Introduction to Vsim:
Vsim Composer
&
Vorpal

Setup, Parameters, Functions, Materials, Geometries,
Fields, Boundary Conditions, Particles, & Histories

Outline

- Simulation Requirements
- Useful Simulation Concepts
- Introduction to VSim
- Walkthrough of VSimComposer
- Basic Implementation of
- Conclusions

Approaching Simulations

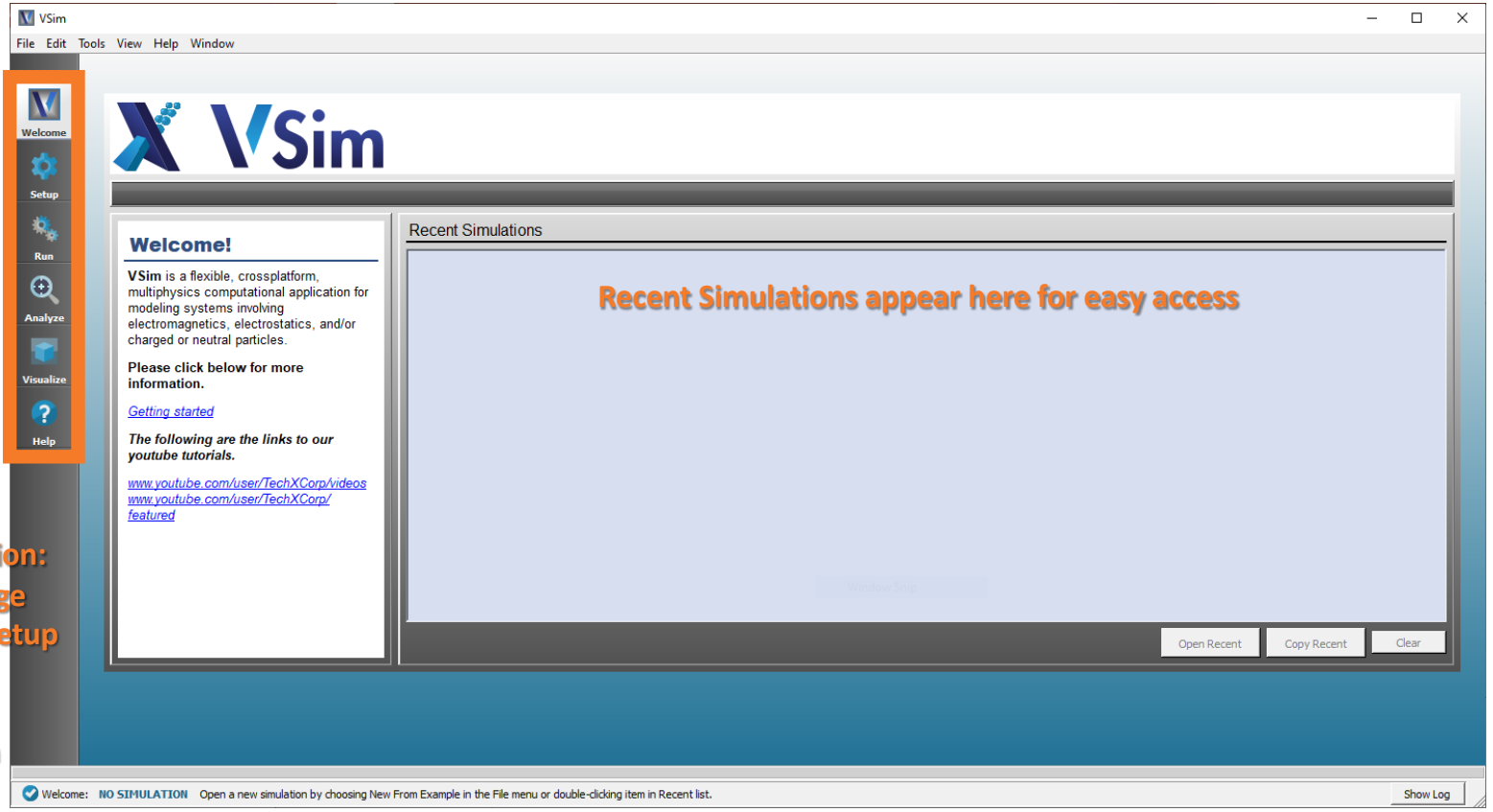
- Can the simulation be done?
  - What are the smallest and largest length scales involved?
  - What about time scales? Are you looking to resolve both ion and electron movement?
  - What is the plasma frequency? That affects the size of your time step
  - What do those requirements mean for the number of cells, number of time steps and time step length, needed to simulate and accurately capture?

- In our case of a Hall Thruster:
  - Smallest characteristic length scale is typically a Debye length (L_D) ~ (KT/nq**2) <- TODO:LATEX
    - In the high electron density locations, this can be of order a few tenths of microns (10**-7 m)
  - Longest characteristic length is typically the size of the device – say a few centimeters (10**-2 m)
- Plasma frequency is of a few GHz (10**9 Hz),
- Time step is a few picoseconds (10**-12 s)

- What is the core physics looking to be explored?
  - Is it field related, particle-particle collisions, Temperature, Thermal velocity?
  - If collisions are important:
    - Compute the collision frequency using the background magnetic field.
    - If the collision frequency is "fc", then make sure time step (DT) is such that DT < 1/fc
- What is the bare minimum required to obtain a physical result?
  - Increase complexity from there

Welcome Screen

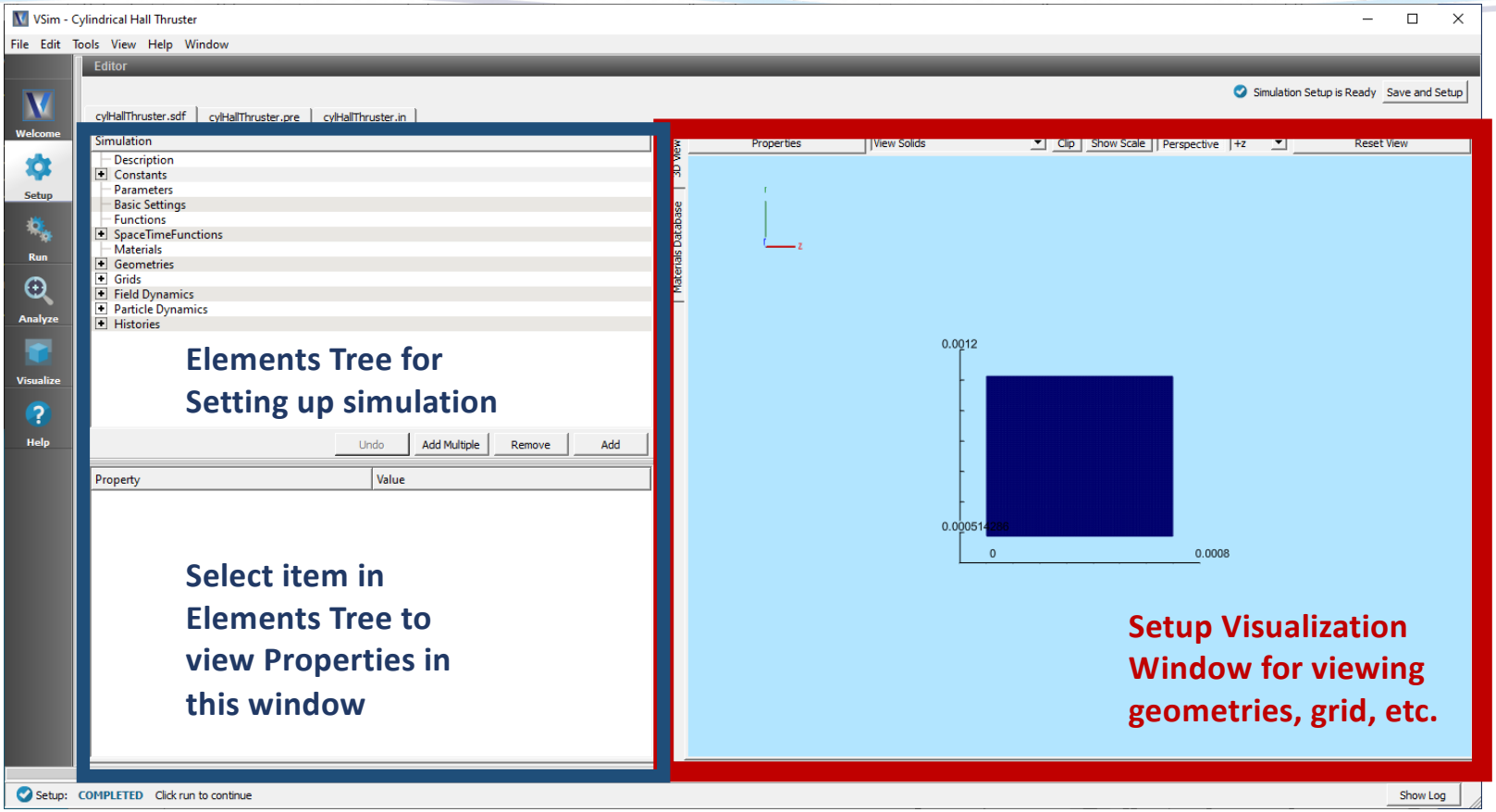
Welcome Tab



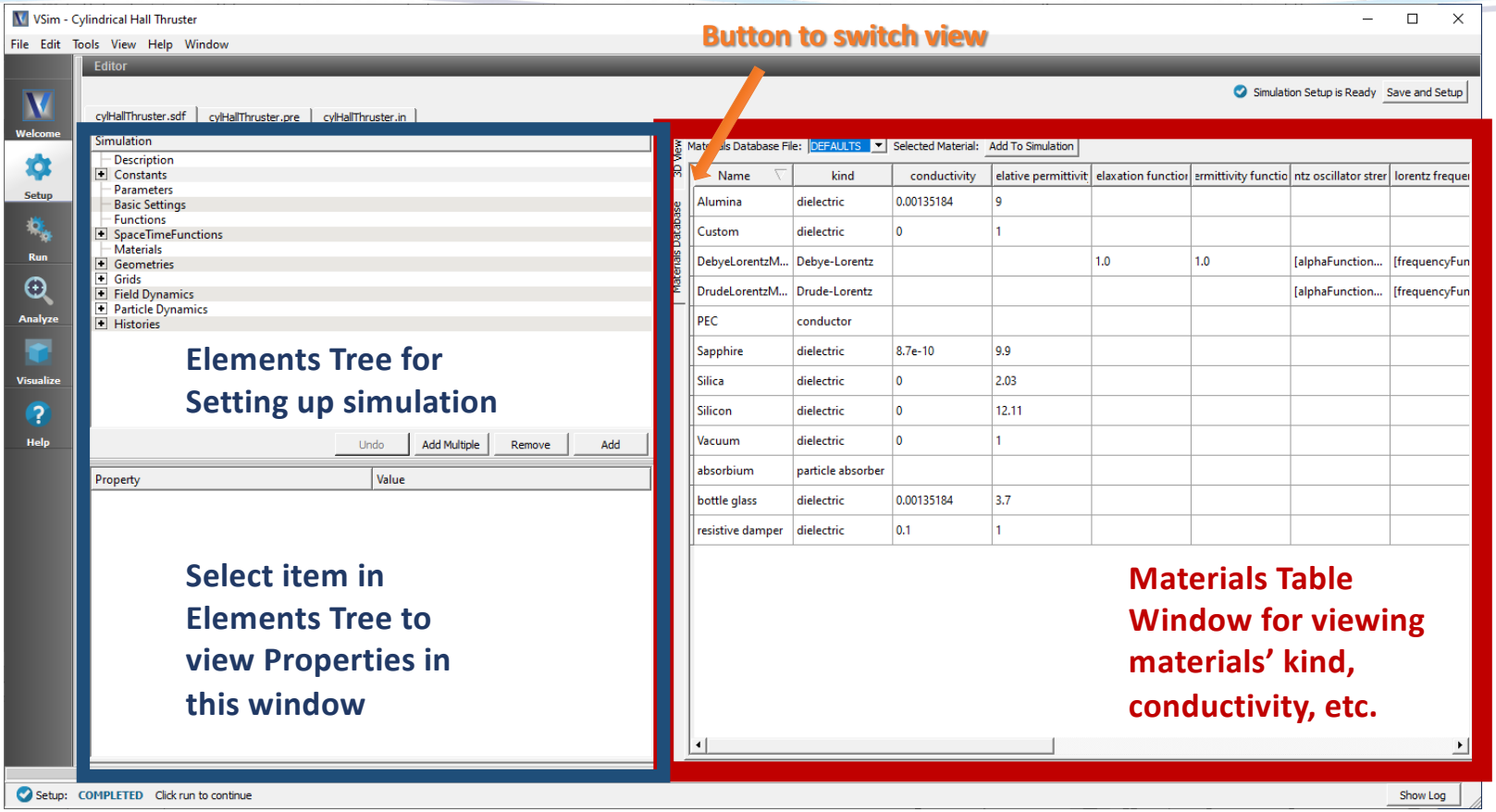
Tabs for navigation:

- **Welcome Page**
- **Simulation Setup**
- **Running**
- **Analysis**
- **Visualization**
- **Help**

Default Setup View

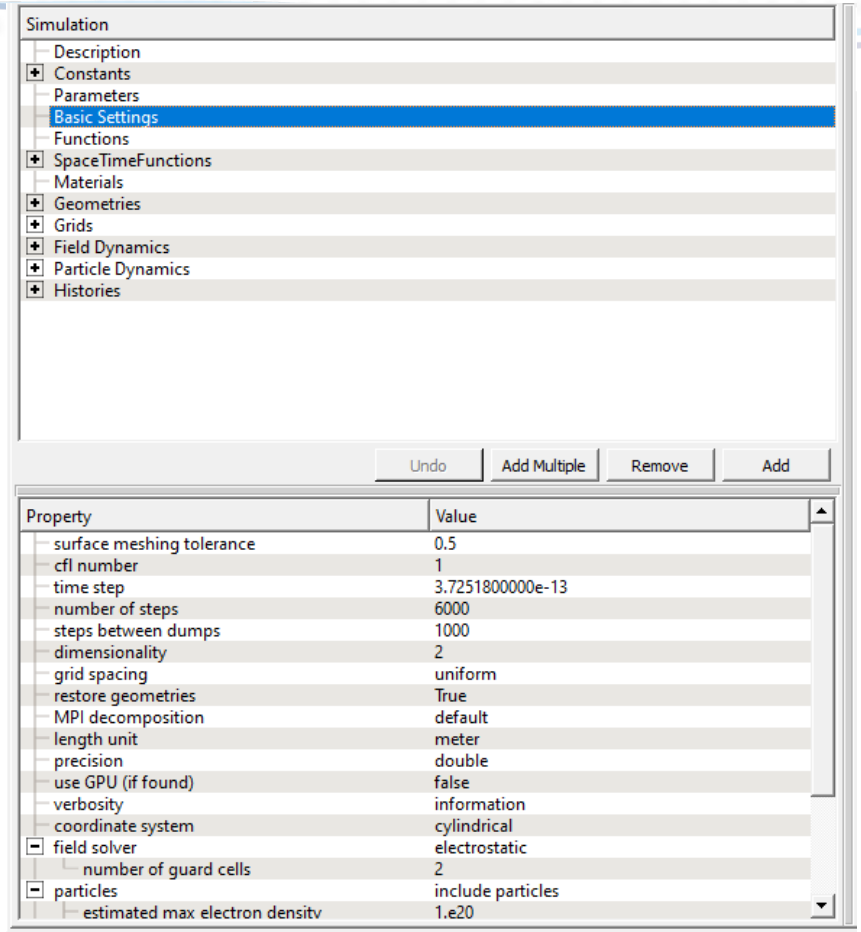


Materials Setup View



Basic Settings

Elements Tree for Setting up simulation



Properties of Selected Element (*Basic Settings*)

Click on *Basic Settings* element in Tree to edit properties here

Basic Settings

Surface Meshing Tolerance

- Determines the relative size at which small cells from a meshed geometry surface are dropped.
- Set to 1.0 for simulations not containing any geometries.

Property	Value
surface meshing tolerance	0.5
cfl number	1
time step	3.7251800000e-13
number of steps	6000
steps between dumps	1000
dimensionality	2
grid spacing	uniform
restore geometries	True
MPI decomposition	default
length unit	meter
precision	double
use GPU (if found)	false
verbosity	information
coordinate system	cylindrical
field solver	electrostatic
number of guard cells	2
particles	include particles
estimated max electron density	1.e20
estimated max electron temperature (eV)	1.0
dump nodal fields	True
collisions framework	reduced
moving window	no moving window
periodic directions	no periodicity

Basic Settings

CFL Number

- If time step is set to zero, the time step is automatically calculated.
- For EM simulations, the time step is reduced proportionately with the CFL number.
- The CFL number is the ratio of time step to Courant limit.

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Basic Settings

Time Step

- If set to a value that is non-zero, this will be used as the simulation time step.
- If set to zero, the time step is calculated for you based on a number of factors.

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Basic Settings

Number of Steps

- The number of time steps to run the simulation.

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dimensionality	2
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Basic Settings

Steps Between Dumps

- The number of time steps between sequential dumps of data to hdf5 format files.

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number of steps	6000
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Basic Settings

Dimensionality

- Set to 1, 2, or 3 to indicate how many dimensions to run the simulation in.

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Basic Settings

Coordinate System

- The type of coordinate system to work in.
  - cartesian
  - cylindrical
- For cylindrical coordinates, only 2 dimensional electrostatic simulations are currently available in visual setup.

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Basic Settings

Field Solver

- The field solver determines which equations will be used to calculate the fields:

1. Electrostatic
   - number of guard cells

2. Electromagnetic
   - Cerenkov Filter
   - Electromagnetic problems allow for the selection of a numerical Cerenkov noise filter.

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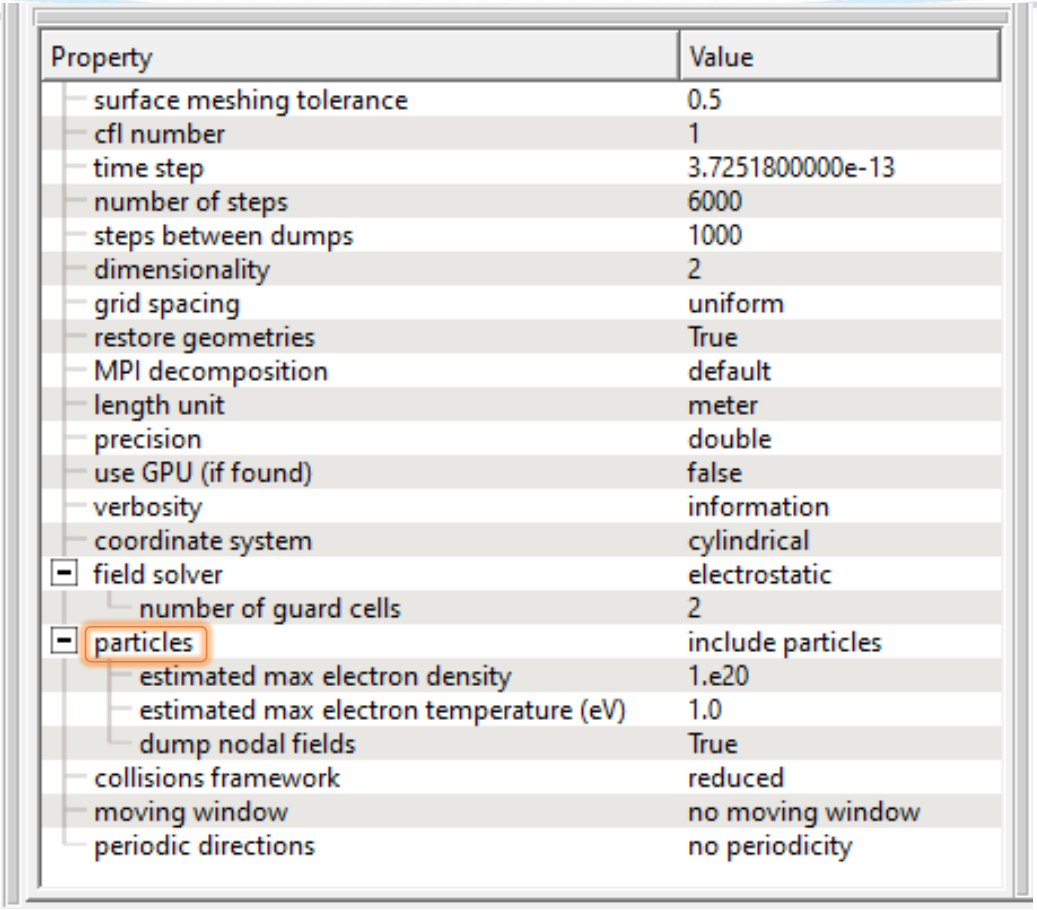
Basic Settings

Particles

- Whether or not to include particles in the simulation.

1. no particles
2. include particles

- If particles are included in the simulation, the following 2 properties are used to help calculate the time step.
  - estimated max electron density
  - estimated min electron temperature (eV)



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Basic Settings

Collisions Framework

- Whether or not to include particles in the simulation.

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2. include particles

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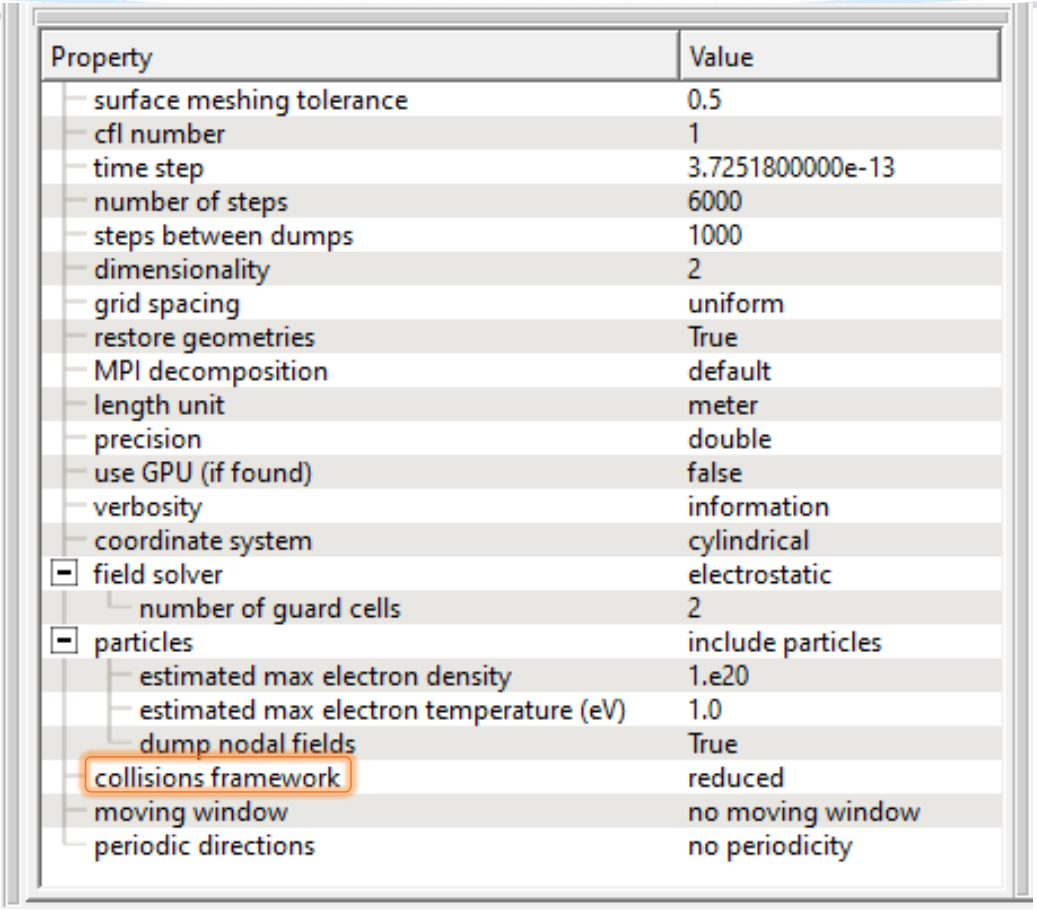
  - estimated max electron density
  - estimated min electron temperature (eV)



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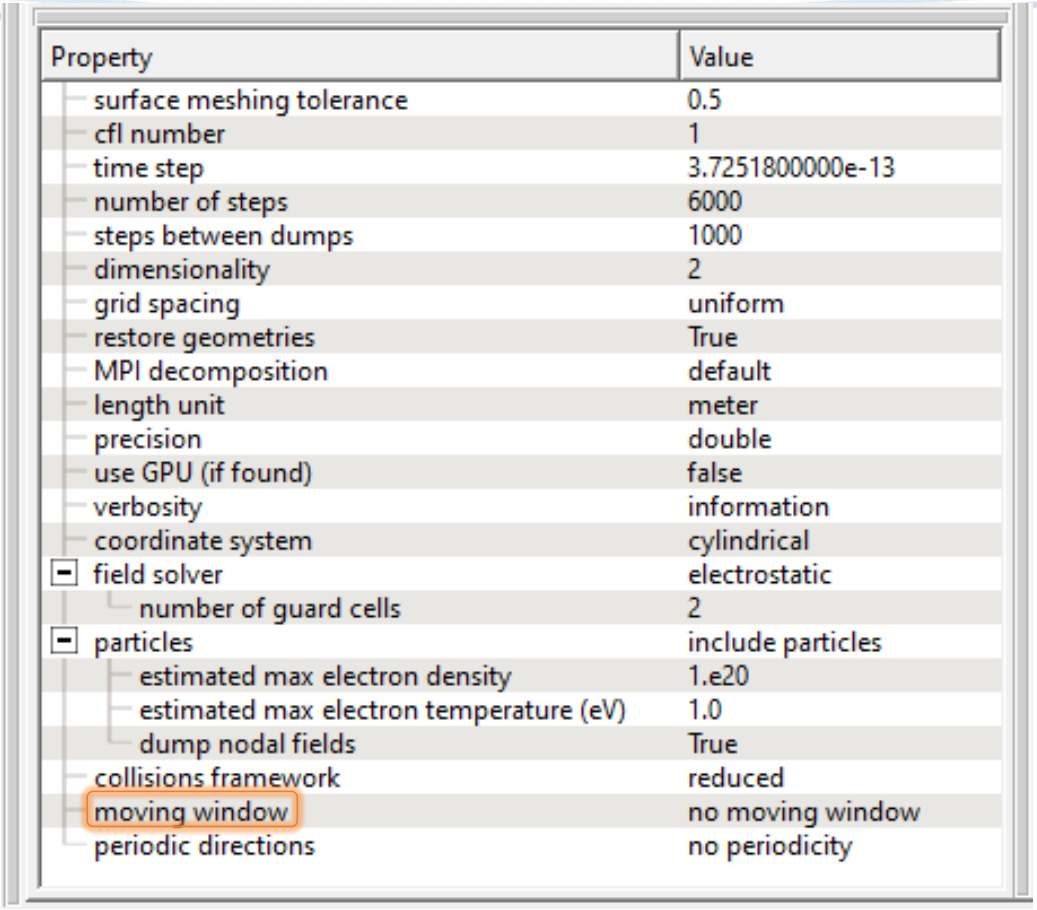
Basic Settings

Moving Window

- Whether or not to use a moving window which allows the simulation window to move at the speed of light in the chosen direction.
- Useful for simulations such as laser pulse or particle beam moving at a velocity close to the speed of light.



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Basic Settings

Periodic Directions

- The directions of the simulation which should be modelled as periodic, if any.

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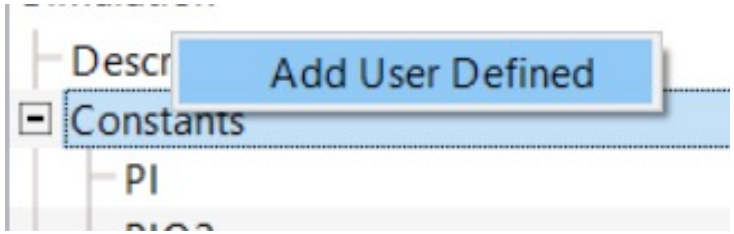
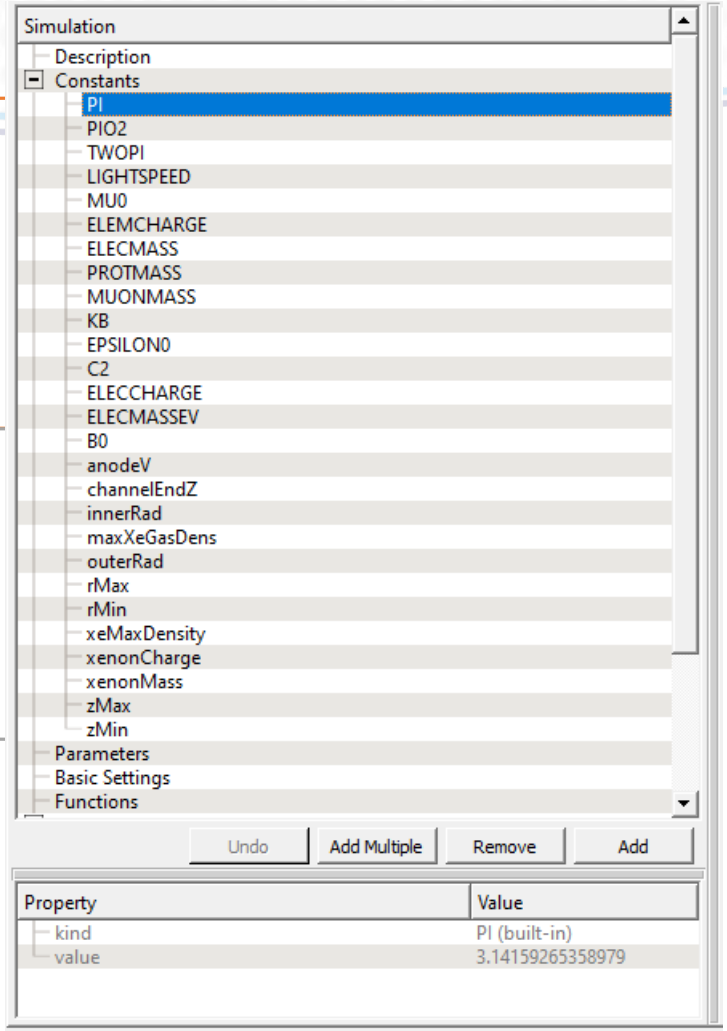
Constants

Built-in universal constants:
π, 2π, c, m_e, e^-, m_p, etc.

User-defined constants:
lengths, frequencies, etc.



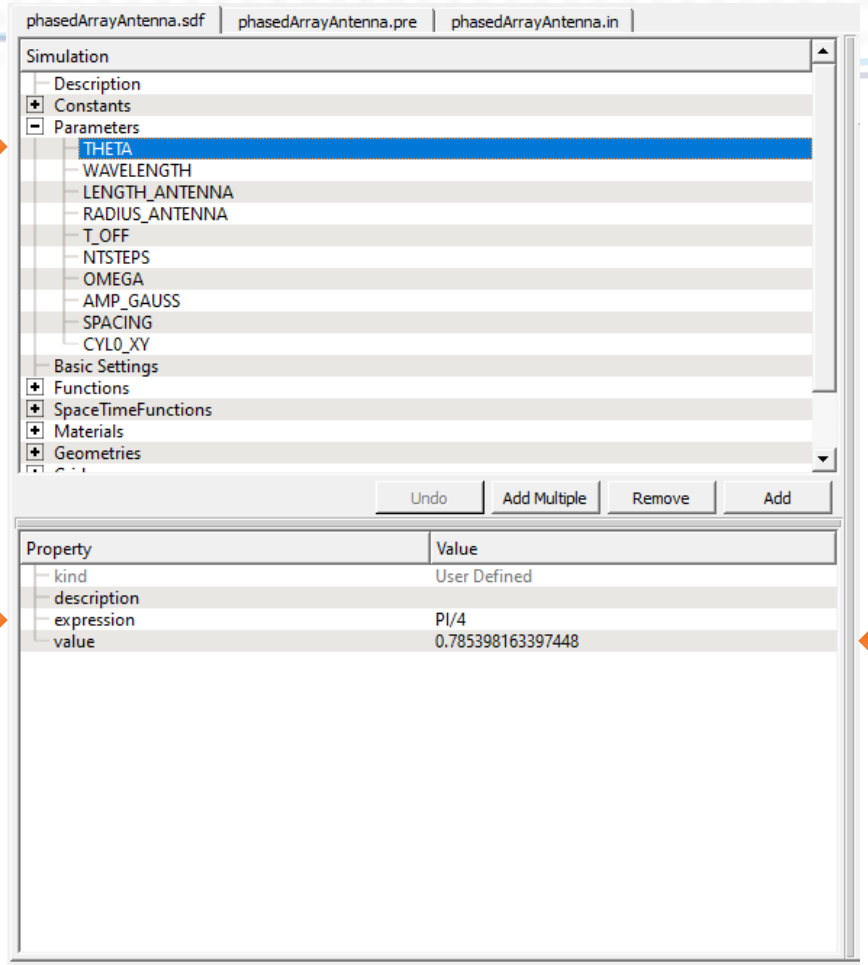
Right-click on element in tree



Derived Parameters

Parameter Name

Parameter Expression

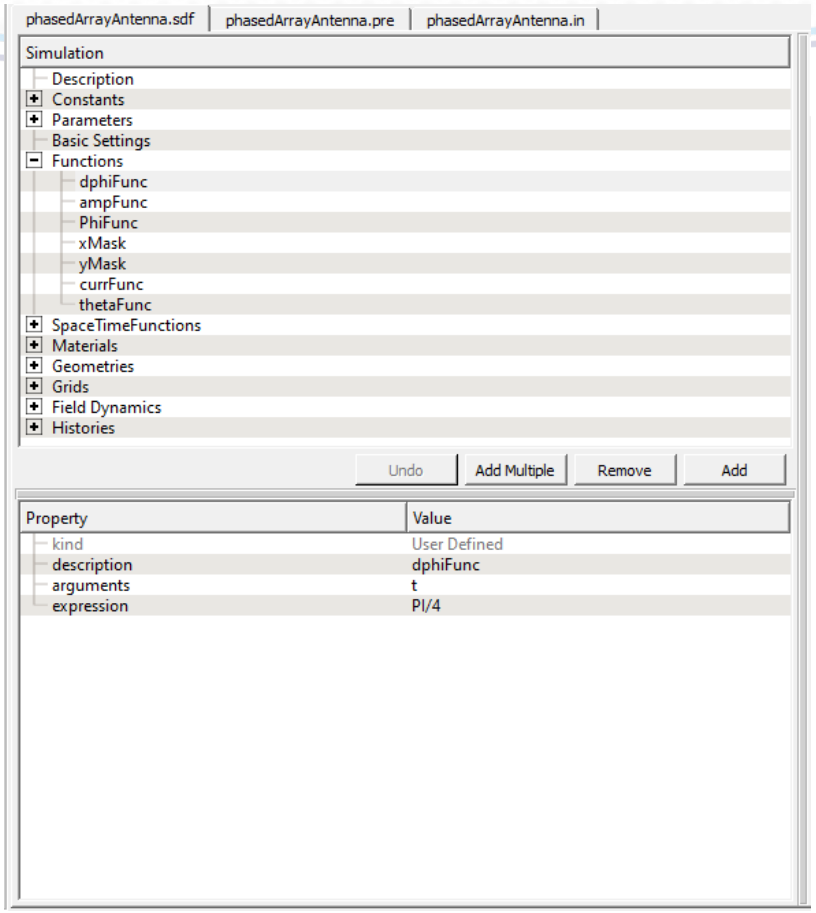


VSim calculates the parameter value from the provided expression

Functions

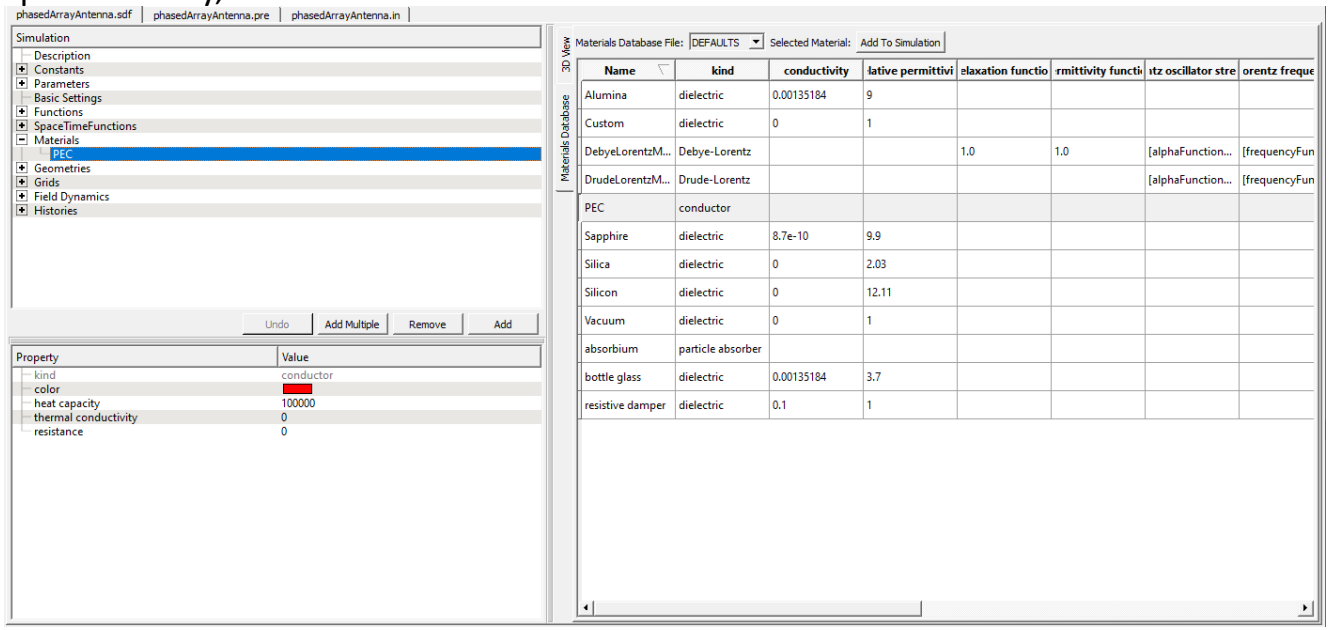
1. Create your own function.
2. Built-in turn on function.

- The function can contain any number of arbitrary arguments and is not limited to the default values of x,y.
- The user-supplied expression is a function of the arguments given in the argument property.
- The expression can include any pre-defined Constants, Parameters, or Functions, as well as real numbers and python operator.



Materials

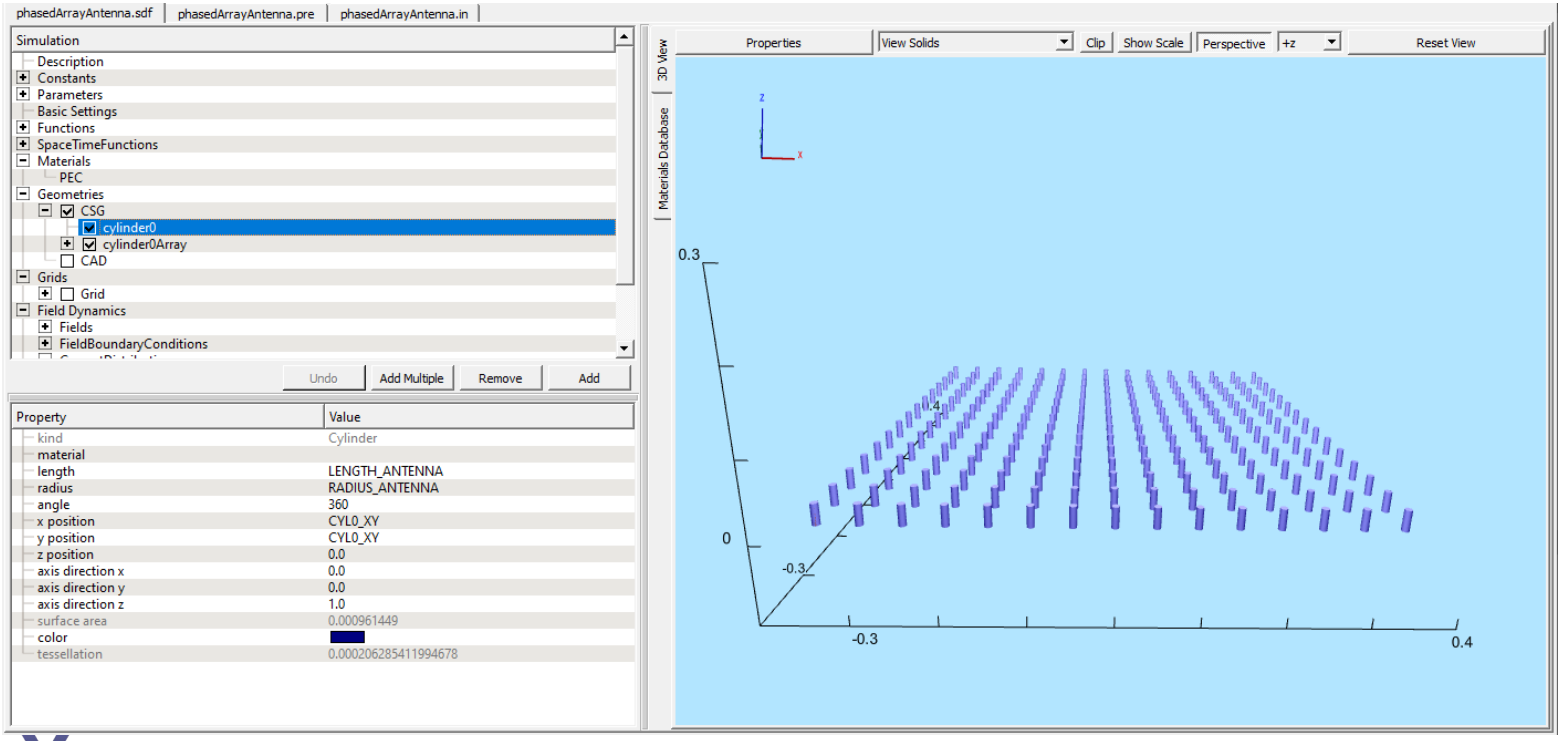
Material Properties: heat capacity, conductivity, permittivity, thermal conductivity, permeability, and resistance.



- See pre-defined materials: switch from *3D View* to *Database.*
- See a wider selection of materials: load the *emthermal.vmat* file by right-clicking on the **Materials** element and selecting *Import Materials*.
- You can also import your own customized material.

Geometries

- Import Files:
  - .stl, .ply, .vtk, .stp, .step, or .p12
- Build complex devices with Constructive Solid Geometries (CSG):
  - sphere, box, cylinder, cone, torus, pipe, wedge, truncated cone



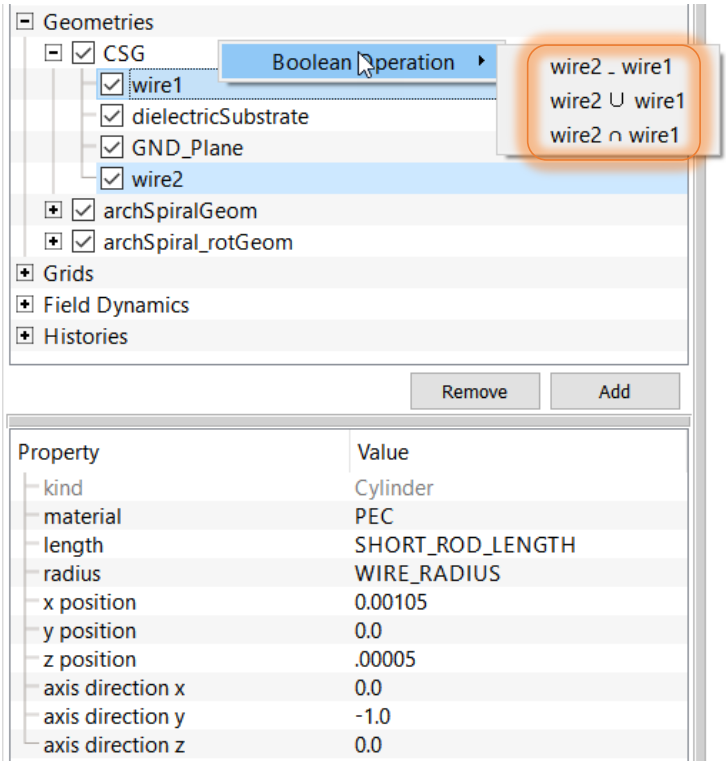
Geometries

- CSG Primitives can be combined:

1. **Subtract**
   - This will subtract the second selected primitive from the first selected primitive.
2. **Union**
   - This will combine the two primitives into a single object. For use if the combined object is set to be a particle sink.
3. **Intersect**
   - This will leave only the volume of the two primitives that intersect as an object.

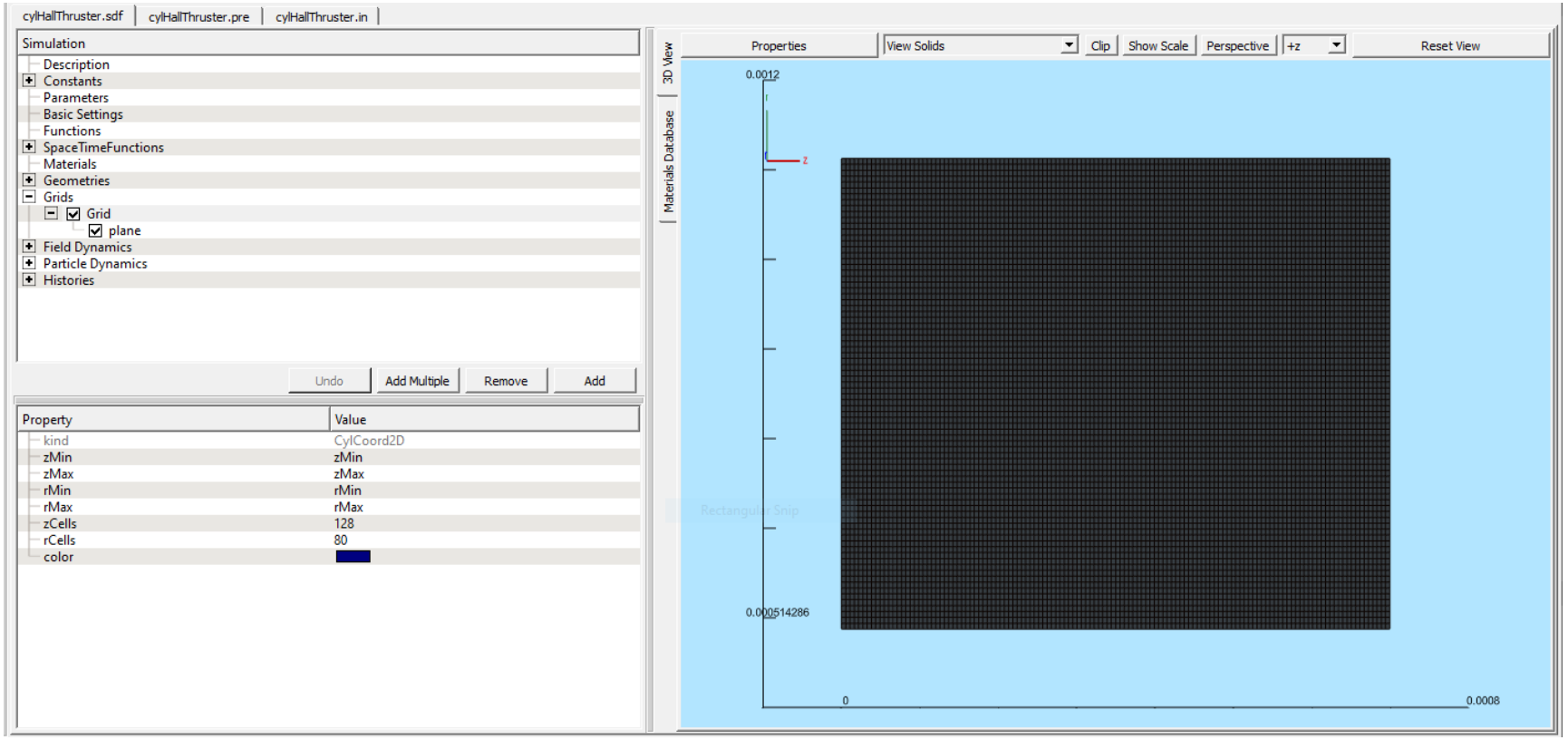
- Boolean operations may be nested.

- For use in the simulation, a Geometries part **MUST** have a material assigned to it, other wise it is ignored (treated as vacuum).



Grid

Determines the simulation size and relationship of physical coordinate to cell indices

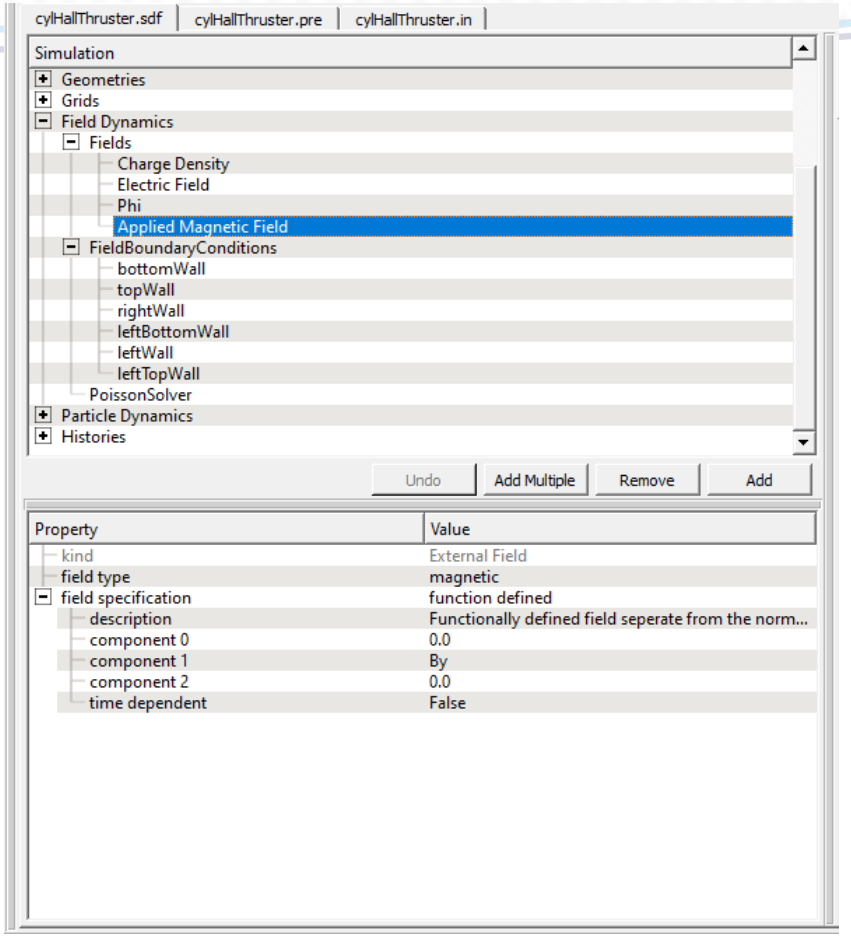


Field Dynamics

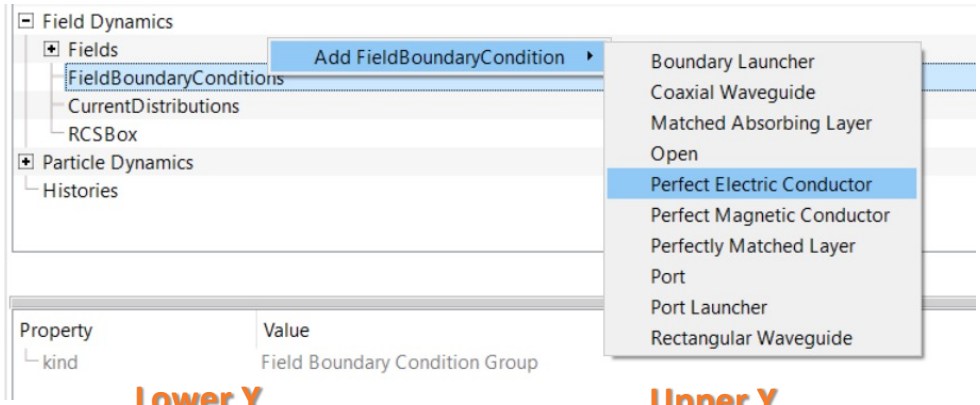
1. **Fields**
   - Initial conditions can be set.
   - External fields can be added.

2. **Field Boundary Conditions**
   - The field solver determines which Boundary Condition are available to add to your simulation.

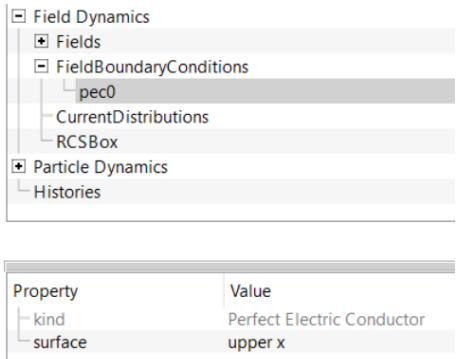
3. **Current Distributions**
   - Dipole
   - Distributed



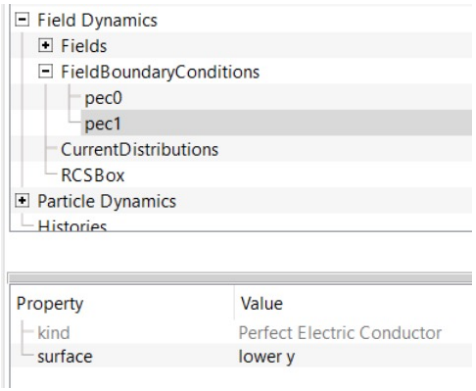
Field Boundary Conditions



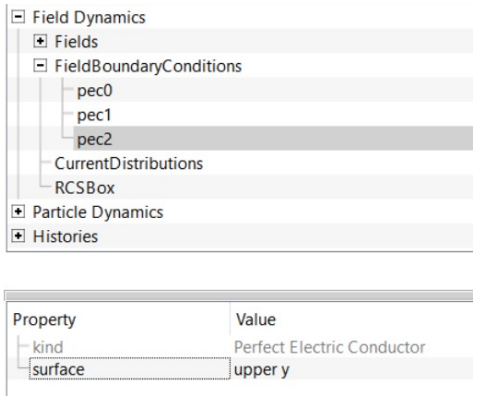
Upper X



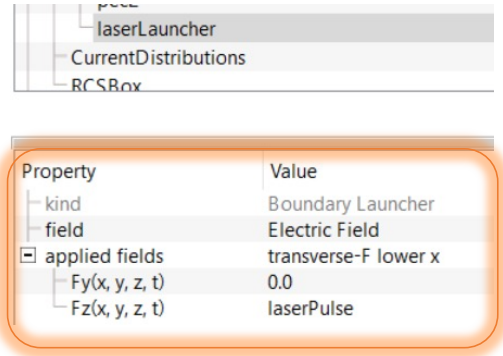
Lower Y



Upper Y

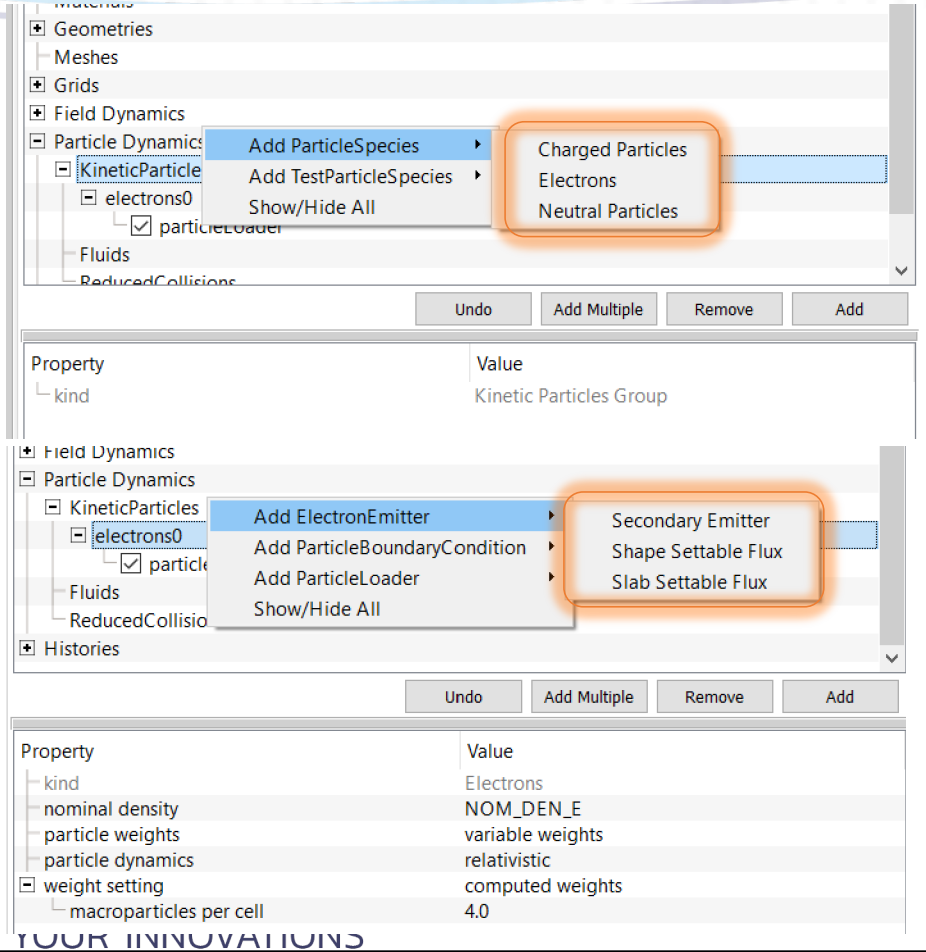


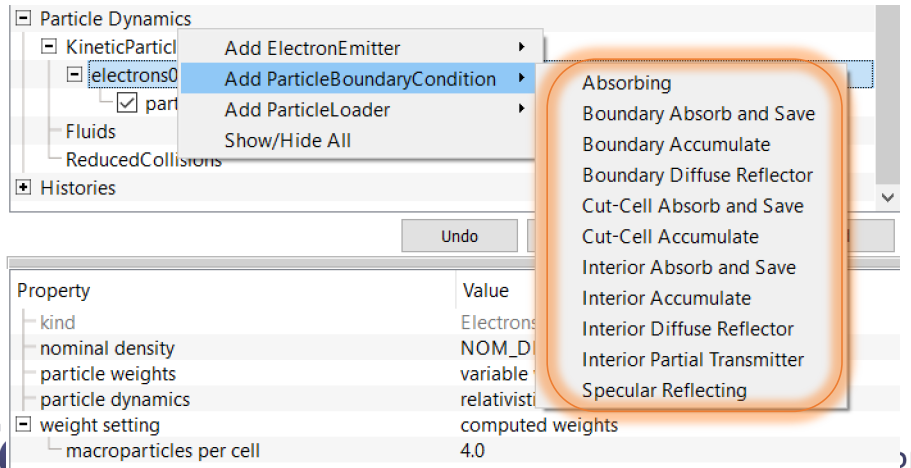
Lower X



Particles

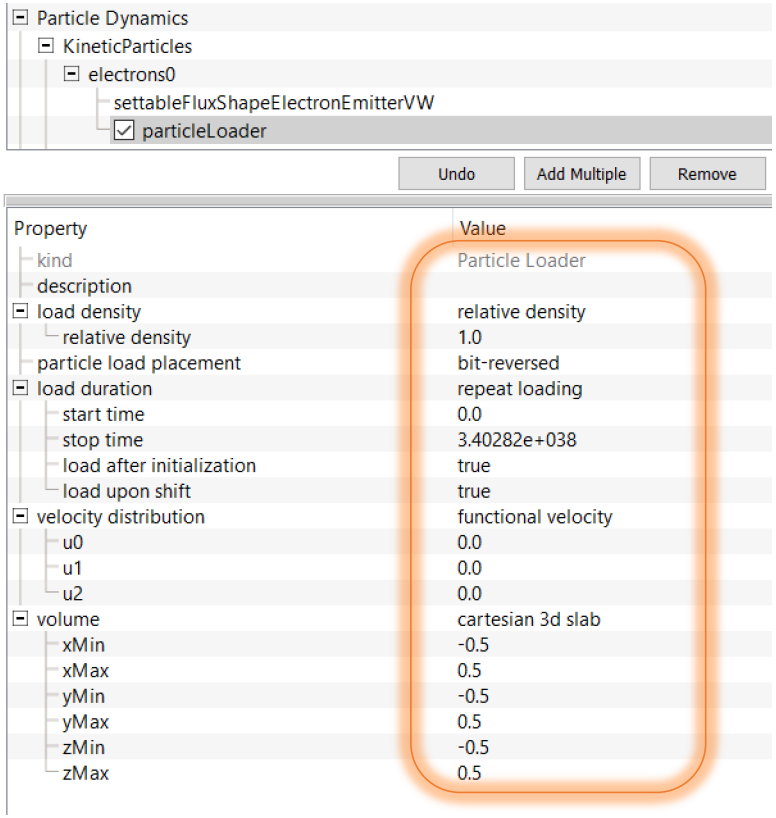
1. **Types**
   - Regular: electrons, ions (or other charged particles), and neutral particles.
   - Test: field-scaled electrons
2. **Loaders & Emitters**
   - Load within a volume
   - Emit from a surface of boundary
   - Emission: primary or secondary
3. **Boundary Conditions**



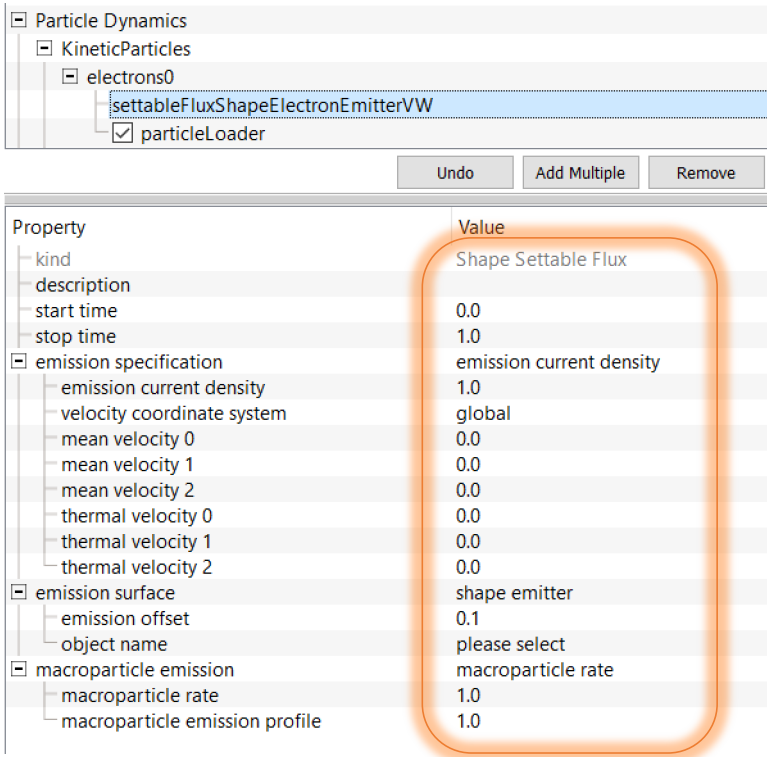


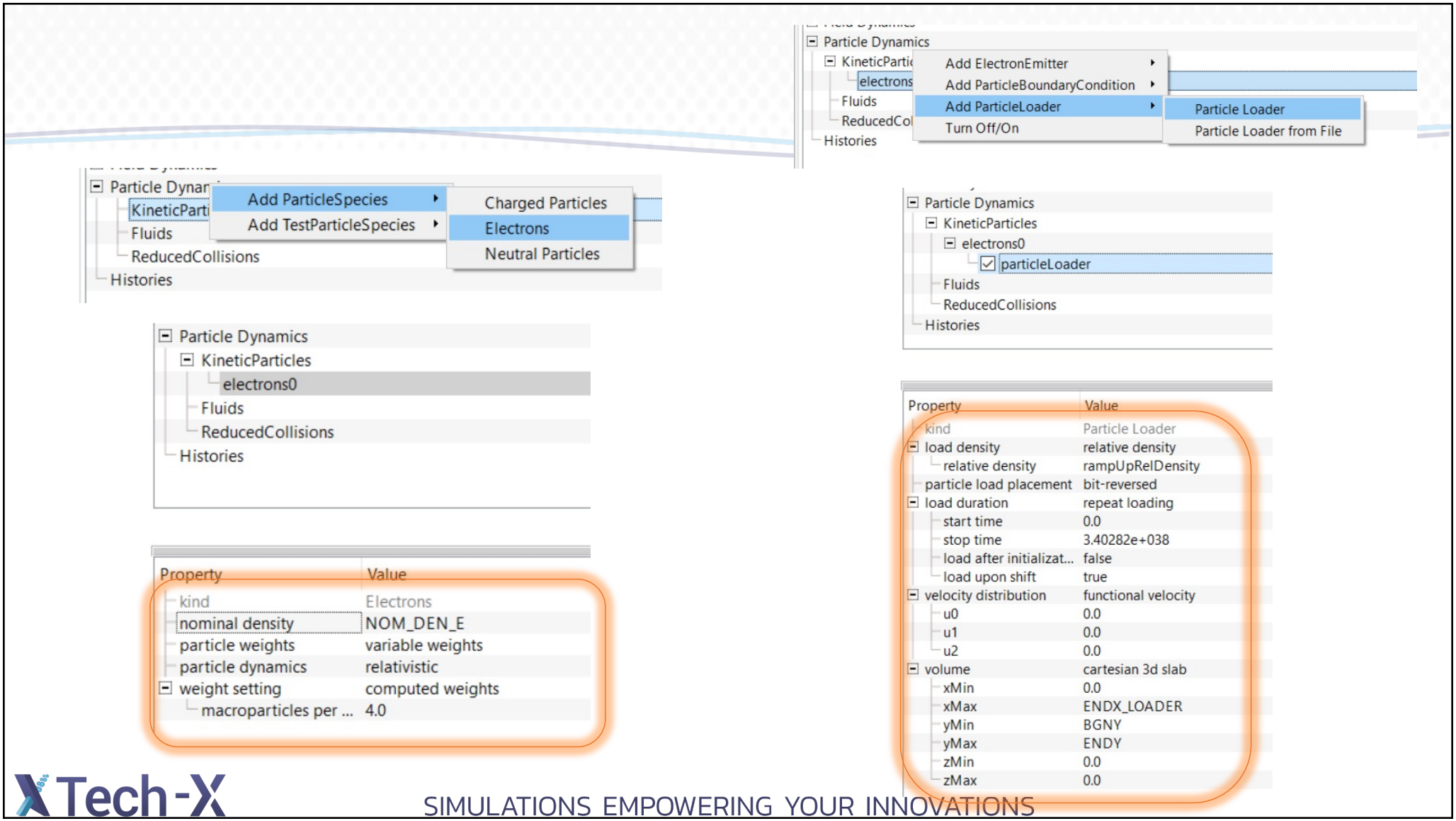
Particles

Loading



Emitting




Particle Dynamics
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Add ElectronEmitter
Add ParticleBoundaryCondition
Add ParticleLoader
Turn Off/On
Particle Loader
Particle Loader from File
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Add ParticleSpecies
Add TestParticleSpecies
Charged Particles
Electrons
Neutral Particles
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particle dynamics
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load density
relative density
relative density
rampUpRelDensity
particle load placement
bit-reversed
load duration
repeat loading
start time
0.0
stop time
3.40282e+038
load after initializat...
false
load upon shift
true
velocity distribution
functional velocity
u0
0.0
u1
0.0
u2
0.0
volume
cartesian 3d slab
xMin
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xMax
ENDX_LOADER
yMin
BGNY
yMax
ENDY
zMin
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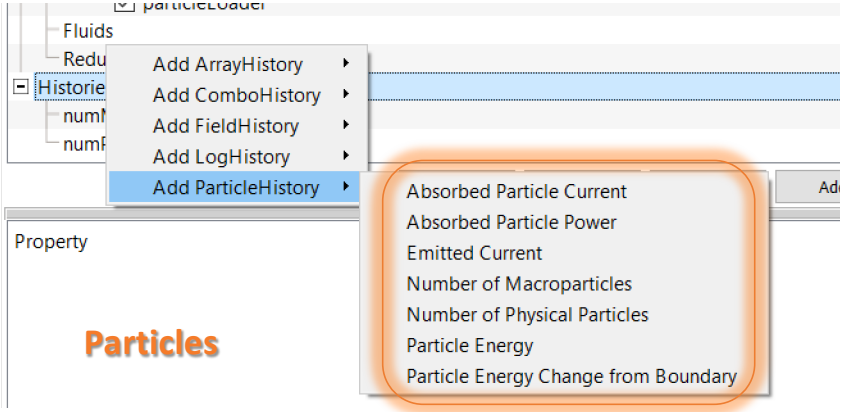
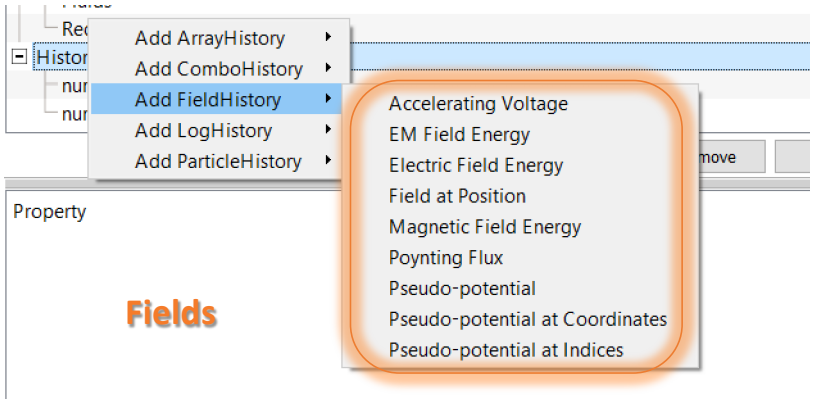
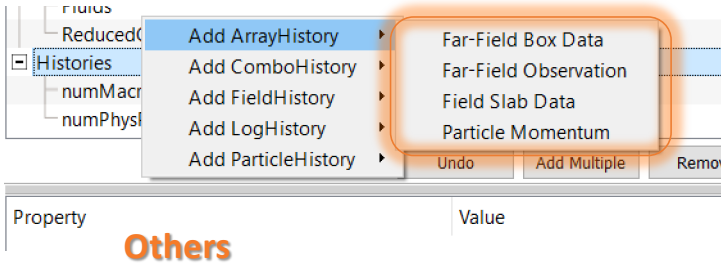
zMax
0.0

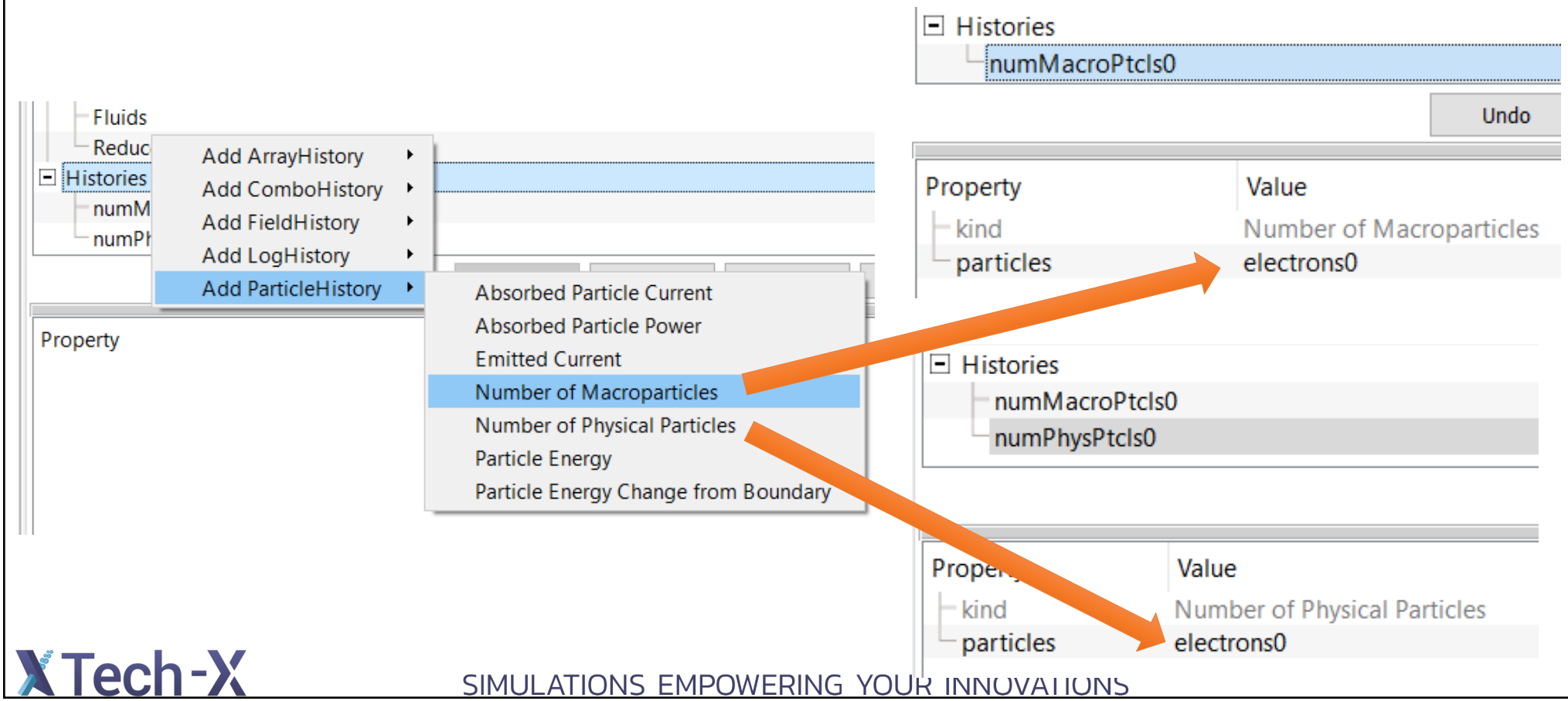
Histories


Fluids
Add ArrayHistory
Add ComboHistory
Add FieldHistory
Add LogHistory
Add ParticleHistory
Absorbed Particle Current
Absorbed Particle Power
Emitted Current
Number of Macroparticles
Number of Physical Particles
Particle Energy
Particle Energy Change from Boundary
Property
Particles


Add ArrayHistory
Add ComboHistory
Add FieldHistory
Add LogHistory
Add ParticleHistory
Accelerating Voltage
EM Field Energy
Electric Field Energy
Field at Position
Magnetic Field Energy
Poynting Flux
Pseudo-potential
Pseudo-potential at Coordinates
Pseudo-potential at Indices
Property
Fields

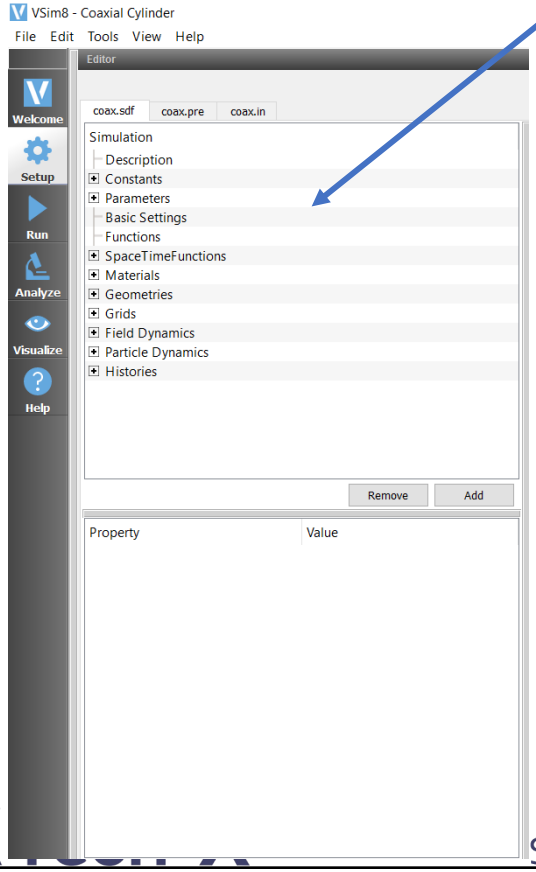

Histories
Add ArrayHistory
Add ComboHistory
Add FieldHistory
Add LogHistory
Add ParticleHistory
Far-Field Box Data
Far-Field Observation
Field Slab Data
Particle Momentum
Undo
Add Multiple
Property
Value
Others

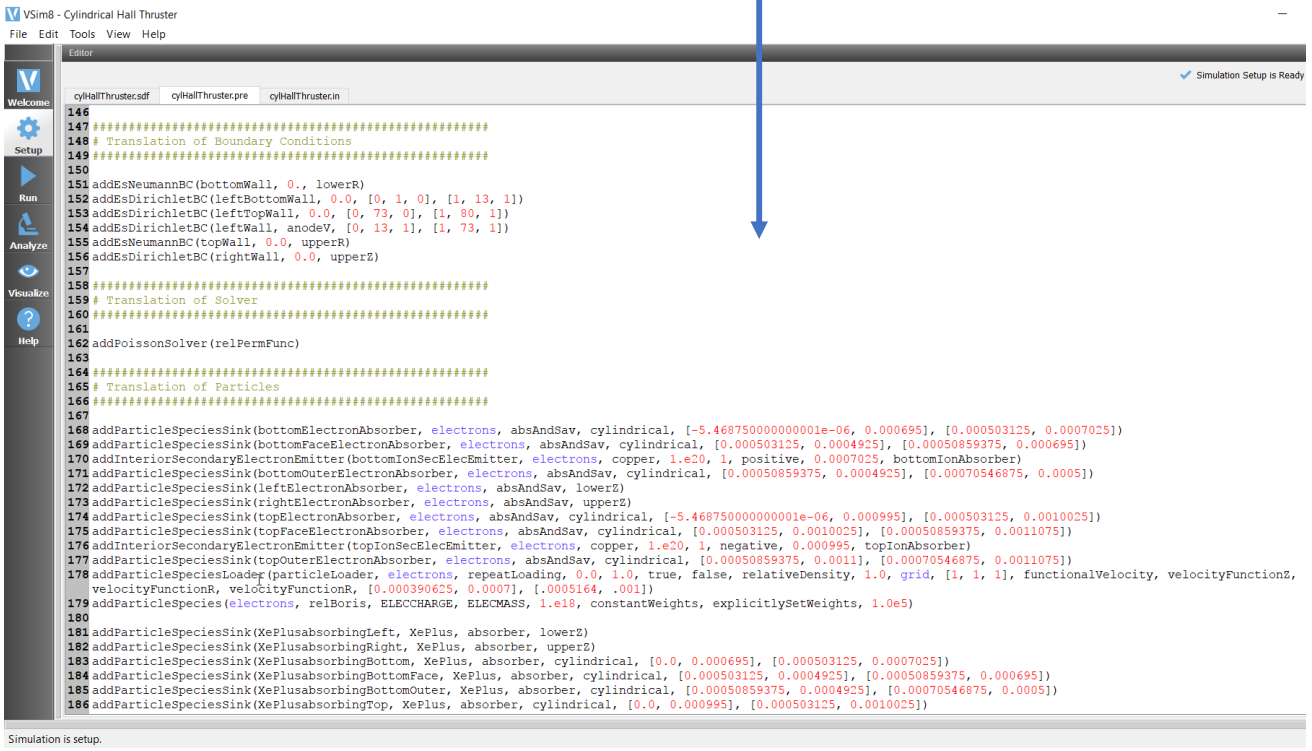
Histories


Fluids
Reduc
Histories
numM
numPh
Add ArrayHistory
Add ComboHistory
Add FieldHistory
Add LogHistory
Add ParticleHistory
Absorbed Particle Current
Absorbed Particle Power
Emitted Current
Number of Macroparticles
Number of Physical Particles
Particle Energy
Particle Energy Change from Boundary
Property
Histories
numMacroPtcls0
Undo
Property
Value
kind
Number of Macroparticles
particles
electrons0
Histories
numMacroPtcls0
numPhysPtcls0
Value
kind
Number of Physical Particles
particles
electrons0

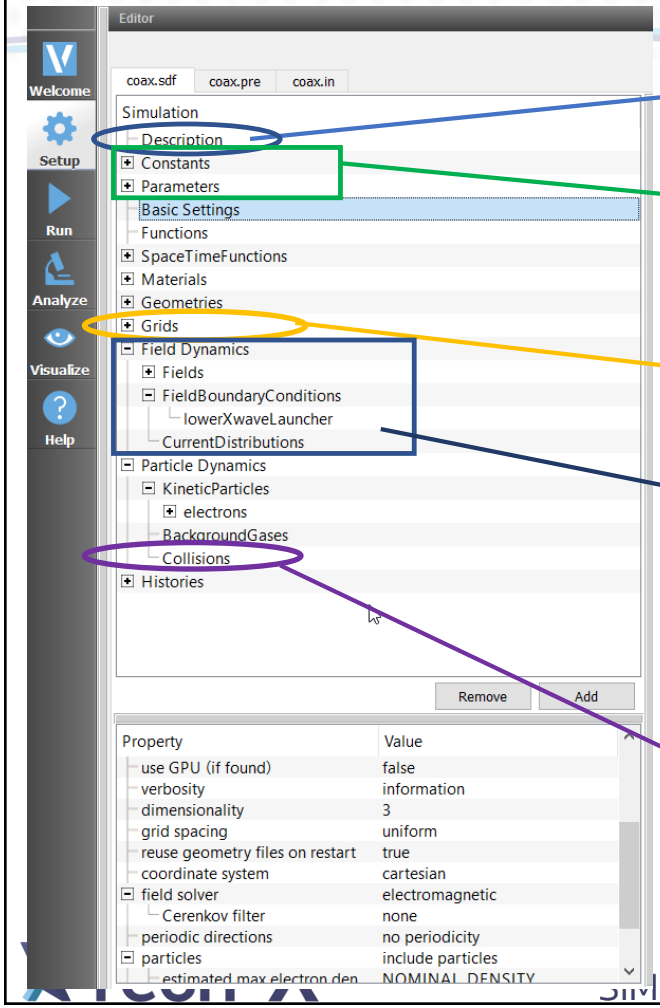
Visual to Text-Based Comparison

File Formats: .sdf and macro-ized .pre



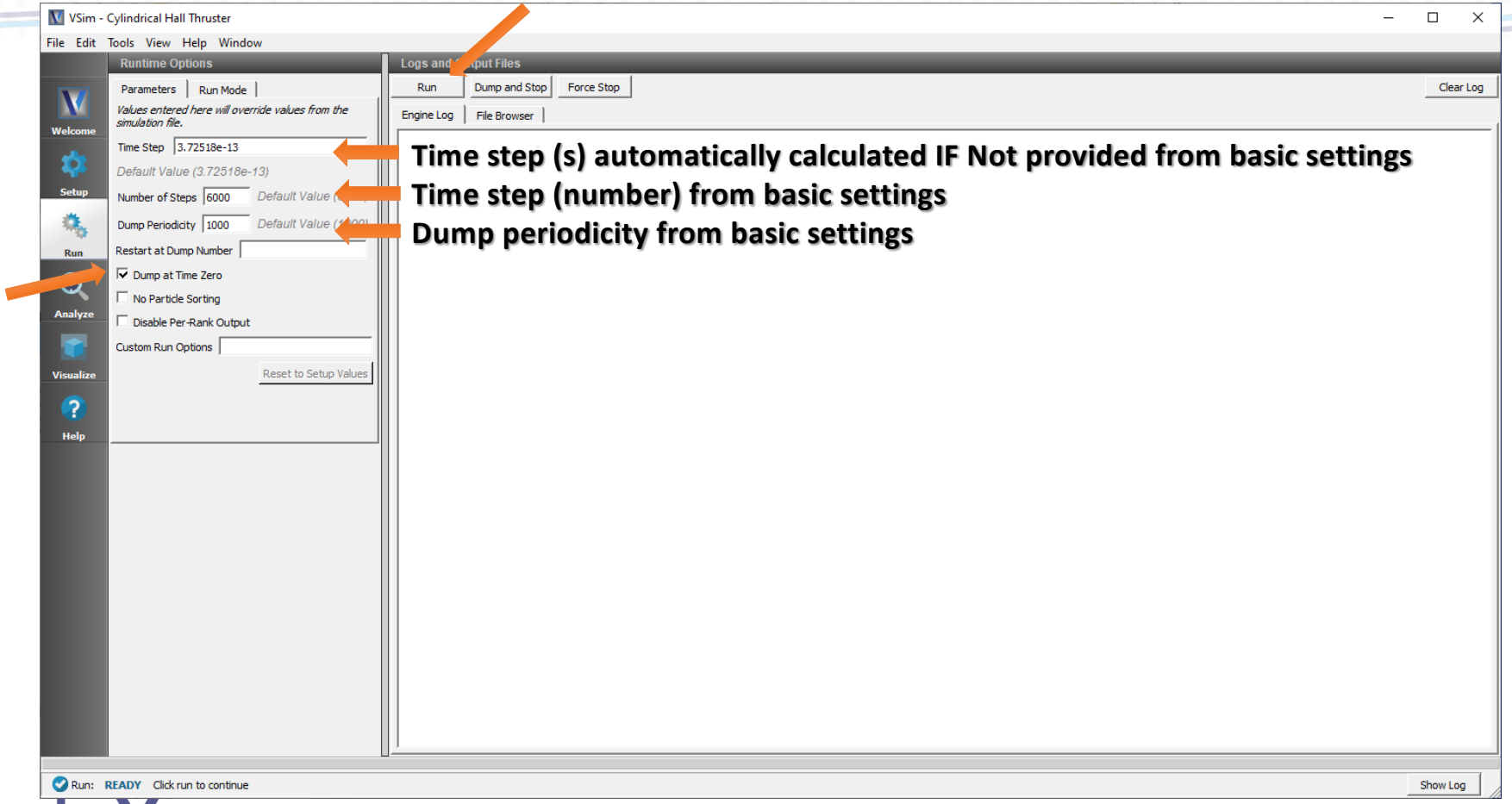


Text-Based and Visual Side-by-Side

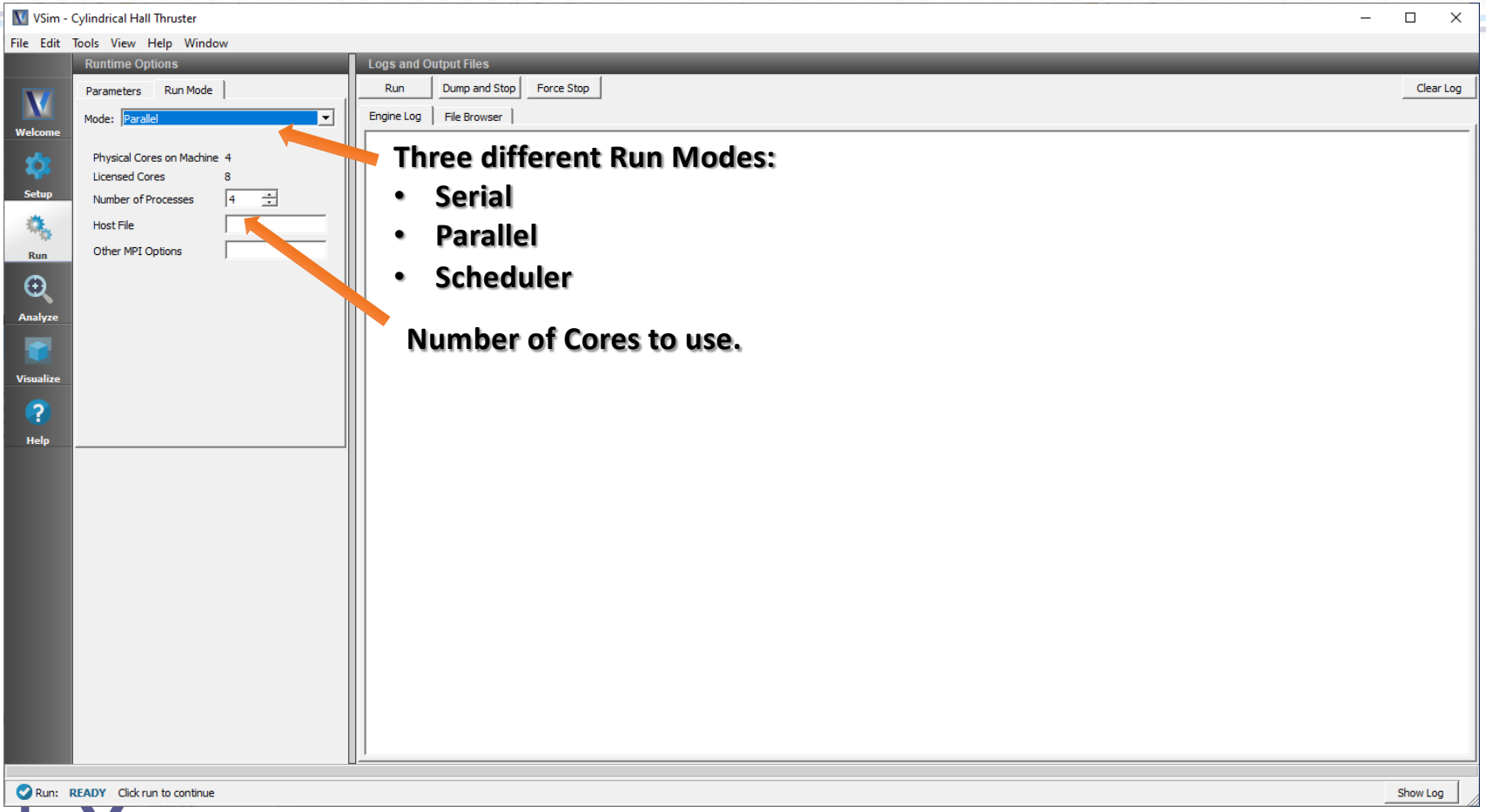



```
<XSim Block>
 -basic description of simulation

<XVars Block>
 -sets the knobs you can turn w/out making big changes to simulation

$ Constants & $ Variables
 -built-in (mathphys)
 -Simulation variables: dump periodicity, NPIM, particle depositors
 -Grid: beginning, end, number of cells
 -physics: debye length estimate, cyclotron frequency, thermal velocity...

$ imports
 -macros, verbosity...

<Grid Block>
 - cylindrical/cartesian
 - variable/uniform

<Decomp Block>
 -usually boring, but lets you manually assign MPI distribution of grid to CPUs

<Multifield>
 -Sets up fields and how they are updated (includes setting up the solver)
 -E, B, rho, phi
 -Boundary Conditions
 -Types of Fields: Edge, Nodal (used to push particles), Face
 -This is generally the 'work-horse/heavy-lifting/beefiest' block

<Species> & <Fluid>
 -Adds particle species or fluid background gas to simulation
    -either explicity modeled kinetically, or implicitly modeled as background fluid
 -Sets up sources and sinks
 -Also can be a heafty block

<Monte Carlo Interactions>
 -sets up particle interactions
 -can set cross-sections from external data files (Hayashi, Tedl, and others)

<Histories>
 -Data to be recorded at every time step
 -Currents into/out of surface, number of particles, field at a point
 -lots of options
```

Running the Simulation



Running the Simulation

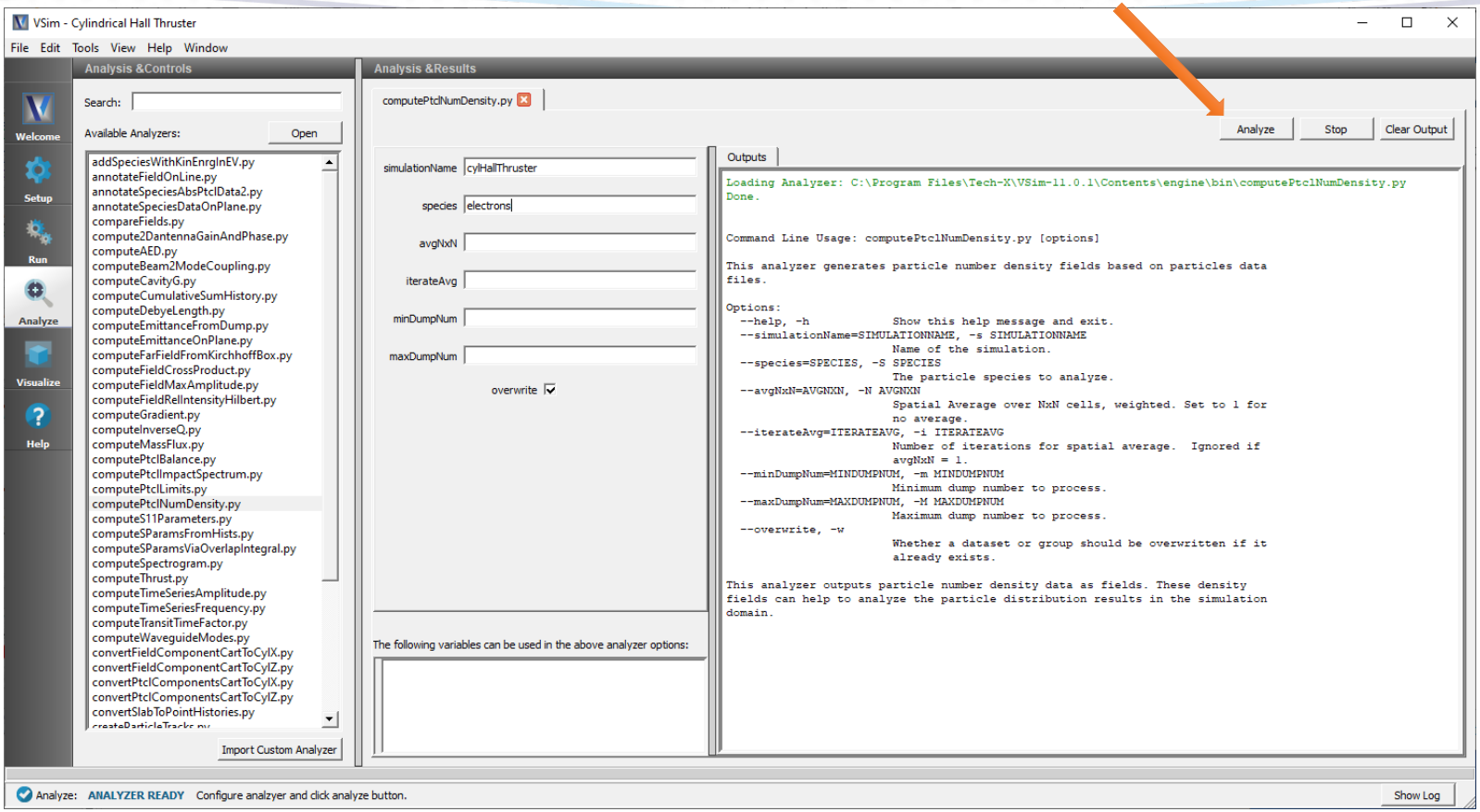


Analyzing Results

Click Analyze button at the top right

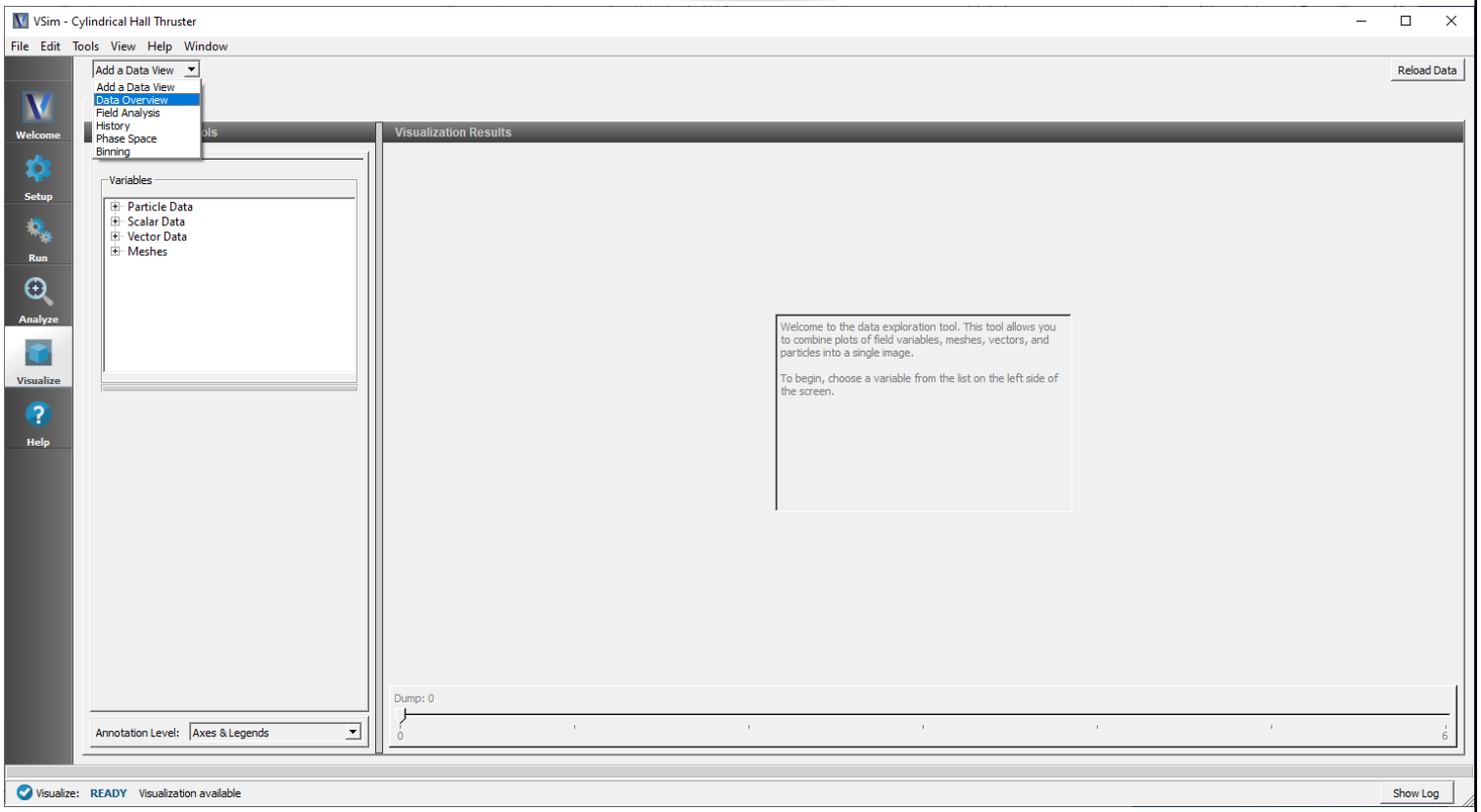
Analyzers, written in python may be used to calculate a variety of items. Custom scripts may be imported for easy use and access.

In this case, computePtclNumDensity.py is being used to calculate the density of the electrons (or ions). To calculate the density of the electrons, set the speciesName to “electrons”.

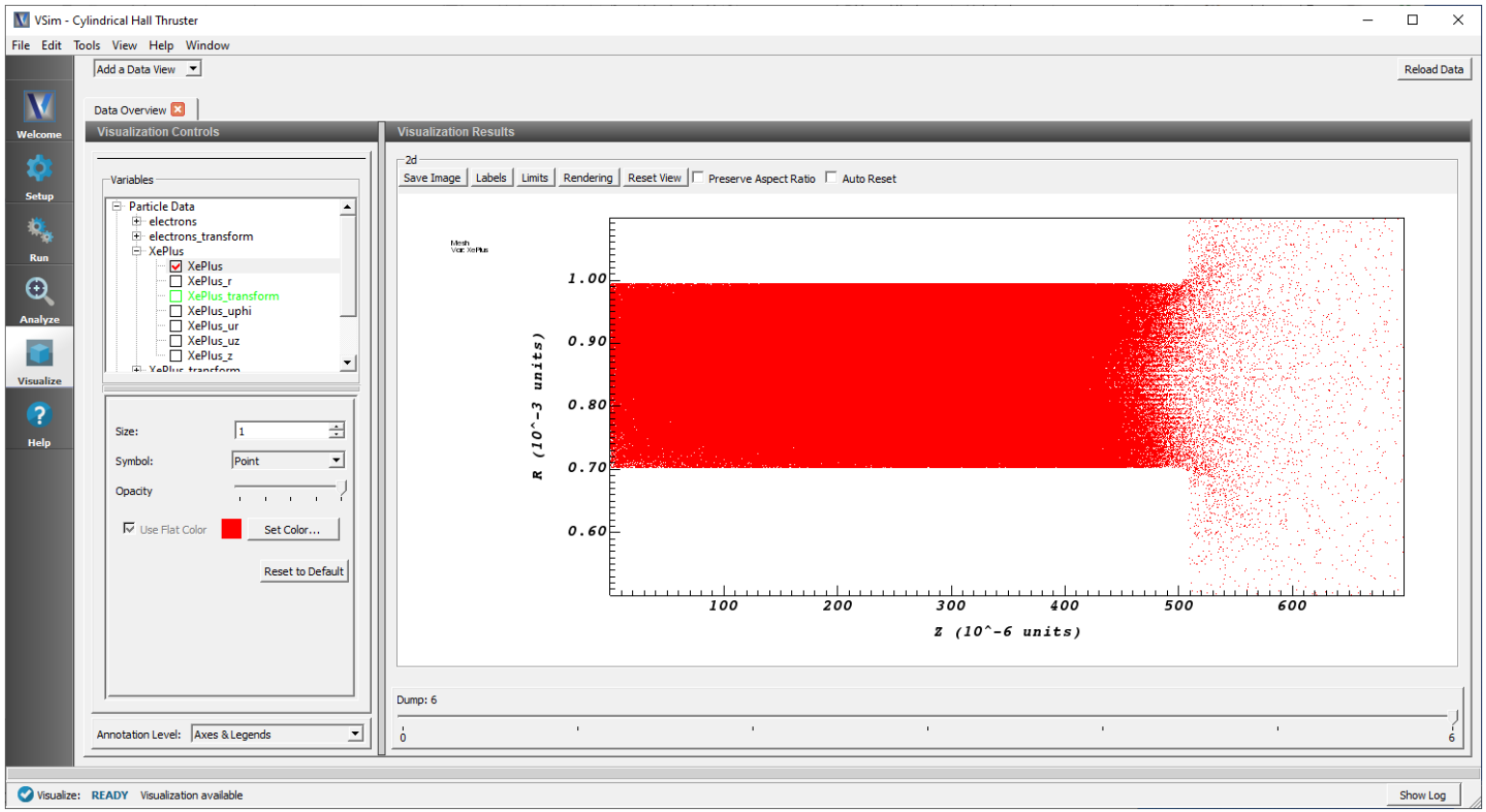


Visualizing Results

1. Data Overview
2. Field Analysis
3. History
4. Phase Space
5. Binning



Data Overview



Field Analysis