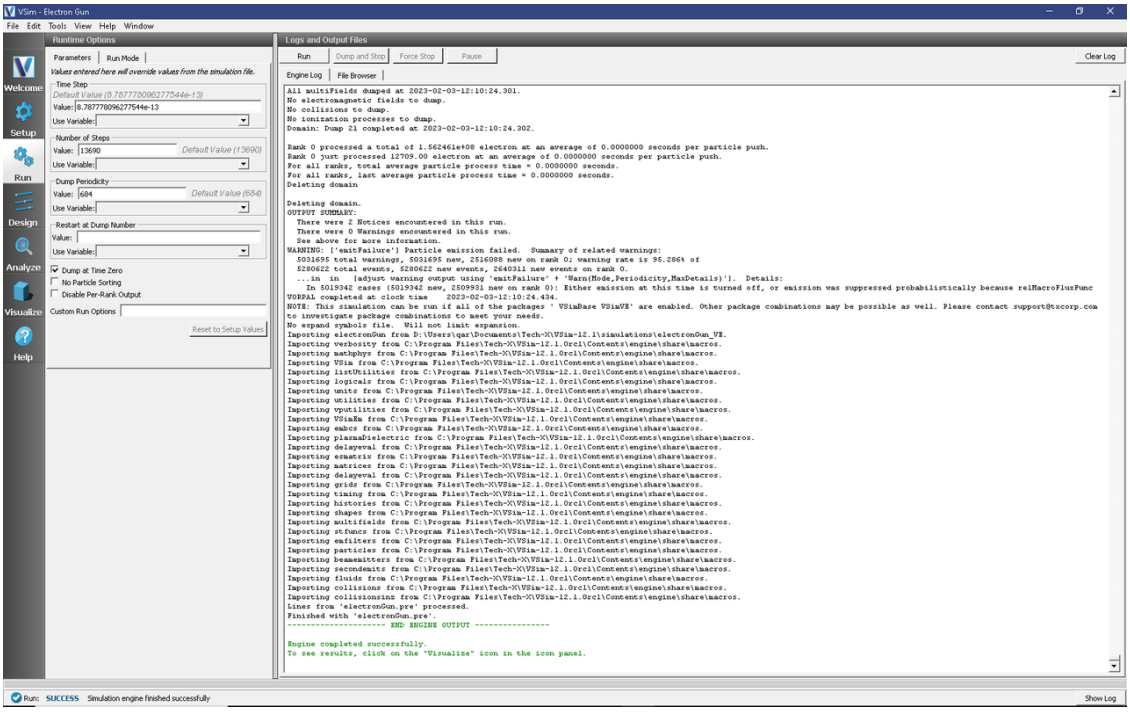


Fig. 4.129: The Run Window at the end of execution.

Visualizing the Results

To reproduce Fig. 4.130 proceed as follows:

- Expand *Particle Data*.
- Expand *electron*.
- Select *electron* in red.
- In the lower part of the right pane, move the Dump slider to dump 14.
- Check the "Clip plot" checkbox.
- Expand *Scalar Data*
- Expand *E*.
- Select "E_magnitude".
- In the lower part of the left pane select "Display Contours".
- Check the "Clip plot" checkbox.
- Expand *Geometries*.
- Select "poly (electronGunPecShapes)".
- Check the "Clip plot" checkbox.

This will show the electron beam and the electric and magnetic fields.

The phase space diagram can also be viewed by choosing *Phase Space* in the *Add Data View* drop down menu in the top left of the main pane.

The voltages and currents at key locations in the simulation are recorded in Histories and can be viewed by selecting the *History* data view.

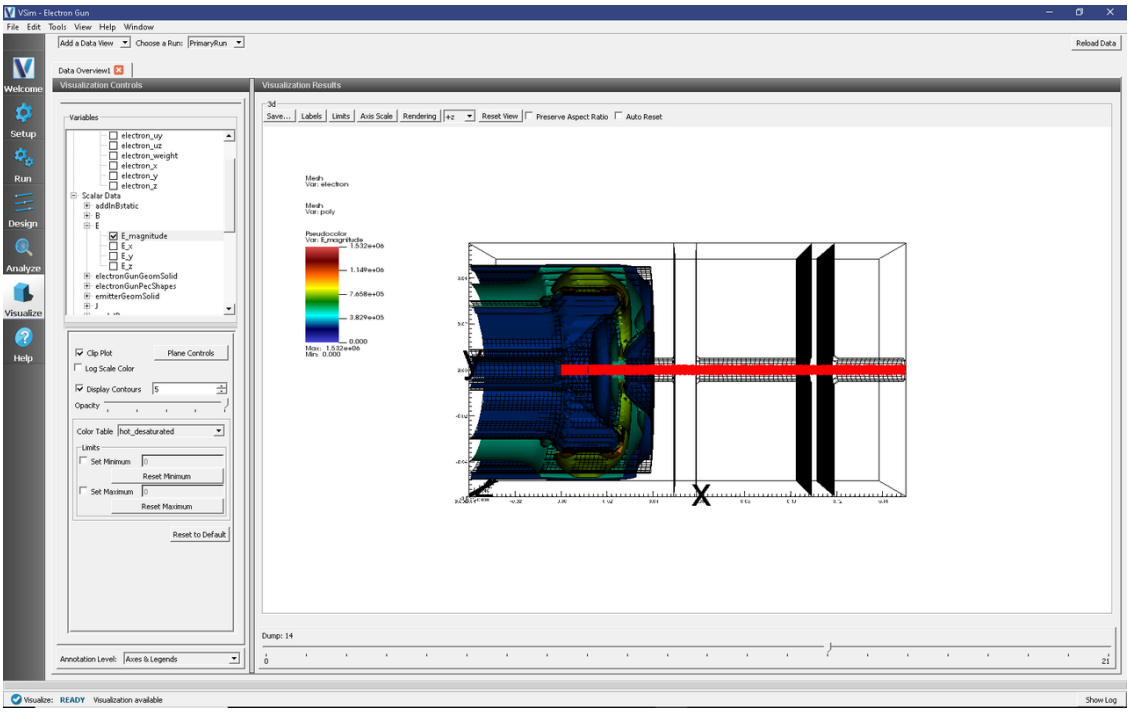


Fig. 4.130: The electron beam and electric field.

Further Experiments

The geometry is extremely important for proper functionality in this example. For example, the angle that the focusing cone makes with the beam axis determines whether the beam will be laminar. If the beam intersects and diverges, the gun can be damaged by its own power. Try altering the dimensions of the geometry and see the effect on the electron beam.

4.6.2 Multistage Collector (multistageCollector.sdf)

Keywords:

`electromagnetics, multistageCollector`

Problem description

Multistage Depressed Collectors (MDCs) are used to recover energy from a spent beam in linear type microwave tubes such as traveling wave tubes (TWTs) and klystrons. VSim provides the capability to simulate these collectors shaped with arbitrarily complex geometries and depressed with different time-dependent voltage profiles to optimize the recovery efficiency of a design. To demonstrate this capability, we show in this example a 4-stage depressed collector. One can adjust the depressed potentials at each electrode individually to see how the performance of the collector is affected.

This simulation can be performed with a VSimVE or VSimPD license.

Opening the Simulation

The Multistage Collector example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Vacuum Electronics* option.
- Expand the *Other VE* option.
- Select "Multistage Collector" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 4.131.

Simulation Properties

The simulation geometry consisting of an S-band 4-stage depressed collector is imported into the computational engine from CAD files in stl format. One can easily create new geometry using any CAD program and output or convert the CAD files into stl files for a new simulation design. The detailed import method is provided in the input file. The spent beam profile is taken from a TWT simulation provided by Prof. H. Song at University of Colorado at Colorado Springs.

An optimized design for a MPM module can be found in reference [1]. Users can set preferred spent beam profiles by employing different emission methods or import data in data format as in this example. A main feature of this input file is that the depressed voltage profiles are time-dependent and are stabilized with a new external circuit model based on special feedback algorithms only available in VSim. Interested users may refer to the publication for a more detailed description and validation. In addition, the convergence of this example is carefully tested.

In this example, the Z coordinate is the direction aligned with the beam axis of the MDC, and the 4 different voltages can be easily assigned at the input panel. Since it is a time domain simulation, the Dey-Mittra algorithm is employed and the accuracy is second-order for the complex boundaries.

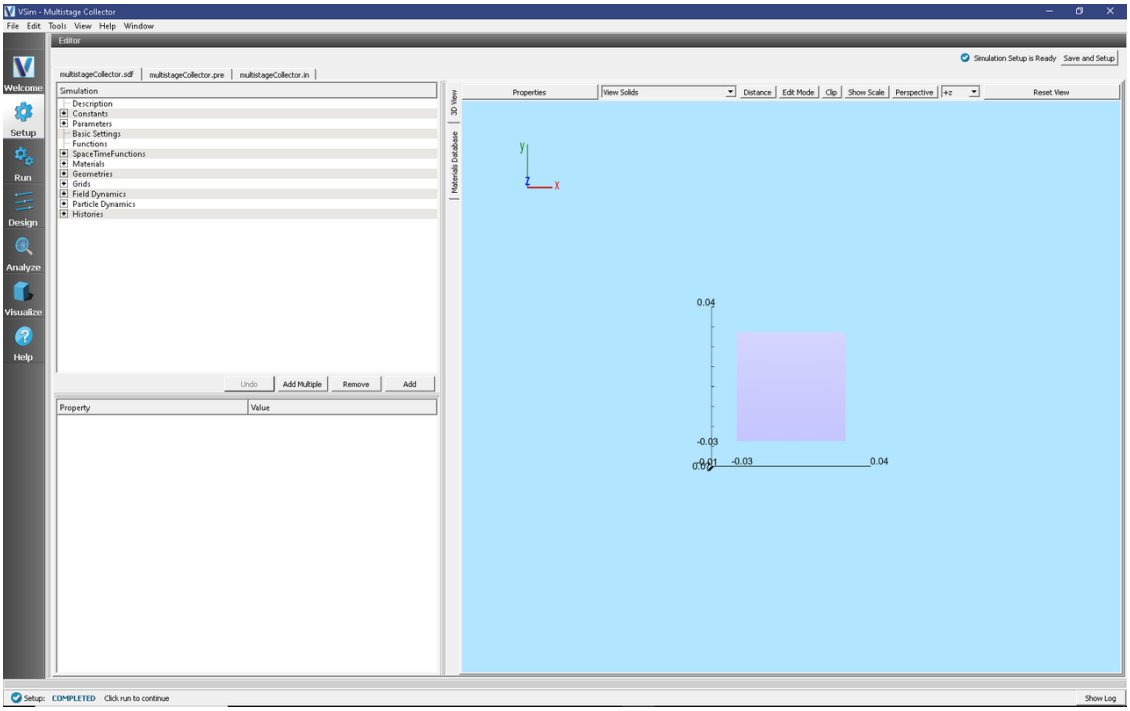


Fig. 4.131: Setup Window for the Multistage Collector example.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.6369582213145e-12
  - *Number of Steps*: 5000
  - *Dump Periodicity*: 250
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 4.132.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

The results are then read from the Data Overview in the Visualize Window:

- Expand *Particle Data*.
- Expand *electrons*.
- Select *electrons* in red.

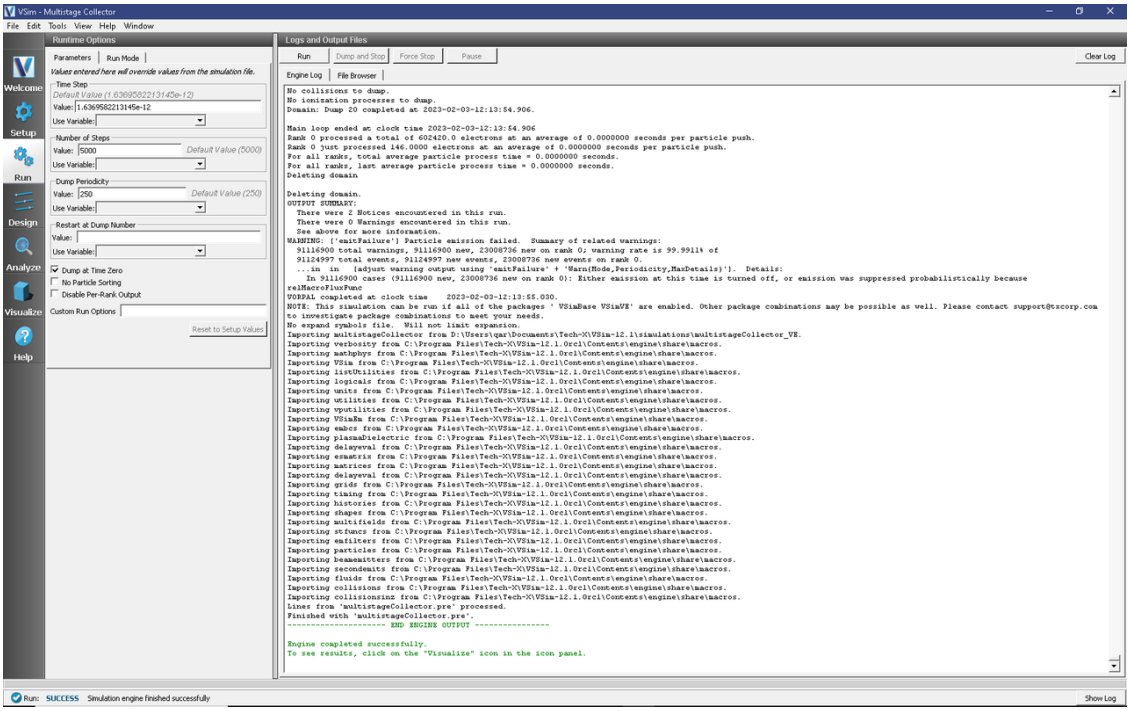


Fig. 4.132: The Run Window at the end of execution.

- Move the Dump slider all the way to the end.
- Check the *Clip Plot* box.
- Click on *Plane Controls* and in the *Clip Plane Control* window, under *Clip Plane Normal* select *X (plane normal to x-axis)*, then click *Ok*.
- Expand *Scalar Data*.
- Expand *E*.
- Select *E_z*.
- Check the *Display Contours* box.
- Check the *Clip Plot* box.
- Click on *Plane Controls* and in the *Clip Plane Control* window, under *Clip Plane Normal* select *X (plane normal to x-axis)*, then click *Ok*.
- Expand *Geometries*
- Select the second option from the top: *multistageCollectorGeomSolidMappedPolysData_surface*.
- Check the *Clip Plot* box.
- Click on *Plane Controls* and in the *Clip Plane Control* window, under *Clip Plane Normal* select *X (plane normal to x-axis)*, then click *Ok*.
- Use the cursor to grab the image and rotate it from right to left to see the image in Fig. 4.133.

The potential of each collector surface is recorded using a history. To visualize these values as shown in Fig. 4.134, do the following:

- Switch *Data View* to “History”.

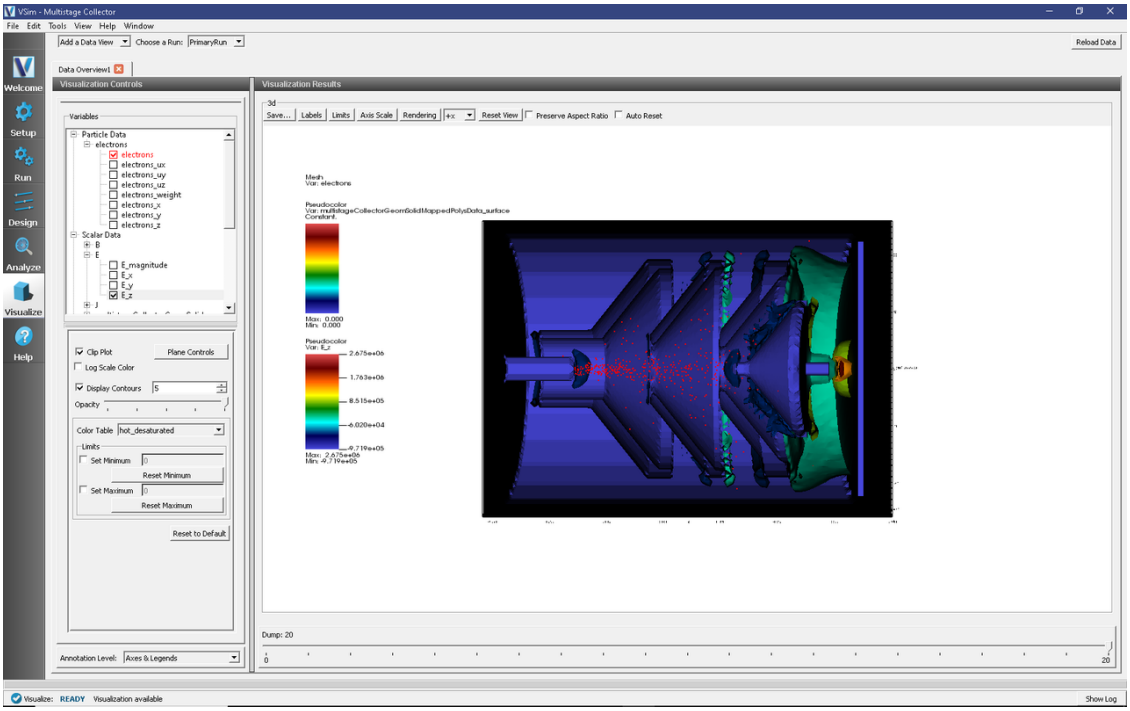


Fig. 4.133: Visualization of the MDC model with a color contour plot of electric fields and electrons in red.

- In the left pane, set Graphs 1-4 to each of the different potential histories: "potential10", "potential20", "potential30", and "potential40", respectively.
- Set the *Location* of each graph to "Window 1".

Further Experiments

The depressed voltages or beam current/radius can be varied in the input panel for testing runs. One can also change the grid cell numbers to see the convergence of the simulations.

References

[1] M. C. Lin, P. H. Stoltz, D. N. Smithe, H. Song, H. J. Kim, J. J. Choi, S. J. Kim, and S. H. Jang, "Design and Modeling of Multistage Depressed Collectors Using 3D Conformal Finite-Difference Time-Domain Particle-In-Cell Simulations ", J. Korean Phys. Soc. 60, 731-738 (2012).

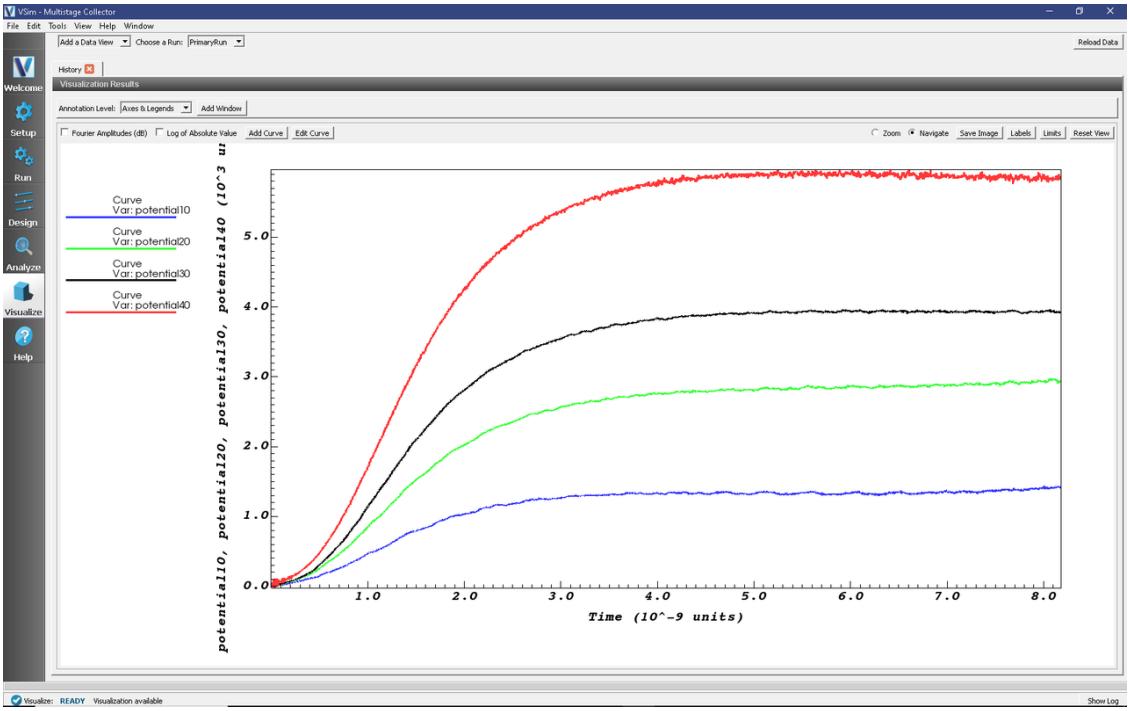


Fig. 4.134: The value of the potential on each of the collectors.

CHAPTER

FIVE

VSIM FOR PLASMA ACCELERATION EXAMPLES

These examples illustrate how to solve complex problems in plasma acceleration.

These examples can be run with a VSimPA license.

5.1 Beam Driven

5.1.1 Electron Beam Driven Plasma Wakefield (electronBeamDrivenPlasma.sdf)

Keywords:

electron driven, plasma wakefield, CLARA, PARS, AWAKE

Problem description

This example demonstrates a method to simulate an electron beam driven plasma wakefield accelerator. The electron beam initializes the field using a speed of light frame Poisson equation solve, then the fields and particles are evolved using FDTD EMPIC. We launch the electron beam from x=0 in the positive x direction using the Lorentz boosted Poisson fields to ensure that the simulation is self-consistent from start. The primary bunch generates a region of high field into which one might inject and accelerate a second bunch of charged particles. The example simulation uses parameters that are appropriate to the plasma acceleration research station (PARS) at the CLARA accelerator at Daresbury Laboratory in the UK.

Opening the Simulation

The Electron Beam Driven Plasma Wakefield example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Beam Drive Acceleration* option.
- Select *Electron Beam Driven Plasma Wakefield* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is shown in Fig. 5.1.

At this stage one can use the element tree on the left-hand side to choose constants such as `LONGITUDINAL_RES` and `TRANSVERSE_RES` which represent the longitudinal and transverse number of cells per RMS bunch size. The minimum of 6 or default of 8, generates a simulation that will complete reasonably quickly, but is not adequate to generate

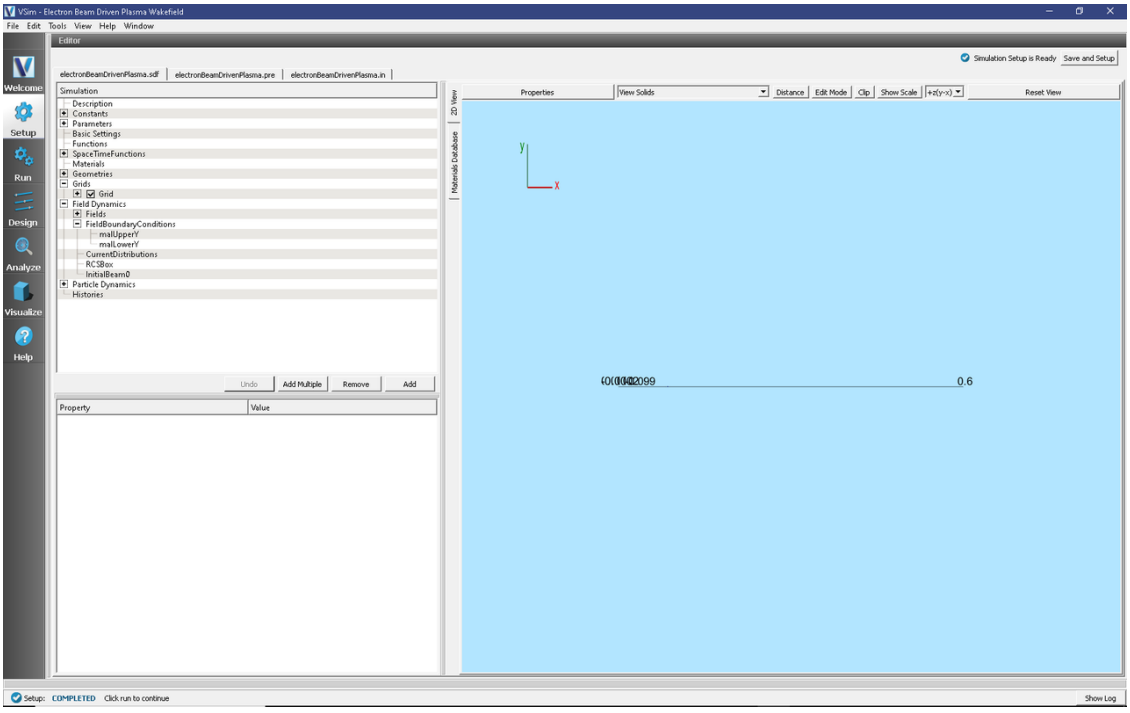


Fig. 5.1: Setup Window for the Electron Driven Plasma Wake example.

good results. Consider 12 or 16 cells in both dimensions to avoid a "checkerboard" pattern of numerical noise from developing.

Input File Features

The simulation setup consists of an electromagnetic solver using the Yee algorithm and uses the initBeam macro to set up the initial beam properties. This takes the beam of variable weight particles and calculates self-consistent fields with which to initialize the simulation. As this beam travels near the speed of light, a moving window that co-propagates with the beam is employed. MALs are used on the transverse sides of the window to absorb outgoing waves. The plasma is represented by macro-particles, and both beam and plasma are moved using the Boris push. The particles in the plasma are variably weighted to represent the density ramp. It is assumed the plasma consists of pre-ionized heavy ions, which do not move in the time frame of the simulations.

One can specify the size of the region to be simulated through the constants `LONGITUDINAL_EXTENT` and `TRANSVERSE_EXTENT`, which are measured relative to the longitudinal RMS size `BEAM_LRMS` and transverse RMS size `BEAM_SIGMAR` of the beam. The number of cells is determined by the settings of `LONGITUDINAL_RES` and `TRANSVERSE_RES`, as shown in the figure.

The plasma density is ramped up using a flat top cosine function, by default, over a quarter of the longitudinal size of the simulation window. This can be modified by editing the `STARTRAMP` and `RAMPLEN` parameters.

Running the Simulations

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 8.057451509102428e-15
  - *Number of Steps*: 3000
  - *Dump Periodicity*: 300
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 5.2.

You can expect a 2 core laptop to take a few minutes at the default resolution and run time.

To produce real significant results, a higher resolution is required by changing LONGITUDINAL_RES and TRANSVERSE_RES. Doing so will greatly increase the amount of time to run this simulation. It should also be run for a longer time than the default 3000 steps.

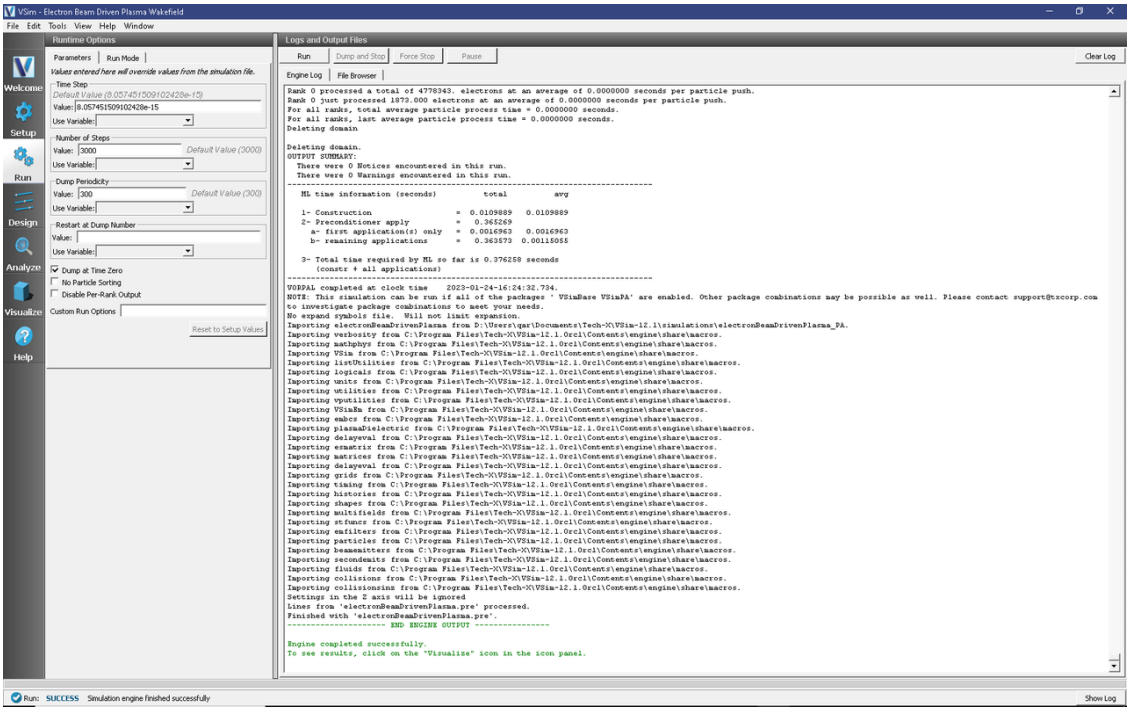


Fig. 5.2: The Run Window.

Visualizing the Output

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize Tab in the left column of buttons.

View the electric field generated by the plasma as shown in Fig. 5.3 by doing the following:

- Select *Field Analysis* in the drop down *Add a Data View* Controls pane
- Set the *Field* to *E_x*
- Choose the *Horizontal* tab in *Lineout Settings* set the intercept to zero, and click *Perform Lineout*
- Check the *Auto Reset* buttons on both the 2d and the Lineout plots. Sometimes it is necessary to expand the plot size in order for the box to appear. You can do this by pulling the divider between "Visualization Controls" and "Visualization Results" to the left and hiding it. Both the 2d and the Lineout plots should be larger now.
- Move the dump slider forward in time.

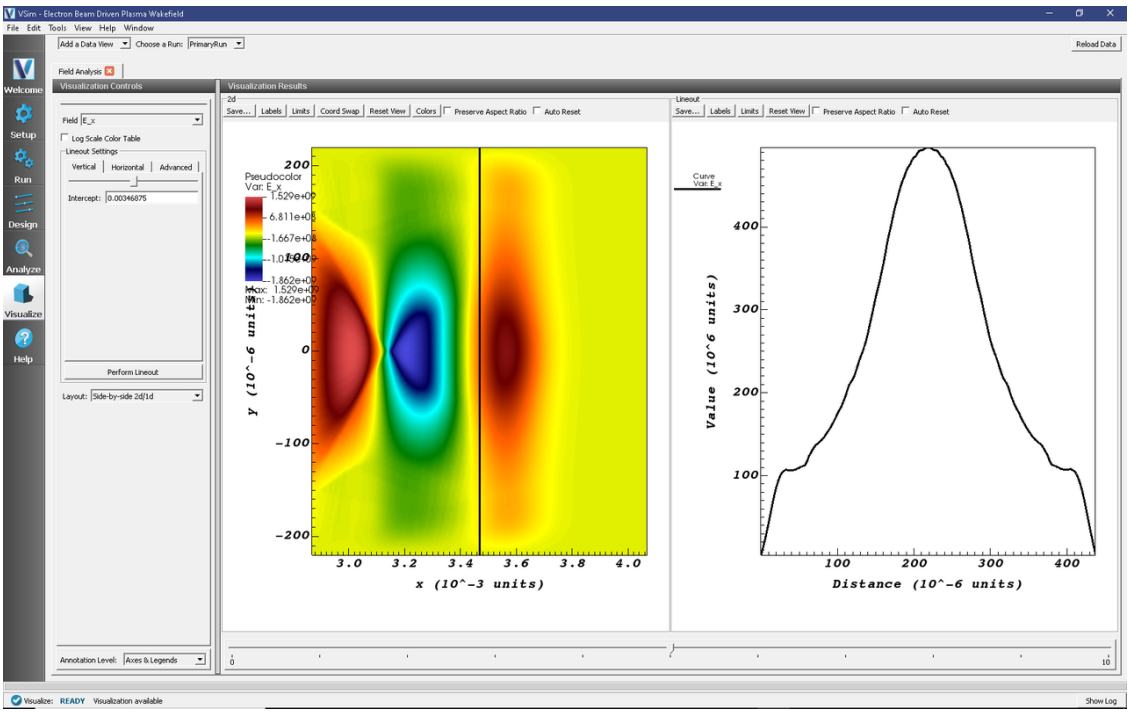


Fig. 5.3: Visualization of the longitudinal electric field as a color contour plot and longitudinal lineout.

The plasma density can be seen as shown in Fig. 5.4 by doing the following:

- Switch to *Data Overview* in the *Data View* drop down
- Expand *Scalar Data*
- Select *rhoBeam*
- Click *Auto Reset*
- Move the slider all the way to the right.

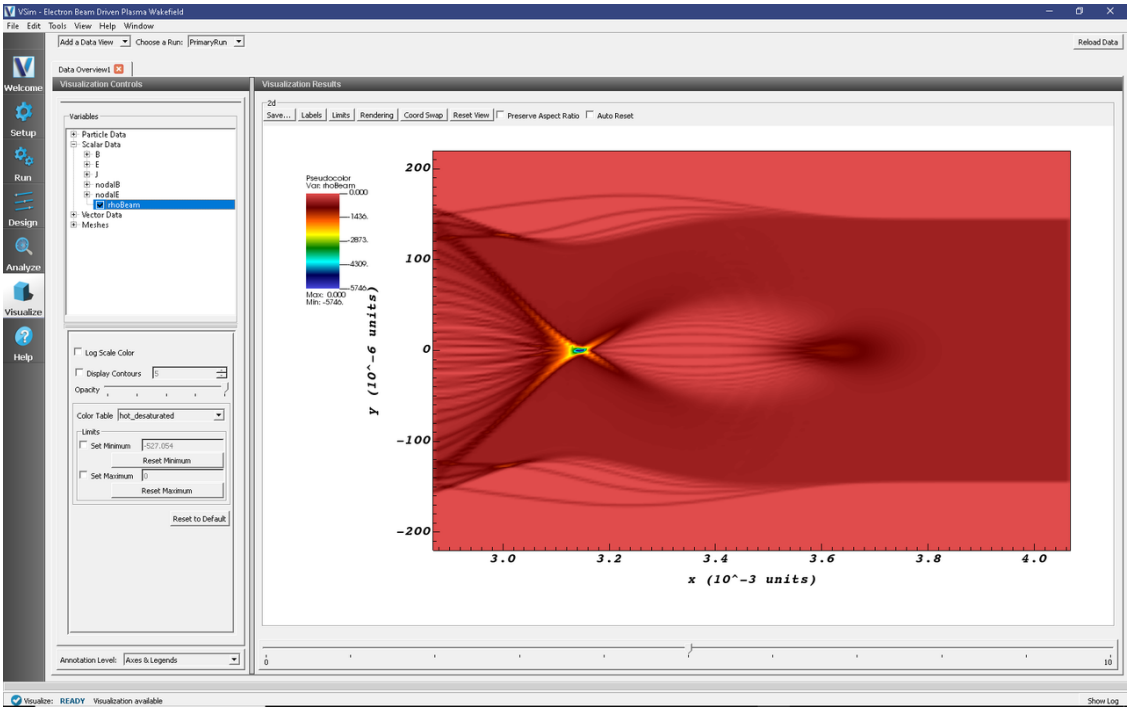


Fig. 5.4: Visualization of the longitudinal plasma density field as a color contour plot.

5.2 Beam Driven (text-based setup)

5.2.1 Dielectric Wall Wakefield Acceleration (dielectricwallacceleration t.pre)

Keywords:

electron driven, plasma wakefield, CLARA, PARS, AWAKE

Problem description

An alternative to a full particle in cell approach for accelerator computations is to use a prescribed beam, that is to set the J field directly without using a vector deposition of the current associated with the charge. This is demonstrated in this example which computes the wakefields in a dielectric lined waveguide. The electron beam initializes the field using a custom python technique, which can be adapted for cases where the Poisson solve might not be appropriate (due to memory limitations for example) then the fields (and effective) particles are evolved using FDTD. We launch the electron beam from x=0 in the positive x direction. The primary bunch generates a region of high field into which one might inject and accelerate a second bunch of charged particles. This simulation broadly follows the approach reported on in [MPSC11]

Opening the Simulation

The Dielectric Wall Wakefield Acceleration example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Beam Driven Acceleration (text-based setup)* option.
- Select *Dielectric Wall Wakefield Acceleration (text-based setup)* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 5.5.

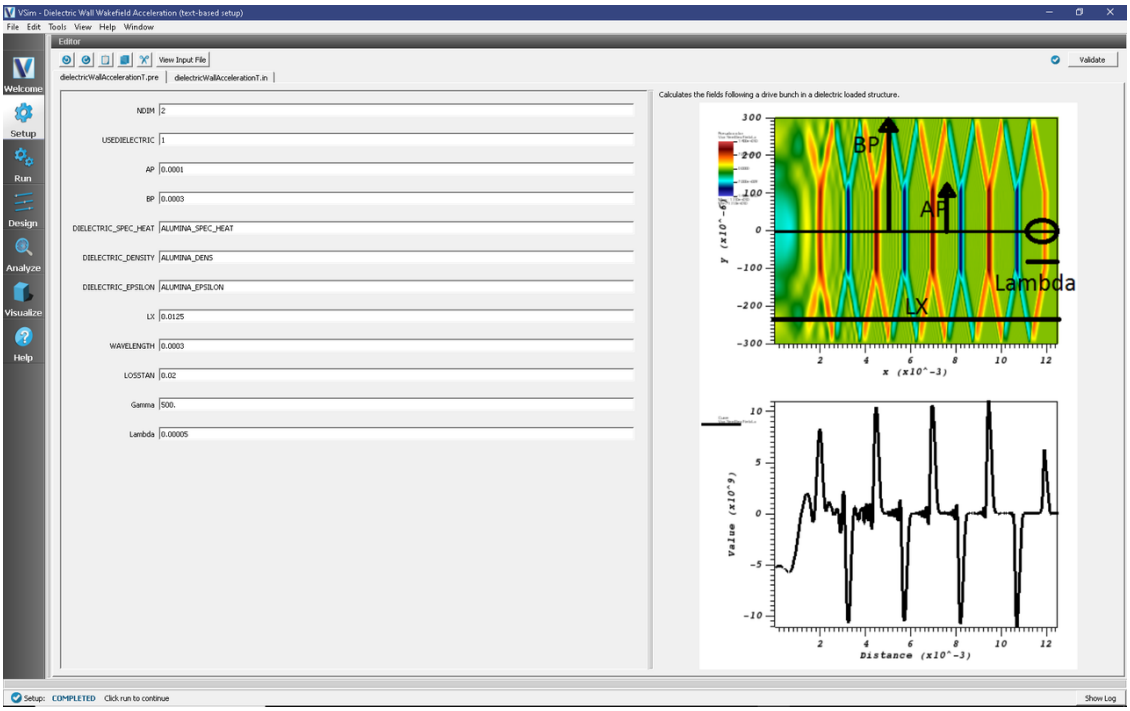


Fig. 5.5: Setup Window for the Dielectric Wall Wakefield Acceleration example.

Input File Features

The simulation setup consists of an electromagnetic solver using the Yee algorithm and takes advantage of a prescribed current source to avoid computationally intensive particle pushes. The 'top' and 'bottom' y extents of the simulation are metal, and we see the behavior in a dielectric lined waveguide, using a first order accurate dielectric algorithm for the walls.

- `BP` is the beampipe half-width
- `AP` is the dielectric aperture half-width
- `DIELECTRIC_EPSILON` allows the user to experiment with different materials
- `LX` sets the length of the structure and simulation
- `Gamma` sets the relativistic velocity of the beam to be used.

Inside the .pre file, which you can reach by pressing *View Input File*, there are various other settings for modeling this with a laser drive, or with PIC particles.

Running the Simulations

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.5330471121731 93e-14
  - *Number of Steps*: 12500
  - *Dump Periodicity*: 250
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 5.6.

Running in 2D, you can expect a 2 core laptop to take a few tens of minutes at the default resolution and run time.

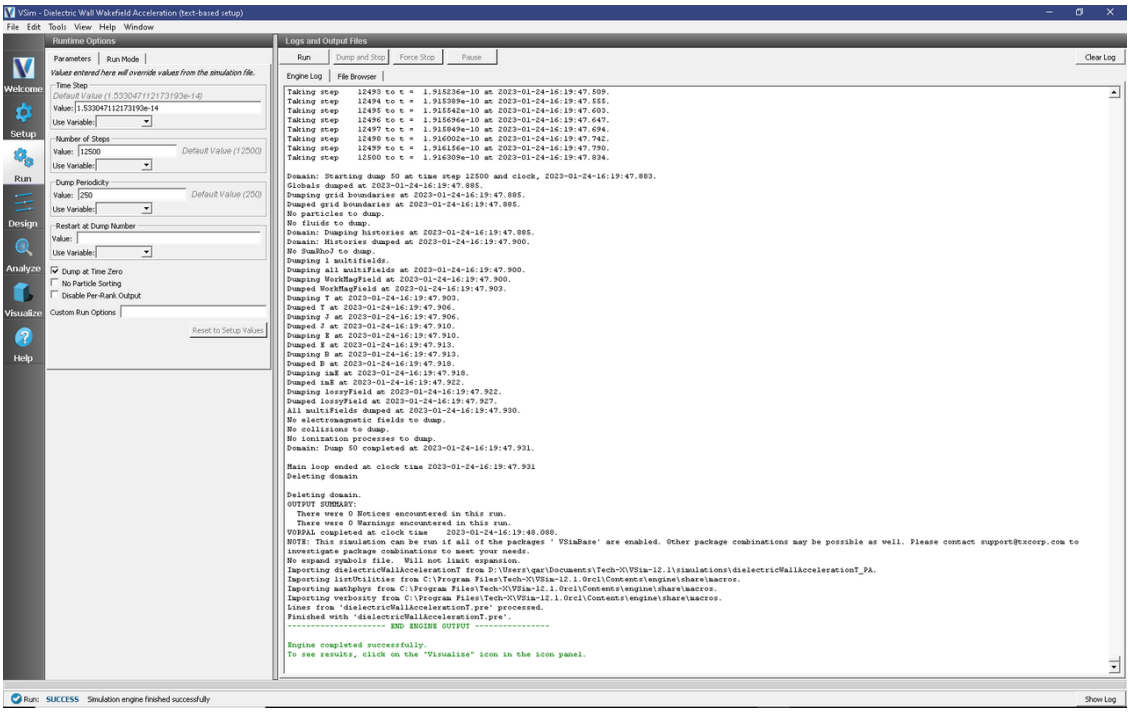


Fig. 5.6: The Run Window.

Visualizing the Output

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize tab in the left column of buttons.

View the electric field generated by the plasma as shown in Fig. 5.7 by doing the following:

- Switch to *Field Analysis* in the *Data View* Controls pane
- Set the *Field* to *E_x*
- Choose the *Horizontal* tab in *Lineout Settings* set the intercept to zero, and click *Perform Lineout*
- Below *Perform Lineout* in the *Layout:* drop down menu, Select stacked 2d/1d view.
- Check the *Auto Reset* buttons on both the 2d and the Lineout plots. Sometimes it is necessary to expand the plot size in order for the box to appear. You can do this by pulling the divider between "Visualization Controls" and "Visualization Results" to the left and hiding it. Both the 2d and the Lineout plots should be larger now.
- Move the dump slider forward in time.

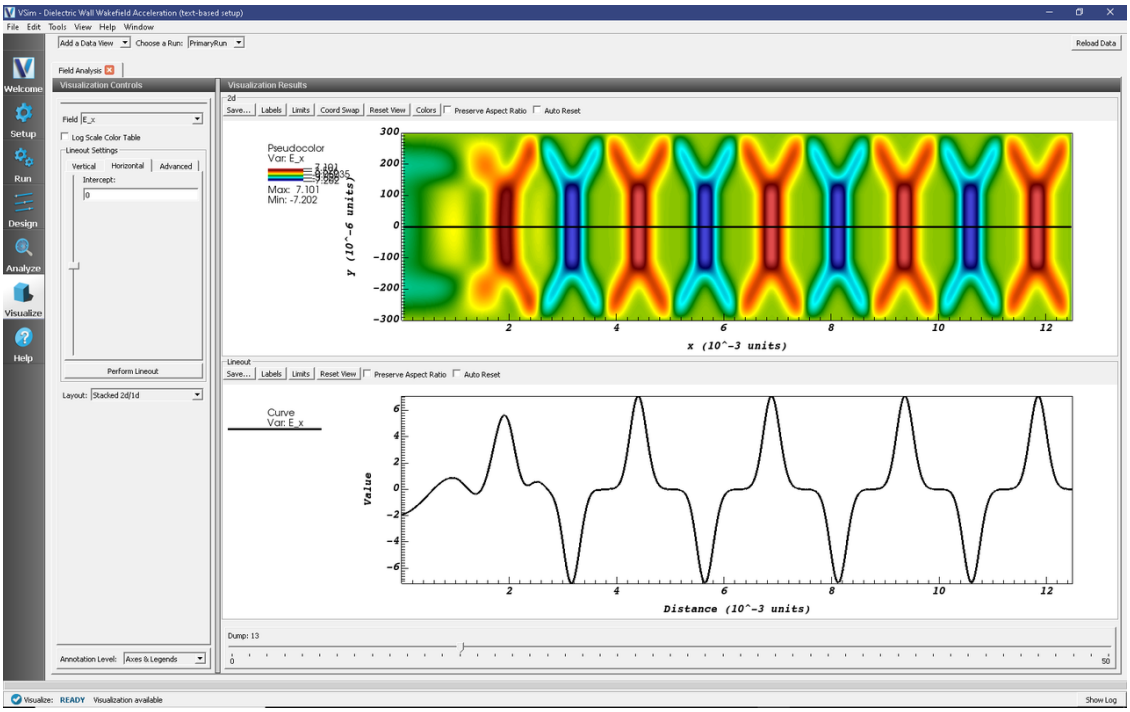


Fig. 5.7: Visualization of the longitudinal electric field as a color contour plot and longitudinal lineout.

Further experiments

There are two bunch shapes provided to start with, you can look at the effect of harmonics in the bunch in the longitudinal field output. There is also a commented block of code that can be switched in that shifts the dielectric into the domain a little, so one can see the process of the electrons beam forming the pattern.

Also, one may add a species propagating from the left hand side to witness the wake, and observe the behavior of particles in or out of phase with the wake.

5.2.2 Electron Beam Driven Plasma Wakefield with Seperable Fields (eBeamDrivenPlasmawSeperableFieldsT.pre)

Keywords:

electron driven, plasma wakefield, CLARA, PARS, AWAKE

Problem description

This example demonstrates a method to simulate an electron beam driven plasma wakefield accelerator. The electron beam initializes the field using a speed of light frame Poisson equation solve, then the fields and particles are evolved using FDTD EMPIC. We launch the electron beam from x=0 in the positive x direction using the Lorentz boosted Poisson fields to ensure that the simulation is self-consistent from start. The primary bunch generates a region of high field into which one might inject and accelerate a second bunch of charged particles. The example simulation uses parameters that are appropriate to the plasma acceleration research station (PARS) at the CLARA accelerator at Daresbury Laboratory in the UK.

Opening the Simulation

The Electron Beam Driven Plasma Wakefield example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Beam Drive Acceleration (text-based setup)* option.
- Select *Electron Beam Driven Plasma Wakefield (text-based setup)* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 5.8.

At this stage one can choose parameters such as `LONGITUDINAL_RES` and `TRANSVERSE_RES` which represent the longitudinal and transverse number of cells per RMS bunch size. The minimum of 6 or default of 8, generates a simulation that will complete reasonably quickly, but is not adequate to generate good results. Consider 12 or 16 cells in both dimensions to avoid a "checkerboard" pattern of numerical noise from developing.

Input File Features

The simulation setup consists of an electromagnetic solver using the Yee algorithm and uses the initBeam macro to set up the initial beam properties. This takes the beam of variable weight particles and calculates self-consistent fields with which to initialize the simulation. As this beam travels near the speed of light, a moving window that co-propagates with the beam is employed. MALs are used on the transverse sides of the window to absorb outgoing waves. The plasma is represented by macro-particles, and both beam and plasma are moved using the Boris push. The particles in the plasma are variably weighted to represent the density ramp. It is assumed the plasma consists of pre-ionized heavy ions, which do not move in the time frame of the simulations.

One can specify the size of the region to be simulated through `LONGITUDINAL_EXTENT` and `TRANSVERSE_EXTENT`, which are measured relative to the longitudinal RMS size `BEAM_LRMS` and transverse RMS size `BEAM_SIGMAR` of the beam. The number of cells is determined by the settings of `LONGITUDINAL_RES` and `TRANSVERSE_RES`, as shown in the figure.

The plasma density is ramped up using a flat top cosine function, by default, over a quarter of the longitudinal size of the simulation window. This can be modified by viewing the input file and editing the `STARTRAMP` and `RAMPLEN` variables.

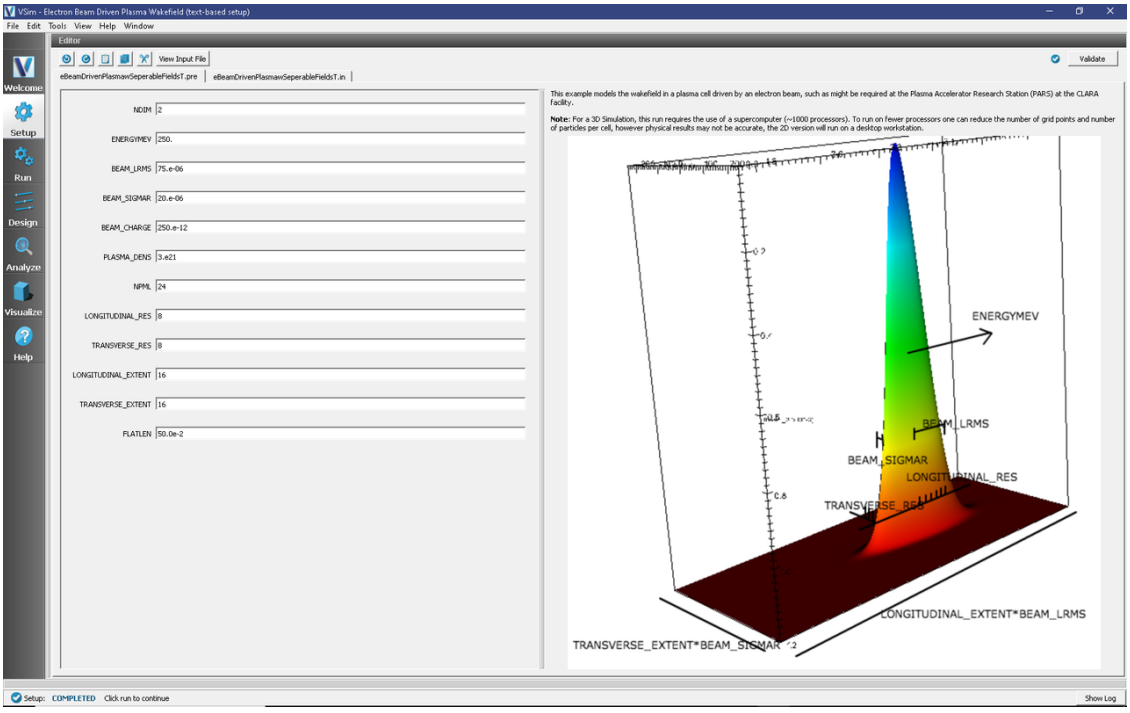


Fig. 5.8: Setup Window for the Electron Driven Plasma Wake example.

Running the Simulations

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.533047112173193e-14
  - *Number of Steps*: 12500
  - *Dump Periodicity*: 250
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 5.9.

Running in 2D, you can expect a 2 core laptop to take a few minutes at the default resolution and run time.

To produce real significant results, a higher resolution is required by changing LONGITUDINAL_RES and TRANSVERSE_RES. Doing so will greatly increase the amount of time to run this simulation. It should also be run for longer than the default 3000 time steps.

The 3D simulation is about 100 times bigger, so 256 cores for a few hours is needed.

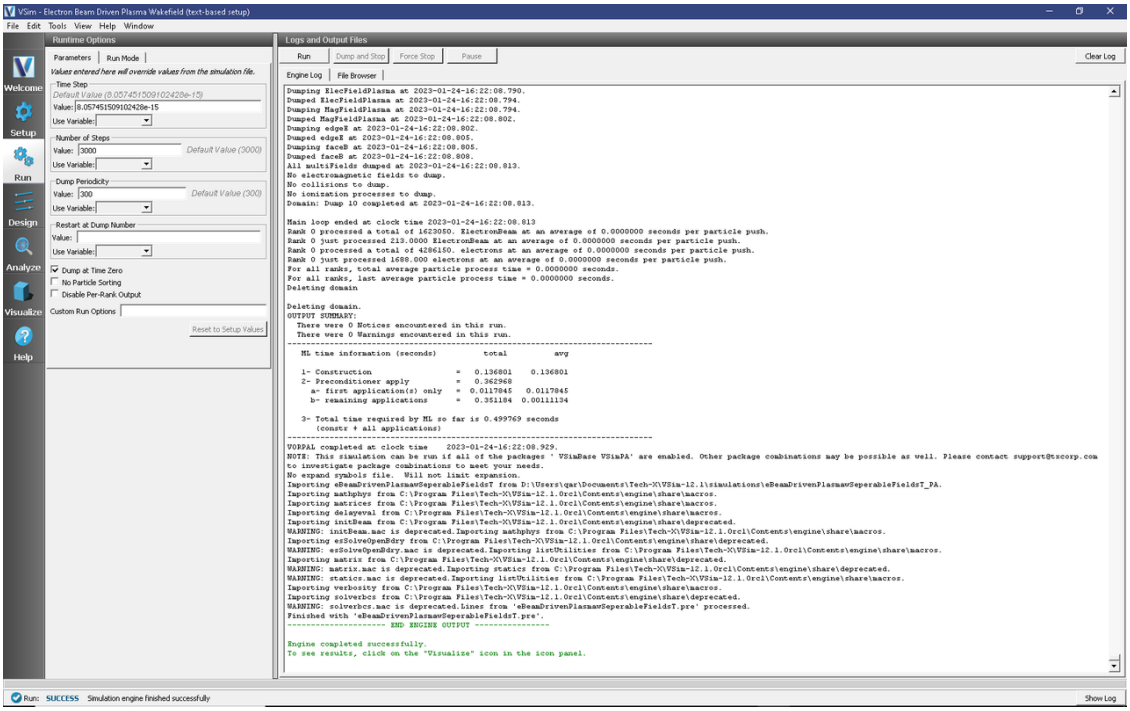


Fig. 5.9: The Run Window.

Visualizing the Output

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize tab in the left column of buttons.

View the electric field generated by the plasma as shown in Fig. 5.10 by doing the following:

- Switch to *Field Analysis* in the *Data View* Controls pane
- Set the *Field* to *ElecFieldPlasma_x*
- Choose the *Horizontal* tab in *Lineout Settings* set the intercept to zero, and click *Perform Lineout*
- Check the *Auto Reset* buttons on both the 2d and the Lineout plots. Sometimes it is necessary to expand the plot size in order for the box to appear. You can do this by pulling the divider between "Visualization Controls" and "Visualization Results" to the left and hiding it. Both the 2d and the Lineout plots should be larger now.
- Move the dump slider forward in time.

The plasma density can be seen as shown in Fig. 5.11 by doing the following:

- Switch to *Data Overview* in the *Data View* drop down
- Expand *Scalar Data*
- Select *rhoPlasma*
- Click *Auto Reset*
- Move the slider all the way to the right.

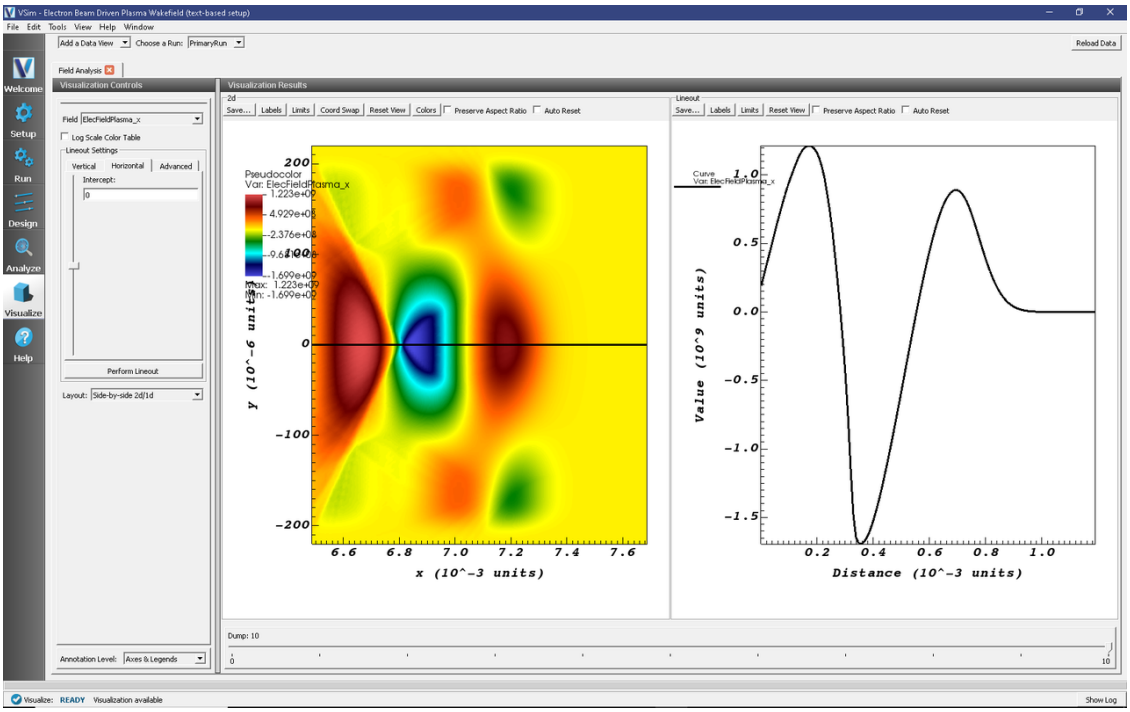


Fig. 5.10: Visualization of the longitudinal electric field as a color contour plot and longitudinal lineout.

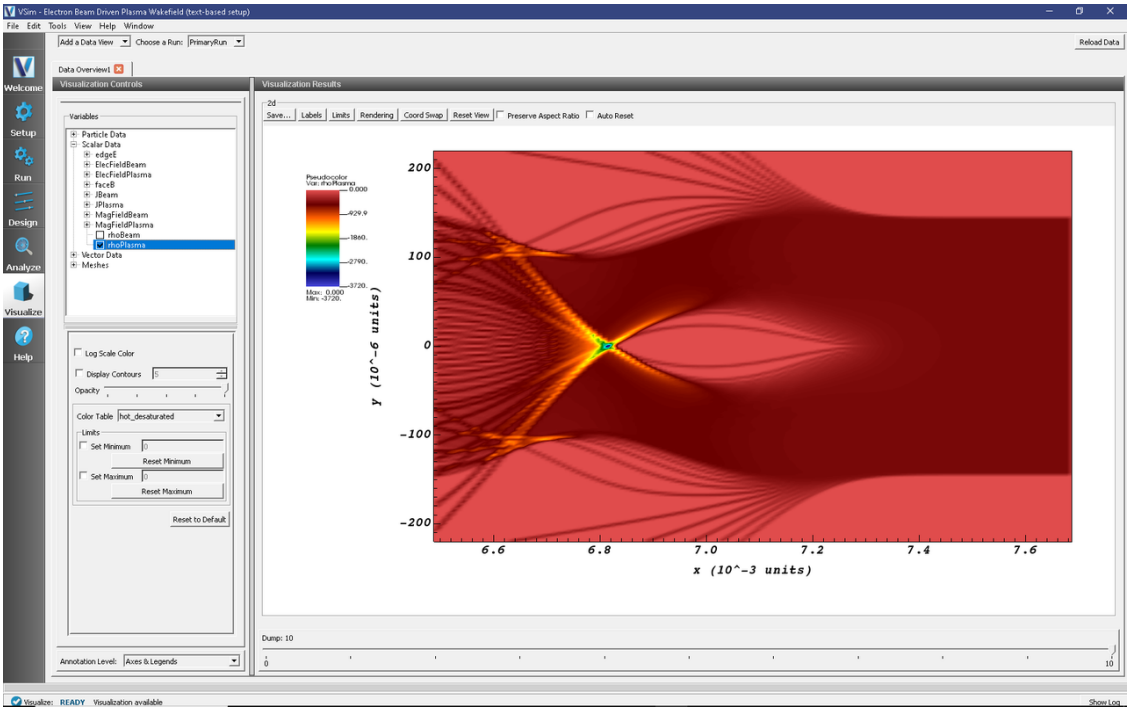


Fig. 5.11: Visualization of the longitudinal plasma density field as a color contour plot.

5.3 Laser Driven

5.3.1 Laser Ionization (laserIonization.sdf)

Keywords:

electromagnetic, particle in cell, field ionization, moving window

Problem description

This example launches an electromagnetic laser pulse into a homogeneous volume of neutral argon gas. The field strength is significant enough to ionize the argon to multiple ionization states, which are included in the simulation. The neutral gas density is depleted as the ionization occurs, with layers of argon atoms at increasing ionization levels towards the center of the Gaussian beam.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Laser Ionization example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Laser Driven Acceleration* option.
- Select "Laser Ionization" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 5.12. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to Grid.

Simulation Properties

Constants are set up to allow setting the laser amplitude and the neutral argon density (1/m^3).

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.1875451751110668e-16
  - *Number of Steps*: 1000
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

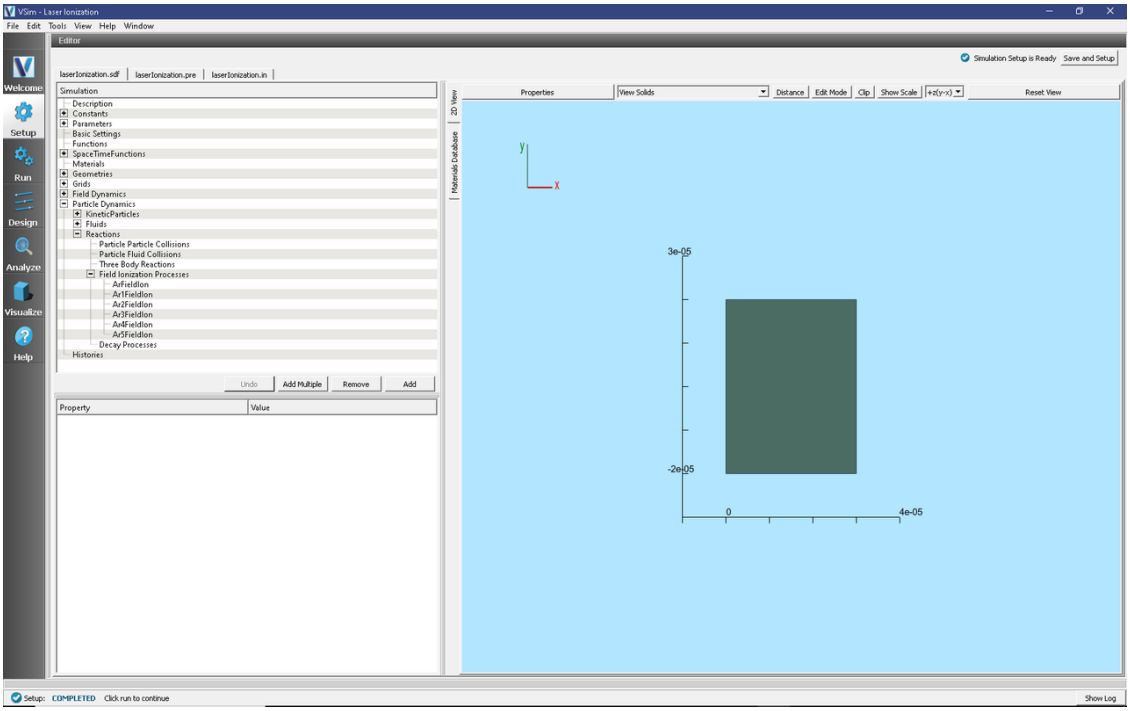


Fig. 5.12: Setup Window for the Laser Ionization example.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 5.13.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize Tab in the left column of buttons.

View the electric field magnitude, by doing the following:

- Expand *Scalar Data*, expand *E* and select *E_magnitude*.
- Scrolling through time (by moving the slider at the bottom of the window) will show the laser pulse propagating across the simulation domain.
- It may be useful to check the *Auto Reset* button in the 2d plot.
- Next, untick the *E_magnitude* and instead tick *neutralArgon*. You can now see the depletion of the neutral background gas as the laser passes through. This will appear the same as in Fig. 5.14.

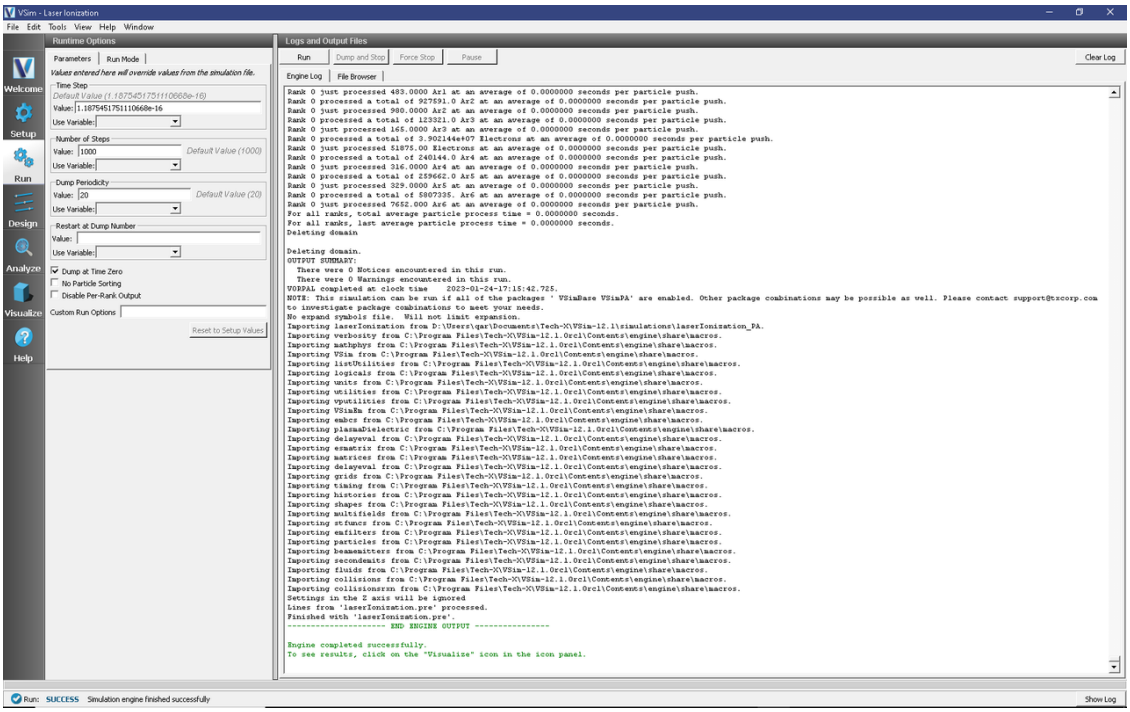


Fig. 5.13: The Run Window at the end of execution.

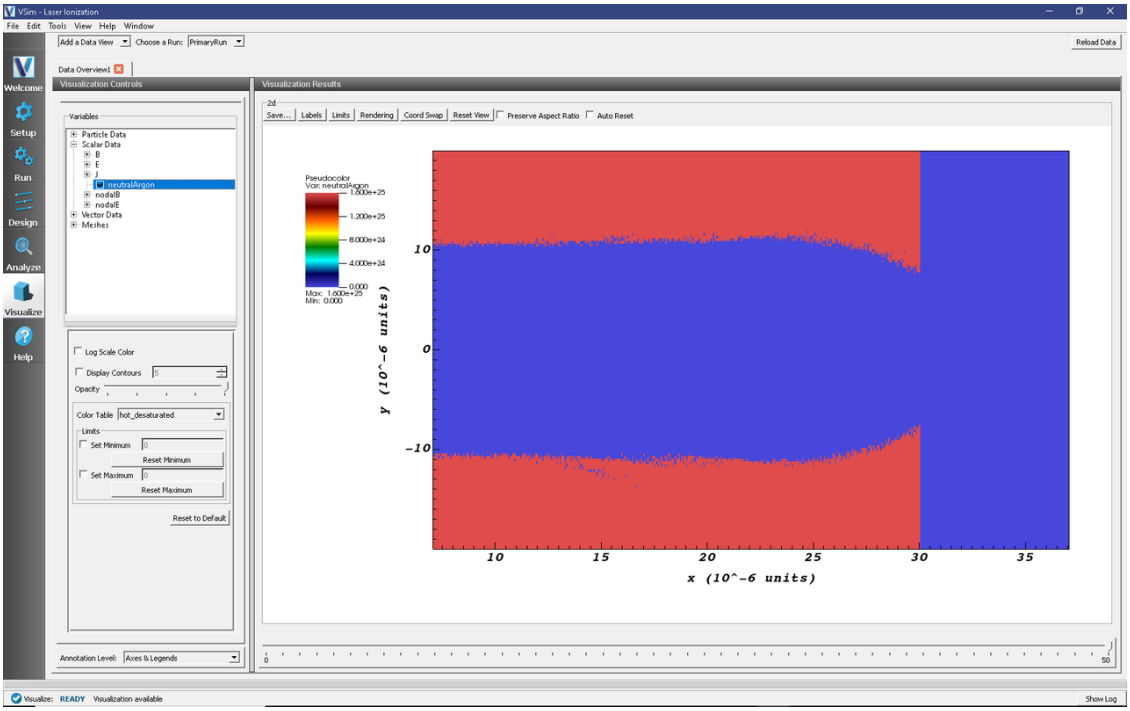


Fig. 5.14: The ionized charge states of argon during laser pulse propagation

Further Experiments

Try adding more charge states of Argon (past 6+) and find the limit of ionization that is achievable with this laser pulse.

5.3.2 Laser Plasma Accelerator (laserPlasmaAccel.sdf)

Keywords:

`Laser Plasma Accelerator`

Problem description

This example demonstrates the use of VSim to simulate a simple laser-plasma accelerator problem using the full PIC algorithm.

An intense, short laser pulse propagating through a plasma can lead to the separation of electrons and ions capable of producing accelerating electric fields of hundreds of GV/m [GTVT+04]. VSim is capable of simulating laser plasma accelerators (laserPlasmaAccel) using several different models: envelope, fluid and full particle-in-cell (PIC).

Here we look at the full PIC model with a 1-mm long plasma with uniform density of $1.e25$ m^{-3}. A gaussian laser pulse, defined by the transverse electric field

$$E_y = E_0(0.5 - 0.5\cos(\pi t/T))H(T-t)\exp(-(y^2+z^2)/(w_0^2 D_y D_z))\cos(\omega t + \phi_y + \phi_z)$$

where w_0 is the radius at which the wave amplitude drops to $1/e$, T is the temporal duration of the pulse,

$$D_y = 1 + (F/Z)^2$$
$$D_z = 1 + (F/Z)^2$$

are the squares of amplitude reductions from being the launching at a distance, F, from the focus, Z is the Rayleigh length, and

$$\phi_y = -(F/Z)(y/w_0)^2/D_y$$
$$\phi_z = -(F/Z)(z/w_0)^2/D_z$$

are the Gouy phases.

The laser is launched from the left side of the box. The laser amplitude is determined through the normalized vector potential $A_0 = eE_0/\omega m_e c$, where ω is the laser angular frequency.

The simulation setup consists of an electromagnetic solver using the Yee algorithm. The laser pulse is launched from the left side of the window using the pre-defined gaussian pulse launcher at the left boundary. Simple conducting boundary conditions are used at the top and sides. As such, one must ensure that waves reflected off the top or bottom do not get into the simulation, and that no waves hit the right boundary to be reflected back into the simulation.

The plasma is represented by macro-particles which are moved using the Boris push. The particles are variably weighted to represent the density ramp.

The input file allows one to set up plasma and laser parameters. The simulation box size is determined as a function of the laser length and spot size. The resolution was set to have about 24 cells per wavelength longitudinally and 3 transversely. The time step is chosen to be very close to the Courant condition limit in order to have good dispersion.

This simulation can be performed with a VSimPA license.

Opening the Simulation

The Laser Plasma Accelerator example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Introductory Examples* option.
- Select "Laser Plasma Acceleration" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 5.15. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

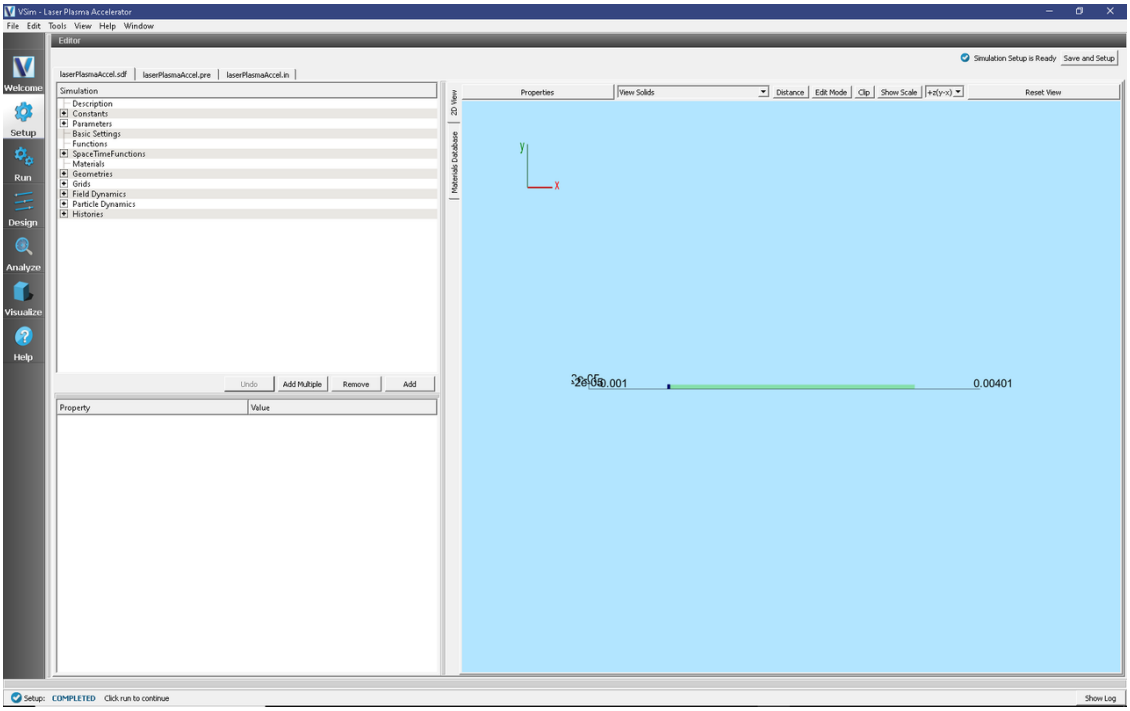


Fig. 5.15: Setup Window for the Laser Plasma Acceleration example.

The Setup Window shows a very long simulation. However, the full length is not simulated at any one time. Instead a moving window is used to simulate only the region where dynamics is occurring. The moving window can be seen in Fig. 5.16 as a small box on the left end of the electron loader.

To see this view: * First toggle off the axes by clicking the *Toggle Axes* button, if it is not visible, click the *Properties* button and then uncheck *Toggle Axes*.

- Then expand the *Particle Dynamics* → *KineticParticles* → *electrons0* item in the setup tree and click *particleLoader*. Finally, zoom in and translate to the left to see the left edge of the particle loader and the darker grid. If one wishes to simulate this for longer distances, one can set the Parameter, `NUM_XLENGTHSS`, to a larger number; 400 is more than enough.

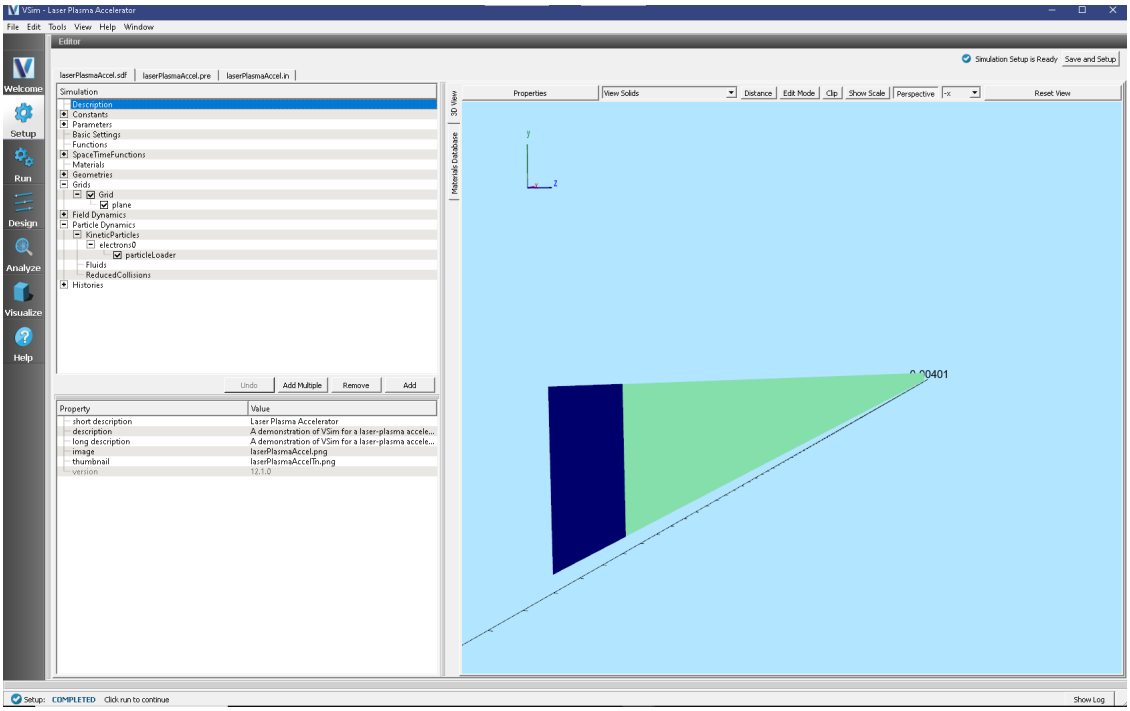


Fig. 5.16: Setup Window, zoomed in on the moving window, for the Laser Plasma Acceleration example showing size of grid.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.0920358205802013e-16
  - *Number of Steps*: 20000
  - *Dump Periodicity*: 250
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 5.17.

Running in 2D, this simulation uses around 225,000 cells and nearly 200,000 particles for 20,000 time steps. The run takes about an hour on a 4-core 2.5 GHz I7.

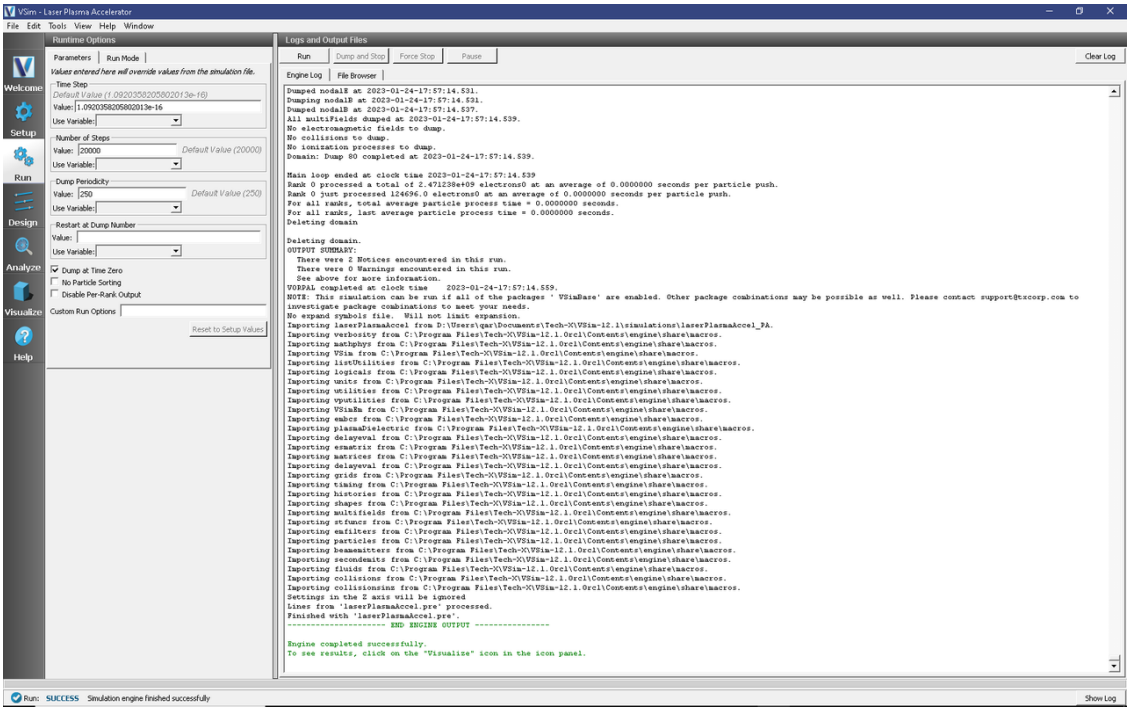


Fig. 5.17: The Run Window at the end of execution.

Visualizing the results

After performing the above actions, click on the *Visualize* Tab in the column of buttons at the left. For all plots, it is useful to keep Auto Reset on so that the window moves with the data. If the *Auto Reset* box is not visible, click on the *Controls...* button and then select *Auto Reset* from the drop down menu.

To view the electric field, switch to Field Analysis in the Data View drop-down menu. From the Field drop-down menu, choose the desired component of the electric field, `E`. The `depField` field is the current density.

To obtain Fig. 5.18:

- Select Field `E_x`
- Select Horizontal and Intercept of 0 for the lineout.
- Select *Perform Lineout* and then select Dump: 80.

The acceleration of the particles can be seen by viewing the (x) component of the velocity. To do this:

- Switch to the Phase Space Data View in VSimComposer
- Set the *X-axis* variable to `electrons0_x`, and the *Y-axis* variable to `electrons0_ux`.
- Set the *color* variable to `electrons0_ux`
- Then click Draw.

You will see a color-coded picture of particle velocity like in Fig. 5.19.

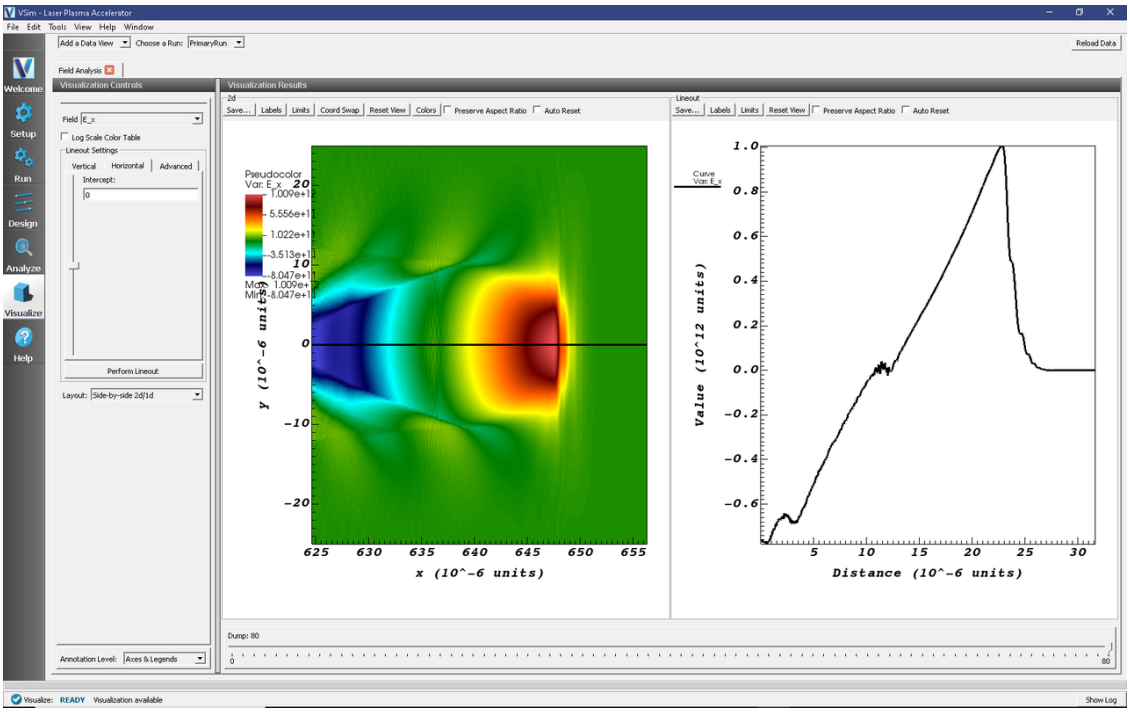


Fig. 5.18: The output of the run shows the accelerating field E_x after about 2 picoseconds.

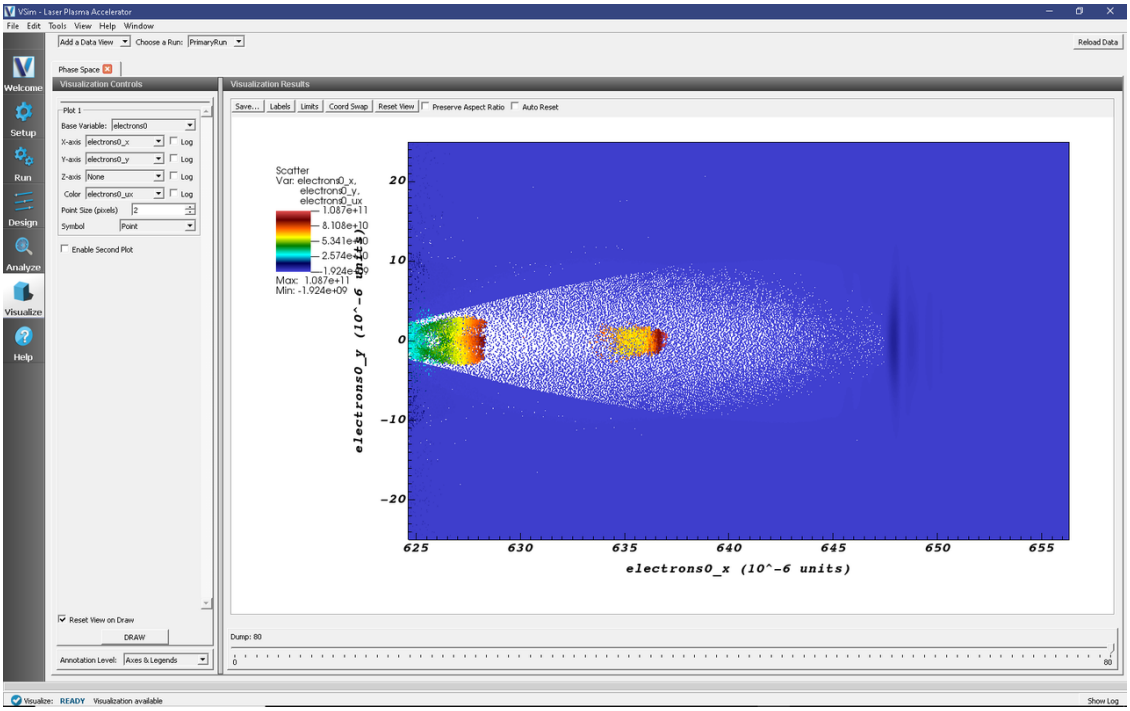


Fig. 5.19: Phase-space plot of plasma electrons at t = 2.1 picoseconds.

Further Experiments

Try increasing or decreasing the intensity of the laser pulse through the parameter `A_0` and see the effect on the shape of the plasma wakefield.

5.4 Laser Driven (text-based setup)

5.4.1 Colliding Pulse Injection (collidingPulseInjT.pre)

Keywords:

laser plasma accelerator, controlled injection, colliding laser pulses

Problem description

This example demonstrates the use of VSim to simulate controlled injection in a laser-plasma accelerator using colliding laser pulses [CMRB+10]. Two laser pulses are launched from opposite sides (one from the left side and the other one from the right side of the box) and propagate in opposite directions. The laser pulse coming from the left side is the main pulse that drives the plasma wake. The laser pulse coming from the right is the collider pulse, with much lower intensity than the main pulse. It can also propagate with a small angle with respect to the main pulse propagation axis. When the two lasers collide they create a slow beat wave, which allows electrons of the background plasma to be trapped and be accelerated by the wakefield driven by the main pulse.

In this example, the laser pulses are polarized in the y direction and both have a Gaussian profile defined by

$$E_y = E_{\mathrm{pump\_(L,R)}} \exp(-x^2/\mathrm{LPUMP\_(L,R)}^2) \exp(-(y^2+z^2)/\mathrm{W0\_(L,R)}^2)$$

where L and R refer to the left and right pulse respectively. The laser intensity is defined through the normalized vector potential

$$\mathrm{APUMP\_(L,R)} = eE_{\mathrm{pump\_(L,R)}}/\omega_{\mathrm{(L,R)}} m_e c$$

where $\omega = 2\pi c/\mathrm{WAVELENGTH\_(L,R)}$ is the laser frequency.

The pulses enter a plasma channel with density on axis `DENSITY0` through a density ramp of length 20 μ m.

This simulation can be performed with the VSimPA or VSimPD license.

Opening the Simulation

The Colliding Pulse Injection example is accessed from within VSimComposer by the following actions:

- Select the *New* $\rightarrow$ *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Laser Driven Acceleration (text-based setup)* option.
- Select *Colliding Pulse Injection (text-based setup)* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem can now be changed via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 5.20.

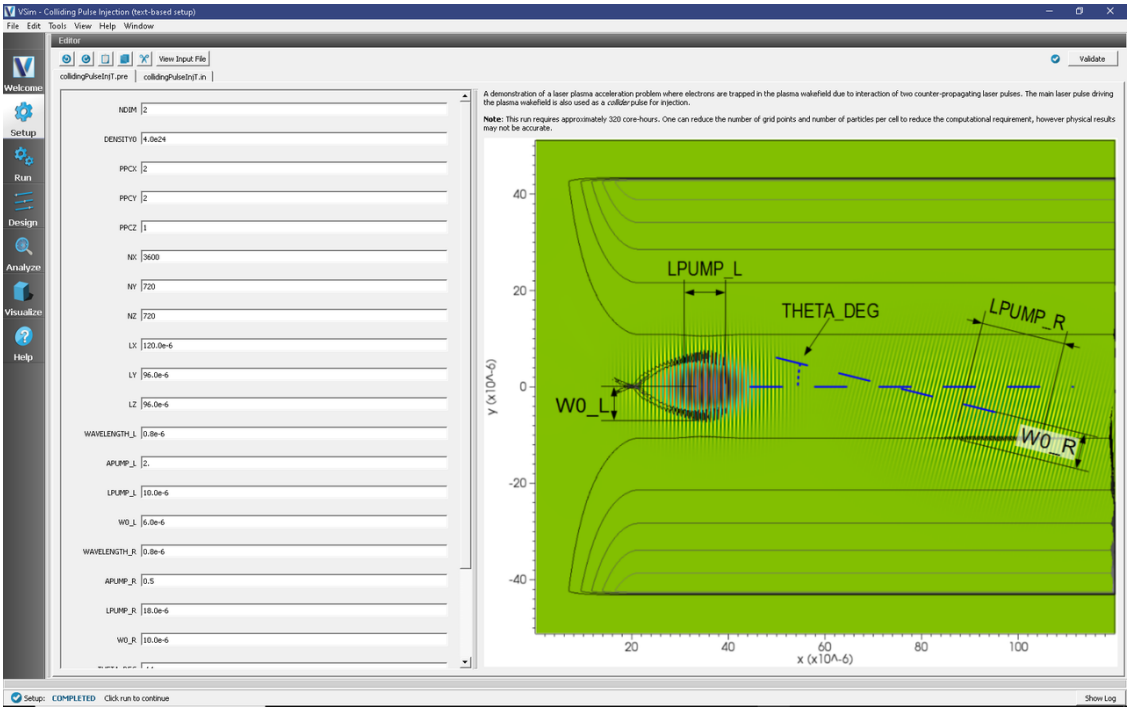


Fig. 5.20: Setup Window for the Colliding Pulse Injection example.

Input File Features

The simulation setup consists of an electromagnetic solver using the Yee algorithm. Two laser launchers are used, one from the left edge and the other from the right edge of the window. PMLs are used on the transverse sides of the window to absorb outgoing waves. The plasma is represented by macroparticles which are moved using the Boris push. The particles are variably weighted to represent the density ramp, and they have a unique tag. The current deposited by the particles is smoothed using four passes of the 1-2-1 filter and subsequently applying a compensator.

The input file allows one to set up both lasers, plasma and grid parameters.

Running the Simulations

Running in 2D, this simulation uses around 2,600,000 cells and nearly 10^7 particles. This run requires about 320 core-hours for the full 156,000 steps on a 2.5 GHz I7. On less powerful hardware, one can reduce the number of steps to 15000 see just the collision or one can reduce the number of grid points and number of particles per cell to see more of the evolution, but physical results may not be accurate.

To run on local hardware do

- Proceed to the Run Window by pressing the Run Tab in the left column of buttons.
- Set the number of steps to 5000 and the dump periodicity to 500 in order to see the initial evolution. The collision occurs at step 4500 (dump 9).
- Run in parallel with as many physical cores as are on your machine, because this is a computationally intense problem. Even with the reduced number of steps, this run can take up to 7 hours on four cores for 5000 steps, depending on the processor.

- To run the file, click on the *Run* button in the upper left This is shown in Fig. 5.21. The run has completed when you see the output, "Engine completed successfully." in this same pane.

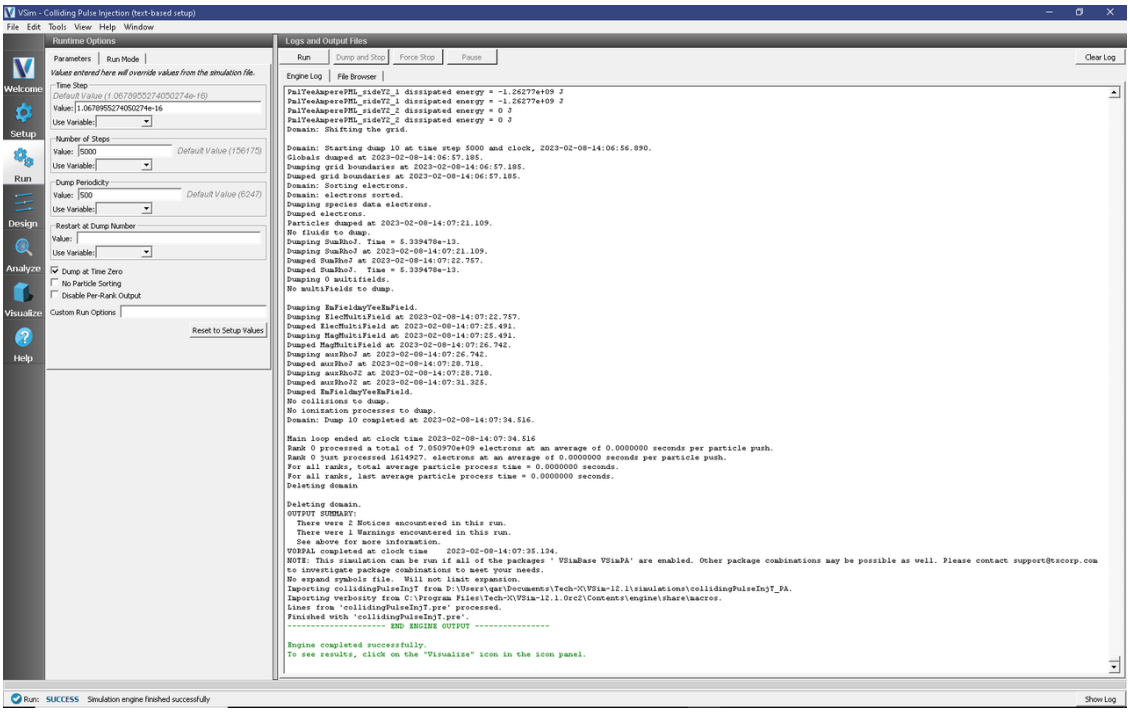


Fig. 5.21: The Run Window.

Alternatively, copy collidingPulseInjT.pre to your more powerful hardware and run it through the command line or submit it to your job queue.

Visualizing the Output

If you have run the job on a remote computer, you would now need to copy back the files that you want to visualize locally into the local directory in which one has the input file open. E.g.,

```
for dmpnum in 0 8 9 10; do
  scp mybigcomputer.mydomain:myspace/collidingPulseInjT_*_${dmpnum}.h5 .
done
```

Then proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

- To view the transverse electric field, switch to the *Data Overview* in the Visualization Controls pane.
- Under *Visualization Controls*, *Variables*, From the Field drop down menu, choose the y component of the `ElecMultiField`.
- Set the color scale by checking the *Set Minimum* and *Set Maximum* boxes in the *Color Table* subwindow under *Visualization Controls*. Then set the minimum to -2e12 and the maximum to 2e12.
- Click the Auto Reset check box.
- Move the dump slider to position 8, then 9, then 10 to see the pulses collide.

The collision of the pulses is then seen as shown in Fig. 5.22 below.

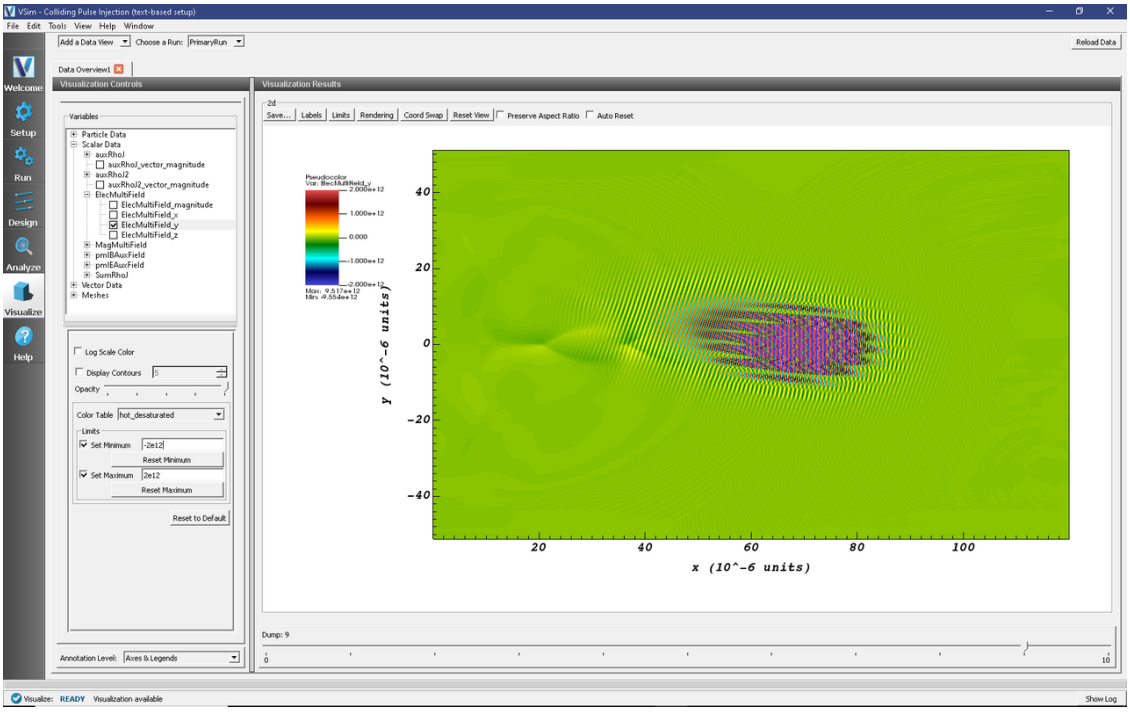


Fig. 5.22: Visualization of the transverse electric field as a color contour plot and longitudinal lineout.

The x-component shows the wake field of the left incoming pulse and some of the electromagnetic field of the incoming collider pulse. The wake field can be better seen by clicking on the *Colors* button and setting the min and max to be -+ 1.e11. The plasma density can be seen in the zeroth component of the SumRhoJ field.

Particle phase-space can be seen by switching to the *Phase Space Data View* in the Controls pane. Fig. 5.23 shows the particle longitudinal momentum as a function of the longitudinal coordinate just after the collision.

Continuing the simulation

The simulation to this point has allowed one to study the initial injection of particles up to high energy, so that they can be trapped by the wake. One can now continue this simulation to study the acceleration in the wake. Since this simulation stopped at dump 10, one can now set the additional Runtime Options to unclick *Dump at Time Zero* and then set *Restart at Dump Number* to 10. Since at this point, the evolution changes more slowly, one can set the *Number of Steps* to 10000 and the *Dump Periodicity* to 5000. Again hit *Run*.

At any time one sees that another data dump has occurred, one can switch over to the Visualize pane and hit *Reload Data* to view the new available data, any of the fields or particles as before.

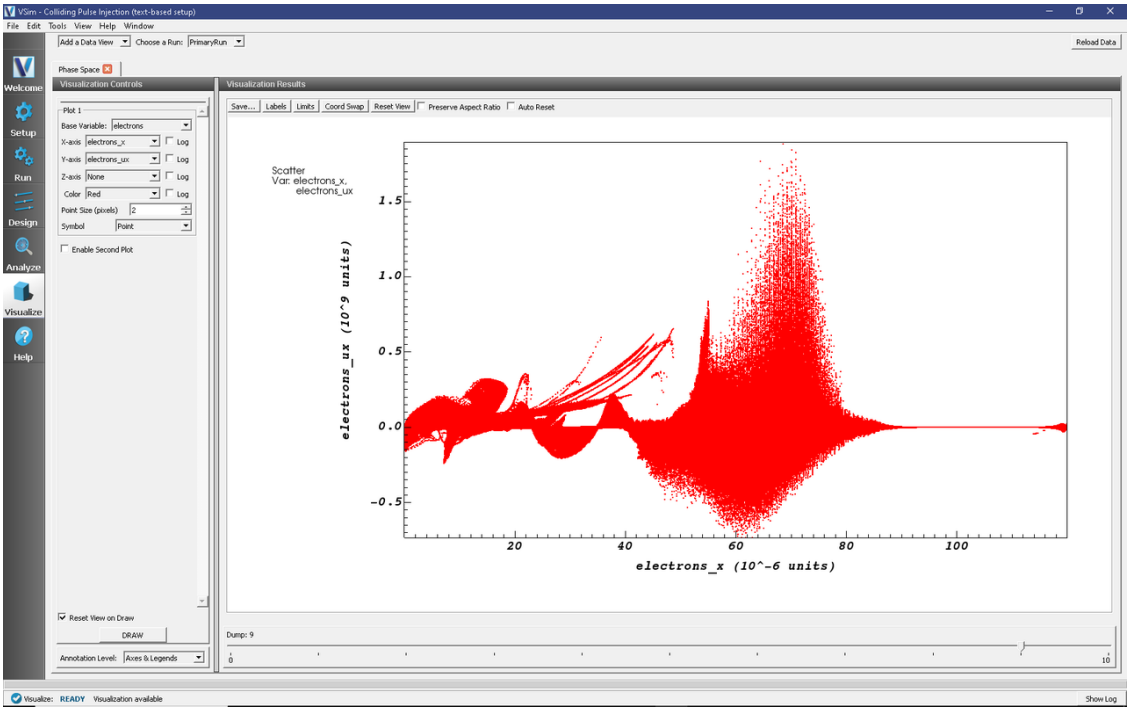


Fig. 5.23: Visualization of the particle longitudinal phase-space during collision. Particles kicked up into the trapped region by the colliding pulses. One can see the acceleration of particles to high energy in later dumps.

5.4.2 Ionization Injection (fieldIonizeT.pre)

Keywords:

laser plasma accelerator, controlled injection, ionization of high-Z gas

Problem description

This example demonstrates the use of VSim to simulate ionization-induced injection in a laser plasma accelerator [CES+12]. An intense laser pulse propagates up a plasma density ramp into a uniform plasma, which creates a wakefield. Neutral nitrogen atoms are added to the pre-ionized gas at the beginning of the plasma, where the laser pulse field ionizes them. If the electrons released from the nitrogen ionization are at the correct position relative to the wakefield phase, they can be trapped and accelerated to high energy [CCMG+13].

The laser envelope has a Gaussian profile defined at the waist position by (`X_0_LASER`):

$$E_z = E_0 \exp\left(-x^2/LPUMP^2\right) \exp\left(-(y^2+z^2)/W\_0^2\right) \sin\left(\omega_0 t\right)$$

where $\omega_0 = 2\pi c$ / `WAVELENGTH` is the laser frequency. The laser amplitude is defined through the normalized vector potential `A_0` = $eE_0/\omega_0 m_e c$.

This simulation can be performed with a VSimPA license.

Opening the Simulation

The Ionization Injection example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Acceleration* option.
- Expand the *Laser Driven Acceleration (text-based setup)* option.
- Select "Ionization injection (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 5.24.

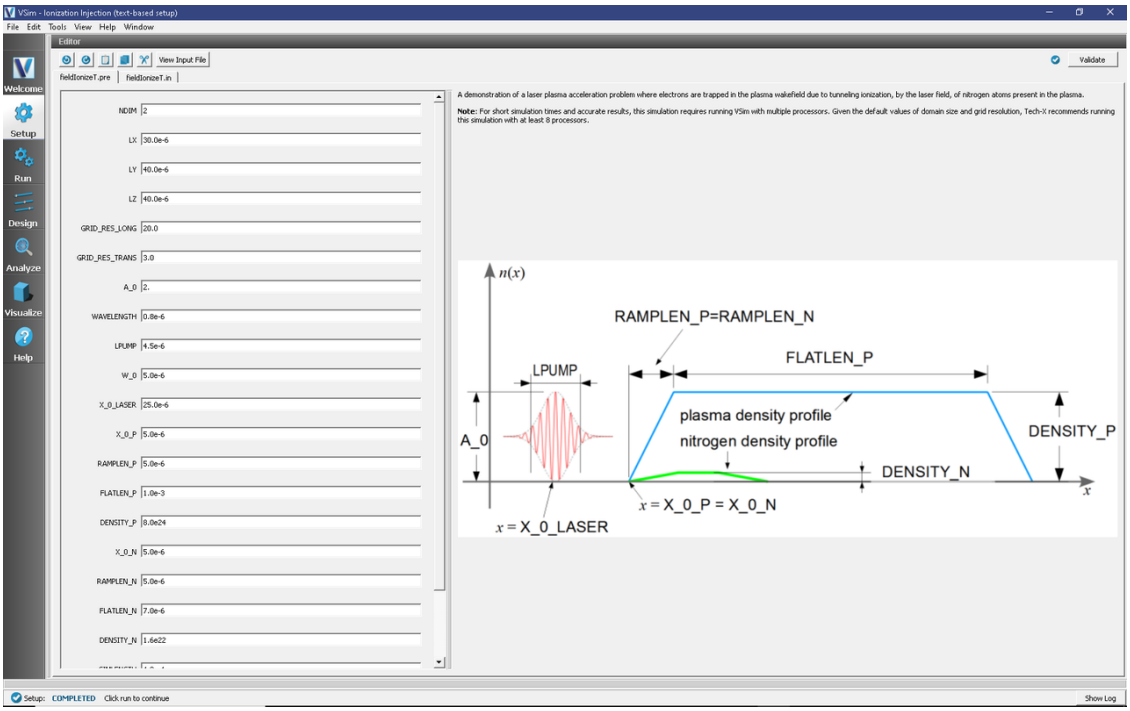


Fig. 5.24: Setup Window for the Ionization injection in Laser Plasma Accelerator example.

Input File Features

The simulation setup consists of an electromagnetic solver using the Yee algorithm. The laser pulse is launched from the left side of the window using an expression launcher at the boundary. MALs are used on the transverse sides of the window to absorb outgoing waves. The plasma is represented by macro-particles which are moved using the Boris push. The particles are variably weighted to represent the density ramp. The nitrogen atoms are represented using a fluid neutral gas. The different excited levels of the nitrogen and electrons product of the ionization are represented through variably weighted macro-particles. The ionization process takes place in MonteCarlo interactions, using the modified time-resolved ADK formula [CES+12].

Running the Simulations

After performing the above actions, continue as follows:

- Proceed to the Run Window by pressing the Run button in the left column of buttons.
- This run is computationally intensive, so you click *Run in Parallel* and select a number of cores equal to the number of physical cores on your machine.
- To see the initial evolution, set the *Number of Steps* to 1000 and the *Dump Periodicity* to 500.
- To run the file, click on the *Run* button in the upper left corner of the Logs and Output Files pane on the right. of the window. You will see the output of the run in that same pane. The run has completed when you see the output, "Engine completed successfully." This is shown in Fig. 5.25.

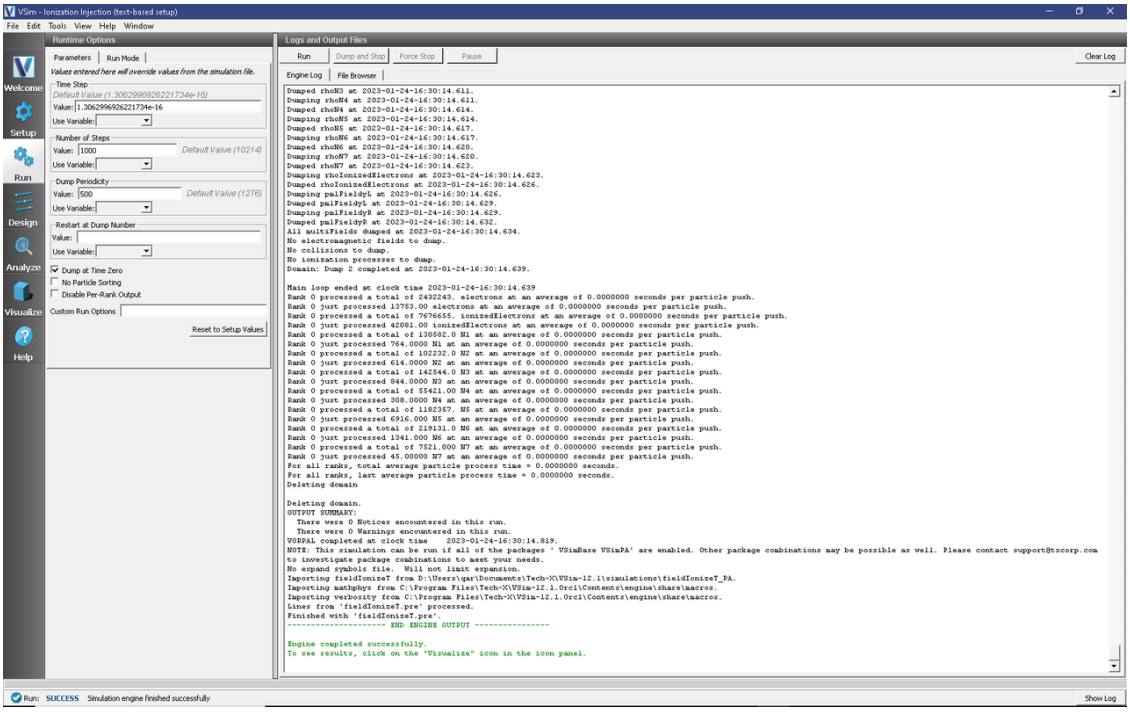


Fig. 5.25: The Run Window at the end of the first execution.

At this point, one can skip ahead to the visualization section to see whether the fields look reasonable. If they do, you can restart:

- Set the *Number of Steps* to 9000 and *Restart at Dump Number* to 2.
- Click on the *Run* button. The run has completed when you see the output, "Engine completed successfully."

This run takes about 70 minutes on a 4 core, 2.5 GHz Intel I7. To run on less powerful hardware one can reduce the number of grid points and number of particles per cell, however physical results may not be as accurate.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize window by pressing the Visualize Tab in the left column of buttons.

The laser pulse is the z component of the field, while the accelerating field is the x component. The plasma density can be seen in `rho`.

Fig. 5.26 shows the longitudinal laser field along the beam axis. To reproduce:

- Set *Data View* to *Field Analysis*
- Select *edgeE_x* from the Field drop down menu
- Select the *Horizontal* tab in the lineout settings
- Set the intercept to `0`
- Click "Perform Lineout
- Click *Auto Reset* on both the pseudocolor and lineout plots so that the window updates the plot region as one moves the slider. You may need to expand your visualization window for the *Auto Reset* checkbox to appear.
- Move the dump slider forward in time

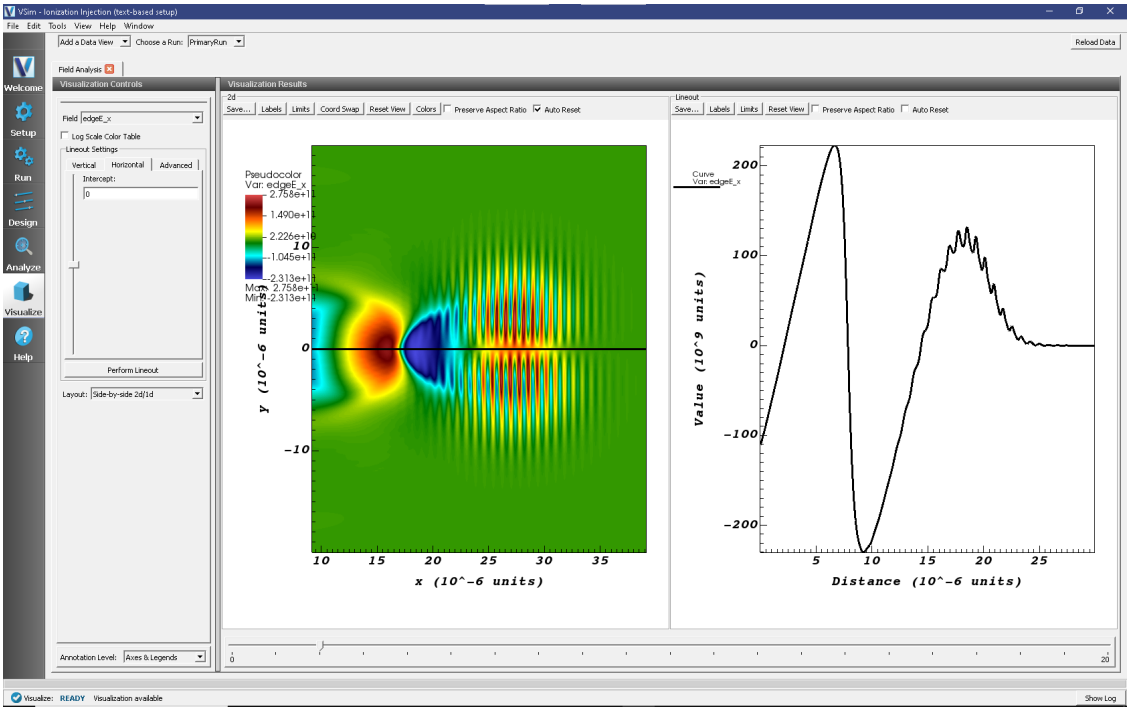


Fig. 5.26: Left: Longitudinal electric field $E_x(x, y)$ at t=1.3 picoseconds. Right: Line-out of field plot at y = 0.

The acceleration of the particles can be seen by viewing the (x) component of the velocity as shown in Fig. 5.27

- Set *Data View* to *Phase Space*
- Set *Base Variable* to *electrons*
- Set the X-axis variable to *electrons_x*, the Y-axis variable to *electrons_ux*
- Check *Enable Second Plot*

- Set *Base Variable* to *ionzedElectrons*
- Set the X-axis variable to *ionizedElectrons_x*, the Y-axis variable to *ionizedElectrons_ux*
- Click *Draw*
- Click *Reset View* or Click *Auto Reset* on the plot so that the window updates the plot region as one moves the slider. You may need to expand your visualization window for the *Auto Reset* checkbox to appear.

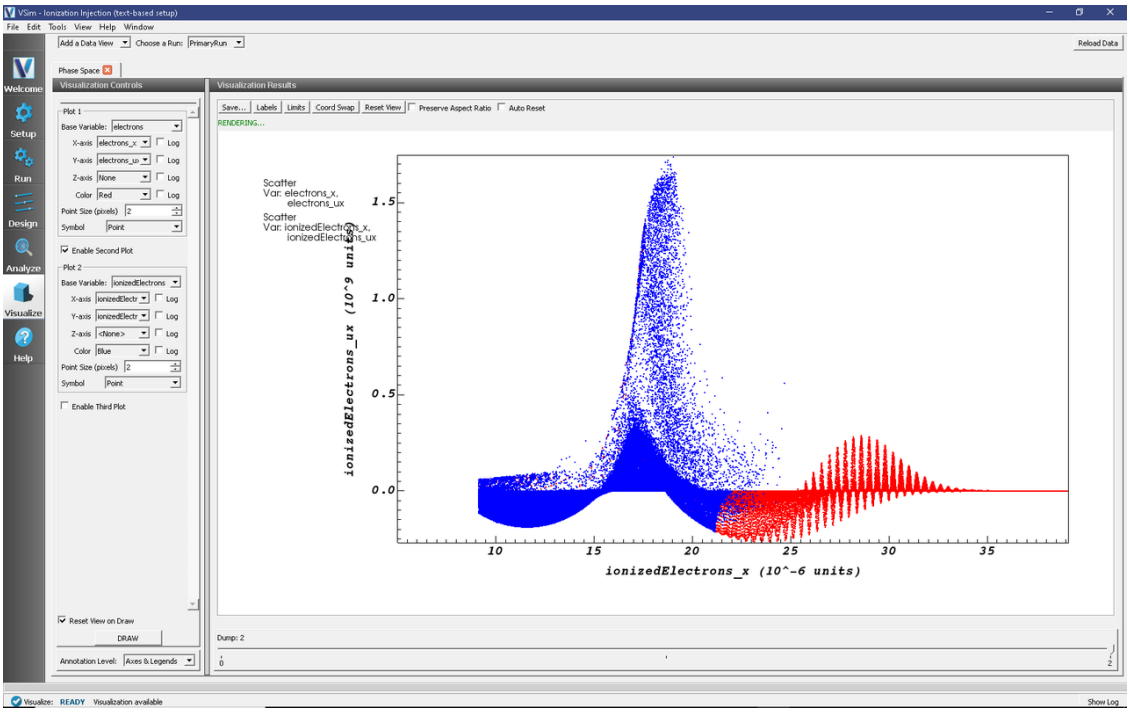


Fig. 5.27: Phase-space plot (x, $\gamma\ v_x$) of plasma electrons at t=0.33 picoseconds.

CHAPTER

SIX

VSIM FOR PLASMA DISCHARGES EXAMPLES

These examples illustrate how to solve complex problems in plasma discharge modelling.

These examples can be run with a VSimPD license.

6.1 Capacitively Coupled

6.1.1 1D Capacitive Argon Plasma Discharge (capacitivelyCoupledArPlasma1D.sdf)

Keywords:

CCP discharge, secondary emission, elastic collision, excitation, ionization.

Problem description

The capacitively coupled plasma (CCP) is one of the most common types of industrial plasma sources. The discharges usually take place between metal electrodes in a reaction chamber and are driven by a radio-frequency (RF) or DC power supply. The plasma is sustained by ohmic heating in the main body and stochastic heating through a capacitive sheath.

This example demonstrates the generation of a capacitively coupled plasma inside two parallel conducting plates separated by 0.05 m. A background Ar neutral gas at approximately 6 mTorr (a number density of approximately $2.0 \times 10^{20}\ m^{-3}$) is filled between the electrodes. The right electrode is grounded, while the left one is connected to a voltage source of 200 V at 60 MHz.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The 1D Capacitively Coupled Plasma Discharge example is accessed from within VSimComposer by the following actions:

- Select the *New* $\rightarrow$ *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Capacitively Coupled Plasmas* option.
- Select "1D Capacitive Plasma Chamber" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* and elements tree with all the implemented physics and geometries, is shown in Fig. 6.1.

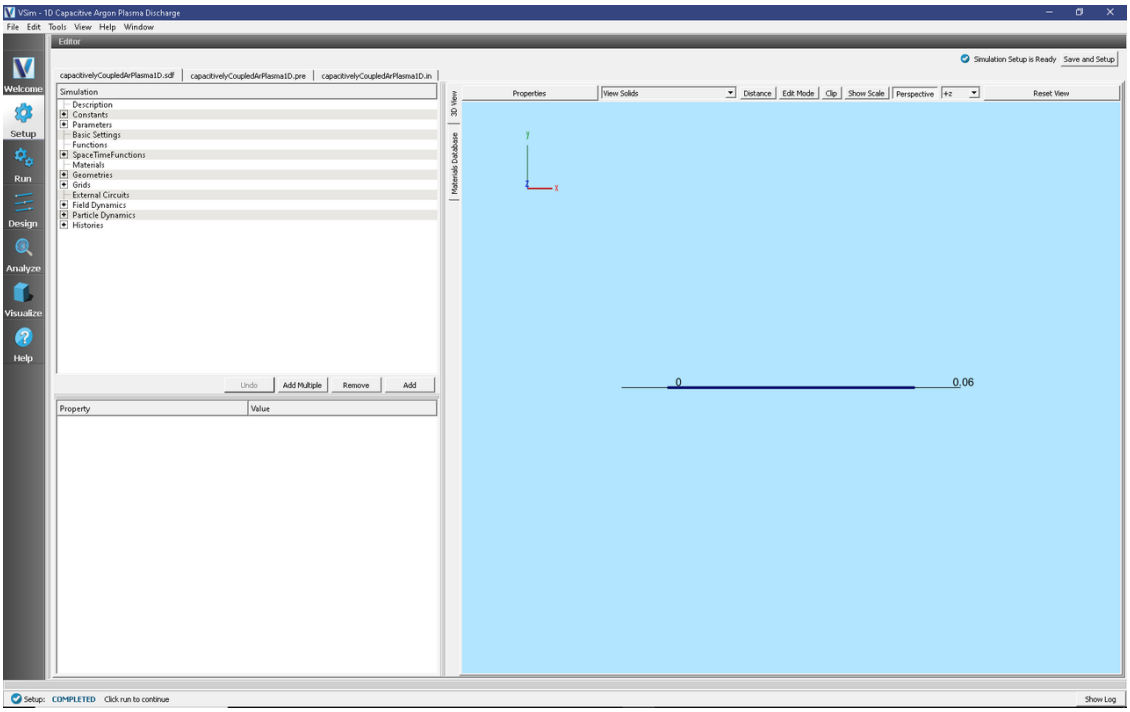


Fig. 6.1: Setup Window for the 1D Capacitively Coupled Plasma Discharge example.

The time step DT should sufficiently resolve the plasma frequency and collision frequency. The default time step used in this example is (TIMESTEP_FACTOR * 0.1) / PLASMA_FREQUENCY to ensure stability. The initial primary electrons are gradually loaded into the simulation domain over a period of LOADSTEPS timesteps, which has a default value of 5000.

Simulation Properties

This simulation includes some constants and parameters for easy adjustment of the simulation properties. These include:

Constants

- NEUTRAL_ARGON_DENSITY: number density of the background neutral argon gas (number/m^3).
- FREQUENCY: sets the frequency of the driving voltage set on the lower X boundary.
- VOLTAGE: sets the amplitude of the driving voltage set on the lower X boundary.
- NOMINAL_DENSITY: this adjusts the number of physical particles loaded into the simulation.
- LOADSTEPS: Timestep when particle loading will end.
- NSTEPS: How many timesteps to simulate.
- STEPS_PER_DUMP: number of steps to take between data dumps.
- BMAG: sets the strength of the magnetic field (default = 0T).

Time-dependent Dirichlet boundary conditions are used to set up the boundaries of electric fields around the reaction chamber walls, and are set in *Field Dynamics -> FieldBoundaryConditions*. The self-consistent electric field is solved from Poisson's equation by the Generalized Minimum Residual (gmres) electrostatic solver in Cartesian coordinates. For more information on the solver, see the Reference Manual. This solver is chosen under *Field Dynamics -> PoissonSolver.*

The plasma is represented by macroparticles which are moved using the Boris pusher in Cartesian coordinates and interact with the background neutral argon gas through collisions set up with the Reactions framework. The particles, background gas, and collisions are set up in the *Particle Dynamics* Element.

The simulation includes two electron species: Primary electrons which are electrons loaded into the simulation, and Secondary electrons which are created through physical processes. Both species are managed weight particle species, which will combine or split macro particles based on user choices. See the Charged Particles section of the Reference Manual for further information on managed weight particles.

Elastic collisions between electrons and the background gas, excitation collisions in which an electron will lose energy to the background gas, and ionization collision in which electrons create argon ions from the background gas are all included. The cross-sections for these collisions are imported from 2-column data files.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.000038212234171e-12
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 200
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.2.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

From the "Data View" option, select "History". There are 6 histories that can be plotted in this window: the number of physical particles and the number of macro particles for each of the three particle species (argon ions, primary electrons, and secondary electrons). To produce the plot in Fig. 6.3 follow these steps:

- Within Graph 1, select Add Curve to plot.
- Plot the 'numArgon' history in Graph 1.
- Plot the 'numPrimaryElec' history in Graph 1.
- Plot the 'numSecondaryElec' history in Graph 1.
- Select Add Window to add a second graph.
- Within Graph 2, select Add Curve to plot.
- Plot the 'numPhysArgon' history in Graph 2.

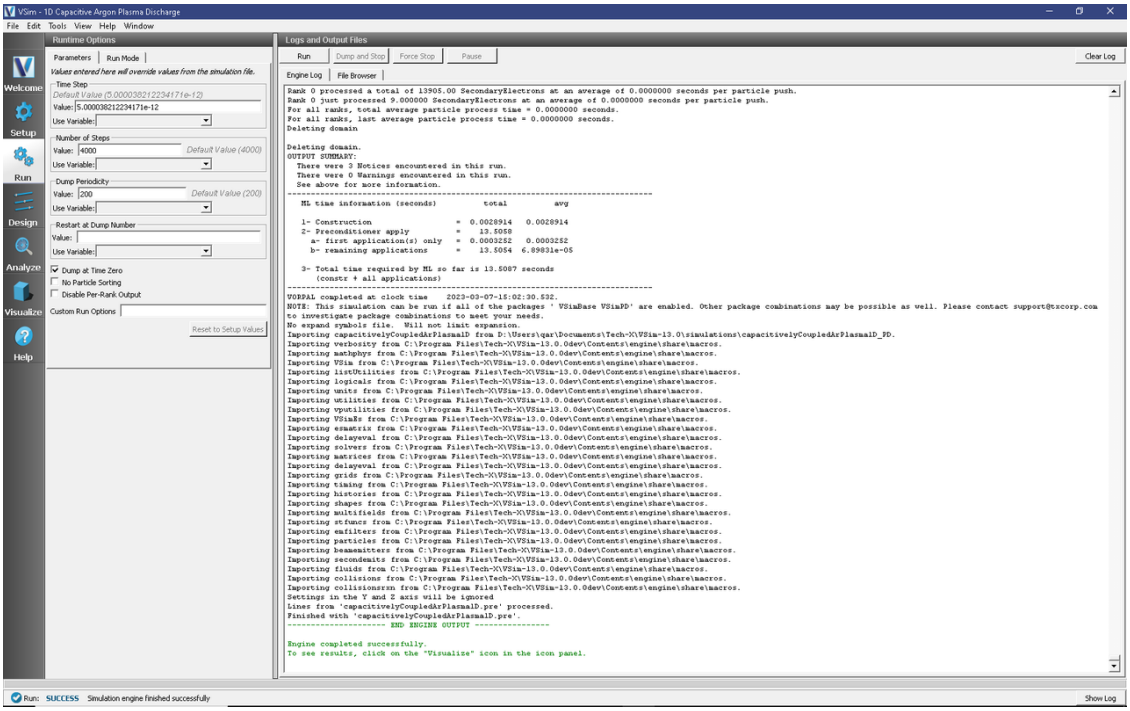


Fig. 6.2: The Run Window at the end of execution.

- Plot the 'numPhysPrimaryElec' history in Graph 2.
- Plot the 'numPhysSecondaryElec' history in Graph 2.

The simulation converges as the number of secondary electrons approaches a constant, indicating a steady state plasma. With the default number of time steps (4000, or 20 nanoseconds), the simulation does not reach steady state (see the black, numPhysSecondaryElec history curve). To reach steady state, the simulation must run for approximately 100 microseconds.

Further Experiments

Set up a History that records the electron current flowing into the left and right sides of the simulation. Right click on the "Histories" element in the *Setup Window* and under "Add ParticleHistory" select "Absorbed Particle Current." You can change the name of the history by double clicking on the new "absorbedPtclCurrent0" element in the tree. Then be sure to pick the particle absorber from which you would like to collect data.

The Reactions framework allows one to set up collision interactions flexibly. The collisions involved in this example are electron-neutral collisions that lead to ionization and ohmic heating. As a further experiment, ion-neutral collisions, such as elastic scattering and charge exchange, can also be added to the simulation.

The VSim interface can import any cross sections that are in a 2-column format. There should be NO headings in the data file. The LXcat scattering database (https://fr.lxcat.net/data/set_type.php) and EEDL cross section database contain cross section data for around one hundred different materials. As another experiment, change the cross-section used in the simulation or change the species of the background gas and import new cross-sections.

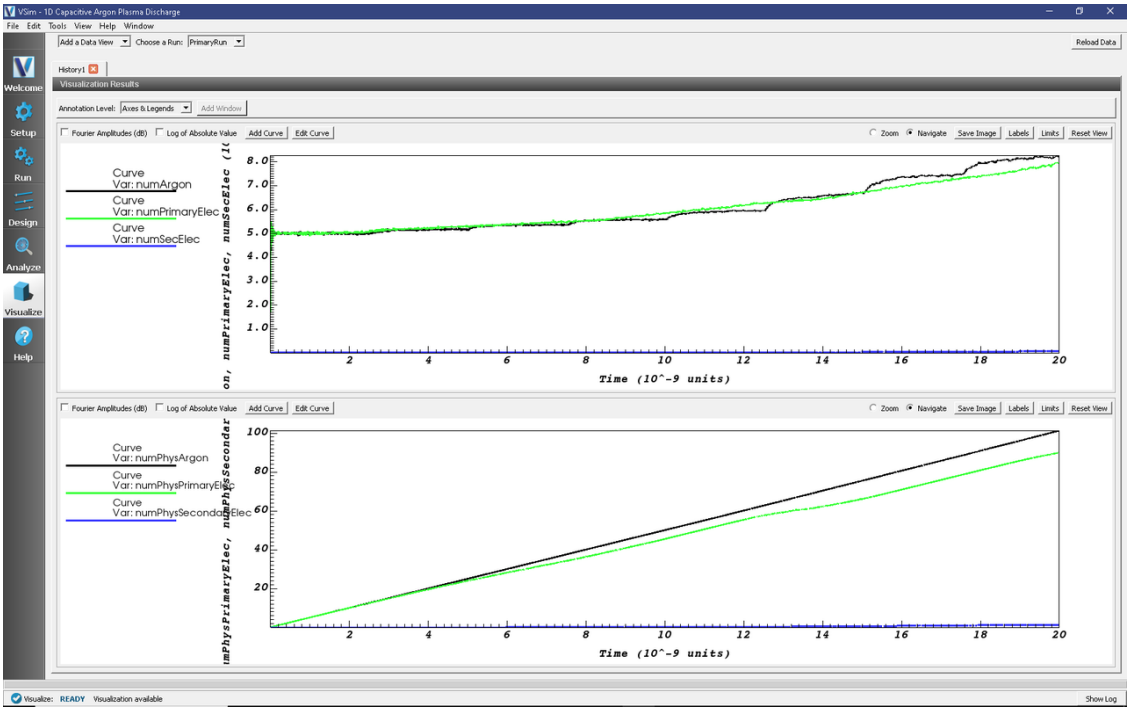


Fig. 6.3: Visualization of number histories of ion, primary electron, and secondary electrons for 4000 steps or 20 nanoseconds.

6.1.2 1D Capacitive Helium Plasma Discharge (capacitivelyCoupledHePlasma1D.sdf)

Keywords:

capacitively coupled plasma, CCP, discharge, steady state, Turner

Problem Description

In this example we demonstrate VSim's ability to simulate capacitively coupled helium plasma discharges in 1D. The example is patterned after case 2 of the work of Turner et al. [TDD+13]; the Turner benchmarks outlined in that work are also discussed more thoroughly in a separate (newer) VSimPD example called "Turner". This example uses older VSim infrastructure (ImpactColliders) to model the interaction of charged particles with a neutral background gas. The newer "Turner" example in VSimPD models the same discharge using VSim's more general Reactions framework.

This simulation can be performed with a VSimPD license.

A video (wherein this example is referred to as "Turner case 2" rather than "capacitivelyCoupledHePlasma1D", consistent with older Tech-X nomenclature) is available for this simulation here: https://www.youtube.com/watch?v=qRX_KnhEekY&list=PLottQ0Bg2M-3ATV5O9IP-3TEC4toVYPAK&index=6

Opening the Simulation

The capacitivelyCoupledHePlasma1D example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item from the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Capacitively Coupled Plasmas* option.
- Select *capacitivelyCoupledHePlasma1D* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.4. In this image, we have unclicked the electrons' particleLoaderE and the HeNeutralFluid so that they will not hide the basic grid. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`. This is a one-dimensional problem, which is shown by having the grid have only a single cell above and below the x-axis.

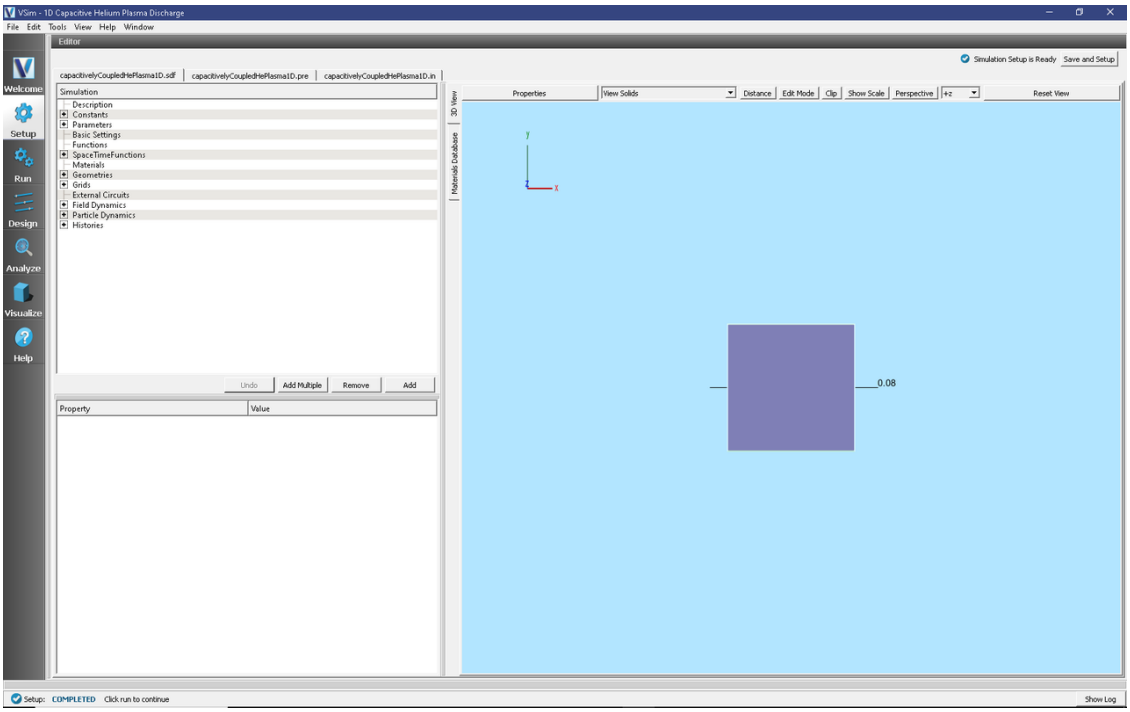


Fig. 6.4: Setup Window for the capacitivelyCoupledHePlasma1D example.

Clicking the electrons' particleLoaderE shows that the electron loader is defined to exist over a cartesian 3d slab, even though this is a one-dimensional simulation. The dimensions that do not apply are ignored, with the coordinate set to zero, but this allows easy conversion from a 1D simulation to a 2D simulation.

Simulation Properties

The basic physics of this simulation is a balance between collisional processes and wall losses; a one-dimensional box of length 6.7 cm contains neutral helium gas at room temperature (300 K) and density 3.21e21/m^3 (1 Torr of pressure at that temperature). The gas is weakly ionized, resulting in a population of free electrons and singly ionized helium atoms at density 5.12e14/m^3. The helium ions are also at room temperature, while the electrons are considerably hotter (30,000 K). The left wall of the box is grounded, while the right wall oscillates with a bias voltage of 200 V at frequency 13.56 MHz.

Charged particles are lost upon collision with the wall and are replenished by ionization of the background neutral gas by the hot electrons; the latter process repopulates both the electrons and helium ions in the plasma (the background neutral gas is treated as an infinite source). Plasma sheaths form near the walls, containing electric fields which are strong relative to those elsewhere in the plasma; the particle density profiles adjust in response to the fields in the sheath. The sheath transit time, for ions, is much longer than the period of the oscillating potential; thus, multiple RF cycles occur while an ion crosses the sheath. A steady state is attained when the loss rate of particles to the wall comes into balance with the ionization rate for a particular profile shape.

In our initial run we are not going to model the full evolution of the discharge to its steady-state parameters; rather, we will explore the basic physics of the discharge and modify the simulation accordingly (with the aim of ultimately hastening convergence to this steady state, while exploring VSim capabilities).

Running the Simulation

The original runs by Turner were for about 4,000,000 steps. To illustrate how to run this problem, we will run for only 10,000 steps, which takes about 5 minutes on a 4-core i7 Windows workstation.

To run the simulation, continue as follows:

- Proceed to the Run Window by pressing the Run button in the left column of buttons.
- Select the 'Run Mode' drop down menu and change it to parallel.
- Set 'Number of Processes' corresponding to your VSim license, shown above as the 'Licensed Cores'
- Check that you are using these run parameters:
  - *Time Step*: 9.218289085545723e-11
  - *Number of Steps*: 10000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- To run the file, click on the *Run* button in the upper left corner of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run during execution is shown in Fig. 6.5.

Analyzing the Results

We are going to run a postprocessing script, computePtclNumDensity.py, which builds density profiles from the particle data generated by VSim, so that we can look at these profiles and their evolution. To do so, we do the following:

- Click the *Analyze* beneath the *Run* button in the leftmost pane.
- From the Available Analyzers, choose *computePtclNumDensity.py*. Then click *Open*.
- Fill in the text boxes
  - The simulationName should be already filled in, but if it is not, type in the name of the .sdf file without the .sdf extension.

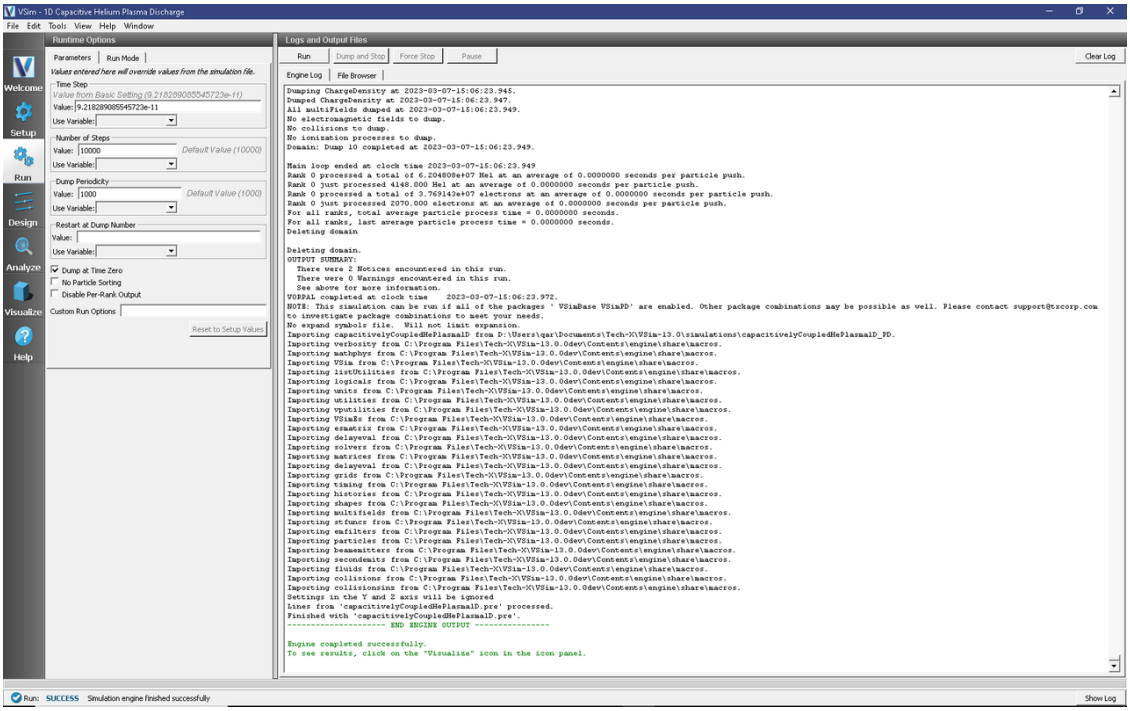


Fig. 6.5: The Run Window during execution.

  - For the speciesName, type in 'electrons' without the quotes.
- Click *Analyze* (in the Analyze Window); this will generate the electron density profiles.
- Now replace 'electrons' in the speciesName box with 'He1', for the helium ions.
- Click *Analyze* (again in the Analyze Window) to generate the ion density profiles.
- The name of the resulting data is *electronDensity* and *He1Density*, which will be visualized in the next section.

Visualizing the Results

Now that we have all of our data, let's look at it.

- Click the *Visualize* button beneath the *Analyze* button in the leftmost pane.

After a brief moment the visualization options for this data should appear.

We will first look at the time evolution of some fundamental one-dimensional quantities. From the *Add a Data View* pulldown menu on the top left, select *History*. The default view here should contain four plots, namely, the electron and ion currents to the left wall and the number of electron and ion macroparticles in the simulation. A number of notable physics effects can be seen here:

- **After a sharp initial decrease in the electron population, both ion and electron populations decline at approximately the same rate.** This is not as apparent from the separate numElec and numIons plots, but with some selection of the plot controls we can combine and reduce the number of plots. In Graph1, select "numElec" as the variable to plot and select "Black" as the color. In Graph 2, select "numIons" to plot, "Window 1" as the Location, and "Green" as the color. In Graph 3 and Graph 4, select "None" as the variable to plot. This should produce the view seen in Fig. 6.6. The initial decrease in electron population arises when rapid electron wall losses create a charge imbalance in the plasma and establish plasma sheaths near the walls. Thereafter, this charge imbalance is preserved and the transport of both electrons and ions to the wall becomes ambipolar.

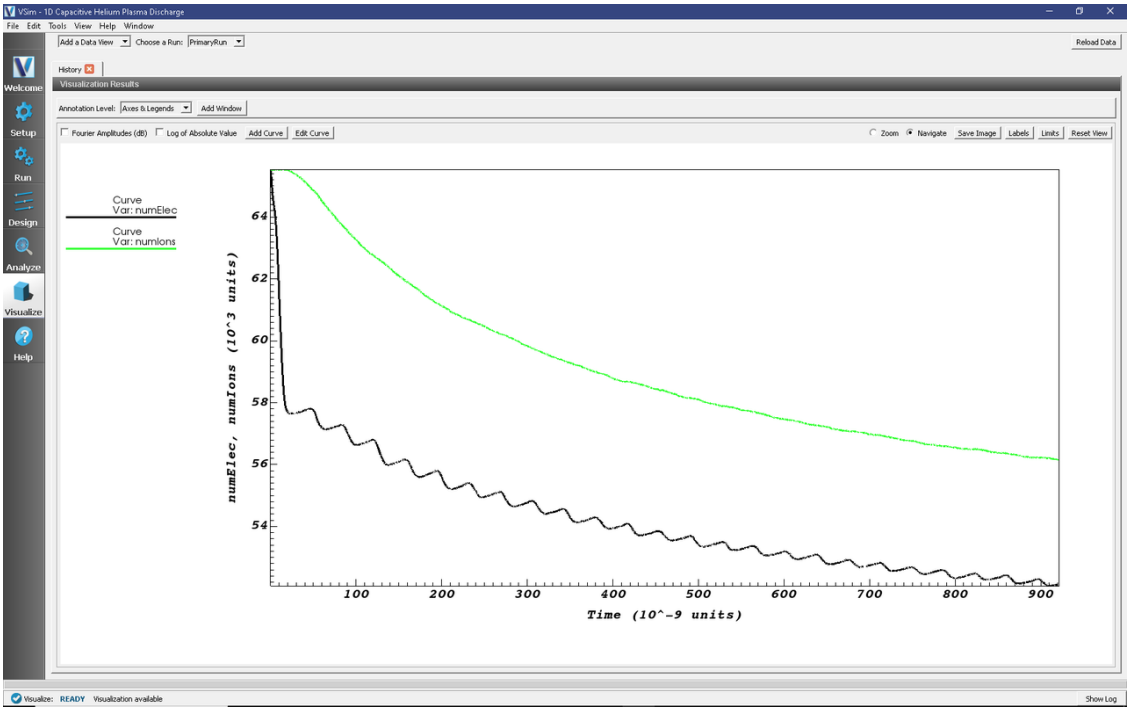


Fig. 6.6: The electron and ion populations versus time.

- **The electron wall currents are quasi-periodic.** The oscillating potential drives the highly mobile electrons alternately into the left and right walls. In the plot variable menu, change "numElec" to "leftElecCurr" in Graph 1 and "numIons" to "rightElecCurr" in Graph 2. The impacts of the electron cloud on the left and right walls, and their phasing in time, can be seen in response to the potential oscillations. A history of the electron currents can be seen in Fig. 6.7
- **The ion currents are non-periodic.** Ions, being much heavier than the electrons, exhibit relatively little response to the oscillating potentials. In the plot variable menu, change the Graph 3 quantity "None" to "leftIonCurrent" and the location to "Window 1", then change the Graph 4 quantity "None" to "rightIonCurrent" and the location again to "Window 1". The ion currents do not have the quasi-periodic structure of the electron currents; rather, ions diffuse outward to the walls in response to the DC sheath potentials, which are established by the initial departure of electrons and may also be rectified by the RF. A history of all the particle currents can be seen in Fig. 6.8
- **Ion losses are negligible before the initial establishment of the sheath.** Change the plot quantity in Graph 3 from "leftElecCurr" to "None". Change the plot quantity in Graph 4 from "rightElecCurr" to "numElec" and for the first two graphs change the "Location" to "Window 3". It is clear that the dominant loss of ions to the wall only begins after the initial decrease in electron population (which corresponds to the establishment of the sheath). A history of the electron population against the ion currents can be seen in Fig. 6.9

We can also look at the plasma sheath and the ensuing changes in density profiles directly. In the "Add a Data View" menu at the top left of the Composer window, select "1-D fields". The plot controls here are similar to those of the history window. Select "E_x" for the plot variable in Graph 1. Select "Phi" for the plot variable in Graph 2. Select "electronsDensity" for the plot variable in Graph 3. Select "He1Density" for the plot variable in Graph 4, and select "Window 3" for the location of this plot. The evolution of the discharge in time can be viewed by moving the time slider below the plots. Slide the bar to dump 10 to view the data at time step 10000 (the data was saved every 1000 time steps).

A number of additional physics features can be seen:

- **Sheath effects are present.** Regions of sharp potential variation, corresponding to strong electric fields, arise

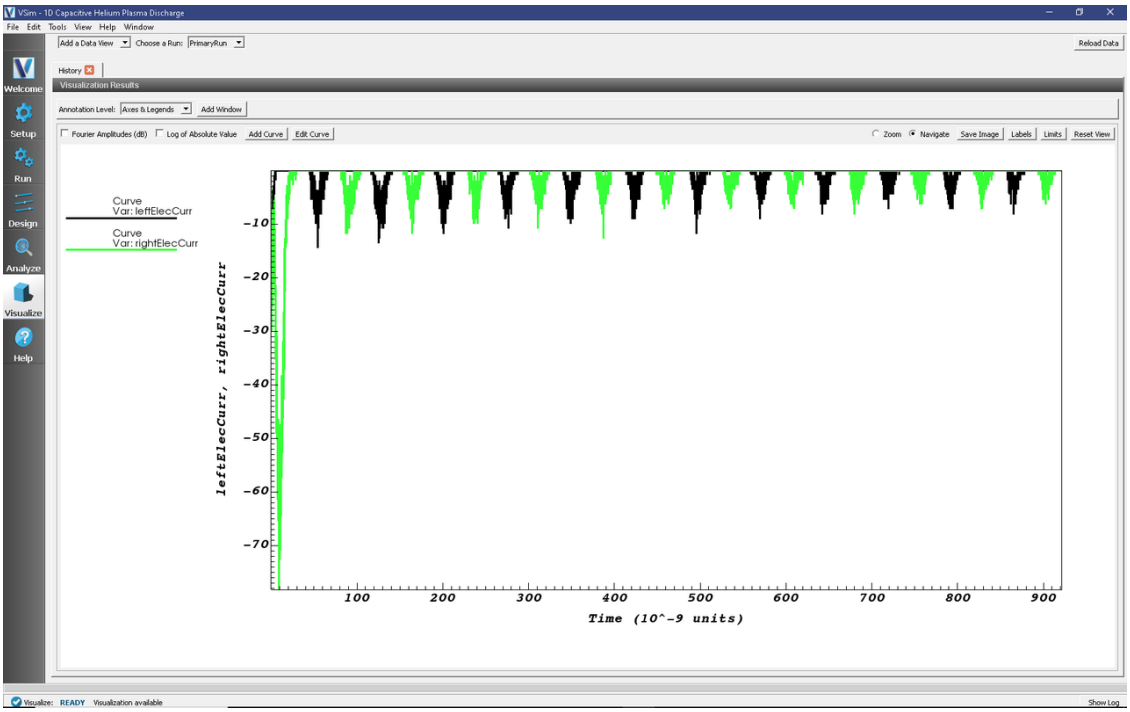


Fig. 6.7: Electron currents on the left (black) and right (green) walls versus time

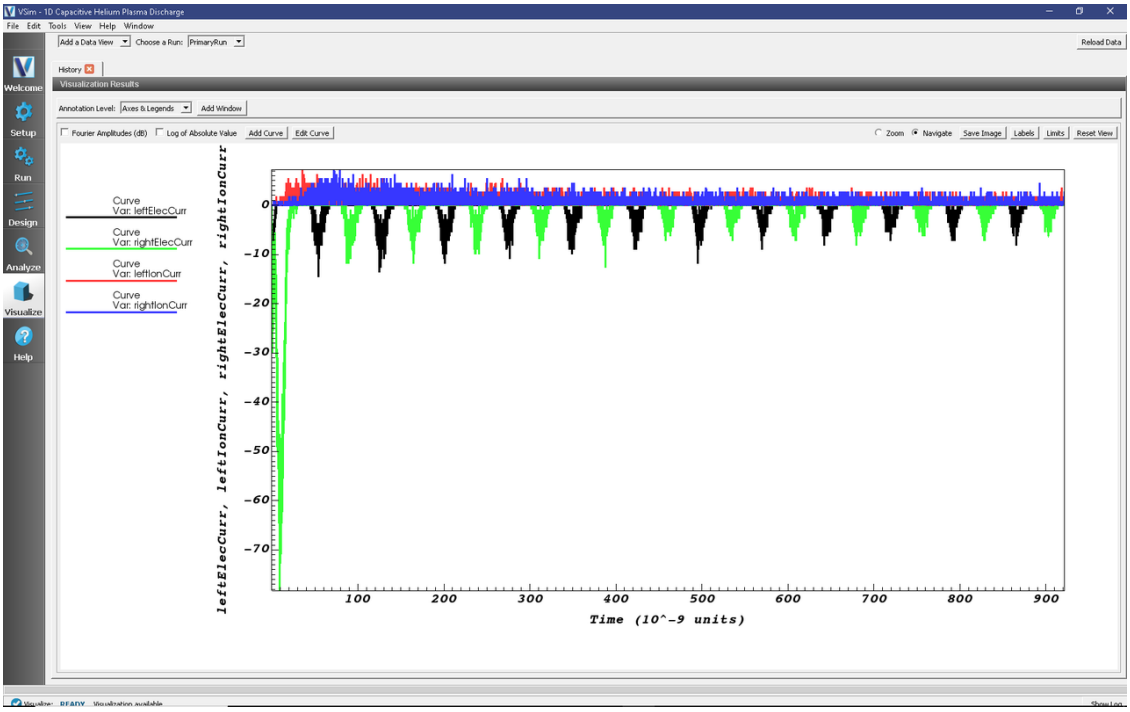


Fig. 6.8: Electron and ion currents on the left and right walls versus time

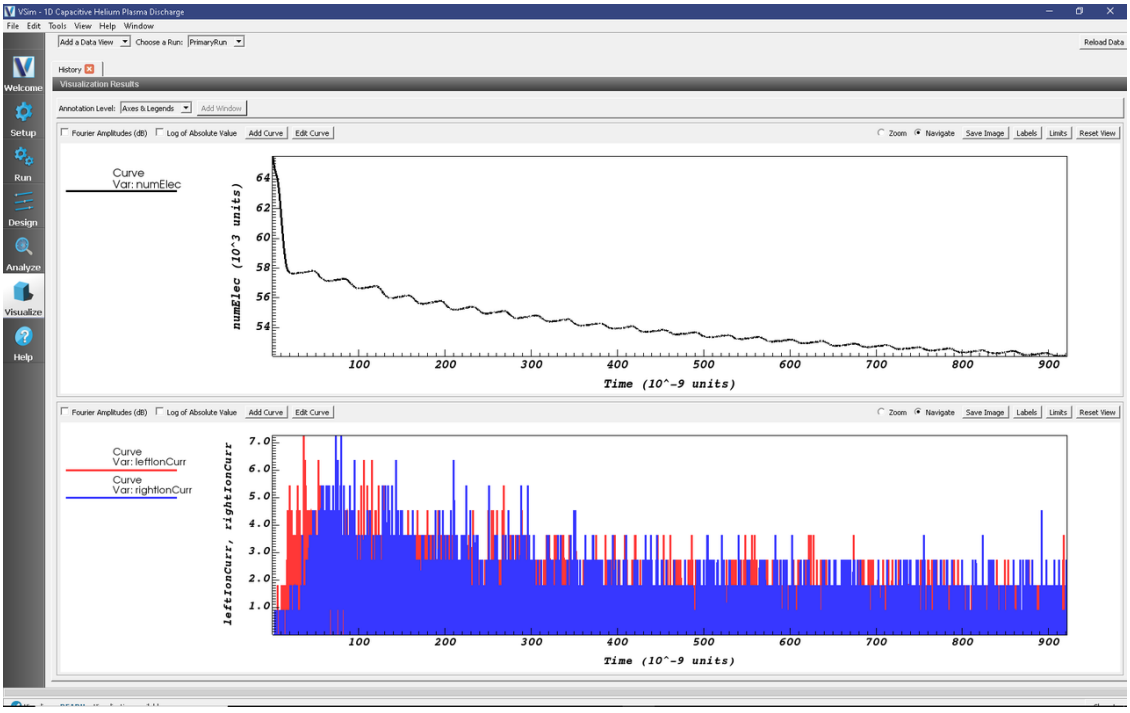


Fig. 6.9: History plots showing the majority of the ion current to the walls only begins after initial decrease in electron population

near the walls, but such fields are screened out in the bulk plasma. Moving the time slider, it is clear that this sheath behavior persists regardless of the phase of the oscillating wall potential.

- **Electron profiles are altered much faster than ion profiles.** Both ions and electron profiles are initially constant (5.12e14 1/m^3), but by the time the first nontrivial dump file is produced (at time dumpPeriodicity * dt, approximately 1/3 of the way through the period of the first wall oscillation), electron-poor regions corresponding to the sheaths have already been established in the electron profile, while the ions have barely begun to respond to the presence of the sheath. Moving the slider forward in time, one observes that the electron profile predominantly oscillates in response to the wall potential, while the ion profile evolves considerably more slowly, particularly outside the sheath regions. The 1-D fields at time step 10000 (dump 10) can be seen in Fig. 6.10

Further Experiments

Now that we understand some of the basic physics of the discharge, we are in position to apply physics-based particle loading methods to hasten its eventual convergence to steady-state. The underlying principle here is to identify the 'slow' processes involved in the evolution of the discharge toward steady state, and then alter the loading to more closely mimic the state to which the plasma is being driven. While we cannot entirely predict the parameters of the steady-state, it is not difficult to at least get some idea of how the simulation is evolving and adjust the particle loads accordingly. We have already observed a number of physical processes of possible relevance:

- initial electron loss and the establishment of ambipolarity
- the slow decay of the total ion and electron population following the initial electron loss
- the rapid response of electrons to applied electric fields, particularly in the sheath region
- the slow evolution of ion density profiles.

Of these, we will primarily consider the ion profiles; the high mobility of the electrons suggests that electron profiles will adjust correspondingly on much shorter timescales. Additionally, since the strong electric fields in the plasma sheath

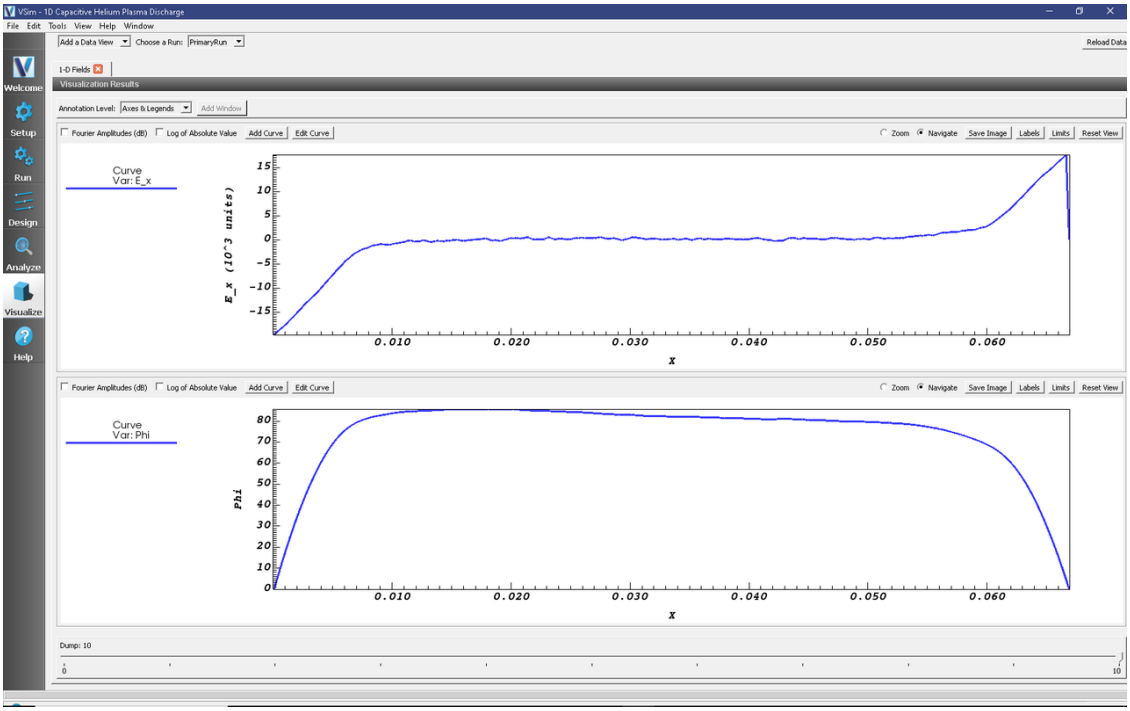


Fig. 6.10: Plots of various 1-D field quantities showing the final state of the run at time step 10000.

region are screened out via Debye shielding as we move away from the walls, it seems clear that profile adjustments in the bulk plasma (where the driving electric fields are weakest) will ensue more slowly than in the plasma edge. We therefore concentrate our attention first on obtaining an approximately correct value for the ion density at the center of the domain.

In the '1-D Fields' tab, set the plot variable to 'None' in plots 2, 3, and 4. In Graph 1, set the plot variable to 'He1Density' and again move the timeslider on the bottom right of the window. The central ion density steadily rises; from its initial value of 5.12e14/m^3, it rises to 6e14/m^3 by the end of our comparatively short run. In addition, a rapid decrease in density near the walls (associated with the plasma sheath) has lowered the edge densities to about 1e14/m^3. The ion density can be seen in Fig. 6.11

Additional Studies

It is possible to try other techniques to more quickly converge to steady state. Initially loading the particles with a non-uniform profile that better resembles the outcome is one such technique. Yet another is to leave a gap near the walls when loading electrons and ions. What happens in the discharge? The electrons, being highly mobile, rush to fill the gap, but rather than immediately being lost to the wall, they instead produce strong electric fields at the plasma edge which begin to modify the ion profile and bring about ambipolarity. If the gap is sufficiently large, the collisional production of ions and electrons will begin before appreciable wall losses ensue, and we can thus assess the relative rates of production and loss fairly early in the simulation. Since the electrons are highly mobile, one can treat the average electron population as a measure of how well we've achieved this balance; net electron production as we move into the ambipolar phase means that our gap is too wide (we have removed too much density), while net losses mean that our gap is insufficiently wide. Because the profile shapes near the walls tend to adjust themselves fairly quickly (due to the larger electric fields in this region), we can in this manner obtain approximately correct values for the total ion and electron populations at the simulation outset.

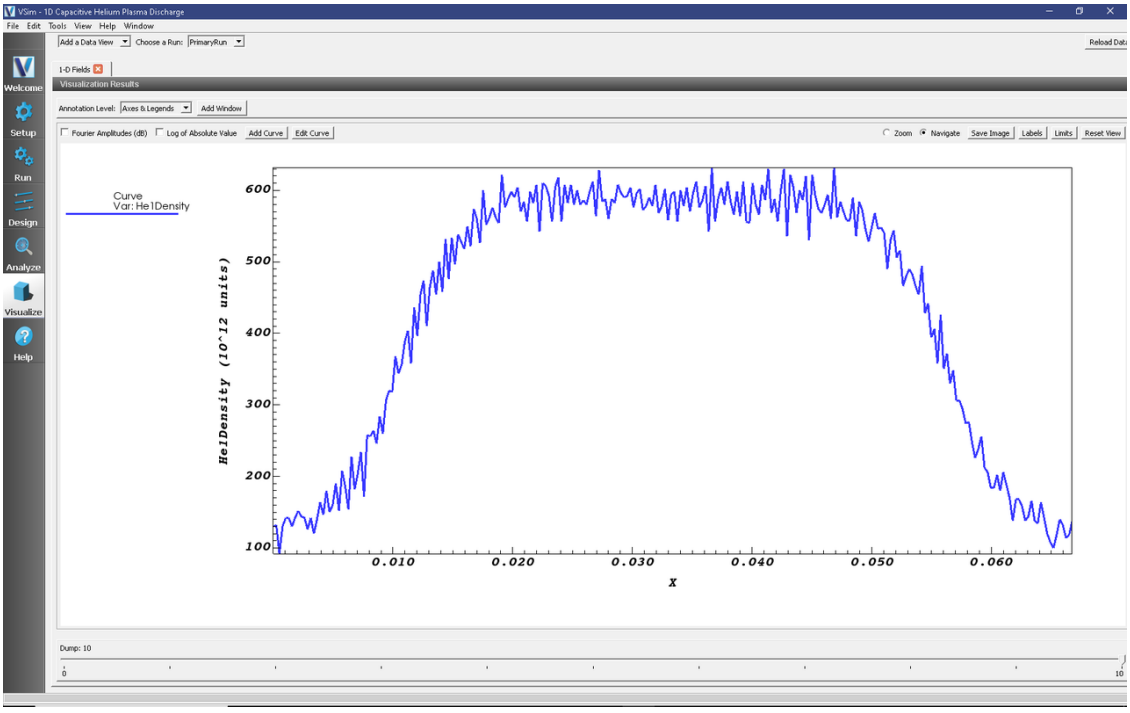


Fig. 6.11: The He ion density at the end of the run (time step 10000).

6.1.3 Turner Low Pressure Benchmarks (Turner.sdf)

Keywords:

capacitively coupled plasma, CCP, discharge, steady state, Turner

Problem Description: Overview of the Turner benchmarks

The physics of a capacitively coupled low-temperature plasma discharge can be quite complex. Sustainment of such a discharge involves a balance between multiple physical effects - losses of charged particles to the chamber walls, production of charged particles via ionizing collisions, and the formation of plasma sheaths (in response to disparate ion and electron mobilities) which mitigate both particle loss and production processes. Accurate numerical models of a capacitively coupled plasma discharge must capture physics associated with:

- Electron-neutral collisions (elastic/ inelastic/ ionizing)
- Ion-neutral collisions (isotropic/ backscattered)
- Particle loss, sheath formation, and imposed voltages at conducting surfaces
- Electrostatic potentials (from existing charge densities and boundary conditions)
- Electric fields (from potential gradients) and responsive charged particle motion

Inaccurate numerical predictions will be made by a particle-in-cell code which cannot accurately represent these basic processes. Even if the inaccuracy is small, its effect on the steady-state properties of the discharge can be significant.

In a notable paper published by M. M. Turner *et al.* [TDD+13] in 2013, modeling benchmarks for capacitively coupled plasmas were proposed which exercise each of the physics capabilities listed above. Turner's paper documents the successful benchmarking of five independently developed particle-in-cell codes (not including VSim) in modeling low-temperature capacitively coupled plasma discharges at four different background pressures. A set of 'accepted results'

for the steady-state ion density produced by the discharge, reproducible to within a specified, statistically-rigorous error tolerance by each of the five codes considered, is provided for each of the four cases. Numerical parameters for each case (e.g. sizes of discrete timesteps or finite grid cells) are also specified, with sufficient detail provided that other numerical models can attempt to reproduce the accepted results for each case to within the specified tolerance. VSim has been run for each of Turner's cases in an effort to make such comparisons; in this example we will demonstrate various results from this modeling. Case 1 will be discussed extensively, and will be shown to pass Turner's rigorous statistical benchmark. An explanation of how to reconfigure this example input file to run Turner's Cases 2-4 will also be provided.

It should be noted that the modeling of physical plasma discharges is in fact not the objective of Turner's work; no comparisons of Turner's 'accepted results' with experimental data are ever made. Rather, the goal is to establish basic standards for codes that will model low-temperature plasma discharges. Agreement with the Turner benchmarks does not guarantee a code's fitness for modeling arbitrary plasma discharges. It does, however, ensure that basic features of that code - e.g. its ability to push charged particles in response to electric fields, to determine the electrostatic potential from a given charge distribution, and to model charged-particle collisions with neutral atoms - are consistent with accepted practices, and that this consistency persists over a broad range of discharge parameters. At the end of this example we will discuss ways in which these simulations could be modified to more closely align with physical plasma discharges.

Problem Description: Physical description of Turner's Case 1

In Turner's Case 1, a capacitively coupled plasma discharge is sustained via a balance between collisional processes (source) and wall losses (sink). A one-dimensional box of length 6.7 cm contains neutral helium gas at room temperature (300 K) and density $9.64 \times 10^{20}/m^3$ (30 mTorr of pressure at that temperature). The helium gas is weakly ionized, resulting in a population of free electrons and singly ionized helium atoms initially at density $2.56 \times 10^{14}/m^3$. Initially, the helium ions are assumed to be at room temperature, while the free electrons are assumed to be considerably hotter (30,000 K). The left wall of the box is grounded, while the right wall oscillates with a bias voltage of 450 V at frequency 13.56 MHz. The oscillating voltage drive rapidly shifts the free electrons back and forth in the domain, but has little direct effect on the ions since their large mass leads to slow response times (much longer than the oscillation period).

Charged particles are lost upon collision with either the left or right wall, and are replenished by ionization of the background neutral gas by the hot electrons. These ionizing collisions repopulate both the electrons and helium ions in the plasma; the background neutral gas is treated as an infinite source. Plasma sheaths form near the walls, containing electric fields which are strong relative to those elsewhere in the plasma, and the particle density profiles adjust in response to the fields in the sheath. The sheath transit time, for ions, is much longer than the period of the oscillating potential; thus, multiple RF cycles occur while an ion crosses the sheath.

A quasi-steady state is attained when the loss rate of particles to the wall comes into balance with the ionization rate for a particular density profile shape. For ions, this density profile is essentially static in time; it is also highly sensitive to the physics of the discharge. Collisional processes represent an effective friction which impedes the outward transport of charged particles within the discharge, and even minor alterations to collision rates or scattering angles will locally modify these frictional forces to yield reshaped density profiles. Details associated with the underlying numerical implementation of individual collisional processes - e.g. the degree to which two-body elastic scattering in the center-of-mass frame is isotropic - thus also influence the steady-state solution.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Turner example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item from the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Capacitively Coupled Plasmas* option.
- Select *Turner* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.12.

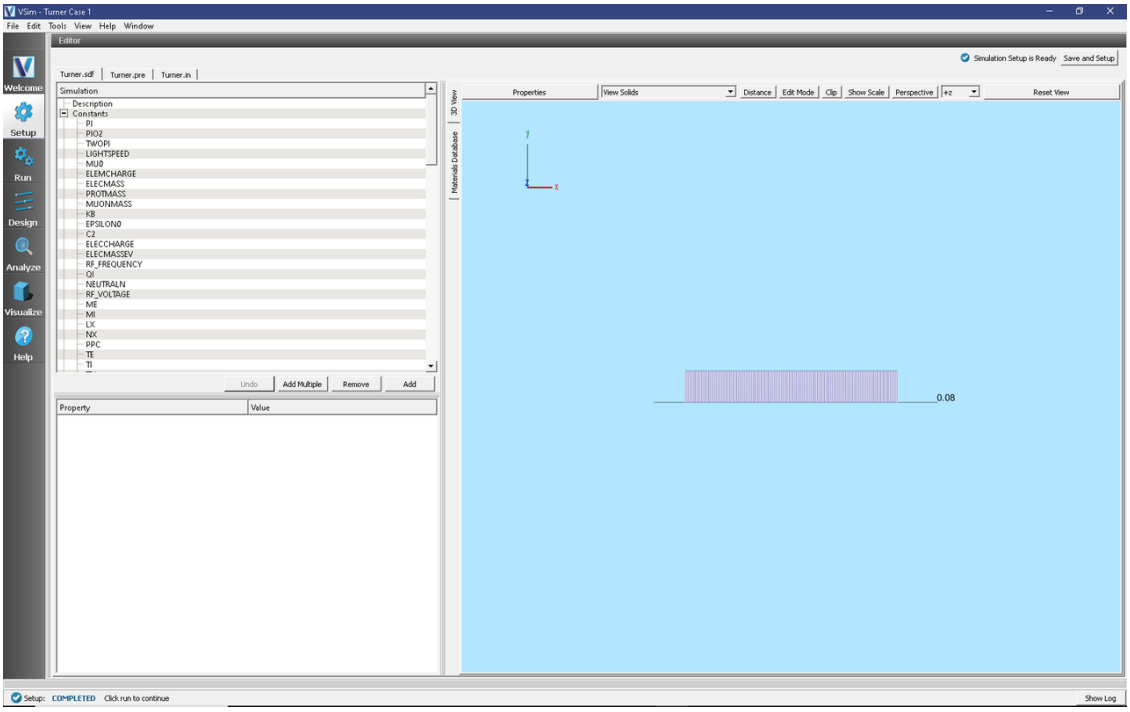


Fig. 6.12: Setup window for the 1D Turner example.

Modifying the Simulation: Turner's Cases 2-4

This VSim example models Turner's Case 1. If desired, VSim users can modify the example input file to instead model other cases in Turner's benchmark paper. Users should be aware of the computational resources that will be needed to run each case and make comparisons with Turner's benchmark data; the required resources are summarized in *Computational Resources Needed For Turner Cases*. Case 1 (this example) can be run to completion in approximately 8 core-hours (e.g. 8 hours in serial, or in about 30 minutes on a 16-core linux cluster). The higher neutral gas pressures used for the other Turner cases lead to shorter collisional mean free paths, and thus increase both the spatial and temporal resolution requirements of the simulations.

Computational resource requirements for Cases 3-4 are substantial. Tech-X strongly recommends the use of a parallel computing cluster (minimum 32 cores) for users who wish to run these cases.

Table 6.1: Computational Resources Needed For Turner Cases

	Neutral Pressure (Torr)	Computing Resources (core-hours)
Case 1	0.03	~8
Case 2	0.1	~170
Case 3	0.3	~750
Case 4	1.0	~4700

To change the example input file to model a different Turner case, users will need to adjust the following simulation parameters in the input file from the Case 1 defaults:

Table 6.2: Input Parameters For Turner Cases 1-4

	Case 1	Case 2	Case 3	Case 4
DT	RF_PERIOD/400.0	RF_PERIOD/800.0	RF_PERIOD/1600.0	RF_PERIOD/3200.0
NEUTRALN	9.64e20	3.21e21	9.64e21	3.21e22
RF_VOLTAGE	450.0	200.0	150.0	120.0
NX	128	256	512	512
PPC	512.0	256.0	128.0	64.0
NDENS	2.56e14	5.12e14	5.12e14	3.84e14
NSTEPS	512000	4096000	8192000	49152000

The number of simulation dumpfiles that will be created for each case, when run with these parameters, is as follows:

Table 6.3: Number of dumpfiles created

	Case 1	Case 2	Case 3	Case 4
Number of dumpfiles	125	1,000	2,000	12,000

The Turner examples proceed by first running the discharge out to steady-state, and then restarting the simulation (using a more frequent dump periodicity) to statistically sample the properties of this steady-state. The restart/sampling procedure will be explained below, and will use the data from the *Number of dumpfiles created* table.

Running the Simulation: Getting to Steady-State

After choosing which of Turner's cases we will run, and making any needed changes to the input file, we are ready to run the simulation. This is done as follows:

- Proceed to the Run Window by pressing the Run button in the left column of buttons.
- Select the 'Run Mode' drop down menu and change it to parallel.
- Set 'Number of Processes' corresponding to your VSim license, shown above as the 'Licensed Cores'.
- Check that you are using these run parameters:
  - *Time Step*: 1.8436578171091448e-10
  - *Number of Steps*: 512000
  - *Dump Periodicity*: 4096
  - *Dump at Time Zero*: Checked

- To run the file, click on the *Run* button in the upper left corner of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully." A snapshot of the simulation run during execution is shown in Fig. 6.13.

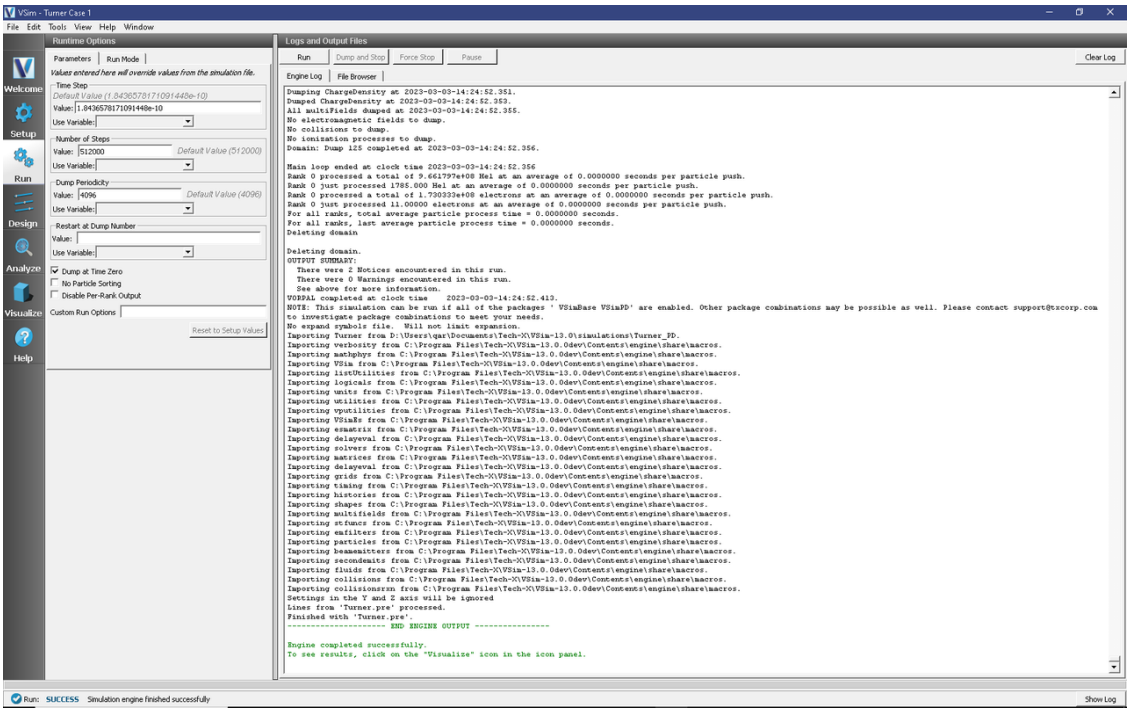


Fig. 6.13: Run window for the Turner example. Simulation runtime will depend on the number of cores available and on which of the Turner cases the user chooses to run (higher pressures yield longer runtimes).

Visualizing the Results: Basic Simulation Output

After the simulation has completed, we should quickly check to verify that the discharge has come to steady-state (at least to the degree that visual inspection permits; we will carry out more detailed mathematical/statistical analysis of the steady-state later in the example). To do so, click the *Visualize* button beneath the *Run* and *Analyze* buttons in the leftmost pane.

After a moment the visualization options for this data should appear.

We are going to look at a very basic metric for steady-state - is the number of simulation macroparticles for each species in the discharge both (a) nonzero, and (b) roughly constant in time? To do so, we will plot a time history of the macroparticle population of each species. This is done as follows:

- In the *Visualization* window, click the *Add a data view* → *History* menu. This will open a *History* tab.
- In the *History* tab, click on the *Add Curve* button. In the dropdown menu that appears (listing various 1D time histories that one might plot), select *NumElec* and then *OK*. A plot showing the variation of the electron macroparticle population in time should appear in the window.
- Click on the *Add Curve* button again, and this time select *NumIons* in the dropdown menu, and then *OK*. Another plot (of ion macroparticle population) should appear in the same window.
- Though it may already be apparent, we can adjust the y-axis limits to more convincingly show that the species macroparticle populations are both nonzero and approximately constant. To do so, click the *Limits* button, and adjust the Y-Axis range to be [0,25000].

From the resulting plot (also shown in Fig. 6.14), we can see that both the electron population and the (slightly higher) ion population have come to a nontrivial steady state. It is also reassuring that the average ion macroparticle population is higher than the average electron macroparticle population (given that the number of physical particles in a macroparticle is the same for both ions and electrons in this example). The higher mobility of the electrons allows them to be more easily lost at the simulation outset, and the formation of plasma sheaths is a direct consequence of the ensuing charge imbalance.

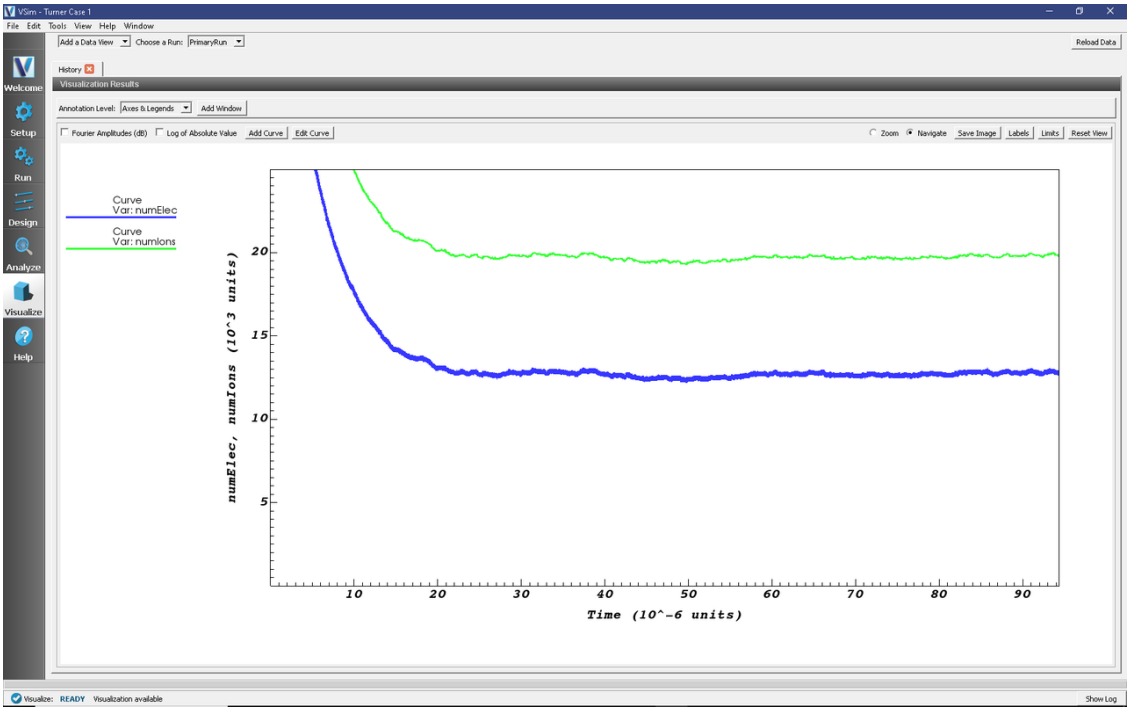


Fig. 6.14: Visualization window for the Turner example, demonstrating that the simulation has come to a nontrivial steady state.

As an exercise in using the *Visualization* window capabilities, users might demonstrate these same results by plotting the number of physical particles of each species, rather than the number of macroparticles. The new plot could be made in a separate window (use the *Add Window* button), or by deleting curves from the existing window (using the *Edit Curve* button) and thereafter adding new ones. The approximate Turner Case 1 steady-state values for ions and electrons are $5.1 \times 10^{12}/m^3$ and $3.2 \times 10^{12}/m^3$ respectively.

Running the Simulation: Sampling the Steady-State

Now that we have reasonable confidence that a steady-state discharge has been achieved, we will need to sample the properties of the steady-state. To do so, return to the Run window by clicking the *Run* button in the leftmost pane.

We will be restarting the simulation using a more frequent dump periodicity to sample the properties of the steady-state. In this manner we generate the data needed for the mathematical/statistical steady-state analysis.

The *Restart Parameters* table contains the parameters needed for the restart.

Table 6.4: Restart Parameters

	Case 1	Case 2	Case 3	Case 4
Number of Steps	13200	26400	52800	105600
Dump Periodicity	12	24	48	96
Restart at Dump Number	125	1000	2000	12000
Total Number of Dumps	1225	2100	3100	13100

Conceptually, we will be restarting the simulation from the final (presumably steady-state) dumpfile generated in the initial run (which is why the last entry of *Restart Parameters* has a corresponding entry in *Number of dumpfiles created*.) We will run the restarted simulation for 33 RF periods, and will sample the properties of the steady state every 0.03 RF periods. In this manner we obtain 11 datapoints at each fractional phase (T/100) of the RF period, yielding 1100 datapoints altogether (1100 dumpfiles are generated in the restart/sampling run). We will average over these datapoints to determine the properties of the steady state.

[**Note:** this averaging/sampling procedure is slightly different than the averaging procedure described in Turner's paper. In that approach, very large quantities of data are generated since every timestep in a 32-period sequence is sampled. We have compared the two approaches and determined that the results are comparable; to use Turner's procedure, one would set the *Dump Periodicity* of the restart run to 1, and modify the *Number of Steps* parameter to run over 32 RF periods instead of 33. Subsequent analysis would then need to take into account the much larger number of dumpfiles that will ensue.]

To restart the simulation and carry out the necessary sampling, do the following in the Run window:

- Change the *Number of Steps* value to match the value in the *Restart Parameters* table corresponding to the Turner case you are doing.
- In the Run window, change the *Dump Periodicity* value to match the value in the *Restart Parameters* table corresponding to the Turner case you are doing.
- In the Run window, change the *Restart at Dump Number* value to match the value in the *Restart Parameters* table corresponding to the Turner case you are doing.
- To run the file, click on the *Run* button in the upper left corner of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully."

A brief discussion of Turner's chi-squared statistical metric

For each of Turner's benchmark cases, a metric for agreement with the predicted physics results (in a statistical sense) has been provided. This statistical metric is based on the time-averaged ion density profile (a slowly-evolving quantity which is quite stable in steady-state) and takes the form $\chi^2 = \sum_{j=0}^{NX} \frac{(n_j - \bar{n}_j)^2}{\sigma_j^2}$. In this expression, n_j is the time-averaged ion density at the j-th gridpoint in the simulation and will be computed from the VSim data produced in the restart/sampling phase of this example. The expressions $\bar{n}_j$ and σ_j are (respectively) Turner's prediction for the time-averaged ion density at the j-th gridpoint, and a statistically computed population standard deviation for $\bar{n}_j$ at this point. The simulation is assumed to have NX grid cells (the number of grid cells for each Turner case is listed in *Input Parameters For Turner Cases 1-4*) and thus has $NX + 1$ gridpoints; the uniform grid spacing is $\Delta x = LX/NX$.

Heuristically, a VSim prediction for n_j at a given point that is less than one standard deviation σ_j away from Turner's predicted value $\bar{n}_j$ at that point will contribute only negligibly to the χ^2 sum; the contribution of this term to the sum will always be less than unity. VSim predictions that deviate from Turner's predicted values by more than one standard deviation will contribute much more significantly to the sum. The expected values of χ^2 given by Turner for each case are:

Table 6.5: Expected Chi-Squared Values

	Case 1	Case 2	Case 3	Case 4
95%	55-303	177-435	405-693	417-665
99%	48-405	160-548	382-798	392-730

For a given case, *Expected Chi-Squared Values* asserts that if VSim is statistically indistinguishable from the five codes used in Turner's benchmark, then the value of χ^2 computed from VSim data will fall within the 95% range with 95% probability (no more than one simulation in 20 should fall outside this range). Likewise, the value of χ^2 will fall within the 99% range with 99% probability (no more than one simulation in 100 should fall outside this range). When VSim predictions fall consistently within the ranges specified by Turner, we can have confidence in its predictive value for the case considered - at least, we can have confidence that it is capturing physics identical to the physics used by the other five codes in the benchmark.

In the following section we will use a VSim analyzer to compute the value of χ^2 for the run we have just completed.

Analyzing the Results: Comparing with Turner chi-squared diagnostic

To determine whether VSim has statistically matched the Turner benchmark, return to the VSim analysis window by clicking on the *Analyze* tab in the leftmost pane.

In the list of available analyzers, find and select *computeTurnerChi.py*. A window should appear at right showing the default input parameters for this analyzer. The *case* option allows users to switch between Turner's cases 1, 2, 3, or 4. If this parameter is changed, the user should also change the *start_dump* and *end_dump* options to be consistent with the data in the *Restart Parameters* table. The correct *start_dump* option is obtained by adding 1 to the *Restart at Dump Number* value found in the table, for the Turner case under consideration. The correct *end_dump* option is the same as the *Total Number of Dumps* option in the table, for the Turner case under consideration.

Clicking the *Analyze* button computes a time-averaged value for χ^2 using all dump files in the interval *start_dump* to *end_dump*. Output for this analyzer is shown in Fig. 6.15; for this particular run, a value of $\chi^2 = 96.16$ was obtained. This number should be compared with the ranges for Case 1 shown in *Expected Chi-Squared Values*.

For this run, the computed χ^2 value falls within both the 95% and 99% allowable ranges of the *Expected Chi-Squared Values* table for Turner's Case 1. The value of χ^2 will almost certainly differ when this example is run on other computing platforms, or even when this example is repeated on the same platform; users should not be alarmed if their values do not precisely match the values shown here. Nevertheless, statistical agreement with Turner's benchmark can be claimed if the computed χ^2 values deviate from Turner's 95% range no more often than one run in twenty (on average), or from Turner's 99% range no more often than one run in a hundred (on average). This result should be independent of computing platform.

Analyzing the Results: Comparing with Turner electron energy distribution function

In this section, we will construct an electron energy distribution function (EEDF) from our steady-state simulation data. Afterwards, we will compare this function to the EEDF predicted by Turner.

Return to the VSim analysis window by clicking on the *Analyze* tab in the leftmost VSim Composer pane. Then, double-click on the *computeTurnerEEDF.py* analyzer in the list of available analyzers on the left of the window. A window should appear showing the default input parameters for this analyzer.

This analyzer operates on the macroparticle data which VSim periodically dumps. Given a macroparticle dumpfile corresponding to a particular time in the simulation, one can extract from this file a histogram of the particle energies at that time. Because the Turner discharges are periodic, the distribution of particle energies will varies slightly in time based on the phase of the periodic driving voltage, so we will need to sample over a sequence of dumpfiles which sample the EEDF uniformly in the different phases. This is done in just the same manner as we sampled other

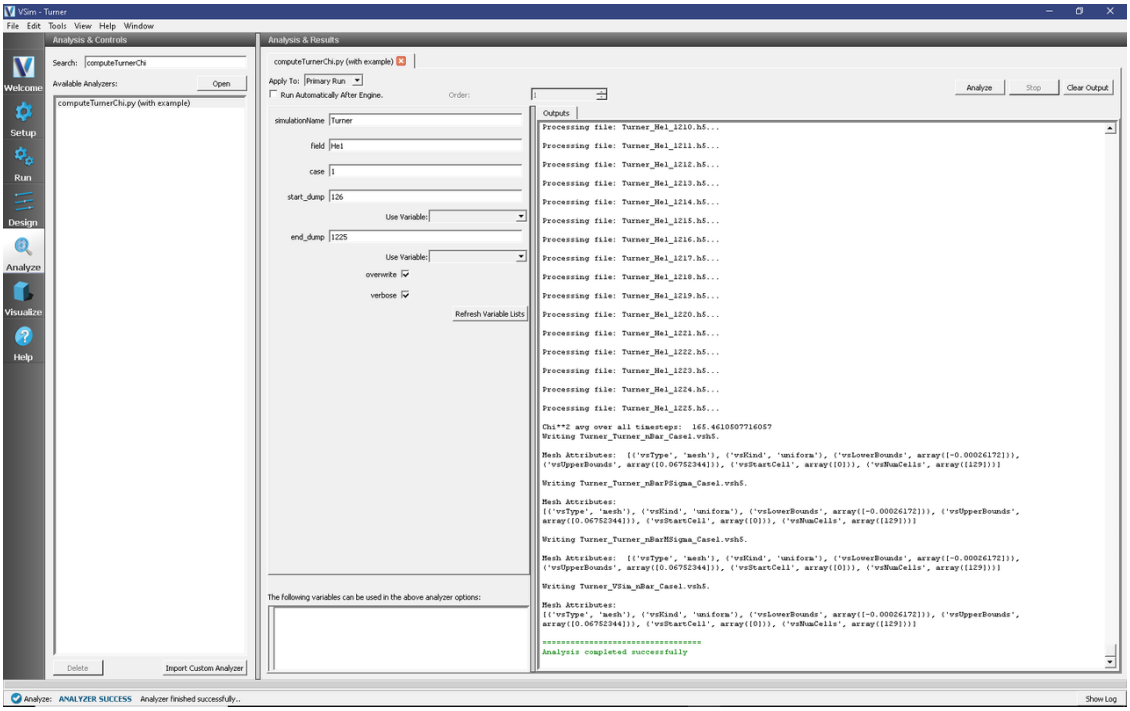


Fig. 6.15: Analysis window for the Turner example, showing input parameters for, and output from, the computeTurnerChi.py analyzer for Turner's Case 1. The computed value for χ^2 falls within Turner's predicted ranges, indicating that these VSim results are statistically indistinguishable from those generated by the five other codes used in the benchmark.

properties of the steady-state above; we will use the same *start_dump* and *end_dump* values for the analyzer as we did for the *computeTurnerChi.py* analyzer above. In doing so, we will sample the EEDF associated with the steady-state discharge. The default *start_dump* and *end_dump* values assume that files from Turner's Case 1 are being analyzed using the less data-intensive sampling method described previously.

The analyzer constructs a normalized histogram $[\epsilon, f(\epsilon)]$ of particle energies, with energy given in units of electron-volts, for all particles within the specified range of dumpfiles. The normalization follows that of Turner; we require that $\int_0^\infty \sqrt{\epsilon} f(\epsilon) d\epsilon = 1$ for the desired distribution $f(\epsilon)$.

After adjusting the *start_dump* and *end_dump* values (if needed), click on the *Analyze* button at the top of the right panel to run this analyzer.

When the analyzer is finished, it will display the histogram bins and the histogram data in the log window at right, and report that the "Analysis completed successfully". For large datasets (such as the one we will construct), only abbreviated representations of the bin and the data arrays will be shown. Representative output for the analyzer, together with its default input parameters, is shown in Fig. 6.16.

The analyzer output is written to a file *Turner1_EEDFelectrons.vsh5* which contains the full bin and data arrays (normalized) of the computed histogram. This file can be viewed in the *Visualize* window, which we will now do.

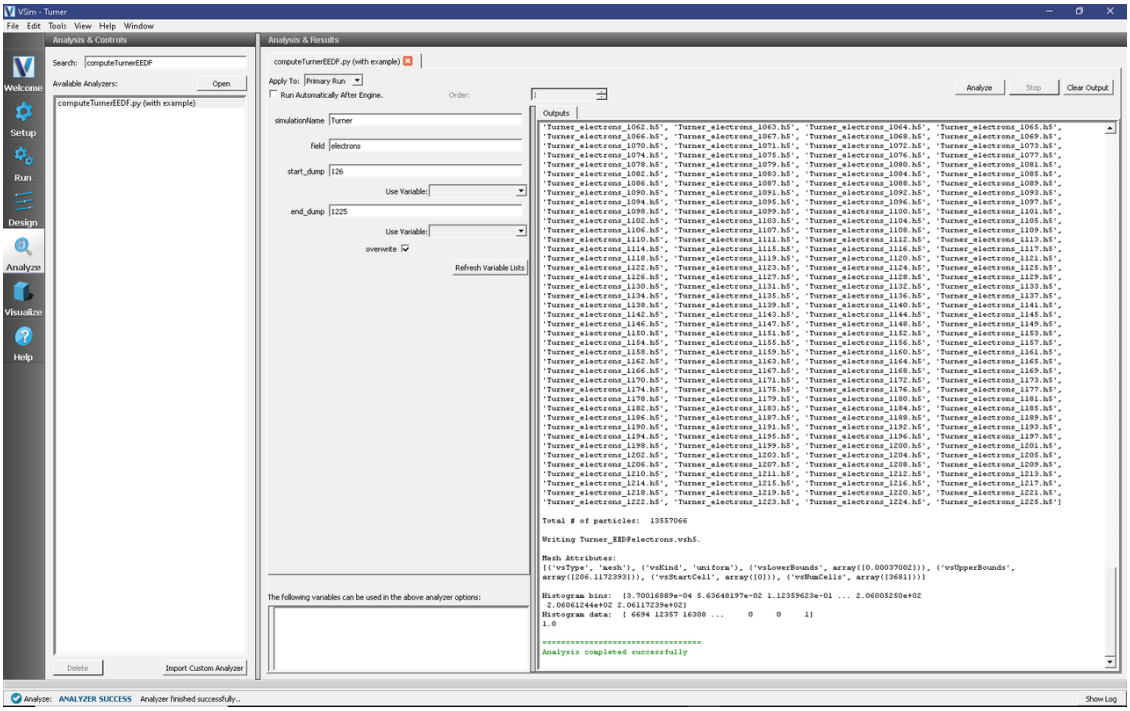


Fig. 6.16: Analysis window for the Turner example, showing input parameters for, and output from, the computeTurnerEEDF.py analyzer for Turner's Case 1.

Visualizing the Results: Comparing with Turner electron energy distribution function

Return to the VSim visualization window by clicking on the *Visualize* tab in the leftmost VSim Composer pane.

The histogram plotted in the previous section is a 1D plot of probability as a function of energy. To view it, click the *Add a Data View* tab in the top left of the visualization window, and select *1-D Fields*. A new tab with this designation will open in the window below.

Click the *Add Curve* button in the plot window. From the dropdown menu that appears, select the *electrons_EEDF variable* and click *OK*. A plot should appear in the window.

We will be comparing with Figure 6 of Turner's paper, which is plotted on a log-linear scale. To make our plot look like Turner's plot, do the following:

- Switch the y-axis to a logarithmic scale by clicking the *Log of Absolute Value* checkbox at the top of the plot window.
- Change the plot limits by clicking the *Limits* box at the top right of the plot window. The X-Axis values should be changed to cover the range 0 (Min) to 60 (Max), while the Y-Axis values should be changed to cover the range -5 (Min) to -1 (Max). (On the logarithmic scale, these values represent the powers of ten spanned by the plot on the y-axis.)

The resulting plot is shown in Fig. 6.17, and can be compared with Figure 6 of Turner's paper [TDD+13].

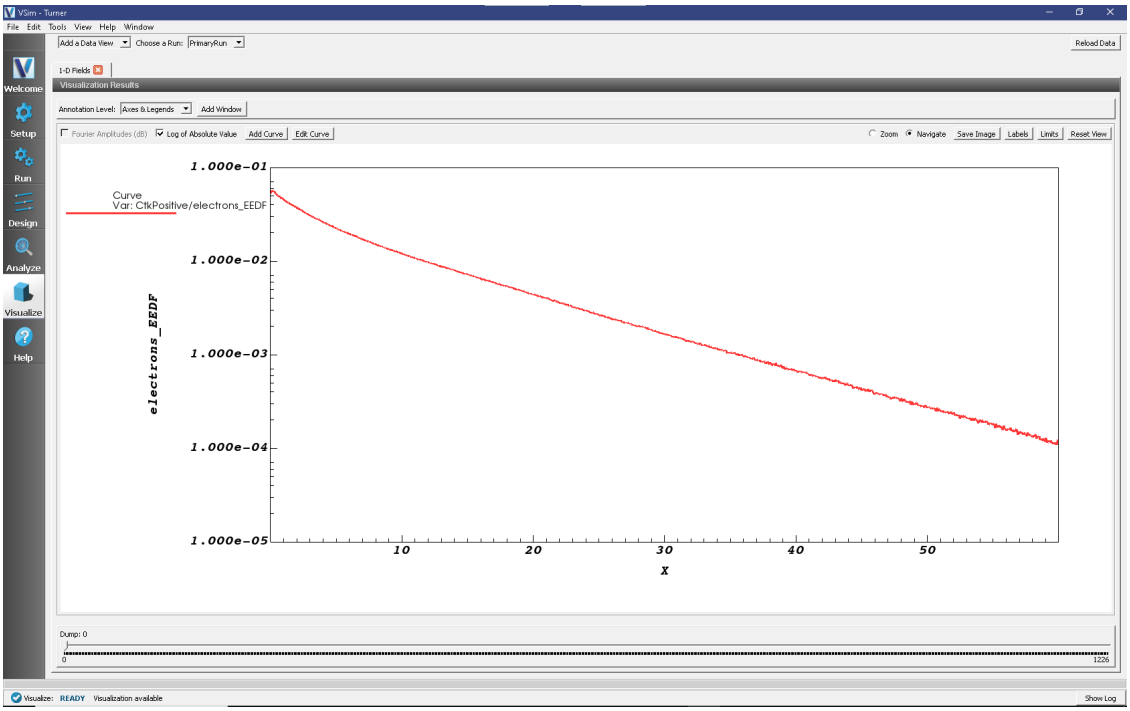


Fig. 6.17: Visualization window for the Turner example, showing a plot of the normalized steady-state electron energy distribution function for Turner's Case 1. This plot can be compared with Figure 6 of Turner's benchmark paper, noting that in that plot the EEDF distributions are normalized inconsistently from what the text indicates [a multiplicative factor of approximately 0.414 reduces the value of $f(\epsilon)$ below the properly normalized VSim result].

Analyzing the Results: Comparing with Turner power deposition diagnostic

In this section, we will construct time-averaged power density profiles $\langle \mathbf{E} \cdot \mathbf{J}_\alpha \rangle$ for each species (α = electrons, ions). Thereafter, we will compare these profiles to the power density profiles predicted by Turner.

Return to the VSim analysis window by clicking on the *Analyze* tab in the leftmost VSim Composer pane. Then, double-click on the *computeTurnerJdotE.py* analyzer in the list of available analyzers on the left of the window. A window should appear showing the default input parameters for this analyzer.

This analyzer operates on the electric field profiles and species current density profiles which VSim periodically dumps. Although these are vector field quantities, for this example only the x-coordinate will be relevant. Electric field components in the ignored directions (y and z) are zero in this simulation.

The analyzer computes a time-averaged $\langle \mathbf{E} \cdot \mathbf{J}_{electron} \rangle$ and $\langle \mathbf{E} \cdot \mathbf{J}_{ion} \rangle$ using the same averaging procedure as was used to plot the EEDF above; it should use the same *start_dump* and *end_dump* values that were used in *computeTurnerChi.py* and *computeTurnerEEDF.py* above to sample the power density profiles associated with the steady-state discharge. The default *start_dump* and *end_dump* values for this analyzer assume that files from Turner's Case 1 are being analyzed using the less data-intensive sampling method described previously.

After adjusting the *start_dump* and *end_dump* values (if needed), click on the *Analyze* button at the top of the right panel to run this analyzer.

When the analyzer is finished, it will display in the right-hand window the full arrays containing the computed power density profiles, in units of kiloWatt per cubic meter. The number of points in these arrays is equal to the number of grid cells for the particular Turner case chosen, i.e. the NX value in *Input Parameters For Turner Cases 1-4*. An "Analysis completed successfully" message should also appear in the log window at right.

Representative output for the analyzer, together with its default input parameters, is shown in Fig. 6.18.

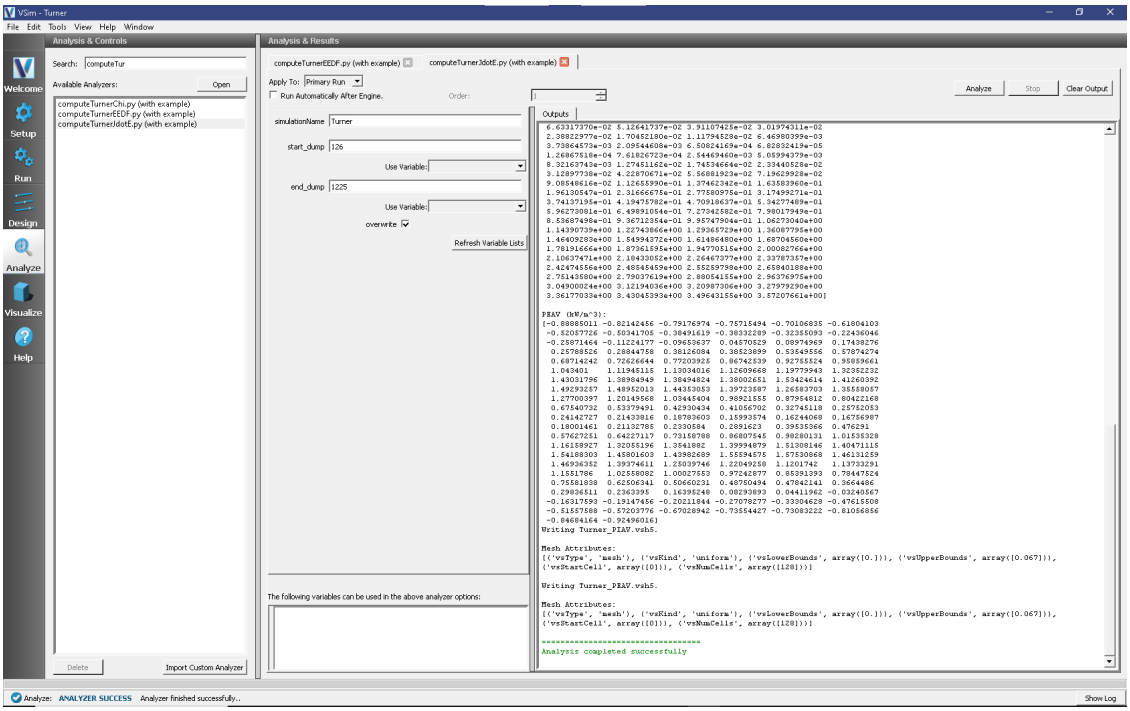


Fig. 6.18: Analysis window for the Turner example, showing input parameters for, and output from, the computeTurnerJdotE.py analyzer for Turner's Case 1.

The analyzer output is written to two files, *Turner1_PEAV.vsh5* and *Turner1_PIAV.vsh5*, which are respectively the electron and ion power density profiles averaged over the specified time interval. These files can be viewed in the *Visualize* window, which we will now do.

Visualizing the Results: Comparing with Turner power deposition diagnostic

Return to the VSim visualization window by clicking on the *Visualize* tab in the leftmost VSim Composer pane.

The power density profiles generated in the previous section are, like the EEDF, 1D plots that can be viewed from the *1-D Fields* tab of the visualization window. You may need to click the *Reload Data* button at the top right of the window to enable these files to be seen in the window. Any existing plots in the *1-D Fields* panel can be erased by clicking the *Edit Curve* button, and thereafter the *Remove Selected Curve* button.

We are going to look at the electron power density profile first. Click the *Add Curve* button in the plot window. From the dropdown menu that appears, select the *PEAV* variable and click *OK*. A plot should appear in the window.

We will be comparing this plot with Figure 4 of Turner's paper. To make our plot look like Turner's plot, change the plot limits by clicking the *Limits* box at the top right of the plot window. The X-Axis values should be changed to cover the range 0 (Min) to 0.067 (Max), and the Y-Axis values should be changed to cover the range -2 (Min) to 9 (Max). (Turner plots x/LX, with LX = 0.067 meters; we are plotting x directly in the range $[0, LX]$.)

The resulting plot is shown in Fig. 6.19; the data compares favorably with Figure 4 of Turner's paper [TDD+13].

We will now look at the ion power density profile. Click the *Edit Curve* button, and thereafter the *Remove Selected Curve* button, to clear the electron power density profile plot. Then click the *Add Curve* button in the plot window. From the dropdown menu that appears, select the *PIAV* variable and click *OK*. A new plot should appear in the window.

We will be comparing this plot with Figure 5 of Turner's paper. To make our plot look like Turner's plot, change the plot limits by clicking the *Limits* box at the top right of the plot window. The X-Axis values should again be changed

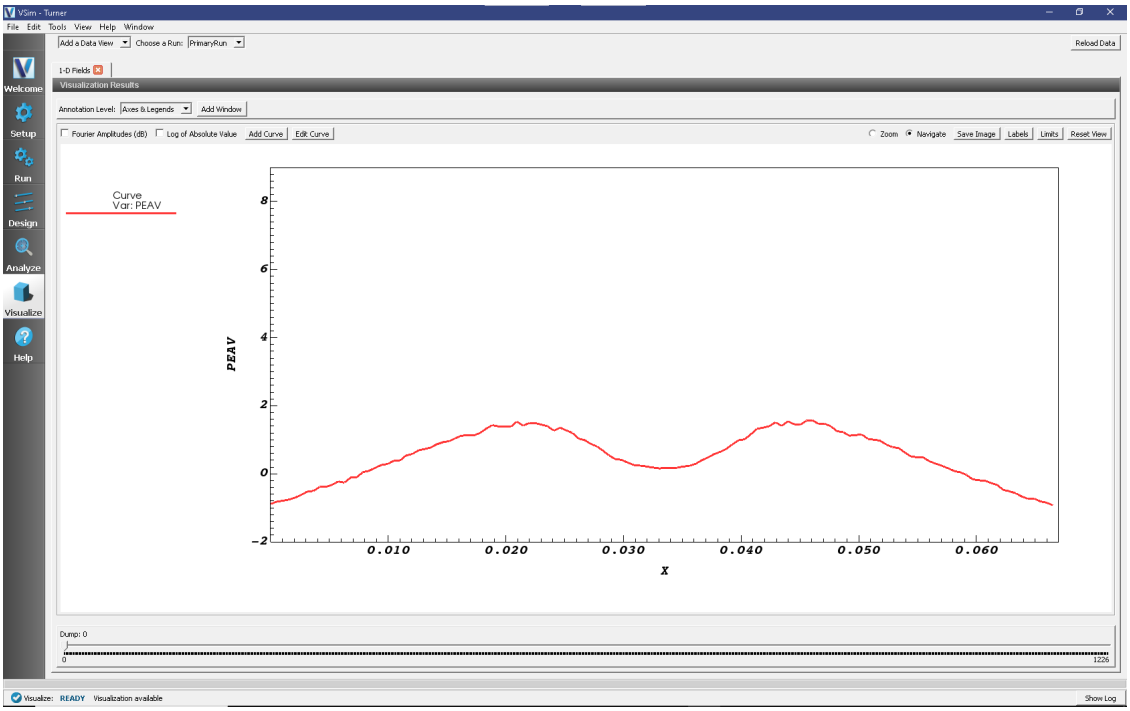


Fig. 6.19: Visualization window for the Turner example, showing a plot of the normalized steady-state electron power density profile for Turner's Case 1. This plot can be compared with Figure 4 of Turner's benchmark paper.

to cover the range 0 (Min) to 0.067 (Max), and the Y-Axis values should be changed to cover the range 0 (Min) to 4.5 (Max). (Again, Turner plots x/LX, with LX = 0.067 meters; we are plotting x directly in the range $[0, LX]$.)

The resulting plot is shown in Fig. 6.20, and the data compares favorably with Figure 5 of Turner's paper [TDD+13].

Further Experiments

As we have noted, the Turner benchmarks provide useful metrics for assessing whether or not basic features of a PIC-MCC code - its ability to push charged particles in response to electric fields, to determine the electrostatic potential from a given charge distribution, and to model charged-particle collisions with neutral atoms - are consistent with accepted practices. The benchmarks do not guarantee a code's fitness for modeling arbitrary low-temperature plasma discharges, though the features listed above are certainly necessary for such modeling.

Nevertheless, given confidence in the benchmark model, one can then move toward a more physically representative model of a given plasma discharge by incrementally altering the benchmark file to include additional physics. Some alterations might be simple and require little additional verification; for example, Turner's benchmark stipulates an electron mass of 9.109×10^{-31} kg (exactly), and equal ion and neutral masses of 6.67×10^{-27} kg (exactly). VSim's underlying code infrastructure works the same way even if we adjust these values to include more significant digits, and/or to more carefully account for the mass difference between neutral and ionized helium atoms. No additional verification would be needed to make such a change, but the steady-state discharge profiles and the other plots we have made will change slightly due to the added physics. In a similar way, adding a new collision process to the discharge (using an appropriate cross-section data file, as documented in the "Obtaining Cross-sections from LXCat" in the Reference Manual. adds only additional physics processes to the discharge whose numerical implementation we trust.

Other alterations to the input file cannot rely directly on the consistency argument established by passing Turner's benchmarks. Changes that alter the underlying physics of a particular collision, e.g. switching the electron-neutral ionization scattering type to *VahediSurendra default* instead of *Turner*, can no longer be checked against the collisional interaction physics of Turner's model. While it is believed that the Vahedi-Surendra scattering model more closely

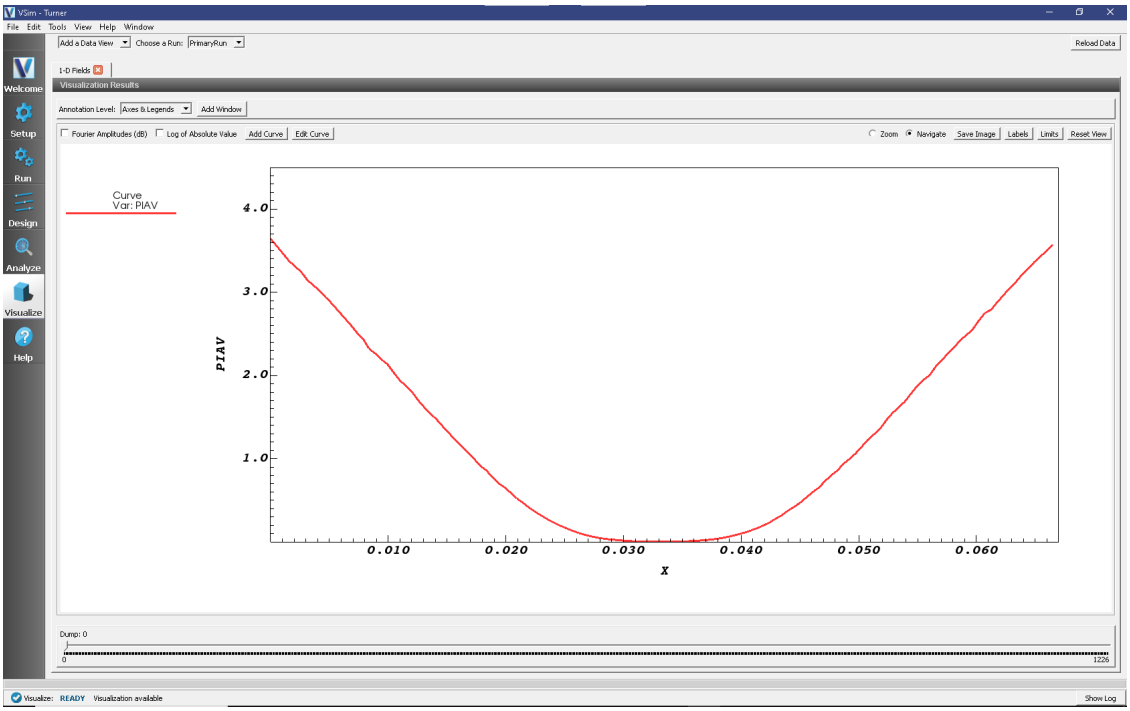


Fig. 6.20: Visualization window for the Turner example, showing a plot of the normalized steady-state ion power density profile for Turner's Case 1. This plot can be compared with Figure 5 of Turner's benchmark paper.

approximates physical reality than the model used in the benchmark (and Tech-X further believes that this scattering model is implemented correctly in VSim, consistent with Ref. [VS95]), the new steady-state of the discharge cannot be compared with Turner's directly. (In such cases, it may be of interest to the user to verify that the physics of the new collision process, as calculated by VSim, matches up with what the user expects. This could be done by constructing a reduced example that models only the new collision process; a modified version of the *Townsend Discharge (townsend.sdf)* example could work well for this purpose.)

6.2 Capacitively Coupled (text-based setup)

6.2.1 2D Capacitive Plasma Chamber (capacitivelyCoupledPlasma2DT.pre)

Keywords:

capacitively coupled plasma discharge under RF and DC voltage in 2D cylindrical system.

Problem description

The capacitively coupled plasma (CCP) is one of the most common types of industrial plasma sources. These plasma discharges typically take place between metal electrodes in a reaction chamber and are driven by a radio frequency (RF) or direct current (DC) power supply. The plasma is sustained by ohmic heating in the main body and stochastic heating through the capacitive sheath.

This example demonstrates the generation of a capacitively coupled plasma inside an axially symmetric reaction chamber with a 50 mm radius and 50 mm length. The top ($r = 0.050$ m) and right ($z = 0.050$ m) boundaries are grounded at zero potential. A target located at the bottom of the chamber (along the $z = 0$ boundary) is connected to a 60 MHz AC voltage source at 200 V. There is a small gap of 5 mm between the target and the grounded wall which is modeled via Neumann boundary conditions. The $r = 0$ boundary also invokes a floating potential using Neumann boundary conditions. The chamber is filled with a background gas of neutral Argon at about 0.005 Torr $\left(2.0 \times 10^{20}\ \mathrm{m}^{-3}\right)$. An initial spatially averaged electron and Ar+ density of $5 \times 10^{11}\ \mathrm{m}^{-3}$ is seeded to start the discharge. The particles are loaded with a density of $5 \times 10^{11}\ \mathrm{m}^{-3}$ every time step for the first 5000 time steps.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Capacitively Coupled Plasma 2D example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Capacitively Coupled Plasmas (text-based setup)* option.
- Select "2D Capacitive Plasma Chamber (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in figure Fig. 6.21.

Input File Features

The self-consistent electric field is solved from Poisson's equation by an electrostatic solver in cylindrical coordinates. Time-dependent Dirichlet boundary conditions are used to set up the boundaries of electric fields around the reaction chamber walls.

The plasma is simulated with macroparticles which are moved using the Boris pusher in cylindrical coordinates. Various types of elastic and inelastic collisions of the particles are calculated.

The Setup Window has various parameters available for easy manipulation including the density of the argon background gas (DENSITY_Ar), the voltage (VOLTAGE), and the frequency (FREQ).

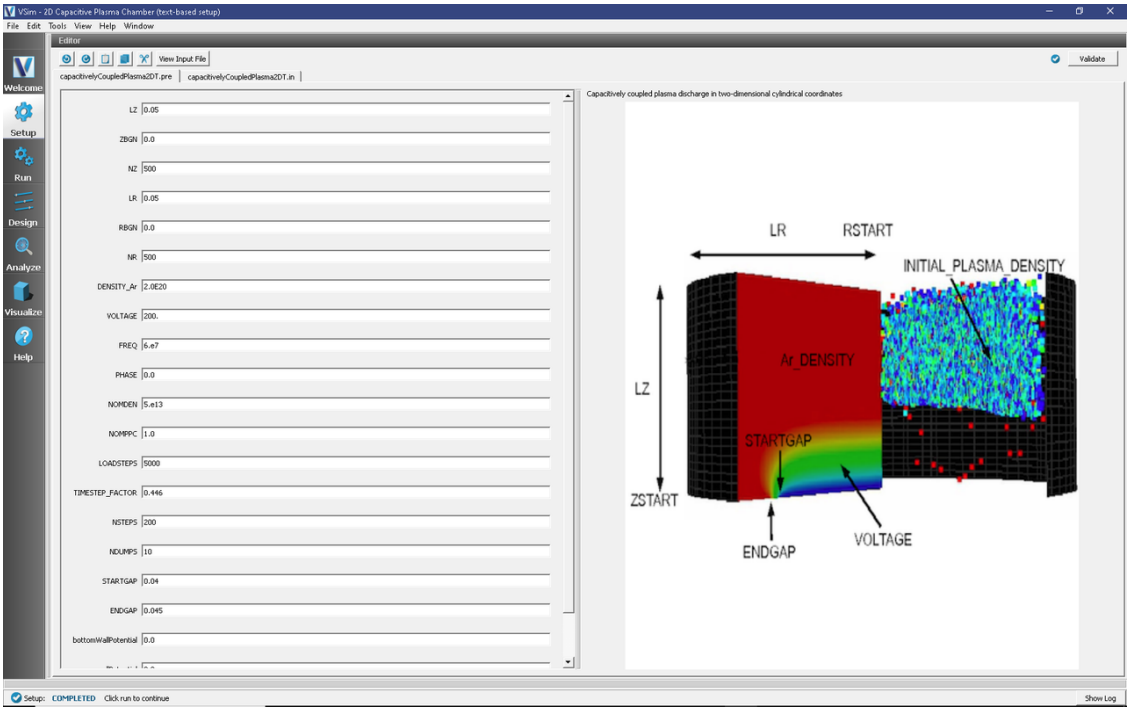


Fig. 6.21: Setup Window for the Capacitively Coupled Plasma 2D example.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.0002665506631895e-11
  - *Number of Steps*: 200
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.22.

Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by clicking the **Visualize** button in the left column of buttons.

To plot the potential:

- In the *Visualization Controls* pane, click on the *Data Overview* tab and expand *Scalar Data*
- Select *phi*
- Move the dump slider at the bottom of the *Visualization Results* pane to the right to move forward in time.

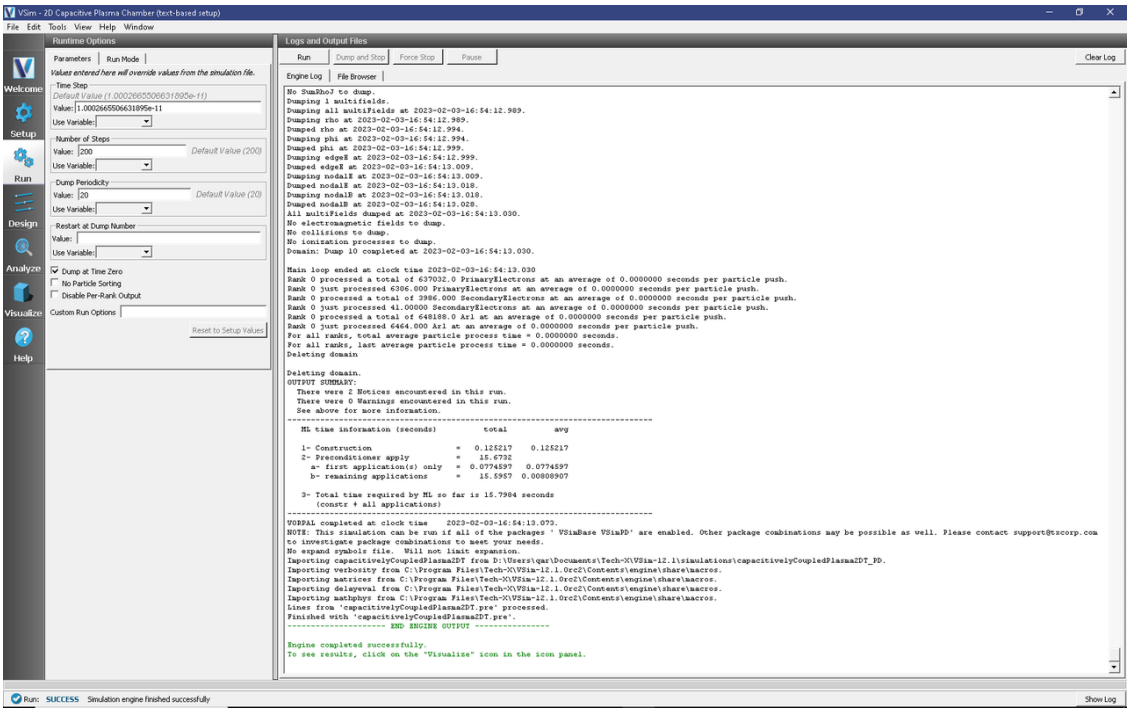


Fig. 6.22: The Run Window at the end of execution.

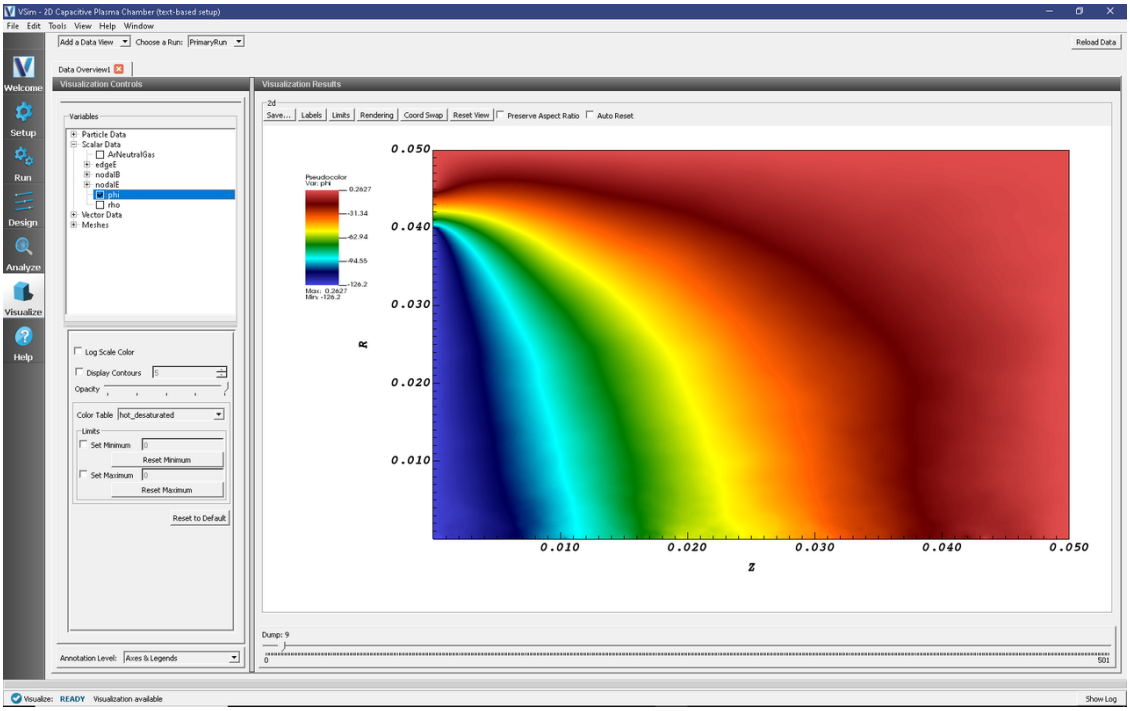


Fig. 6.23: Visualization of the electric potential in r-z coordinates.

Further Experiments

With a time-step of 10^{-11} seconds, running this simulation for the default 200 time-steps will only capture part of the first oscillation. With the frequency set to 6×10^7 Hz, the oscillation period is 1.667×10^{-8} seconds, which corresponds to 1,667 time-steps. To see the approximate steady-state behavior of this example, set the number of time-steps to 10,000 or more and restart or re-run the simulation. When running in parallel on 4 processors, this should take approximately two hours to complete.

After 5×10^{-8} seconds, or 5000 dumps, the plasma sheath starts to exhibit oscillating steady-state behavior. To view the behavior of the oscillating plasma sheath, take the following steps:

- In the *Data Overview* tab, expand *Scalar Data*
- Select *rho*
- At the top of the *Visualization Results* pane, click *Colors* to open the *Color Options* window
- Select "Fix Minimum" and set the minimum to `-0.0005`, then select "Fix Maximum" and set the Maximum to `0.0005` (or experiment with minimum and maximum values for best results) and click *OK*
- Move the dump slider at the bottom of the *Visualization Results* pane to dump 250.

After 250 time-steps, the plasma density should appear as shown in Fig. 6.24. The green areas at approximately zero charge density denote the quasi-neutral plasma bulk, while the red areas (positive charge density) denote the non-neutral plasma sheath.

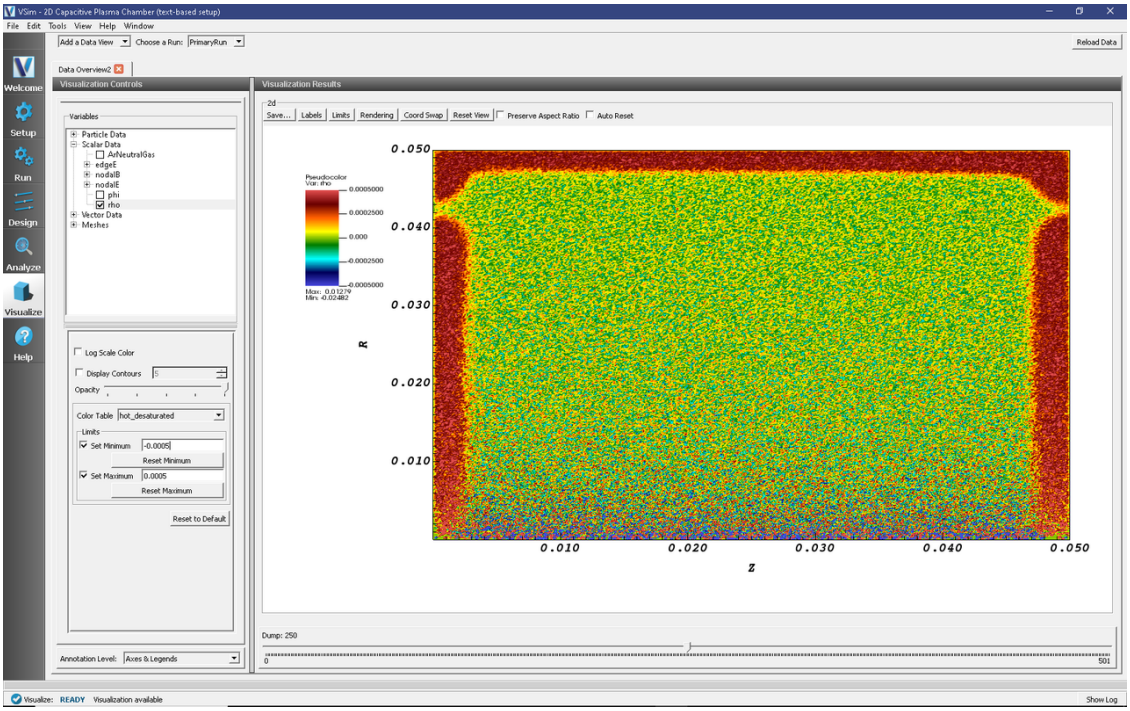


Fig. 6.24: Visualization of the plasma sheath via the charge density.

To view the plasma sheath potential profile, take the following steps:

- In the *Visualize* window, select *Field Analysis* from the *Add a Data View* drop-down menu
- In the *Field Analysis* tab, click on the *Fields* drop-down menu and select *phi*
- Under *Lineout Settings* click on the *Horizontal* tab, and change the intercept value if desired

- Click *Perform Lineout*

The electric potential as well as the axial potential profile should now be visible as shown in Fig. 6.25. Move the slider to the right to see how the plasma sheath potential oscillates in time.

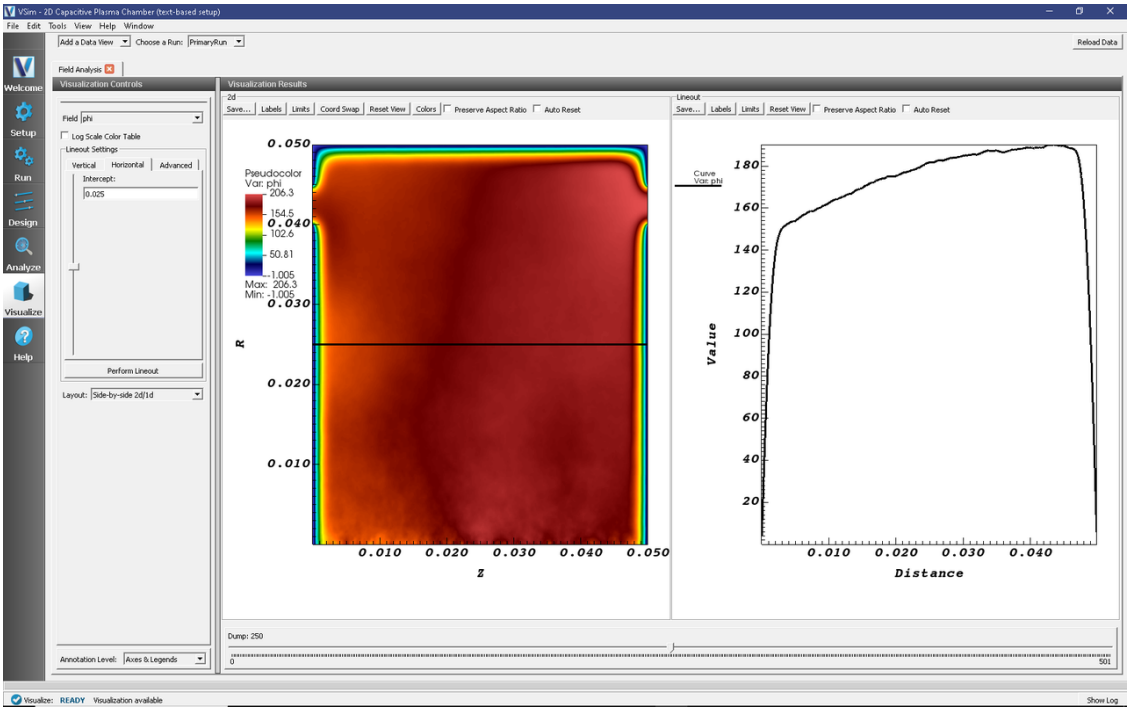


Fig. 6.25: Visualization of the plasma sheath via the charge density.

6.3 DC Plasmas

6.3.1 Drifting Electrons (driftingElectrons.sdf)

Keywords:

electron transport, electron mobility, monte carlo, electrostatic

Problem description

VSim may be used to model charged particles drifting in a background neutral gas. When charged particles, such as electrons, are injected into a background neutral gas, collisions between gas atoms and electrons eventually lead to thermal equilibrium, and electrons will reach the same temperature as the background gas. However, when an external electric field is applied across the neutral gas, the electron collisions and distribution will change due to this applied field. Electrons will gain energy from the applied electric field. The energy loss due to electron-atom collision is small, and most of the energy ends up heating the electrons. Assuming only elastic collisions take place between electrons and atoms, the electron mobility is defined as

$$\mu_e = \left(\frac{\pi\lambda}{2mE}\right)^{\frac{1}{2}}$$

which describes the relation between electron drifting velocity and applied electric field.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Electron Drifting example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *DC Plasmas* option.
- Select "Drifting Electrons" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 6.26.

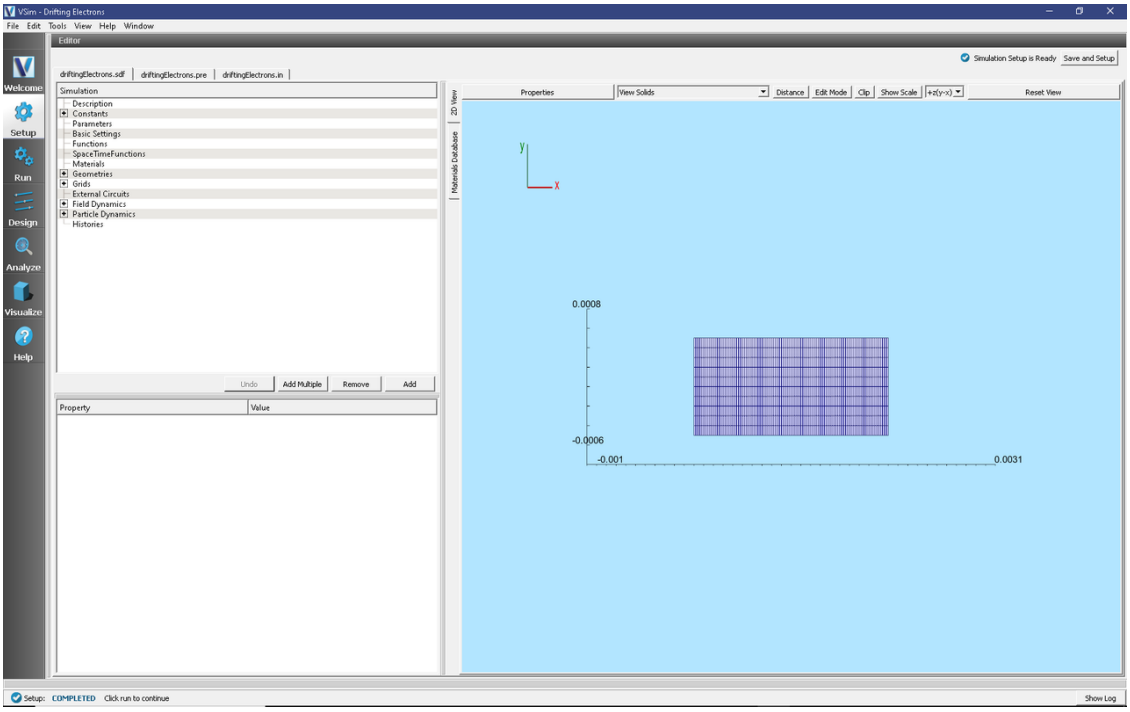


Fig. 6.26: Setup Window for the Electron Drifting example.

Simulation Properties

This input file contains electron as kinetic species as well as a background fluid description of a gas. Elastic collisions between kinetic particles and the background gas are described by Monte Carlo interaction blocks of kind impactIonization.

The fields are solved for electrostatically at each time step, including the fields due to all charged particles, subject to the boundary conditions specified in the input file. There are a number of histories that record the number of particles for electrons.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.53e-12
  - *Number of Steps*: 500
  - *Dump Periodicity*: 50
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.27.

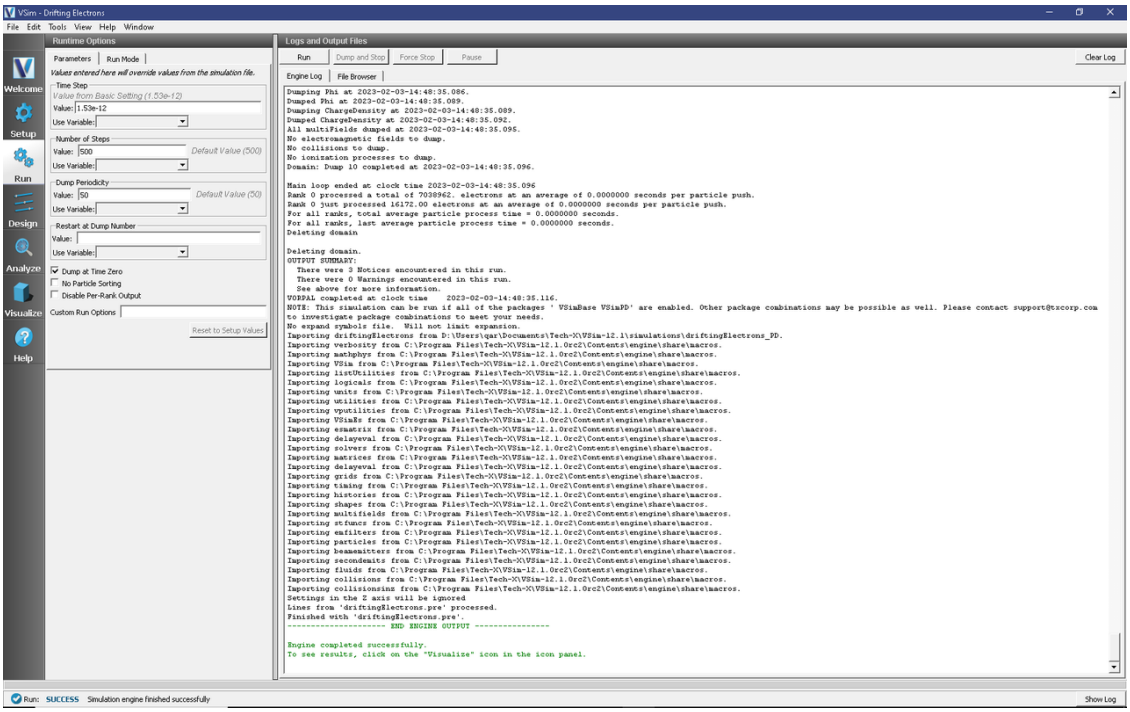


Fig. 6.27: The Run Window at the end of execution.

Visualizing the Results

After run completion, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the phase space distribution for the drifting electrons, select *Phase Space* from the drop down *Add a Data View* tab. This will open a new tab called *Phase Space*. In *Base Variable*, select *electrons*. Select *electrons_x* for *X-axis* and *electrons_ux* for *Y-axis*. Click *DRAW* and move the *Dump* slider to view electron accelerating and scattering when they drift over the space. The electron phase space at dump number 10 is shown in Fig. 6.28.

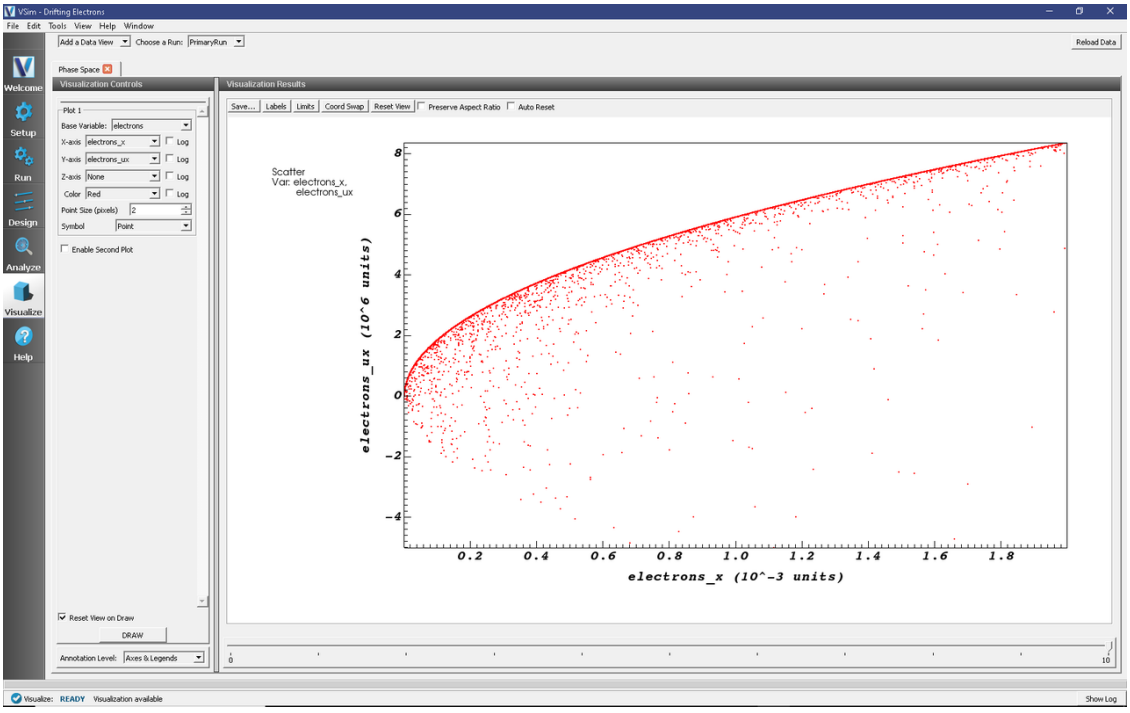


Fig. 6.28: Electron phase space at Dump 10.

Further Experiments

At lower applied electric fields, electrons are more collisional due to increased cross section. Try reducing the CATHODE_POTENTIAL, and observe more scattered electron distribution when drift over space.

At higher applied electric fields, not only elastic collisions, but also inelastic collisions will take place between electrons and atoms, which further reduce electron drifting velocity and mobility. For further experiments, try adding other collision types, such as excitation and ionization, and observe the effects to electron drifting velocity.

6.3.2 Langmuir Probe (langmuirProbe.sdf)

Keywords:

`electrostatics, particle in cell, sheath, box bounding, internal boundary`

Problem description

This example computes the fields and particles in a box, with an interior probe, modeled as a particle absorber and a constant-voltage (Dirichlet) boundary condition. There is an immobile, background neutralizing charge density. The electrons move to the walls and the probe, creating sheaths at all interfaces.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Langmuir Probe example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *DC Plasmas* option.
- Select "Langmuir Probe" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.29. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to Grid.

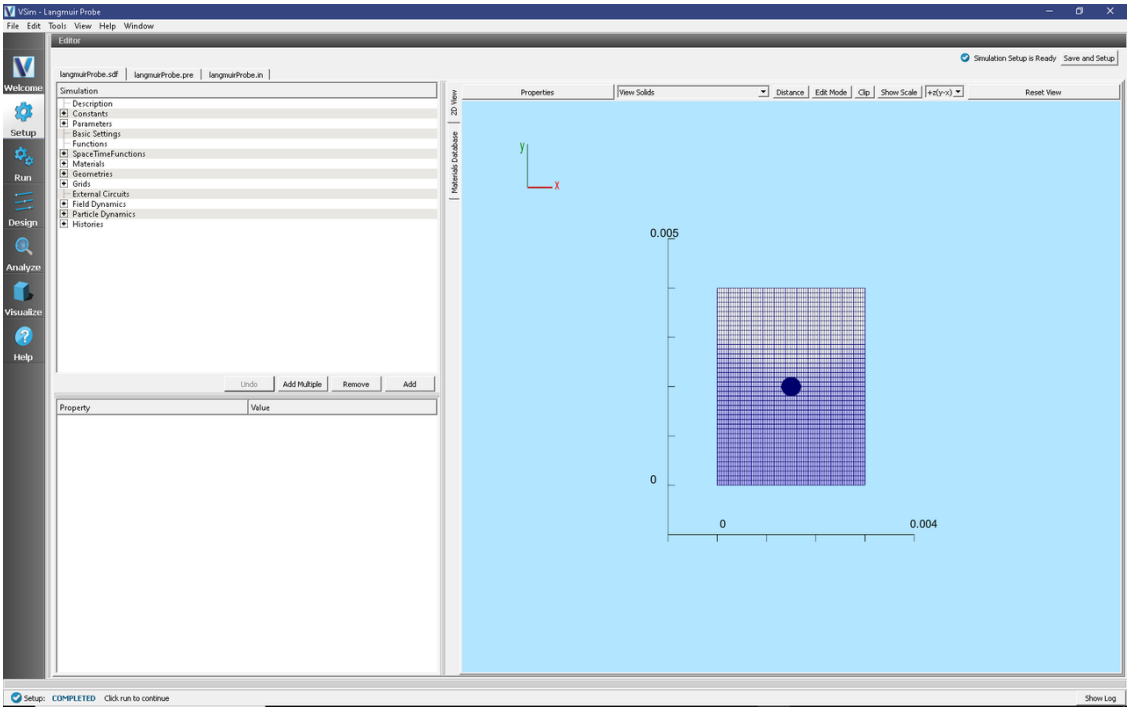


Fig. 6.29: Setup Window for the Langmuir Probe example.

Simulation Properties

Constants are set up to allow setting the electron temperature in eV (ELEC_TEMP_EV), the electron density (NOM_DENS_E), the number of cells (NCELLS_X, NCELLS_Y) in the x and y directions, the number of particles per cell (PPC), and the size of the simulation (LEN_X, LEN_Y) in the x and y directions.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3e-12
  - *Number of Steps*: 400
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.30.

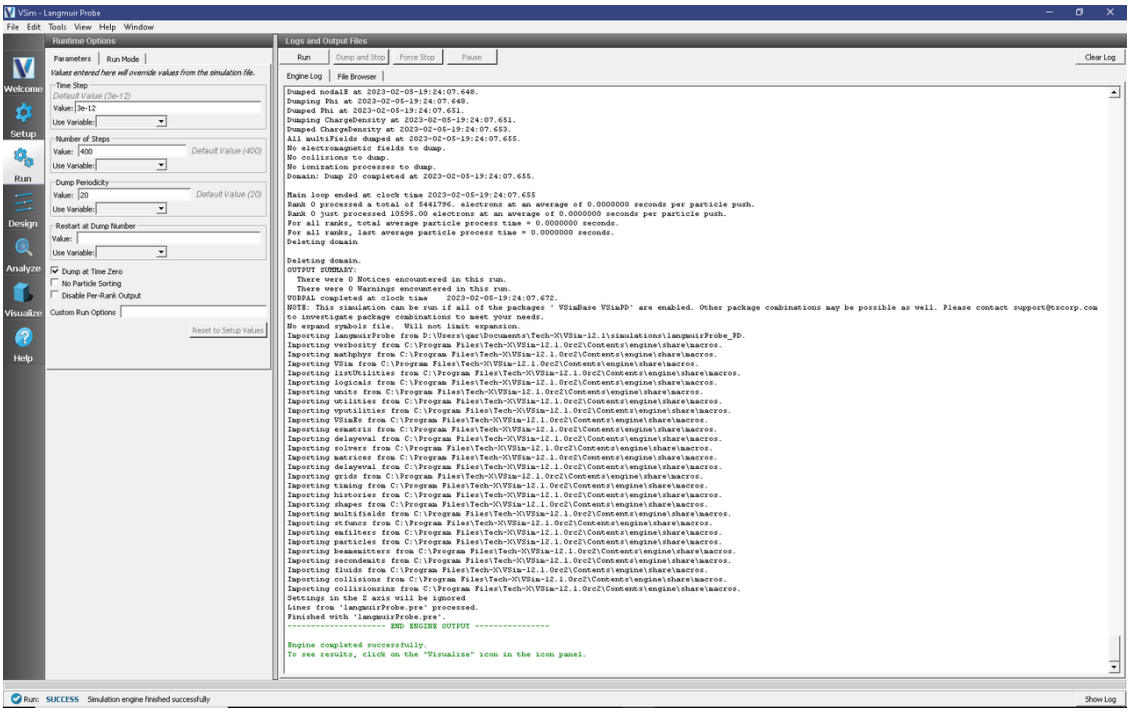


Fig. 6.30: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

To view the electric potential, expand *Scalar Data* in the *Data Overview* tab and select *Phi*. The potential in the visualization window resembles that shown in Fig. 6.31.

To view the electrons and sheaths, expand the *Particle Data*, expand *electrons* and select *electrons*. Move the dump slider forward in time to see the formation of the sheaths as seen in Fig. 6.32.

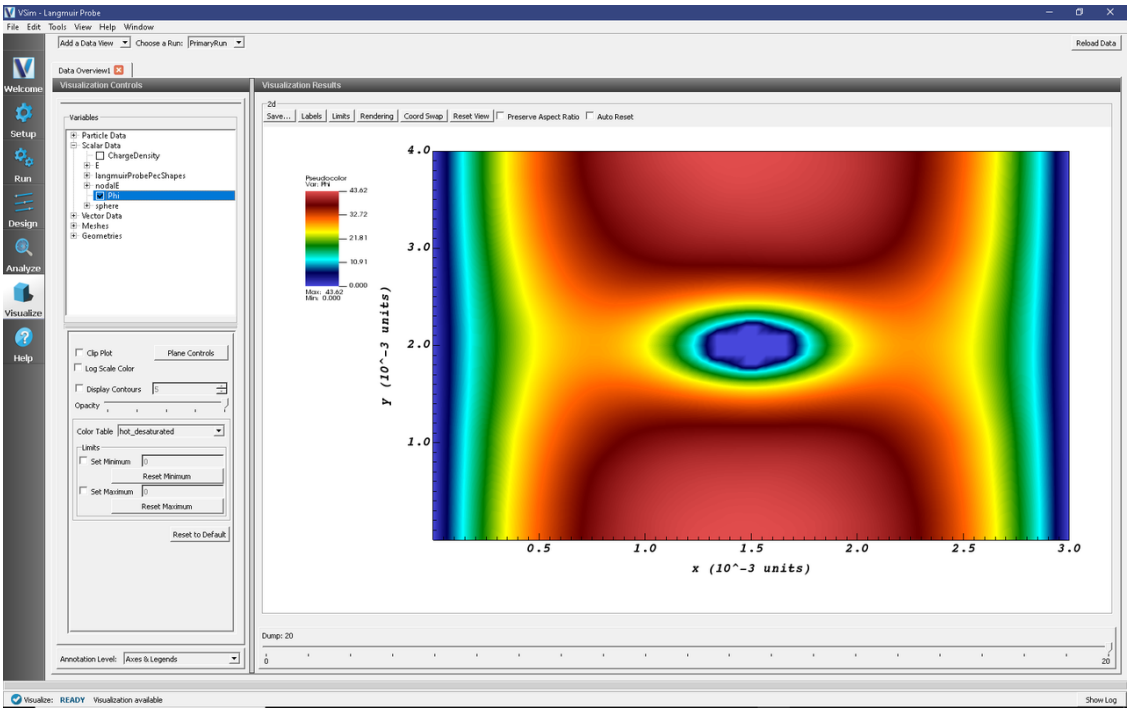


Fig. 6.31: The electrostatic potential

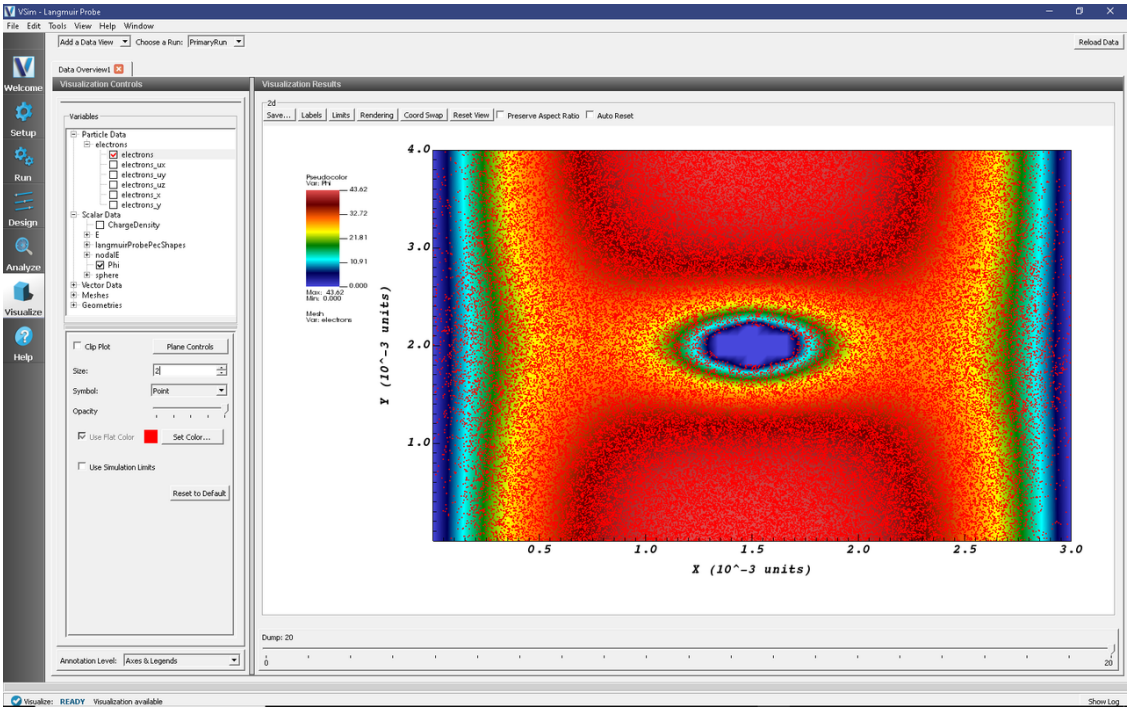


Fig. 6.32: The sheath formation

Further Experiments

Try adding in another geometry for inclusion of the support rod or try changing the geometry to represent a different probe.

6.4 Inductively Coupled

6.4.1 2D Inductively Coupled Plasma Chamber (icpCyl.sdf)

Keywords:

inductively coupled plasma, ICP, discharge, steady state

Problem Description

This VSimPD example illustrates how to simulate an inductively coupled plasma (ICP) in 2D cylindrical coordinates using the VSim Software. ICPs are one of the most common sources used to generate low temperature plasmas, and are extensively used in the semiconductor manufacturing industry. A typical ICP chamber has an antenna external to the plasma powered by an RF current. The plasma is sustained primarily through elecromagnetic induction.

Simulating an inductively coupled plasma is a complex problem. The plasma is electromagnetically driven and inherently three-dimensional. Ordinarily, kinetic modeling of these plasmas would require taking time steps to resolve the speed of light on the computational mesh. These issues are addressed in this example by using a proprietary 2D implicit electromagnetics solver to efficiently model the inductive power source.

This simulation can be run with a VSimPD license.

Opening the Simulation

The 2D Inductively Coupled Plasma Chamber (icpCyl.sdf) example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Inductively Coupled Plasmas* option.
- Select *2D Inductively Coupled Plasma Chamber* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 6.33.

Simulation Properties

This example contains many user defined *Constants* and *Parameters* which help simplify the setup and make it easier to modify. The following constants or parameters can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* or *Parameters* and all the constants or parameters used in the simulation will be displayed. To add your own constant or parameter, right click on *Constants* or *Parameters* and left click on *Add User Defined*. Below is an explanation of a few of the constants and parameters used. There are several more constants and parameters included in the simulation.

- **I0_RF**: Amplitude of RF current source (A)

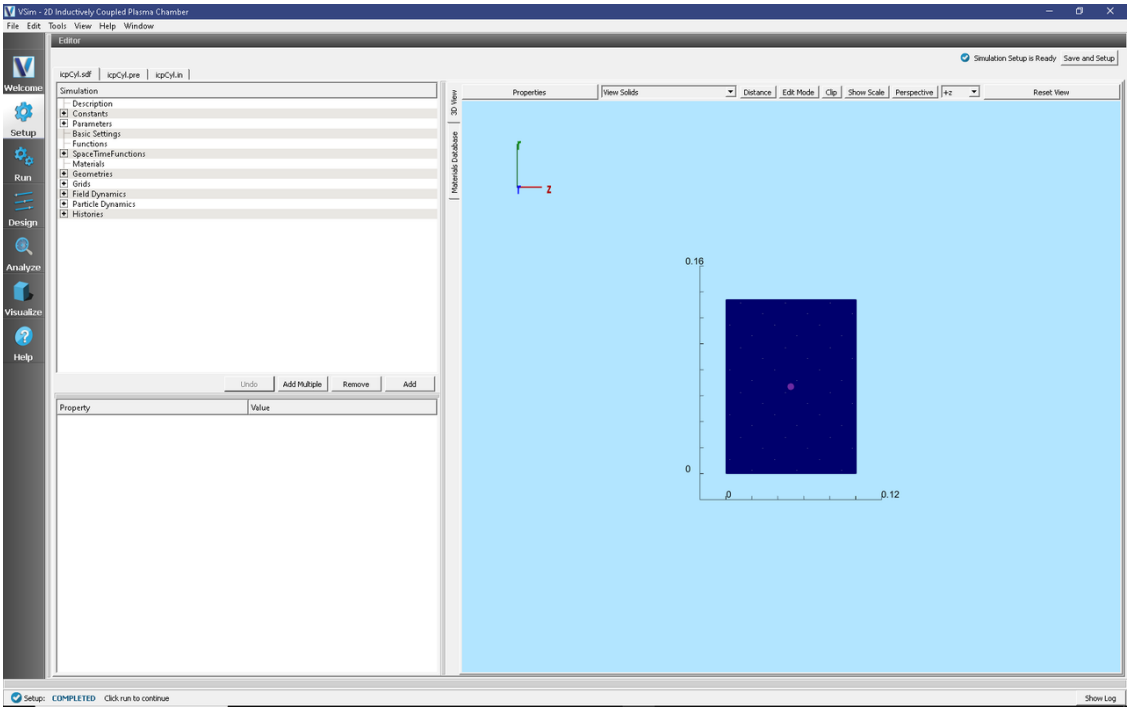


Fig. 6.33: Setup Window for the icpCyl example.

- **RF_VOLTAGE**: Amplitude of RF voltage source (V)
- **RF_FREQUENCY**: Frequency of the RF sources, same frequency used for current and voltage sources
- **NDENS**: Initial plasma density (#/m^3)
- **BGNZ_ANTENNA, ENDZ_ANTENNA, BGNR_ANTENNA, ENDR_ANTENNA**: Location of the antenna in spatial coordinates.
- **NEUTRALN**: Number density of neutral background gas. This determines the mean free path.

There are also many *SpaceTimeFunctions* (*STFunc*) defined in this example. *BIAS_VOLTAGE* and *RFsourceSTFuncJ0* are the space-time functions which set the sinusoidal bias voltage and current sources respectively. Note that *RFsourceSTFuncJ0* is more complex than *BIAS_VOLTAGE* to give a smooth ramp for stability.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.218289085545724e-11
  - *Number of Steps*: 800
  - *Dump Periodicity*: 40
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.34.

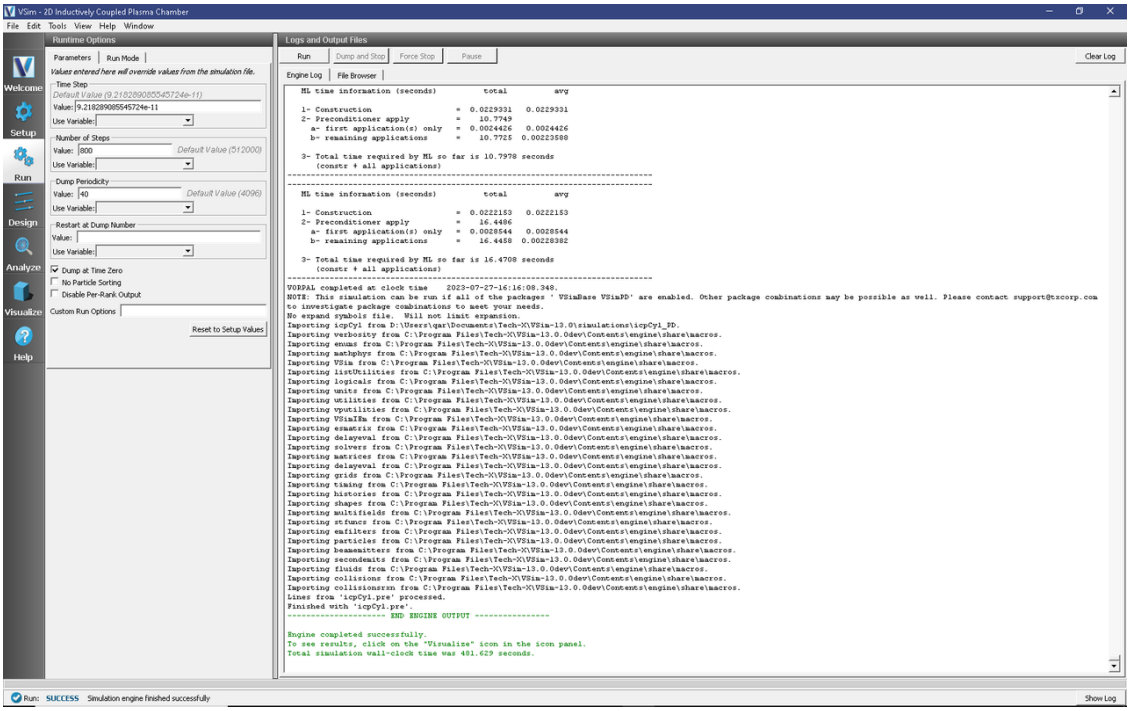


Fig. 6.34: The Run Window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Click on the *Add a Data View* dropdown menu and select *Field Analysis*.
- A new tab called *Field Analysis1* should automatically open.
- In the *Visualization Controls* pane, select the field for analysis, e.g. E_theta.
- Perform a lineout by clicking on the *Horizontal* button and set the intercept to 0.067.
- Click the *Perform Lineout* button and move the *Dump* silder to progress through time.

The resulting visualization is shown in Fig. 6.35 for dump 20.

To visualize the electric potential:

- Go to the *Field Analysis1* tab.
- In the *Visualization Controls* pane, select a different field for analysis, this time Phi, the electric potential.
- Perform a lineout by clicking on the *Horizontal* button and set the intercept to 0.067.
- Click the *Perform Lineout* button and move the *Dump* silder to progress through time.

The resulting visualization is shown in Fig. 6.36 for dump 20.

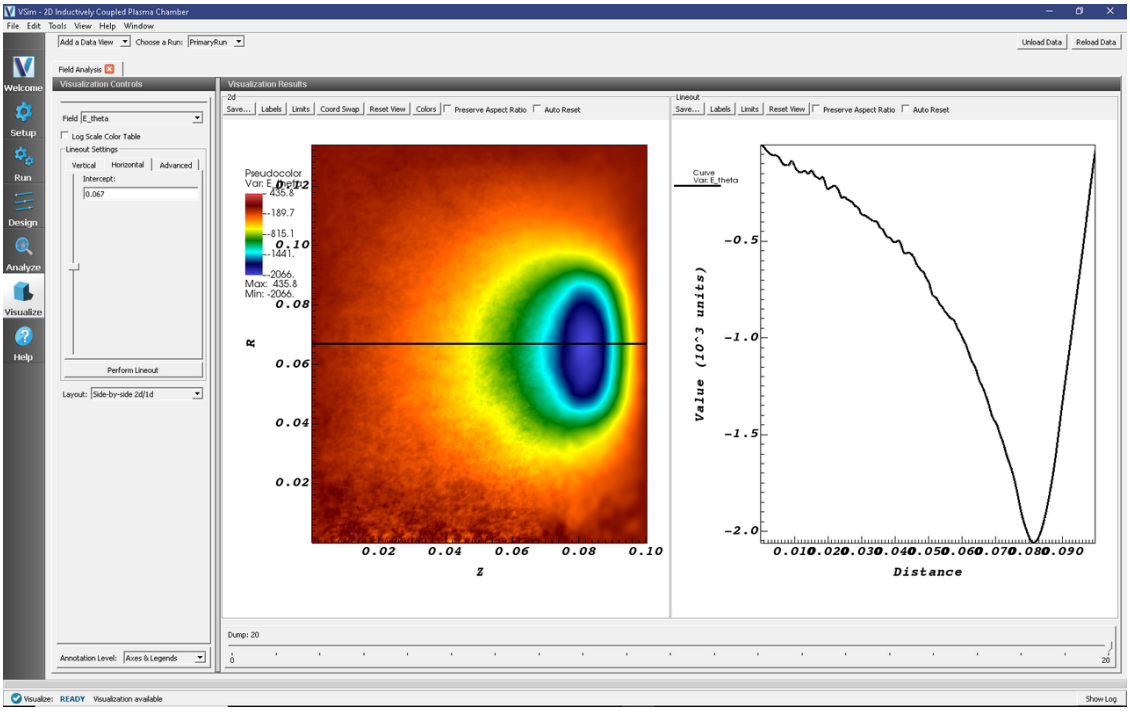


Fig. 6.35: The azimuthal electric field (E_theta) with a lineout at R = 0.067. Magnitude of the electric field is largest in the current source (antenna) and decays into the plasma as power is absorbed.

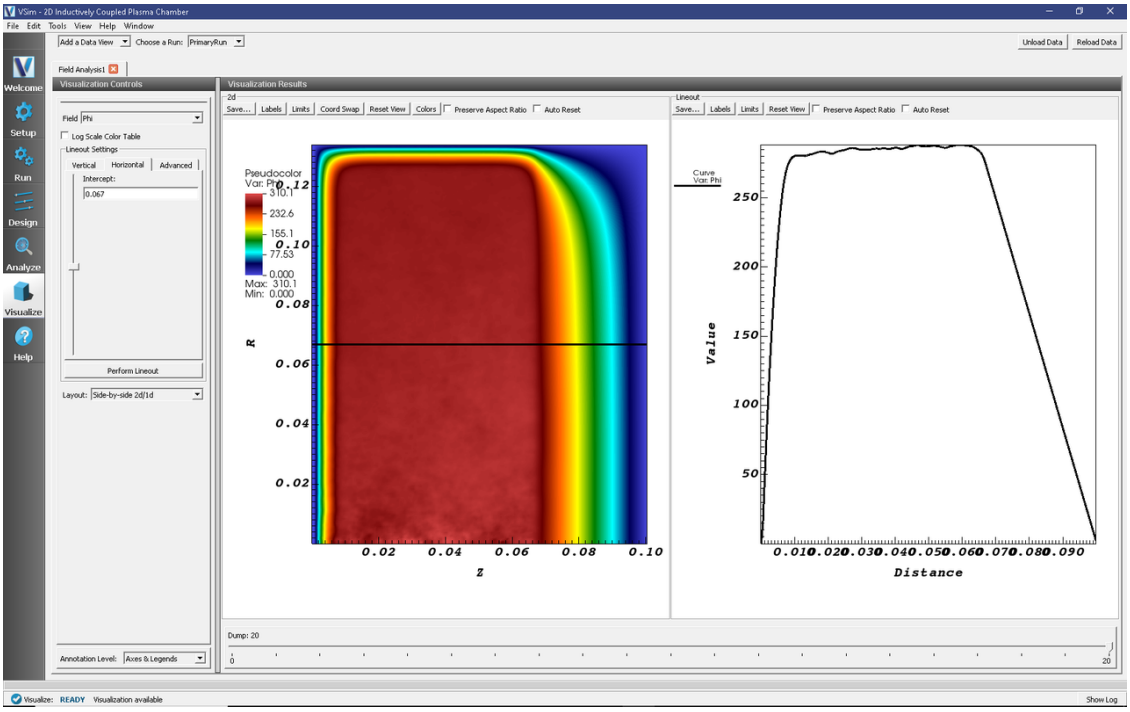


Fig. 6.36: The electric potential field (Phi) with a lineout at R = 0.067. Sheaths form at the plasma/material boundary surfaces.

Addition of Bias Voltage

Many inductively coupled plasmas also feature an RF bias, which is simple to add using VSimPD.

- Return to the *Setup* tab.
- Under the *Simulation* window, expand the *Parameters* menu.
- Under *Parameters*, select **RF_VOLTAGE** and change the *expression* from 0. to 100.
- Click *Save and Setup*
- Rerun the simulation by going to the *Run* tab and clicking the *Run* button.

The resulting visualization is shown in Fig. 6.37 for dump 20.

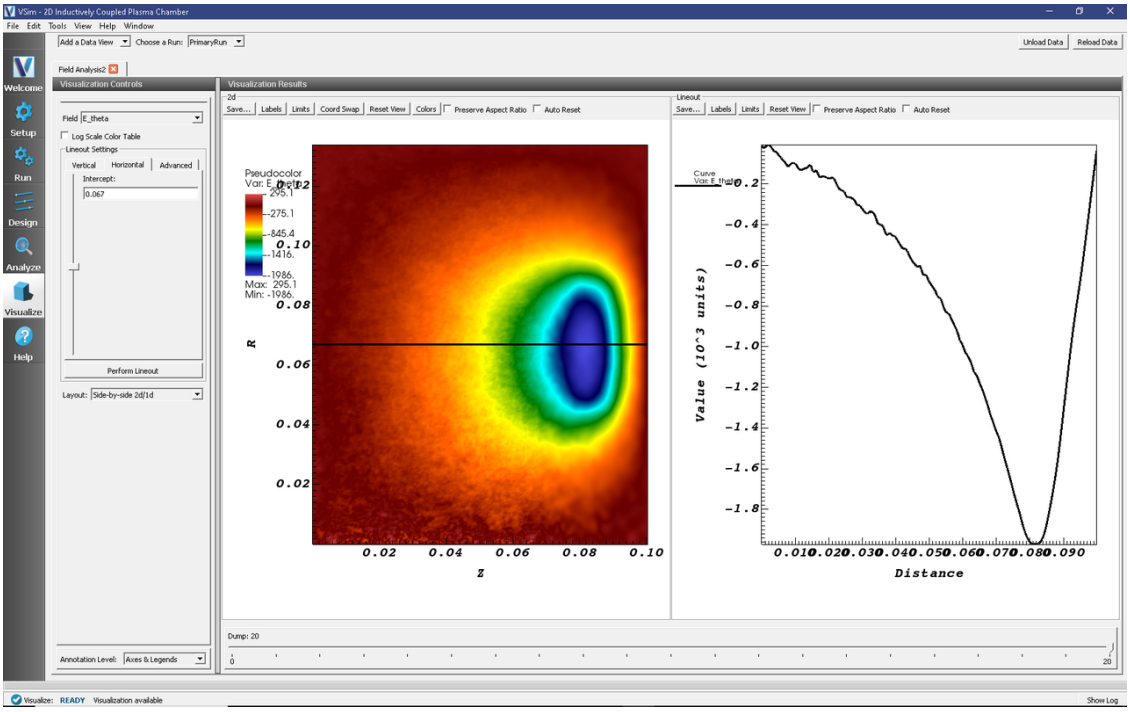


Fig. 6.37: The azimuthal electric field (E_theta) with a lineout at R = 0.067. Magnitude of the electric field is largest in the current source (antenna) and decays into the plasma as power is absorbed.

The resulting visualization is shown in Fig. 6.38 for dump 20.

The addition of an RF bias can improve the functionality of an ICP chamber by increasing the energy which ions hit surfaces (Reactive Ion Etching).

Further Experiments

Some of the easier parameters to modify are the **RF_VOLTAGE** and antenna current, **I0_RF**. However, it is important to note that the time step and necessary mesh resolution heavily depend on the plasma density for stability. Increasing the antenna current or rf bias voltage can greatly increase the plasma density leading to unstable simulations.

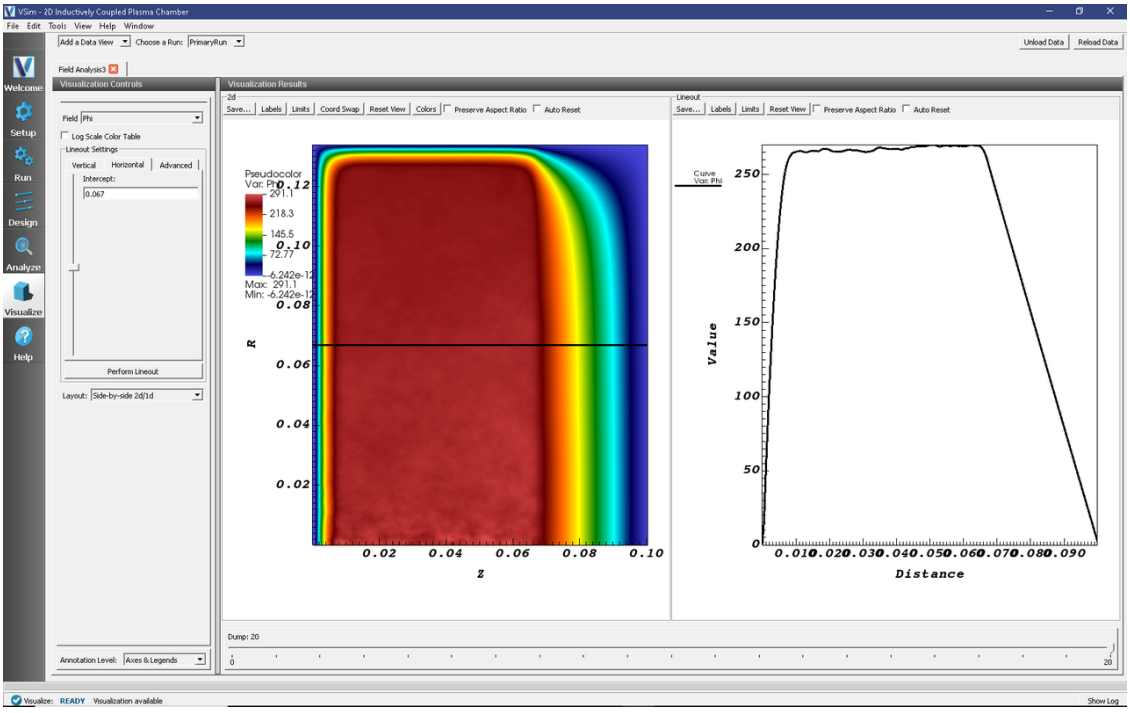


Fig. 6.38: The electric potential field (Phi) with a lineout at R = 0.067. Sheaths form at the plasma/material boundary surfaces.

6.4.2 2D Inductively Coupled Plasma Chamber With Shapes (icpCylShapes.sdf)

Keywords:

inductively coupled plasma, ICP, discharge, steady state

Problem Description

This VSimPD example illustrates how to simulate an inductively coupled plasma (ICP) in 2D cylindrical coordinates using the VSim Software. ICPs are one of the most common sources used to generate low temperature plasmas, and are extensively used in the semiconductor manufacturing industry. A typical ICP chamber has an antenna external to the plasma powered by an RF current. The plasma is sustained primarily through elecromagnetic induction.

Simulating an inductively coupled plasma is a complex problem. The plasma is electromagnetically driven and inherently three-dimensional. Ordinarily, kinetic modeling of these plasmas would require taking time steps to resolve the speed of light on the computational mesh. These issues are addressed in this example by using a proprietary 2D implicit electromagnetics solver to efficiently model the inductive power source.

This example is an extension of the 2D Inductively Coupled Plasma Chamber, icpCyl.sdf, with the addition of complex material boundary conditions (Shapes) to better define the simulation.

This simulation can be run with a VSimPD license.

Opening the Simulation

The 2D Inductively Coupled Plasma Chamber with Shapes (icpCylShapes.sdf) example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Inductively Coupled Plasmas* option.
- Select *2D Inductively Coupled Plasma Chamber with Shapes* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 6.39.

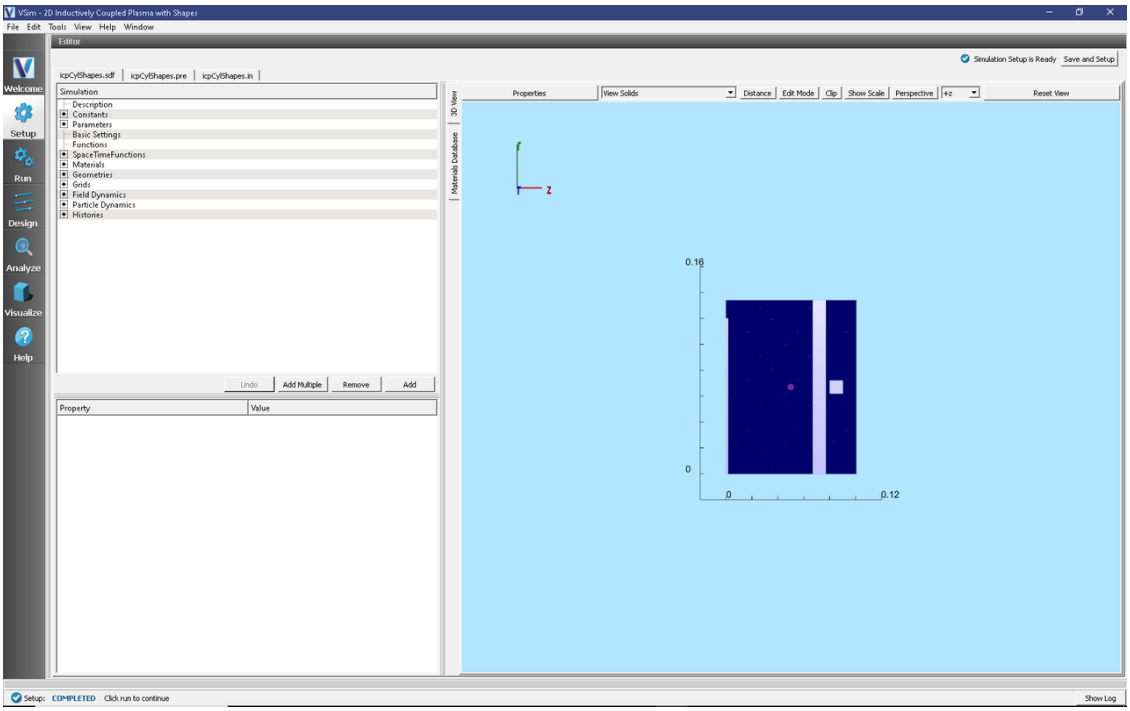


Fig. 6.39: Setup Window for the icpCylShapes example.

Simulation Properties

This example contains many user defined *Constants* and *Parameters* which help simplify the setup and make it easier to modify. The following constants or parameters can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* or *Parameters* and all the constants or parameters used in the simulation will be displayed. To add your own constant or parameter, right click on *Constants* or *Parameters* and left click on *Add User Defined*. Below is an explanation of a few of the constants and parameters used. There are several more constants and parameters included in the simulation, but will not be discussed here for brevity.

- **`I0_RF`**: Amplitude of RF current source (A)
- **`RF_VOLTAGE`**: Amplitude of RF voltage source (V)
- **`RF_FREQUENCY`**: Frequency of the RF sources, same frequency used for current and voltage sources
- **`NDENS`**: Initial plasma density (#/m^3)

- **NEUTRALN**: Number density of neutral background gas. This determines the mean free path.
- **BGNZ_ANTENNA, ENDZ_ANTENNA, BGNR_ANTENNA, ENDR_ANTENNA**: Location of the antenna in spatial coordinates.
- **antLength, antWidth, antXPOS, antYPOS**: Parameters used to define CSG geometry position of antenna.

There are also many *SpaceTimeFunctions* (*STFunc*) defined in this example. *BIAS_VOLTAGE* and *RFsourceSTFuncJ0* are the space-time functions which set the sinusoidal bias voltage and current sources respectively. Note that *RFsourceSTFuncJ0* is more complex than *BIAS_VOLTAGE* to give a smooth ramp for stability.

This example contains 6 specified CSG Geometries, corresponding to a wafer (Silicon dielectric), focusRing (Alumina dielectric), groundShield (Perfect Electric Conductor (PEC)), window (dielectric modeled as bottle glass), antenna (PEC), and biasElectrode (PEC).

These CSG Geometries are defined within VSimComposer by specifying four parameters: Length, Width, XPOS, and YPOS. The type of material needs to also be set. Voltages can be specified on PEC materials as a FieldBoundaryConditions under the Field Dynamics drop down menu. This has been done in icpCylShapes.sdf as dirichletBias - an Electrostatic Dirichlet boundary condition, set to the *STFunc BIAS_VOLTAGE* for the shape surface object named 'biasElectrode'.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.218289085545724e-11
  - *Number of Steps*: 1600
  - *Dump Periodicity*: 40
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.40.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list of *Available Analyzers*, select *computeAED.py*
- The analyzer fields should be filled as below:
  - simulationName :: icpCylShapes [string]
  - speciesName :: He1 [string]
  - startTime :: 7.374631e-08 [float]
  - endTime :: 1.474926e-07 [float]
  - lowerPos :: 0.001 [float]
  - upperPos :: 0.1 [float]

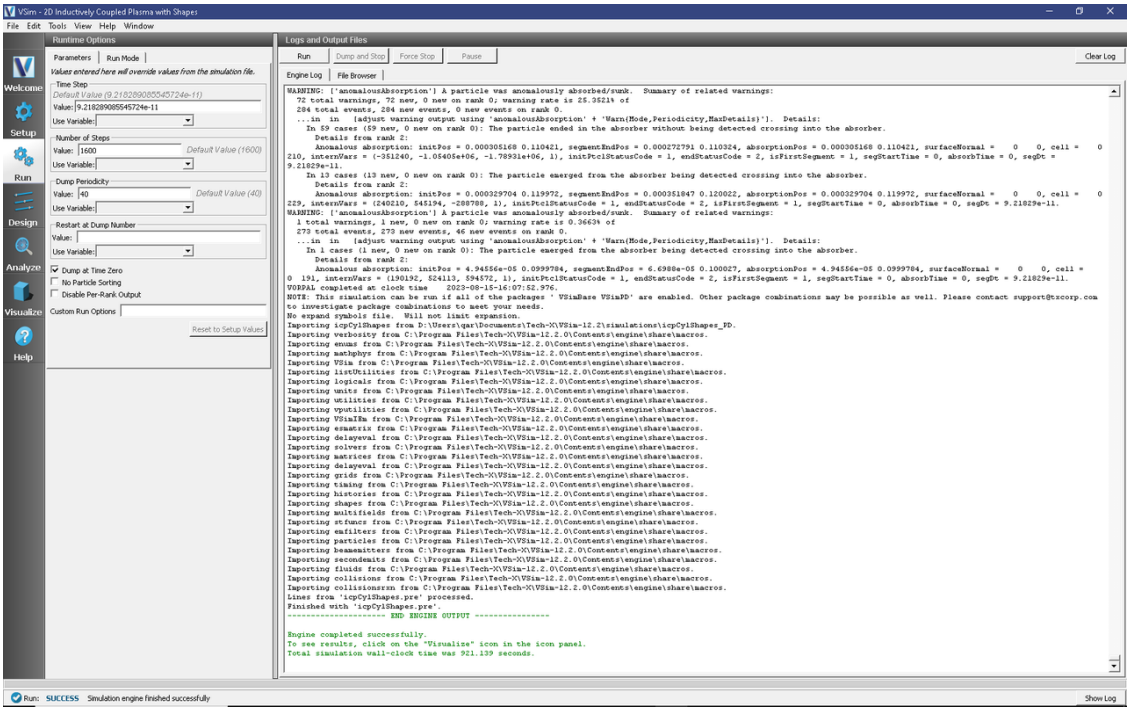


Fig. 6.40: The Run Window at the end of execution.

  - historyName :: computeAEDHe1 [string]
  - numEnergyBins :: 50 [int]
  - numAngleBins :: 50 [int]
  - lowerEnergy :: 0 [float]
  - upperEnergy :: 130 [float]
  - lowerAngle :: -10 [float]
  - upperAngle :: 10 [float]
  - NDIM :: 2 [int]
  - perpDir :: +z [string]
  - normTan :: False [bool]
  - compMajorC :: False [bool]
  - overwrite :: True [bool]

- Click *Analyze* in the top right corner.
- The analsis is completed when you see the output shown in successfully." This is shown in Fig. 6.41.

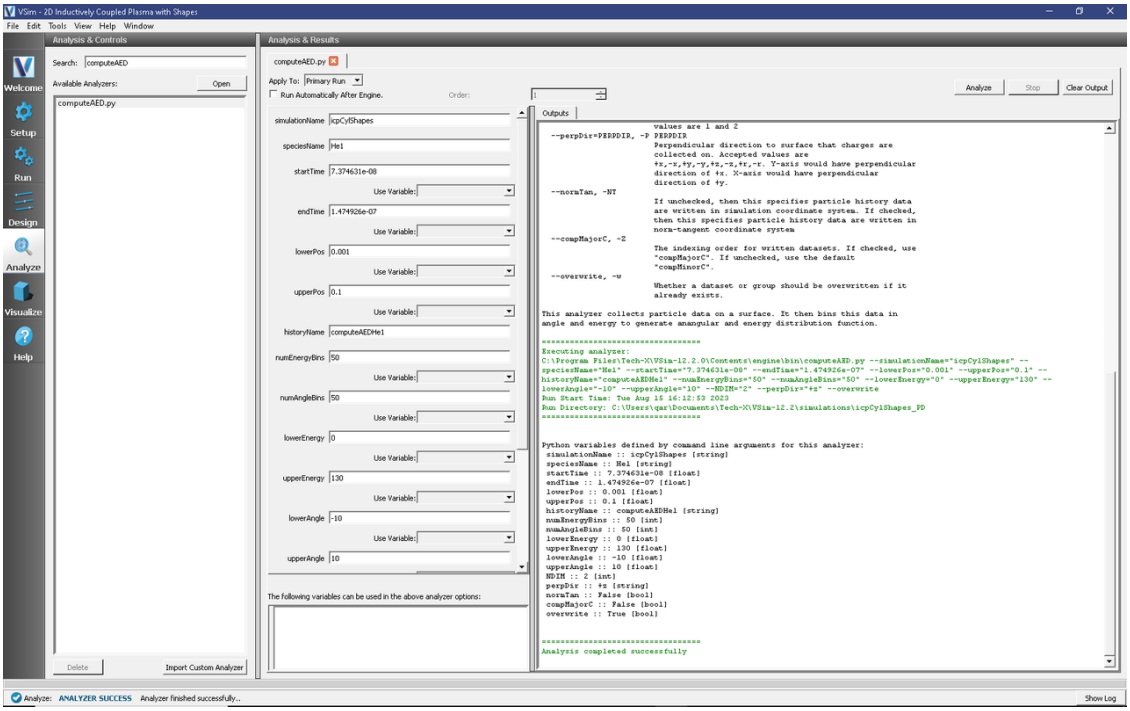


Fig. 6.41: The Analysis Window at the end of execution.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Click on the *Add a Data View* dropdown menu and select *Data Overview*.
- A *Data Overview* tab should open, if not already present.
- In the *Visualization Controls* pane, we can select variables for analysis.
- View the shapes that are in the simulation by expanding the *Geometries* menu, and selecting the desired shapes to be drawn (poly (antenna), poly (biasElectrode), poly (focusRing), poly (groundShield), poly (wafer), and poly (window)).
- Expand the *Scalar Data* menu, expand *E*, and select *E_theta* to plot the induced azimuthal electric field.
- Expand the *Particle Data* menu, expand the *electrons* menu, and select *electrons_uphi* for plotting.

The resulting visualization is shown in Fig. 6.42 for dump 40.

Additional analysis of the simulation results can be performed as follows:

- From the Visualize Window, click on the *Add a Data View* dropdown menu and select *Field Analysis*.
- A new tab called *Field Analysis1* should automatically open.
- In the *Visualization Controls* pane, select the field for analysis, e.g. E_theta.
- Perform a lineout by clicking on the *Horizontal* button and set the intercept to 0.067.
- Click the *Perform Lineout* button and move the *Dump* silder to progress through time.

The resulting visualization is shown in Fig. 6.43 for dump 40.

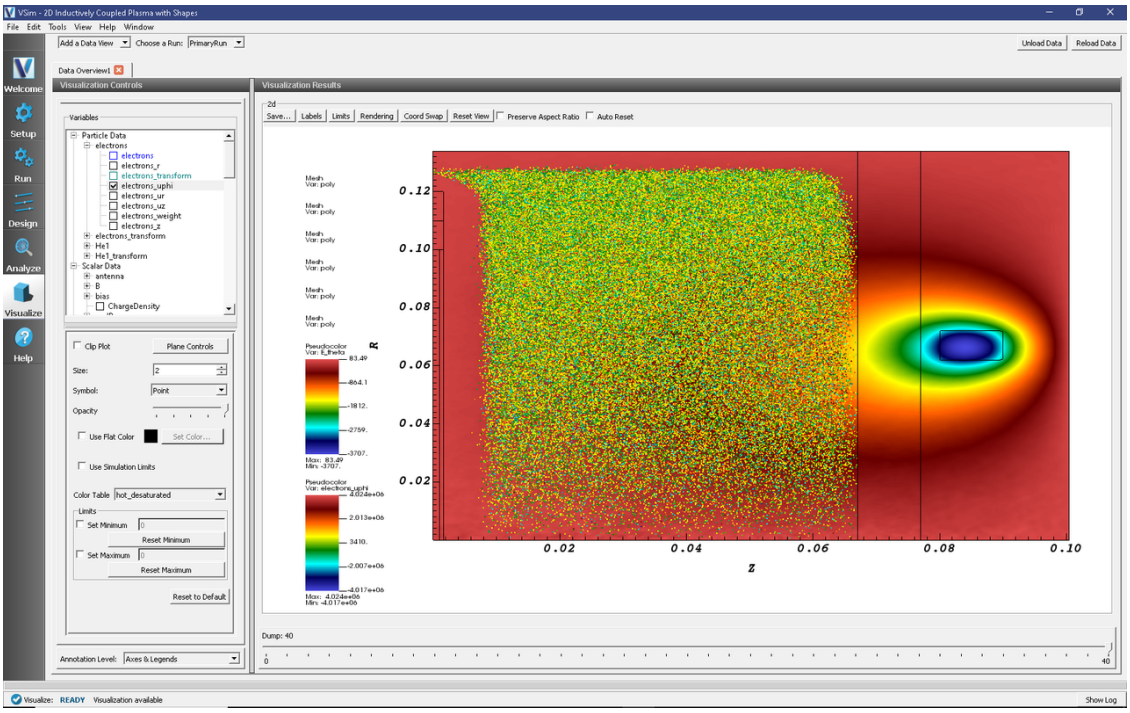


Fig. 6.42: The azimuthal electric field (E_theta) with electron particle data. Magnitude of the electric field is largest in the current source (antenna) and decays into the plasma as power is absorbed. Electrons are colored by azimuthal velocity.

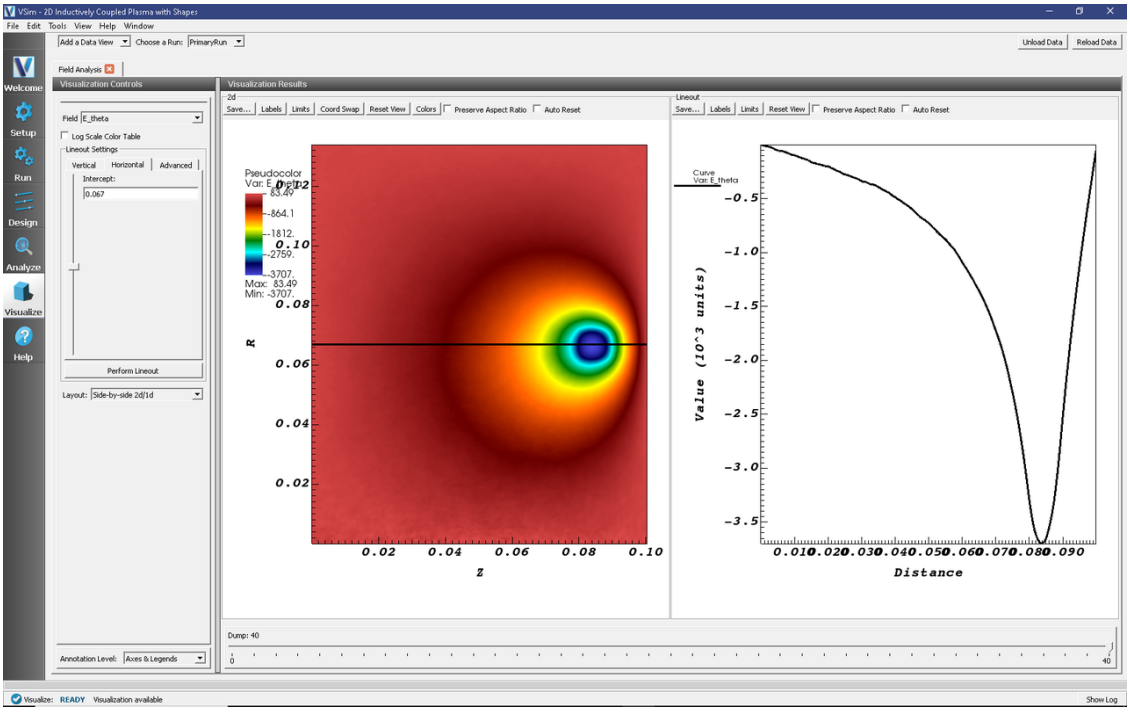


Fig. 6.43: The azimuthal electric field (E_theta) with a lineout at R = 0.067. Magnitude of the electric field is largest in the current source (antenna) and decays into the plasma as power is absorbed.

To visualize the electric potential:

- Go to the *Field Analysis1* tab.
- In the *Visualization Controls* pane, select a different field for analysis, this time Phi, the electric potential.
- Perform a lineout by clicking on the *Horizontal* button and set the intercept to 0.067.
- Click the *Perform Lineout* button and move the *Dump* silder to progress through time.

The resulting visualization is shown in Fig. 6.44 for dump 35.

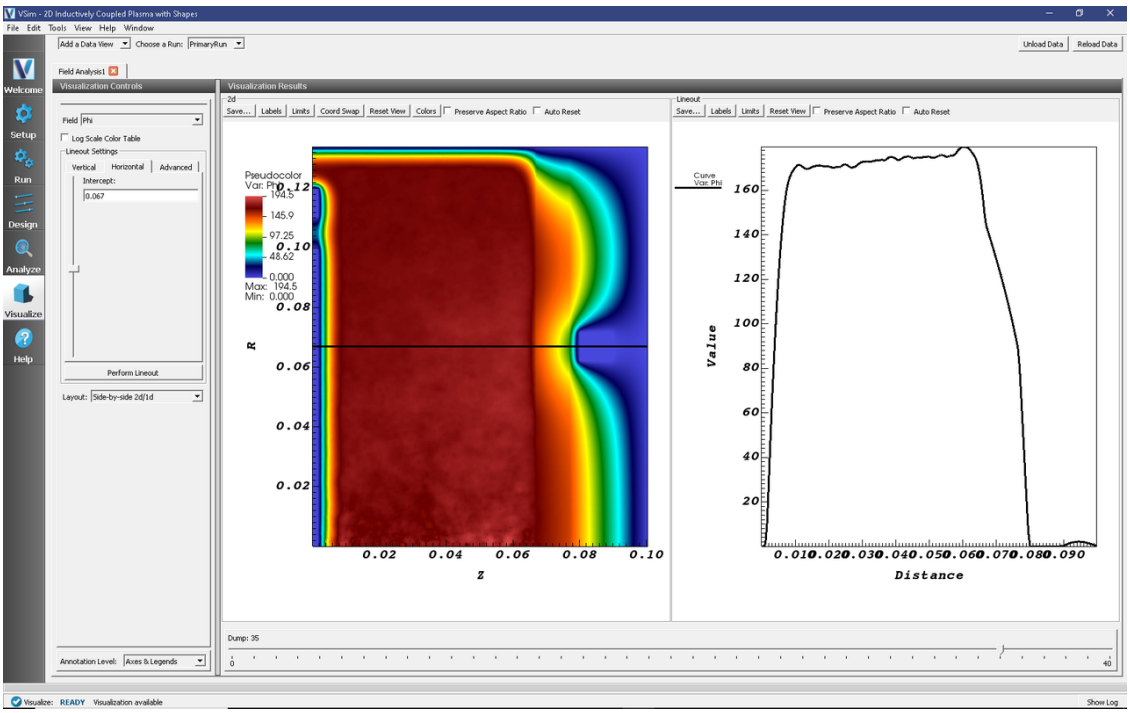


Fig. 6.44: The electric potential field (Phi) with a lineout at R = 0.067. Sheaths form at the plasma/material boundary surfaces.

Additional data from the simulation was saved as a history file, and can also be viewed:

- From the Visualize Window, click on the *Add a Data View* dropdown menu and select *History*.
- A new tab called *History* should automatically open.
- In the *Visualization Results* pane, click the *Add Window* button to add a second window for plotting.
- In the top plotting pane, select the *Add Curve* button.
- In the drop down menu, pick the variable for plotting by selecting probePhi.
- In the lower plotting pane, select the *Add Curve* button.
- In the drop down menu, pick the variable for plotting by selecting probeE_2.

The resulting visualization is shown in Fig. 6.45.

The data generated by the computeAED.py Analyzer can also be visualized:

- From the Visualize Window, click on the *Add a Data View* dropdown menu and select *1-D Fields*.
- A new tab called *1-D Fields* should automatically open.
- In the *Visualization Results* pane, click the *Add Window* button to add a second window for plotting.

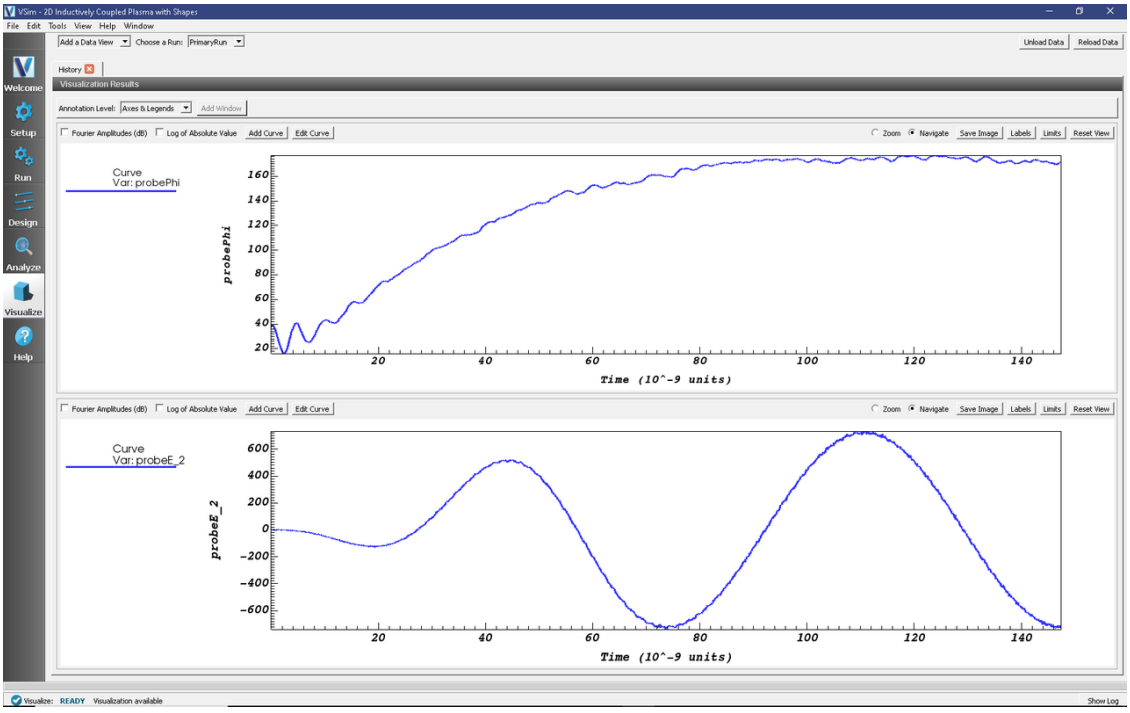


Fig. 6.45: A time-history of the electric potential (Phi) and the azimuthal electric field at a probe position Z = 0.05 m, R = 0.067 m.

- In the top plotting pane, select the *Add Curve* button.
- In the drop down menu, pick the variable for plotting by selecting *He1ED*.
- In the lower plotting pane, select the *Add Curve* button.
- In the drop down menu, pick the variable for plotting by selecting *He1AD*.

The resulting visualization is shown in Fig. 6.46.

Addition of Bias Voltage

Many inductively coupled plasmas also feature an RF bias, which is simple to add using VSimPD.

- Return to the *Setup* tab.
- Under the *Simulation* window, expand the *Parameters* menu.
- Under *Parameters*, select **RF_VOLTAGE** and change the *expression* from 0. to 100.
- Click *Save and Setup*
- Rerun the simulation by going to the *Run* tab and clicking the *Run* button.
- Plots of the new results can be regenerated following the prior instructions.

The visualization of the Etheta field is shown in Fig. 6.47 for dump 40.

The electric potential field is shown in Fig. 6.48 for dump 35.

The addition of an RF bias can improve the functionality of an ICP chamber by increasing the energy which ions hit surfaces (Reactive Ion Etching). Voltage for the antenna is set to 0. V, but an applied voltage can additionally be specified if values are known.

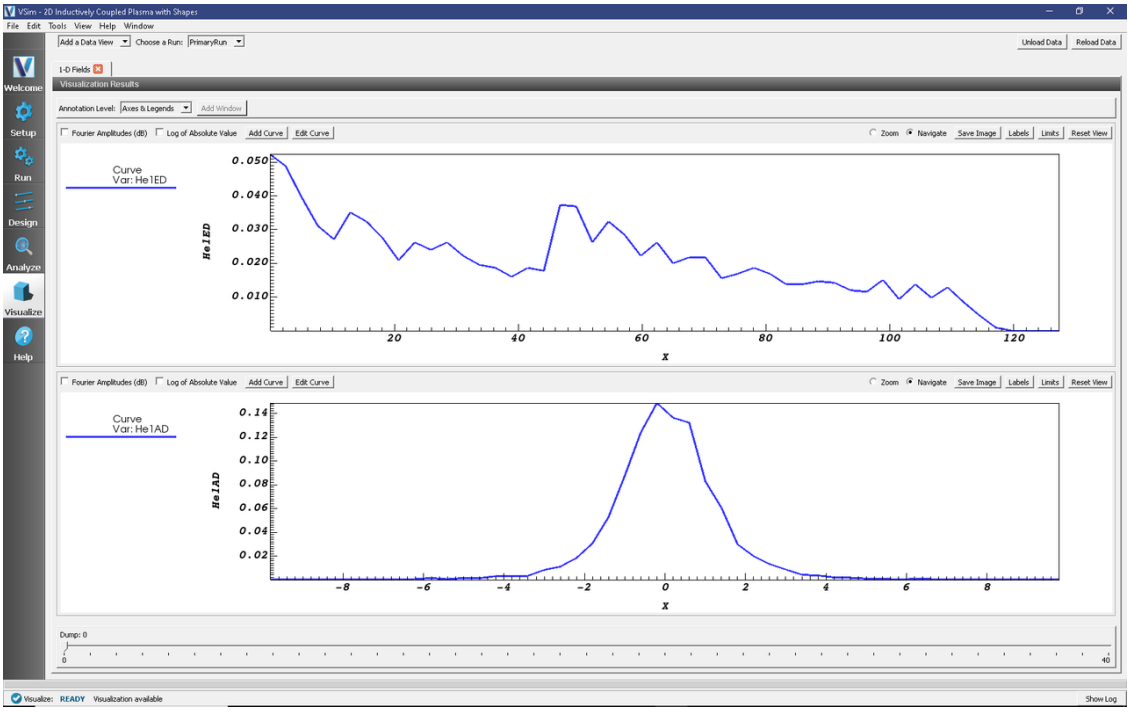


Fig. 6.46: Images of the Energy Distribution (Top) and the Anguluar Distribution (Bottom) of He1 ions impacting the wafer.

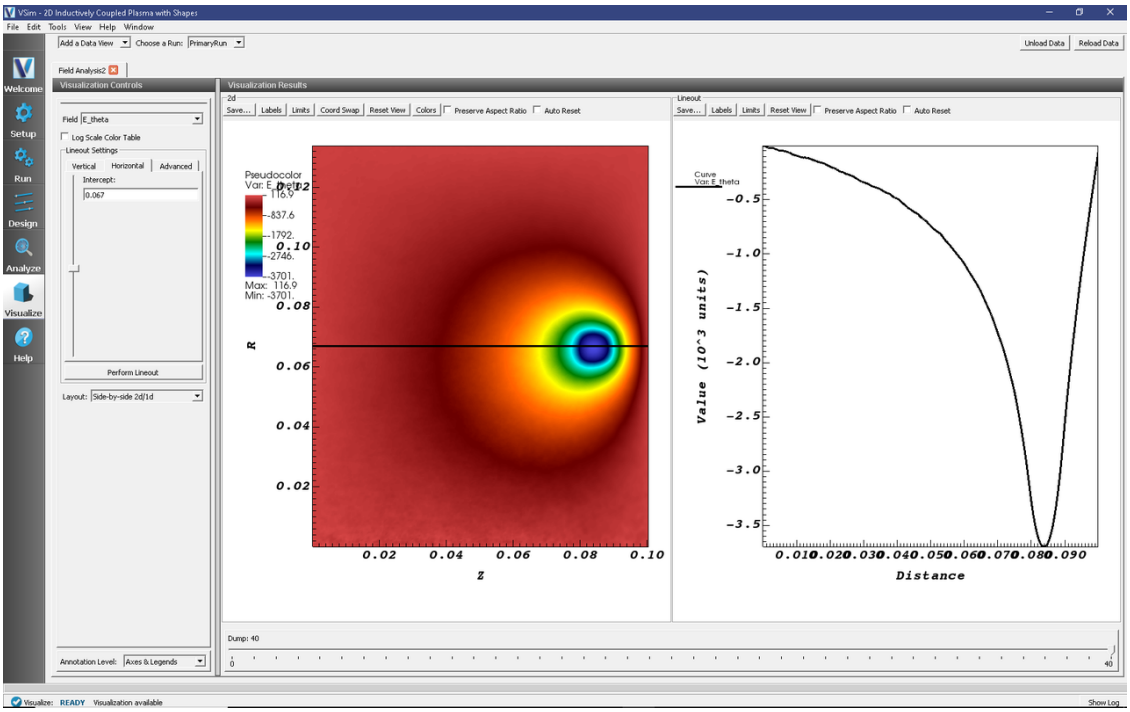


Fig. 6.47: The azimuthal electric field (E_theta) with a lineout at R = 0.067. Magnitude of the electric field is largest in the current source (antenna) and decays into the plasma as power is absorbed.

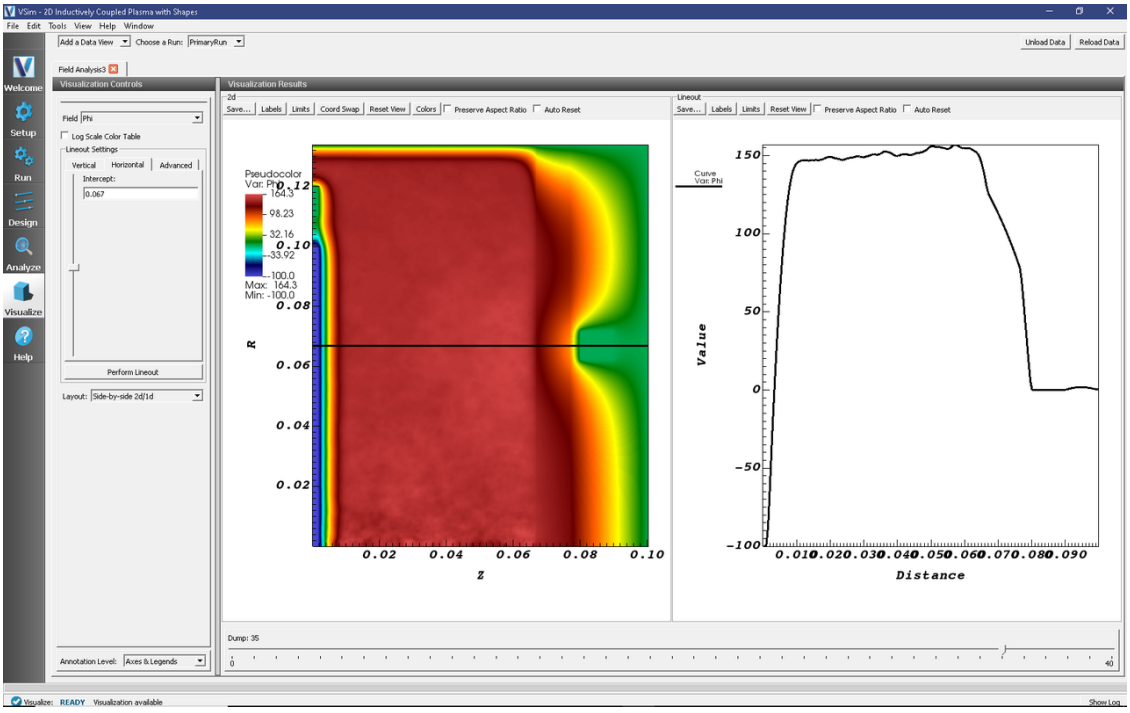


Fig. 6.48: The electric potential field (Phi) with a lineout at R = 0.067. Sheaths form at the plasma/material boundary surfaces. Dump 35 shows the RF voltage at a minimum, with the lineout showing the potential varying from -100 V on the lower Z boundary, increasing up to 150 V in the plasma, and decreasing inside the dielectrics to 0 V at the uppper Z boundary.

The probe at position Z = 0.05 m, R = 0.067 m can also give valuable information about the electrical characteristics of the plasma, and the time series plot is shown in Fig. 6.49.

Further Experiments

Some of the easier parameters to modify are the **RF_VOLTAGE** and antenna current, **I0_RF**. However, it is important to note that the time step and necessary mesh resolution heavily depend on the plasma density for stability. Increasing the antenna current or rf bias voltage can greatly increase the plasma density leading to unstable simulations.

An additional test is to change the placement of the antenna CSG geometry. The position can easily be seen by plotting the poly geometries after a single time-step. The position of the antenna will change where the maximum in the azimuthal E-field occurs, and change how the plasma density profile develops.

6.5 Ion Sources

6.5.1 Simple Ion Source (simpleIonSource.sdf)

Keywords:

coherent ion beam, electron emitters, electron-neutral collisions, plasma source

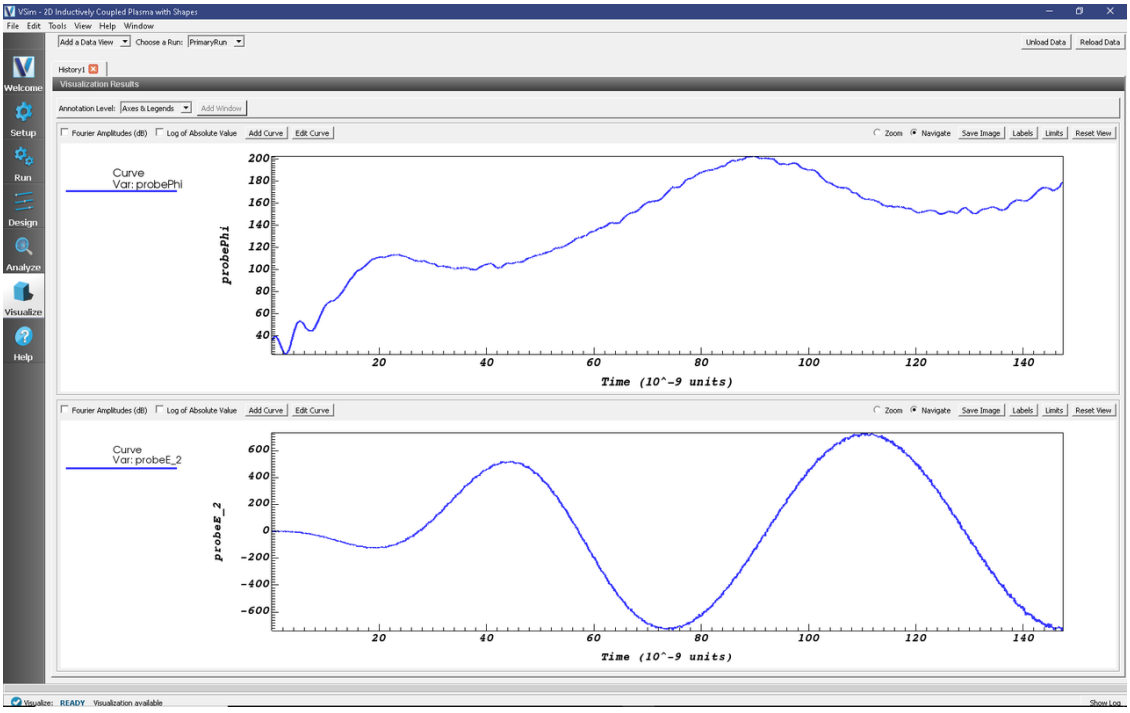


Fig. 6.49: A time-history of the electric potential (Phi) and the azimuthal electric field at a probe position Z = 0.05 m, R = 0.067 m. The addition of a 100. V RF bias causes the electric potential at the probe position to osciallate and reach a maximum of 200 V compared to 165 V without an applied bias.

Problem Description

This simple ion source example illustrates how to generate an electron population by emitting electrons off of a cathode. The charge neutral plasma forms due to electron-neutral collisions which ionizes the neutral fluid to generates a second electron (in each collision) and a singly charged positive ion. The ions are then extracted from the plasma source with two extraction plates biased to a large negative potential. The two extraction plates accelerate the ions out of the plasma generating an ion beam which is focused to a small width according the space between the two extraction plates. To further focus the ion beam, absorbing plates are placed above the extraction plates which further focuses the ion beam to a smaller width. A magnetic field can also be imposed to further restrict the motion of the ions. For the example shown here a SpaceTimeFunction is used to define the magnetic field but we have not included the magnetic field in the simulation. The user is free to add this magnetic field to perform further tests on the setup.

This simulation can be run with a VSimPD license.

Opening the Simulation

The simple ion source example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Ion Sources* option.
- Select *Ion Source* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.50. You can expand the tree elements and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on option. The right pane shows a 3D view of the geometry as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

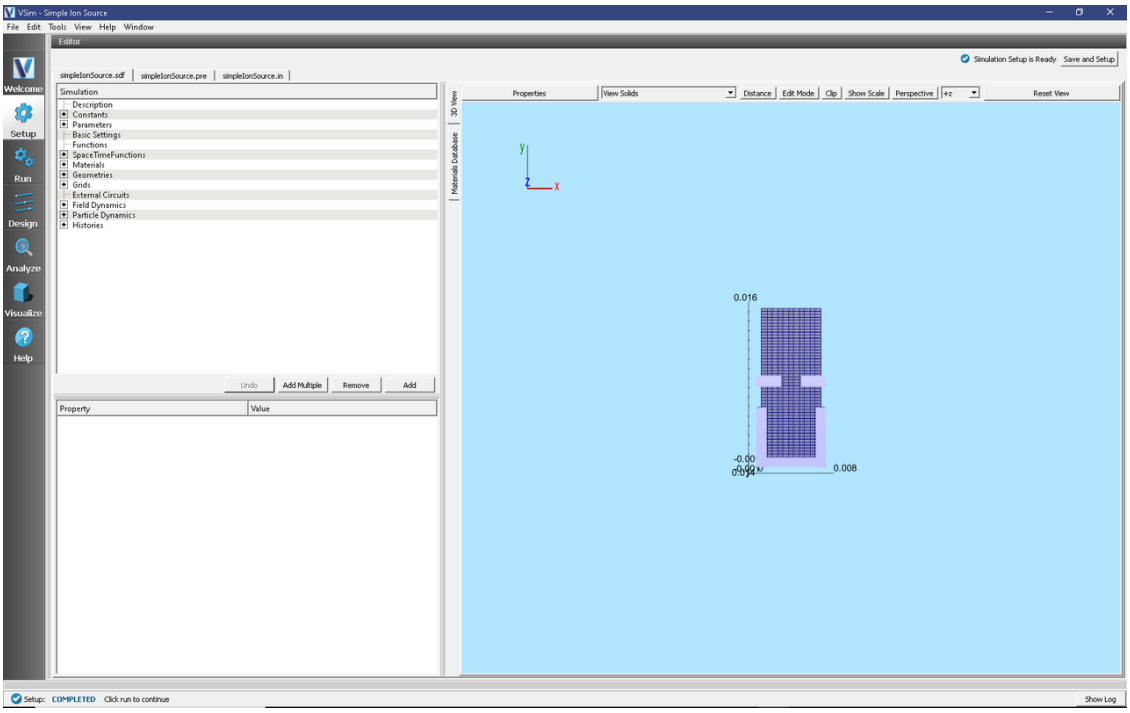


Fig. 6.50: Setup window for the Simple Ion Source example.

Simulation Properties

This example contains many user defined *Constants* which help simplify the setup and make it easier to modify. The following constants can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* and all the constants used in the simulation will be displayed. To add your own constant, right click on *Constants* and left click on *Add User Defined*. Below is an explanation of a few of the constants used. There are several more constants included in the simulation.

XMIN/XMAX,YMIN/YMAX,ZMIN/ZMAX: Physical dimensions of simulation in meters.

CATHPOT: Potential of electron source from which electrons are emitted

B0: Magnetic of external magnetic field (if you choose to include this)

T0: Time that the electrons are emitted from the electron source.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.36e-11
  - *Number of Steps*: 400
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.51.

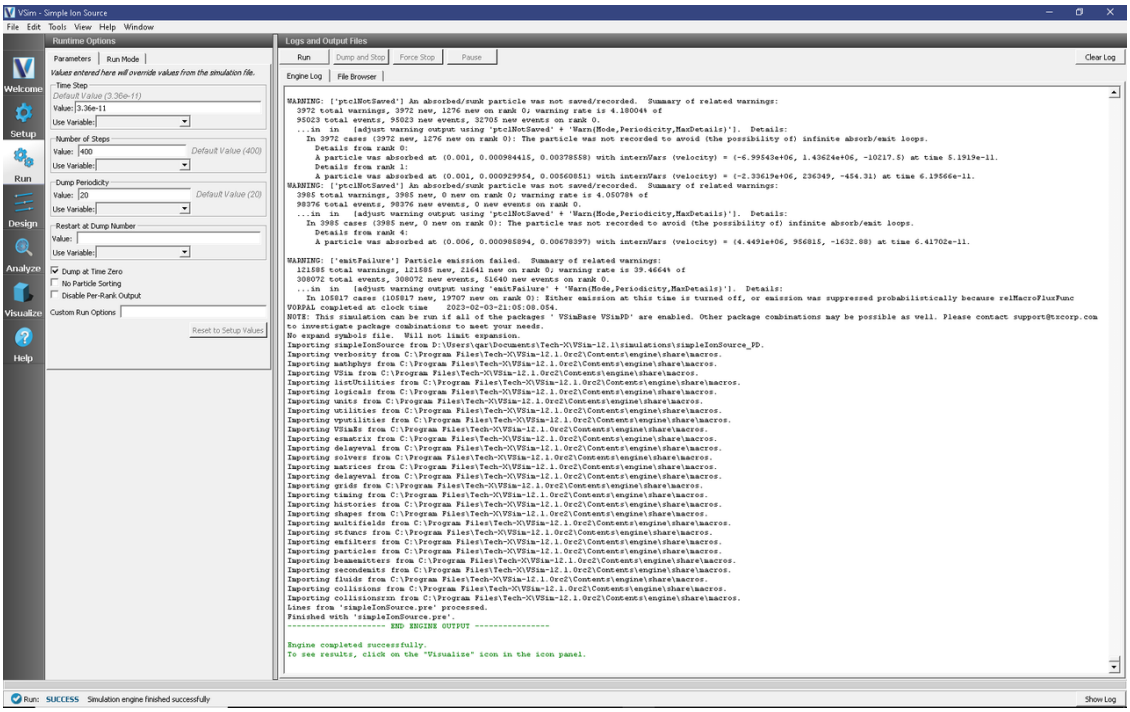


Fig. 6.51: The Run Window at the end of execution.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the list of *Available Analyzers* , select *computePtclNumDensity.py* and press *Open** The analyzer fields should be filled as below:
  - *simulationName*: simpleIonSource
- Fill in *SpeciesName* with "electrons" or "Ions" which are the names of the two species in the "Particle Dynamics" tab in the visual setup.

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.52.

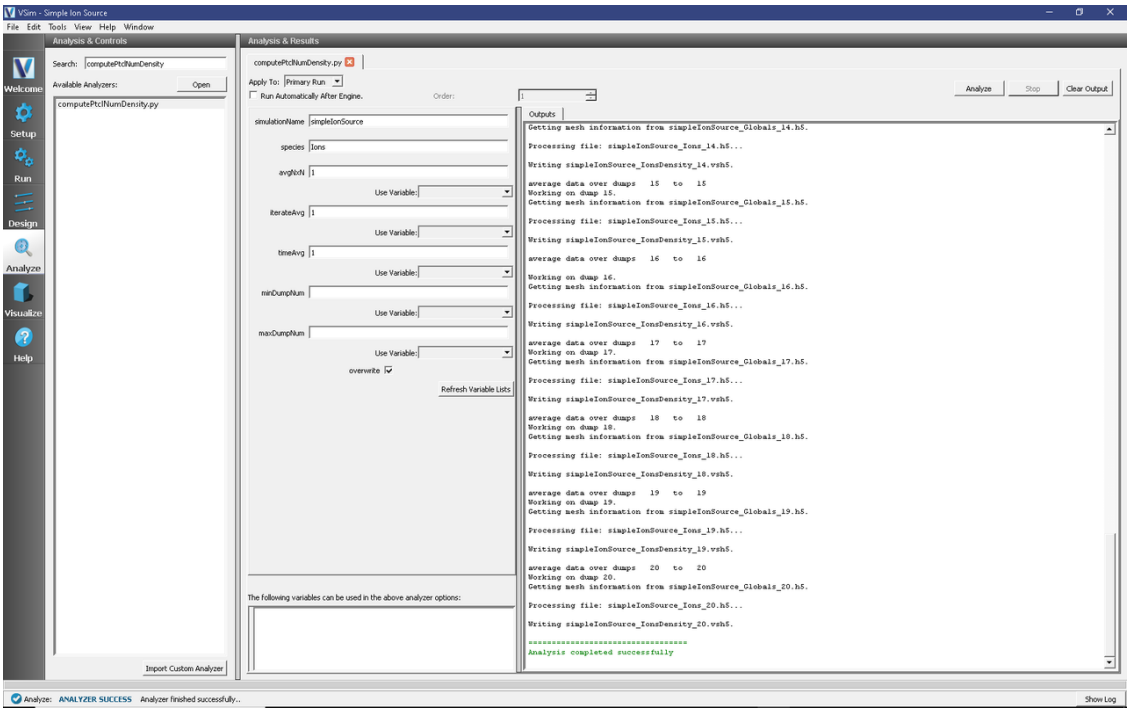


Fig. 6.52: The Analyze Window at the end of a successful run.

The resulting data is called *electronDensity* and *IonDensity* and shows the number density in the 3D simulation domain in units of #/m^3.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Clicking on the *Data View* dropdown menu shows there are many different types of data to visualize.
- To get started, lets visualize the formation of the plasma at the bottom near the cathode and the resulting ion beam.
- Click on *Data View* then click on *Data Overview*
- Under *Variables*, click on “Particle Data”, “electrons” and the top most box (“electrons”)
- Click on “Ions” then click on the top most box (“Ions”)
- Finally, to visualize the plasma species in the context of the geometries in the simulation, click on “Geometries”, “poly(extractionPlate1)”, “poly(extractionPlate2)”, and “poly(electronSource)”.
- You can rotate the figure by holding down the right mouse button and moving the mouse.

The resulting visualization is shown in Fig. 6.53.

This plot shows that the ions have been extracted from the plasma reservoir to form a coherent ion beam.

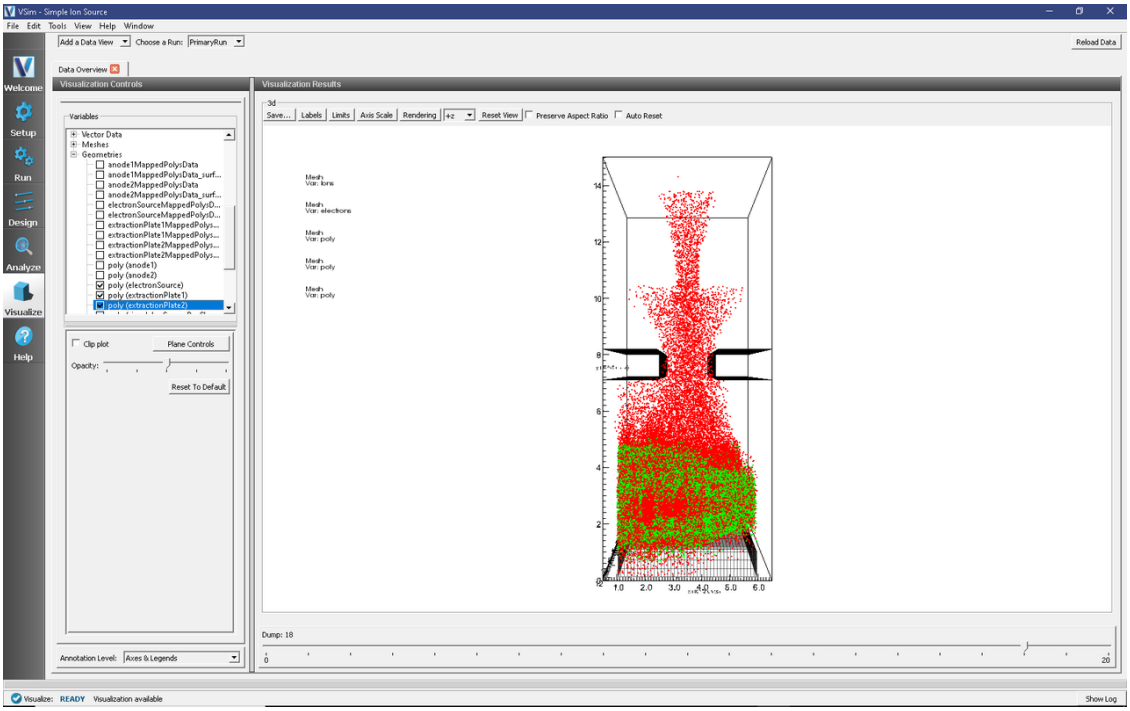


Fig. 6.53: The evolved ion beam near the end of the simulation.

Next you can visualize the potential. Click on "Data View" at the top left of the Visualization window. Then click on "Field Analysis". A new tab will open called "Field Analysis". In the "Field Analysis" tab, click on the arrow next to the "Field" option and you will see all the available fields for visualizing. Click on "Phi", which is the potential. To get a 2D view with a 1D slice of the data click on "Side-by-side 2d/1d" next to the *Layout* option. Under "Slice Settings", change the value from 0 to 0.005, then hit Enter. Now the data is being shown in the 2D plane at z=0.005 m. Finally, you can slide the bar under the "Vertical,Horizontal,Advanced" tabs to change the 1D slice that is shown. You need to click on "Perform Lineout" to see the new slice. To change the axis labels, click on "labels" in the respective plots.

The visualization window showing the potential is shown in Fig. 6.54.

Further Experiments

In this example simulation, we have reduced the ion mass to illustrate some key aspects of the capabilities in VSim. For example, we illustrate the formation of the plasma in the plasma source region. As the plasma builds up, the ions are extracted from the plasma source region by the "extraction plates". The ions will also be attracted to electrons in the plasma source region due to the ambipolar electric field which is created by the spatial separation between the ions and electrons. This example can be used to design an experimental setup with realistic ion masses. With larger masses, the ambipolar electric field makes it more difficult for the ions to escape. Therefore, the following modifications can be performed to test more realistic scenarios. (1) Change ion species to hydrogen. (2) Modify "T0" which is the time that the electrons are emitted from the electron source. Increasing T0 means that the ions source becomes more dense. For heavy ions, you will need to modify this so that the ambipolar electric field does not become too large thus pulling the ions back in to the plasma source region. (3) Modify "EPYPosition" which is the distance along the y-axis the extraction plates are plates.

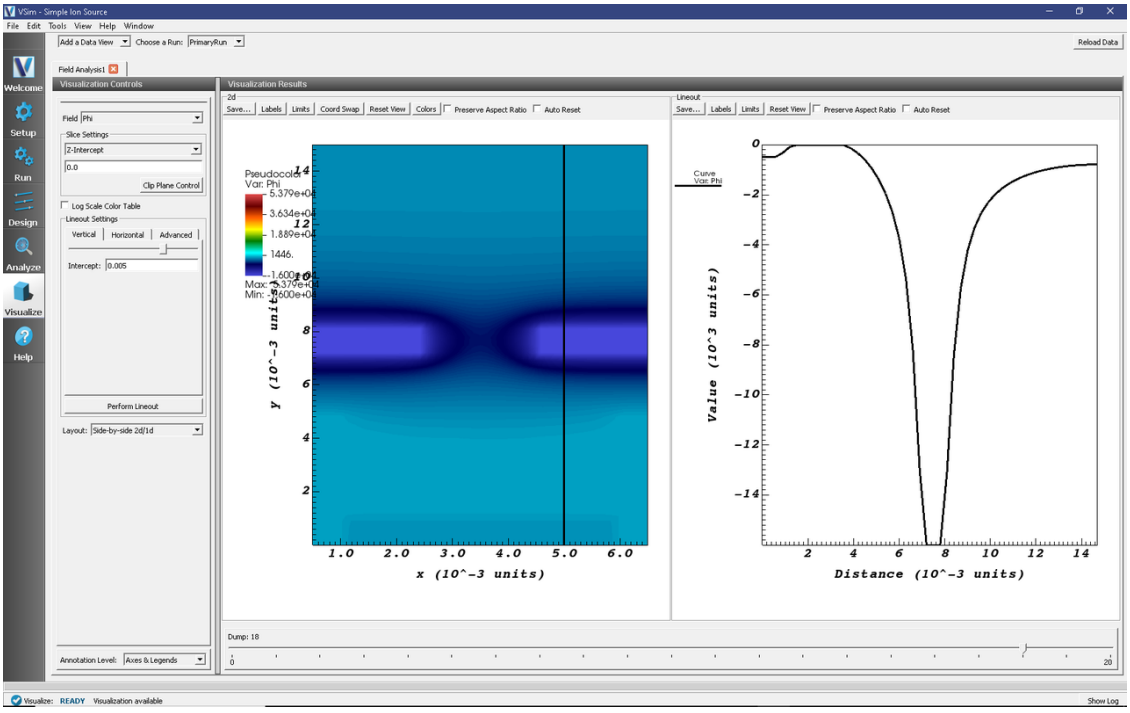


Fig. 6.54: Plot showing the 2D potential in the z=0.005 m plane along with a 1D plot along the y-axis (at a fixed value of x).

6.5.2 Penning High Intensity Ion Source (PenningSource.sdf)

Keywords:

coherent ion beam, electron emitters, electron-neutral collisions, plasma source

Problem Description

This Penning Source example illustrates how to generate an electron population by emitting electrons off of a cathode using VSim's Settable Flux Shape Emitter model. The plasma forms due to impact ionization from electron-neutral collisions which ionizes the neutral Argon gas to generate a second electron (in each collision) and a singly charged Argon ion. This simulation also includes impact excitation and elastic collisions between electrons and Argon gas. The various types of elastic and inelastic collisions of the particles are calculated with the Vorpal engine's Reaction Framework package. The plasma particles, background gas, and collisions are set up in the *Particle Dynamics* Element. The cross-sections for these collisions are imported from 2-column data files. The electrons are attracted in to the plasma chamber by charging the anode (filled with Argon gas) to a positive potential. Secondary electrons are emitted off the anode due to the primary electrons interacting with the anode walls. This is set up using a *Secondary Emitter* model in VSim.

The Argon ions are then extracted from the plasma source with two extraction plates biased to a large negative potential. The two extraction plates accelerate the ions out of the plasma generating an ion beam which is focused to a small width according to the space between the two extraction plates. To further focus the ion beam, absorbing plates are placed below the extraction plates which are part of the anode. A 0.16 Tesla magnetic field in the $y-$ direction is imposed to restrict the motion of the electrons in the Anode region. For the example shown here a Space Time Function is used to confine the magnetic field to a specified region using a Heaviside Step function. The electric field is solved via Poisson's equation using a Generalized Minimal Residual (GMRES) linear solver. This solver is chosen under *Field Dynamics -> PoissonSolver*. A combination of Dirichlet and Neumann boundary conditions involving the shapes and simulation

boundaries are imposed. Field boundary conditions are imposed under *Field Dynamics* -> *FieldBoundaryConditions*. The plasma is represented by macro-particles which are moved using the Boris scheme in a 3D Cartesian coordinate system.

One challange to modeling ion sources using PIC methods is the need to resolve the electron Deybe length to avoid a numerical grid heating instability when the most common PIC methods are used. In this example, the electron density exceeds $10^{17}\mathrm{m}^{-3}$ and the electron temperature is about 3-5 eV. This results in a Debye length that is about 5×10^{-5} m, which would require a grid size ≈ 10 times smaller that what we use in this example (which in 3D would mean the simulation would need a 1000 times more cells than what we use). We avoid this issue by using an energy conserving particle deposition scheme discussed in Reference [1].

This simulation can be run with a VSimPD license.

Opening the Simulation

The Penning Source example is accessed from within VSimComposer by the following actions:

- Select the *New* $\rightarrow$ *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Ion Sources* option.
- Select *Penning High Intensity Ion Source* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.55. You can expand the tree elements and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on an option. The right pane shows a 3D view of the geometry as well as the grid. To show or hide the grid, expand the "Grid" element and select or deselect the box next to `Grid`. You can also show or hide the different geometries by expanding the "Geometries" element and selecting or deselecting "anodePlasmaPlate", "cathode" and/or "extractionPlates". Note that these three shapes are unions of the other more basic shapes included in this simulation.

Simulation Properties

To demonstrate how to set up the energy conserving particle deposition scheme [1], click on "basic settings" in the elements tree. Under the basic settings option, you will see that the simulation is setup to use an electrostatic field solve, that particles are enabled and that we are invoking the Reactions collisions framework. To create a particle deposition scheme that conserves energy, we have chosen the "particle to field deposition" which we call "smoother energy conserving". This allows you to run simulation in which the grid size is larger than the electron Debye length and still maintain a physical electron temperature (less than 10 eV). In addition, this example contains many user defined *Constants* which help simplify the setup and make it easier to modify. The following constants can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* and all the constants used in the simulation will be displayed. To add your own constant, right click on *Constants* and left click on *Add User Defined*. Below is an explanation of a few of the constants used. There are several more constants included in the simulation.

XSTART/XEND,YSTART/YEND,ZSTART/ZEND: Physical dimensions of simulation in meters.

CATHODE_VOLTAGE: Potential of electron source from which electrons are emitted

ANODE_VOLTAGE: Potential of anode which attracts the electrons from the cathode

PENNING_MAGNETIC_FIELD: Magnetic of external magnetic field used to confine the ion beam

T1: Time that the electrons are emitted from the electron source.

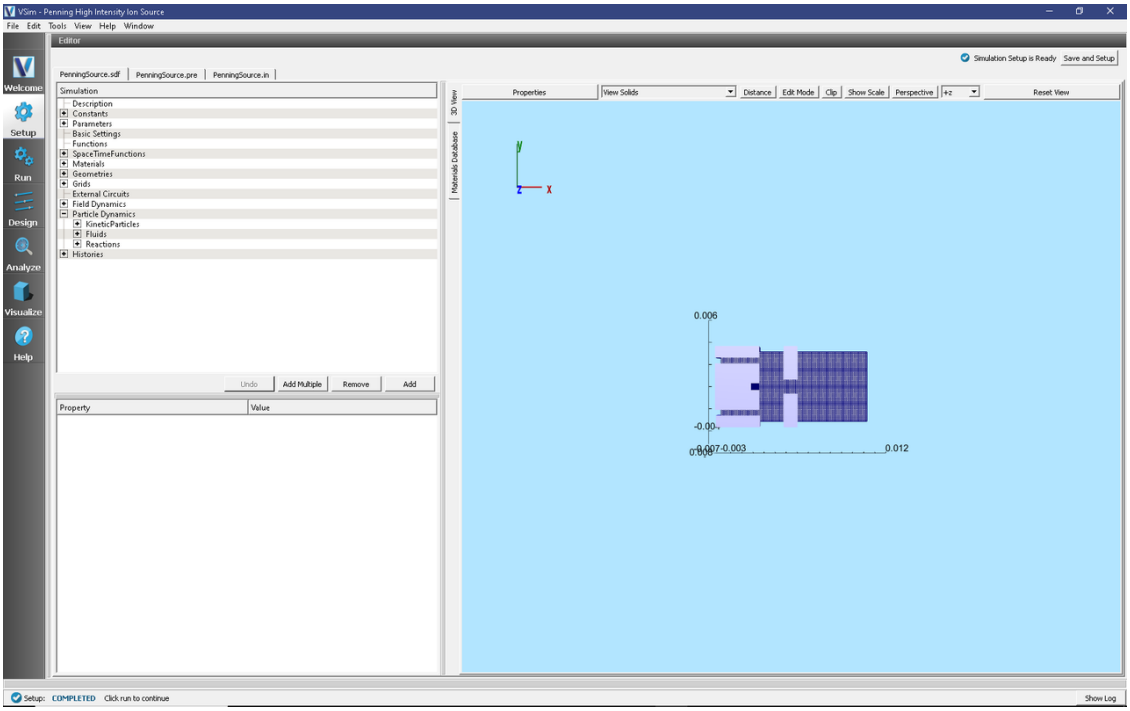


Fig. 6.55: Setup window for the Penning Source example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.36e-11
  - *Number of Steps*: 5000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.56.

Analyzing the Results

After performing the above actions, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list of *Available Analyzers*, select *computePtclNumDensity.py* and press *Open*
- The analyzer fields should be filled as below:
  - *simulationName*: penningSource

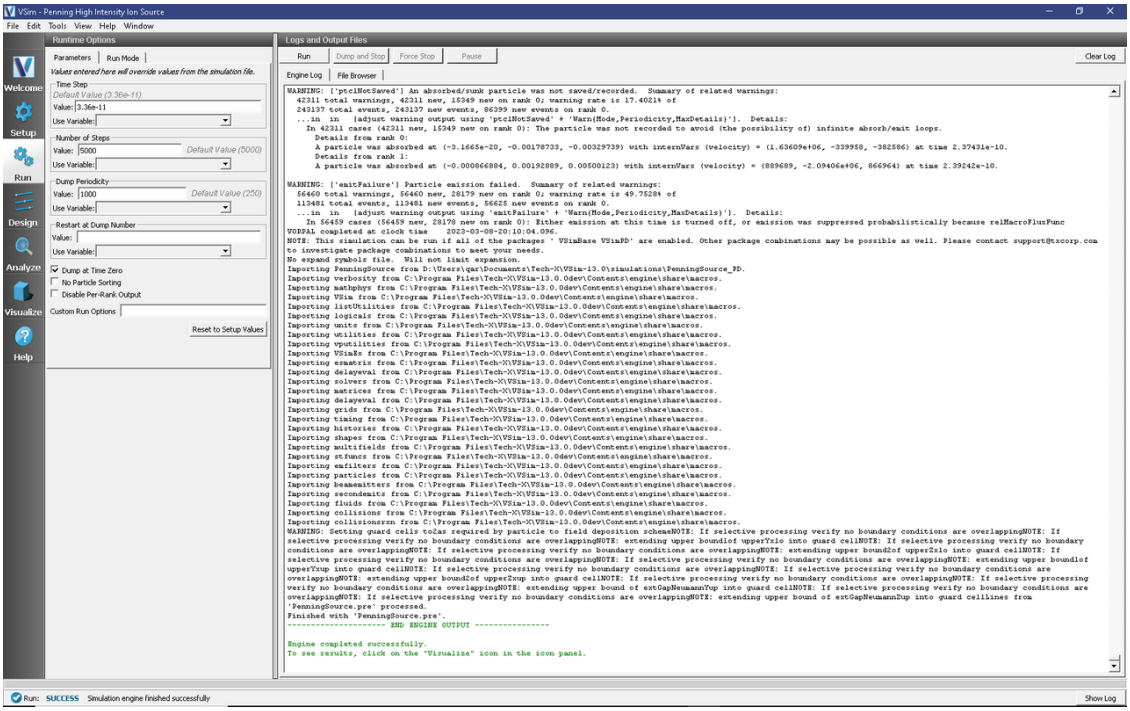


Fig. 6.56: The Run Window at the end of execution.

  - *speciesName* with “electrons” or “Ar1” which are the names of the two species in the “Particle Dynamics” tab in the visual setup.

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.57.

The resulting data is called *electronDensity* and *Ar1Density* and shows the number density in the 3D simulation domain in units of #/m^3.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Clicking on the *Add a Data View* dropdown menu shows there are many different types of data to visualize.
- To get started, lets visualize the formation of the plasma in the anode and the resulting ion beam.
- Click on the *Data Overview* tab which is a default tab already loaded in the “Visualize” section of VSim.
- Under *Variables*, click on “Particle Data”, “electrons” and the top most box (“electrons”)
- Click on “Ar1” then click on the top most box (“Ar1”)
- Finally, to visualize the plasma species in the context of the geometries in the simulation, click on “Geometries”, “poly(cathode)”, “poly(extractionPlates)”, and “poly(anodePlasmaPlate)”.
- You can rotate the figure by holding down the left mouse button and moving the mouse.
- Slide the bar to the right at the bottom of the display window to watch the ions form and accelerate out of the anode.

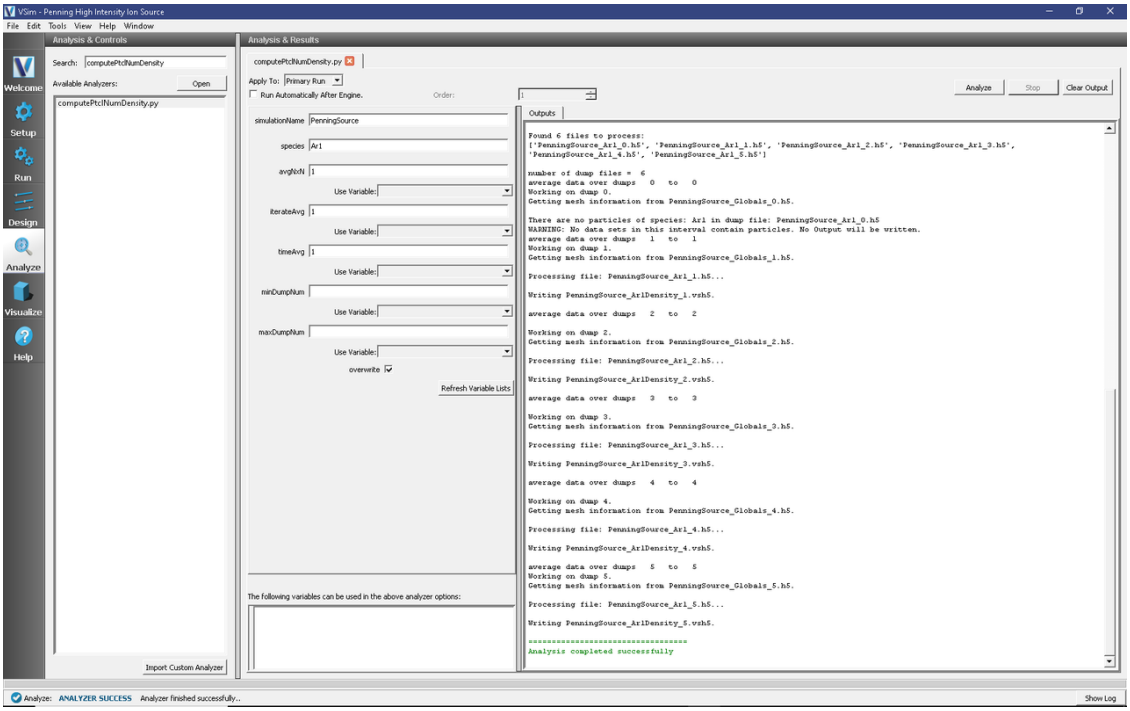


Fig. 6.57: The Analyze Window at the end of a successful run.

The resulting visualization is shown in Fig. 6.58.

This plot shows that the ions have been extracted from the plasma reservoir to form a coherent ion beam.

Next you can visualize the electron density which was generated when you ran computePtclNumDensity.py. To view this dataset, click on "Add a Dataview", then click on "Field Analysis". This will open a new plotting window. Click on the region with the "Field" icon, and choose "electronDensity". You can view this with various configuration. One configuration is to choose "side-by-side 2d/1d" under the "layout" option. This setup is shown in Fig. 6.59. The option "Preserve Aspect Ratio" is chosen. If you slide the "Lineout Settings" so that a lineout goes through the dense electron region, then you can see that the electron density is $\approx 10^{16}\mathrm{m}^{-3}$.

The visualization window showing phase space is shown in Fig. 6.59.

Further Experiments

The default example runs for only 5000 time steps. However, the simulation takes 50000 time steps to reach steady state. Therefore, one experiment would be to run the simulation to time step 50000. You should see that the electron density increases to $\approx 10^{17}\mathrm{m}^{-3}$. Since the grid size is ≈ 0.1 mm, the grid size is several times times the electron Debye length. Therefore the energy conserving particle deposition allows for considerable speed up in this calculation.

Set up a History that records the Ar1 current flowing out of the plasma chamber on to the x=XEND boundary. Right click on the "Histories" element and under "Add ParticleHistory" select "Absorbed Particle Current." You can change the name of the history by double clicking on the new "absorbedPtclCurrent0" element in the tree. Then be sure to pick the particle absorber from which you would like to collect data. Note that to add a history on a boundary, that boundary needs to be of type "Absorb and Save".

The Reactions framework allows one to set up collision interactions flexibly. The collisions involved in this example are electron-neutral collisions that lead to ionization and ohmic heating. As a further experiment, ion-neutral collisions, such as elastic scattering and charge exchange, can also be added to the simulation.

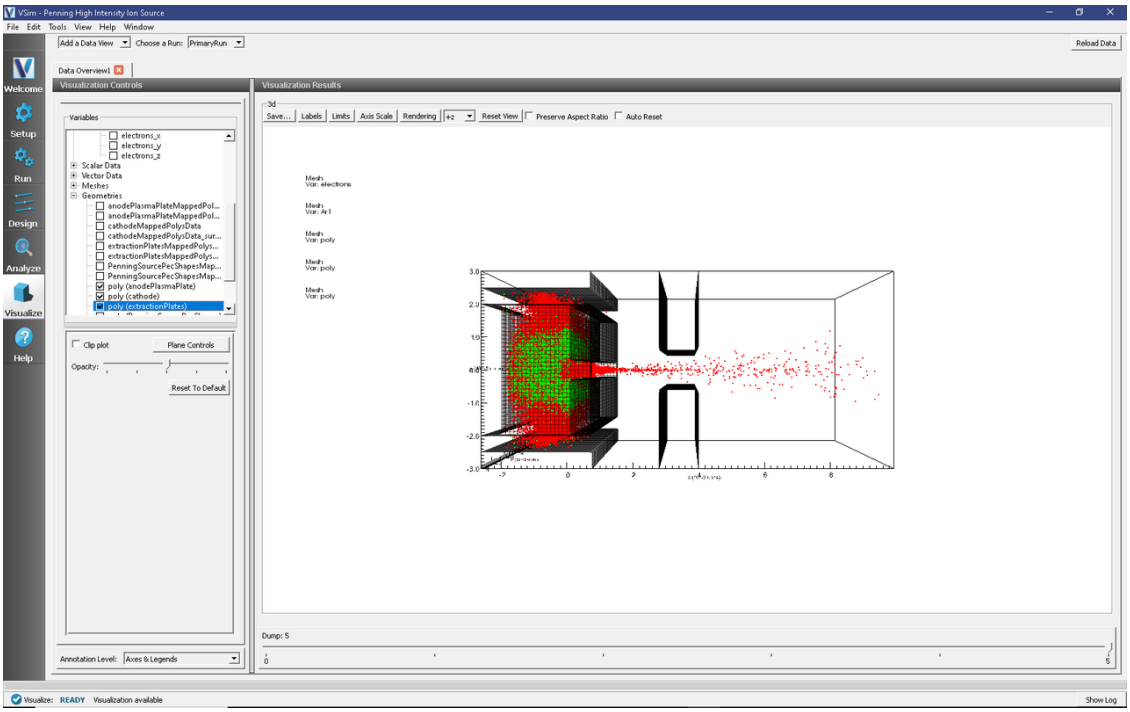


Fig. 6.58: The evolved ion beam at time step 5000.

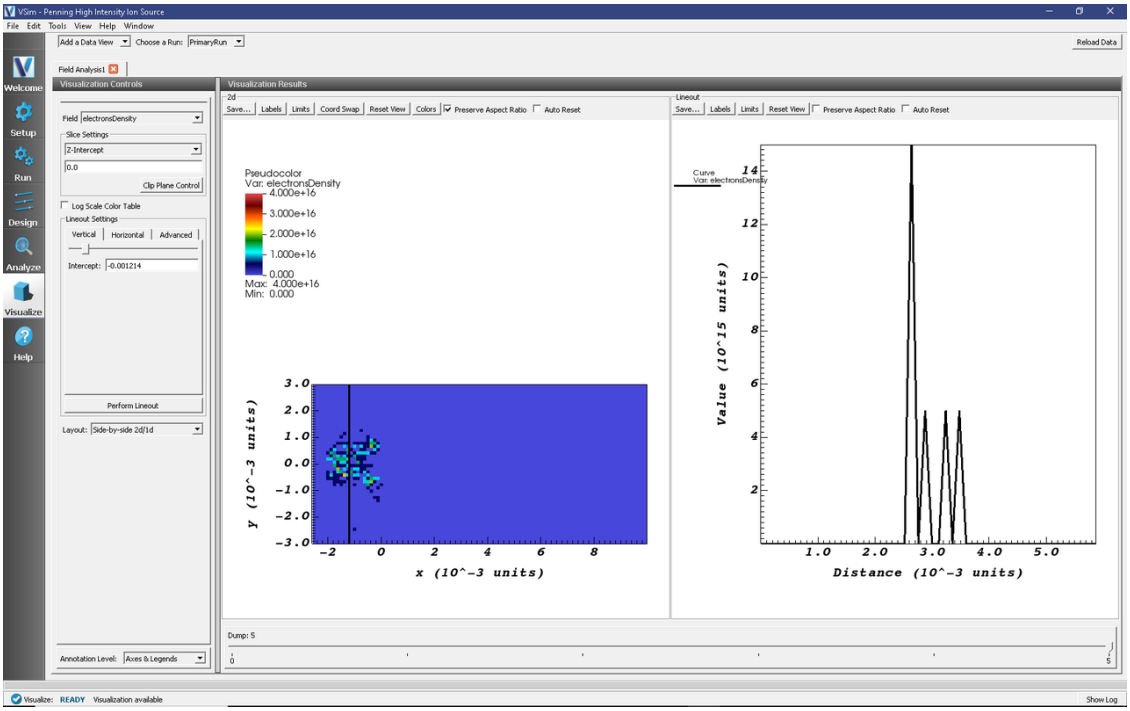


Fig. 6.59: Plot of electron density at time step 5000 in m^{-3}

Optimizing Simulation Runtime via Parallelism and Decomposition

As noted above, the default example runs for only 5000 time steps. With 32 cores, these 5000 steps take roughly 30 minutes. Extending the experiment out to 50,000 steps, doubling the cells in each direction, etc. without modifications could become resource intensive. This is where domain decomposition can play a significant role. For a more in-depth primer on Parallelism and Decomposition, see the "Parallelism and Decomposition" section in the UserGuide Manual. The core concept is to place more resources (cpus), where the heavier computational load is located within the simulation.

Tech-X has an analyzer (computeLoadBalancedDecomp.py) that can more evenly distribute the computational load across all available resources. For the full specifications of the analyzer, see the Parallelism and Decomposition section in the UserGuide Manual. The analyzer achieves this by writing out a custom domain decomposition block that dictates what cpu gets which region of the grid; for HPC resources this can include both intra- & inter-nodal decomposition. This analyzer requires two pieces of information: The total number of cells in the simulation, and the number of particles per cell.

Turning On Particle Per Cell Dumping

VSim does not automatically dump the number of particles per cell and so the user will have to turn on that capability. To do so, follow the instructions below:

- Proceed to the Setup Window by pressing the *Setup* button in the navigation column.
- In the Simulation sub-pane of the sdf, Expand the *Particle Dynamics* option.
- Select the *KineticParticles* option.
- Set the KineticParticles->"dump particles per cell" option to "yes".

This will add the attribute to all kinetic particle species. This is shown in Fig. 6.60.

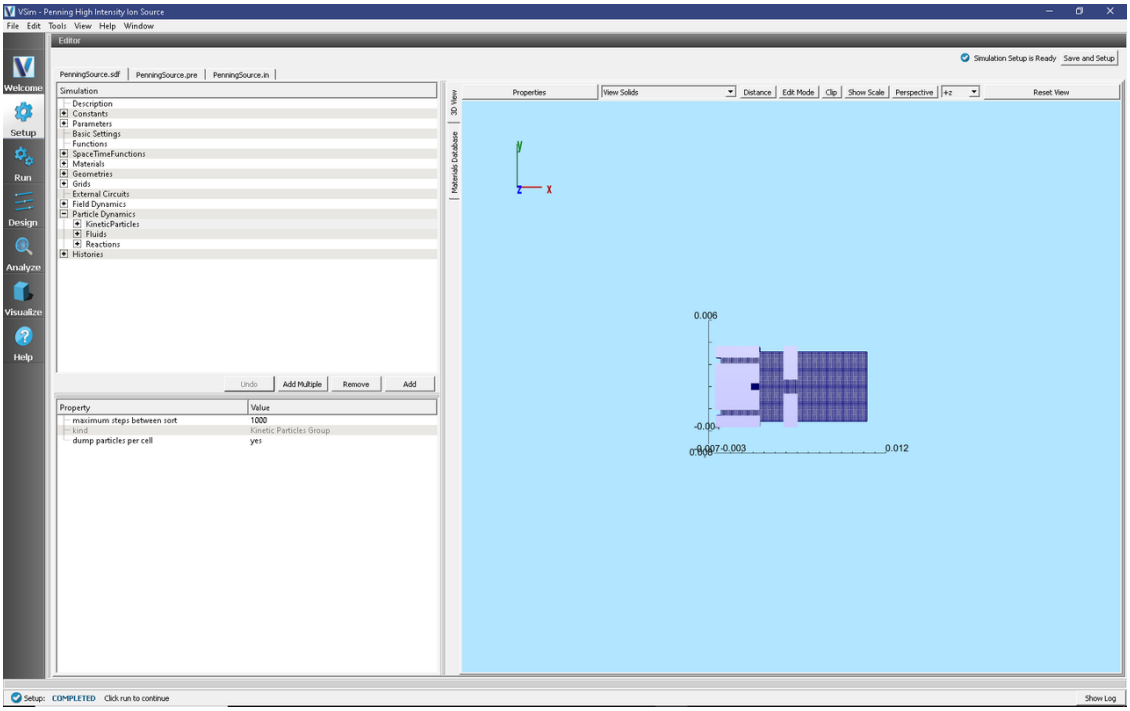


Fig. 6.60: Location of the flag to turn on tracking and dumping the number of particles per cell.

Using the Analyzer to Create a Custom Decomposition

After turning on tracking the PPC for the simulation, and running it. There should be a dump file with the naming scheme: *simulationName_speciesPPC_dumpNumber.h5* Once there is, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list of *Available Analyzers*, select *computeLoadBalancedDecomp.py* and press *Open*
- The analyzer fields should be filled as below:
  - *simulationName*: PenningSource
  - *species*: Blank. Typically will be "electrons" or "Ar" which are the names of the two species in the "Particle Dynamics" tab in the visual setup.
  - *nnodes*: Blank. This value is 1, unless using more than one node on a HPC.
  - *ncores*: Blank. This value is the number of cores you would like to use.
  - periodic_dirs: 2. This example has 2 periodic boundaries.
  - *dump_number*: 0. This is the dump you wish to perform the analysis upon. Preferably the most recent one.
- Note, unless you wish to have slab decomposition, leave intra- & inter-slice unchecked.
- Click *Analyze* in the top right corner.
- The analysis is completed when you see output similar to that shown in Fig. 6.61.

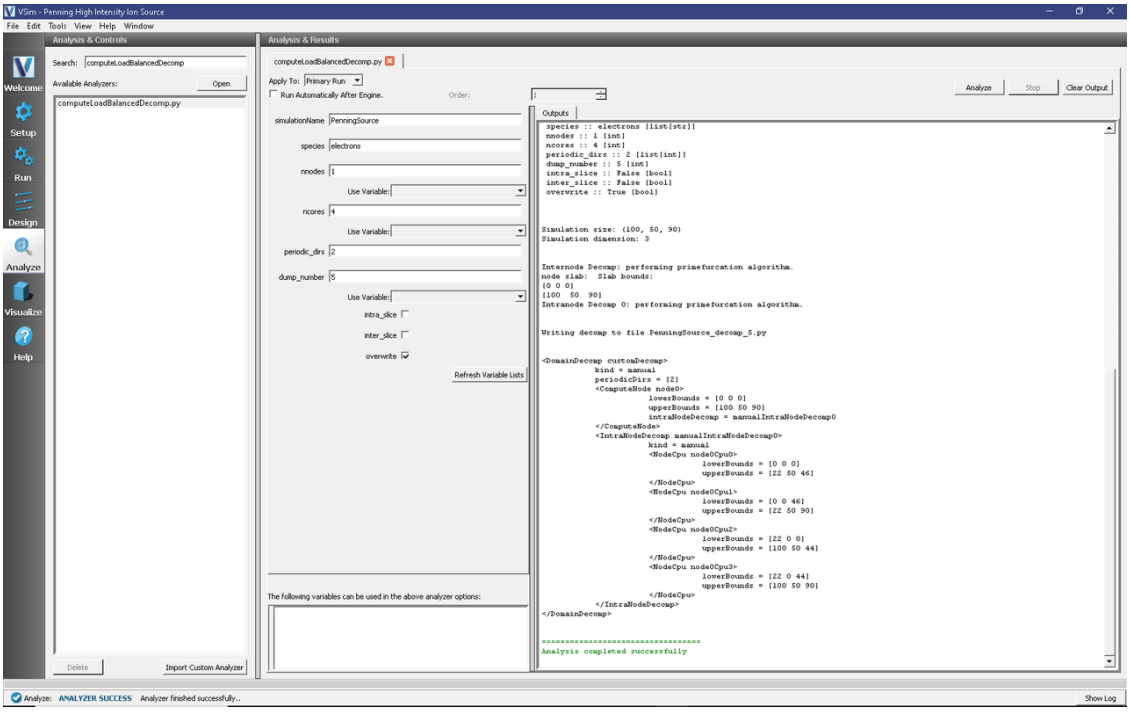


Fig. 6.61: Output of the computeLoadBalancedDecomp analyzer for a 32 core run on 1 node (i.e. workstation or 1 node of a hpc) at time step 5000.

Along with the screen readout, the analyzer also writes a file to disk, with the naming convention *<simulationName>_decomp_<dumpNumber>.mac*, using values from their respective fields.

Loading the Custom Decomposition into the Simulation

This custom decomposition file can be loaded into VSimComposer to then be used. To do this, proceed as follows:

- Proceed to the Setup Window by pressing the *Setup* button in the navigation column.
- In the Simulation sub-pane of the sdf, Expand the *Basic Settings* option.
- Select the *domain decomposition* property to see the drop-down menu.
- Select *manual*
- Enter the filename of the custom decomposition file. If from the analyzer, recall it has a form of *<simulationName>_decomp_<dumpNumber>.mac*

This is shown in Fig. 6.62.

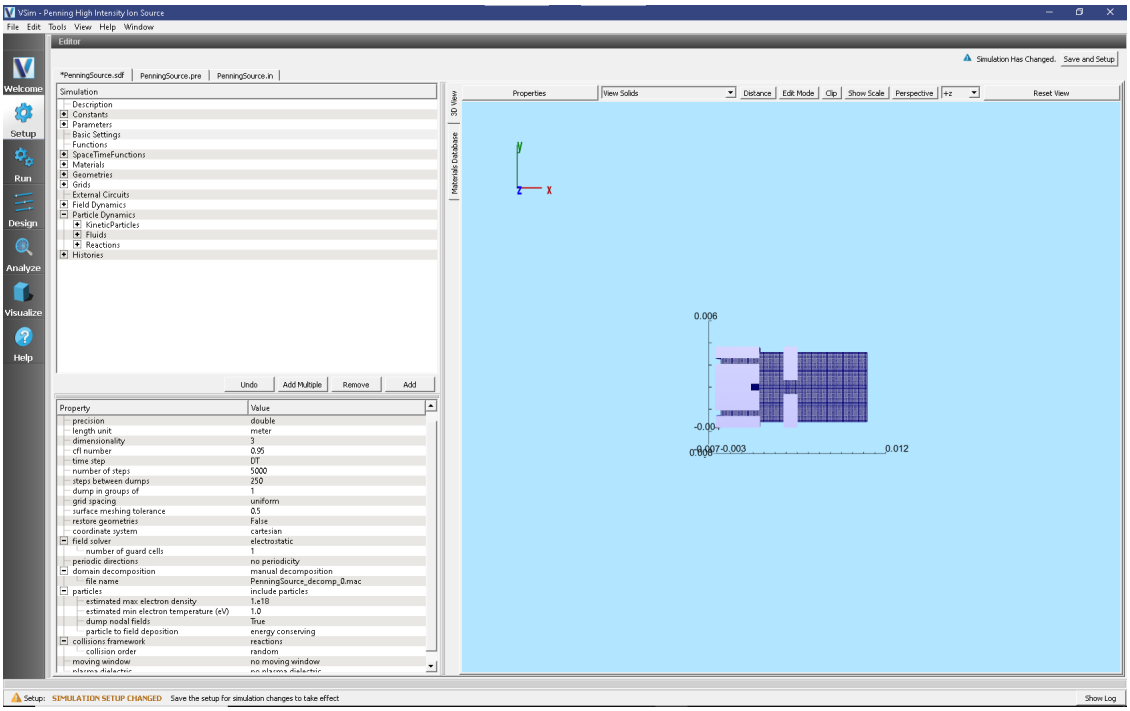


Fig. 6.62: Location of the drop-down menu to import a custom decomposition file.

References

[1] Birdsall, C. K., & Langdon, A. B. (1985). Plasma Physics via Computer Simulation. New York: McGraw-Hill.

6.6 Processes

6.6.1 Corona Discharge 3D (coronaDischarge3D.sdf)

Keywords:

seed electron population, ionization collisions, poisson solver, dielectric, cascade

Problem Description

This example illustrates how to use VSim to model corona discharge, which is a problem that can occur in a variety of conditions including the manufacturing of dielectrics. In the scenario which we simulate, and which represents many situations, a potential difference is established between two boundaries. In many cases there may also be a dielectric present that can modify the field solution. Furthermore, there will also be an electric field within the dielectric, which VSim correctly calculates. When a potential difference exists between two boundaries, a free electron will be accelerated in the resulting electric field. Free electrons often form due to the ionization of a neutral atom from a stray cosmic ray or UV light. When no potential difference exists, the electron is reabsorbed by surrounding neutrals. However, if a potential difference does exist, this free electron will be accelerated and collide with surrounding neutrals. If the electron ionizes another neutral before being reabsorbed, then a cascade condition is established and more free electrons form due to ionization collisions. This process has been considered by Paschen, who calculated the potential difference required for a cascade of electrons to form. Paschen simplified the process by lumping the contribution from all the collisions into a few terms. However, with VSim, we can consider the effect of each collision separately.

This example illustrates how to set up collisions, and establish a seed electron population (which represents the free electrons that form due to UV light or cosmic rays). We also illustrate a new capability in VSim, which is the ability to create a CSG geometry and assign a dielectric to it.

This simulation can be run with a VSimPD license.

The video attached here provides a full walkthrough of this example: https://www.youtube.com/watch?v=OTBm459OAUo&list=PLottQ0Bg2M-3ATV5O9IP-3TEC4toVYPAK&index=13

Opening the Simulation

The corona discharge example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Plasma Processing* option.
- Select *Corona Discharge* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.63. You can expand the elements tree and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on an option. The right pane shows a 3D view of the geometry as well as the grid. To show or hide the grid, expand the "Grid" element and select or deselect the box next to `Grid`. You can also show or hide the different geometries by expanding the "Geometries"

element and selecting or deselecting the various geometries. "cylinderConductorUnionpipe0" is created by performing a boolean union operation between "cylinderConductor" and "pipe0".

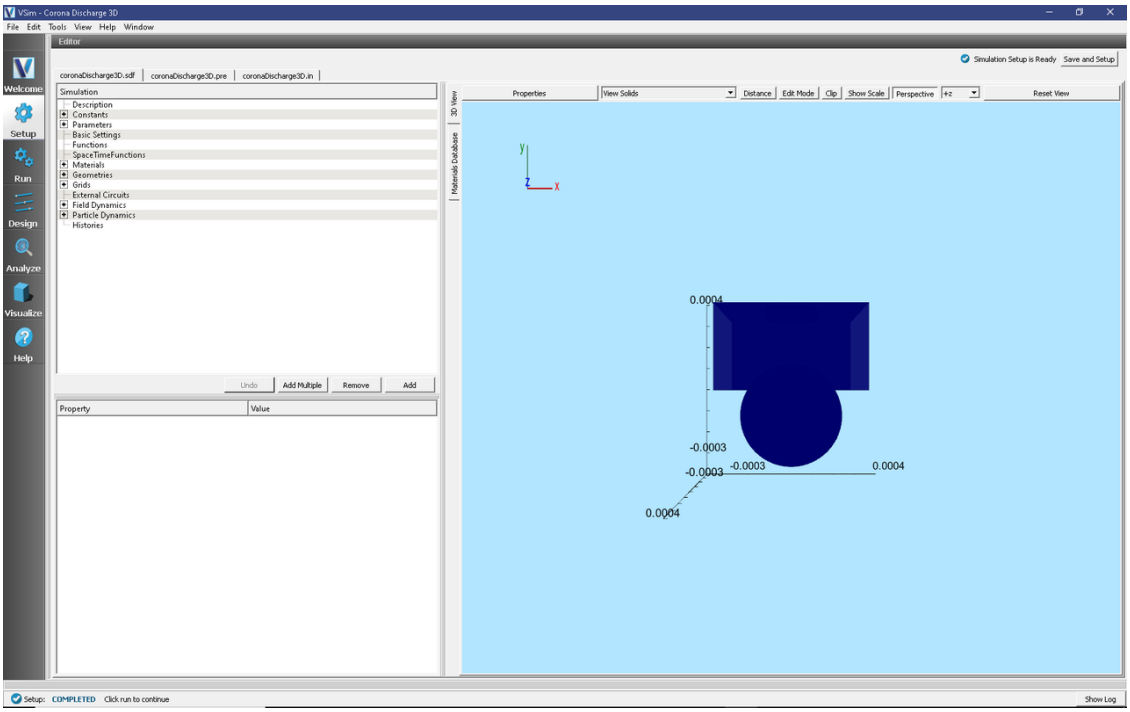


Fig. 6.63: Setup window for the corona discharge example.

Simulation Properties

This example contains many user defined *Constants* and *Parameters* which help simplify the setup and make it easier to modify. The following constants or parameters can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* or *Parameters* and all the constants or parameters used in the simulation will be displayed. To add your own constant or parameter, right click on *Constants* or *Parameters* and left click on *Add User Defined*. Below is an explanation of a few of the constants and parameters used. There are several more constants and parameters included in the simulation.

- **MAX_SIGMA**: Largest cross-section for all collisions that are included in simulation. This sets necessary grid size
- **GAS_PRESSURE_TORR**: Pressure of neutral gas. Mean Free Path (MFP) depends on this
- **MFP**: Smallest Mean Free Path based on GAS_PRESSURE_TORR and MAX_SIGMA. DX/DY/DZ should be less than MFP.
- **FCOLL**: Largest collision frequency. Time step should be smaller than 1/FCOLL
- **XC_SPHERE/YC_SPHERE/ZC_SPHERE/RADIUS_SPHERE**: Coordinates for center of sphere and radius of sphere
- **CYLINDER_YPOS/CYLINDER_LENGTH/CYLINDER_RADIUS**: Coordinates and dimensions for cylindrical dielectric
- **PIPE_LENGTH/PIPE_OUTER_RADIUS**: Dimensions of conductor which surrounds cylindrical dielectric
- **CYLINDER_CONDUCTOR_YPOS**: Y-position of cylindrical conductor that sits on top of the cylindrical dielectric.

Basic Settings

Before creating your own simulation or running an example, a good place to look is the "Basic Settings" in the elements tree. In Basic Settings, you will be able to set the dimensions of the simulation (3D in this case), the type of field solve (electrostatic which is explained more below), whether to include particles and reactions and any periodic directions. You should notice that the x and z directions are periodic in this example.

Importing Materials

All geometries which are included in the simulation must be assigned a material. In VSim 11, a new feature is possible, which is the ability to import a dielectric and assign that dielectric to a geometry. To import a material click on the "Materials Database" button which is below the "3D View" button. I've highlighted this window in Fig. 6.63. To add PEC (for example), click on PEC and the click on "Add to Simulation" at the top of the table. You don't need to do this since this material is already added, which can be seen by expanding the "Materials" option in the elements tree. We have also added Sapphire, which is the dielectric we have chosen to use. Once these materials are added, they can be assigned to geometries

Geometries Created Using CSG

An important part of this simulation is the creation of several geometries. To view the geometries, left click on the + sign next to Geometries in the *Setup* window, then left click the + sign next CSG. To view the geometries clearly, you can expand *Grid* and unclick the box next to *Grid*. However, there may still be a box present. This is most likely the neutral fluid (which I will explain below). Therefore, expand *Particle Dynamics*, then expand *Fluids* and uncheck the box next to "N2". All the geometries should now be easily viewed. Right clicking anywhere in the "3D View" and moving the mouse allows you to rotate the geometries. A new feature to VSim 11 is the ability to change the scale of the grid which is visualized. At the top of the 3D View, click on "Show Scale". This will create a scale slider bar at the bottom. Sliding the bar changes the scale that the grid is displayed in. In this simulation, there are two PEC (Perfectly Electrical Conductors) and one dielectric geometry. The two PEC geometries are "sphere0" and "cylinderConductorUnionpipe0". The latter geometry is created by pressing the "Shift" button and clicking "pipe0" and "cylinderConductor" which highlights the two geometries. Once highlighted, right click and you will see the option to perform a boolean operation. We have already done this to create "cylinderConductorUnionpipe0". If you click on "cylinderConductorUnionpipe0" or "sphere0", you will see that the material assigned is PEC. If you click on "cylinderDielectric", you will see that the material assigned to Sapphire. Assigning a dielectric to a geometry is new to VSim 11 and uses a new electric field solve called cutCellPoisson, which requires a PD license.

Field Boundary Conditions

This simulation solves for the self consistent electric field only (the self consistent magnetic field is not solved for and therefore this field solve is called an "electrostatic field solve"). To solve for the self consistent electric field, the charged particles are interpolated on to a grid, the charge density is computed, and Poisson's equation is solved at each time step. In order to do this, boundary conditions must be set for all 6 boundaries (since this is a 3D simulation). Since the simulation is periodic along x and y, which we set in Basic Settings, we need to set up boundary conditions at YMIN, YMAX and all PEC geometries. This is done by expanding "Field Dynamics", then expanding "FieldBoundaryConditions". Here you will see four Dirichlet boundary conditions, which set the potential along these surfaces. You also have the freedom to set YMIN or YMAX as Neumann (which sets the electric field). Note that either YMIN or YMAX has to have a potential specified in order to invert the Poisson matrix.

Creating Particles

To explore the kinetic species that are included in this simulation, expand "Particle Dynamics", then expand "KineticParticles". Here you will see three kinetic species which are "N2Plus", "seedElectrons", and "SecElec". This simulation begins with one seed electron which begins the cascade process that creates the secondary electrons and ionized nitrogen molecules. The seed electrons is called "seedElectrons". If you expand "seedElectrons", you will see "particleLoader0". If you click on "particleLoader0", you will see that we load one particle on the grid. You can load many more particles if you would like by increasing "macro particles per direction" from (1,1,1) to something larger. Or you can change particle load placement from "grid" to "bit-reversed", which will load particles randomly in a cell within the region that you establish by expanding "volume". There are two other kinetic particles that are not initially present. N2Plus and SecElec are both created in the ionization collision *seedElectrons + N2 –> N2Plus + SecElec* and *SecElec + N2 –> N2Plus + SecElec*. Both of these collisions can be found by expanding *Reactions*, then expanding *Particle Fluid Collisions* and you will see two ionization collisions present. Note that in reality, this simulation should also include elastic collisions and several excitation collisions. We have not included elastic collisions because the mean free path is much smaller than ionization collisions and would therefore require around 20-40 processors to efficiently process. However, in 1D or 2D, including elastic collisions is much more feasible. Finally, we have modeled the N2 is a fluid. You can model a neutral species as either a kinetic particle or fluid.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.8173521285034863e-13
  - *Number of Steps*: 500
  - *Dump Periodicity*: 50
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.64. The simulation takes about 2 hours on 6 cores.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Clicking on the *Add a Data View* dropdown menu shows there are many different types of data to visualize.
- To get started, lets visualize the self-consistent potential.
- Click on the *Data Overview* tab which is a default tab already loaded in the "Visualize" section of VSim.
- Under *Variables*, expand "Scalar Data" then check the box called "Phi"
- To view the potential at a slice through the simulation domain, check the box next to "Clip Plot"
- Finally, to visualize the potential superimposed with the geometries in the simulation, expand "Geometries", and check the boxes next to "poly(cylinderConductorUnionpipe0)", "poly(cylinderDielectric)" and "poly(sphere0)".
- Slide the bar to the right at the bottom to view the potential as a function of time.

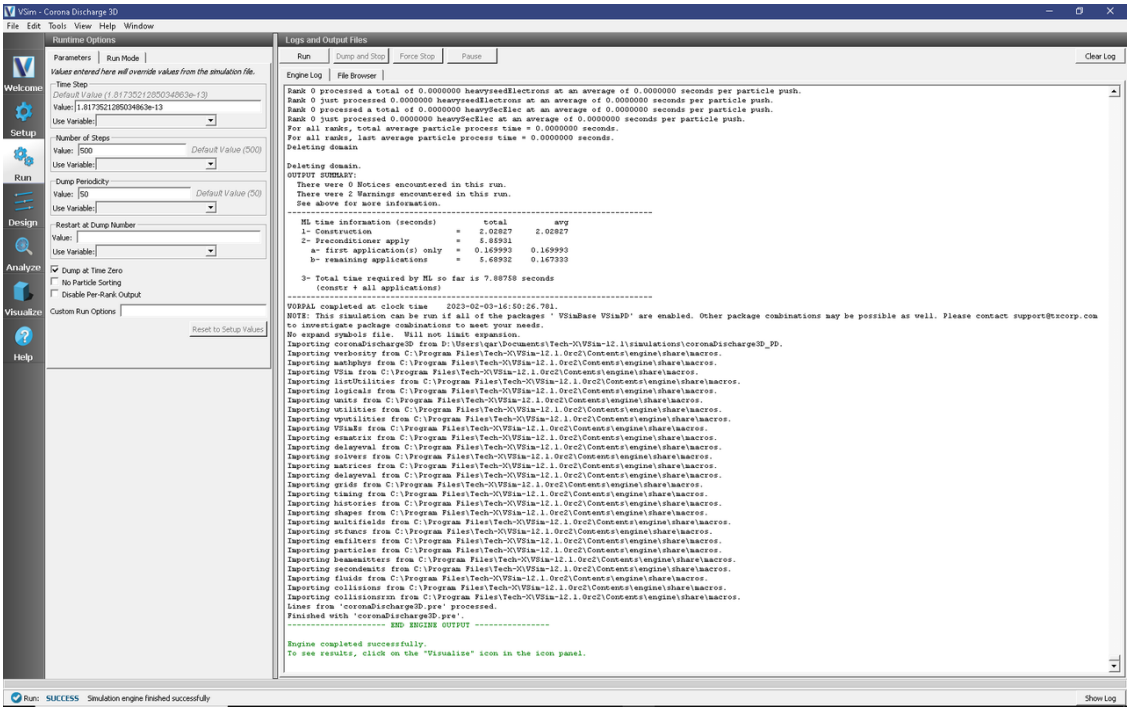


Fig. 6.64: The Run Window at the end of execution.

- Particles can be superimposed on this plot by expanding "Particle Data" and clicking the species you want to visualize.

The resulting visualization is shown in Fig. 6.65.

Further Experiments

One way to make the simulation more realistic is to add elastic collisions between N2 and electrons. This will require a smaller cell size to resolve the smaller mean free path. Other collisions that you could add are excitation collisions between N2 and electrons. Examples of excitation collisions can be found in the Townsend Discharge example. If you add more collisions, you will need to add more seed electrons. The reason is that in a given time step, a particle undergoes only one collision (this is an assumption in our model). If you add elastic collisions, the most likely collision to occur will be elastic. Therefore, to increase the likelihood of an ionization collision, you most likely will need to start with several hundred seed electrons. Finally, you can add secondary emission of ions hitting the sphere, which will most likely require several hundred thousand time steps for ions to travel back to the sphere. To include other collisions and a different neutral fluid background, the LXcat scattering database (https://fr.lxcat.net/data/set_type.php) can be used.

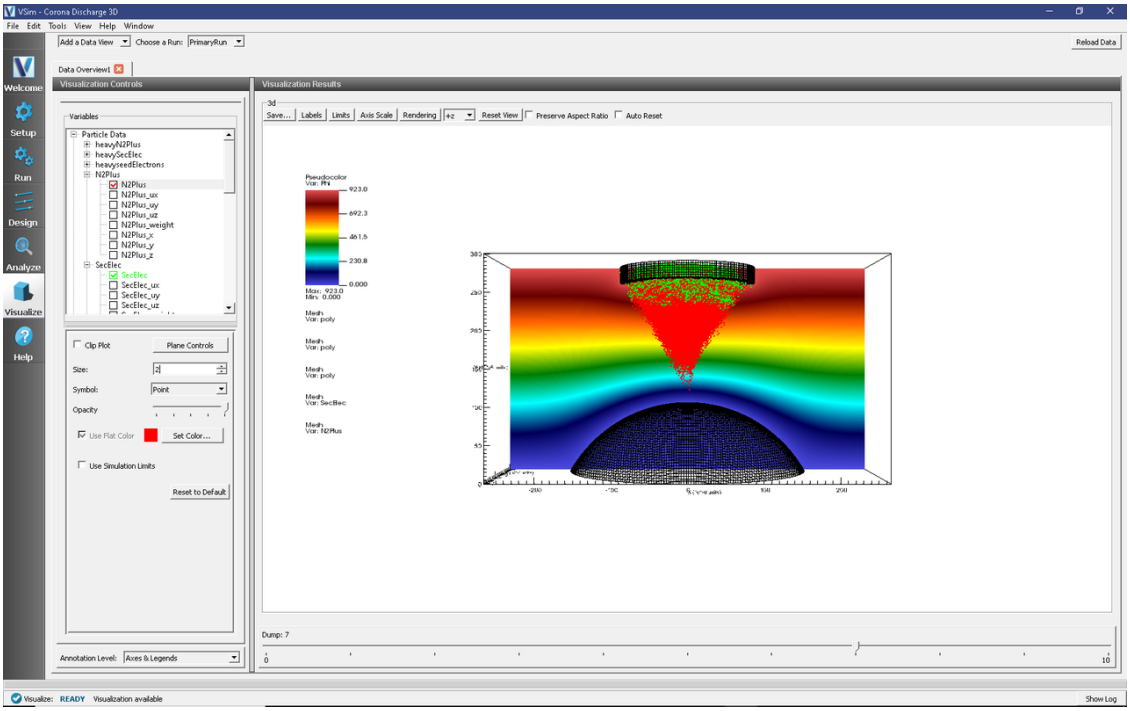


Fig. 6.65: The evolved potential with the geometries and particles superimposed.

6.6.2 Negative Ion Beam (negativeIonBeam.sdf)

Keywords:

ion beam, beam transport, reactions, electrostatic

Problem description

VSim may be used to model ion beam transport and particle dynamics where the beam is represented by kinetic simulation particles. Low density background gasses can cause instabilities in the beams due to collisions between the beam particles and the background gas.

In this simulation, a beam of H- ions propagates through a background H2 gas. Collisions between the beam ions and the background gas produce electrons, H2+, and neutral H through the following reactions:

$H^- + H_2 \rightarrow H^- + H_2^+ + e^-$ (ion impact ionization)

$e^- + H_2 \rightarrow H_2^+ + 2e^-$ (electron impact ionization)

$H^- + H_2 \rightarrow H + H_2 + e^-$ (detachment)

$H^- + e^- \rightarrow H + 2e^-$ (stripping)

There are other reactions that are not included in this tutorial simulation. Typically these reactions have low cross sections. Fig. 6.66 shows the cross sections for the above reactions as a function of incident energy.

This simulation can be performed with a VSimPD license.

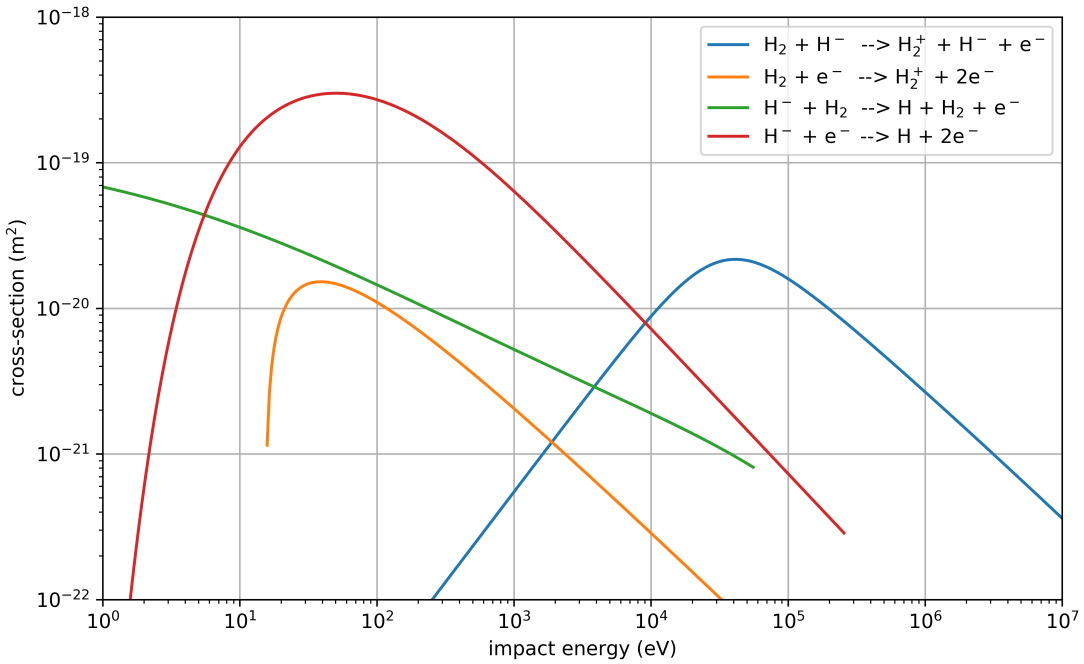


Fig. 6.66: Cross sections for the four collision reactions included in this example.

Opening the Simulation

The Kinetic Collisions example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes* option.
- Select "Negative Ion Beam" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is now shown with all the implemented physics and geometries, if applicable. See Fig. 6.67.

Simulation Properties

This input file contains a number of different kinetic species as well as a background fluid description of a gas. Ionization collisions between kinetic particles and the background gas are described by Monte Carlo interaction blocks of kind impactIonization, and detachment of electrons due to a collision with the background gas are of kind negativeIonDetachment. Collisions between kinetic particles and other kinetic particles are described in the input file by an interaction of kind binaryIonization.

The fields are electrostatically solved for at each time step, including the fields due to all charged particles, subject to the boundary conditions specified in the input file. There are a number of histories that record the number of particles for different species, their energies, as well as currents absorbed at the boundaries.

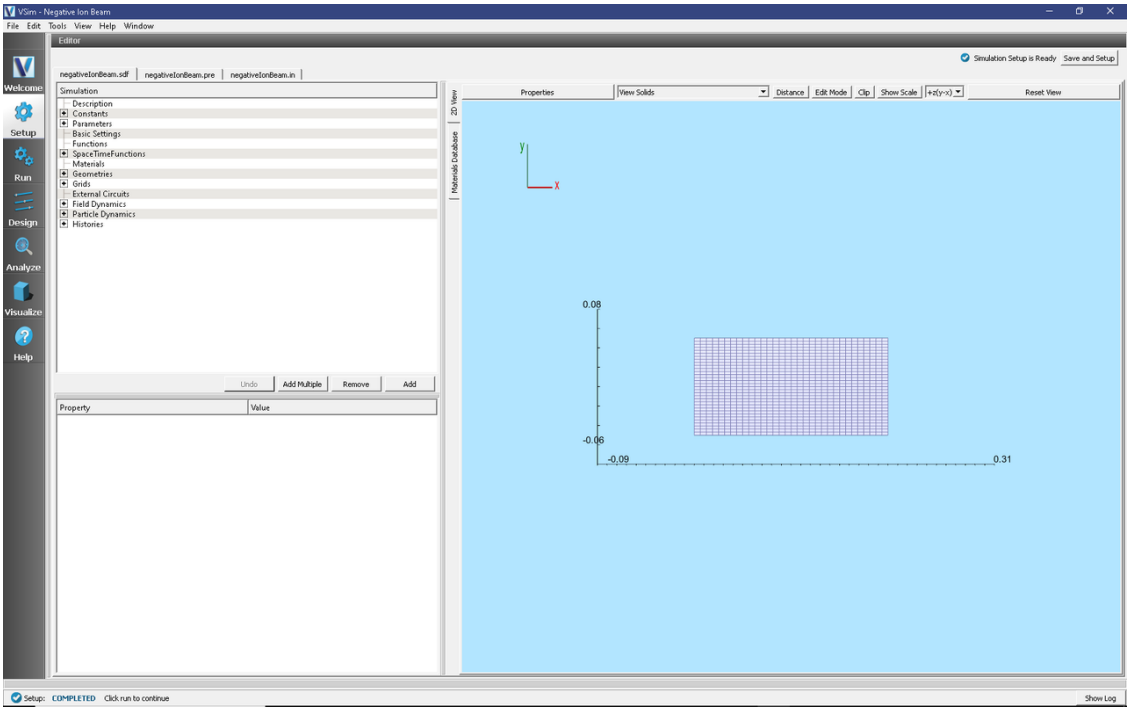


Fig. 6.67: Setup Window for the Negative Ion Beam example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 9.230165897488955e-12
  - *Number of Steps*: 6100
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.68.

Analyzing the Results

If it is desired to calculate the density of the electrons the analysis script *computePtclNumDensity.py* must be used.

- First click on the *Analyze* Tab.
- From the list of *Available Analyzers* and choose *computePtclNumDensity.py*. Then click *Open* at the bottom of the *Analysis Controls* pane.
- Ensure that the "simulationName" field is "negativeIonBeam" and enter "Electrons" in the "speciesName" field. Leave the "aveNxN" and "iterateAve" with their default values.

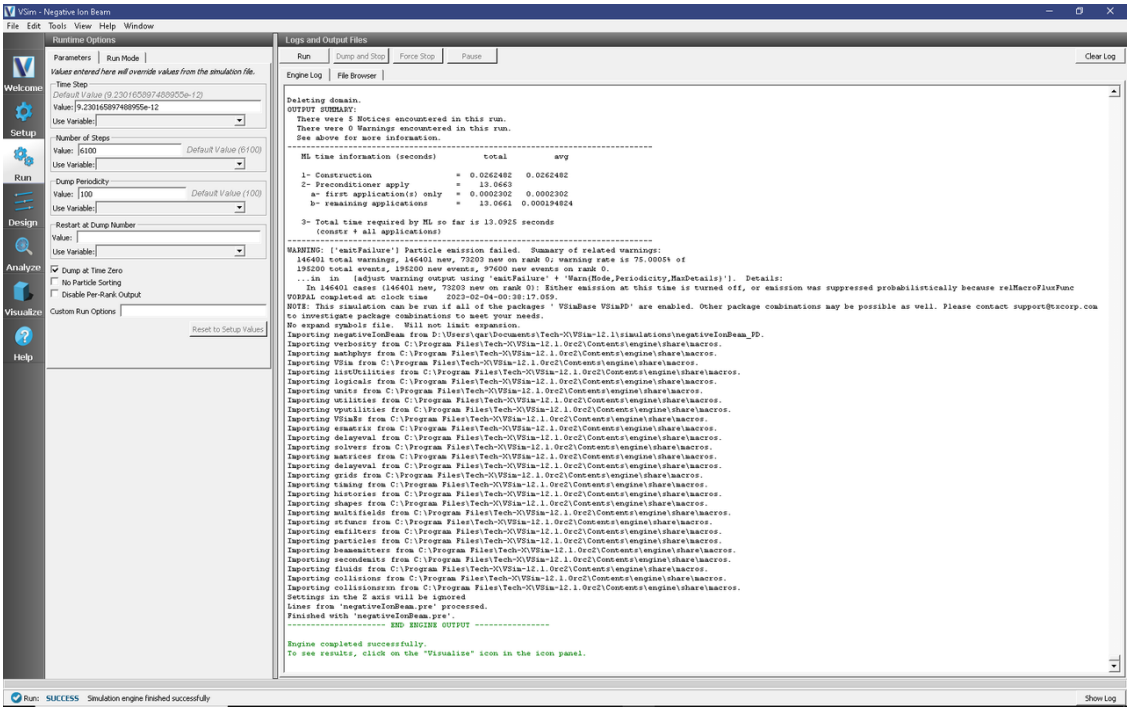


Fig. 6.68: The Run Window at the end of execution.

- Press the *Analyze* button on in the upper right corner of the window to run the analysis. Below, the Analyze Tab is shown at the end of a successful run.

The resulting data can be visualized as "ElectronsDensity" under the Scalar Data menu in the *Visualize* Tab. A plot of this data is shown below in Fig. 6.70. The density of H2plus, Hminus or Hneutral can also be calculated if those species names are used in place of "Electrons" and the analyzer is re-run. If you have previously navigated to the *Visualize* Tab, you will need to press the *Reload Data* button at the bottom of the *Visualize* Tab to view the data.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.
- Expand "Particle Data" and select "Electrons," "H," "H2Plus," and "Hminus".
- Then expand "Scalar Data" and select "Phi."
- Check the *Display Contours" box, which is below the *Variables* box in the *Visualization Controls* pane.
- Set the "# of Contours" to 20. The scroll through the dumps to produce the image in Fig. 6.71.

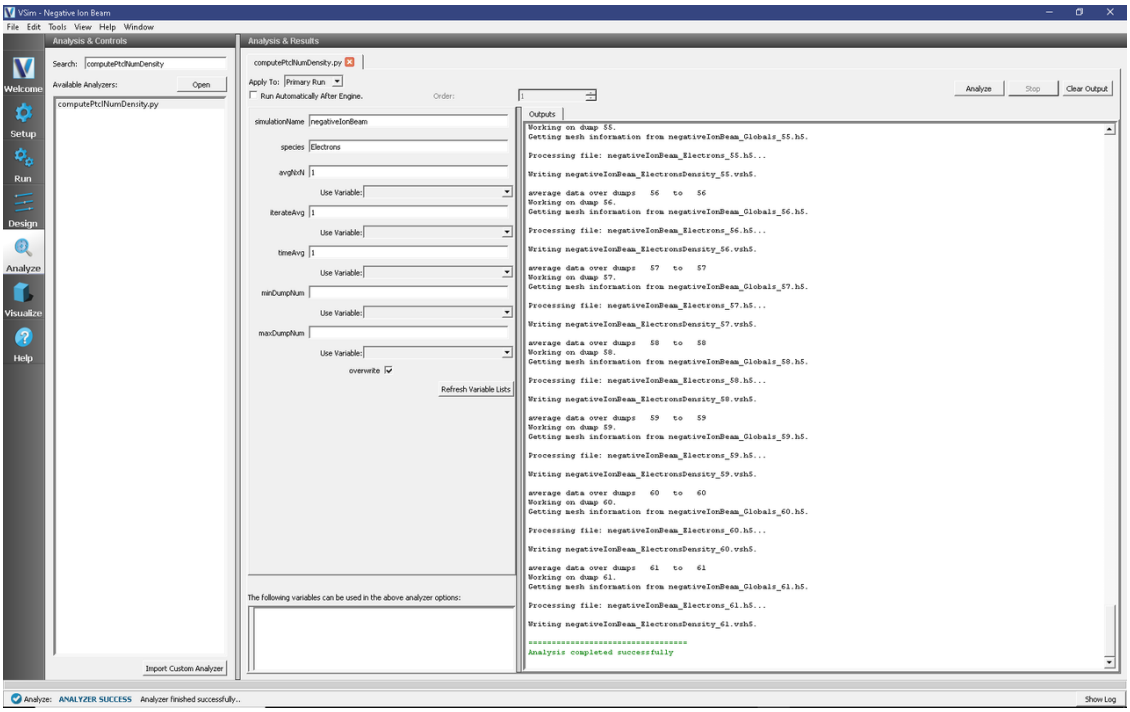


Fig. 6.69: The Analyze Window at the end of execution.

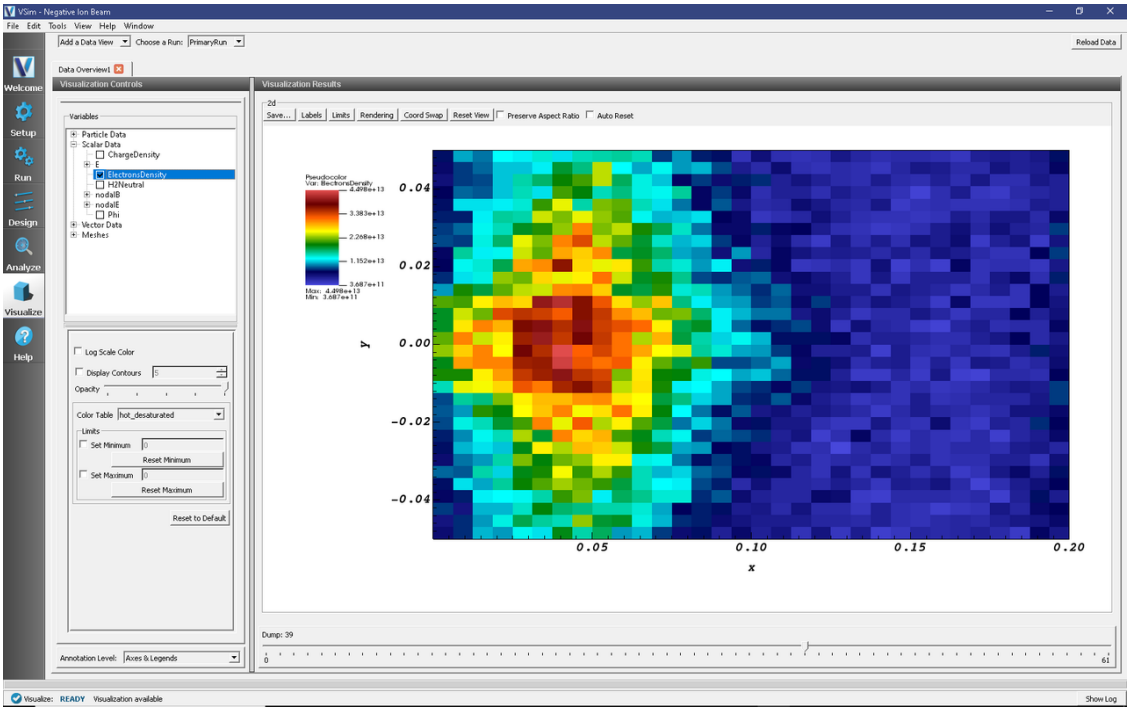


Fig. 6.70: Plot of the electron density at dump 39.

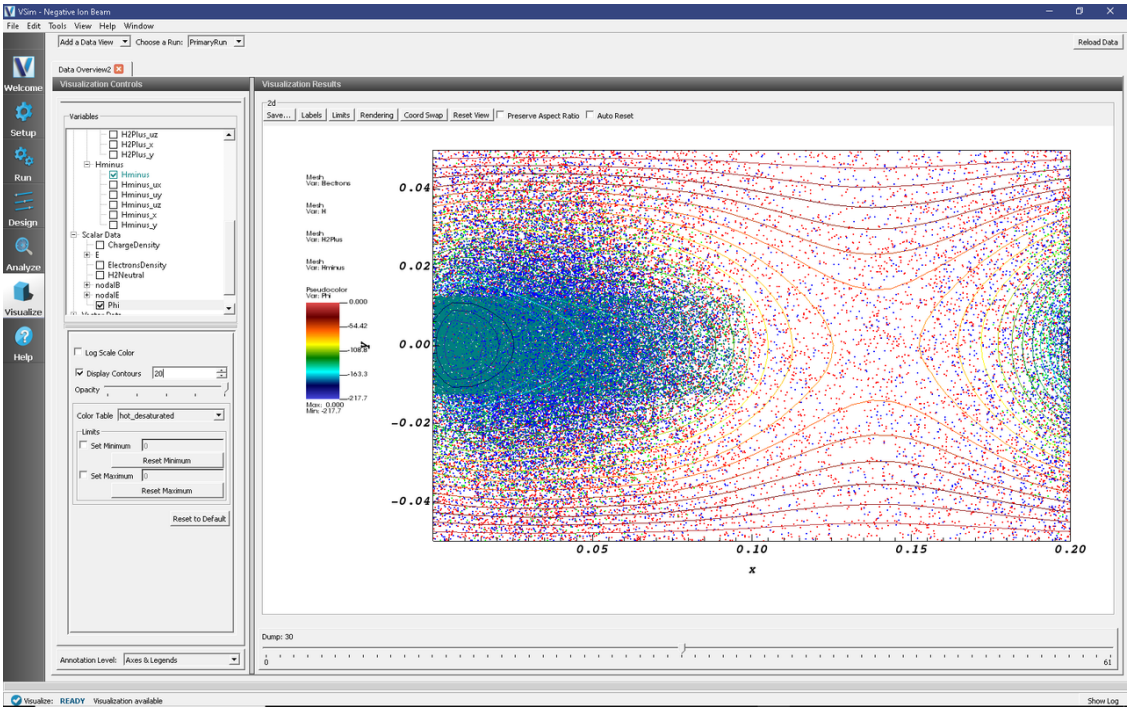


Fig. 6.71: Visualization of particle densities as a color contour plot, overlaid with a scatter plot of the particle positions.

Further Experiments

The background gas pressure is higher than one would typically see in an accelerator in this example so that the example will produce results quickly. Decreasing the pressure will give the same results, but over longer time scales.

Since this beam is negatively charged, it repulses electrons from the region near the beam. Decreasing the beam current will produce more neutralizing H2+ near the beam as the electrons can more effectively ionize the background H2 gas in that area.

6.6.3 Neutral Heat Transport DSMC (neutralHeatTransport.sdf)

Keywords:

`heat transport, DSMC, elastic collisions, reactions`

Problem description

VSim may be used to model the heat flux through a neutral gas confined between two plates of different temperatures. This problem is a common benchmark for DSMC simulations, and is described by Bird in "Molecular gas dynamics and the direct simulation of molecular gas flows" (1994) on page 280. In this example, we model the heat transport between cold (250K) and hot (1000K) plates separated by a meter. Between the plates is a volume of neutral Argon gas that transports the heat through either free-molecular motion (in the case of lower pressure) or through collisional transport via elastic collisions (in the case of higher pressure). The simulated heat flux can then be compared to the analytic result, validating the reactions framework in VSim.

This simulation can be performed with a VSimPD license.

Two videos are available demonstrating this example: https://www.youtube.com/watch?v=FFgqtJASseM&list=PLottQ0Bg2M-3ATV5O9IP-3TEC4toVYPAK&index=8 https://www.youtube.com/watch?v=WWbQ6uq1LOo&list=PLottQ0Bg2M-3ATV5O9IP-3TEC4toVYPAK&index=7

Opening the Simulation

The Neutral Heat Transport example is accessed from within VSimComposer by the following actions:

- Select the *New –> From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes* option.
- Select "Neutral Heat Transport" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is shown with all the implemented physics and geometries in Fig. 6.72.

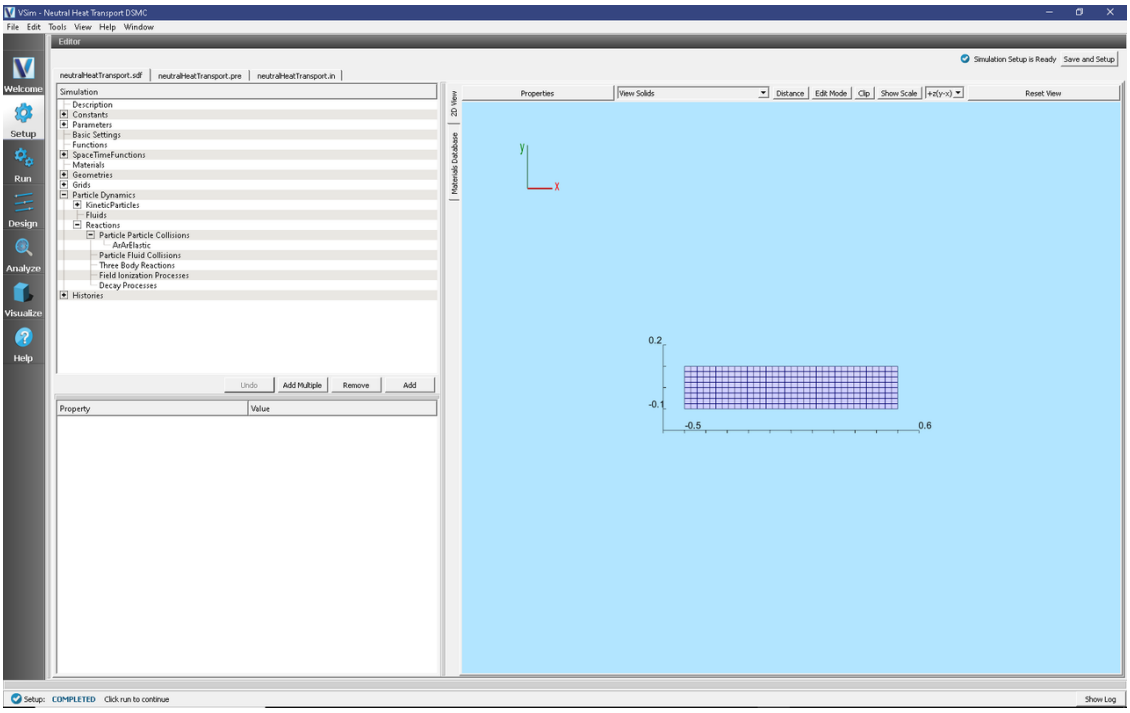


Fig. 6.72: Setup Window for the Neutral Heat Transport example.

Simulation Properties

This input file contains one kinetic species of neutral Argon, the required thermalizing boundary conditions for the hot and cold plates, and the Ar-Ar elastic collisions. The constants and parameters are set up so that the Argon pressure (ARPRES) in Pa can be changed, and the simulation grid will adjust resolution to ensure that the mean-free path is always resolved. This means that multiple simulations can be run to match the analytic result for a variety of pressures/collisionality.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.626591923643533e-06
  - *Number of Steps*: 15000
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.73.

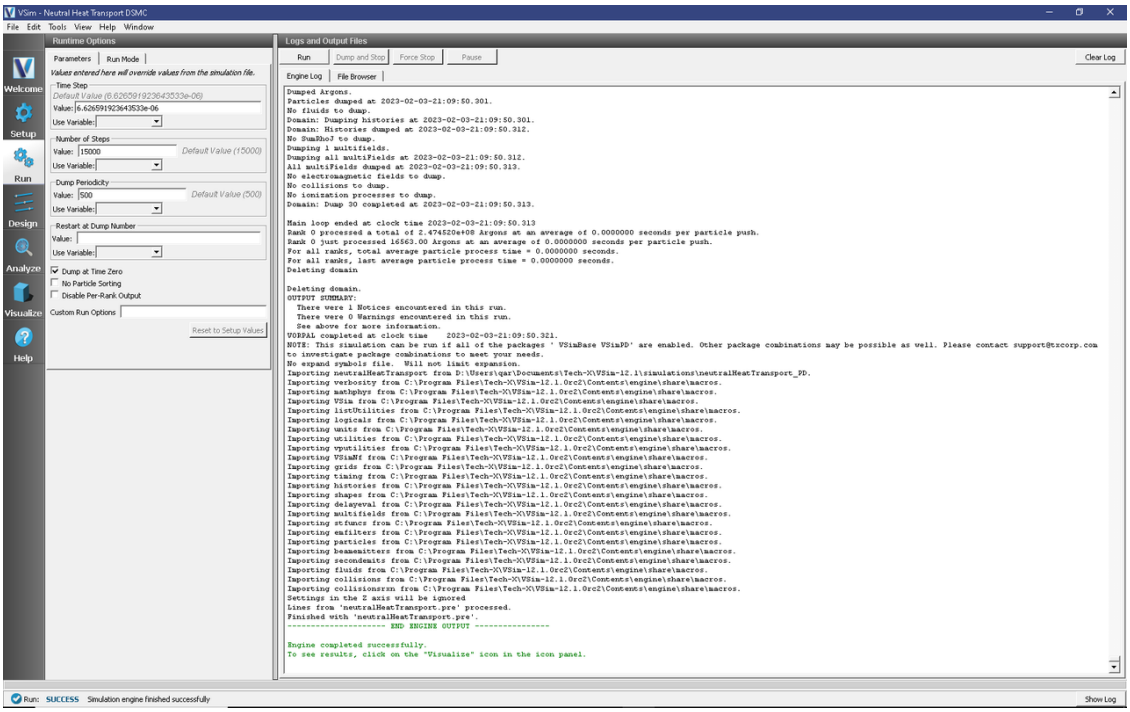


Fig. 6.73: The Run Window at the end of execution.

Visualizing the Results

After run completion, continue as follows:

- Proceed to the *Visualize* Tab by pressing the Visualize button in the left column of buttons.
- Select "History" from the *Data View* drop down menu, which is located in the upper right corner the window.

Two graphs will be shown in the resulting window (see Fig. 6.74). The first graph, ArEnergy, shows the total kinetic energy of the argon species. The second, AverageEnergyExchange, shows the average energy transferred between the particles and the plates as a function of time. The AverageEnergyExchange plot divided by the cross-sectional area of a plate gives the average heat flux. A python script, validation.py, is provided to calculate this heat flux from the

simulation data, and plot the heat flux versus the analytic heat flux. To run this script, go to the examples directory and run python from the command line (using the command "python validation.py"). The first plot is the same histories seen in the VSim Composer visualization. The second plot is the validation.

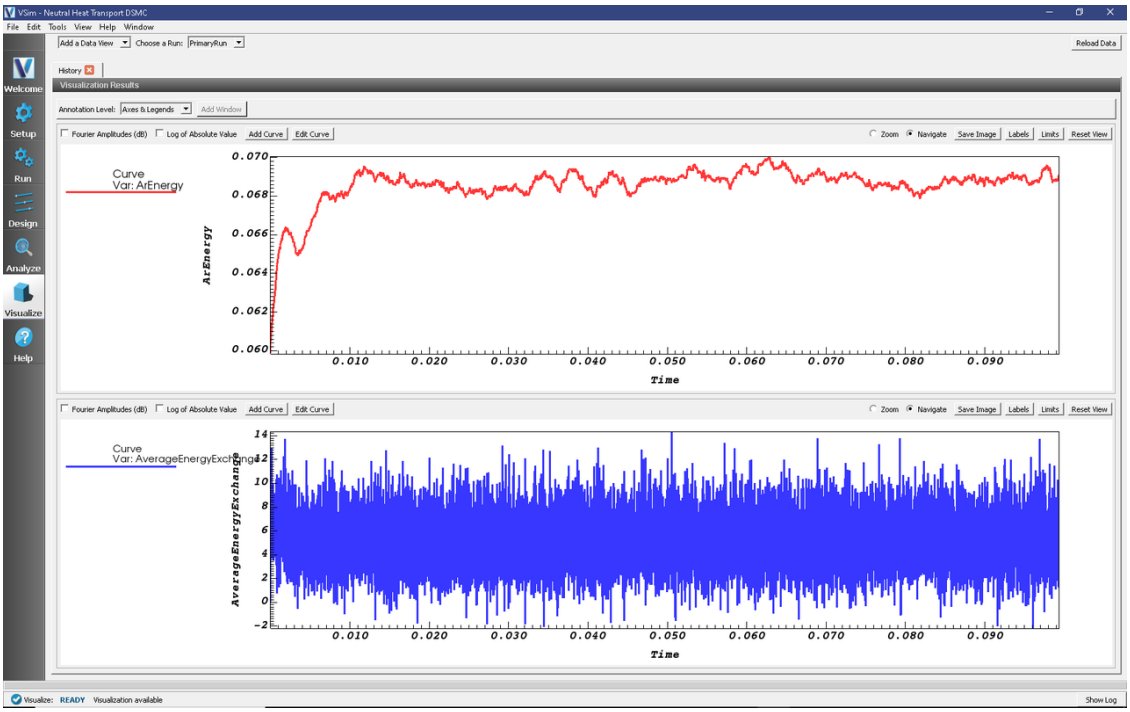


Fig. 6.74: Results from the history data collected in the simulation.

Further Experiments

As stated in the simulation properties section, simulations can be run with varying pressures (maintaining all else constant) and the resulting heat fluxes plotted against the analytic result, as shown in Fig. 6.75. The provided python script will only plot one simulation result at a time, but it can be modified easily to overplot multiple simulations. Each simulation should lie on the analytic green line. It is important to ensure that the statistics of the collisions are good enough, so when moving to lower collisionality (pressure) the number of macro particles per cell should be increased. Additionally, it is useful to switch the kinetic particle type so that it is variable weight with managed weights. This allows an isotropic macroparticle density while accounting for a variable physical particle density. Alternatively, the temperature of the plates, distance between them, species of neutral gas, etc. can all be modified to test the generality of the model and collisions.

6.6.4 Proton Beam (protonBeam.sdf)

Keywords:

electromagnetic, particle in cell, material boundary, reactions, particle emitter

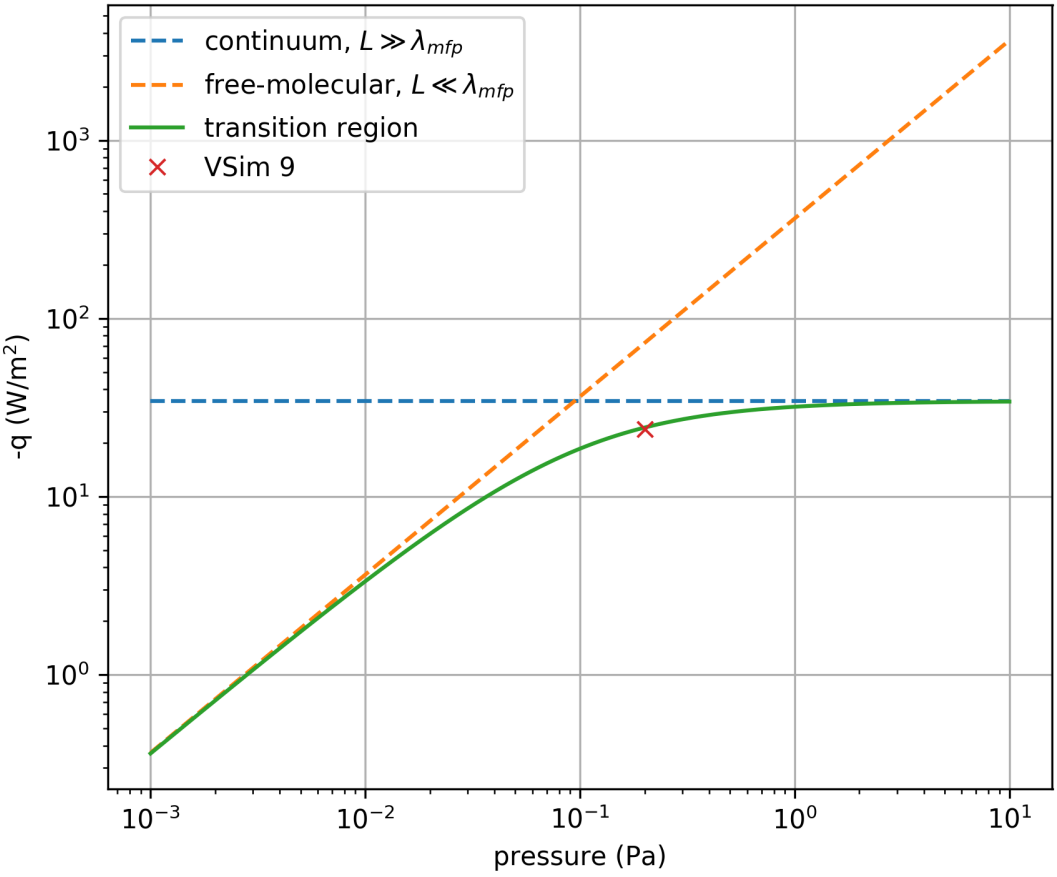


Fig. 6.75: Analytic result of heat flux compared with simulation.

Problem description

This example injects a proton beam into a column of neutral H2 gas. The geometry is setup like an electron column in an accelerator beamline (i.e. external solenoidal B-field and negative electrodes on either end for electron confinement). Upon entering the neutral gas multiple reactions begin to occur including ionization, charge exchange, dissociation, H3+ formation, and others. The beam leaves the column, leaving behind a combination of ions, electrons, and neutrals that are either confined or ejected by the background electrode potential.

In this simulation, a beam of H+ ions propagates through a background H2 gas. Collisions between the beam ions and the background gas produce electrons, H2+, neutral H, and H3+ through the following reactions:

$H^+ + H_2 \rightarrow H^+ + H_2^+ + e^-$ (ion impact ionization)

$e^- + H_2 \rightarrow H_2^+ + 2e^-$ (electron impact ionization)

$H^+ + H_2 \rightarrow H^+ + H_2$ (elastic)

$H^+ + H_2 \rightarrow H + H_2^+$ (charge exchange)

$H_2^+ + H_2 \rightarrow H_3^+ + H$ (H3+ formation)

$H_2^+ + H_2 \rightarrow H_2^+ + H_2$ (charge exchange)

$H_2 + e^- \rightarrow H^+ + H + 2e^-$ (dissociative ionization)

$H_3^+ + H_2 \rightarrow H_3^+ + H_2$ (elastic)

Fig. 6.76 shows the cross sections for the above reactions as a function of incident energy.

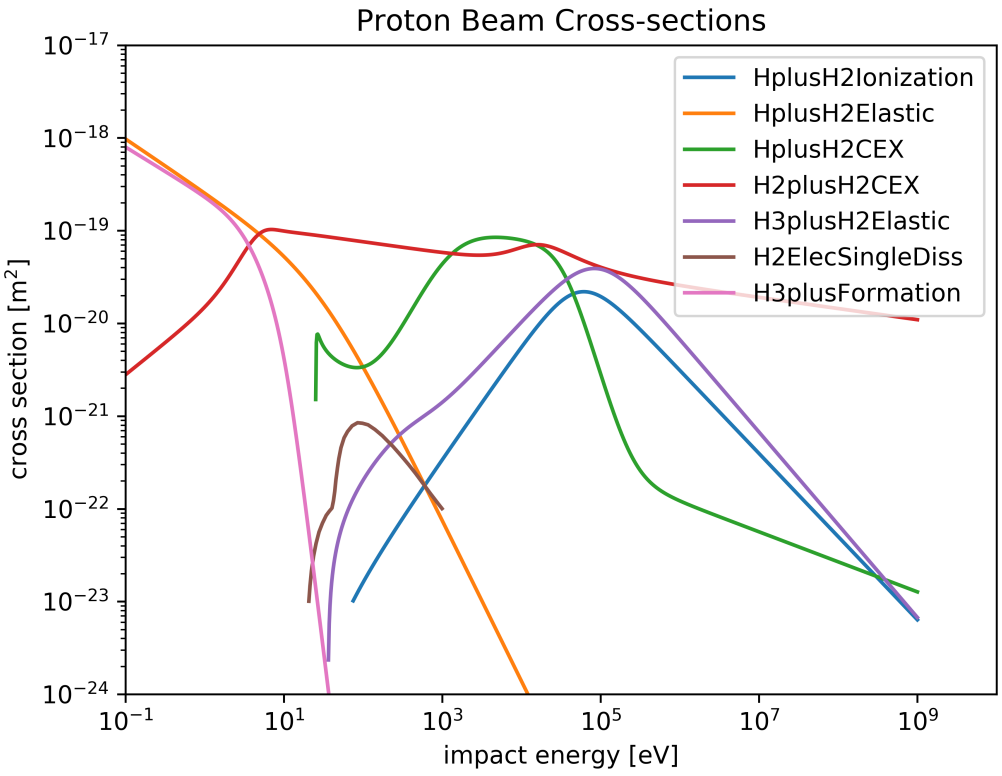


Fig. 6.76: Cross sections for the collisions included in this example.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Proton Beam example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes* option.
- Select "Proton Beam" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.77. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to Grid.

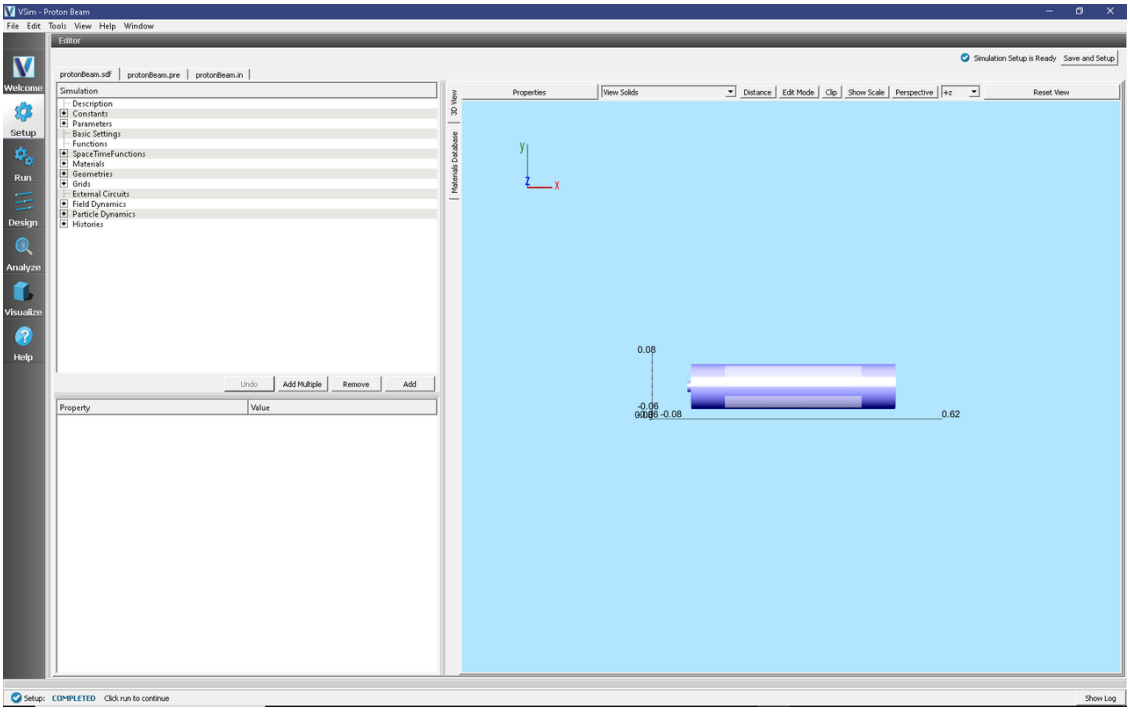


Fig. 6.77: Setup Window for the Proton Beam example.

Simulation Properties

Constants are set up to allow setting the proton beam energy and current, the background H2 pressure and temperature, and the cross-sectional size of the beam emission.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.6116568744463712e-11
  - *Number of Steps*: 5500
  - *Dump Periodicity*: 100
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.78.

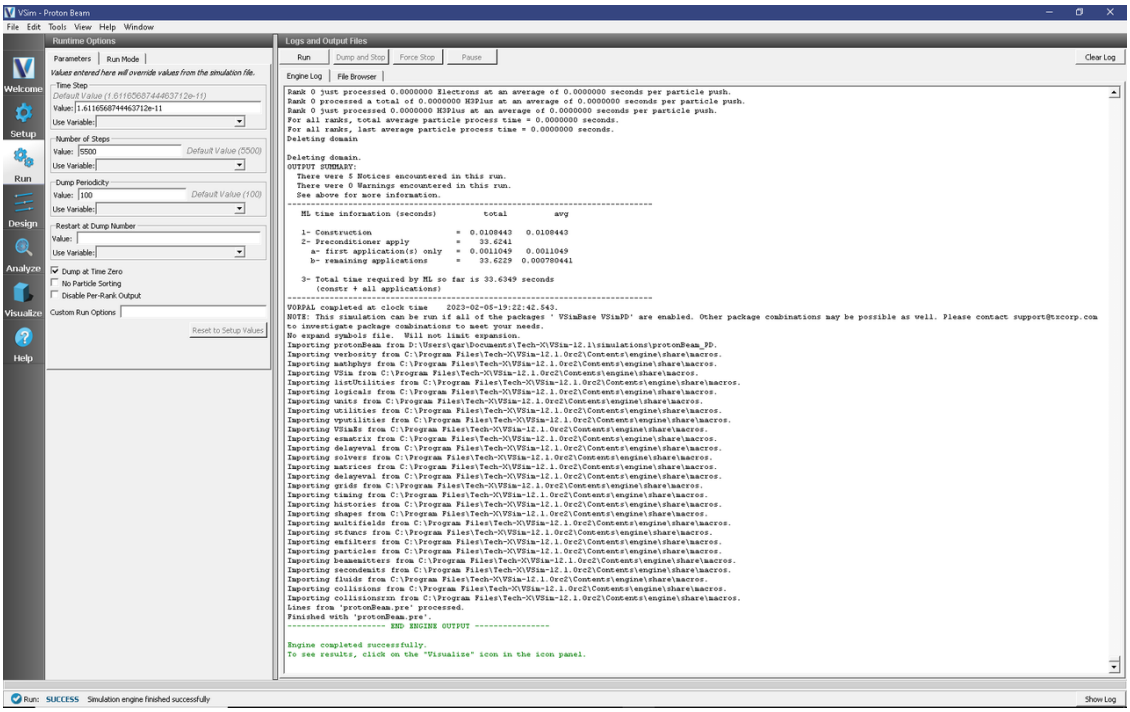


Fig. 6.78: The Run Window at the end of execution.

Visualizing the Results

We can now visualize all of the particles at a particular time slice. To do this:

- Proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons
- Expand *Particle Data* and select Electrons, H2Plus, and Hplus.
- Slide the time slider to advance the simulation in time (step 50 is shown in Fig. 6.79)

Next we can visualize the potential due to the particles and the electrodes:

- Unselect the particle data (Electrons, H2Plus, and Hplus).

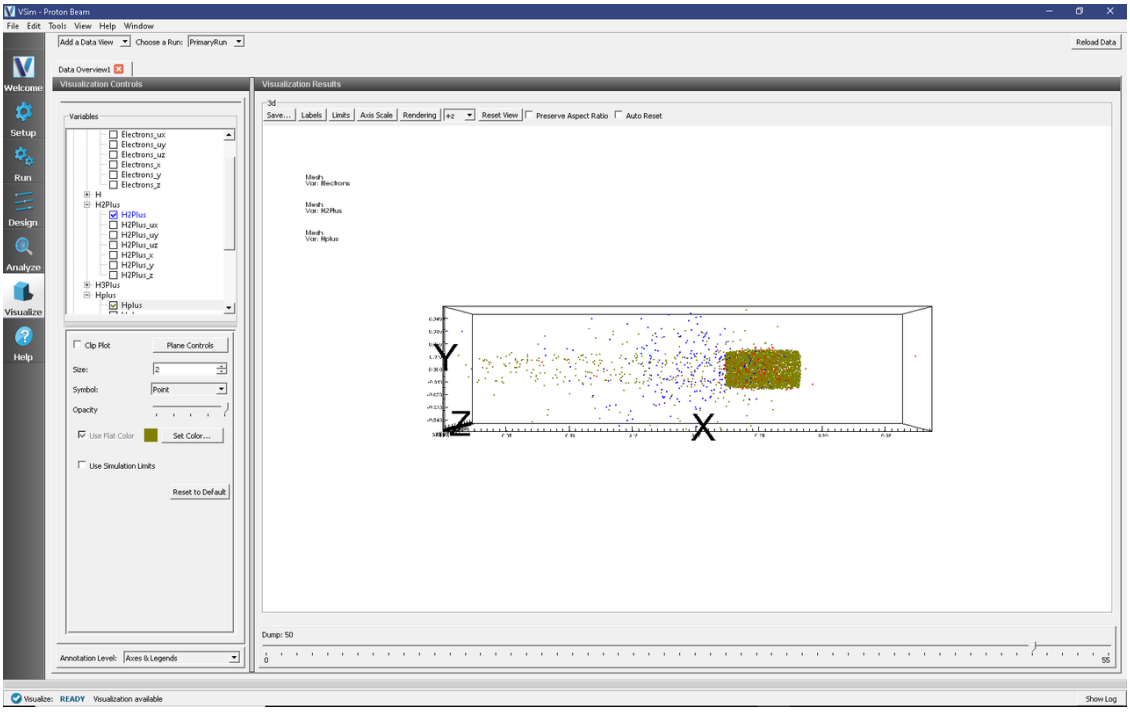


Fig. 6.79: Plot of all the particles at timestep 50. Notice that the electrons are confined by the magnetic field to the inner radius of the device. Some will also be confined by the electrodes to oscillate along the device.

- Expand *Scalar Data* and select *Phi*.
- Check the *Clip All Plots* box and scroll through the dumps.

The potential shown in Fig. 6.80 is the total potential, that is, the potential due to the static electrodes, the proton beam, and other charged species resulting from the reactions.

Further Experiments

Try changing the neutral gas pressure (which in turn will modify its density). At higher densities more reactions will occur and the proton beam will not be able to traverse the column intact. For lower densities, which are more in line with experiment, the proton beam will cause small amounts of ionization in the background gas, generating an electron cloud that is confined by the electrodes that can provide space-charge compensation for the beam. Lowering the beam energy will allow some lower energy reactions, such as H3+ formation, to occur.

6.6.5 Single Particle Circular Motion (singleParticleCircularMotion.sdf)

Keywords:

`single particle, circular motion, finite difference effects`

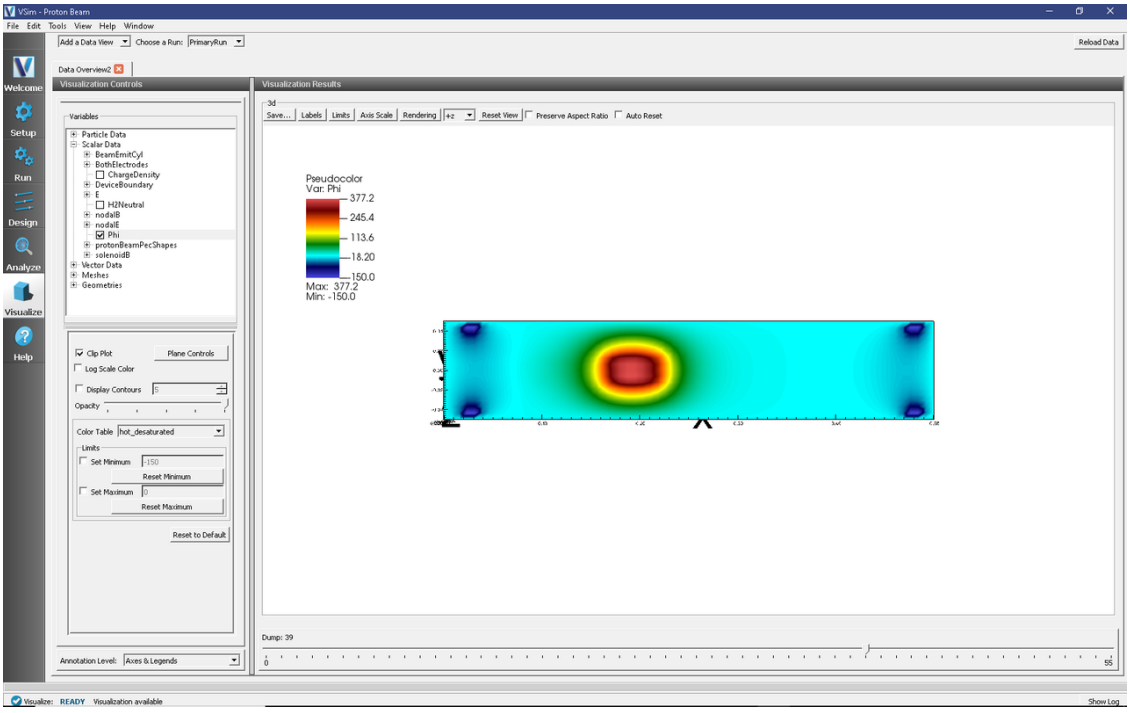


Fig. 6.80: The electrostatic potential

Problem Description

This example shows how to simulate the uniform circular motion of a single electron in a constant, uniform magnetic field in VSim. The electron is loaded inside a cylindrical capacitor with grounded walls to eliminate any stray electric fields. The electron is loaded far from the walls to reduce any effects from image charges. The magnetic field points down the positive z-axis.

Due to the finite difference algorithm utilized by VSim, two corrections must be made in order to get the electron to take a true circular trajectory. The first correction is to the cyclotron frequency. In the finite difference world of VSim, the electron does not move along a circular arc from time step to time step, instead it moves along a straight line. To correct for this we need to set our $\omega_{cyclo_{FD}} = \frac{2}{\Delta T} \arctan\left(\frac{\omega_{cyclo}\Delta T}{2}\right)$ [1] (see chapter 4 section 3).

The next correction is to account for the implementation of the Boris Method [1], the algorithm used in VSim to push particles. In the Boris Method, the position of the particle, $\vec{x}(t)$, is defined at full time steps, while the velocity, $\vec{v}(t)$, is defined at half time steps. This scheme of 'well-centered' derivatives means that VSim is automatically accurate to second order, but it means we have to be careful about our initial conditions for the electron's velocity. The initial velocity is set under Particle Dynamics → Kinetic Particle → electrons0 → particleLoader0 then velocity distribution. VSim will assume that this is the particle's velocity a **ONE HALF** time step before the start of the simulation, so we must load the particle with the velocity it would have a half time step before the start of the simulation.

This simulation can be performed with a VSimBase license.

Opening the Simulation

The Single Particle Circular Motion example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes* option.
- Select *Single Particle Circular Motion* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.81. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

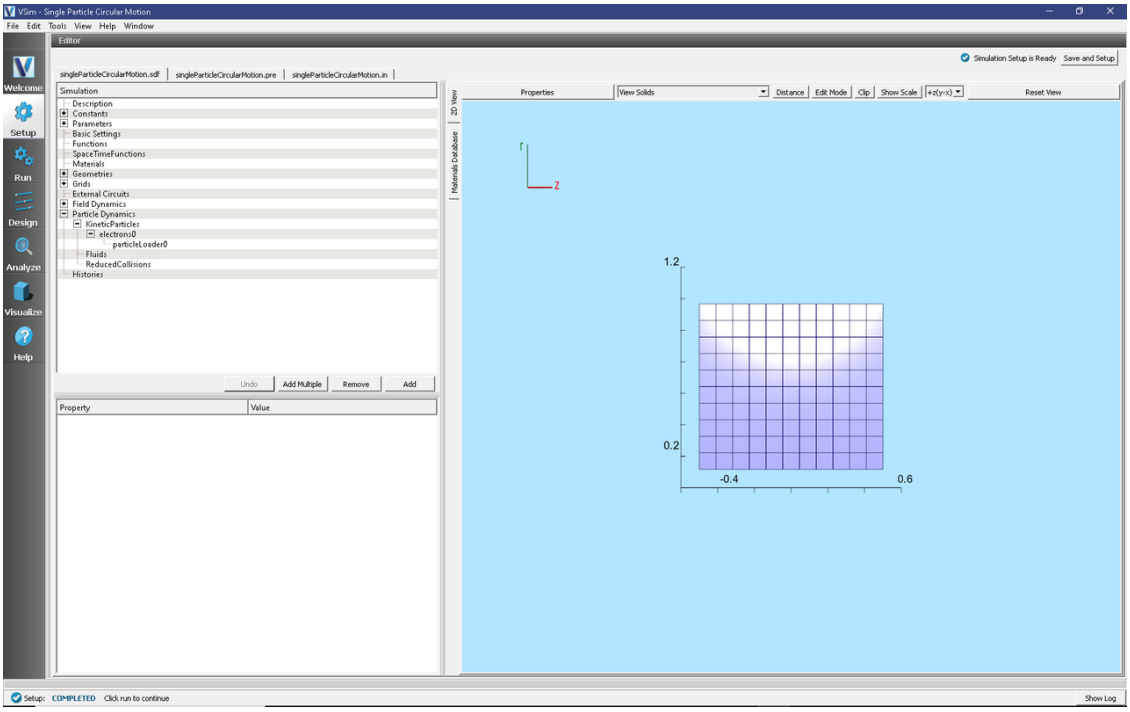


Fig. 6.81: Setup Window for the Single Particle Circular Motion example.

Simulation Properties

The Single Particle Circular Motion example includes some constants for easy adjustment of simulation properties:

- B0: The magnitude of the magnetic field
- VOLTAGE_OUTER and VOLTAGE_INNER: sets the value of the radial electric field experienced by electron (default value for both is zero)

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 5.685630103565723e-07
  - *Number of Steps*: 100
  - *Dump Periodicity*: 1
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.82

In serial, this simulation only takes seconds to run.

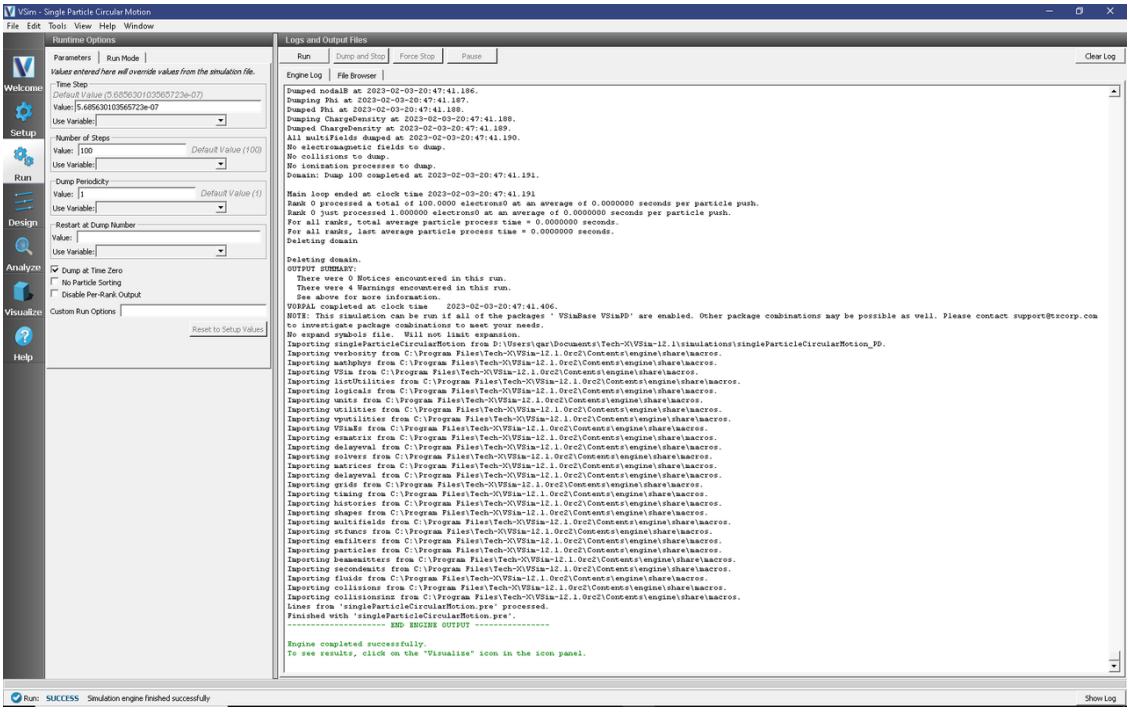


Fig. 6.82: The Run Window at the end of execution in serial.

Visualizing the results

After performing the above actions, continue as follows:

Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

- In the Visualize Window, expand 'Particle Data' then 'electrons0' and check the box next to the red 'electrons0.' This will plot our single electron.
- Expand 'Meshes' then 'globalGridGlobal' and check the box next to 'globalGridGlobal (ChargeDensity)' as shown in Fig. 6.83.
- Scroll through the dump slider (found below the plot), the electron will be stationary because the axial coordinate (phi) has been compressed. This means the electron remains at the same r and z coordinate (this is a 2D simulation).

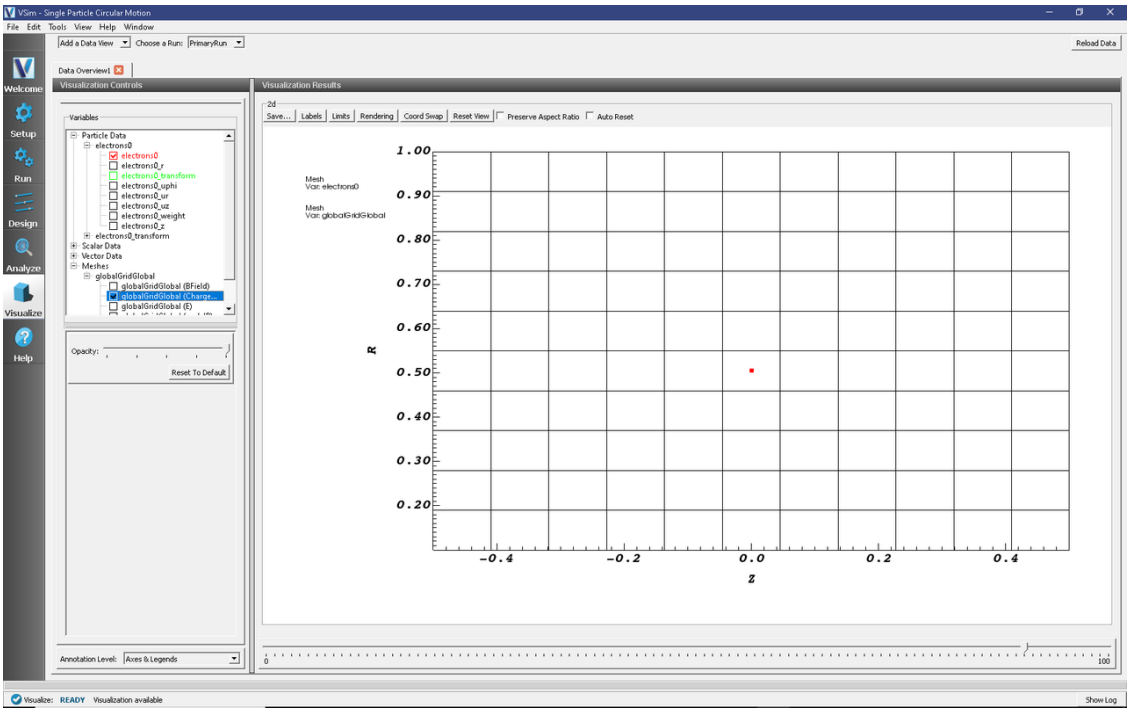


Fig. 6.83: Visualization of Single Particle Circular Motion at dump 100.

Further Experiments

Simulations are correct only to some accuracy. The corrections we made to the cyclotron frequency and the initial velocity make this simulation correct to second order. By looking at the phase space plot, we can explore the second order accuracy of this simulation. Navigate to the Visualize Window, select 'Phase Space' from the 'Data View' drop down menu, and plot 'electrons0_r' vs 'electrons0_ur.'

As you scroll through the dumps for the first time (with the 'Auto Reset' box UN-checked), the axes will adjust. The particle is taking an elliptical path in phase space. In a perfect simulation, the electron would remain at the same position in phase space with constant radius and zero radial velocity. Instead, the electron oscillates between the positions $r = 0.50500$ m and $r = 0.50542$ m for a $\Delta r = 0.00042$ m. Cut the time step in half and double the number of timesteps taken (so that the simulation runs through the same amount of time). Now look at the phase space plot again. By approximately what factor did Δr drop? Since the simulation is correct to second order, dropping the time step by a factor of 2 should drop the error by a factor of 4.

Other things you can play around with:

- Reset the electron speed, electron loading position, or the cyclotron frequency, OMEGA, back to the uncorrected versions and redo the error analysis described above.
- Change the values for VOLTAGE_INNER and VOLTAGE_OUTER to see the effects of a radial electric field on the single electron.

References

[1] Birdsall, C. K., & Langdon, A. B. (1985). Plasma Physics via Computer Simulation. New York: McGraw-Hill.

6.6.6 Townsend Discharge (townsend.sdf)

Keywords:

background gas, particle emission, ionization, inelastic anisotropic scattering

Problem Description

In a Townsend avalanche, electrons are accelerated by an electric field and ionize a background gas of neutral atoms or molecules. Each ionization event creates an additional electron that will also be accelerated and eventually produce more ionization events of its own. This process of repeated doubling results in an exponential increase in the number of electrons. The Townsend avalanche occurs when the electron and ion densities are too low to behave collectively and form a plasma.

This type of discharge is named after John Townsend who first proposed (c. 1897) the ionization model to explain the phenomena. In his experiments, Townsend measured the current across a gas-filled chamber with a pair of parallel plates on the two ends. Townsend illuminated the cathode plate with X-rays which produced electrons via the photo-electric effect. Townsend noticed that the current between the plates depended on the strength of the electric field between the plates and the pressure of the gas.

His observations lead to the conclusion that electrons were ionizing the gas and causing an exponential increase in the measured current. The current measured across the discharge chamber is described by the following formula:

$$\frac{I(x)}{I_0} = \frac{e^{\alpha(x-x_0)}}{1-\gamma(e^{\alpha(x-x_0)}-1)}$$

where I_0 is the photo-current produced by the X-rays, $I(x)$ is the current through the chamber as a function of the plate separation, x. The parameter x_0 is a characteristic distance that a collection of electrons has to travel away from the cathode before an equilibrium is reached. The parameters α and γ are the first and second Townsend coefficients, respectively. The first Townsend coefficient, α is a measure of how many ionization events a single electron will produce per unit length, and γ is a parameter accounting for electron generation from secondary processes, like ion impact at the cathode.

In this example simulation, we will loosely follow the experimental setup of L.M. Chanin and G.D. Rork who measured the first Townsend coefficient for Helium [CR64a], Neon, and Hydrogen [CR64b] in the 1960s. For low voltage discharges, the factor γ is negligible and the equation above reduces to:

$$I(x) = I_0 e^{\alpha(x-x_0)}.$$

In reality, α is a complicated function of pressure, accelerating field, and the species of background gas molecule/atom. Chapter 14 section 3 of *Principles of Plasma Discharges and Materials Processing*, [LL05] presents an analytical model for α as a function of pressure and electric field and provides the fitting constants for different gases. This simulation will estimate a value for α for a Helium gas keeping the electric field and pressure constant at $E = 2.12e5$ V/m and

$p = 21.2$ torr. It should be noted that Chanin and Rork [CR64a] measure to find α/p_0, rather than α directly. At this pressure and electric field, the accepted value for α/p_0 is 1.3 [CR64a], [LL05].

This simulation can be run with a VSimPD license.

Opening the Simulation

The Townsend Avalanche example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes* option.
- Select *Townsend Avalanche* and press the *Choose* button.
- In the resulting dialog box, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

The resulting Setup Window is shown Fig. 6.84.

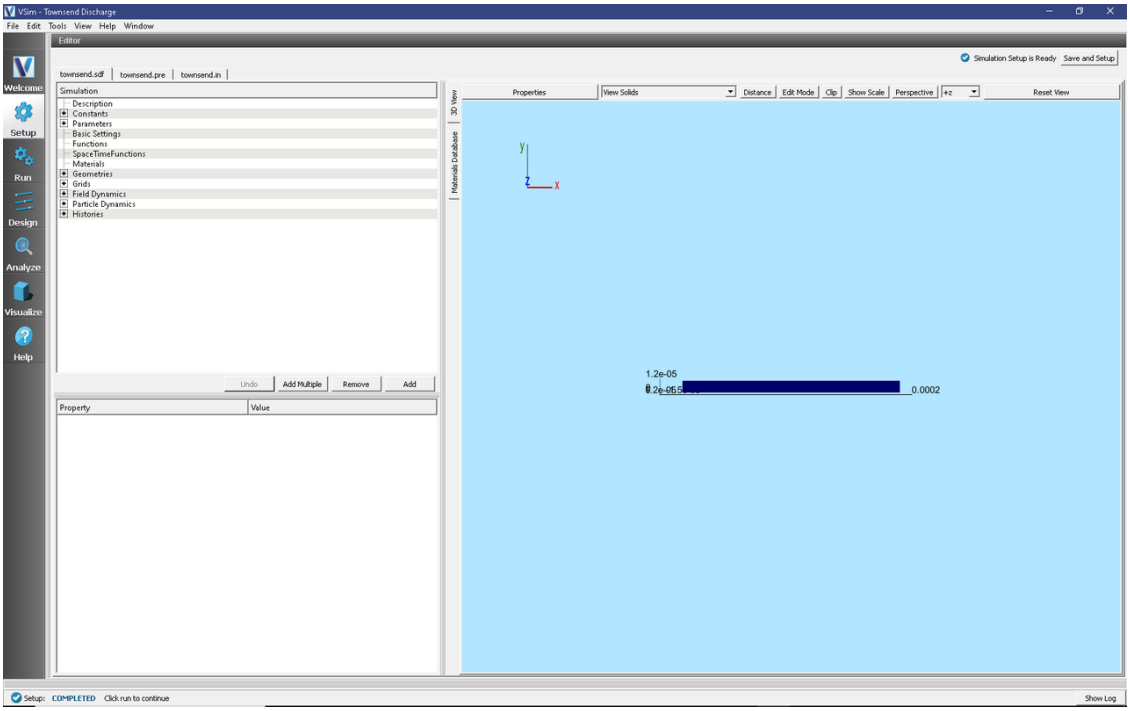


Fig. 6.84: Setup Window for the Townsend Avalanche example.

Simulation Properties

In order to calculate a value for the Townsend coefficient, this simulation will need to be run multiple times at different plate separations while keeping the electric field and pressure constant. This parameter scan of plate separations can be done within the Design Tab, which is explained in *Parameter Scan*.

The data points from these multiple runs will be used in a least squares fit to an exponential function of the form:

$$F(x) = Ae^{\alpha(x-\beta)}$$

where α and β are the constants being fitted, with α being the Townsend coefficient of interest. Details on how to fit the data yourself is covered in the section **Computing the Townsend Coefficient** below.

The simulation input file is set up to allow for rapid iteration on the multiple plate separations. The *voltageDifference* actually controls the separation of the two plates in such a way that keeps the electric field constant; it is also used to calculate an estimate for the maximum electron speed which goes into determining the time step.

In **Basic Settings** the field solver is set to *prescribed fields*. This means we manually set the electric field as a function of space (and have an option to add time dependence). In the **Field Dynamics** element, under `Fields` is where we actually set the value for the constant electric field present between the two plates at either end of the discharge tube. In the `externalElectricField` element we set `component0`, the x-component of the electric field to a value calculated from the parameters in [CR64a].

The **Particle Dynamics** element is where we set up the which particle species the simulation will contain, how particles of each species get added and removed from the simulation, and in what processes/interactions they participate.

This simulation contains an electron species, a positive helium ion species, and a background gas of helium neutral gas. The `settableFluxSlabElectronEmitterCW0` is set up to emit a total of 100,000 physical electrons. Both the electron and helium ion species have been set up such that each macro particle corresponds to a single physical particle.

The electric field points from upper x (right side of screen) to lower x (left side of screen). The electrons are emitted into the simulation from the lower x and are accelerated to the right. There are seven interactions in which an electron can be involved as it crosses the simulation grid. These processes are set in the `Reactions` element, which has been enabled by choosing *include particles* and *reactions* in **Basic Settings.**

The processes included in this simulation are electron/neutral helium elastic scattering, five different electron/neutral helium excitation processes in which electrons lose some energy to putting a neutral helium atom into an excited state, and an electron/neutral helium ionization process which is the crucial bit of physics for this simulation. We found that the it was important to use the reaction type `Inelastic Electron Scattering` with `scatter type` set to *VahediSurendra* for getting an accurate value for the Townsend coefficient.

To add collision processes to VSim, cross-sections data must be supplied by the user. To get the most accurate results from this validation study, we used cross sections from the LXCat database. According to the terms of the database, we are not permitted to distribute data obtained from the database, so the data included as part of this example is less accurate. The "Obtaining Cross-sections from LXCat" section in the Reference Manual contains a set of instructions for obtaining the more accurate cross-section data for yourself.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: DT: 1.32369e-12
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 40

  - *Dump at Time Zero*: Checked

- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.85.

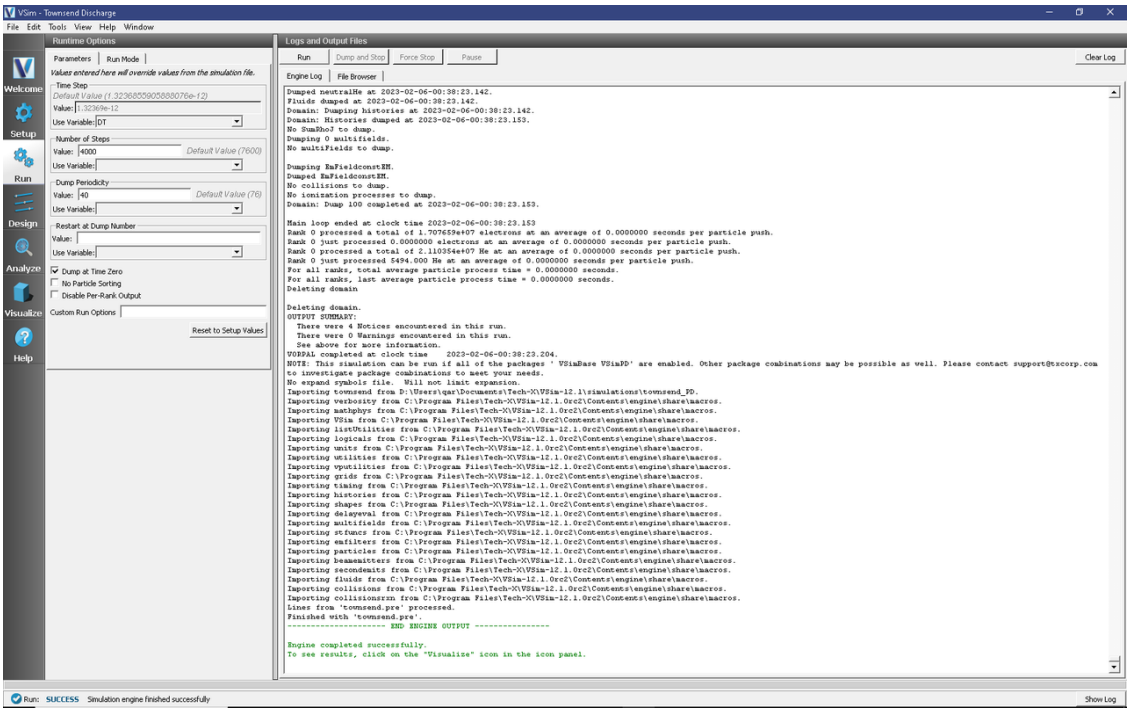


Fig. 6.85: The Run window at the end of execution.

Parameter Scan

In order to start a parameter scan

- Proceed to the design window by pressing the Design button in the left column of buttons.
- The left sub-panel, Runtime Options, of the Design window contains several sub-elements
- Within the Setup sub-element we can edit the Scan Name and we can Add Parameter(s) to iterate over.
- Here we are iterating over the constant *voltageDifference*
- The Model Choice drop-down menu has two options: List and Range.
  - For the *voltageDifference* constant, the model choice has been set to List.
  - The list should have seven (7) values to scan over (40, 60, 80, 100, 120, 140, 160).
- Below the Model Choice and options, is the Run Settings sub-element.
  - Here you can set the scan/run parameters, including how many cores to run with.
- The Default settings is to do serial runs for each parameter choice with the max concurrent runs equal to the licensed number of cores.
- When you are finished setting run parameters, click on the *Run* button in the upper left corner. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully." This is shown in Fig. 6.86.

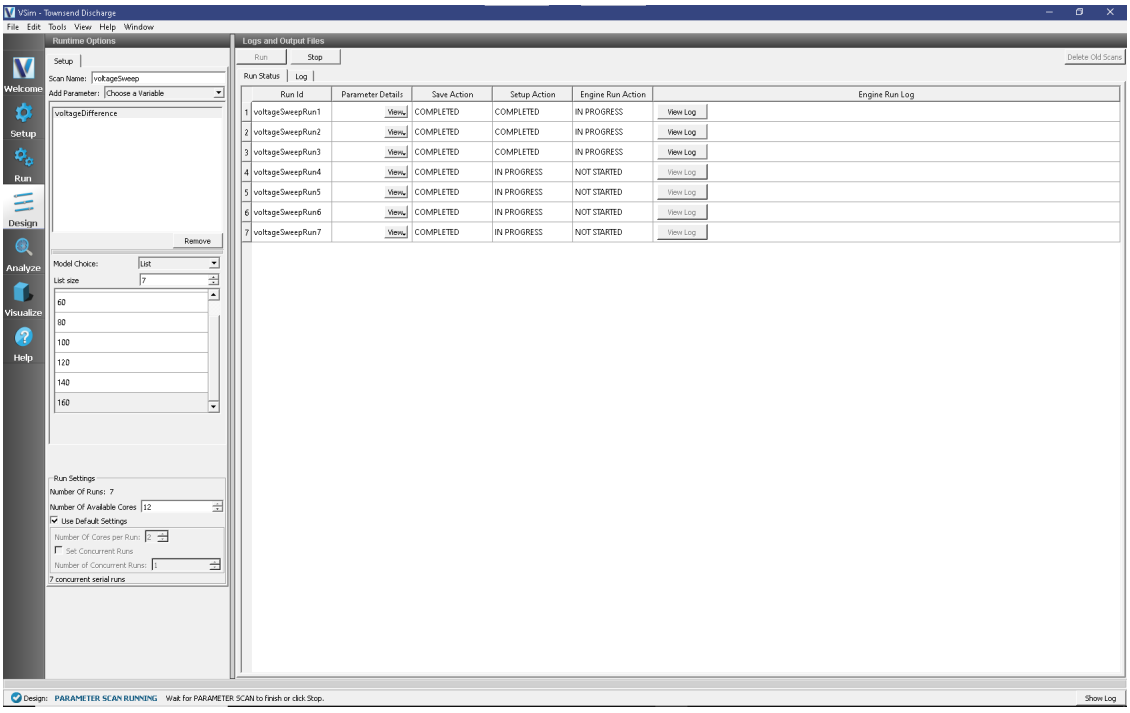


Fig. 6.86: The Design window at the end of execution.

Computing the Townsend Coefficient

To collect enough data and make a fit to

$$\frac{I(x)}{I_0} = e^{\alpha(x-x_0)}$$

this simulation will need to be run multiple times with different plate separations. Since the electric field is constant, different plate separations correspond to different voltage differences between the right and left plates. As the plates get further apart, electrons will have more space to accelerate and ionize the neutral helium gas. Since the total number of helium ions created in collisions with electrons depends on the total number of electrons in the space between the two electrodes, the exponential form of the equation above is expected.

The Design Tab allows for easy modification of the the plate separation and running of multiple concurrent simulations.

If the user prefers to modify these values by hand:

> To adjust the plate separation, change the *voltageDifference* constant which is under **Constants** in the setup tree. The simulation will open with this constant set to 40 volts. When we performed this study, we ran at voltages of 40, 60, 80, 100, 120, 140, and 160 volt differences.

Following the generation of this data for volt differences, we then ran *scanAnalyzerTownsend.py* which can extract the data from the simulation folders generated via a Scan. The scan analyzer will then produce $\frac{\alpha}{p_0}$. as seen in Fig. 6.87.

scanAnalyzerTownsend.py requires the scanName and the number of simulations run in the scan, along with some other values; it then computes the townsend coefficient. This is done by obtaining several values from each simulation:

- The voltage difference between plates,
- The electron current on the upper X absorber (i.e. downstream of the ionizing reactions).
- The step size, dt

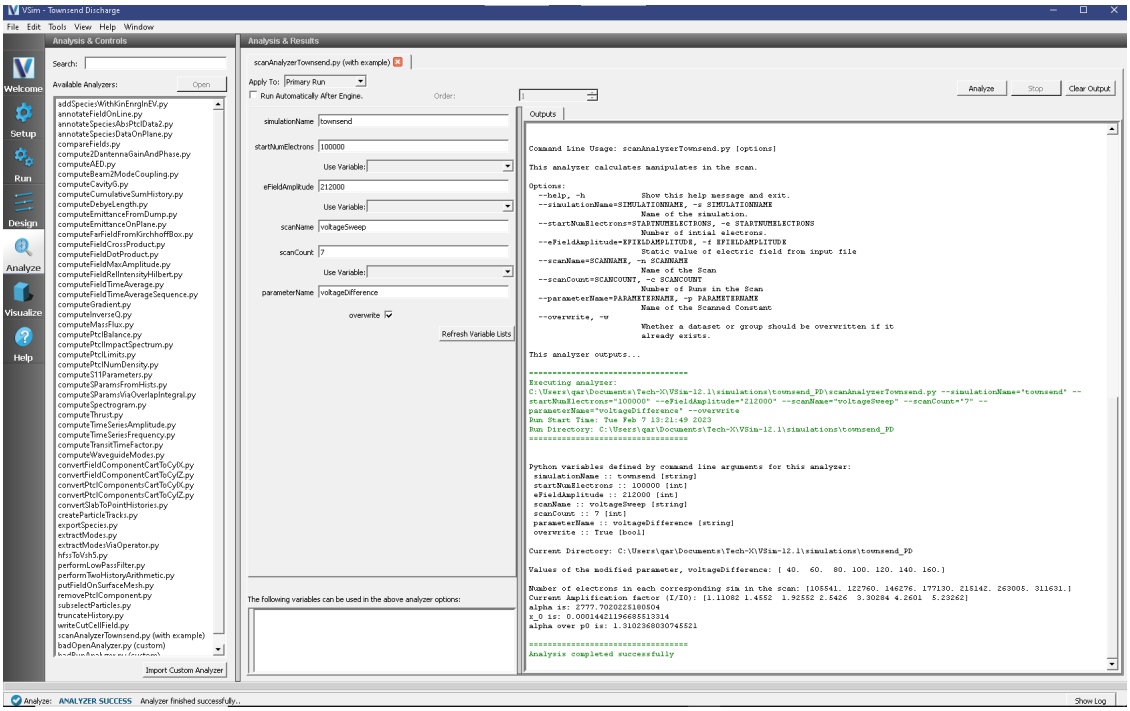


Fig. 6.87: The Analyzer window at the end of execution.

Using the electron current on the upperXAbsorber, dt, the initial number of electrons and the elemental charge, we can calculate the number of electrons that are produced. Note, we consider each particle to represent one "unit" of current, in that $I_{unit} = Q_{elementary}/dt$.

The number of electrons produced is useful as we can then determine the current amplification factor associated with each voltage difference.

The analyzer then calculates α and x_0 from the separation between plates and the current amplification factor. It does so via statistical averages of those values in order to determine a slope and intercept, similar to $y = m * x + b$. The slope, m is our α, while x_0 is the negative of the intercept over the slope. The analyzer prints both α and x_0 before printing the value of interest, $\frac{\alpha}{p_0}$. As a reminder to the reader, we are looking to compare to Chanin/Rorks' $\frac{\alpha}{p_0}$, as those are the experimentally provided values.

Further Experiments

1. Run the simulation at a different pressure to measure the Townsend coefficient in a different regime.
2. Change the gas type by switching the ion species, gas species, and cross-sections.

6.7 Processes (text-based setup)

6.7.1 Neutral Heat Transport DSMC (text-based setup) (neutralHeatTransportT.pre)

Keywords:

heat transport, DSMC, elastic collisions, reactions, reaction diagnostics

Problem description

VSim may be used to model the heat flux through a neutral gas confined between two plates of different temperatures. This problem is a common benchmark for DSMC simulations, and is described by Bird in "Molecular gas dynamics and the direct simulation of molecular gas flows" (1994) on page 280. In this example, we model the heat transport between cold (250K) and hot (1000K) plates separated by a meter. Between the plates is a volume of neutral Argon gas that transports the heat through either free-molecular motion (in the case of lower pressure) or through collisional transport via elastic collisions (in the case of higher pressure). The simulated heat flux can then be compared to the analytic result, validating the reactions framework in VSim. The text-based version of this example includes the ability to monitor collision frequencies across the domain as the simulation progresses.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Neutral Heat Transport example is accessed from within VSimComposer by the following actions:

- Select the *New –> From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Processes (text-based setup)* option.
- Select "Neutral Heat Transport (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* is shown with all the implemented physics and geometries in Fig. 6.88.

Simulation Properties

This input file contains one kinetic species of neutral Argon, the required thermalizing boundary conditions for the hot and cold plates, and the Ar-Ar elastic collisions. The constants and parameters are set up so that the Argon pressure (ARPRES) in Pa can be changed, and the simulation grid will adjust resolution to ensure that the mean-free path is always resolved. This means that multiple simulations can be run to match the analytic result for a variety of pressures/collisionality.

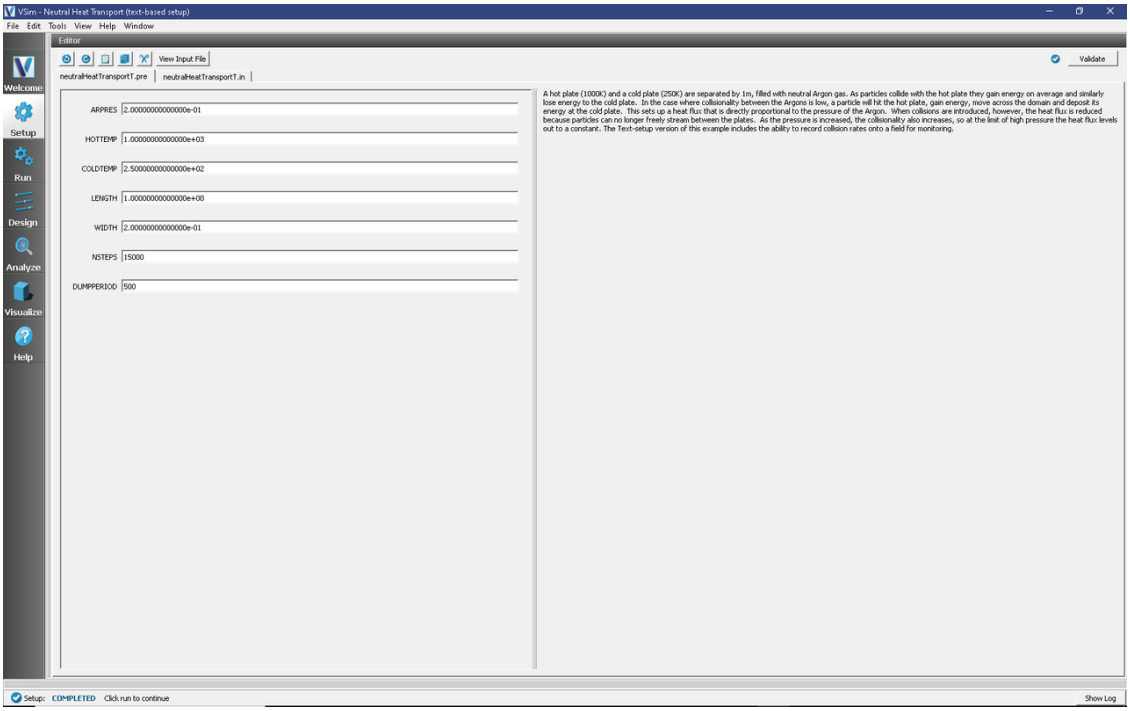


Fig. 6.88: Setup Window for the Neutral Heat Transport example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.626591923643533e-06
  - *Number of Steps*: 15000
  - *Dump Periodicity*: 500
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.89.

Visualizing the Results

After run completion, continue as follows:

- Proceed to the *Visualize* Tab by pressing the Visualize button in the left column of buttons.
- Select "History" from the *Data View* drop down menu, which is located in the upper right corner the window.

Two graphs will be shown in the resulting window (see Fig. 6.90). The first graph, ArEnergy, shows the total kinetic energy of the argon species. The second, AverageEnergyExchange, shows the average energy transferred between the particles and the plates as a function of time. The AverageEnergyExchange plot divided by the cross-sectional area of a plate gives the average heat flux. A python script, validation.py, is provided to calculate this heat flux from the

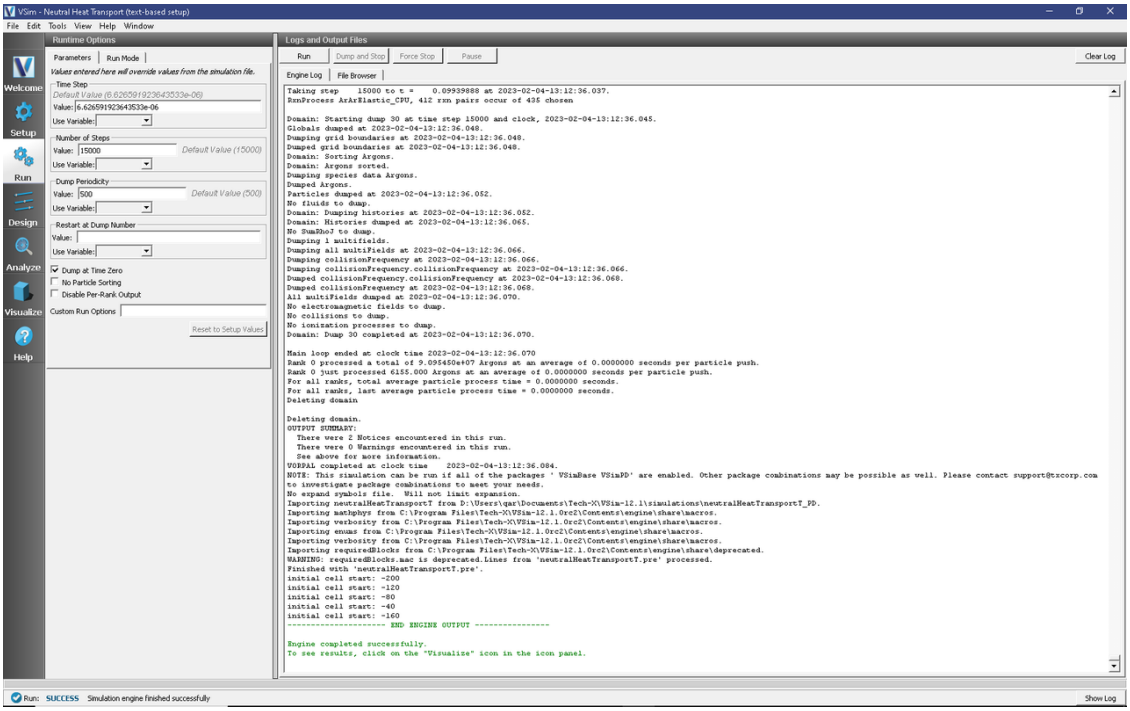


Fig. 6.89: The Run Window at the end of execution.

simulation data, and plot the heat flux versus the analytic heat flux. To run this script, go to the examples directory and run python from the command line (using the command "python validation.py"). The first plot is the same histories seen in the VSim Composer visualization. The second plot is the validation.

To visualize collision frequencies, return to the *Visualize* Tab and select the "Data Overview" tab next to the "History" tab. In the *Variables* box, expand the "Scalar Data" menu and check the box labeled "collisionFrequency". A plot of the elastic collision frequency, in collisions/m^3*s, will appear on the right (see Fig. 6.91). To visualize the collision frequency as the simulation progresses, drag the slider at the bottom of the screen to the right. After the first few dumps, the collision frequency field will stabilize to a quasi-steady state, with the highest collision frequency being near the hot plate.

Further Experiments

As stated in the simulation properties section, simulations can be run with varying pressures (maintaining all else constant) and the resulting heat fluxes plotted against the analytic result, as shown in Fig. 6.92. The provided python script will only plot one simulation result at a time, but it can be modified easily to overplot multiple simulations. Each simulation should lie on the analytic green line. It is important to ensure that the statistics of the collisions are good enough, so when moving to lower collisionality (pressure) the number of macro particles per cell should be increased. Additionally, it is useful to switch the kinetic particle type so that it is variable weight with managed weights. This allows an isotropic macroparticle density while accounting for a variable physical particle density. Alternatively, the temperature of the plates, distance between them, species of neutral gas, etc. can all be modified to test the generality of the model and collisions.

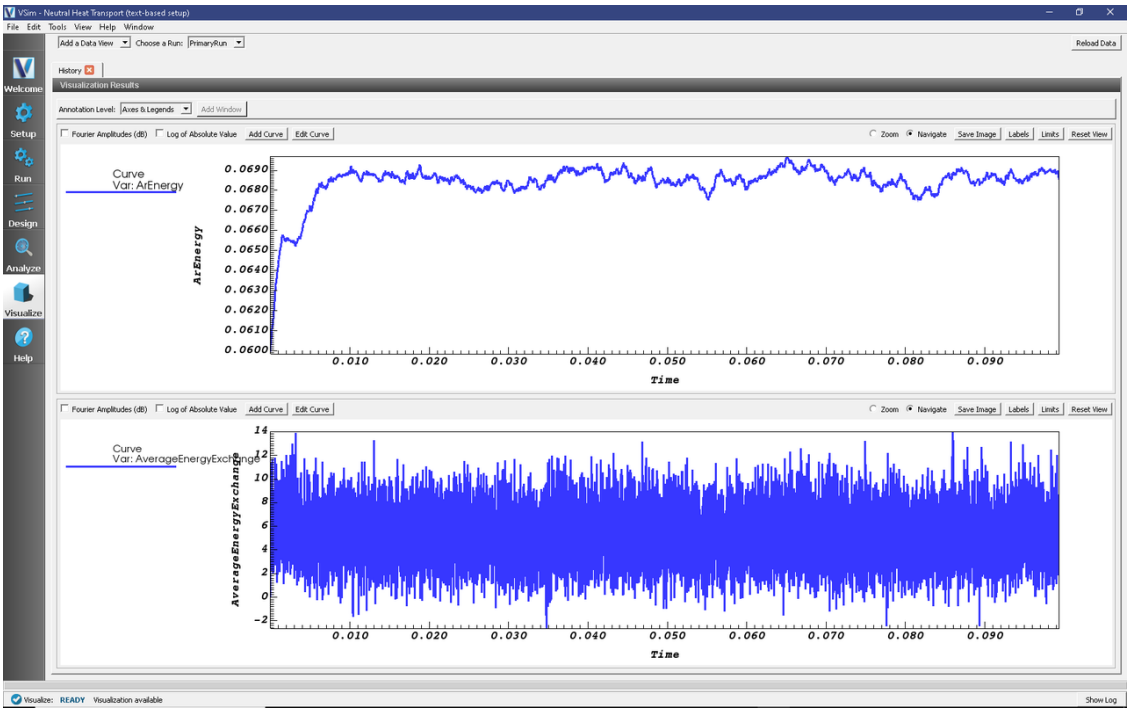


Fig. 6.90: Results from the history data collected in the simulation.

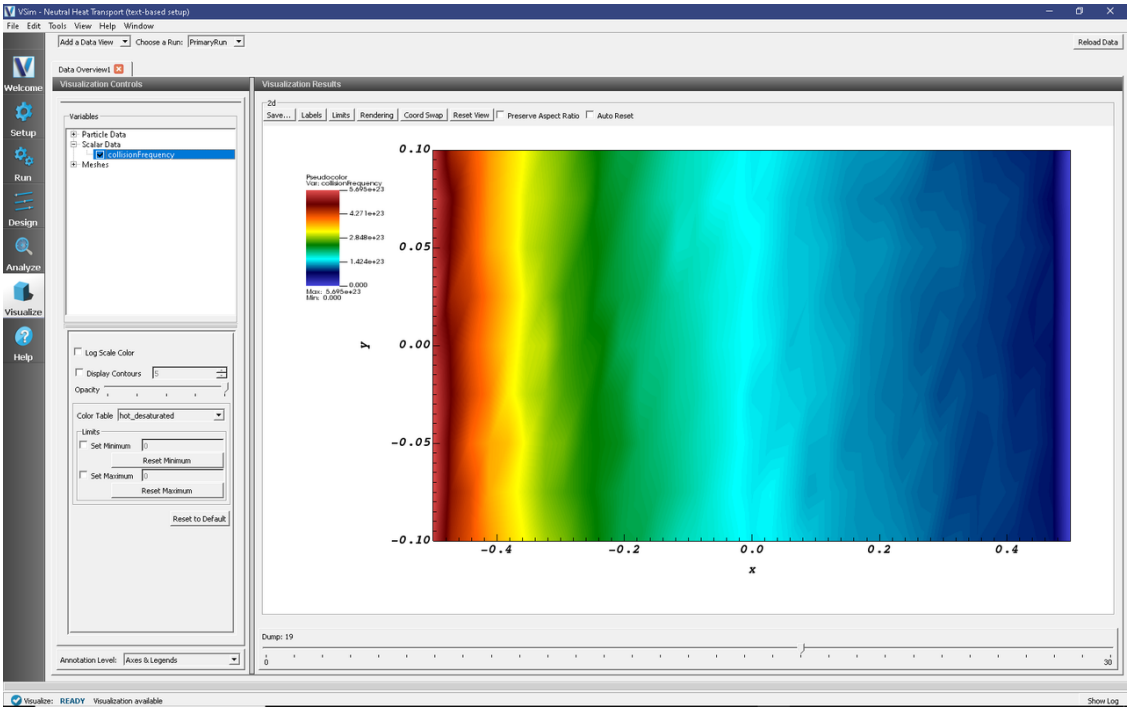


Fig. 6.91: Visualization of collision frequencies.

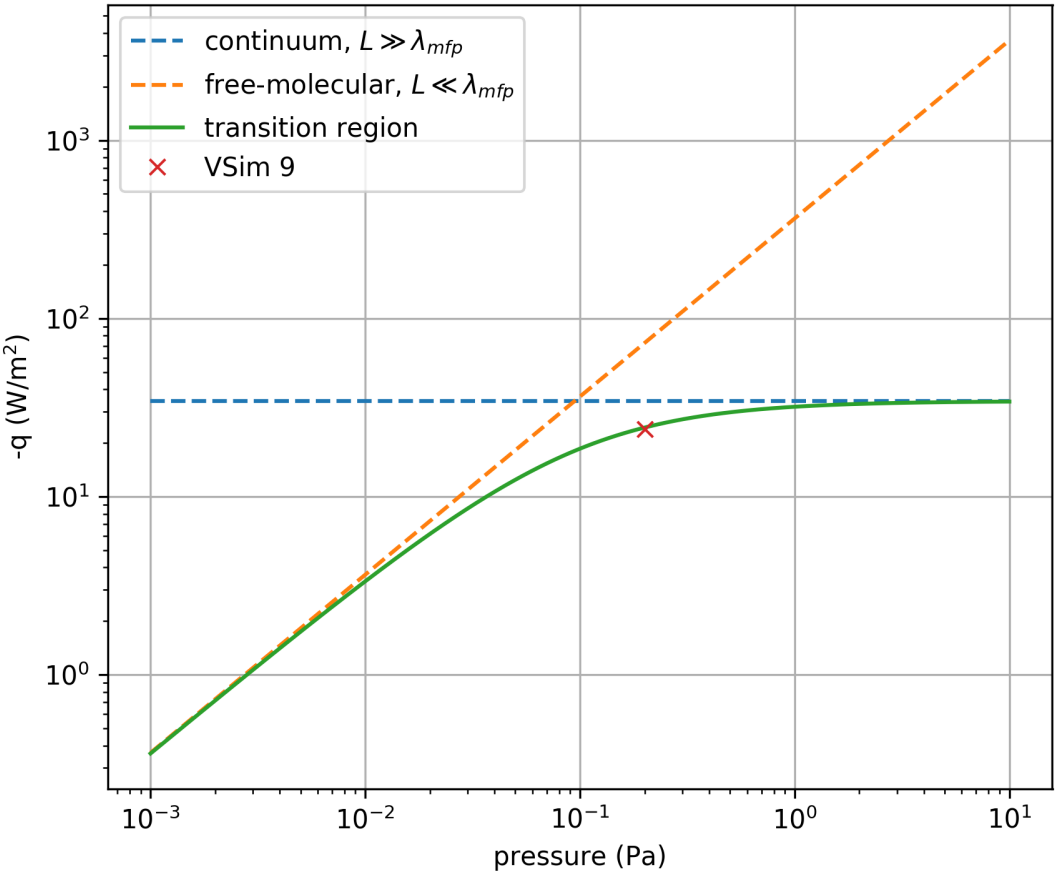


Fig. 6.92: Analytic result of heat flux compared with simulation.

6.8 Spacecraft

6.8.1 Coupon Array Charging (couponArrayCharging.sdf)

Keywords:

solar wind, electrostatics, surface charging

Problem description

In orbit, insulating outer surfaces of satellites will develop a surface charge due to the impinging solar wind. If enough surface charge accumulates electric breakdown can occur across or through the satellite and damage the craft.

This simulation models the accumulation of solar wind particles on an array of solar cells (coupons). The array includes 6 coupons, a kapton backing, and 6 metal busbars. Using post-simulation analysis, the component of the electric field normal to the surface of the satellite is calculated.

With additional data specific a particular spacecraft and materials, this simulation can indicate locations where breakdown is likely to occur.

NOTE: The simulation runs in serial and on 4 cores out of the box in Windows. On Linux, the example runs on up to 12 cores (testing above 12 cores has not been done).

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Electron Drifting example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Spacecraft* option.
- Select "Coupon Array Charging" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The *Setup Window* as seen after opening the example is shown in Fig. 6.93.

Simulation Properties

The geometry for the busbars and coupon array are imported from stl files. Material properties are set on the geometries: perfect electrical conductor (PEC) for the busbars, and absorbium, an insulating particle absorbing material, on the array of cells.

A voltage of 5 volts is set on the busbars. The upper z boundary is set as the $V = 0$ point, a Neumann boundary condition is set on the lower z boundary of the simulation grid, which enforces that the gradient of the electric field normal to this surface is zero. Periodic boundary conditions (for particles and fields) are set on all other simulation boundaries.

The solar wind is emitted off the upper z boundary of the simulation domain with a number density of 1.e7 particles per meter cubed. The masses of the ions are artificially set to 100x the mass of the electrons. Particle accumulation boundary conditions are set on the insulating surface of the coupons, and a particle absorbing boundary condition is set on the metal busbars.

Histories save the absorbed particle energy deposited onto the satellite surface.

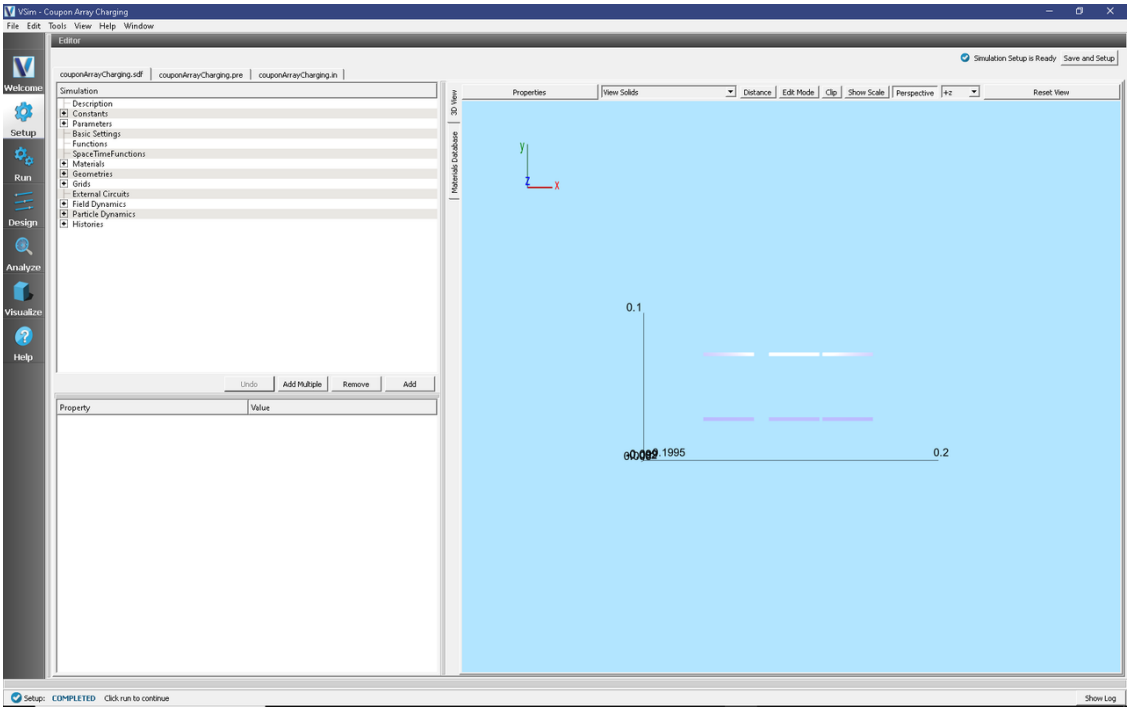


Fig. 6.93: Setup Window for the Coupon Array Charging example.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.4899999999999997e-10
  - *Number of Steps*: 4000
  - *Dump Periodicity*: 400
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.94 below.

Analyzing the Results

The physics engine, vorpal, inside VSim only calculates field values on edges, nodes, or faces of grid cells. The *putFieldOnSurfaceMesh.py* analyzer can interpolate the values calculated on the grid to the surface of a geometry in the simulation.

To calculate the normal component of the electric field on the surface of the array, proceed to the *Analyze* Tab. The *putFieldOnSurfaceMesh.py* analyzer is included by default to this simulation. Click on the text "putFieldOnSurfaceMesh.py (Default)" to highlight it, then click the "Open" button at the bottom of the *Analysis Controls* pane. Ensure the following is entered into each field:

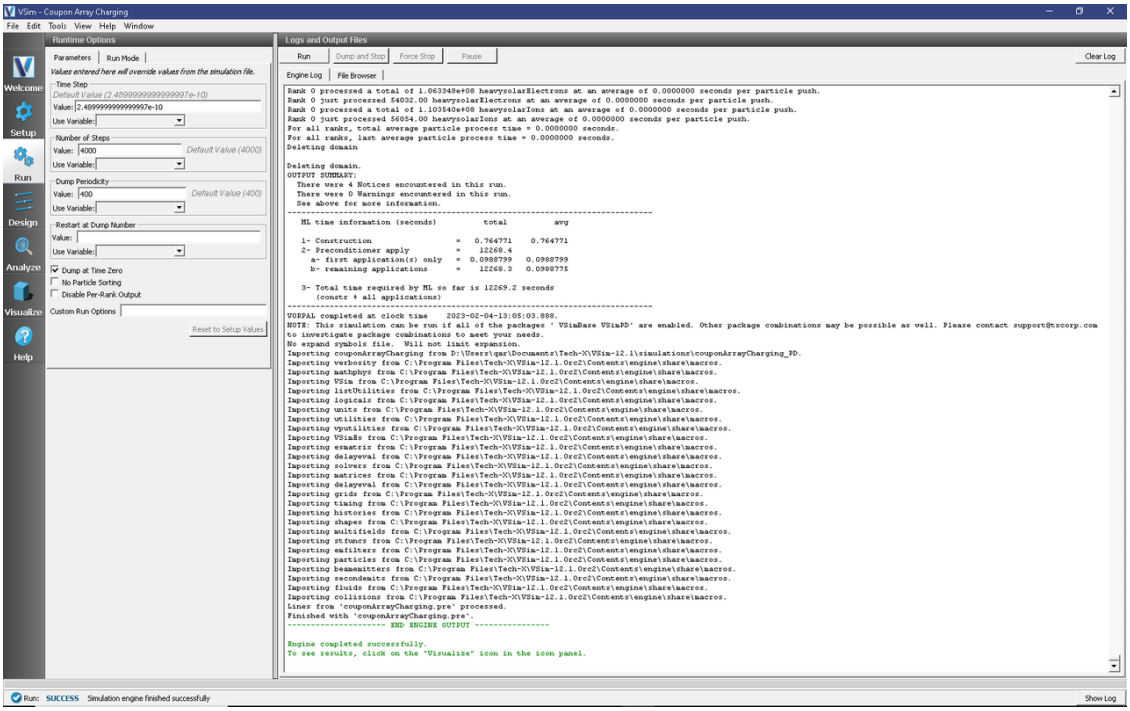


Fig. 6.94: The Run Window at the end of execution.

- **simulationName:** "couponArrayCharging"
- **geometryName:** "satelliteSurfaceGeomSolid"
- **fieldName:** "E"
- **beginDump:** "1"
- **endDump:** "9"
- **outputFileName:** "elecFieldOnSurface"
- Click *Analyze* in upper right corner of the window. When the analysis is finished, you should see a window similar to Fig. 6.95.

Visualizing the Results

After run completion, continue as follows:

Proceed to the Visualize Tab by pressing the Visualize button in the left column of buttons. To view the normal component of the electric field on the surface of the array follow the following steps.

- If you have previously switched to the Visualize Tab, you will have to click the *Reload Data* button at the bottom of the *Visualization Controls* pane.
- In the upper left corner of the Visualization window, click on "Add a Data View" and select "Data Overview" (note: there may already be a "Data Overview" tab opened. If so, skip this step.)
- In the "Data Overview" tab, expand "Scalar Data" then expand "elecFieldOnSurface" and check the box for "elecFieldOnSurface_magnitude" to plot the component of the electric field normal to the surface of the coupon array. It is also possible to plot the two tangential components of the field, as well as the magnitude.
- To compare to the satellite geometry, expand "Geometries" then select "poly (satelliteSurfaceGeomSolid)".

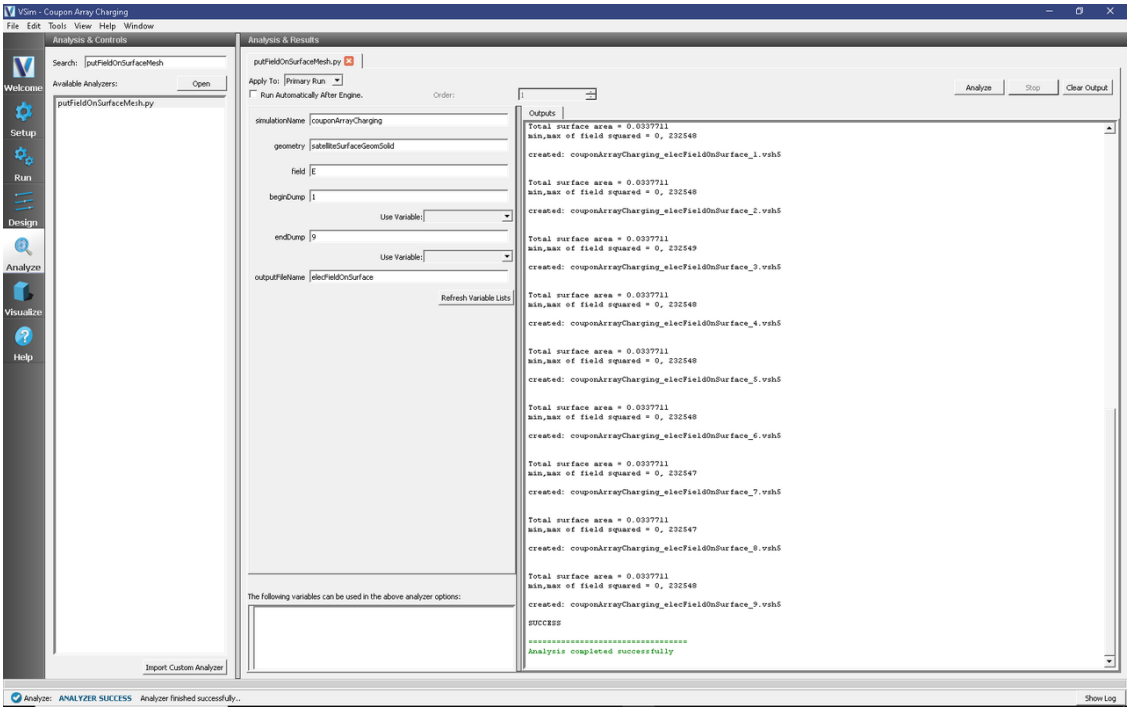


Fig. 6.95: The Analyze Window at the end of execution.

- To see the fields more clearly, select "Log Scale Color"
- The resulting visualization is shown in Fig. 6.96.

We can see the accumulation of electric charge by unselecting "elecFieldOnSurface_magnitude" and viewing "ChargeDensity" instead. To view the charge density on the surface of the geometry, click on "Plane Controls" with your mouse. A new window will pop open. In the new window, make sure that the "Z (plane normal to z-axis)" is checked and that "Origin of Normal Vecor" is such that Z=0. Also make sure that the box next to "Clip Plot" is checked. Note that we are plotting the data on a log color scale. Move the dump slider to view the accumulation of charge over time, as shown in Fig. 6.97.

Further Experiments

Perform the same analysis done above for the electric potential, "Phi," and charge density, "ChargeDensity," to create plots of those fields on the surface of the satellite geometry.

Import your own geometry and reset the materials, grid size, and particle absorbers as necessary.

Increase the grid resolution to get finer data on the electric field that develops on the surface of the spacecraft.

Change the number density and speeds of the incident particles to values for orbits at different altitudes.

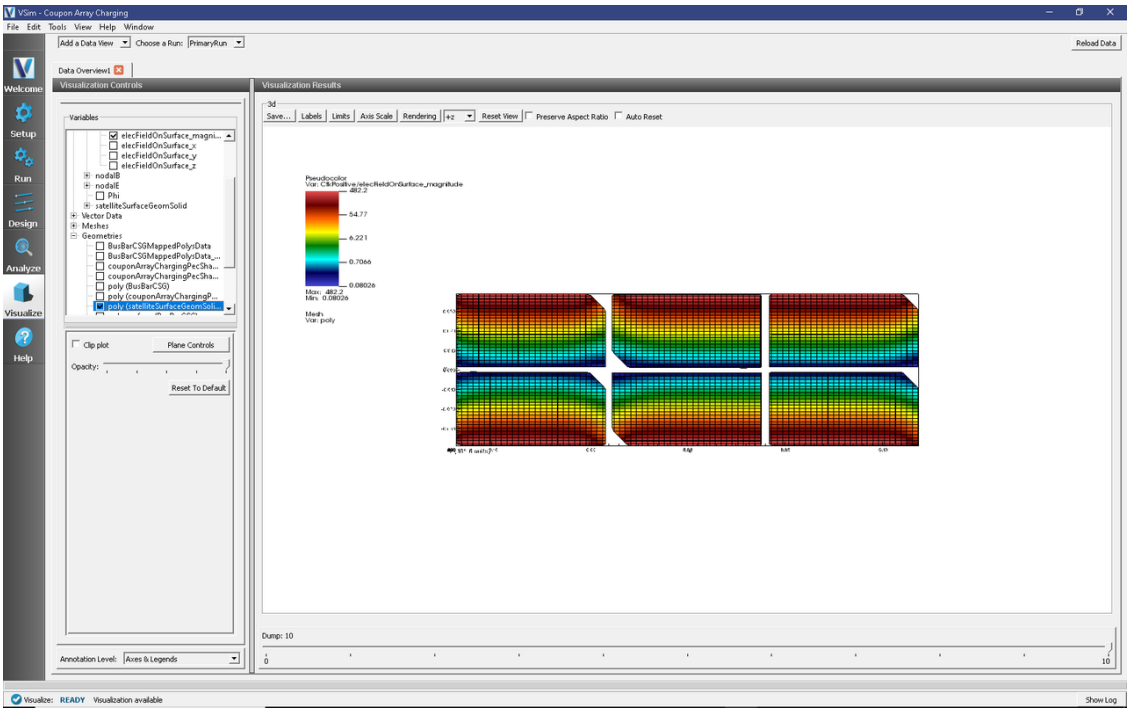


Fig. 6.96: Visualization of the Electric Field on the Satellite Surface.

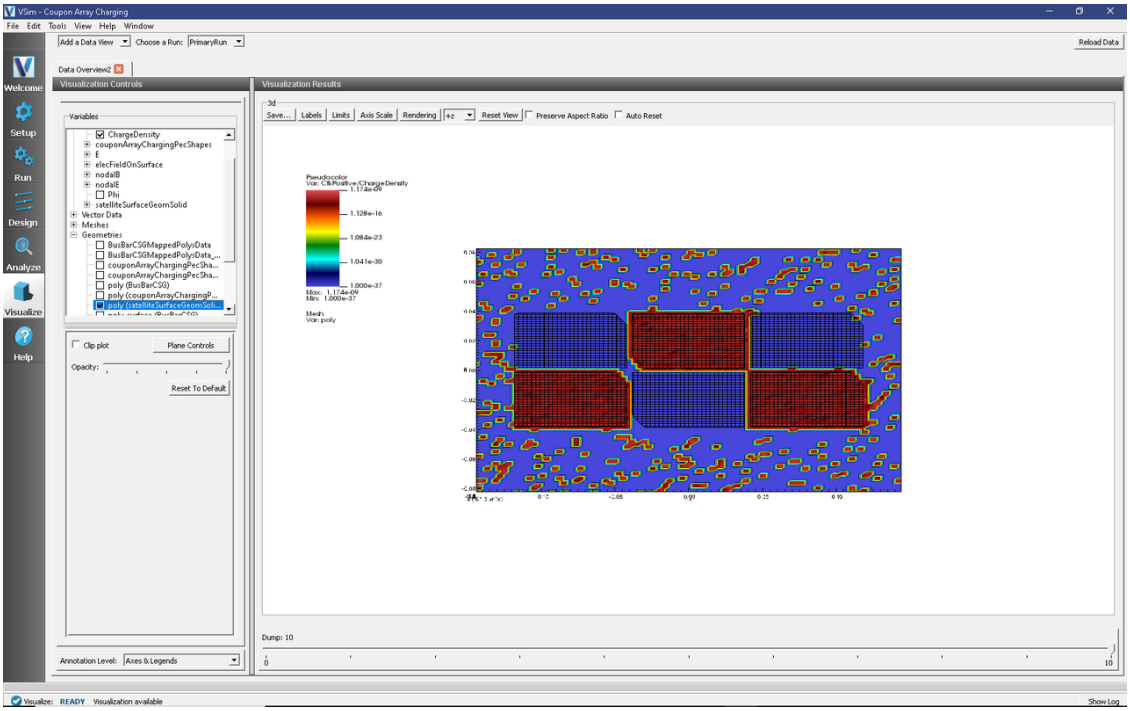


Fig. 6.97: Visualization of the Charge Density

6.8.2 Cylindrical Hall Thruster (cylHallThruster.sdf)

Keywords:

electric propulsion, Hall thruster channel, erosion models.

Problem description

Electric Hall thrusters are used for in-space propulsion and satellite station-keeping needs. The discharge plasma inside the Hall thruster channel is produced by the ionization of electrons with a neutral propellant gas such as xenon. The electrons are emitted from the neutralizer cathode placed at the exit of the Hall thruster (cathode end). The neutral gas is fed into the channel from the anode end of the Hall thruster channel. The electrons are confined inside the Hall thruster channel by the radial magnetic field applied through the solenoidal magnetic fields. Plasma xenon ions are accelerated out of the channel at high velocity, which produces the thrust necessary for space propulsion. Recently these thrusters are being designed to support long life time, high-power and high-thrust operations. The channel wall erosion occurring inside of the Hall thruster is one of the main limitations to these design needs. It becomes important to understand the plasma discharge processes occurring inside the Hall thruster channel and predict the lifetime of the Hall thruster based on the calculations of sputtered material from the Hall thruster channel.

This example demonstrates the xenon discharge plasma processes of a Stationary Plasma Thruster (SPT-100) channel. The outer cylinder has a radius of 5 cm and the inner cylinder has a radius of 3.5 cm. The radial channel gap is 1.5 cm. The channel length is 2.5 cm and our simulation domain is extended up to 1 cm outside the channel region (to simulate both channel and plume plasma). The left wall is biased at 300 V anode potential. Both inner and outer cylinders are maintained as dielectric cylinders (with hexagonal boron-nitride dielectric material coating) with a dielectric permittivity ratio of 4.6. The exit boundary is taken at 0 V. An electron source is placed at the channel exit for considering the electron emission from the neutralizer cathode. The cathode emission current is taken as 4.5 A. The xenon neutral gas is considered as a static fluid background. The neutral gas density is taken to be linearly decreasing trend with a maximum gas density is taken at the anode end of the channel. The simulation is initiated from a uniform plasma with both electrons and xenon ions. We enable a self-similar scaling system laws for the simulation of Hall thruster channel described by figure 1 in [Mahalingam2011]. This is based on earlier work by Taccogna [Taccogna2005] [Taccogna2004]. We have taken a scale factor of 1/50, i.e., the thruster dimensions are scaled by 1/50. This scaling is followed so that the kinetic Hall thruster channel plasma simulations can be performed in a reasonable run time. The scaling affects the physical dimensions and external potentials.

This example does demonstrate ionization of neutral fluids in cylindrical geometry.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Cylindrical Hall Thruster example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Spacecraft* option.
- Select *Cylindrical Hall Thruster* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.98. You can expand the tree elements and navigate through the various properties, making any changes you desire. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. To show or hide the grid, expand the Grid element and select or deselect the box next to `Grid`.

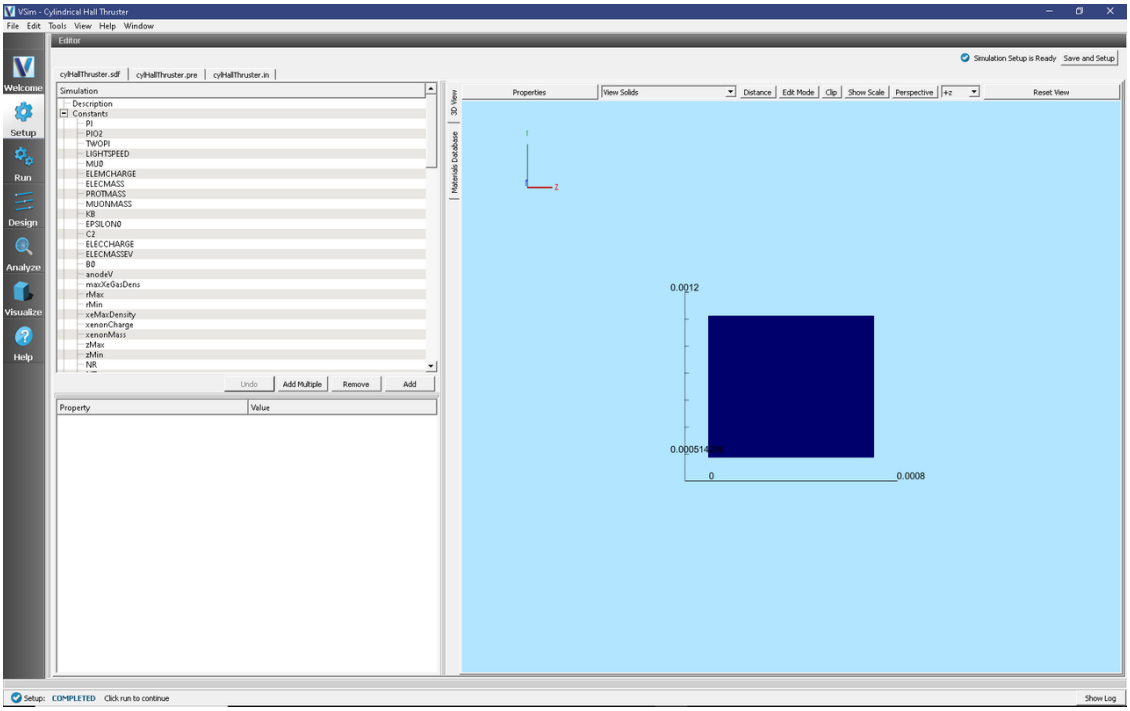


Fig. 6.98: Setup Window for the Cylindrical Hall Thruster Channel example.

Simulation Properties

This example contains many user defined *Constants* which help simplify the setup and make it easy to modify. These include constants such as:

- B0: The amplitude of the background magnetic field
- anodeV: the anode voltage
- innerRad and outerRad: inner and outer cylinder radius
- xeMaxDensity: the maximum density of the background Xe fluid

There are also several *SpaceTimeFunctions* that are used to define spatially and/or temporally varying inputs to other properties. These include:

- By: the magnetic field profile
- initialGasDensity: the profile for the background gas density

The self-consistent electric field is solved from Poisson's equation by the electrostatic solver in a cylindrical coordinate system. The simulation is performed in axisymmetric 2-D fashion. The plasma is represented by macro-particles which are moved using the Boris pusher in cylindrical coordinate system. Various types of elastic and inelastic collisions of the particles are also taken into account.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 3.72518e-13
  - *Number of Steps*: 60000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.99.

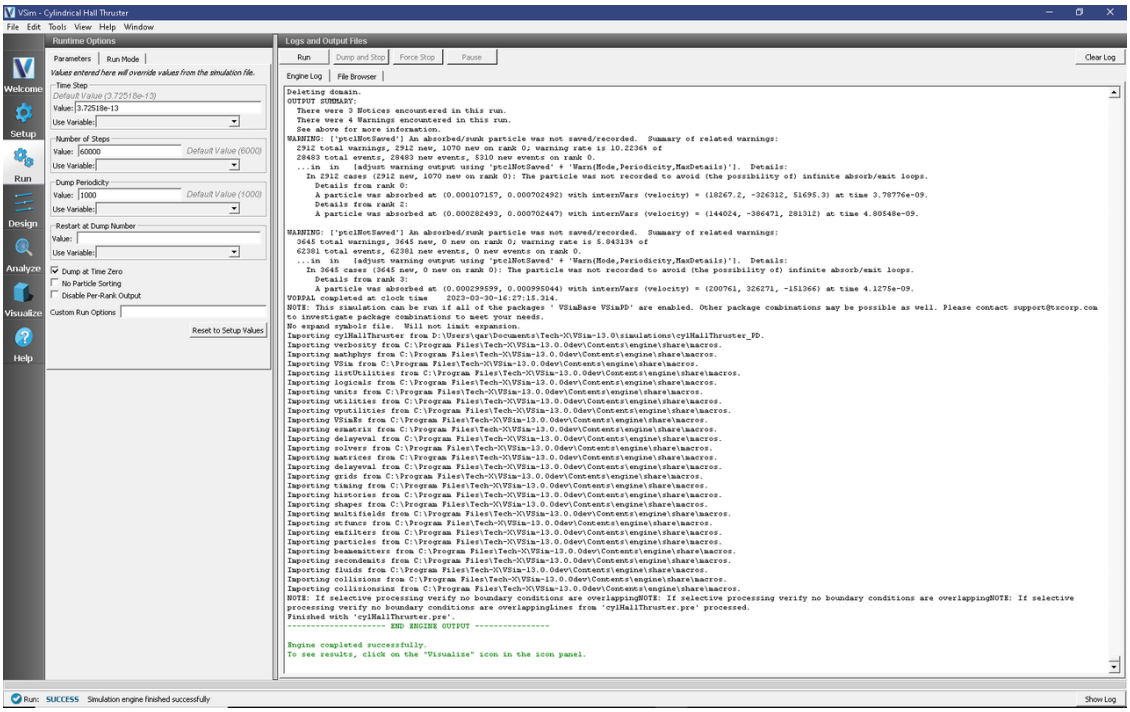


Fig. 6.99: The Run Window at the end of execution.

Analyzing the Results

If it is desired to calculate the density of the electrons or ions the analysis script *computePtclNumDensity.py* must be used.

- First click on the *Analyze* Tab.
- From the *Available Anaylzers* list, choose *computePtclNumDensity.py*. Then click *Open*.
- This script accepts the *simulationName* (Name of the input file) and *speciesName* to be calculated (species of particles).

- To calculate the density of the electrons, set the simulationName to “cylHallThruster” and the speciesName to “electrons”.
- Click on the *Analyze* button at the top right of the *Analysis Results* pane.
- A snapshot of the simulation run completion is shown in Fig. 6.100.

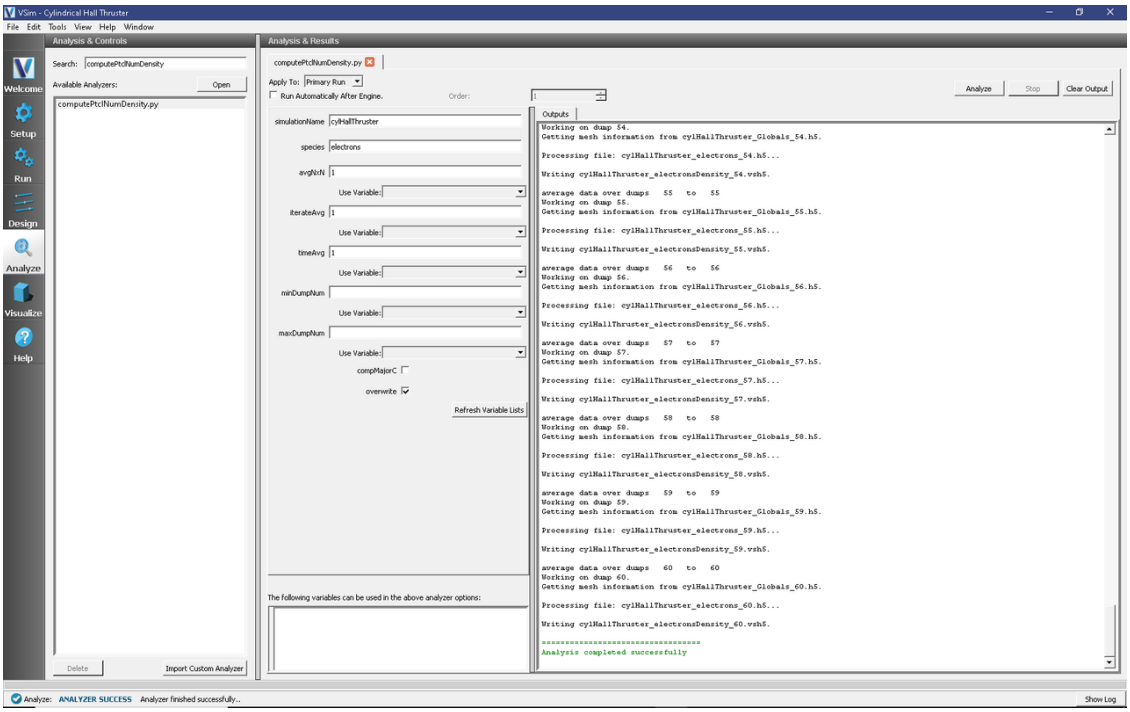


Fig. 6.100: The Analyze Window at the end of execution.

The resulting data will be visualizable as *electronsDensity* under the *Scalar Data* menu in the *Visualize* Tab. The density of other particles such as heavyIons, or Xeplus can also be calculated if those species names are used in place of electrons.

Visualizing the Results

To visualize the results, continue as follows:

- Proceed to the Visualize Window by pressing the Visualize button in the left column of buttons.

There are many different fields, particles, and histories that can be visualized in this example. The horizontal axis represents Z direction and the vertical axis represents R direction.

To view the electric potential, click on “Add a Data View” in the upper left corner of Composer. Then click on “Field Analysis”. This will open a new field analysis tab. In the new tab, click on the down arrow next to “Field” and choose “Phi”. Scroll the dump slider to view the potential at different times. In the Field Analysis tab, you can view the data as a 2D color contour plot and also look at slices of the data. Fig. 6.101 shows the visualization seen for the electric potential of the cylindrical Hall thruster channel and in the exit region.

In the Hall thruster channel plasma, the electrons injected from the right end (i.e., exit of the channel) are accelerated towards the anode biased wall at the left end. In VSim it is possible to plot particle data superimposed with a field quantity. To plot both particles and fields, click on “Add a Data View” and select “Data Overview”. In the “Data Overview” tab, expand *Scalar Data* and select “Phi”. Next expand “Particle Data” and select the “electrons” and “XePlus” check boxes. To view particle data superimposed with field data, it is best to use black and white particles.

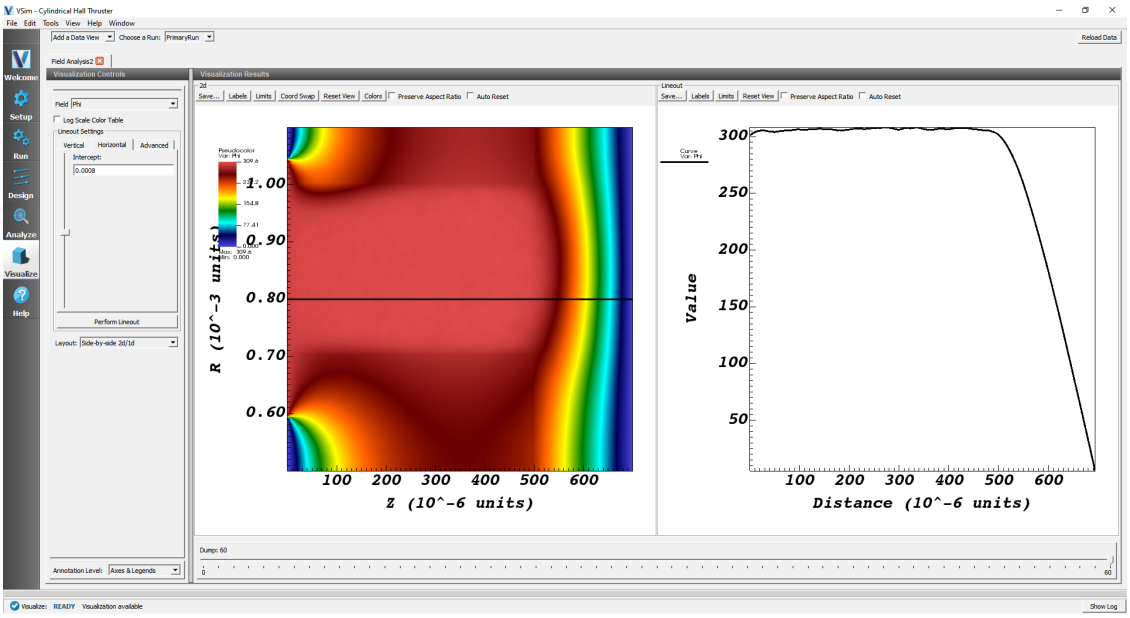


Fig. 6.101: Visualization of the cylindrical Hall thruster electric potential with a line-out showing the axial sheath structure.

Therefore, choose the electrons to be white and the XePlus ions to be black. Finally, scroll the dump slider to dump 60 to view the evolved plume and sheath which develops to the right. The figure below, Fig. 6.102, shows the spatial distribution of positively charged xenon ions (black dots), electrons (white dots) and potential.

The static radial magnetic field distribution considered for the SPT-100 Hall thruster channel set up is shown in Fig. 6.103. To reproduce this plot, Open a new Field Analysis tab, click on area next to the Field option, and choose "nodalB_r". Slide "intercept" to the right so that the lineout goes through the region of the strongest magnetic field. The magnetic field is strong near the inner cylinder and has a Gaussian bell-shaped field distribution both inside and at the exit of the channel.

The background xenon neutral fluid density distribution (plottable as *XeNeutralFluid* in a Field Analysis tab) used in the simulation set up is shown in Fig. 6.104. The maximum neutral fluid density is taken at the left end of the channel near the anode wall. A linearly varying neutral fluid density is assumed.

Finally, we show the electron current impacting the anode and the ion current exiting through the plume. These data are saved in histories called "electronAnodeCurrent" and "absorbedIonCurrent" which are setup in Composer. To view how the histories are created, click on "Setup" on the left hand side of Composer. "Histories" is the bottom-most option in the elements tree. By expanding "Histories" you will see multiple histories already created including "electronAnodeCurrent" and "absorbedIonCurrent". To view the data, click on "Visualize". Then click on "Add a Data View" and choose "History". In the History tab click on "Add Curve" and choose "AbsorbedIonCurrent". Once the data are plotted, you can add "AbsorbedAnodeCurrent" by clicking on "Add Curve" again and following similar steps.

The resulting data plot is shown in Fig. 6.105.

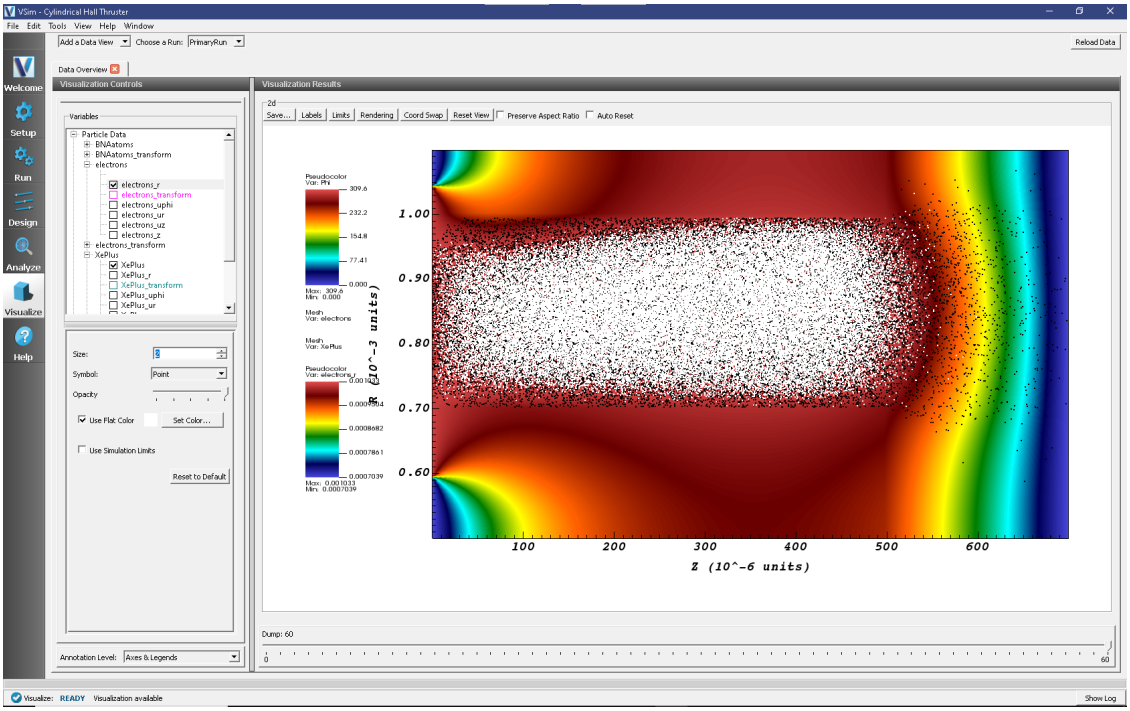


Fig. 6.102: Visualization of electrostatic potential with the spatial distribution of electrons and ions superimposed.

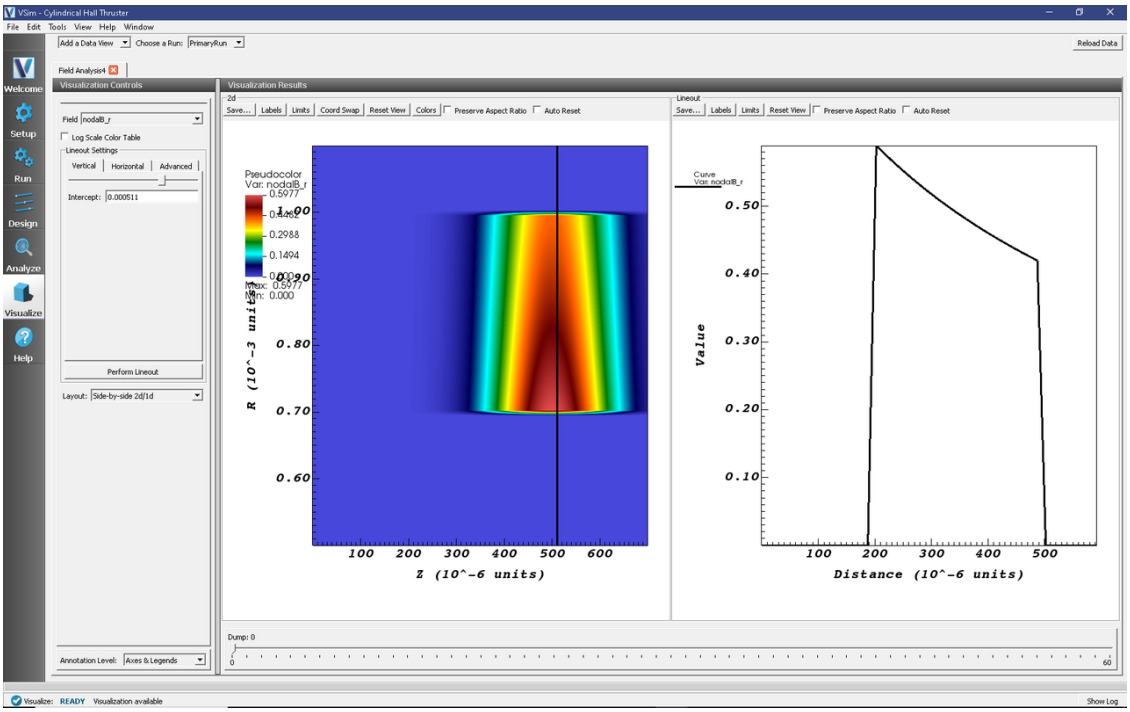


Fig. 6.103: Visualization of radial magnetic field in the Cylindrical Hall thruster channel. The left panel shows the color contour plot and the right panel shows the lineout.

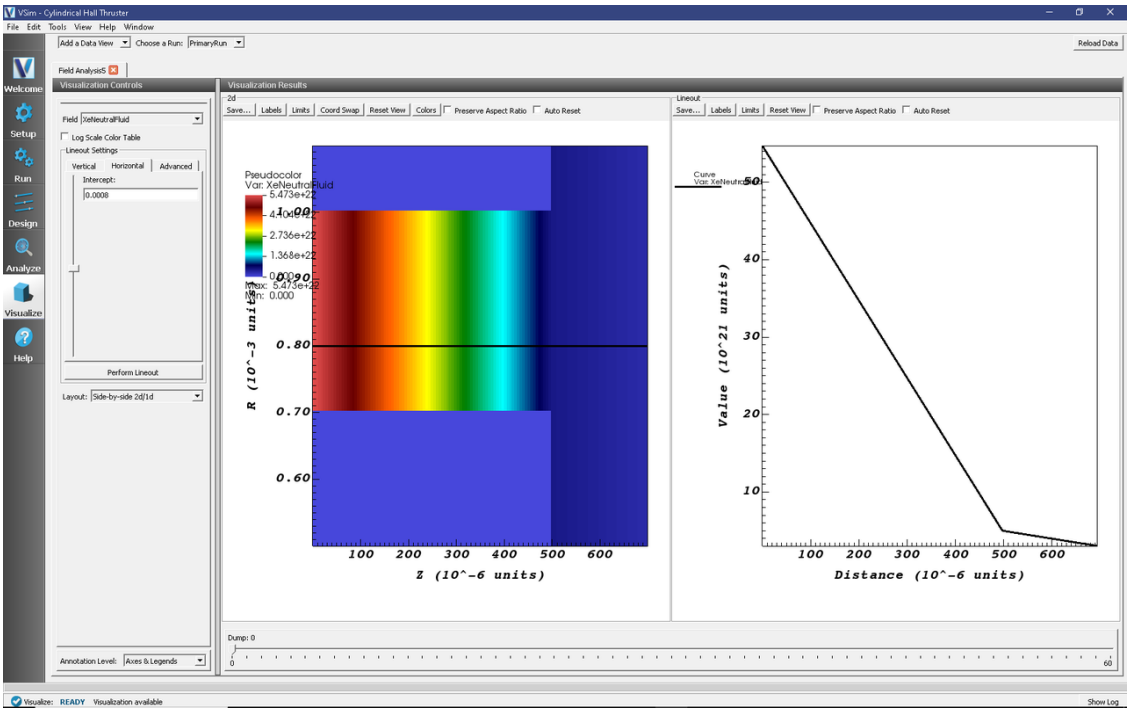


Fig. 6.104: Visualization of xenon neutral fluid density in the Cylindrical Hall thruster channel.

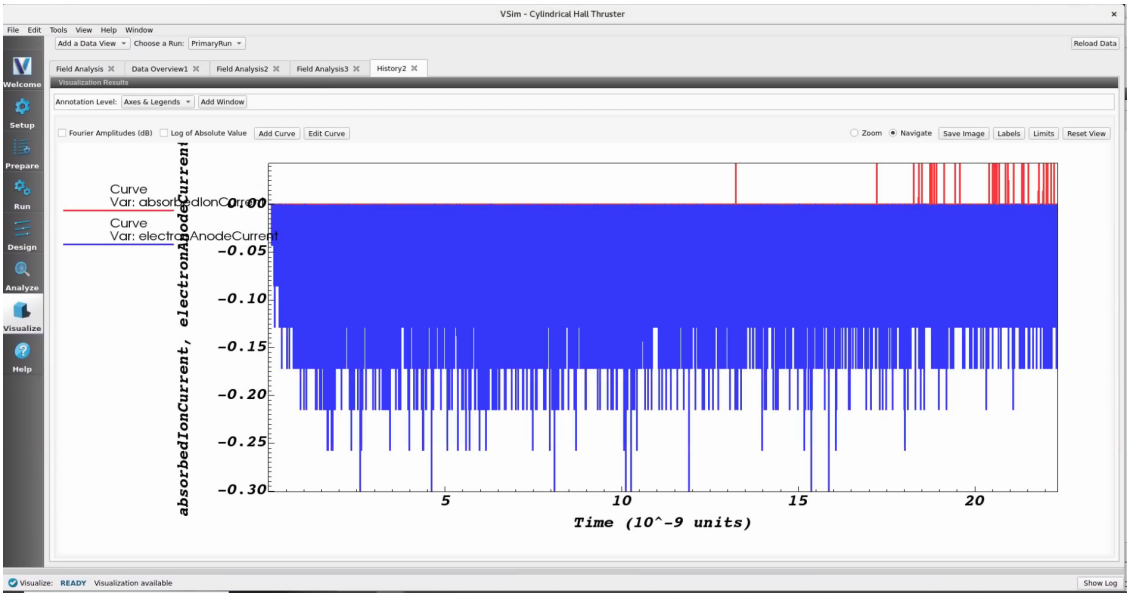


Fig. 6.105: Visualization showing electron current impacting the anode and ion current leaving through the plume.

Further Experiments

This example can be modified to test different design parameters such as varying anode voltages, varying background neutral gas densities and varying electron emission currents. This will allow users to study high-to-low power and high-to-low throttle levels.

Also the background fluid type can be changed to investigate other fluid species' in this simulation set up.

6.8.3 Satellite Surface Charging (satelliteSurfaceCharge.sdf)

Keywords:

`electrostatics, surface charges, Poisson solver`

Problem description

Satellites and other spacecraft operating in the space environment often suffer arcing and breakdown problems due to surface charging. Charged particles buildup on the spacecraft surfaces (such as solar panel arrays and other components) leading to localized arcing/breakdown discharges that can critically fail a component or the entire unit. This problem is made worse as the demand for high power space missions in both satellite and deep-space applications rises. These high-power spacecraft are outfitted with high-voltage solar panels. These panels minimize the overall payload requirements and offer other advantages over more massive, low-voltage arrays. However, they are also more vulnerable to surface charge related arcing. It therefore becomes important to predict the surface charge buildup on spacecraft bodies operating in different space environments, where the ion sources may be natural solar wind or human-made space plasma resulting from electric thruster plasma plumes.

This example demonstrates a satellite body operating in the solar wind environment where the space plasma consists of ions and electrons. The simulation box is set up with dimensions of 15 m x 30 m x 15 m. The satellite system is placed in the middle of the domain. It has a 3 m radius x 5 m long cylindrical central unit connected to solar panels at either end. Each solar panel has a total span length of 6 m and a width of 4 m. The satellite central unit has a 5-volt equipotential circular body with radius of 2 m and length of 3 m. The satellite system is treated as a conductor floating in free space which acquires the plasma potential. The system domain boundaries are assumed to have zero perpendicular electric field, i.e. Neumann boundary conditions. The solar wind plasma is introduced in the simulation domain from the positive x direction. The solar wind density is set to $1 \times 10^7 \mathrm{m}^{-3}$ with a temperature of 10 eV. The number of particles per cell introduced at each time step is 5. The number of physical particles per macro particle is automatically computed by the computational engine (Vorpal). Both electrons and ions are introduced from the source based on the solar wind density and temperature. The electrons and ions and emitted from the XMIN boundary using a particle emitter called a "slab settable flux". With this emitter, there are many options for specifying the emission quantity such as "emission current density", "emission flux" and "emission current". We have chosen to specify the emission current density. For a cold (0 temperature) plasma, the emission current density is $n0 \times q \times v_d$, where n0 is the number density, q is the charge of the emitted species and v_d is the drift velocity. For a warm plasma, v_d must be found as the first moment of the distribution function, which is a drifting Maxwellian. Since the electron thermal velocity is much greater than the ion thermal velocity, this means that the electron current density is also greater than the ion current density. To state this another way, to maintain plasma uniformity within finite bounds, the electron source rate is somewhat larger than the ion source rate because electrons are lighter and leave the system more quickly than do ions. At the same time, the positive ions are imbued with a lighter mass to speed up the simulation. All simulation boundaries are set up to absorb particles. The charges collected in the satellite system are counted by emitting a heavy electron or heavy ion at the point where an electron or ion was absorbed. The heavy electron/ion is not a physical concept, it is a computational trick whereby any charged particle striking the satellite gets converted to a new species, one with equivalent charge but with a much larger mass (1 kg in this case) and suppressed energy (suppressed by a factor of 10 billion). In this way, the heavy particles do not propagate from their point of origin, effectively sticking to the satellite surface. The collected electron and ion currents on the satellite surfaces are output as histories.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The satellite surface charging example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Spacecraft* option.
- Select "Satellite Surface Charging" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.106. You can expand the tree elements and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on an option. The right pane shows a 3D view of the geometry as well as the grid. To show or hide the grid, expand the "Grid" element and select or deselect the box next to `Grid`. You can also show or hide the different geometries by expanding the "Geometries" and "CSG" elements. Under "CSG", you will see all the geometries which are created using VSim's primitive geometry creation capabilities. Selecting a box next to a geometry shows that geometry in the 3D view.

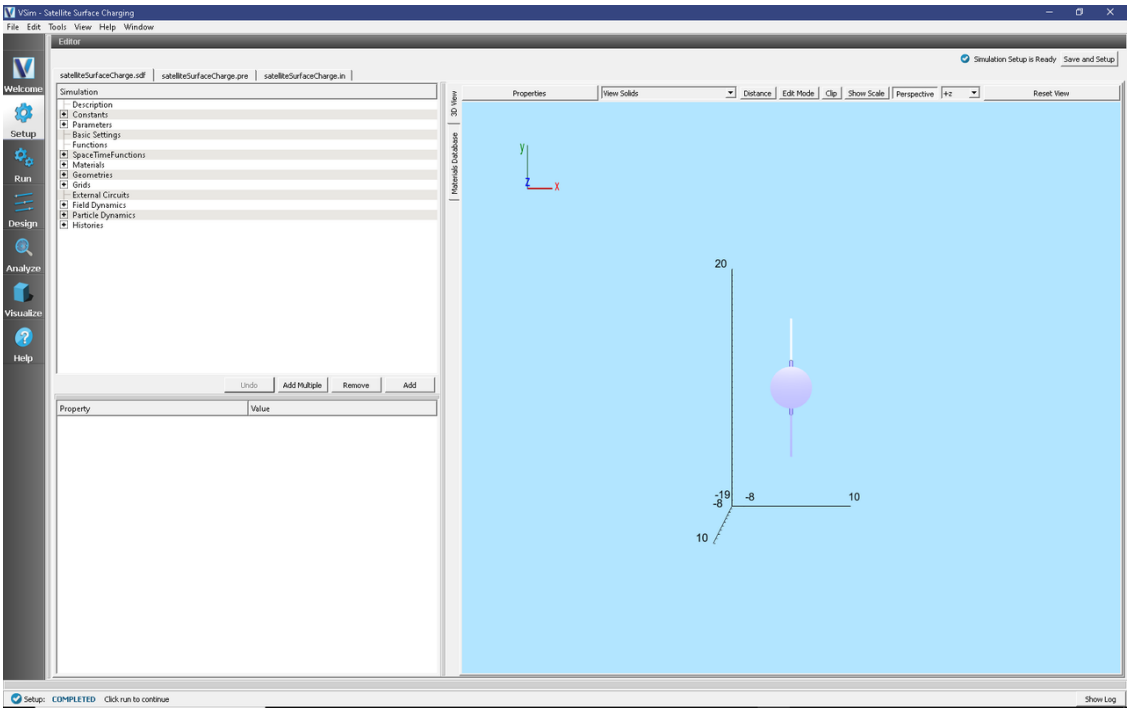


Fig. 6.106: Setup Window for the Satellite Surface Charging example.

Input File Features

The input file allows a choice of space environment parameters (number density, plasma temperature, drift speed), satellite body voltage, simulation domain size, and resolution (number of cells in each direction). Note, however, that "ION_CURRENT_DENSITY" and "ELECTRON_CURRENT_DENSITY" (which are two parameters that can be found by expanding the "Parameters" option) are computed outside of VSim. These are found by computing the first moment of the drifting Maxwellian which is the kinetic drift velocity that takes in to account the thermal spread of each species. Therefore, if you change the number density, plasma temperature and/or drift speed, "ION_CURRENT_DENSITY" and "ELECTRON_CURRENT_DENSITY" will need to be recomputed. The current density for species s can be found with the following formula: $n0 \times q_s \times \int_{-\infty}^{0} v f(v) \mathrm{d}v$, where $f(v)$ is the kinetic distribution function which is represented as a drifting Maxwellian in this example. Note that the integral extends from $-\infty$ to 0 since this is the range of particles that get injected from the XMIN boundary.

The self-consistent electric field is solved from Poisson's equation by the electrostatic solver. The far-field space boundaries are handled with Neumann boundary conditions. The satellite inner body is set up with an equipotential boundary. The surface charges collected on the satellite system make the satellite body float at a slightly lower voltage than the space plasma.

The plasma is represented by macro-particles which are moved according to the Boris pusher.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2.2838270097897377e-08
  - *Number of Steps*: 2000
  - *Dump Periodicity*: 200
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.107.

Analyzing the Results

If the electron density is desired, then proceed as follows:

- In the leftmost panel, click the *Analyze* button and then select *computePtclNumDensity.py* from the list of analyzers, then click *Open* at the top of the Analysis Controls pane.
- Enter the following parameters in the appropriate fields:
  - simulationName = satelliteSurfaceCharge
  - speciesName = solarWindElectrons
  - avgNxN = 1
  - iterateAvg = 1
- Click the *Analyze* button in the upper right corner of the window.

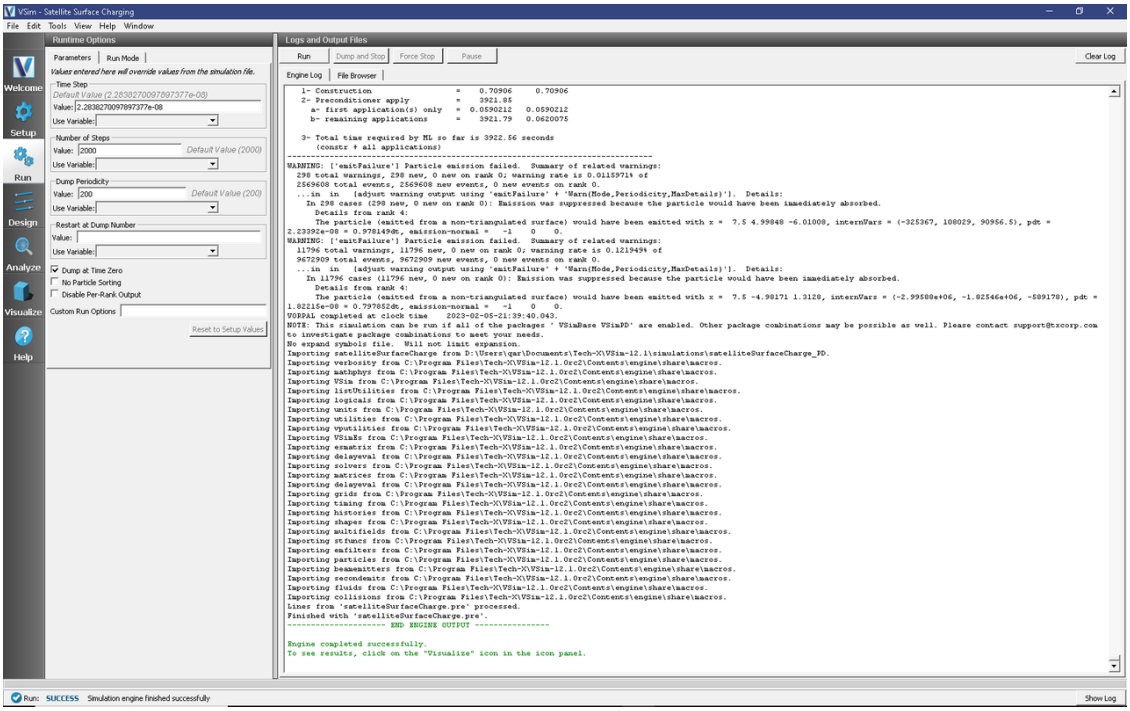


Fig. 6.107: The Run Window at the end of execution.

See Fig. 6.108.

The resulting data can be visualized as *solarWindElectronsDensity* under the *Scalar Data* menu in the *Visualize* Tab. The density of solarWindIons can be calculated in the same way by substituting that species name in place of *solarWindElectrons*.

Visualizing the results

After performing the above actions, proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

To visualize the satellite geometry with electrons proceed as follows:

- Open a *Data Overview* tab.
- Expand *Particle Data*.
- Expand *heavySolarWindElectrons*.
- Select “heavySolarWindElectrons” in red.
- Expand *solarWindElectrons*.
- Select “solarWindElectrons” in green.
- Expand *Geometries*.
- Select “poly_surface (satelliteWithRodsUnionsatelliteBothCells)”.
- Move the Dump slider to dump 7.

The resulting plot is shown in Fig. 6.109. In order to view the data as shown in Fig. 6.109, you need to take a slice in the z=0 plane. To do this, click on “Plane Controls”, then select Z(plane normal to z-axis) to be the plane normal.

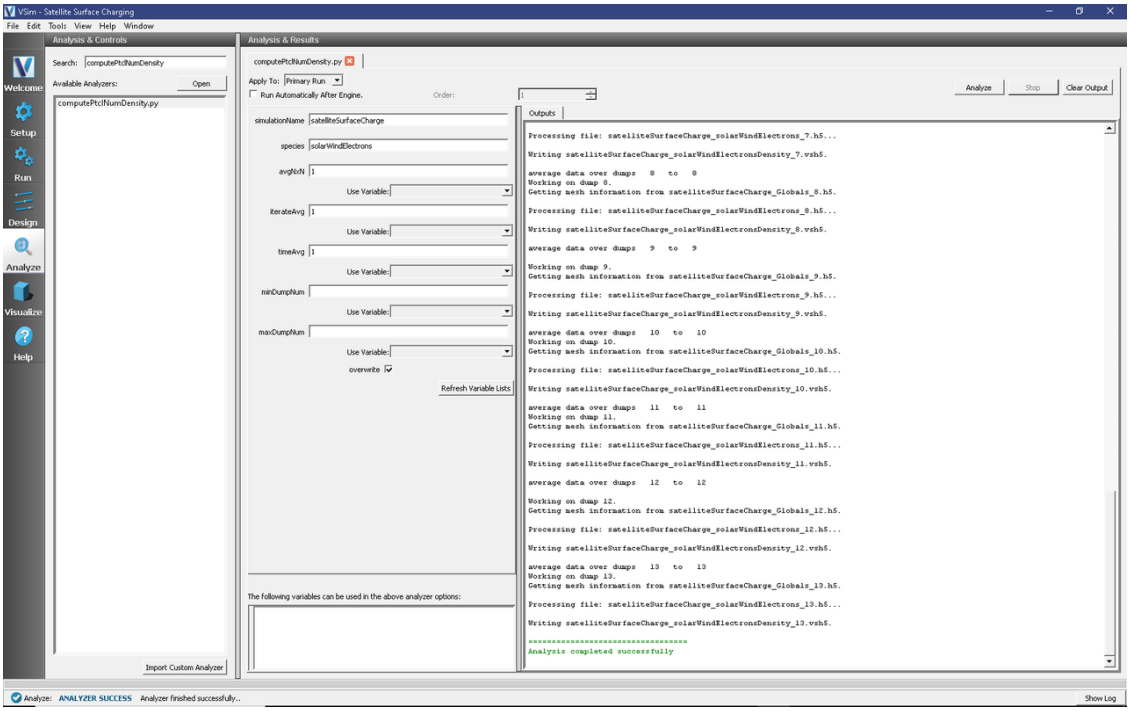


Fig. 6.108: The Run Window at the end of execution.

Finally, set the Origin of Normal Vector to be 0.0 and click OK. You need to follow these steps for all the data shown. Therefore, do this after selecting "heavySolarWindElectrons" and "solarWindElectrons".

Here are some things to try:

- Under *Data Overview* you can access plots of the electric field, charge density (ChargeDensity), and electric potential (Phi). To view these data sets, expand *Scalar Data* option. After selecting any field quantity, to view a slice in plane, click on "Plane Controls" as discussed above
- To view the phase space distribution for the electrons and ions, click on the *Add a Data View* drop down menu and select *Phase Space*. Click the *Draw* button to generate a plot.
- Also from the *Data View* menu select *History* to observe the satellite currents and the time history results for the number of macro-particles broken down by species.

To generate Fig. 6.110, that shows the satellite system with the inner equipotential cylindrical body, proceed as follows:

- In the *Data View* pane on the left side select "Data Overview" from the drop-down menu.
- Expand *Geometries*
- Select "poly (satelliteWithRodsUnionsatelliteBothCells)"
- Select "poly_surface (Inner)".

The spatial distribution of the positive ions (solarWindIons species) surrounding the satellite system is shown in Fig. 6.111 which is obtained after running the simulation for 400 time steps. Solar wind plasma enters into the simulation system from the minimum x boundary. If the plane is still clipped from prior plots, uncheck the "Clip plot" box next to the "Plane controls" button. Furthermore, play around with the different colors and opacity options until a plot with the desired look is achieved. There is also an "Annotation levels" option at the bottom of Composer. We have selected "No annotations" so that just the satellite is showing.

The charge density on the satellite system is shown in Fig. 6.112 after running for 2,000 time steps. To view the charge density in the simulation domain, click on "Add a Data View" and choose "Field Analysis". Then click on region next

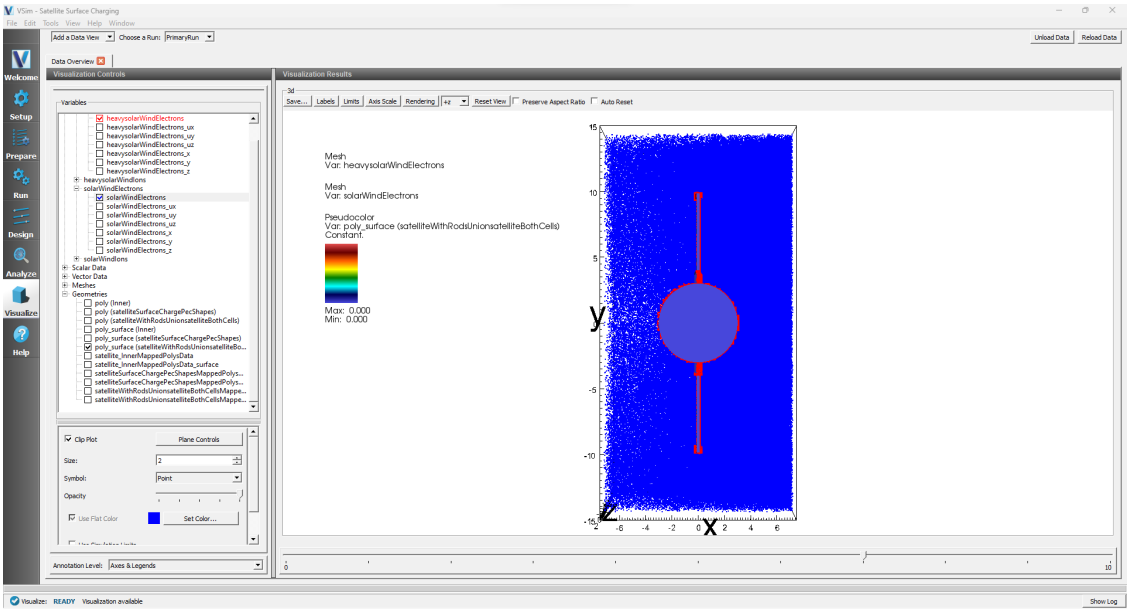


Fig. 6.109: Visualization plot of satellite system with solar wind electrons in green and the electrons that stick to the satellite surface in red.

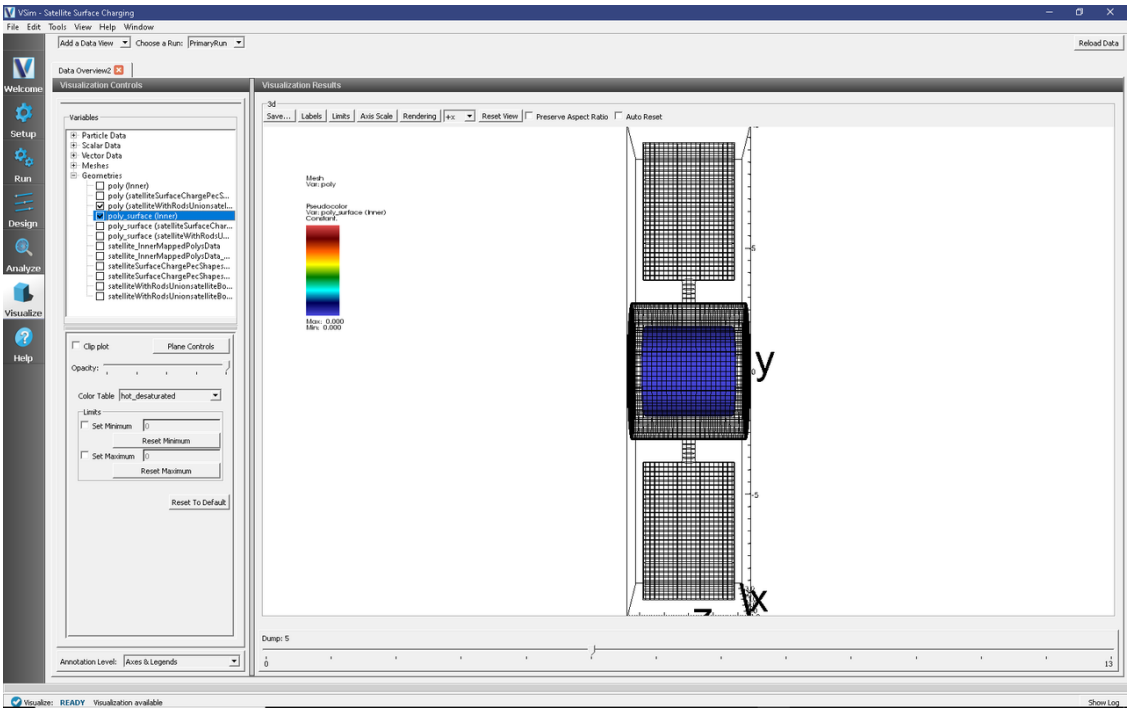


Fig. 6.110: Visualization of the inner body inside the satellite system.

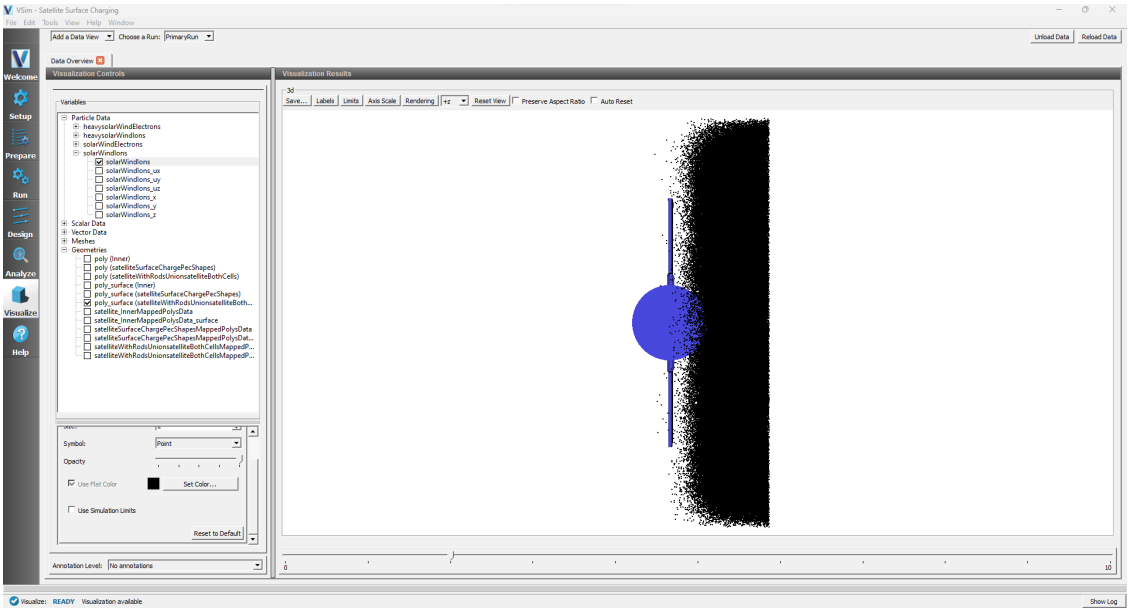


Fig. 6.111: Visualization of the satellite system with solar ions.

to "Field" and choose *ChargeDensity*. The default view will show a 3D, 2D and 1D view (i.e. 3 windows are shown by default). You can choose different slices in the 3D view just as you could in the Data Overview tab. To view the data as shown in Fig. 6.112, click in the region next to "Layout" and choose "Side-by-side 2d/1d". Now we want to make the color scale symmetric with respect to 0. So click on "Colors above the 2D color contour plot. Then check the boxes "Fix Minimum" and "Fix Maximum" and choose the color scale to lie between -2e-11 and 2e-11 (units are in C/m^3). Next, for the lineout setting, click on "Horizontal" and drag the bar to change the location of the lineout. This allows you to quantify the data better. We see in this plot a large negative build-up on the side the solar wind enters from and a smaller build-up on the opposite side of the satellite. We have circled some of the key features in Composer that allow you to customize your plot.

To view the electrostatic potential, check the box next to "Phi" under the Scalar Data in the *Data Overview* pane. The electrostatic potential of the satellite system simulated is shown in Fig. 6.113 after running for 2,000 time steps. The electrostatic potential is plotted in the X-Y-Z domain with clipping in the Z=0 plane. The bulk of the plasma potential in the space region is close to -1 V (red region). The negative surface charge built-up on the solar panels lowers the surface potential about 5 V below the bulk space plasma.

Further Experiments

The geometry and background space plasma parameters of this input file can be modified to test satellite inner body voltages and satellite surface charge collection in a variety of different space environments.

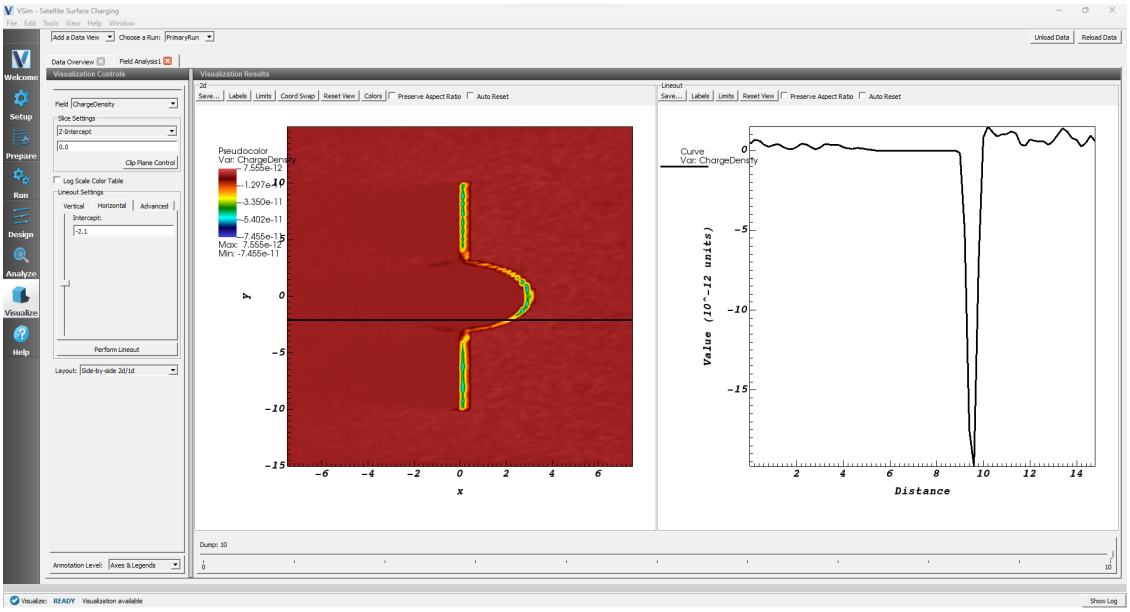


Fig. 6.112: Visualization of the charge density on the satellite system.

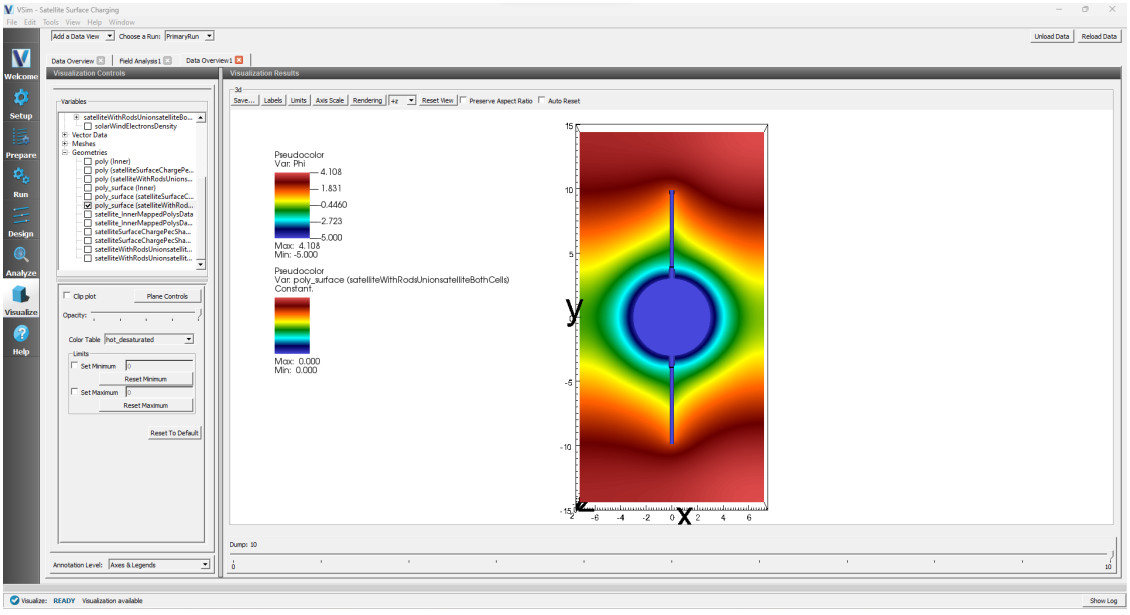


Fig. 6.113: Visualization of the electric potential surrounding the satellite system.

6.9 Spacecraft (text-based setup)

6.9.1 Ion Thruster (ionThrusterT.pre)

Keywords:

electric ion thruster discharge chamber plasma processes in 2D cylindrical system.

Problem Description

Ion thrusters are electric propulsion devices used for in-space propulsion and satellite station-keeping. In this device, a propellant gas (xenon in this example) is ionized into a plasma state inside a cylindrical discharge chamber. The plasma ions are accelerated out of the chamber through an electrostatic grid optics system to produce thrust. The device consists of the following components: an anode-biased discharge chamber, a discharge hollow cathode assembly, permanent magnet rings, a neutral propellant feed system, grid optics (screen and accelerator plates), and a neutralizing hollow cathode. The discharge hollow cathode is placed in the center of the discharge chamber and emits energetic electrons (primary electrons) into the system. Primary electrons undergo ionizing collisions with the neutral propellant gas inside the chamber to produce plasma ions and secondary electrons. An energetic electron impacting a xenon atom that is already singly ionized may cause another electron to detach, resulting in a doubly ionized xenon atom. The permanent magnetic rings within the discharge chamber confine the electrons, increasing their time of flight in the chamber, and thus their chances of ionizing neutrals before collection at the anode-biased discharge chamber walls. The plasma ions produced in the chamber leave primarily through the screen grid plate with some losses to the cathode biased walls. To ensure long discharge cathode lifetimes, a protective enclosure called a cathode keeper (generally kept between 3 and 5 volts above the discharge cathode voltage) is used to shield the cathode plate from plasma ion collisions. The bombardment of singly charged and doubly charged ions during thruster operation will over time erode the face of the cathode keeper and expose the discharge cathode to energetic ions. Thus, it becomes important to model the ion flux around the cathodes. Recently ion thrusters have been designed to meet high-power and high-thrust-to-power space propulsion requirements. Numerical discharge chamber plasma simulations provide a detailed understanding of the plasma processes that go on inside a discharge chamber and help with the calculation of electron discharge currents, ion beam currents, and ion current losses to the chamber walls.

This example demonstrates the xenon discharge plasma processes inside of a cylindrical discharge chamber with a three-ring magnetic circuit arrangement. One magnetic ring is mounted on the forward wall (seen as the left wall in the geometry of the example) and two magnetic rings are mounted to the exterior wall of the cylindrical discharge chamber (seen as the top wall in the example setup). The radius of the cylindrical chamber is 20 cm and it is 18 cm long. The screen grid plate has a radius of 18 cm and is placed at the aft end of the discharge chamber (far right in the example setup). The discharge hollow cathode assembly is placed at the center of the discharge chamber. The radius of the cathode keeper assembly is taken to be 0.75 cm and its orifice protrudes out 7 cm from the forward wall (from the left wall in the example diagram). An electron particle source is implanted next to the cathode keeper orifice to model the electron emission of the discharge cathode. In this simulation the cathode emission current is taken as 10 A. The same cathode emission source location is also used for modeling the neutral propellant flow from the discharge cathode. The main xenon neutral propellant source is modelled along the exterior wall (top wall in the example diagram). We have taken neutral propellant flow rates of 4.5 sccm and 43.5 sccm for the discharge cathode neutral source and main neutral source respectively. The anode biased discharge chamber walls are kept at 25 V. The discharge cathode keeper is biased at 5 V and the screen grid plate is kept at 0 V. Finally, we enable a self-similar scaling system for the simulation of discharge chamber plasma described by figure 1 in [MCL+11]. This is based on earlier work by Taccogna [TLCS04, TLCS05]. By default the shrink scale factor is 200, i.e., the thruster dimensions are scaled by 1/200. This scaling ensures that simulations can be performed in a reasonable run time but it requires use of an inflated permittivity scale factor, i.e. the permittivity of free space is artificially inflated so that numerical parameters like grid spacing and time step values satisfy the smaller plasma frequency and Debye length.

The simulation is initiated with the chamber pre-filled with xenon neutrals. This is because the neutrals are heavy and slow, and it would take a great many time steps at the start of every run to populate an empty chamber. To view the initial distribution of neutrals, the input file can be run with particle sources turned-off. To do this, switch the

TURN_THRUSTER_OFF parameter to 1 and run for one time step. Then, in the Visualize window, select XeNeutrals under Particle Data.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The ion thruster example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item from the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Spacecraft (text-based setup)* option.
- Select *Ion Thruster (text-based setup)* and click the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 6.114.

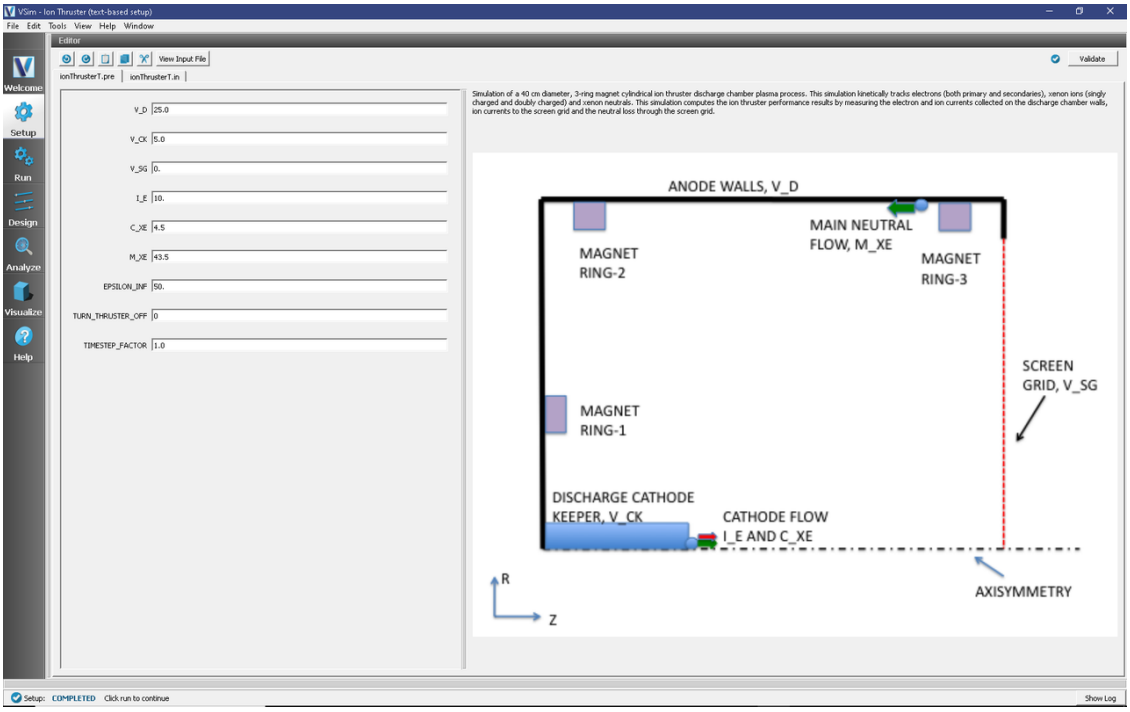


Fig. 6.114: Setup Window for the Ion Thruster example.

Input File Features

The input file allows the user a choice of ion thruster operating parameters such as discharge voltage, cathode keeper voltage, screen grid voltage, discharge cathode electron emission current, cathode neutral flow rate, and main neutral flow rate. Also it gives the user an option to specify the inflated permittivity scale factor by which the real permittivity of free space is scaled.

The self-consistent electric field is solved from Poisson's equation by the electrostatic solver in cylindrical coordinates. Because this simulation is defined in the *r*-*z* plane, the Laplacian uses a cylindrical geometry involving a 1/r term in the derivative with respect to *r*. The simulation is performed in an axisymmetric 2-D (*r*-*z*) domain. The actual thruster dimensions are reduced by the `SHRINK_FACTOR` variable in the input file (default 200). Correspondingly the physical parameters such as electric fields, magnetic fields, and particle densities are scaled by the shrink factor to maintain consistent physical effects (e.g. Larmor radius, Knudsen number).

The plasma is represented by macro-particles which are moved via the Boris pusher in cylindrical coordinates. Various types of elastic and inelastic particle collisions are calculated with the computational engine's Monte Carlo package. In this simulation the propellant xenon neutrals are tracked as kinetic particles and undergo collisions with electrons. The simulation employs variable-weight particle splitting and self-combination via `NullInteraction` blocks to help maintain good particle resolution over orders-of-magnitude variations in density across the domain.

This input file contains an imported magnetic field. The external magnetic field file is in units of Gauss, and is converted into Teslas when imported by VSim.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1e-12
  - *Number of Steps*: 5000
  - *Dump Periodicity*: 1000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.115.

The default number of time-steps for this simulation is 5,000, but to approach steady-state, approximately 500,000 time-steps are required. The *Visualizing the Results* section provides a review of the results at 5,000 time-steps, while the *Further Experiments* section is a review of the results after 500,000 time-steps.

Analyzing the Results

If the electron density is desired the analysis script *computePtclNumDensity.py* may be used.

- In the leftmost panel, click the **Analyze** button. Select *computePtclNumDensity.py* from the list of analyzers, then click *Open* at the top of the Analysis Controls pane.
- Enter "electrons" into the *speciesName* field.
- Click the *Analyze* button near the upper right of the Analysis Results pane.
- Repeat with other particle species if desired ("XeIons", "XeNeutrals")

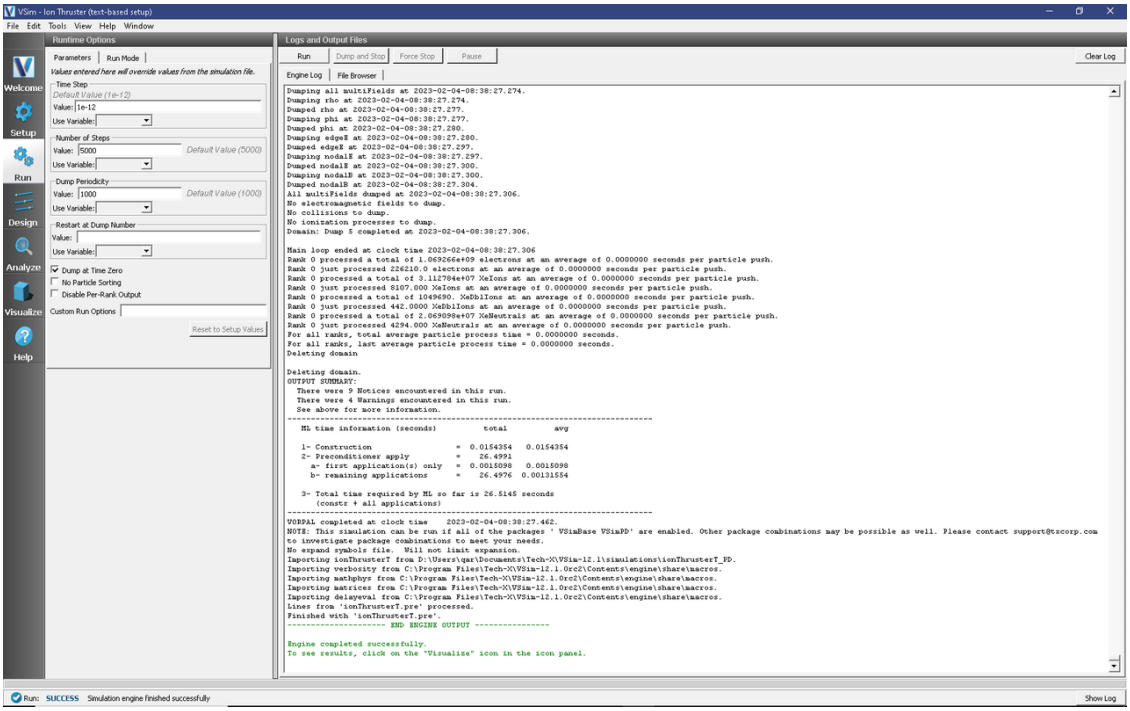


Fig. 6.115: The Run Window at the end of execution.

The analysis results are now viewable in the Visualize window, as shown in the following section.

Visualizing the Results

After performing the above actions, continue as follows:

- Proceed to the Visualize window by clicking the **Visualize** button in the leftmost panel.
- In the top of the *Visualization Controls* pane, click on the *Add a Data View* button then click on *Field Analysis*. This will open a new *Field Analysis* tab next to the existing *Data Overview* tab.
- In the *Field* dropdown menu, select *phi*. A pseudocolor plot of the potential with a radial lineout performed should be displayed as shown in Fig. 6.116.
- To plot the axial potential profile, in the *Lineout Settings* section, select the *Horizontal* tab, change the intercept to `0.00005`, and click *Perform Lineout* to plot the axial accelerating potential as shown in Fig. 6.116. If desired, select the *Advanced* tab to choose arbitrary start and end points for the lineout.
- In the top of the *Visualization Controls* pane, click on the *Add a Data View* button then click on *Phase Space*. This will open a new *Phase Space* tab next to the *Field Analysis* tab.
- In the *Base Variable* dropdown menu, select *electrons*.
- To maintain the same *z-r* convention as the previous electric potential plot, in the *X-axis* dropdown menu select *electrons_z* and in the *Y-axis* dropdown menu select *electrons_r*.
- Near the bottom of the *Visualization Controls* pane click *DRAW* and at the bottom of the *Visualization Results* pane move the *Dump* slider to the right to dump 5. The *z-r* phase space should be visible as shown in Fig. 6.117.

Recall that the electron number density distribution was calculated in *Analyzing the Results*. Plot the results of this analyzer as follows:

- In the top of the *Visualization Controls* pane, switch to the *Data Overview* tab.

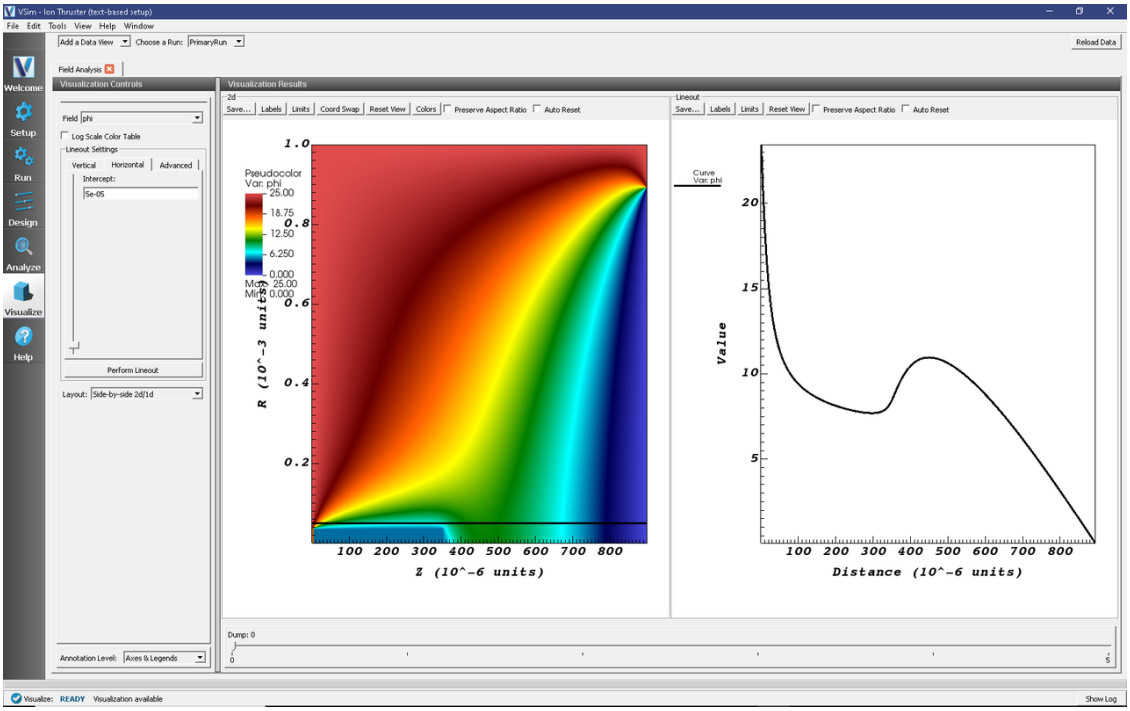


Fig. 6.116: Visualization of the *Field Analysis* result for the electric potential inside the ion thruster discharge chamber at timestep 0. Move the slider to the right with your mouse to view advanced timesteps.

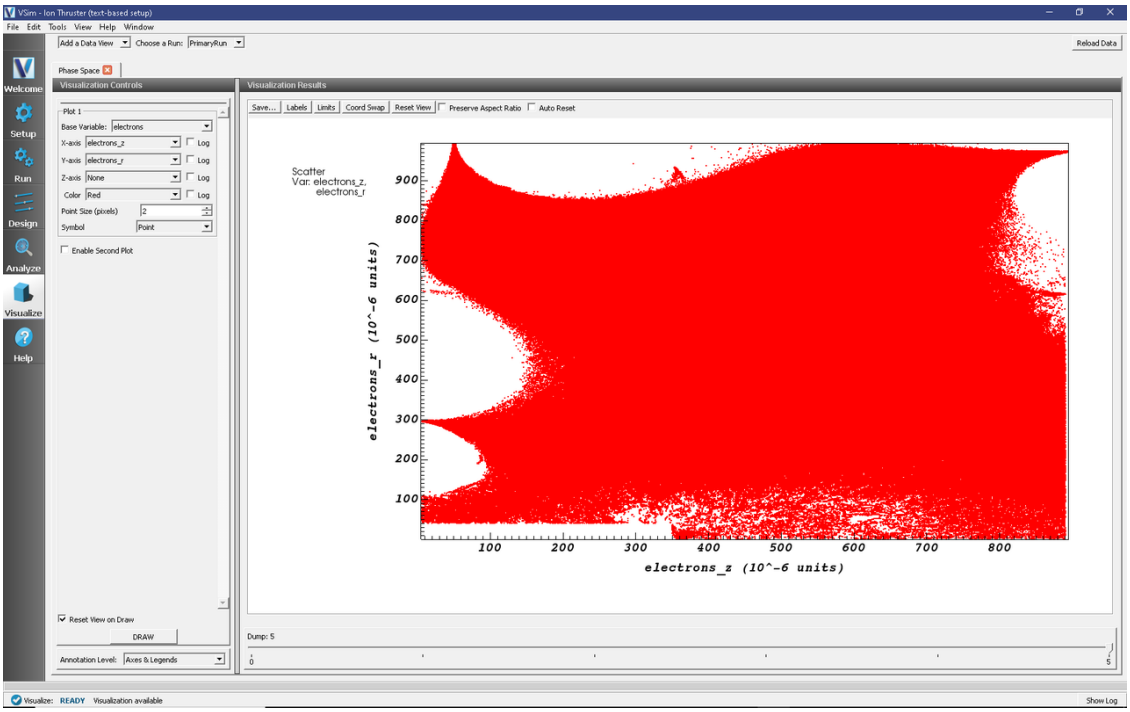


Fig. 6.117: Electron phase-space distribution results after 5,000 steps.

- In the *Variables* section, expand *Scalar Data*.
- Select *electronDensity*. A plot of the electron number density distribution should be displayed, though due to the large variation in densities, only a small portion of the domain will appear to be non-zero
- At the bottom of the variables section of the Visualization Controls pane, select the *Log Scale Color* checkbox.
- At the top of the Visualization Results pane click the *Colors* button, and in the resulting dialog set the limits to a minimum of 1e16 and maximum of 1e22, or experiment with limits as desired. The electron density on a logarithmic color scale should now displayed as shown in Fig. 6.118.

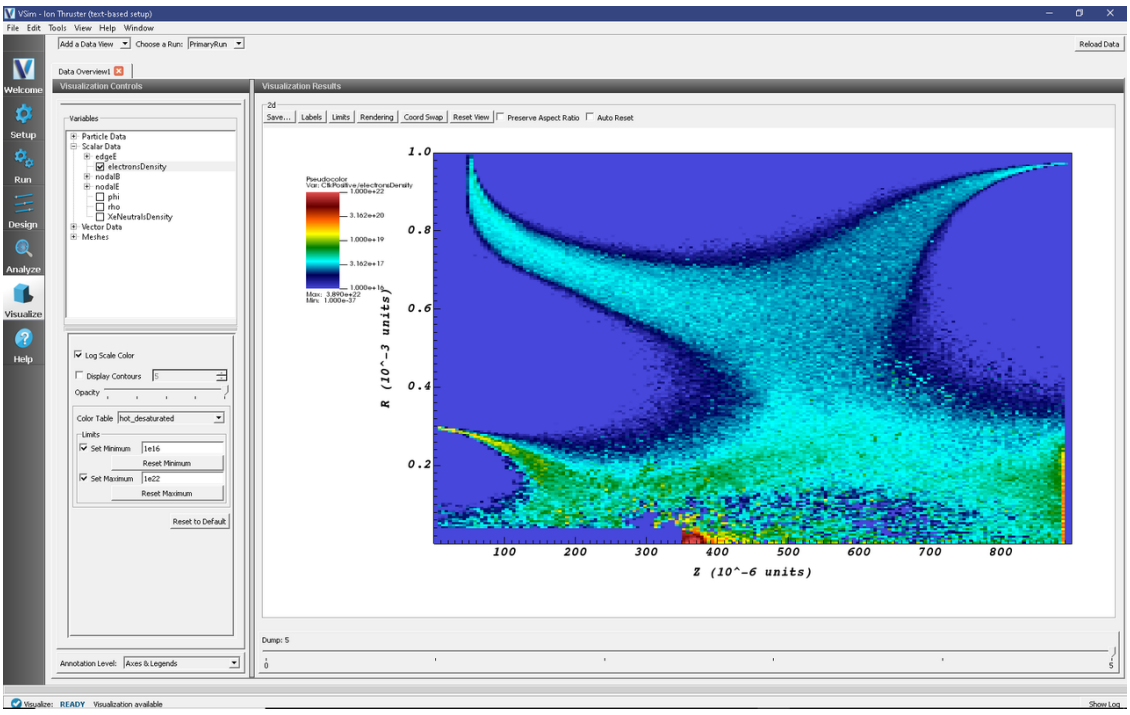


Fig. 6.118: Electron number density distribution results inside the discharge chamber after 5,000 steps.

Further Experiments

Return to the Run window by clicking on the **Run** button in the leftmost panel, change *Number of Steps* to 500,000. To reduce the number of output files, change the *Dump Periodicity* to 5000 and then click the *Run* button at the top of the Logs and Output Files pane. A high-performance computing cluster is recommended for this run, which will require approximately 6 days running on 64 cores. When the run has completed, take the following steps.

- Plot the potential at the final data dump similar to the steps taken in *Visualizing the Results*.
- In the Visualization Results pane, in the *2d* section, click the *Colors* button
- Set the minimum to 0 and the maximum to 25 (Volts). The resulting plot is shown in Fig. 6.119

It can be seen that the ions experience most of their acceleration in the sheath near the right-side boundary of the plasma chamber. Plot the electron and ion densities by taking the following steps:

- Following once again the steps taken in *Visualizing the Results*, run the *computePtclNumDensity.py* analyzer on both *electrons* and *XeIons*.
- Plot the electrons density using the color log scale and the same limits as previous, as shown in Fig. 6.120

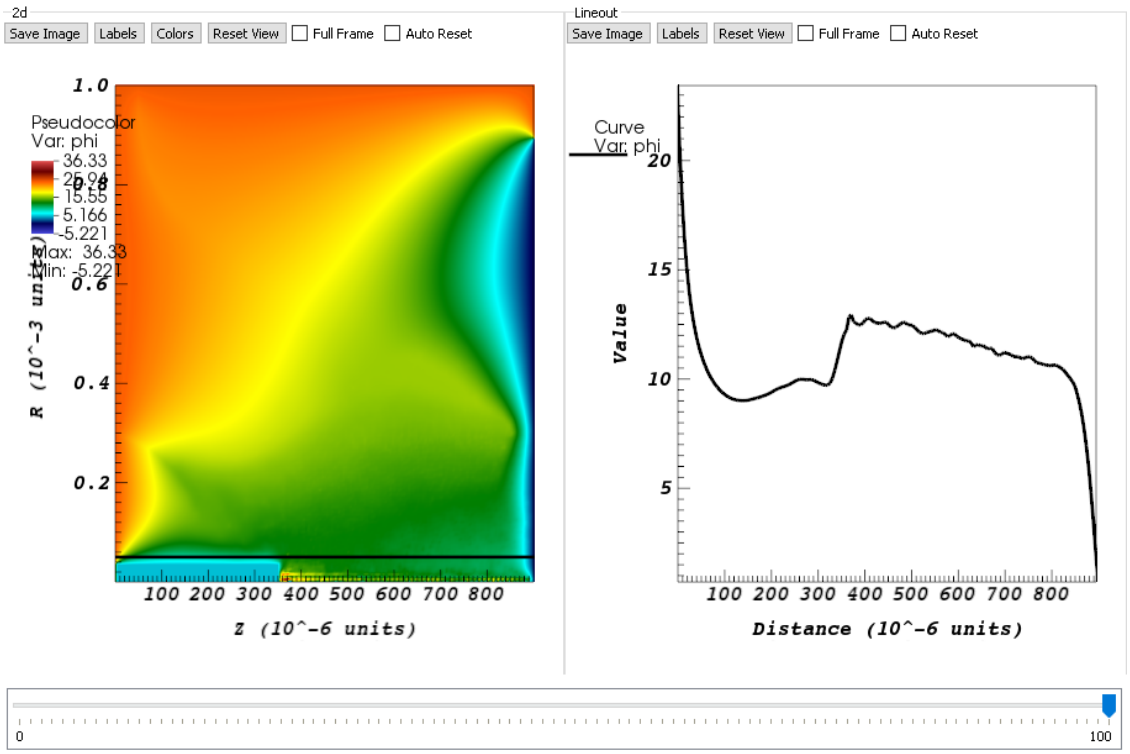


Fig. 6.119: Electric potential of the plasma inside the ion thruster discharge chamber after 500,000 time-steps.

- Plot the ion density using the color log scale with a minimum of 1e18 and a maximum of 1e23 to get the image shown in Fig. 6.121 or experiment with the limits as desired.

It can be seen from Fig. 6.120 and Fig. 6.121 that the electrons are confined by the magnetic field lines while the much heavier ions are not, allowing a more uniform acceleration of ions out the right side of the chamber, resulting in thrust.

Plot the electron and ion macroparticle positions with the following steps:

- In the top of the *Visualization Controls* pane, open a new *Phase Space* tab under the *Add a Data View* button.
- Under *Plot 1* click the *Base Variable* drop-down menu and select *electrons*
- Change *X-axis* to *electrons_z* and *Y-axis* to *electrons_r*, change *Point Size* to 1, and at the bottom of the Visualization Controls pane, click *DRAW* to see the electron macro-particle positions.
- Check the *Enable Second Plot* button.
- Under *Plot 2* change *Base Variable* to *XeIons*, change *X-axis* to *XeIons_z* and *Y-axis* to *XeIons_r*, change *Point Size* to 1, and click *DRAW* once again to see the electron and singly-ionized xenon macro-particle positions.
- Check the *Enable Third Plot* button.
- Under *Plot 3* change *Base Variable* to *XeDblIons*, change *X-axis* to *XeDblIons_z* and *Y-axis* to *XeDblIons_r*, change *Point Size* to 3, and click *DRAW* once again. The ion and electron positions should be displayed as shown in Fig. 6.122.

The electrons appear well confined by the 3-ring magnetic circuit arrangement, and move along the magnetic cusp regions formed between the magnets. Most of the electrons are lost to the discharge chamber walls through the magnetic cusps and are absorbed at the walls in 3 small areas. Only a few electrons are able to cross the strong magnetic field lines and reach the top wall between the cusps.

Singly and doubly ionized xenon are generated inside the discharge chamber through ionizing collisions of electrons

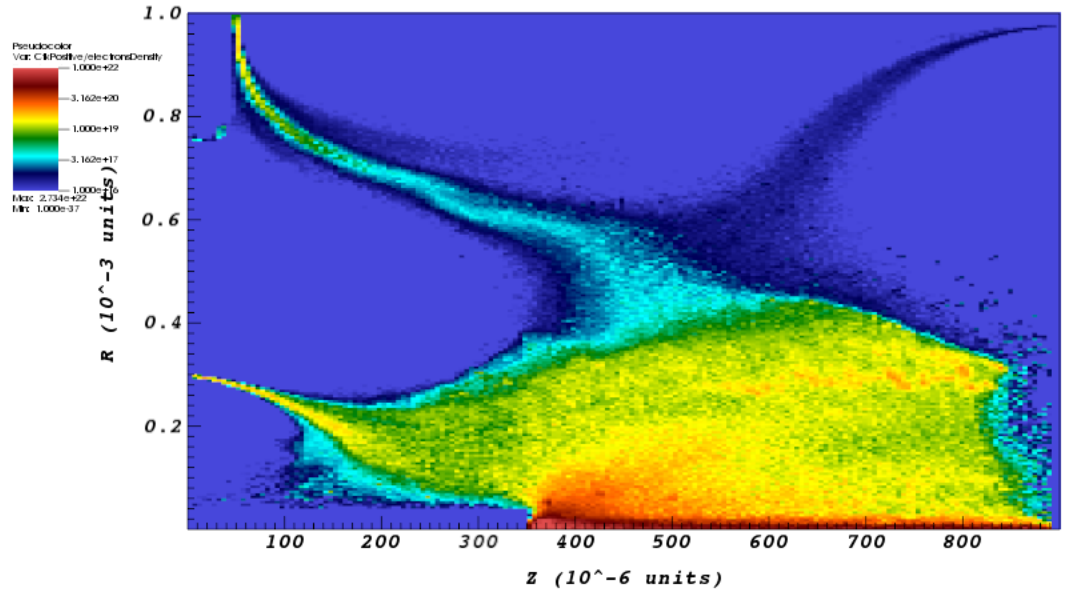


Fig. 6.120: Electron number density distribution results inside the discharge chamber after 500,000 steps.

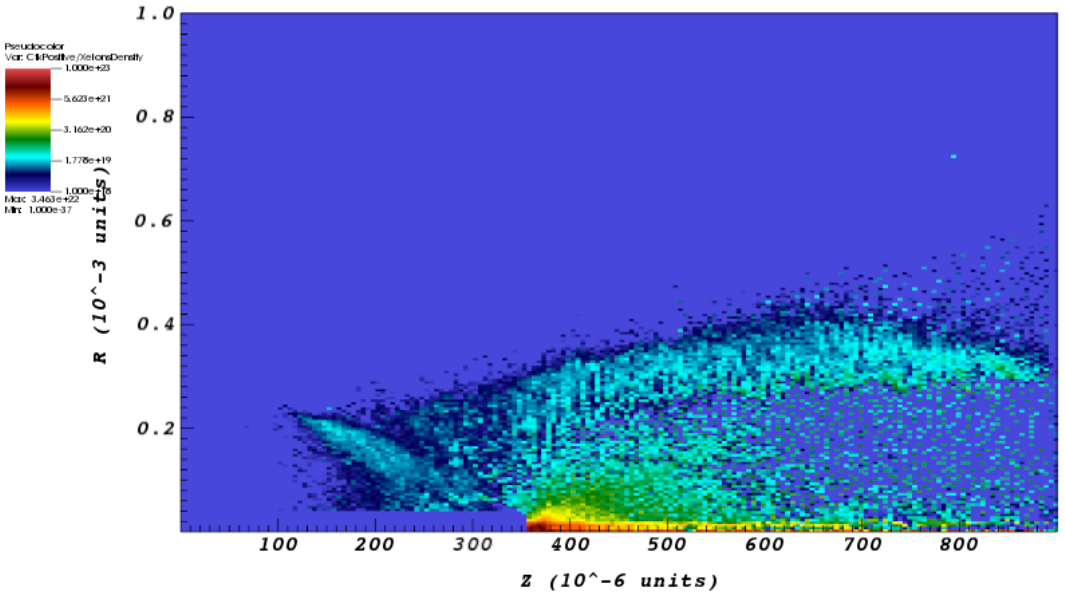


Fig. 6.121: Ion number density distribution results inside the discharge chamber after 500,000 steps.

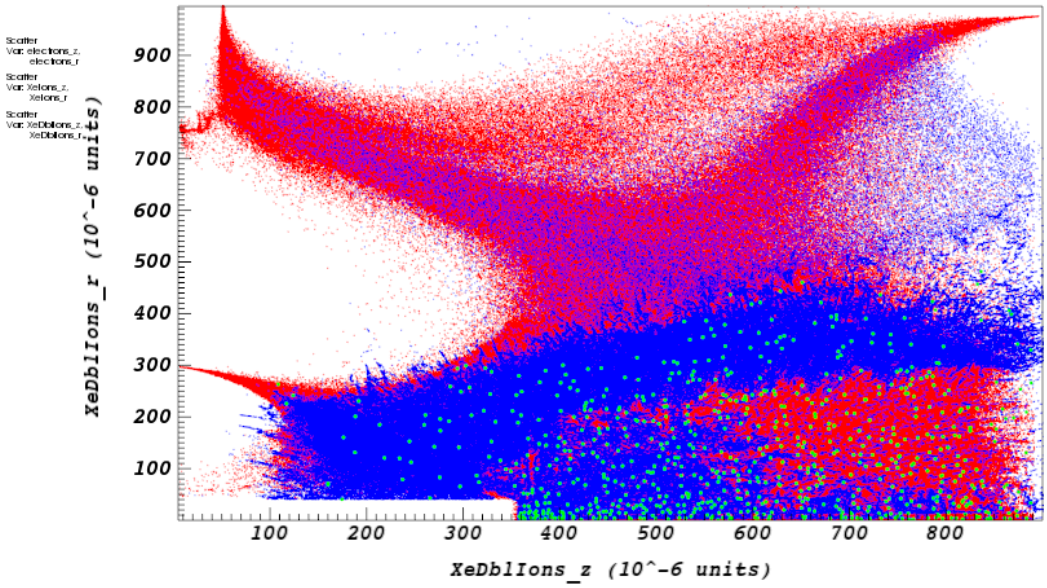


Fig. 6.122: Electron and ion phase-space distribution results after 500,000 steps.

with xenon neutrals. Only electrons with energies above the ionization thresholds (12.1 eV for the first ionization level and 21.25 eV for the second) can ionize neutrals.

This input file can be modified to test different design parameters covering a range of anode voltages, xenon flow rates, and electron emission currents, to allow study of high-to-low power and high-to-low throttle levels.

6.9.2 Satellite Surface Charging (satelliteSurfaceChargeT.pre)

Keywords:

`electrostatics, surface charges`

Problem description

Satellites and other spacecraft operating in the space environment often suffer arcing and breakdown problems due to surface charging. Charged particles buildup on the spacecraft surfaces (such as solar panel arrays and other components) leading to localized arcing/breakdown discharges that can critically fail a component or the entire unit. This problem is made worse as the demand for high power space missions in both satellite and deep-space applications rises. These high-power spacecraft are outfitted with high-voltage solar panels. These panels minimize the overall payload requirements and offer other advantages over more massive, low-voltage arrays. However, they are also more vulnerable to surface charge related arcing. It therefore becomes important to predict the surface charge buildup on spacecraft bodies operating in different space environments, where the ion sources may be natural solar wind or human-made space plasma resulting from electric thruster plasma plumes.

This example demonstrates a satellite body operating in the solar wind environment where the space plasma consists of ions and electrons. The simulation box is set up with dimensions of 15 m x 30 m x 15 m. The satellite system is placed in the middle of the domain. It has a 3 m radius x 5 m long cylindrical central unit connected to solar panels at either end. Each solar panel has a total span length of 7.8 m and a width of 5 m. The satellite central unit has a 5-volt equipotential circular body with radius 2 m and length 3 m. The satellite system is treated as a conductor floating in free

space. The system domain boundaries are assumed to have zero perpendicular electric field, i.e. Neumann boundary conditions. The solar wind plasma is introduced in the simulation domain from the positive z direction. The solar wind density is set to $1 \times 10^7 \mathrm{m}^{-3}$ with a temperature of 10 eV. The number of physical particles per macro-particle is set to 5000. Both electrons and ions are introduced from the source based on the solar wind density and temperature. To maintain plasma uniformity within finite bounds, the electron source rate is inflated slightly because electrons are lighter and leave the system more quickly than do ions. At the same time, the positive ions are imbued with a lighter mass value to speed up the simulation. All simulation boundaries are set up to absorb particles. The charges collected in the satellite system are counted by emitting a heavy electron or heavy ion at the point where an electron or ion was absorbed. The heavy electron/ion is not a physical concept, it is a computational trick whereby any charged particle striking the satellite gets converted to a new species, one with equivalent charge but drastically swollen mass (1 kg in this case) and suppressed energy (suppressed by a factor of 10 billion). In this way, the heavy particles do not propagate from their point of origin, effectively sticking to the satellite surface. To limit the number of macro heavy particles tracked we apply a particle combining algorithm which limits the number of macro particle per cell to one. The collected electron and ion currents on the satellite surfaces are output as histories.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The satellite surface charging example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Spacecraft (text-based setup)* option.
- Select "Satellite Surface Charging (text-based setup)" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the Setup Window, as shown in Fig. 6.123.

Input File Features

The input file allows a choice of space environment parameters (number density, plasma temperature, drift speed), satellite body voltage, simulation domain size, and resolution (number of cells in each direction).

The self-consistent electric field is solved from Poisson's equation by the electrostatic solver. The far-field space boundaries are handled with Neumann boundary conditions. The satellite inner body is set up with an equipotential boundary. The surface charges collected on the satellite system make the satellite body float at a slightly higher voltage than the space plasma.

This is a large domain, 3-D problem, and its resolution is aided by several numerical methods. The plasma is represented by macro-particles which are moved according to the Boris pusher. Variable weight particle treatment is employed on all simulated species, reducing the overall number of macro-particles in the computation. Additionally, null interactions are considered as part of the Monte Carlo analysis to limit the number of macro-particles per cell; macro-particles are eliminated in overcrowded cells by means of inelastic combination.

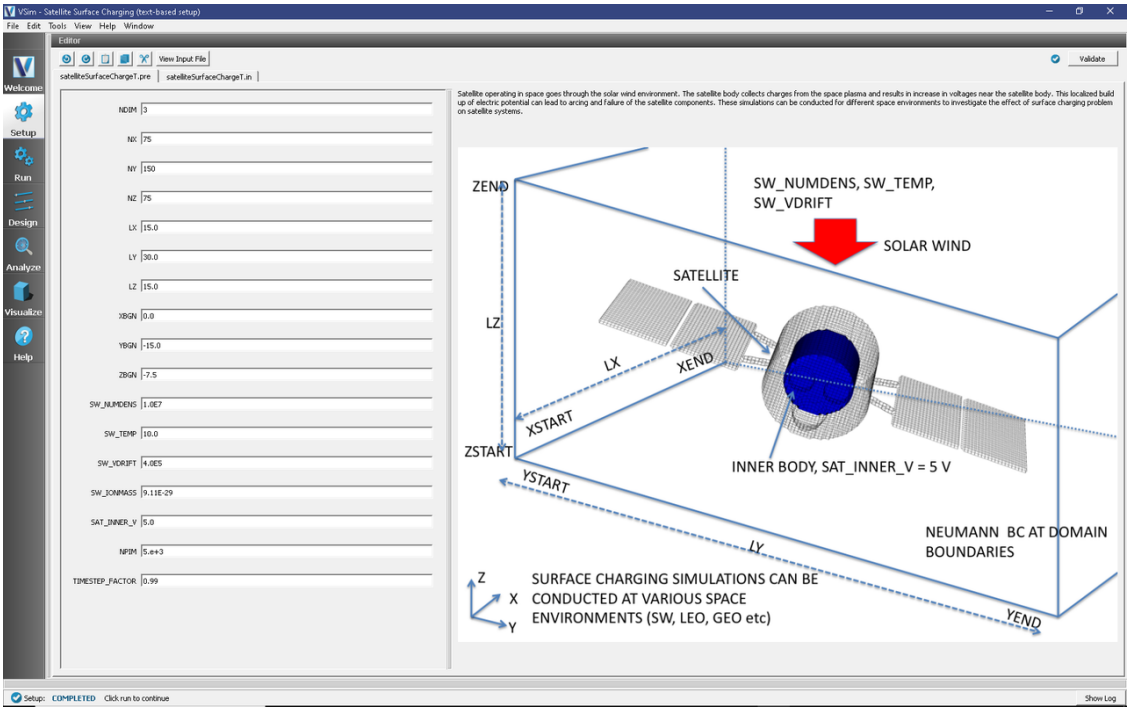


Fig. 6.123: Setup Window for the Satellite Surface Charging example.

Running the simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 2e-08
  - *Number of Steps*: 100
  - *Dump Periodicity*: 10
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.124.

Analyzing the Results

If the electron density is desired, then proceed as follows:

- In the leftmost panel, click the *Analyze* button and then select *computePtclNumDensity.py* from the list of analyzers, then click *Open* at the top of the Analysis Controls pane.
- Enter the following parameters in the appropriate fields:
  - simulationName = satelliteSurfaceChargeT
  - speciesName = solarElectrons

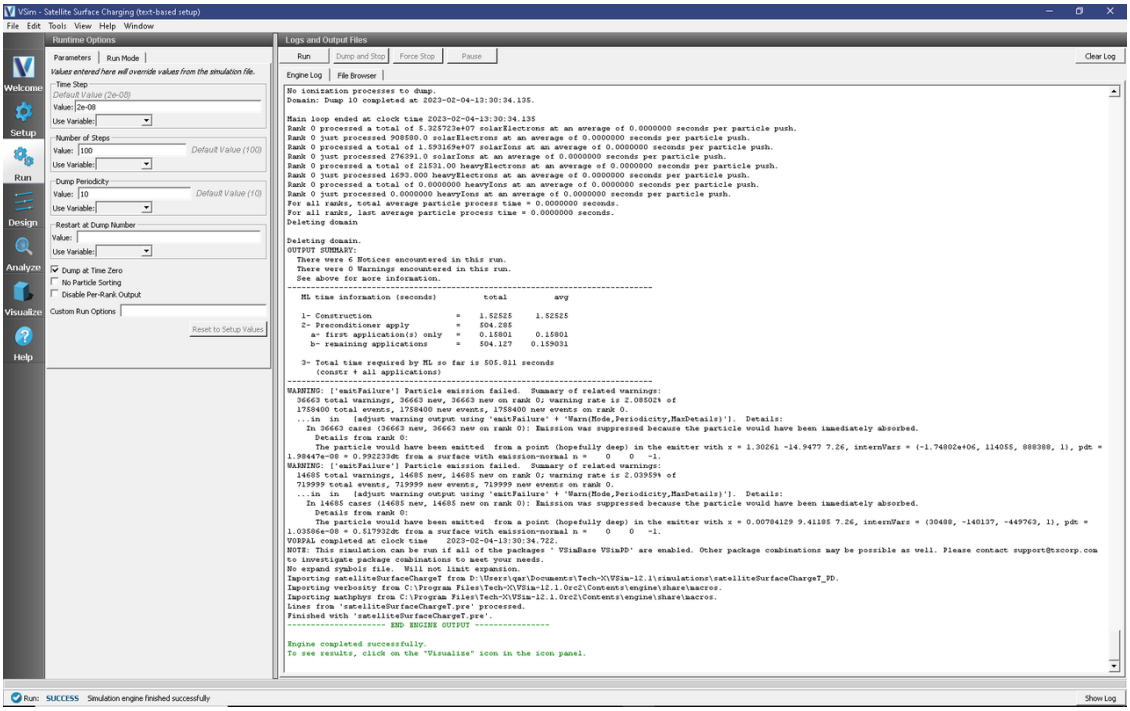


Fig. 6.124: The Run Window at the end of execution.

  - avgNxN = 1
  - iterateAvg = 1

- Click the *Analyze* button in the upper right corner of the window.

See Fig. 6.125.

The resulting data will be visualizable as *solarElectronsDensity* under the *Scalar Data* menu in the *Visualize* Tab. The density of solarIons can be calculated in the same way by substituting that species name in place of *solarElectrons*.

Visualizing the results

After performing the above actions, proceed to the Visualize Window by pressing the *Visualize* button in the left column of buttons.

To visualize the satellite geometry with electrons Fig. 6.126, proceed as follows:

- Expand *Particle Data*.
- Expand *heavyElectrons*.
- Select “heavyElectrons” in red.
- Expand *solarElectrons*.
- Select “solarElectrons” in green.
- Expand *Geometries*.
- Select “poly_surface (Satellite)”.
- Move the Dump slider to dump 7.

Here are some things to try:

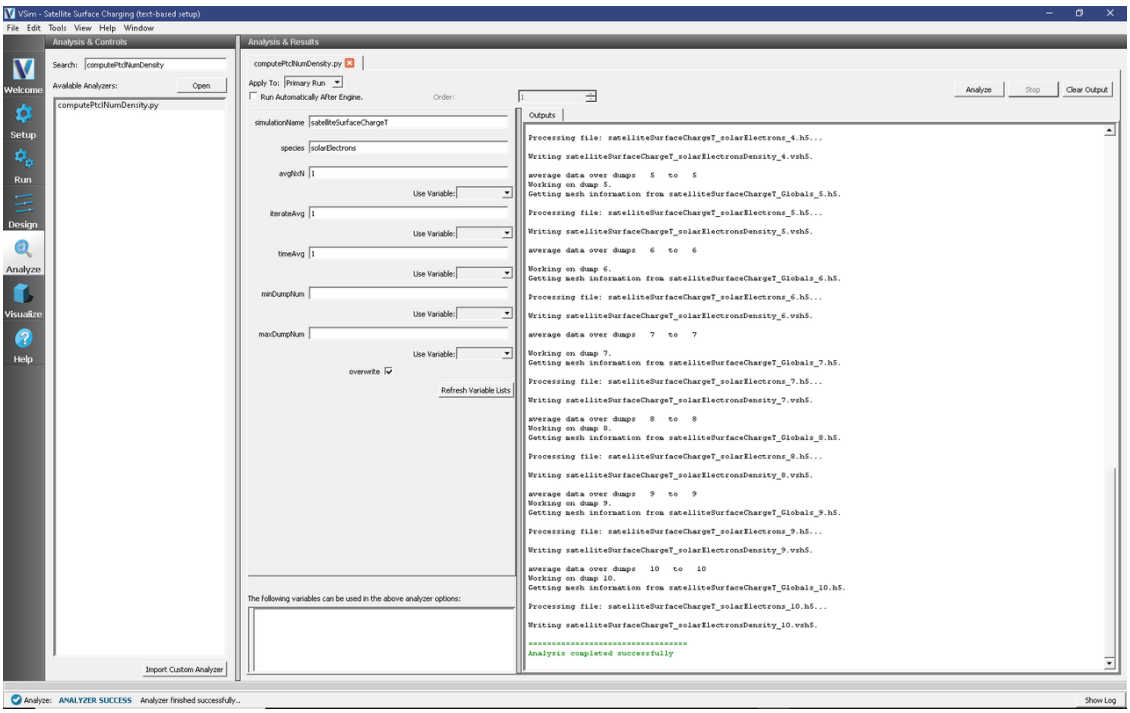


Fig. 6.125: The Run Window at the end of execution.

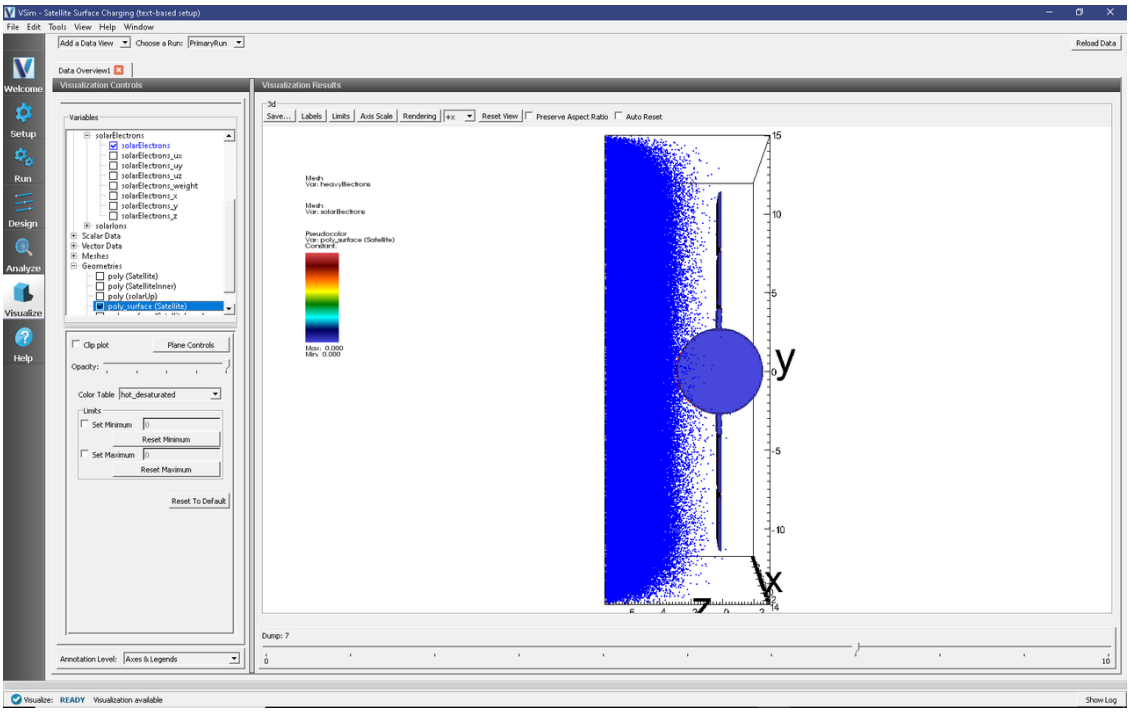


Fig. 6.126: Visualization plot of satellite system with solar wind electrons in green and the electrons that stick to the satellite surface in red.

- Under *Data Overview* you can access plots of the electric field, charge density (rho), and electric potential (phi). Select the *Display Contours* check box for viewing these.
- To view the phase space distribution for the electrons and ions, click on the *Data View* drop down menu and select *Phase Space*. Click the *Draw* button to generate a plot.
- Also from the *Data View* menu select *History* to observe the satellite currents and the time history results for the number of macro-particles broken down by species.

To generate Fig. 6.127, that shows the satellite system with the inner equipotential cylindrical body, proceed as follows:

- In the *Data View* pane on the left side select "Data Overview" from the drop-down menu.
- Expand *Geometries*
- Select "poly (Satellite)"
- Select "poly_surface (SatelliteInner)".

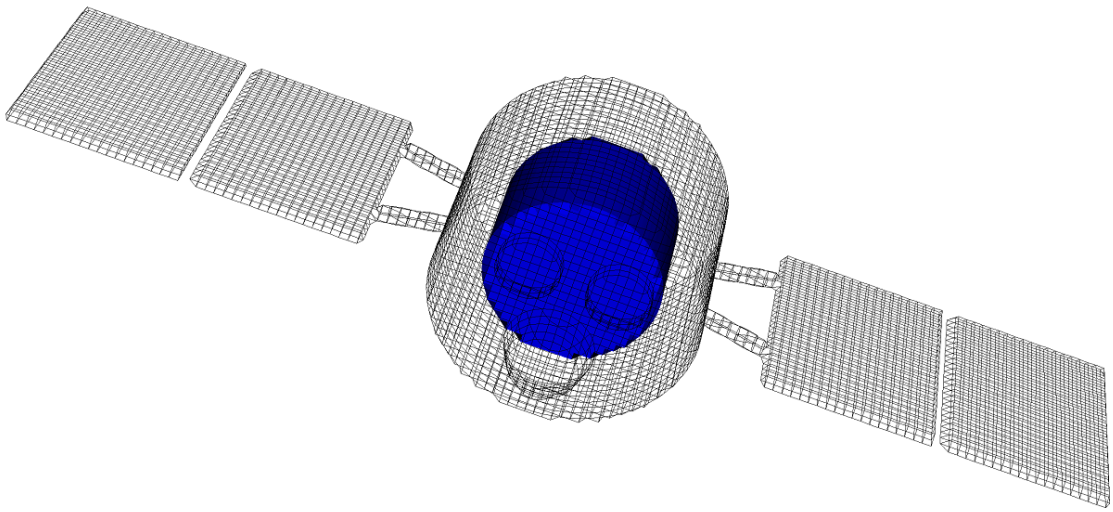


Fig. 6.127: Visualization of the inner body inside the satellite system.

The phase-space distribution of the positive ions (solarIons species) surrounding the satellite system is shown in Fig. 6.128 which is obtained after running the simulation for 500 time steps. Solar wind plasma enters into the simulation system from the top z boundary, i.e. above the satellite body.

Surface charge accumulation on the satellite body after 93,000 time steps is shown in Fig. 6.129. The red dots indicate electrons and the green dots ions. The surface charges on the satellite body can be viewed in VSimComposer by turning on Particle Data –> heavyElectrons and ParticleData -> heavyIons under the Data Overview pane.

The charge density built-up on the satellite system is shown in Fig. 6.130 after running for 93,000 time steps. To view the charge density in the simulation domain, turn on the Scalar Data -> rho field in the *Data Overview* pane. In this figure the satellite body is also included by turning on the Geometries -> poly_surface(Satellite) option in the *Data Overview* pane. The charge density appears net positive in most regions of the solar panels.

To view the electrostatic potential, turn on phi under the Scalar Data in the *Data Overview* pane. The electrostatic potential of the satellite system simulated is shown in Fig. 6.131 after running for 93,000 time steps. The electrostatic potential is plotted in X-Y-Z with domain clipping in the X and Z directions. The bulk of the plasma potential in the space region is close to 0 volts (blue contours). The surface charge built-up on the solar panels raises the surface potential by up to 4 to 5 volts above the bulk space plasma.

The magnitude of the electric field distribution on the satellite surface after 93,000 time steps is shown in Fig. 6.132. The peak of the distribution coincides with regions on the solar array where there is net positive charge buildup. The

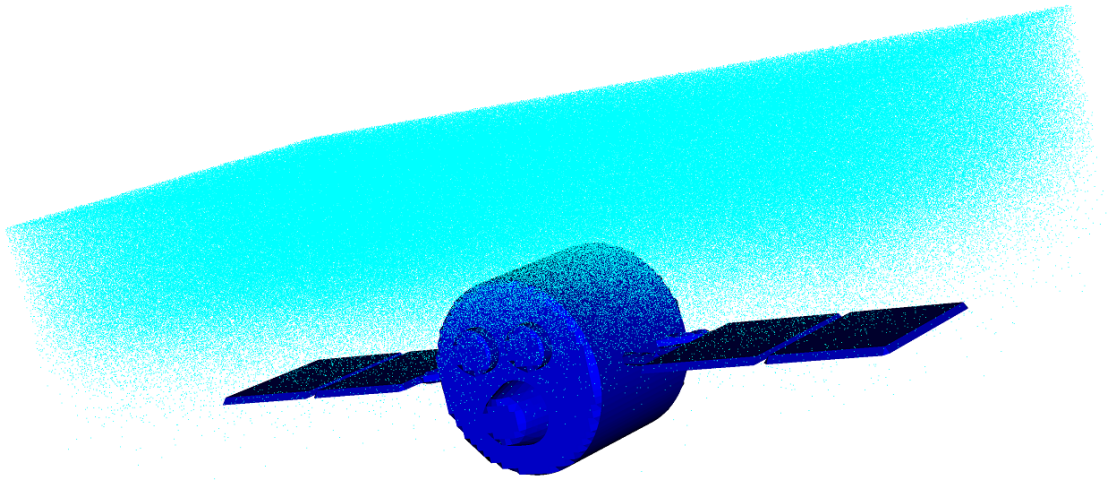


Fig. 6.128: Visualization of the satellite system with solar ions.

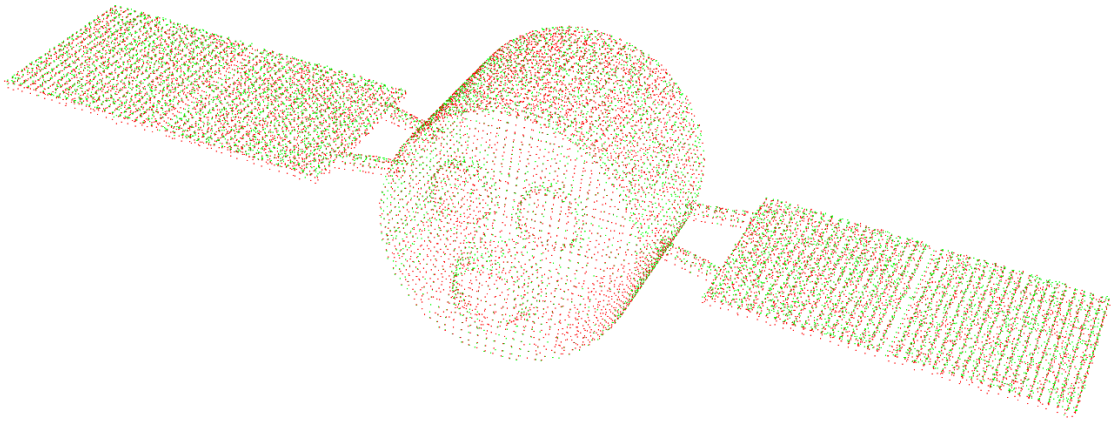


Fig. 6.129: Visualization of surface charge buildup on the satellite system after 93,000 time steps.

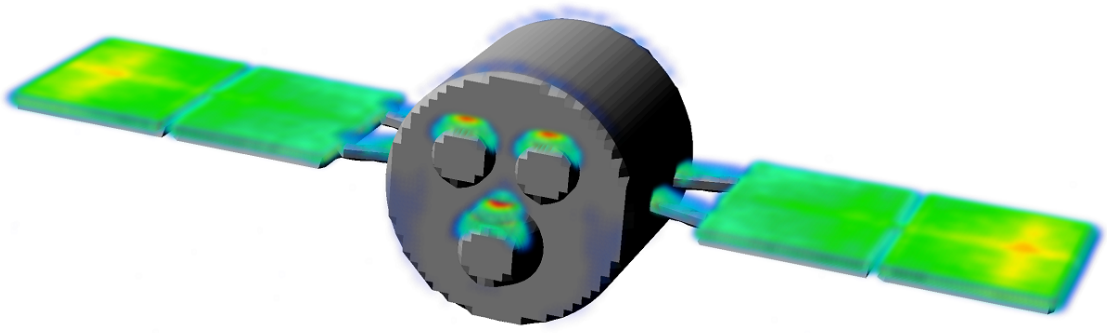


Fig. 6.130: Visualization of the charge density on the satellite system.

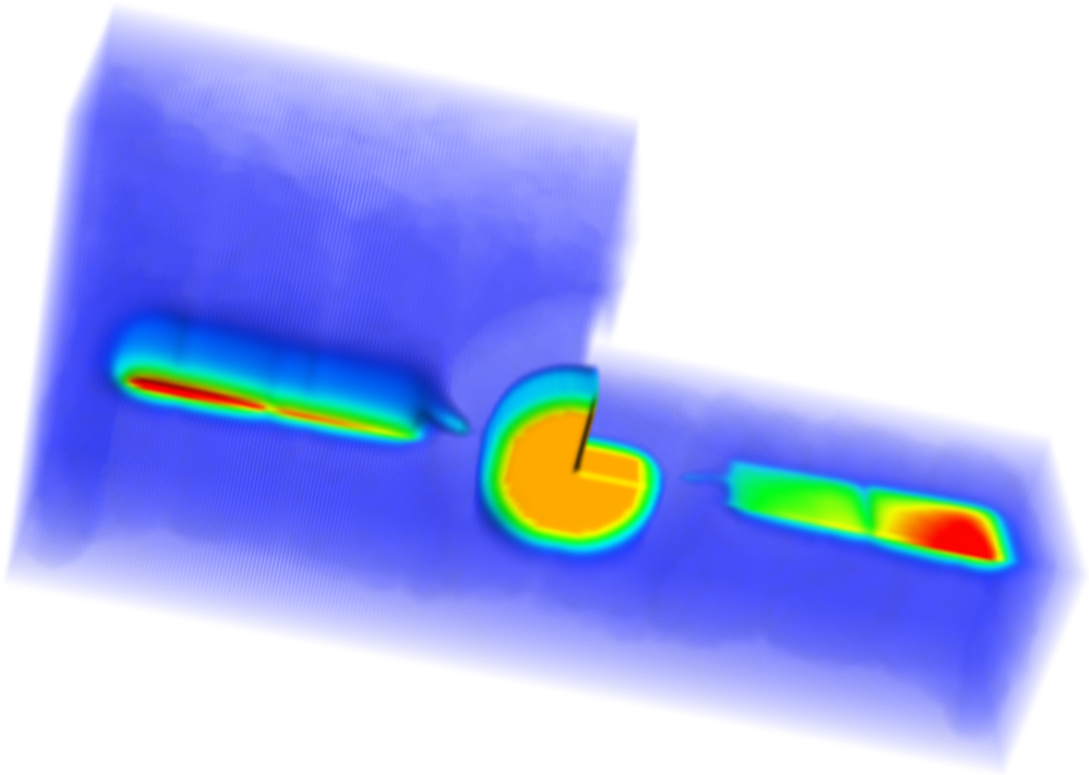


Fig. 6.131: Visualization of the electric potential surrounding the satellite system.

magnitude of the electric field was computed using the *Expressions* function in the Visit interface. Should you wish to get to those calculations, right-click on the plot and select *Open GUI*. (You must have the *Enable VisIt context menu* box check-marked in Visualization Options. Go to Tools -> Settings -> Visualization Options, to enable this.) This will launch the VisIt control panel. From there, go to Controls -> Expressions. You can select any plottable variable to view its mathematical definition.

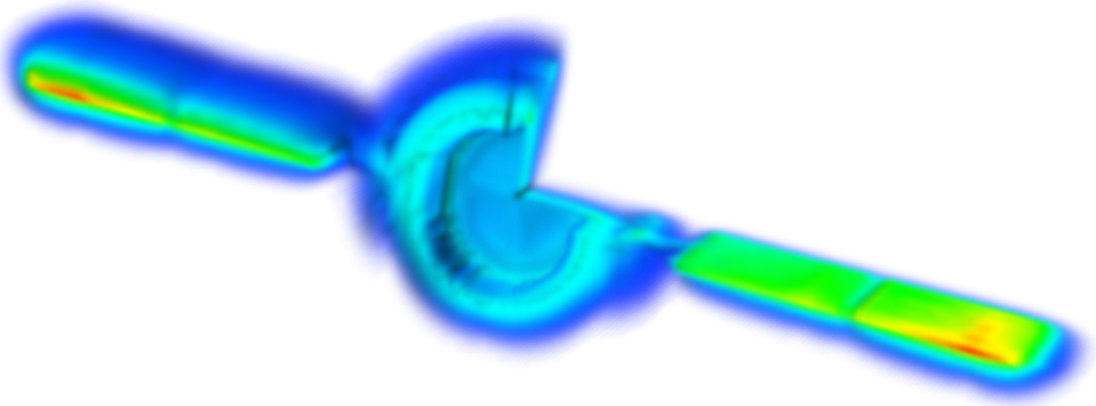


Fig. 6.132: Visualization of the magnitude of electric field surrounding the satellite system.

Further Experiments

The geometry and background space plasma parameters of this input file can be modified to test satellite inner body voltages and satellite surface charge collection in a variety of different space environments.

VSim allows the use of "open" boundary conditions to represent the far-field boundaries in the space environment.

6.10 Sputtering

6.10.1 Ion Beam Sputtering (ionBeamSputtering.sdf)

Keywords:

`sputtering, ion beam, electrostatics`

Problem Description

In this simulation, a 450 eV beam of positively charged argon ions strikes a copper plate (cathode) at -25 volts with respect to the walls on the upper and lower x boundaries of the simulation. A Neumann boundary condition where the slope of the electric potential is zero is placed on the upper and lower y walls of the simulation.

The argon ion beam travels through a vacuum and sputter off neutral copper atoms from the cathode.

This demonstrates how to set up a sputtering interaction through the Visual Setup in VSimComposer.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The Ion Beam Sputtering example can be accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Sputtering* option.
- Select "Ion Beam Sputtering" and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

You can expand the tree elements and navigate through the various properties, making any changes you desire, but the run here is using the setup as is. The right pane shows a 3D view of the geometry, if any, as well as the grid, if actively shown. The setup window, with the *Particle Dynamics* → *Kinetic Particles* → *ArgonIons*, and *neutralCopper* elements expanded is shown in Fig. 6.133.

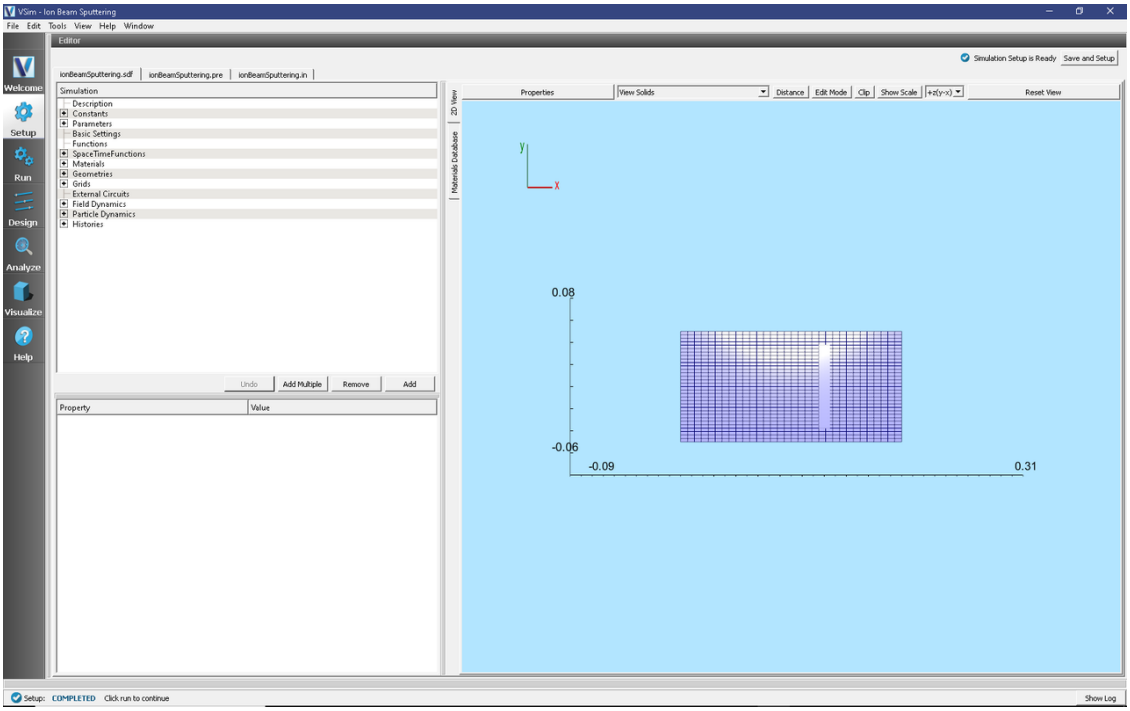


Fig. 6.133: Setup window for the Ion Beam Sputtering example.

Simulation Properties

The Ion Beam Sputtering example includes some constants for easy adjustment of simulation properties:

- **`BEAM_RADIUS`**: sets the radius of the argon ion beam
- **`BEAM_ENERGY`**: sets the energy (and speed) of the ion beam
- **`BEAM_CURRENT`**: sets the emitted current. *Note*: the total current emitted will be less than this value if a mask is applied to the particle emitter (which is the case in this simulation).
- **`CATHODE_VOLTAGE`**: the negative bias for the cathode.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 6.7271460165054675e-09
  - *Number of Steps*: 1000
  - *Dump Periodicity*: 20
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.134.

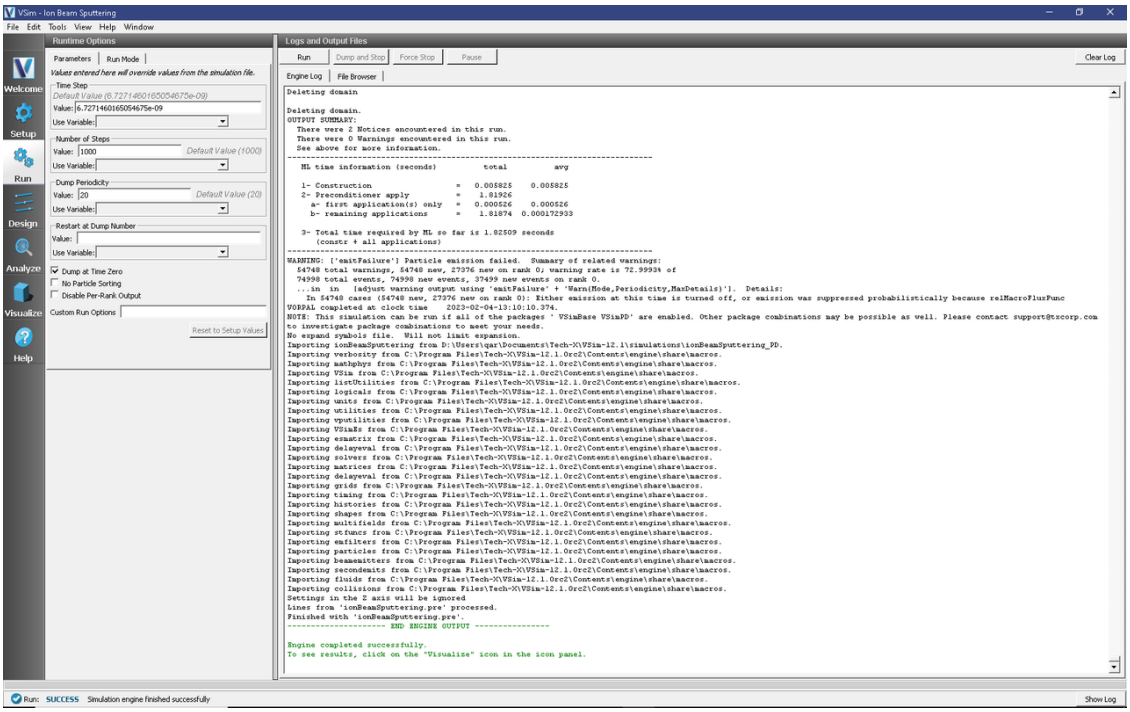


Fig. 6.134: The Run window at the end of execution.

Visualizing the results

After performing the above actions, continue as follows:

1. Proceed to the *Visualize* window by pressing the Visualize button in the left column of buttons. Be sure to press the "Reload Data" button at the bottom of the window if you have previously navigated to the *Visualize* window.
2. Expand "Particle Data" then expand "ArgonIons" and check the red "ArgonIons" box.
3. Expand "neutralCopper" and check the green "neutralCopper" box.
4. Expand "Scalar Data" and check "Phi". Then check the "Display Contours" box.

5. Expand “Geometries” and select poly (cathode).

Scrolling through the dumps, you should see the argon beam expand as it travels towards the cathode, as in Fig. 6.135. Copper atoms will appear after the argon beam strikes the cathode.

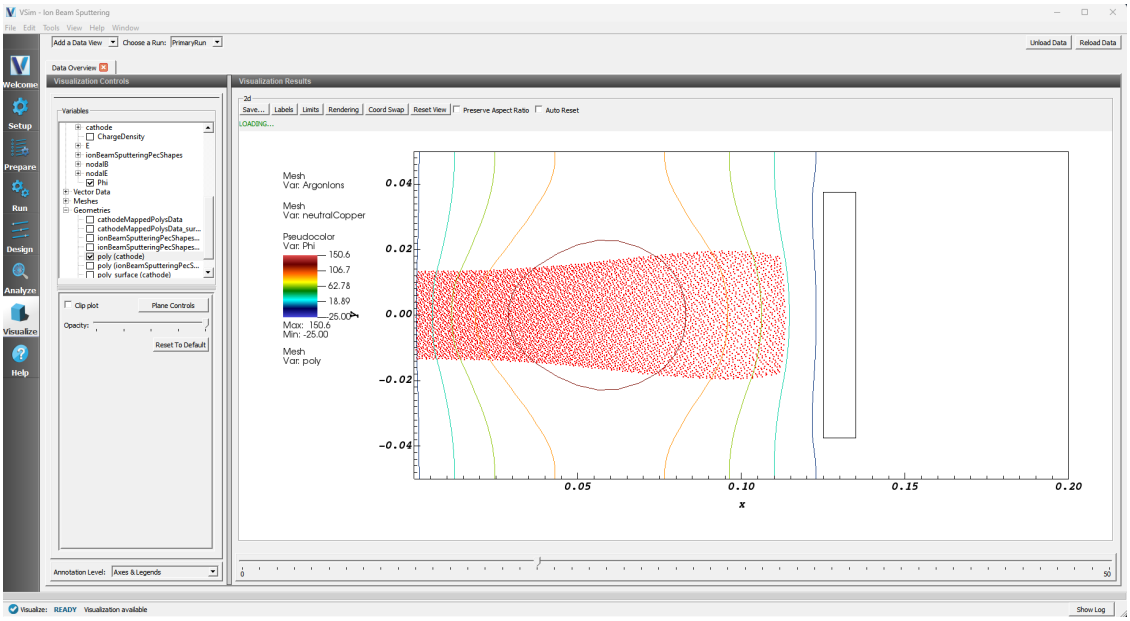


Fig. 6.135: Ion Beam Sputtering an instant before the argon beam strikes the wall.

Next, in the *Data View* drop down menu at the top left of the window, switch from “Data Overview” to “History”. In *Graph 2*, change from “emittedArgonCurrent” to “<None>” to see the plots shown in Fig. 6.136

These plots show the energy deposited onto the cathode from the argon ion species as well as the number of neutral copper macro particles. From these plots its clear that the ion beam strikes the cathode after about 2.5 microseconds. A history for the total number of physical copper atoms is also available to be added to the simulation.

Further Experiments

1. Vary the *BEAM_ENERGY* constant, the species of ions in the beam, and the target material to see how the sputter yield changes in response (see the “numMacroCopper” history available in the *Visualize* Tab).

   To change the material of the target to see the effect on the sputtering yield, expand the *Particle Dynamics* element, then *neutralCopper*. Select the *sputterNeutralEmitter* and choose a new material from the “material properties” dropdown menu.

   Note: Savvy users may notice that the material of the cathode is also set in the *Geometries* element under *CSG → cathode*. This assignment of “PEC” sets the _electromagnetic_ properties of the geometry, not the particle properties.

   ---

2. Add electrons, secondary electron emission, an RF oscillating frequency on the cathode, and possibly an external magnetic field. Add a copperIons species and an electron impact ionization process to create copperIons from neutralCoppers. Add a second copper sputter emitter to the cathode that creates copper neutrals from copperIons to simulate self-sputtering.

3. Modify the beam current to account for the loss in current due to the mask. See the Negative Ion Beam example (*Negative Ion Beam (negativeIonBeam.sdf)*) for an example of how this is accomplished.

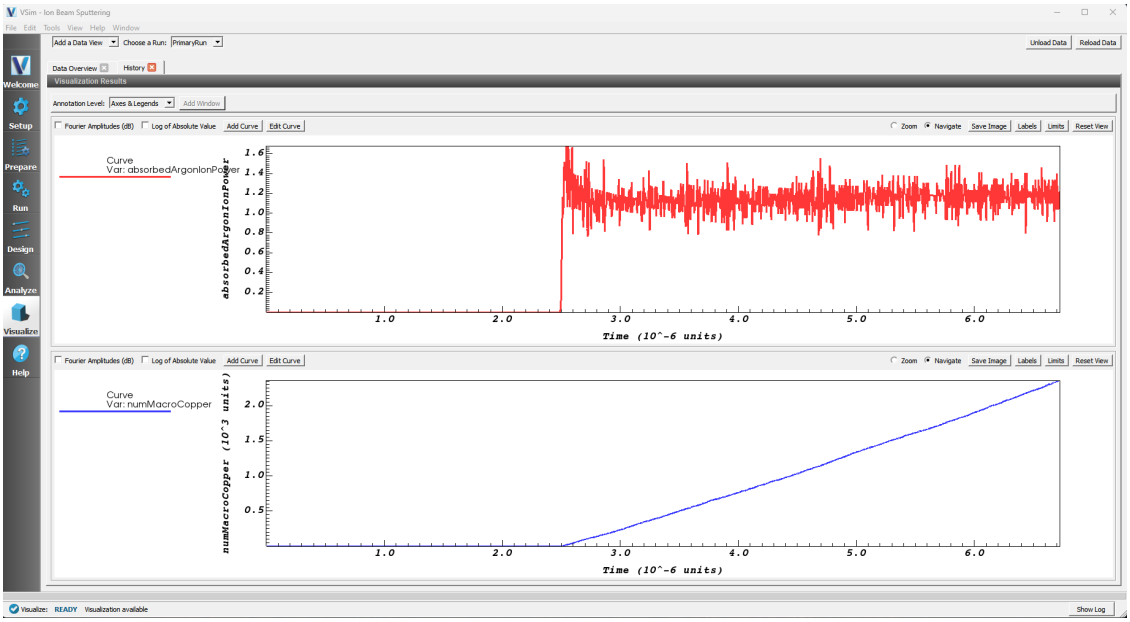


Fig. 6.136: Plots of the absorbed power and neutralCopper macro particle count.

6.10.2 Cylindrical Magnetron Sputtering (cylMagnetronSputtering.sdf)

Keywords:

Poisson solver, secondary electron emission, sputtering, external circuit, external magnetic field, physical vapor deposition, thin film deposition

Problem Description

This example illustrates the use of VSim to model one type of Physical Vapor Deposition (PVD) in which ions are accelerated (via a sheath) onto the cathode leading to the sputtering of the cathode material. The sputtered cathode material (composed of copper) is then dispersed onto the surrounding material uniformly leading to the thin film deposition of copper. There are several key physical concepts which lead to the effective sputtering of copper. The first key concept is that an external magnetic field must supplied in the proper orientation near the cathode. The magnetic field serves to trap some population of electrons which bounce between the north and south poles of two different magnets. The effective trapping of electrons allows for the formation of the sheath. (2) The massive ions are unmagnetized and are accelerated through the sheath onto the cathode. In this process, the ions impart their energy and momentum onto the copper cathode thus releasing copper ions in a process known as sputtering.

In addition, we also seek a steady state solution in this modeling effort. Steady state can be defined in a variety of ways and in this problem, steady state means a near constant number of physical secondary electrons and a near constant cathode potential. The reason for seeking a steady state solution is that PIC models are costly in terms of CPU-hours and many magnetron sputtering industrial setups will run in excess of millisecond time scales. It would take weeks or even months to run on such time scales using a reasonable number of processors. Therefore, if we can find steady state solutions then we can run VSim for 1-10 microsecond on reasonable time scales (less than 24 hours) and on a reasonable number of processors (less than 32) and extrapolate the results to millisecond time scales. Another reason for seeking steady state solutions is physically this will happen in most applications over some time scale. Therefore, by seeking a steady state solution which converges in 1-10 microseconds, we reduce the time it takes to model your problem.

In order to achieve steady state, there are many aspects to this problem which must be balanced. Here we will summarize many of the physical processes which we model and must in turn remain in balance. This problem represents a true

multi-physics simulation, all at your disposal in VSim: (1) Collisions between electrons and neutral Ar (2) Secondary emission of electrons off of the cathode (3) Trapping of electrons in the externally supplied magnetic field (4) Floating potential at the cathode modeled using an external circuit (5) Collection of currents at the cathode (6) Sputtering of neutral copper at the cathode

In the following sections, we will explain each part of the setup in more detail and how to modify this example to suit your individual setup.

This simulation can be run with a VSimPD license.

Opening the Simulation

The cylindrical magnetron sputtering example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Sputtering* option.
- Select *Cylindrical Magnetron Sputtering* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.137. Note that you can change the scale that is shown on the axes in the Setup window. In this case, the axes in Fig. 6.137 are shown in cm. You can change the scale by clicking on the "Show Scale" button at the top of the SetUp window. You can expand the tree elements and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on an option. The right pane shows a 3D view of the geometry as well as the grid. To show or hide the grid, expand the "Grid" element and select or deselect the box next to `Grid`.

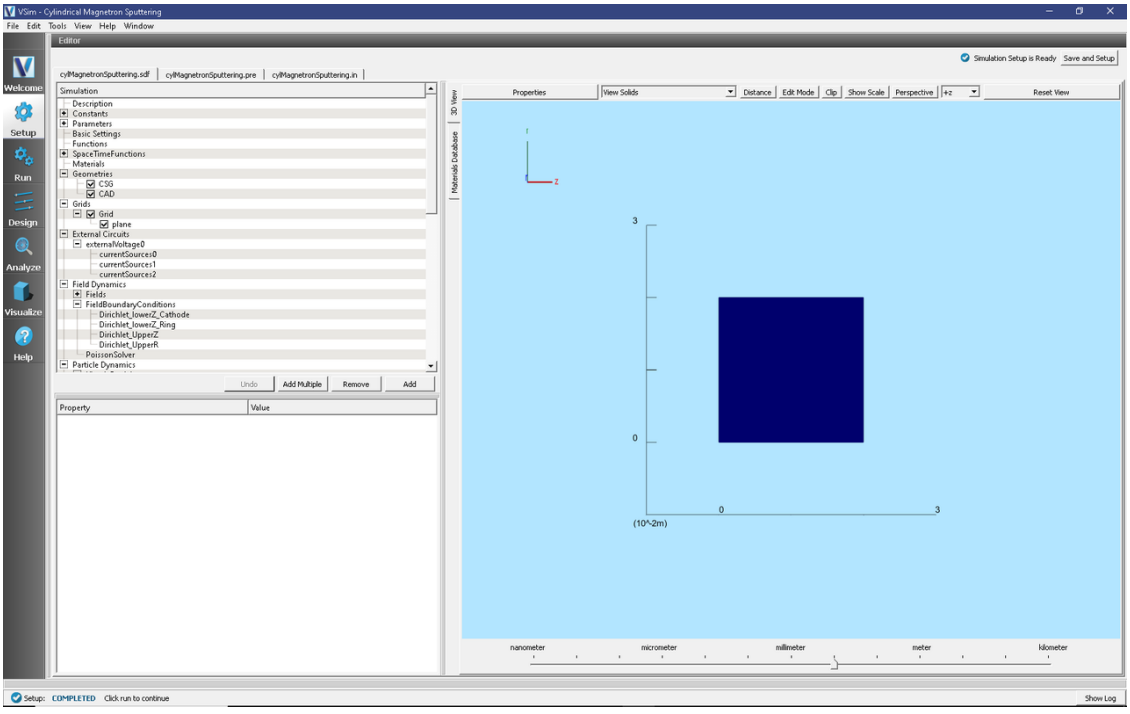


Fig. 6.137: Setup window for the cylindrical magnetron sputtering example.

Simulation Properties

This example contains many user defined *Constants* and *Parameters* which help simplify the setup and make it easier to modify. The following constants or parameters can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* or *Parameters* and all the constants or parameters used in the simulation will be displayed. To add your own constant or parameter, right click on *Constants* or *Parameters* and left click on *Add User Defined*. Below is an explanation of a few of the constants and parameters used. There are several more constants and parameters included in the simulation.

- **VOLTAGE0**: Initial voltage of Cathode. The Anode is set to 0 V (ground). The Cathode voltage can float by imposing an external circuit model.
- **EC_RESISTANCE**: Resistance used in external circuit model
- **AR_DENSITY**: Density of neutral gas (in this case Argon).
- **INITIAL_TE_eV/INITIAL_ARPLUS_TEMP**: Initial temperature of electron and Ar+ in eV. Simulation results should be somewhat insensitive to this parameter.

There are also several *SpaceTimeFunctions* (*STFunc*) defined in this example. *MAXWELLIAN_El* and *MAXWELLIAN_AR* are *SpaceTimeFunctions* used to load the initial Ar+ and electron as Maxwellian velocity distribution functions. In this case the SpaceTimeFunction is actually a function of velocity. *Potential_LowerZ_Ring* is a function which specifies the voltage in a small region separating the cathode and anode. This function allows for a smooth linear transition in the voltage between the anode and cathode.

You want to run this simulation long enough for the ions, electrons and cathode voltage to come to steady state. As stated in the introduction, we have attempted to reach steady state in 1-10 microseconds. However, your particular setup may take longer. This example ran for about 1.5 microseconds, which is long enough to demonstrate that steady state has been reached. The total number of time steps is 120000.

Explanation of Key Parts of Setup

Setting up the External Magnetic Field Because of the complexity of this problem, we will now further explain key components to this example which are needed to model magnetron sputtering. First, one must include an external magnetic field. There are three ways to include an external magnetic field in VSim. One method (which is the simplest and least general) is to provide an analytic expression as a function of position. You then write this analytic expression as a *StFunc*. A second method is to use another program to model the magnetic field and write the output into a text file. Then the user can write a space-time Python functions (*stPyFunc*) to read the data onto VSim and interpolate onto the VSim grid. One example that illustrates this method is the "ionThrusterT" example. A third method is to import a hdf5 file which is vis schema compliant, which is the method we have used in this example. For this example, we used an in-house input file which solves for the magnetic field using a magnetostatic solver via "magnetic charges" and a magnetic scalar potential. The resulting magnetic field can easily be read into VSim by expanding "Field Dynamics" in the setup tree. Under "Field Dynamics", right click on "Fields", then choose "Add Field" and finally choose "external field". This will create a new option under "Fields" with a default name of "externalField0". By double clicking on "externalField0", we renamed the external field to "externalMagField".

Initializing the Plasma If you are creating a simulation from scratch, then you must first enable particles in the simulation. To do this, click on "Basic Settings" in the setup tree. Then find the "particles" option and double click "no particles", and choose "include particles". This will create a new option in the Setup Tree called "Particle Dynamics". By expanding "Particle Dynamics", then "KineticParticles" in the Setup Tree, the user can see the various kinetic species that are included in this simulation. To create a new species, right click on "KineticSpecies", choose "Add ParticleSpecies", and choose either "Charged Particles", "electrons", or "Neutral Particles. The species called "electrons" are initially present to initiate the ionization collisions between Argon and electrons which leads to the formation of secondary electrons (*secElectrons*). The final density of the secElectrons is about 100 times larger than the initial electron density, indicating that the final results in this model are insensitive to the exact initial conditions. The species labeled "ArIons" is used to initialize the simulation in the ionization collision and is also a product in the ionization collisions. Finally, "CuNeut" is the sputtered copper atoms at the cathode. By expanding "electrons", and clicking on

"particleLoader0", the user can see the necessary parameters for the initial condition. One necessary parameter can be seen by expanding "volume", which is the spatial location of the initial electron population. It is necessary for the initial electron population to be contained in the boundaries of the simulation domain. You can place the initial population within any volume of the simulation boundaries, and in this case, we choose to fill the entire simulation domain with particles. The user must also specify the initial velocity distribution (i.e. phase space). By expanding "velocity distribution", the user can see that we have initialized all three velocity components with the same Maxwellian distribution. To population the velocity distribution with a *StFunc*, simply right on the space next to "u0" and choose the option "assign SpaceTimeFunction" (noting again that this particular SpaceTimeFunction is actually a function of velocity). We also note that a species can be defined without having an initial population such as CuNeut and secElectrons. These two populations form as the simulation progresses in time.

Particle Boundary Conditions When using the visual setup, the default particle boundary condition is set to *absorbing* in order to prevent particles from leaving the simulation domain (which leads to segmentation faults due to particles entering a region of memory not controlled by VSim). The exception to this default boundary condition is the lower R boundary condition in an axi-symmetric simulation, which defaults to specular (and does not need to be set up in the visual setup). User supplied boundary conditions can be set up by right-clicking on a species (such as "electrons" or "secElectrons"), clicking on "Add ParticleBoundaryConditions", and choosing one of the many options available. Each specific boundary condition is discussed in greater detail in the Reference Manual. In this model, we have used either "Boundary Absorb and Save" or "Interior Absorb and Save". Cut-Cell boundary conditions can be used on geometries. To set up a particle history, the user must first set up an "Absorb and Save" particle boundary condition. We note one particular particle boundary condition called *electronsabsSaveCathode*, *secElectronsabsSaveCathode*, and *ArIonsabsSaveCathode*. These three boundary conditions are needed to set up the external circuit, which is discussed below. To see where these three particle boundary conditions are used, we now navigate to "Histories".

Setting up Histories A "history" is data collected at every time step. There are several histories set up in this example. By expanding the "Histories" option, the user can see all the histories that are set up in this example. To understand how to set up this history, right click on "Histories" revealing all the different types of histories available in the visual setup. If the user hovers the mouse over "Add ParticleHistory" and clicks on "Absorbed Particle current", a new history will be created. Double clicking on the new history allows the user to change the name of the history. Now left-click on the newly created history and the user will see an option called "particle absorber". Left clicking "please select" reveals all the particle boundaries that have been assigned "Absorb and Save". Therefore, to use the "Absorbed Particle Current" history, the user first has to setup at the "Absorb and Save" particle boundary condition. Three useful histories are called "ionCathCurr", "elecCathCurr", and "secElecCathCurr", which are the currents for the three plasma populations that are collected on the cathode at every time step.

Setting up the External Circuit To specify the field boundary conditions discussed in the next paragraph, we must first discuss the external circuit model. This model can be conceptually understood as an external circuit which connects the cathode and the anode. In the circuit model, we include a resistor, with the value of the resistor specified by the user. Obviously the resistance needs to be greater than 0 to make physical sense. The relation between the cathode voltage and the current is simply given by Ohm's law. Therefore, to fully specify the current, we must compute the current accumulated on the cathode at each time step, which was discussed in the previous paragraph. The external circuit model can be set up by right clicking on "External Circuits", and choosing the option "Add Resistive Voltage Source". This will create a new option called "externalVoltageN", where "N" is some integer. Next right click on "externalVoltageN" and click on "Add Boundary Condition". This will create a new option under "externalVoltageN" called "currentSourcesN". Now click on "currentSourcesN", and choose the boundary condition that contributes to the current on whatever boundary you choose (in our case the cathode). Repeat this process for all the plasma particles that contribute to the current. In our circuit model, we have included the contribution of electron, secElectron, and ArIons currents. Finally, to finish the external circuit model, the user needs to specify the resistance (in Ohms), and a parameter called "Time Constant". This last parameter is used to create a low pass filter. Since particle codes are noisy, we want to average the current over some number of time steps and use this average value to specify the current. "Time Constant" specifies the number of time steps to average over.

Setting up Field Boundary Conditions Next we discuss the field boundary conditions, which are found by expanding "Field Dynamics" then expanding "FieldBoundaryConditions". This simulation is electrostatic which means that we only solve the self-consistent electric field and assume that the self-consistent magnetic field does not contribute to the plasma dynamics. Therefore all boundaries (except lower R) need to be assigned either the value of the potential

(Dirichlet) or the electric field (Neumann). In an axisymmetric simulation (such as this example), lower R is a computational construct and therefore (in almost all simulations) does not represent a real physical boundary. Therefore, lower R is not assigned by the user and is given a default Neumann boundary condition. Right clicking on "Field-BoundaryConditions" exposes either the "Neumann" or "Dirichlet" options. To see where the external circuit model is used, click on "Dirichlet_LowerZ_Cathode", where the user can see "externalVoltage0" populates the "boundary surface" option. Therefore, this potential will float based on the total current at the cathode. To summarize the steps needed to include an external circuit in an electrostatic simulation:

1. Set up particles with "Absorb and Save" boundary condition.
2. Right click on "External Circuit" to add a new external circuit.
3. Right click on the newly created option to add a particle boundary condition. Make sure to do this for every particle impacting a surface.
4. Populate "resistance" and "time constant".
5. This external circuit can now be used as a Dirichlet boundary condition under "Field Dynamics".

NB: Following these steps creates new histories which can be visualized during or after the simulation has run.

Setting up Reactions If you are creating a simulation from scratch, then you must first enable reactions in the simulation. To do this, click on "Basic Settings" in the Setup Tree. Then find the "collisions framework" option and double click "no collisions", and choose "reactions". Note that you must first add particles in order to add collisions. This will create a new option under "Particle Dynamics" called "Reactions". Since we are modeling the Argon as a neutral fluid (as opposed to a neutral particle), then you will notice all the collisions are "Particle Fluid Collisions". The user can add new collisions by right clicking on "Particle Fluid Collisions" and choosing one of the many collisions. All collisions require a user supplied cross-section table. For this example, we have supplied the cross-section tables for the reactions. The cross-section tables in the reactions framework contain two columns. The first column is electron energy in eV. The second column is the cross section in m^2.

Setting up Secondary Emission off Cathode The particle population called *secElectron* is produced from ionization collisions between electrons and neutral Argon and also from secondary emission off the cathode. In this model, we include secondary emission from both electrons and Argon ions impacting the cathode. The secondary electron emission model is based on [FP02]. To setup secondary electron emission, first create the species using the method discussed in the section called *Initializing the Plasma*. Then right click on the newly created species, hover your mouse over "Add ElectronEmitter", then click on "Secondary Emitter". Following these steps will create a new option called "secondaryElectronEmitter0" which can be renamed by double clicking on the newly created option. Under the secondary electron emitter option, double click next to "emitter boundary type" and choose which type of boundary you want to emit from. If you choose "boundary emitter", then "material properties" next to "emission specification", the user can choose either copper or stainless. Finally, the user needs to select which boundary to emit from which is done under "particle boundary condition".

Setting up Sputtered Copper The particle population called "CuNeut" is created from copper sputtering off of the copper cathode. This population can be setup by first creating a kinetic neutral species. Once the neutral species is created, right click on the species name, select "Add NeutralEmitter" and select "Sputter Emitter". A new emitter will be created called "sputterNeutralEmitter0". Click on the newly created sputter emitter and the region next to "particle boundary condition" to select the boundary that you want to emit from. Since this is a sputter emitter, make sure the particle boundary condition corresponds to an ion hitting the boundary.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.1779413261623052e-11
  - *Number of Steps*: 120000
  - *Dump Periodicity*: 3000
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.138.

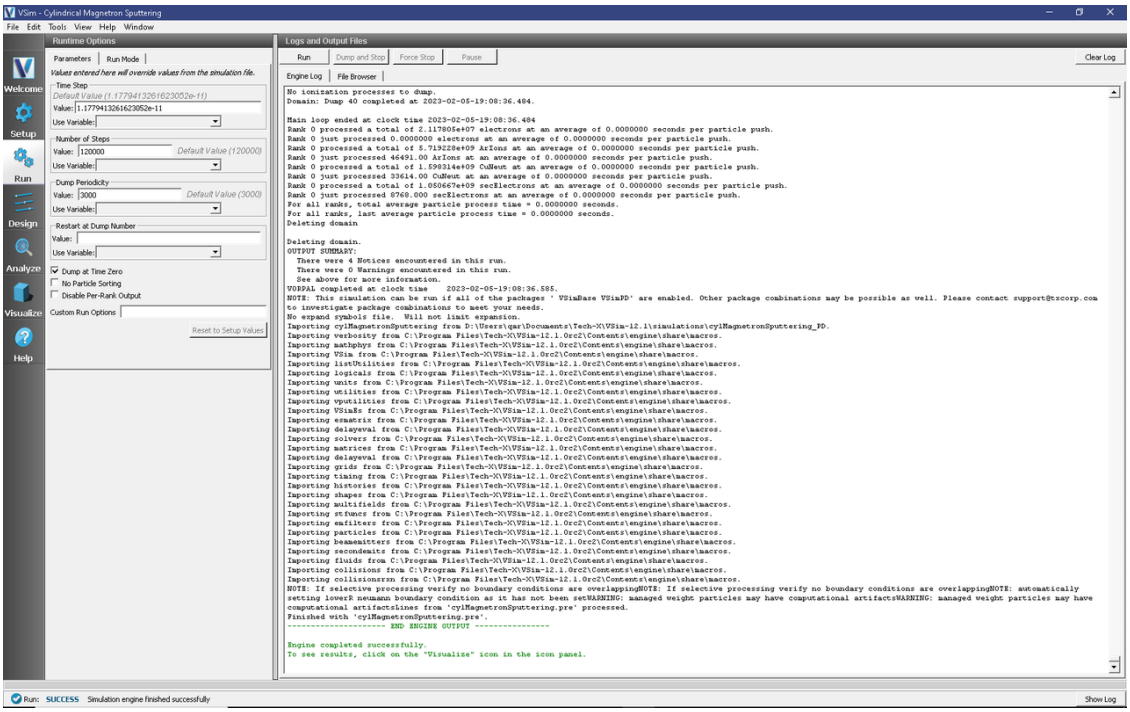


Fig. 6.138: The Run Window at the end of execution.

Analyzing the Results

Every VSim software purchase comes with numerous post-processing routines written in Python which we call analyzers. For this example, we demonstrate the use of 3 analyzers which computes the electron temperature and density, and the copper density. The name and use of each analyzer is discussed below.

Step 1A: After the simulation has completed, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- There should be three pre-selected, pre-populated analyzers already loaded. However, if the this is not the case, follow these steps:

- In the resulting list of *Available Analyzers*, select *addSpeciesWithKinEnrgInEV.py* and press *Open*
- The analyzer fields should be filled as below:
  - **simulationName:** cylSputteringMagnetron
  - **species:** secElectrons
  - **outputSpeciesName:** WithKinEnrg

Select the boxes "Remove", "outputMagnitude", and "overwrite". De-select the boxes "outputXcomponent", "outputYcomponent", and "outputZcomponent". This analyzer creates a new data set called "secElectronsWithKinEnrg" and has a ".vsh5" extension to indicate that this data set is computed with an analyzer (all data sets generated from analyzers have .vsh5 extensions. These files are saved in the hdf5 standard).

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.139.

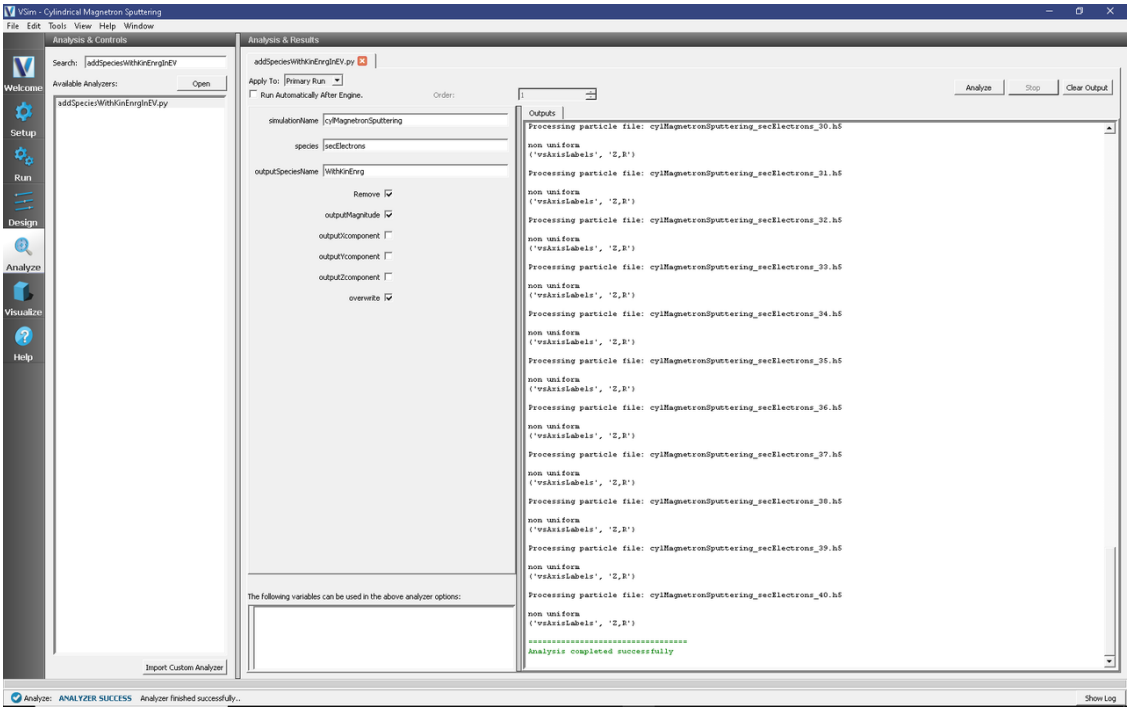


Fig. 6.139: The Analyze Window showing the use of addSpeciesWithKinEnrgInEv.py.

The resulting data set contains the total kinetic energy of each particle appended on the original particle data. If the particle has a small drift, then the total kinetic energy can be used to compute the temperature. *addSpeciesWithKinEnrgInEV.py* needs to be run before the next analyzer can be run.

Step 1B: After running the *addSpeciesWithKinEnrgInEV.py* in Step 1A, continue as follows (Note: if *computeDebyeLength.py* is already open and populated simply click "Analyzer" in the upper right corner).

- In the resulting list of *Available Analyzers*, select *computeDebyeLength.py* and press *Open*
- The analyzer fields should be filled as below:
  - **simulationName:** cylSputteringMagnetron
  - **species:** secElectronsWithKinEnrg
- Click *Analyze* in the top right corner.

- The analysis is completed when you see the output shown in Fig. 6.140.

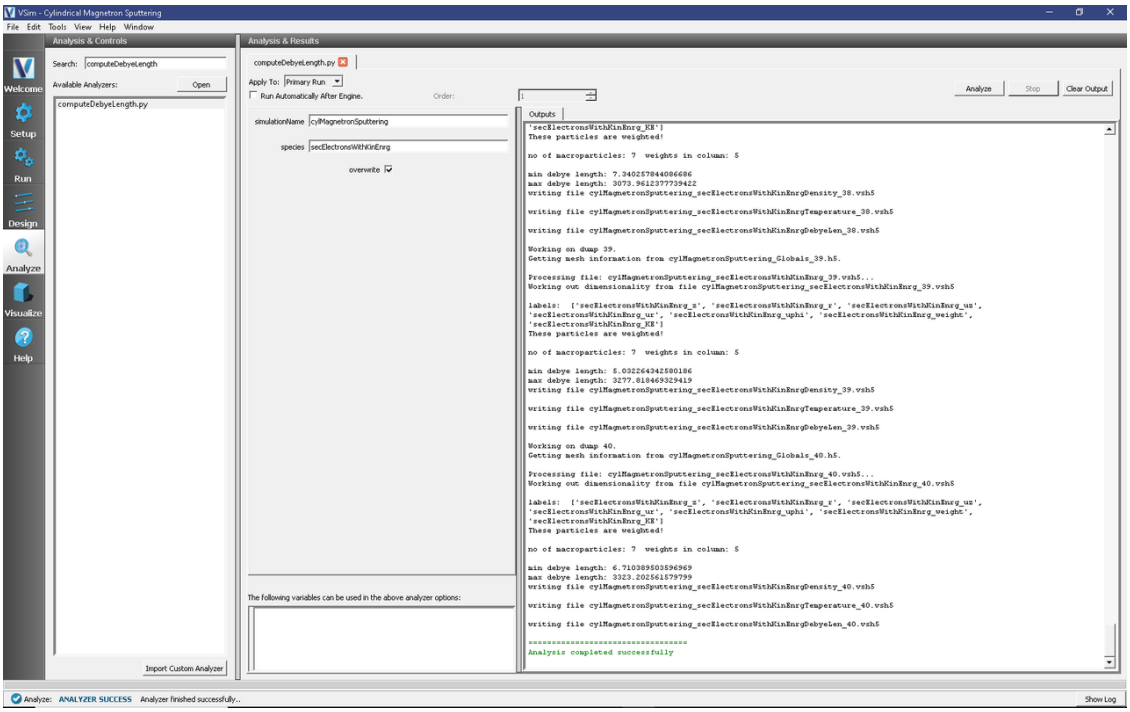


Fig. 6.140: The Analyze Window showing the correct use of computeDebyeLength.py.

This analyzer produces three new data sets. The data set called *secElectronsWithKinEnrgDensity* contains the secondary electron density in MKS units. The data set called *secElectronsWithKinEnrgTemperature* contains the secondary electron temperature in Kelvin. Finally, the data set called *secElectronsWithKinEnrgDebyeLen* contains the ratio of the secondary electron Debye length to the smallest cell size which must be greater than 1 everywhere in order to obtain physically meaningful results. As already stated, Step 1B requires you to first run Step 1A. The next step (Step 2) can be run independently.

Step 2: If the analyzer *computePtclNumDensity.py* is not already open, follow these steps.

- In the resulting list of *Available Analyzers*, select *computePtclNumDensity.py* and press *Open*
- The analyzer fields should be filled as below:
  - **simulationName:** cylSputteringMagnetron
  - **species:** CuNeut
  - **avgNxN:** 1
  - **iterateAvg:** 1
  - **timeAvg:** 1
  - **species:** CuNeut
  - **minDumpNum:** N/A
  - **maxDumpNum:** N/A
- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.141.

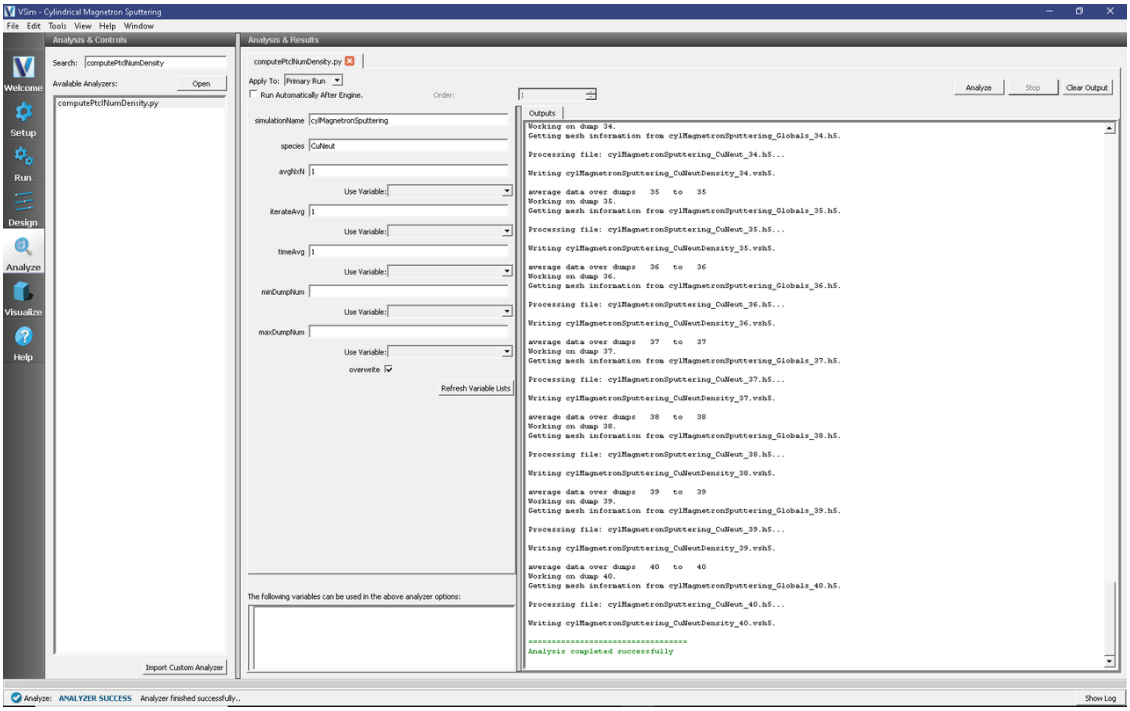


Fig. 6.141: The Analyze Window at the end of computePtclNumDensity.py.

This analyzer computes the copper density in MKS units. It contains several useful features such as the ability spatially and temporally average the data.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Clicking on the *Add a Data View* dropdown menu shows there are many different types of data to visualize.
- To get started, lets visualize two history plots which demonstrate that the simulation has reached steady state.
- If a *History* tab is not already open, then left-click on *History*
- Two windows should be open on the pre-loaded *History* tab which shows cathode voltage on the top plot and number of physical electrons on the bottom plot. If the *History* tab is not pre-loaded, then follow these next steps:
- After opening a new history tab, there should be two windows present.
- On the top plot, left-click on “Add Curve” and add the data set called “externalVoltage0RealVoltage”. This is the cathode voltage
- Then click on “Edit Curve”, and click on “Select Curve” in the window that pops up. If a second data set is plotted, delete that data set.
- For the bottom plot, follow similar steps: Click on “Add Curve” and add the data set called “numPhysElec”. This is the number of physical electrons modeled in the simulation.
- If a second data set is present, click on “Edit Curve” and delete the second data set.
- We used the “Labels” option on the upper right corner to label the y-axis on the cathode voltage history plot

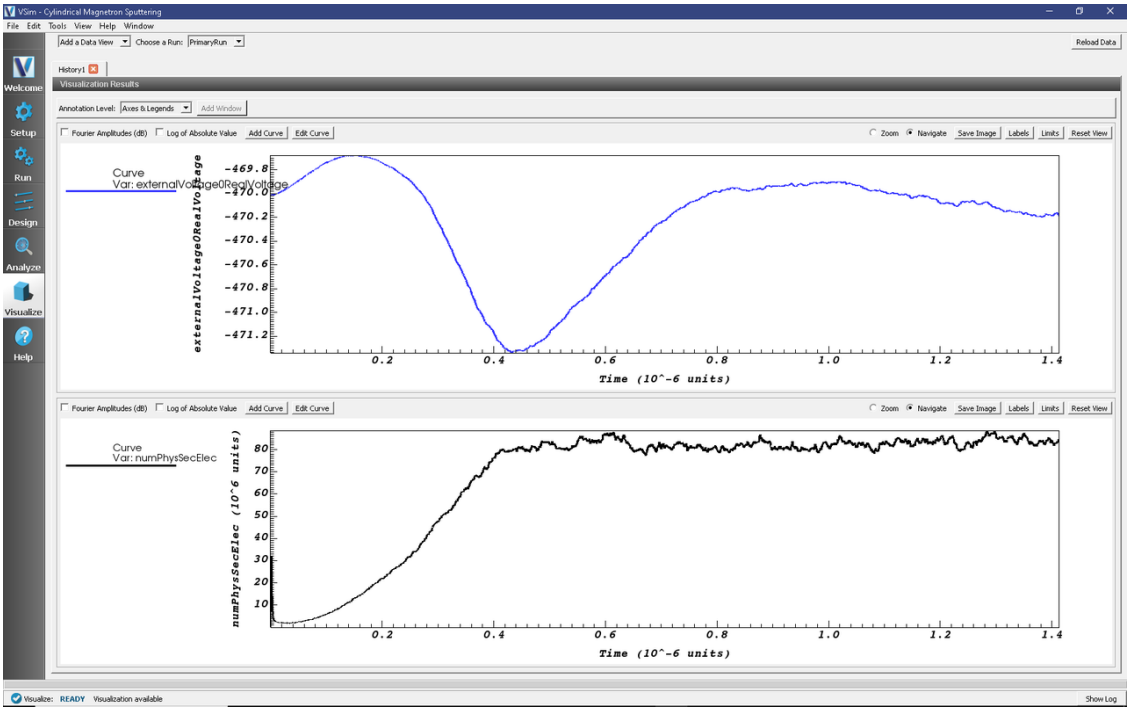


Fig. 6.142: The cathode potential (top) and number of physical secondary electrons (bottom) as a function of time.

The resulting visualization is shown in Fig. 6.142.

These two history data sets are how we determine if the simulation has reached steady state. After the simulation has reached steady state at about 1 microsecond, the number of physical secondary electrons and the cathode potential are nearly constant.

The next data set we visualize is the self-consistent potential with the secondary electrons superimposed. **To plot any field data with particle data superimposed, the user must first plot the field data, then the particle data.** Follow these steps to view both of these data sets. If the data are already plotted you can skip these steps. However, these steps are applicable to lots of data types, so following these steps will allow you to view other data sets:

- Left-click on the "Add a Data View" option in the upper left corner and select "Data OverView". This will open a new tab
- In the new tab expand the "Scalar Data" option and select *Phi*
- Slide the bar to the right at the bottom to view the potential and notice that the sheath thickness varies with time.
- Now expand the "Particle Data" option and expand "secElectrons" options. Check the box "secElectrons"
- You will now see the secElectrons macro particles plotted. To reduce the size of each particle, change the "Size" to 1
- Flip the axes by clicking on "Coord Swap" at the top of the window. This will plot the radial axis along the standard x-axis
- Finally, to preserve the aspect ratio, click the "Preserve Aspect Ratio" box at the top

The data are shown in Fig. 6.143.

Note that in VSim the state of your simulation is saved when you close a simulation. This means that all the visualization windows will re-open automatically when you re-load your simulation. However, the state that is saved might not be exactly what you first did. Therefore, you may need to re-swap the axes and you may need to unclick/re-click the particle data to visualize the particles.

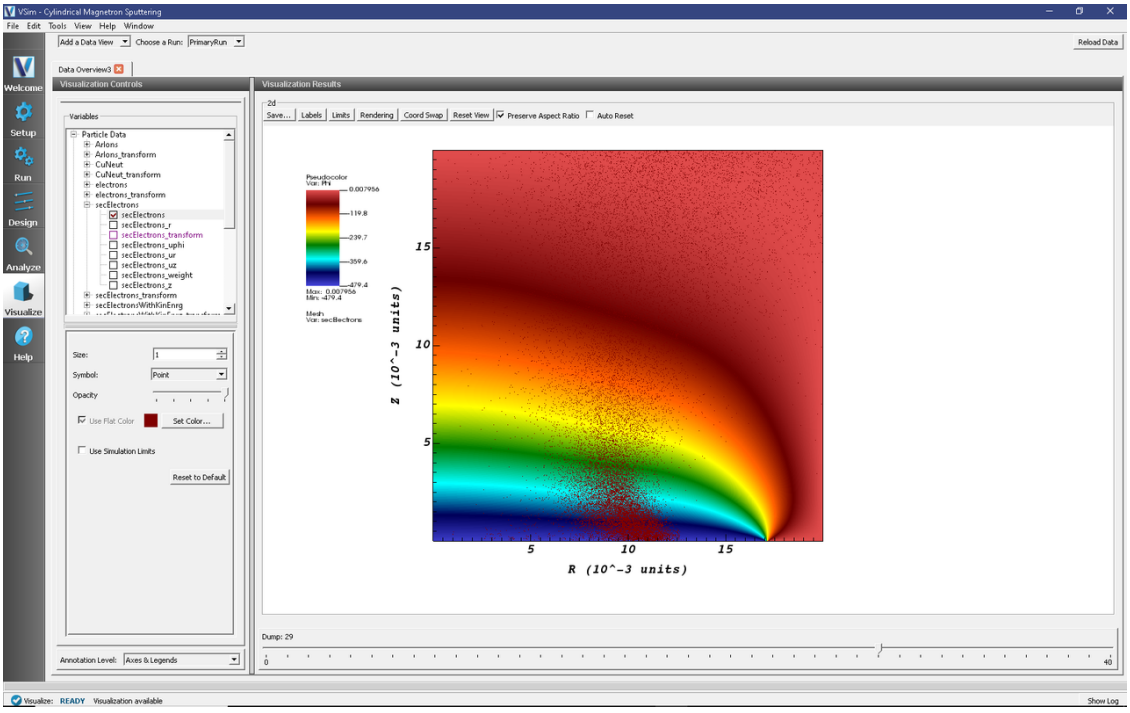


Fig. 6.143: Self-consistent potential with the secondary electrons superimposed.

One vital aspect to this problem is the presence of an external magnetic field which traps some population of electrons near the cathode. To view where the bulk of the secondary electrons form w.r.t. the external magnetic field, we next plot B_r with the secondary electrons superimposed. Follow similar steps to plotting the secondary electrons and the potential. This plot is shown in Fig. 6.144.

Finally, we plot copper density with the argon ions superimposed. This plot illustrates the main purpose of this simulation, which is the formation of Cu atoms that uniformly coat the surfaces in the chamber. To plot this data follow the previously discussed steps (recalling that field data must be plotted first). The copper density peaks where the ions are impacting the cathode the greatest. To visualize the data more easily we took two additional steps. (1) We changed the color scale of the copper density to range from $10^{16}/\mathrm{m}^3$ to $2 \times 10^{21}/\mathrm{m}^3$. We then plotted the data on a log scale. (2) We change the Z-axis to extend from 0 to 5 mm. The plot of copper density with ions superimposed is shown in Fig. 6.145.

There are countless diagnostics that can be computed in VSim using analyzers already built. There are also numerous ways to visualize the data. If you have any further questions regarding this example (or any other example), data visualization in VSim or you need a custom analyzer for your application please contact Tech-X

Further Experiments

This problem involves a complex interaction of sources (secondary emission off of the cathode and ionization collision) and sinks at both the anode and cathode. Furthermore, the magnetic field profile and strength plays a key role in trapping just enough electrons to form a sheath but not too many electrons that then create a cascade of more secondary electrons. There are several parameters the user can change to determine the role of these various parameters in forming the sheath. For example, the user could try a different magnetic field (which the user has to provide). The user could also change the neutral density, the initial cathode voltage, and/or the external circuit parameters. Finally, the user could add more reactions to improve the physics of this example. Remember that one goal to try to maintain physically reasonable results is to reach steady state.

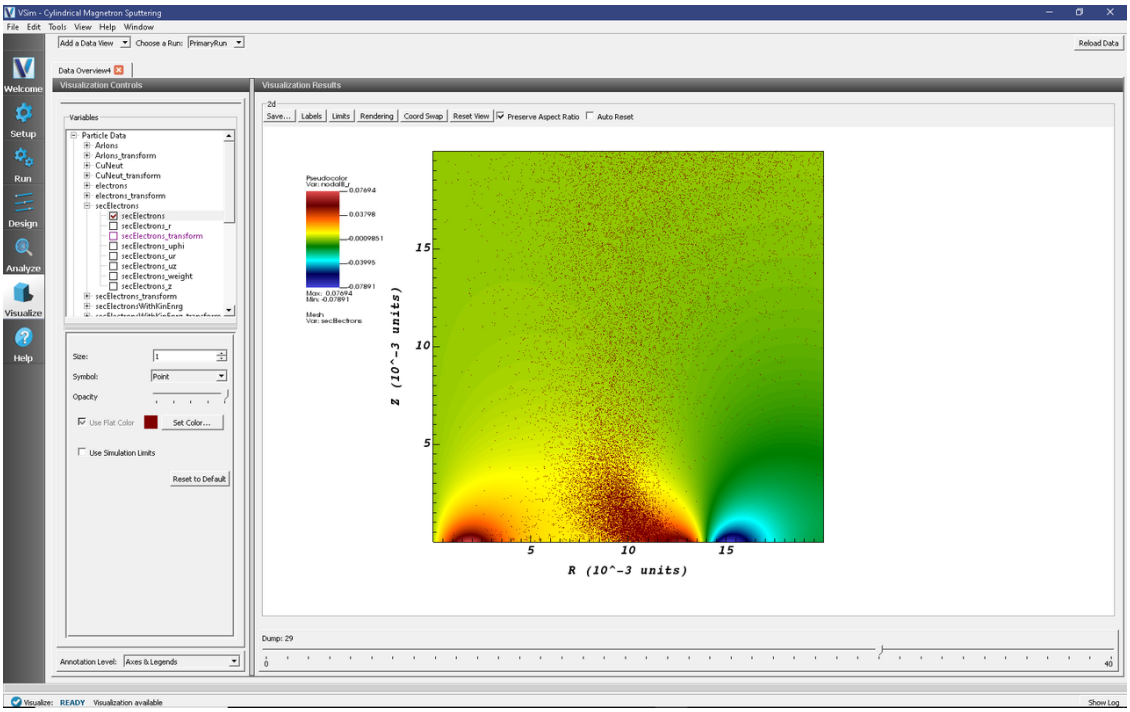


Fig. 6.144: Externally imposed magnetic field with the secondary electrons superimposed.

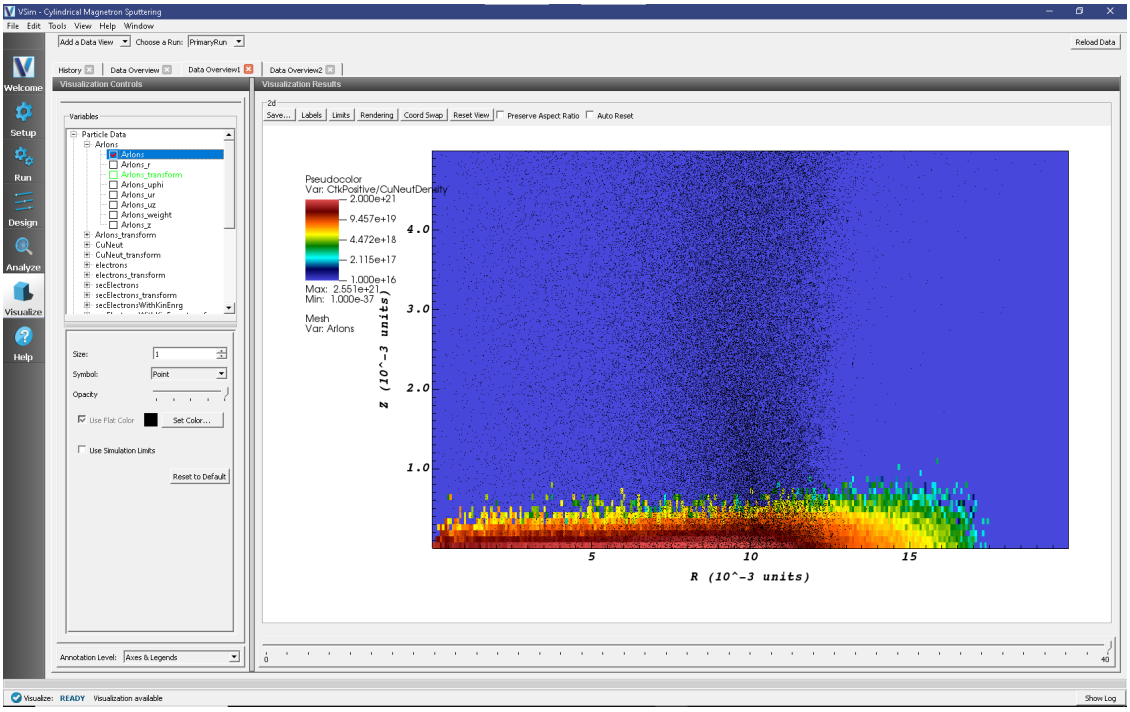


Fig. 6.145: The copper density plotted as a color contour plot with the Ar ions superimposed.

6.11 SputteringT (text-based setup)

6.11.1 2D Cartesian Magnetron Sputtering (cartMagnetronSputteringT.pre)

Keywords:

electrostatics, magnetostatics, magnetron sputtering

Problem Description

The 2D Cartesian Sputtering Magnetron simulation models a simple sputtering chamber. For a more extensive reference on magnetron sputtering modeling, see [MI14]. A constant voltage difference is set between two sheets on the upper and lower y boundaries of the simulation domain. The voltage along the left and right walls of the chamber ramp from -500 volts on the bottom boundary (lower y wall) up to 0 volts at the top boundary (upper y wall). To confine the particles, there is a curl-less, divergence-less magnetic field of the form $\vec{B} = \frac{(y-5*DY)B_0}{x^2+(y-5*DY)^2}\hat{x} - \frac{xB_0}{x^2+(y-5*DY)^2}\hat{y}$. The vertical shift in the y direction moves the singular point of the magnetic field off the origin and below the simulation domain.

The lower x, upper x, and upper y walls are stainless steel, and the lower y wall is copper. A plasma sheath develops above the lower y wall which accelerates argon ions towards the bottom wall. The argon ions strike the lower surface and sputter off neutral copper atoms which ballistically travel through the chamber.

The plasma is sustained through ionization reactions of electrons with a neutral background gas of argon atoms and secondary emission of electrons off all 4 walls of the chamber. The simulation also includes electron-neutral gas elastic and inelastic (excitation) collisions. The Hayashi cross section data from the LXcat database are used with permission from LXcat https://fr.lxcat.net/data/set_type.php.

This simulation can be performed with a VSimPD license.

Opening the Simulation

The cartMagnetronSputteringT example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example...* menu item from the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Cartesian Magnetron Sputtering (Text-based setup)* option.
- Select *cartMagnetronSputteringT* and press the *Choose* button.
- In the resulting dialog, create a New Folder if desired, and press the *Save* button to create a copy of this example.

The basic variables of this problem should now be alterable via the text boxes in the left pane of the *Setup Window*, as shown in Fig. 6.146.

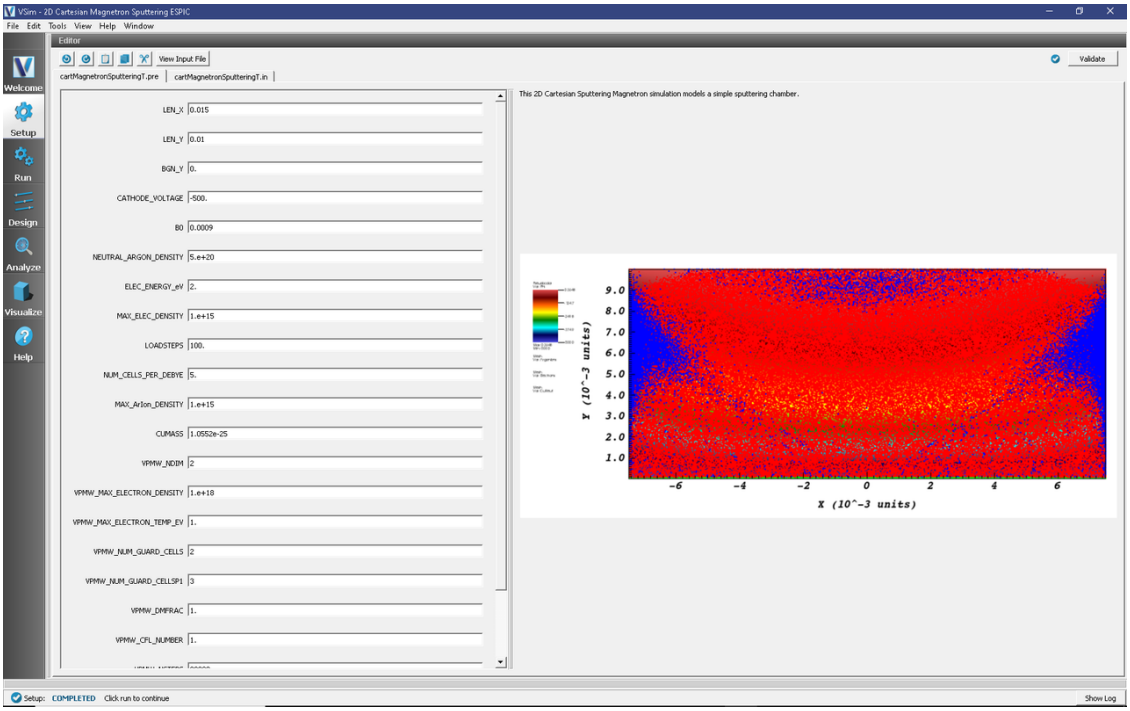


Fig. 6.146: Setup Window for the cartMagnetronSputteringT example.

Input File Features

This VSimPD example simulates a magnetron sputtering in two dimensions in a Cartesian coordinate. The system size is chosen as 1.5cm x 1.0cm. A nonuniform external magnetic field is applied using the functional field in VSim while the negative voltage is appled through the copper cathode with the rest walls set to ground. Argon is used as the working gas and the plasma dischrage is simulated using the Electrostatic Particle-in-Cell (ESPIC) method with collisions described by Monte Carlo Interactions. The sputtered copper atoms are generated when argon ions hit the copper cathode with enough energy to cause a sputtering.

This simulation can be performed with a VSimPD license.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 7.913017481743232e-12
  - *Number of Steps*: 20000
  - *Dump Periodicity*: 200
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, “Engine completed successfully”. This result is shown in Fig. 6.147.

Note: 20,000 steps takes about 40 minutes on a MacBook Pro in serial

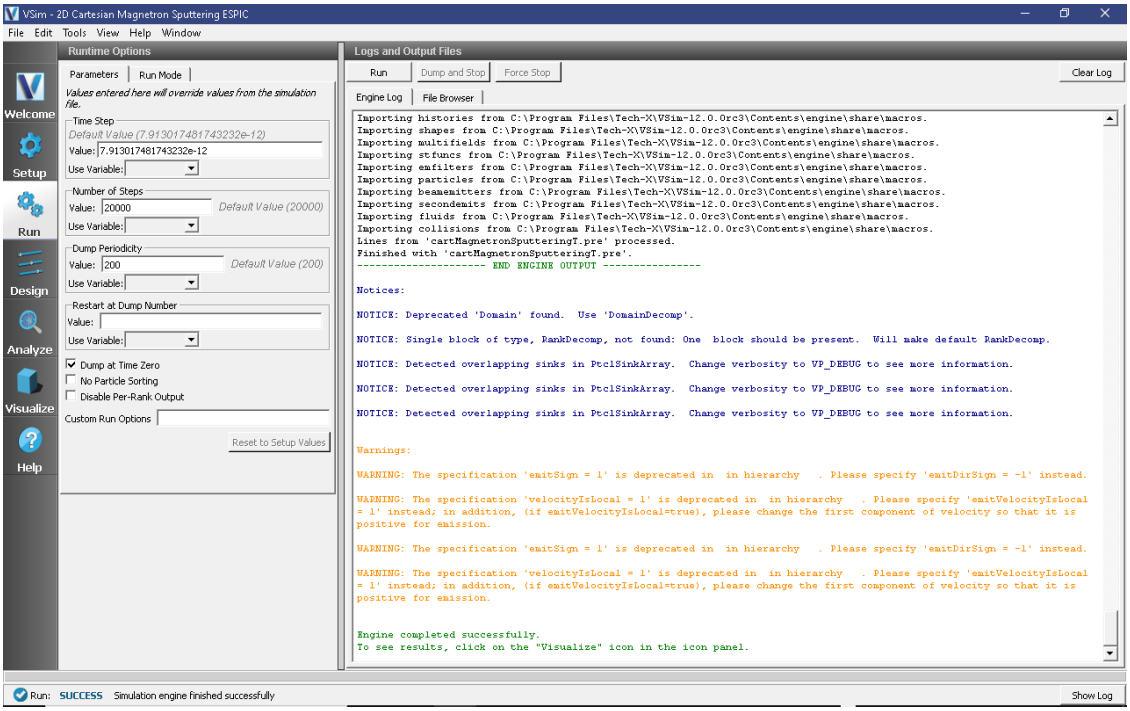


Fig. 6.147: The Run Window during execution.

Visualizing the Results

Now that we've got all of our data, let's look at it.

- Click the *Visualize Window*

After a brief moment the visualization options for this data should appear.

We'll first look at the time evolution of some fundamental one-dimensional quantities. From the *Data View* pulldown menu on the top left, select *History*. The default view here should contain four plots, namely, the electron and ion currents to the left wall and the number of electrons and ions in the simulation. A number of notable physics effects can be seen here:

- **After a sharp initial decrease in the electron population, the electron population is steady while the ion one declines and the sputtered copper atoms generated.** Choose "numMacroArgon", "numMarcoElec", and "numMarcoCu" for Graph 1, 2, and 3, respectively. This is not as apparent from the separate numMacroArgon and numMarcoElec plots, but clicking on the "Location" dropdown window in Graph 2 and selecting "Window 1" as the new rendering destination, places both ion and electron populations in the same plot. (Select "<None>" in the plot variable (the topmost menu) for Graph 4 to resize the Argon Ion/electron and Cu plots.) The initial decrease in electron population arises when rapid electron wall losses create a charge imbalance in the plasma and establish plasma sheaths near the walls. Thereafter, this charge imbalance is preserved and the transport of both electrons and ions to the wall becomes ambipolar. A history of the particle populations can be seen in Fig. 6.148

We can also look at the plasma and the sputtered copper atoms directly. In the "Data View" menu at the top left of the Composer window, continue as follows:

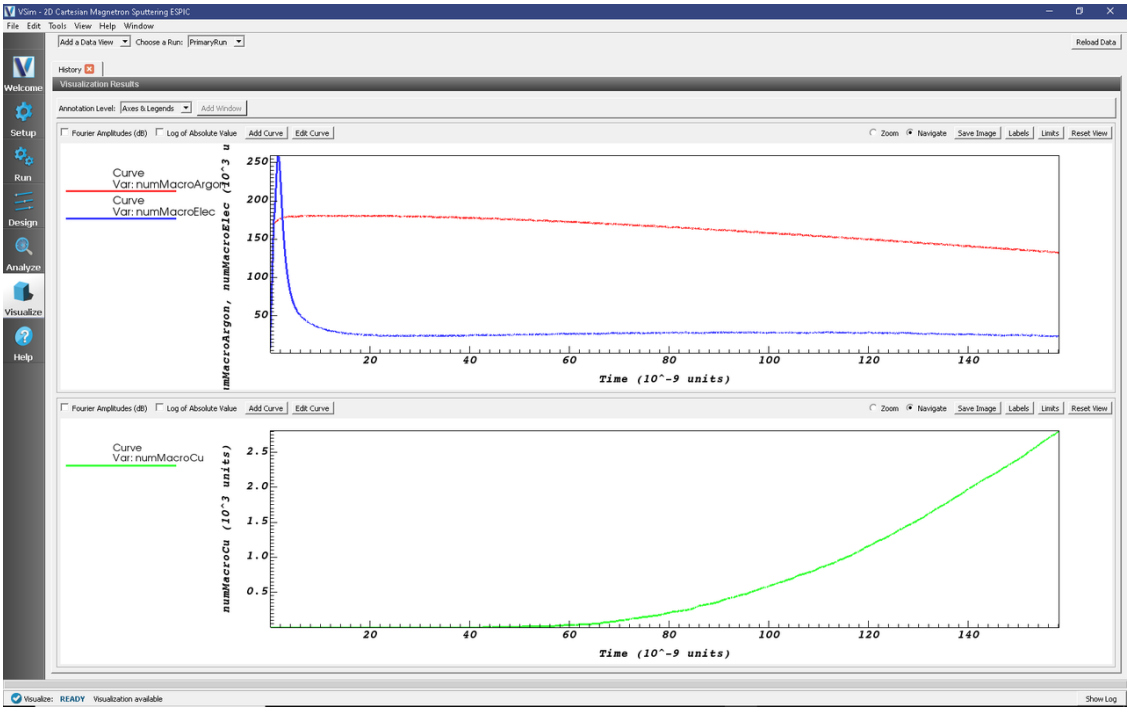


Fig. 6.148: The electron and ion populations versus time.

- Expand *Particle Data*
- Expand *ArgonIons*
- Select *ArgonIons*
- Expand *electrons*
- Select *electrons*
- Expand *CuNeut*
- Select *CuNeut*
- Expand *Scalar Data*
- Select *Phi*

The magnetron sputtering copper atoms can be viewed in the right pane. Use the dump slider on the bottom of the right pane to step through time. After copper atoms are sputtered from the cathode by argon ions, they travel to the anode at their constant inertial velovities as seen in Fig. 6.149.

The detailed magnetron sputtering can be viewed in the Phase Space. From the *Add a Data View* pulldown menu, select *Phase Space*, choose X-axis to CuNeut_x and Y-axis to CuNeut_y and click Draw, as seen in Fig. 6.150.

The external magnetic field can be viewed in the Field Analysis. In the *Add a Data View* menu, select *Field Analysis*, choose Field to BField_x, as seen in Fig. 6.151.

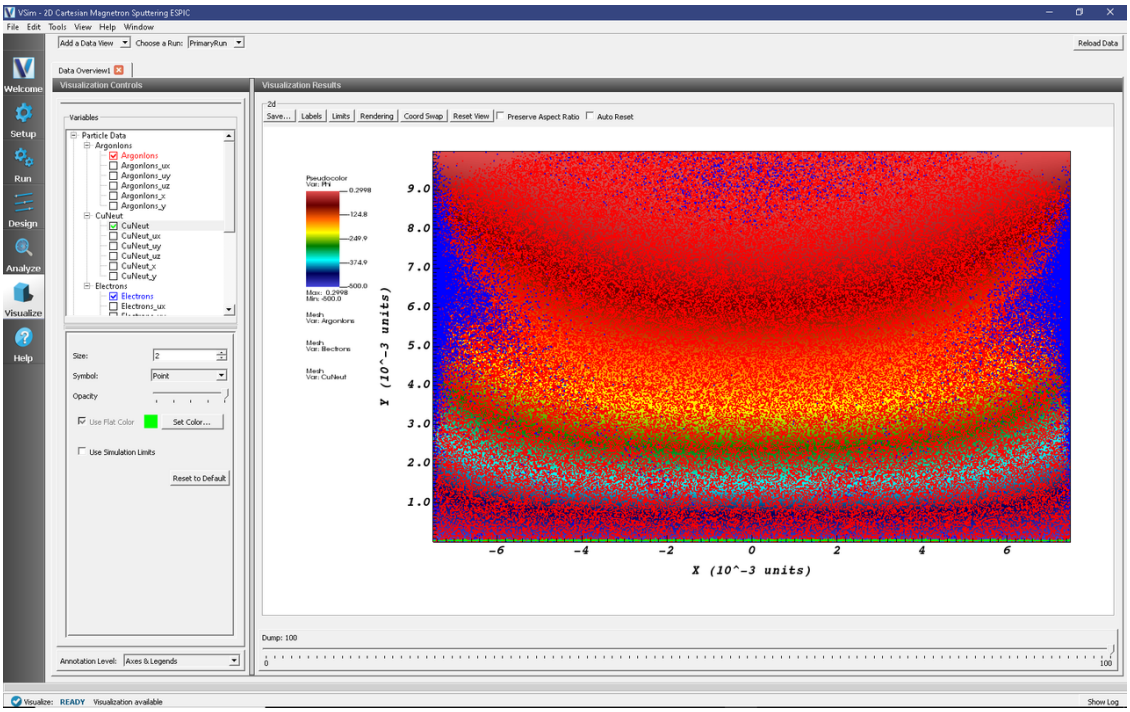


Fig. 6.149: Plots of this Data View showing the sputtered copper atoms.

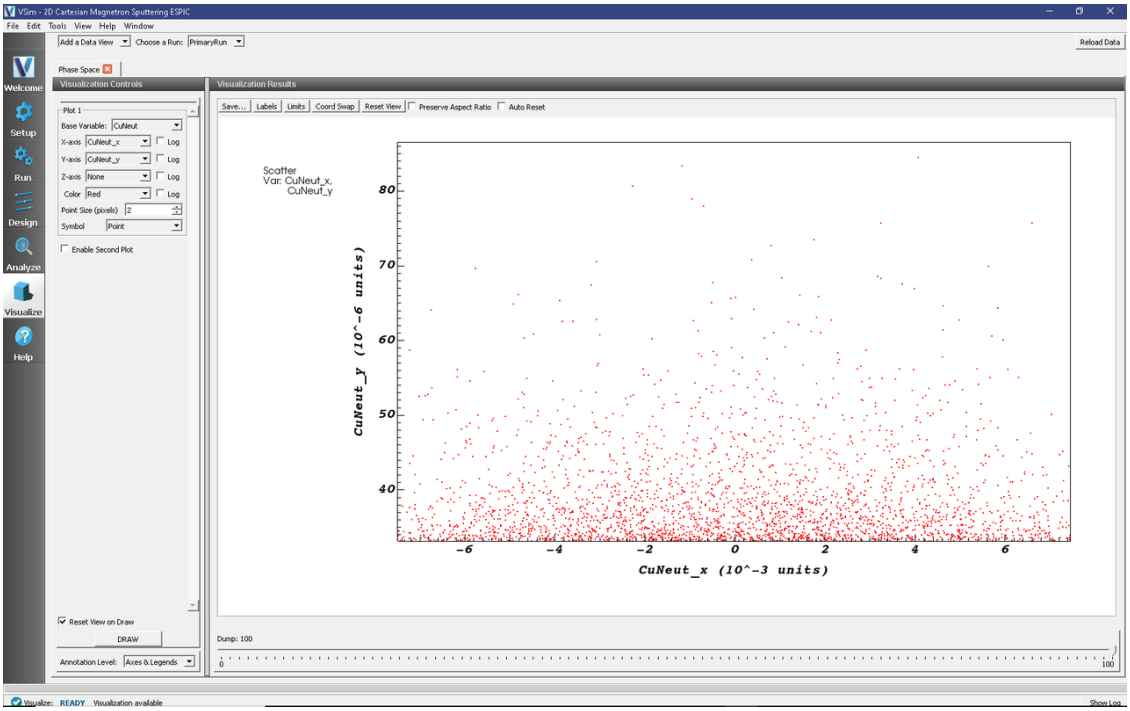


Fig. 6.150: Plots of this Phase Space showing the sputtered copper atoms travel away from the cathode.

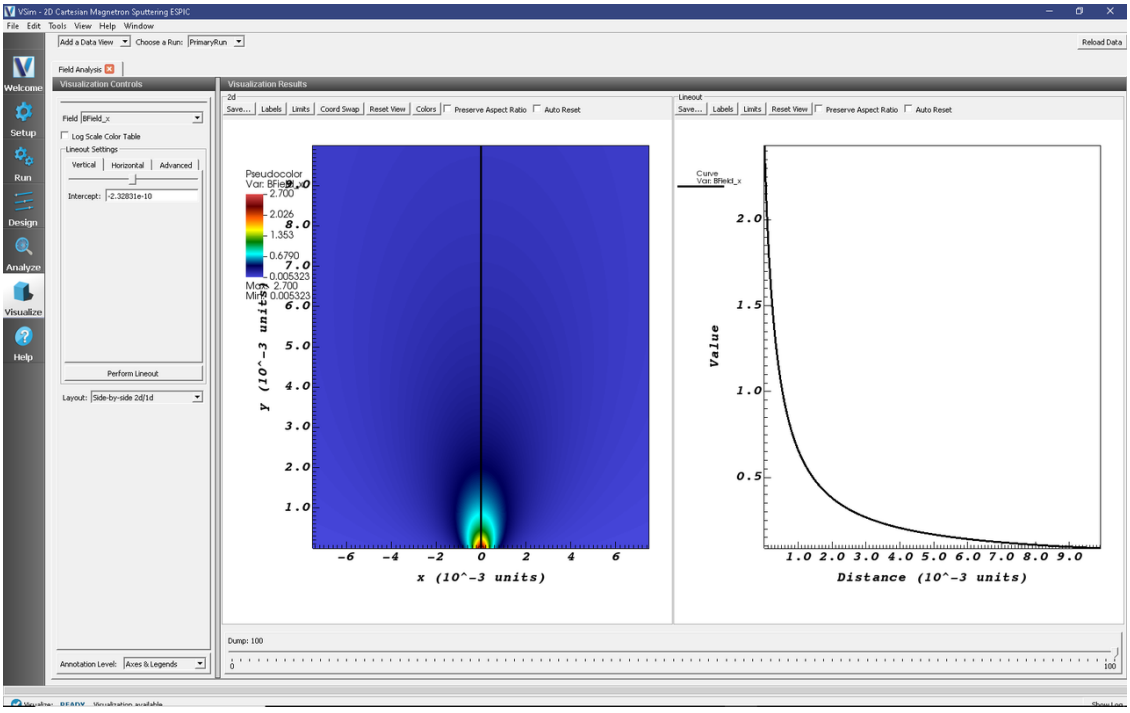


Fig. 6.151: Plots of this Field Analysis showing the external magnetic field component parallel to the cathode used in the magnetron sputtering.

Further Experiments

1. Add a secondary electron species to track the electrons created through physical processes separately from electrons that were loaded during the initialization period. Be sure to add collisions in the Monte Carlo Block for the new species.

2. Get some new cross-section data from the LXcat

3. Changing magnetic field

Describe something they might see as interesting by changing an xvar value or a value in the Run panel.

References

[1] McInerney, E.J. "Computational Explorations in Magnetron Sputtering." San Jose, CA: Basic Numeric Press, 2014.

6.12 Surface Interactions

6.12.1 Wafer Impact in Plasma Processing (waferImpact.sdf)

Keywords:

uniform ion beam, wafer edge, RF voltage source, poisson solver, dielectric

Problem Description

This example illustrates how to use VSim to model a plasma processing problem in which argon ions are used to etch wafers used for microelectronics. In a typical chamber, the plasma is generated by imposing a voltage source at one of the boundaries which oscillates in the radio frequency (RF) range (a few MHz to tens of MHz). The plasma is generated as the electrons oscillate in response to the applied RF voltage and collisionally ionize the neutral Argon ions present in the chamber. In this example we are not interested in how the plasma forms and therefore pre-populate the simulation with electrons and Ar ions. During this process, a sheath forms near the wafer and the thickness of the sheath oscillates with the voltage RF source. The resulting Ar ions are then accelerated toward the wafer primarily by the sheath electric field and thereby etch the wafer. Unlike the electrons, which respond nearly immediately to the RF voltage source, the ions are accelerated more slowly and the motion of the ions can be found by averaging the sheath potential drop over one RF period. A desired outcome would be a uniform plasma sheath and therefore a uniform ion beam along the length of the wafer. One significant obstacle to this process occurs at the edge of the wafer, where changes in the dielectric material lead to modification to the sheath electric field.

The process described above is fundamentally a kinetic process involving processes on electron and ion time scales. However, simulation of the above process is mostly needed near the wafer edge where non-uniformities in the sheath potential cause problems. One solution to this problem is with the use of a so-called "focus ring" which is a second piece of dielectric material (e.g. quartz) of varying height placed next to the silicon wafer which is used to shape the sheath and make it more uniform at the edge of the wafer. Therefore, in this example we only simulate a region near the wafer edge and sufficiently far enough into the bulk of the plasma that the sheath dynamic is adequately resolved. As a result, we do not include most of the plasma far from the wafer and save significant computational time by modeling only the interesting and necessary processes.

Because we are not modeling most of the plasma, we have developed a method of injecting the plasma at the boundary opposite the wafer that is smooth and results in no artificial sheath at the computational boundary. An injection method is necessary to replace the plasma lost to the wafer and focus ring. The electrons and ions are injected using flux conserving particle boundary conditions accomplished through the use of a Space-Time Python Function (*stPyFunc*) which is a flexible way for the user to define their own function via a call external to Python. The particles are injected using a *Slab Settable Flux* boundary condition which correctly computes the initial position and velocity upon injection in the simulation domain.

The dielectric materials are modeled by constructing a CSG geometry in VSim. The user could easily import their own CAD (.stl or .step files) geometries and assign dielectrics to the various parts of the imported geometry. However, for this example, you can view the geometries by expanding "Geometries" and then expanding "CSG". We then assign a dielectric material (and hence a dielectric constant) to each geometry, which is further explained below. A combination of Dirichlet and Neumann boundary conditions on the simulation boundaries are imposed. Field boundary conditions are imposed under *Field Dynamics* -> *FieldBoundaryConditions*. The plasma is represented by macro-particles which are evolved using the Boris scheme in a 2D cylindrical (z-r) coordinate system. The particle boundary conditions are *Cut-Cell Accumulate* which allows the electrons and ions to be absorbed by the dielectric material. The dielectric retains the accumulated charge once a plasma particle hits the dielectric. Averaged over one RF cycle, the total charge accumulation will be near-zero, but over short periods, the dielectric can have a net positive or negative charge.

We have also included critical diagnostics needed to determine the effect of the focus ring, collisions, and other physical processes crucial to this problem. One diagostic is the angular energy distribtuion (AED) function. We find that it is crucial to include collisions (even with a tenuous background gas) in order to obtain an AED function that is well centered around the normal to the wafer. We have also included a flux calculation to determine the uniformity of the ions impacting the wafer. The use of both of these diagnostics is discussed below.

This simulation can be run with a VSimPD license.

Opening the Simulation

The wafer impact example is accessed from within VSimComposer by the following actions:

- Select the *New* → *From Example…* menu item in the *File* menu.
- In the resulting *Examples* window expand the *VSim for Plasma Discharges* option.
- Expand the *Surface Interactions* option.
- Select *Wafer Impact* and press the *Choose* button.
- In the resulting dialog, create a *New Folder* if desired, then press the *Save* button to create a copy of this example.

All of the properties and values that create the simulation are now available in the Setup Window as shown in Fig. 6.152. Note that you can change the scale that is shown on the axes in the SetUp window. In this case, the axes in Fig. 6.152 are shown in cm. You can change the scale by clicking on the "Show Scale" button at the top of the SetUp window. You can expand the tree elements and navigate through the various properties, making any changes you desire. Please note that many options are available by double clicking on an option and also right clicking on an option. The right pane shows a 3D view of the geometry as well as the grid. To show or hide the grid, expand the "Grid" element and select or deselect the box next to `Grid`. You can also show or hide the different geometries by expanding the "Geometries" element and selecting or deselecting "Silicon_WaferUnionCurved_Silicon_End" and/or "quartz_FR". "Silicon_WaferUnionCurved_Silicon_End" is a union of "Curved_Silicon_End" and "Silicon_Wafer".

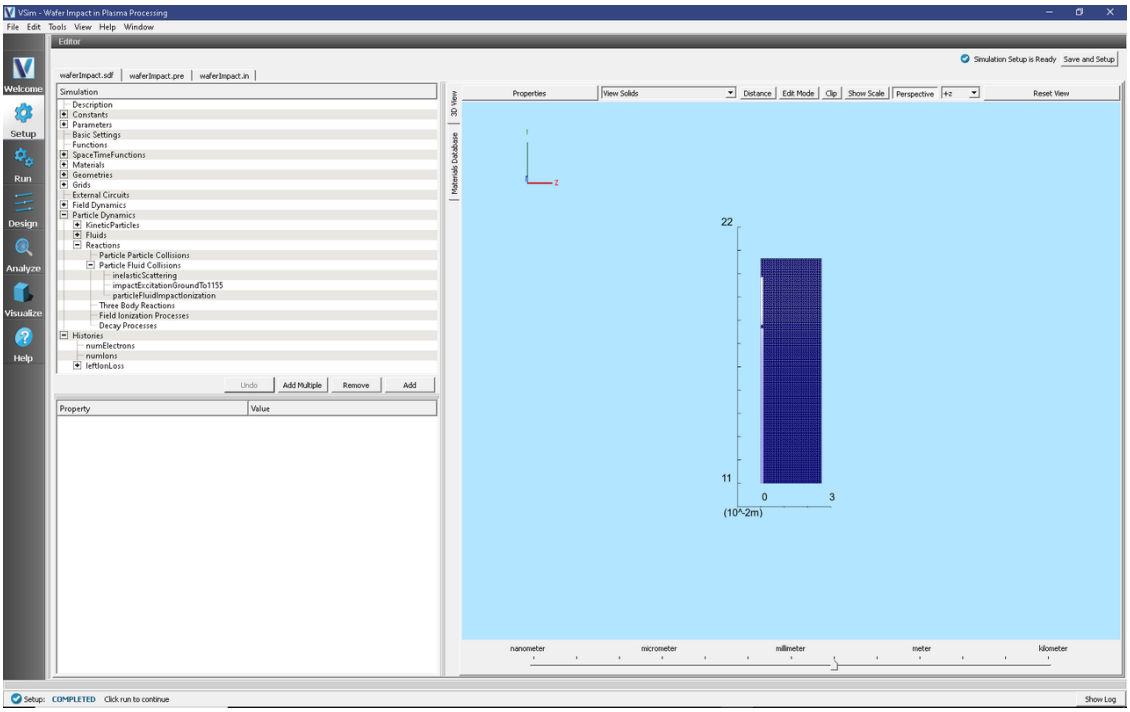


Fig. 6.152: Setup window for the wafer impact example.

Simulation Properties

This example contains many user defined *Constants* and *Parameters* which help simplify the setup and make it easier to modify. The following constants or parameters can be modified by left clicking on *Setup* on the left-most pane in VSim. Then left click on + sign next to *Constants* or *Parameters* and all the constants or parameters used in the simulation will be displayed. To add your own constant or parameter, right click on *Constants* or *Parameters* and left click on *Add User Defined*. Below is an explanation of a few of the constants and parameters used. There are several more constants and parameters included in the simulation.

- **QUARTZ_UPPERX/QUARTZ_LOWERX/QUARTZ_UPPERY/QUARTZ_LOWERY**: Location of quartz focus ring in simulation domain
- **SILICON_UPPERX/SILICON_LOWERX/SILICON_UPPERY/SILICON_LOWERY**: Location of silicon wafer in simulation domain
- **V0**: Amplitude of RF voltage source
- **OMEGA_RF**: Angular frequency of RF source. Linear frequency is OMEGA_RF/2π
- **NEUTRAL_PRESSURE_TORR**: Pressure of neutral background gas. This determines the mean free path.

There are also many *SpaceTimeFunctions* (*STFunc*) defined in this example. *vxRighte* and *vxRighti* are space-time Python functions (*stPyFunc*) called from a Python script called "waferImpact.py". In order for a Python function to be called correctly, the Python script must be given the same prefix as the input file, in this case "waferImpact". The functions that are called are "EmitVxRighte" and "EmitVxRighti". These functions invert the cumulative distribution function [BL04] given by $v_x \times f(v_x)$, where $f(v_x)$ is the initial distribution function which in this example is a drifting Maxwellian with the drift set to the ion acoustic speed. We use Rejection-Sampling theory to invert $v_x \times f(v_x)$ since there is no analytic solution for a drifting Maxwellian.

In addition to the *SpaceTimeFunctions*, there are also several materials that need to be added. To open the materials data base, right click on "Materials", then click on "import materials". This will open a folder that you can use to open the material data base file. The default materials data base file is called "emthermal.vmat". You don't need to add any materials to the simulation for this example to run. The two dielectrics which are included in the simulation are quartz and silicon. However, you can also choose to add your own dielectric using the same format as the other materials already included.

To examine how the silicon wafer and quartz focus ring are modeled, expand "Geometries" by left-clicking on the + sign. Then expand "CSG". There you see two geometries that have been assigned materials. The geometry called "Silicon_WaferUnionCurved_Silicon_End" is a bolean union between "Curved_Silicon_End" and "Silicon_Wafer". This geometry has been assigned the material silicon. The geometry called "quartz_FR" is the focus ring and the dielectric material assigned to it is quartz. The dielectric constants for these two regions are automatically added to the Laplacian matrix used in the Poisson field solve. Note that in order to add dielectrics to your simulation when using the electrostatic field solve requires a VSimPD license.

We find that including collisions is crucial to this problem. Collisions tend to create an ion distribution that is centered around the normal to the wafer. Collision can be added to any VSim simulation by first navigating to "Basic Setting" in Composer. Before adding collisions, you must first double click next to "particles" and choose "include particles". Once particles are added, double click next to "collisions framework" and choose "reactions". Then in the elements tree, you will see a tab called "Particle Dynamics". If you click the "+" icon to expand this options, you will see three options: "KineticParticles", "Fluids", and "Reactions". The plasma particles are added under "KineticParticles". The background Argon gas is modeled as a fluid. Finally, all the reactions we include (ionization, elastic scattering, and excitation) are placed under "Particle Fluid Collisions".

Typically you want to run this simulation long enough for the ions to come to equilibrium, which can take between 10-100 RF cycles. The time step is automatically computed using a parameter called "DT" and the number of time steps in a RF period is computed in a parameter called "NT". Therefore, multiplying NT by 10-100 will allow you to run the simulation for 10-100 RF cycles. In this example, we set the number of time steps to 10037 which is about 15 RF periods.

Running the Simulation

After performing the above actions, continue as follows:

- Proceed to the run window by pressing the Run button in the left column of buttons.
- Check that you are using these run parameters:
  - *Time Step*: 1.391023682183476e-10
  - *Number of Steps*: 10037
  - *Dump Periodicity*: 200
  - *Dump at Time Zero*: Checked
- Click on the *Run* button in the upper left corner of the right pane.

You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully". This result is shown in Fig. 6.153.

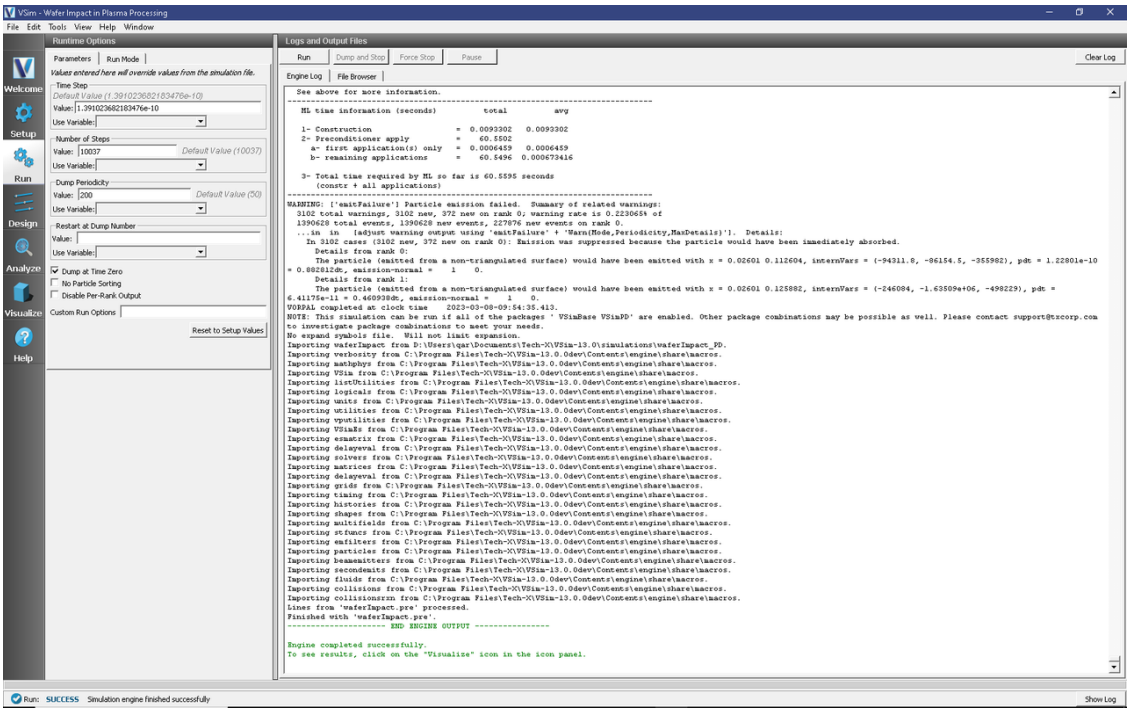


Fig. 6.153: The Run Window at the end of execution.

Analyzing the Results

A quantity of interest for many in plasma processing is the Angular Energy Distribution (AED) function. We have written an analyzer which computes the AED on any surface which saves the particle data in a history. The analyzer uses an "Absorbed Particle Log" history which in this simulation we call "leftIonLoss". This history collects particle data on the silicon wafer at every time step. The Analyzer then specifies the region and time interval in which to bin the data in energy and angle, all of which the user specifies.

After the simulation has completed, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.

- In the resulting list of *Available Analyzers*, select *computeAED.py* and press *Open*
- The analyzer fields should be filled as below:
  - **simulationName:** "waferImpact"
  - **speciesName:** ions
  - **startTime:** 1.1170107212763709e-06
  - **endTime:** 1.3031791748224327e-06
  - **lowerPos1:** 0.155
  - **upperPos1:** 0.176
  - **lowerPos2:** 0 (ignored in 2D)
  - **upperPos2:** 1 (ignored in 2D
  - **historyName:** leftIonLoss
  - **numEnergyBins:** 25
  - **numAngleBins:** 26
  - **lowerEnergy:** 160
  - **upperEnergy:** 240
  - **lowerAngle:** -10
  - **upperAngle:** 10
  - **NDIM:** 2
  - **perpDir:** 0
  - **normTan:** if checked then history data are collected in norm-tangent coordinate system. If unchecked, simulation coordinate system is used.

"endTime" and "startTime" are times over which the AED is calculated in seconds. "perpDir" is the direction normal to the surface you are collecting the data on. A description of each input quantity is found in the VSim "Analyze" window.

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.154.

The resulting data is called *ionsAED* which is the probability distribution function normalized to 1 as a function of angle (in degrees) on the horizontal axis and energy (in eV) on the vertical axis.

Another quantity of interest in plasma processing is the spatial distribution of the number, energy, and charge flux impacting a surface. We have written an analyzer which computes the flux on any surface which saves the particle data in an "Absorbed Particle Log" history. In this simulation, the history is called "leftIonLoss". This history collects particle data on the silicon wafer at every time step. The Analyzer then bins the data in position along the wafer. The user inputs the time interval and spatial region of interest.

After the simulation has completed, continue as follows:

- Proceed to the Analysis Window by pressing the *Analyze* button in the navigation column.
- In the resulting list of *Available Analyzers*, select *computeFlux.py* and press *Open*
- The analyzer fields should be filled as below:
  - **simulationName:** "waferImpact"
  - **speciesName:** ions

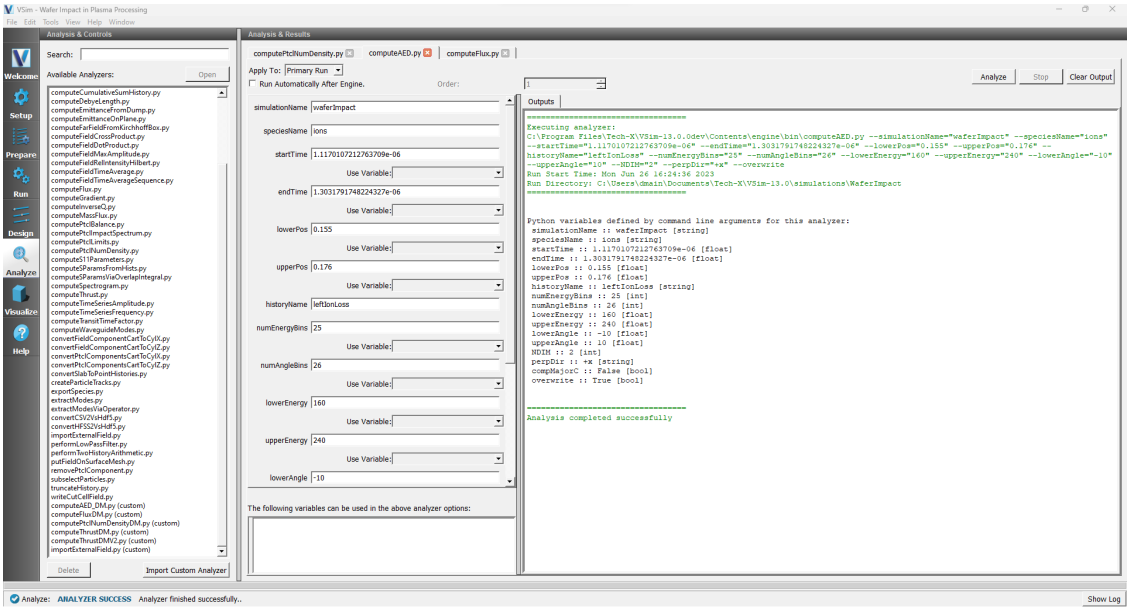


Fig. 6.154: The Analyze Window at the end of a successful run.

- **startTime:** 1.1170107212763709e-06
- **endTime:** 1.3031791748224327e-06
- **lowerPos1:** 0.155
- **upperPos1:** 0.176
- **lowerPos2:** 0 (dummy argument not used in 2D simulation)
- **upperPos2:** 1 (dummy argument not used in 2D simulation)
- **historyName:** leftIonLoss
- **numBins1:** 50
- **numBins2:** 25 (dummy argument not used in 2D simulation)
- **NDIM:** 2
- **perpDir:** 0

"endTime" and "startTime" are times over which the flux is calculated in seconds. "perpDir" is the direction normal to the surface you are collecting the data on. A description of each input quantity is found in the VSim "Analyze" window.

- Click *Analyze* in the top right corner.
- The analysis is completed when you see the output shown in Fig. 6.155.

The resulting data are called *ionsNumFlux*, *ionsEnergyFlux*, and *ionsCurrentFlux*.

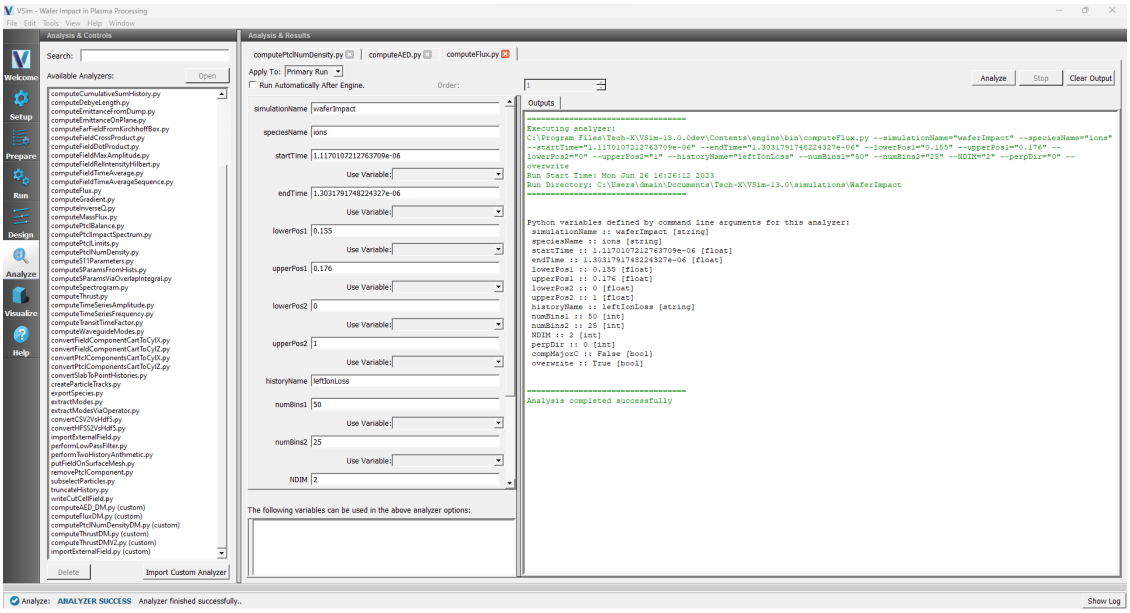


Fig. 6.155: The Analyze Window at the end of a successful run.

Visualizing the Results

After performing the above actions, the results can be visualized as follows:

- Proceed to the Visualize Window by pressing the *Visualize* button in the navigation column.
- Clicking on the *Add a Data View* dropdown menu shows there are many different types of data to visualize.
- To get started, lets visualize the self-consistent potential.
- Click on the *Data Overview* tab which is a default tab already loaded in the "Visualize" section of VSim.
- Under *Variables*, expand "Scalar Data" then check the box called "Phi"
- Finally, to visualize the potential in the context of the geometries in the simulation, expand "Geometries", and check the boxes next to "poly(End)" and "poly(FR)".
- Slide the bar to the right at the bottom to view the potential and notice that the sheath thickness varies with time.

The resulting visualization is shown in Fig. 6.156.

We now visual the Ion Angular Energy Distribution (IAED) function calculated in the previous section. Click on *Add a Data View* then click on *Data Overview*. In the newly created *Data Overview* tab, expand *Scalar Data* and check the box called "ionsAED". The horizontal axis represents angle ranging from -10 degrees to 10 degrees. The vertical axis represents energy in eV ranging from 160 to 240 eV. You can make the color scale more sensitive by changing "Set Maximum" value to 0.01 on the left side of VSim Composer. The data are shown in Fig. 6.157.

When the AED is computed, the 1D Angular Distribution (AD) is computed by integrating over all energies. Likewise the 1D Energy Distribution (ED) is computed by integrating over all angles. These can be plotted by clicking on *Add a Data View* then clicking on *1-D Fields* which will open a new tab. In "Graph 1" select *ionsAD* and in "Graph 2" select *ionsED*. The visualization window with the plots is shown in Fig. 6.158.

Finally we visualize the flux onto the wafer computed with "computeFlux.py" in the previous section. To view this data set, click on *Add a Data View* then click on *1-D fields*. In the newly created 1-D Fields tab, click on "Add Curve" and choose "ionsNumFlux". You will also see two other options corresponding to the energy flux and charge flux (i.e. current) onto the surface. The horizontal axis represents distance along the wafer. The vertical axis represents number flux. The data are shown in Fig. 6.159.

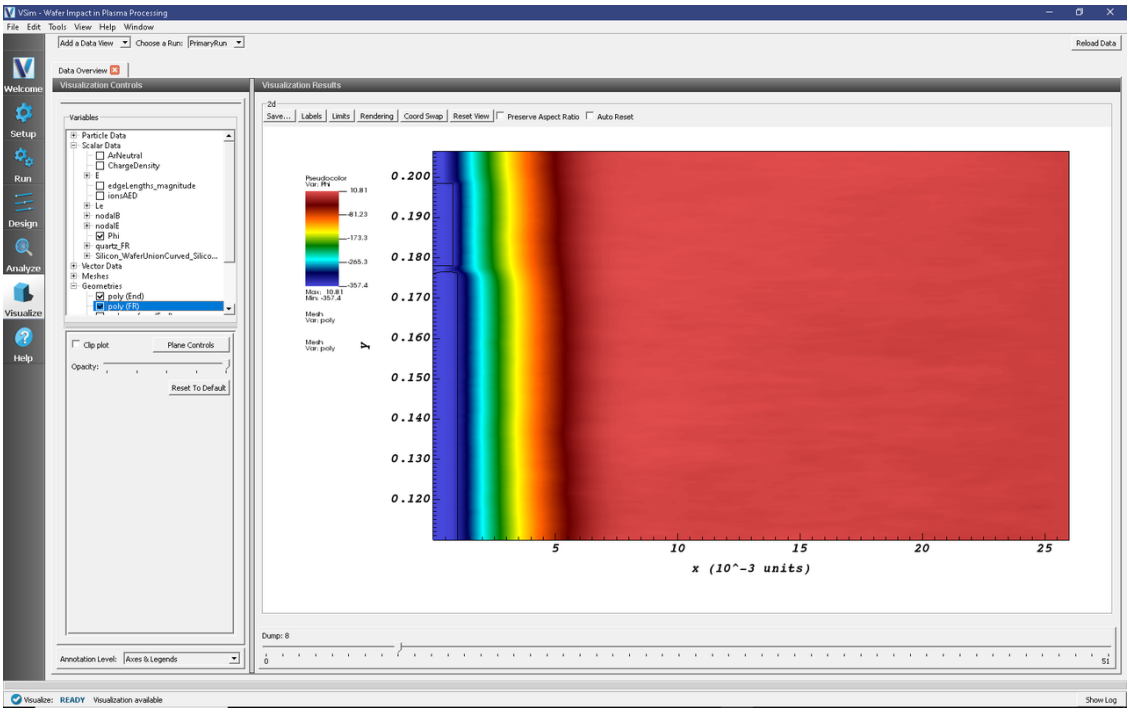


Fig. 6.156: The evolved potential with the geometries superimposed.

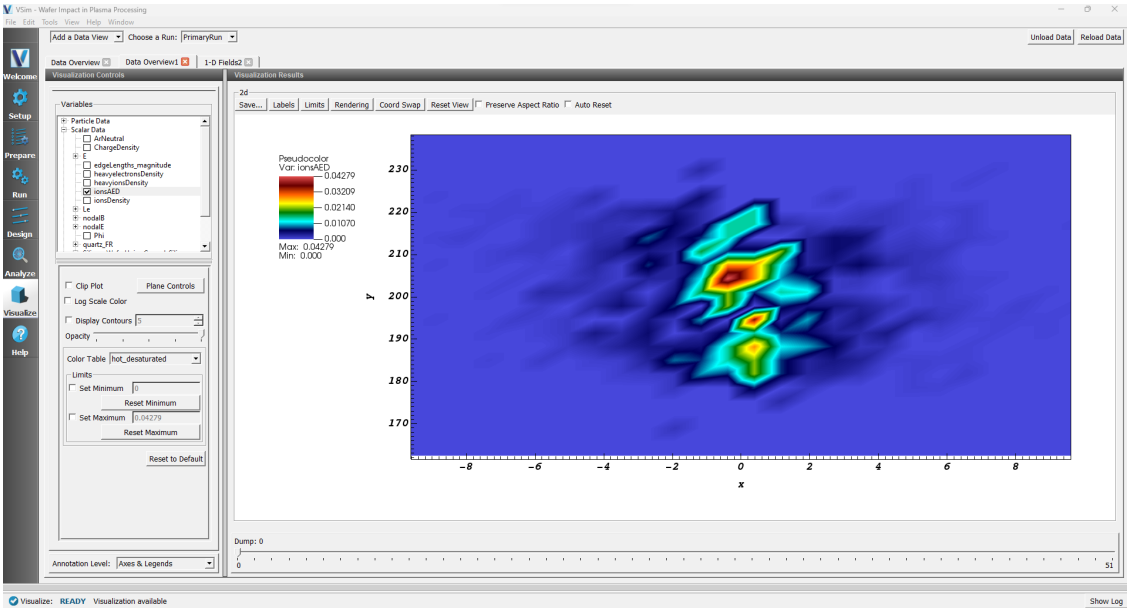


Fig. 6.157: Ion Angular Energy Distribution (IAED) function which was generated in the previous section.

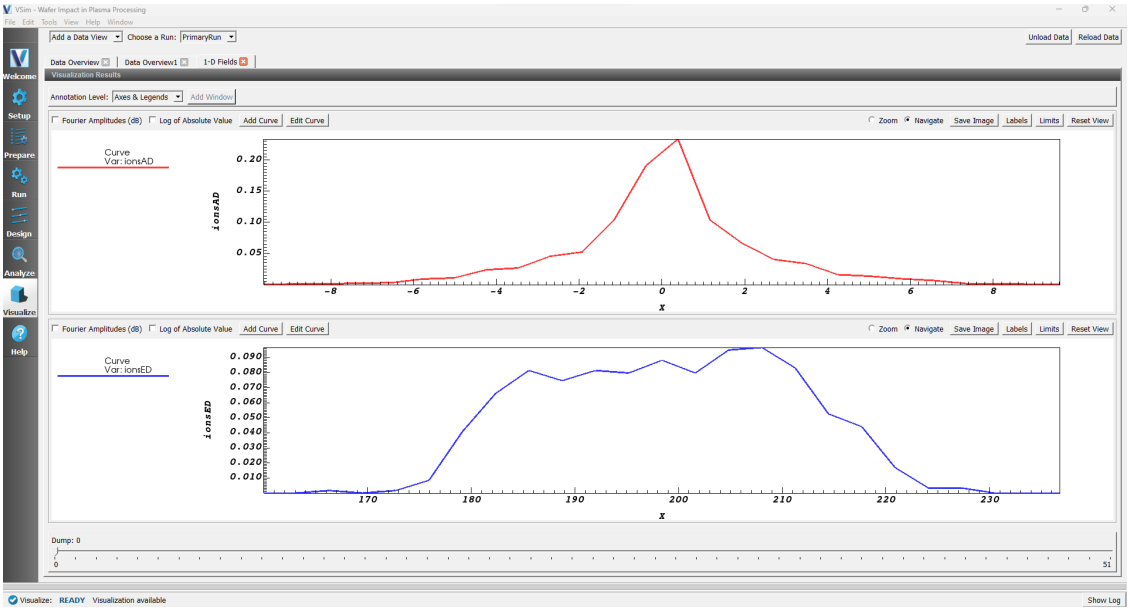


Fig. 6.158: Ion Angular Distribution (AD) and Energy Distribution (ED) functions which were generated in the previous section.

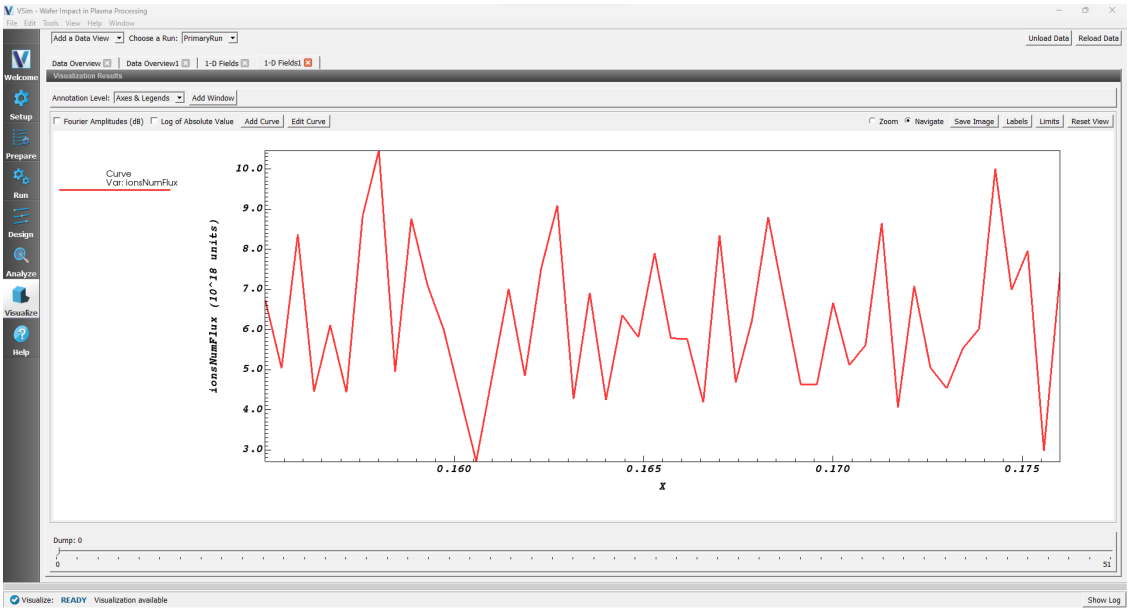


Fig. 6.159: Ion Number flux impacting the wafer. These data were computed with the analyzer computeFlux.py.

Further Experiments

For this simulation, collisions with a background neutral species have been included. You could include more excitation collisions to make the interaction with the background gas more realistic. You can also add secondary electron emission off of the dielectrics. Lastly, you can modify the RF source or add an additional RF source to create a dual frequency RF source.

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