
VSim Installation and Release Notes

Release 9.0.2-r2448

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Nov 29, 2018

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OVERVIEW

This guide shows how to customize VSim [*VSi*], the arbitrary dimensional, electromagnetics and plasma simulation code, to add macros and analyzers.

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.

INSTALLATION DETAILS

2.1 What is Installed with VSim?

Upon completing the installation process (described in *VSim Installation Instructions*), VSimComposer, the VSim Computation Engine, Python, and MPI will be installed on your computer. These are described in detail below.

2.1.1 VSimComposer

VSimComposer is a graphical user interface for

- Creating and editing VSim input files
- Executing VSim
- Analyzing VSim generated data
- Visualizing VSim generated data
- Viewing the documentation.

The VSimComposer editor and validator have built-in functions and graphical components that help you to create input files. Example input files, ranging in complexity from beginning to advanced, are included with VSimComposer. New VSim users can use these examples as templates. Advanced VSim users can use VSimComposer to validate the syntax of their own input files, whether their files have been created using VSimComposer or by using a text editor.

The VSimComposer Run pane invokes the VSim engine with user definable settings for number of steps, number of data dumps, and restart file, if any. It also allows selection of serial versus parallel VSim.

VSimComposer now allows selection of analysis programs, either supplied with VSim or user written.

The visualization in VSimComposer is provided by the graphical analysis tool **VisIt** (see <https://wci.llnl.gov/codes/visit/>). VisIt is embedded within VSimComposer. Data generated by VSim or by analysis programs automatically appears in the Visualization pane.

All documentation can be seen from within VSimComposer, fully cross-referenced.

2.1.2 VSim Computational Engine

The VSim computational engine runs both as a serial (vorpalsr) and parallel (vorpall) application for multi-processor / multi-core systems that support MPI. VSim now comes in the specialized VSim packages. The VSim computational engine is embedded within VSimComposer.

2.1.3 Python

Python is an open-source, interpreted scripting language managed by the Python Software Foundation. For more information about Python (See <http://www.python.org/>).

VSIm uses Python to process input files, allowing users to set up simulations with math functions, variable substitutions, and macros.

VSIm uses its own embedded version of the Python interpreter to pre-process input files and execute any Python code in an input file.

2.1.4 MPI

The Message Passing Interface (MPI) is an application programming interface (API) for communicating between processes that execute in parallel. There are many implementations. The Linux and Mac versions come with the OpenMPI (See <http://www.open-mpi.org/>) implementation of MPI. The Windows versions come with the Microsoft MPI implementation. The appropriate MPI implementation is embedded within VSImComposer.

More Information

More information about VSIm can be found at the VSIm Product Website (<https://www.txcorp.com/vsim>). Send questions about installing or running VSIm to Tech-X Customer Support at support@txcorp.com. For technical questions about the physics, users may wish to email the VSIm discussion list (<https://ice.txcorp.com/mailman/listinfo/vorpal-users>). Extensive assistance in the use of VSIm or simulation in general is available from Tech-X Professional Services. Please contact Tech-X directly for sales, consulting, and other questions at sales@txcorp.com.

2.2 VSIm System Requirements

VSIm runs on 64-bit Windows, Linux, and Mac and has installation procedures that users will be familiar with on their respective operating system. Some of the systems supported are:

- Windows 7, 8, 10, Server 2008 R2, Server 2012
- Linux distributions with glibc 2.11.3 or later (verified on Fedora/RedHat/CentOS, SUSE, Ubuntu)
- A compatibility version will support Linux distributions with glibc 2.5 or later (verified on CentOS and Ubuntu)
- Mac OS X Yosemite, El Capitan, Sierra, and High Sierra
- Cray XC30

Note: The version of glibc can be found with the command: `ldd -version`

The VSIm serial engine (vorpalsr) is available for running on single processor workstations. The VSIm parallel engine (vorpals) is provided for multi-core systems that support the Message Passing Interface (MPI). There is support for running VSIm simulations on Linux clusters with common job schedulers as well as running with the “Windows Clustering” server technology.

VSIm is licensed per compute platform, which may be a workstation or a cluster. For a workstation, creating a license requires the MAC (hardware) address.

A cluster is defined to be “A dynamic collection of compute nodes sharing a common filesystem and a single common queuing system.” For a cluster, all nodes be able to determine their own hardware (or MAC) address and hostname. For a cluster, we also require that there is a method available from each compute node that can determine the list

of compute nodes from the queuing system given to us by the customer. If the customer wants the capability to dynamically change the size of the cluster after licensing, then we require that the compute nodes be able to remote-shell-connect to each other. If a job is running on a collection of nodes, any one of which is licensed, and all of which can see the shared filesystem and are in the nodes list from the queuing system, then we consider the job to be running on the licensed cluster. Otherwise, if one or more job nodes can reach one the licensed nodes and can validate it, and all of the nodes can see the shared filesystem and are in the nodes list from the queuing system, then we also consider the job to be running on the licensed cluster.

VSim is highly scalable, and has been developed to solve the most challenging computational electromagnetics problems of our time. Some example calculations, particularly for plasma acceleration, require a supercomputer to run adequately in 3D, though VSim desktop users may explore how the files work by running them in 2D. Some microwave device examples, such as our Helix Traveling Wave Tube Power Run, could require 12GB RAM or more to run. However, it is possible to set up an input file at lower resolution if you have limited resources.

The VSim 9 Windows installer is around 350MB, and requires around 1.2GB of disk space to install. The Linux installer is slightly over 1GB due to the inclusion of additional system packages, and unpacks into around 2.7GB. Please ensure you have enough additional space to run your simulations.

The visualization in VSim uses OpenGL and requires optimal graphics drivers. The standard Linux distributions may not come with drivers written by the graphics-card manufacturer, which are necessary for full hardware acceleration. You should download and install the latest driver for your graphics card from your graphics card vendor's website. In the case of an NVidia graphics card, you can get the latest driver by going to NVidia's website, selecting the Download Drivers link, and then selecting the Linux Display Drivers link.

The application has a minimum size that does not work well below the resolution of 1280x800 pixels or XVGA. Smaller resolutions will start to lose parts of the user interface of the application.

VSim has GPU computing capability based on the NVidia CUDA Toolkit, currently at version 9.1. This is supported only on 64-bit Linux and 64-bit Windows. One does not need a CUDA-enabled graphics card to use VSim unless the GPU capability is invoked, but if a simulation is configured to run on the GPU, then the graphics card must have CUDA capability and a driver that is compatible with version 9.1 of the toolkit.

Note: To use the GPU capability of VSim, you will need a CUDA-enabled GPU card with a driver that is compatible with the CUDA Toolkit version 9.1. Downloading the developer toolkit is not needed, just the driver, but if you do download the CUDA Toolkit (see <https://developer.nvidia.com/cuda-downloads>, then it will guarantee your driver is compatible.

For large parallel simulations running across nodes in high performance cluster, there are some requirements that can worked out easily with system administrators and depend on the details of the cluster configurations. In general, we don't recommend running VSim on AFS file systems.

Note: The Andrew File System (AFS) is not recommended to run VSim in parallel. The distributed AFS system is optimized for location-transparency over a wide area network rather than the low-latency conditions necessary for high performance in cluster storage. File systems such as Lustre or the General Parallel File System (GPFS) perform better when running VSim.

For installation instructions see: [VSim Installation Instructions](#)

2.3 VSim Installation Instructions

These are instructions on installing the VSim product. Please see the [VSim System Requirements](#) first to make sure your system meets the requirements. There are special instructions for versions of MacOS from El Capitan and later.

2.3.1 Windows VSIm Software Installation

The VSIm distribution package for 64bit Windows is a self-extracting executable installer. Invoke the installer by double clicking on it. The default installation path is:

```
C:\Program Files\Tech-X (Win64)\VSIm-9.X
```

where X is the minor version of your software. To open the VSIm software, go to the Start Menu, click on the Tech-X folder, click on VSIm 9.X, then click on VSImComposer. See Fig. 2.1.

2.3.2 Windows VSIm Software Installation Using a Windows Network Location

These instructions outline how to install VSIm to a shared network location. This method will allow users from multiple machines to access and run this installation of VSIm on their local machines.

To start, you must have a shared network location that you intend to install to. To do this, locally navigate to the location you wish to install to. Right click the target folder and select properties. A window will appear. Select the “Sharing” tab near the top of the window. Click Share and set the permissions appropriately.

Now that this folder is accessible, install to the folder by following the Windows Installation instructions, using the shared location as your installation location. This can be done from the machine where VSIm is being installed, or from another machine with access to the shared folder.

In order to run VSIm from a network location, it is best to map the shared network location to a network drive on any machine where VSIm may be run. To do this, simply right click the shared network drive on the machine where VSIm will be run and select Map Network Drive. At this time you will be prompted to select a drive letter and change settings. Change the settings as desired and press Finish. The user should use this path rather than the Network path when starting VSIm. When running VSIm from a shared network location, we suggest using the VSIm executable directly by navigating to:

```
Contents\bin\VSImComposer.exe
```

For convenience, a shortcut can be made on the machine in which VSIm is run. Ensure that the shortcut uses the mapped network drive.

To ensure all users have access to the license, the license should go in:

```
Contents\engine\bin\
```

inside the installation of VSImComposer.

2.3.3 Linux VSIm Software Installation

The VSIm distribution package for Linux is a gzipped tarball. Unpack the gzipped tarball into the directory in which you wish to install VSIm. A typical location would be

```
/usr/local/VSIm-9.0
```

The unzip and untar command is

```
$ cd /usr/local
$ tar xf VSIm-9.0.0-Linux64.tar.gz
```

Or, if your Linux machine does not have OpenGL rendering support then you may want to install the “offscreen” version, in which case the file would be “VSIm-9.0.0-Linux64-offscreen.tar.gz. After untarring, the user interface is started with the command:

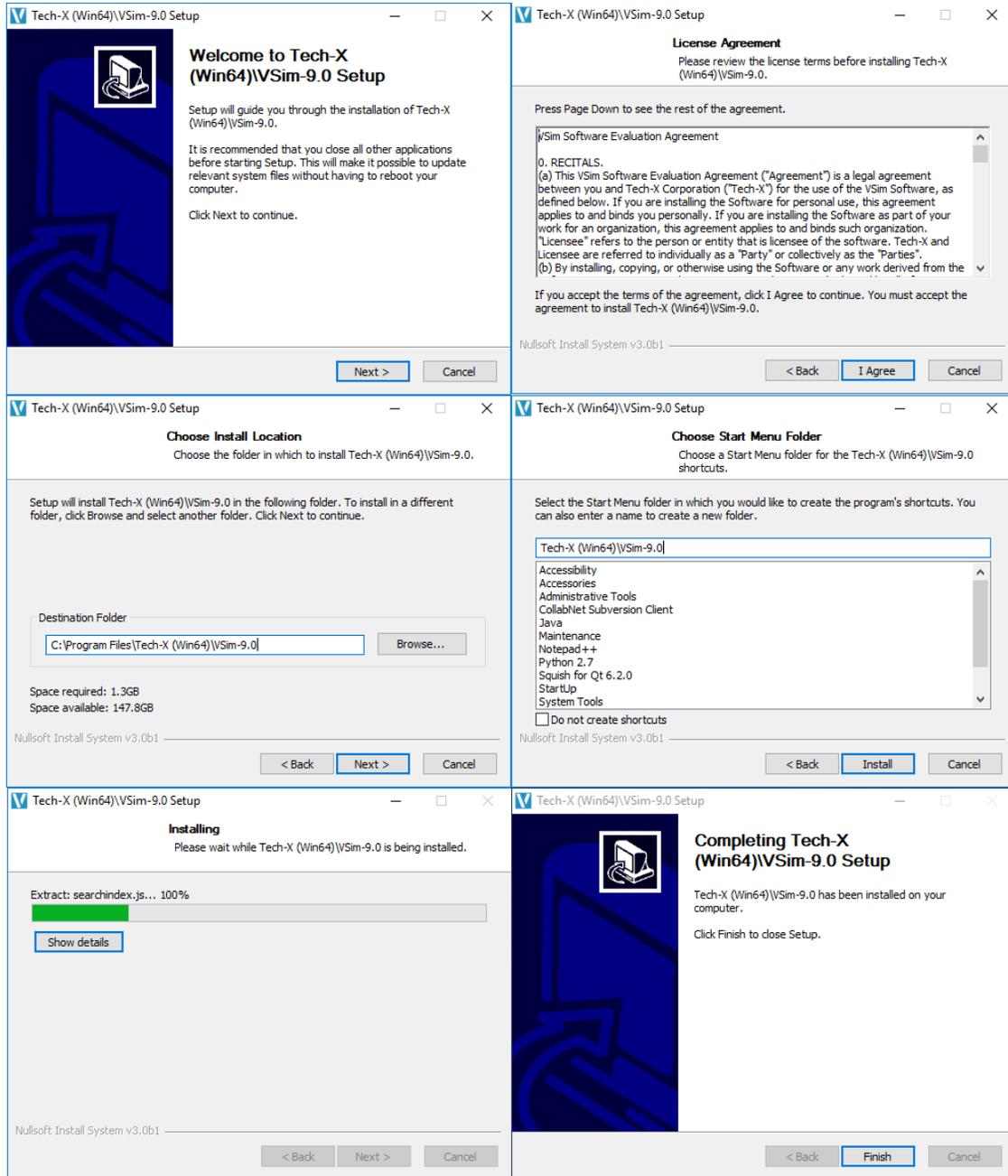


Fig. 2.1: Dialogs for Windows installation

```
$ cd VSIm-9.0
$ ./VSImComposer.sh
```

If you plan to run the simulation engine or any other executable from the command-line then you will need to source the startup script:

```
$ source /usr/local/VSIm-9.0/VSImComposer.sh
<execute engine, analyzers, etc.>
```

See VSIm User Guide: Running Vorpak from the Command Line for more instructions on command-line operations.

2.3.4 Mac OS X VSIm Software Installation

MacOS Yosemite or previous Users:

The VSIm distribution package for Mac OS X is a .dmg installer. Invoke the installer by double clicking on it. Drag the VSIm-9.0 folder into your Applications folder (visible in the installer window). From the Application folder, double click on the VSImComposer icon in the VSIm-9.0 folder. See [Fig. 2.2](#). This default installation path is:

```
/Applications/VSIm-9.0
```

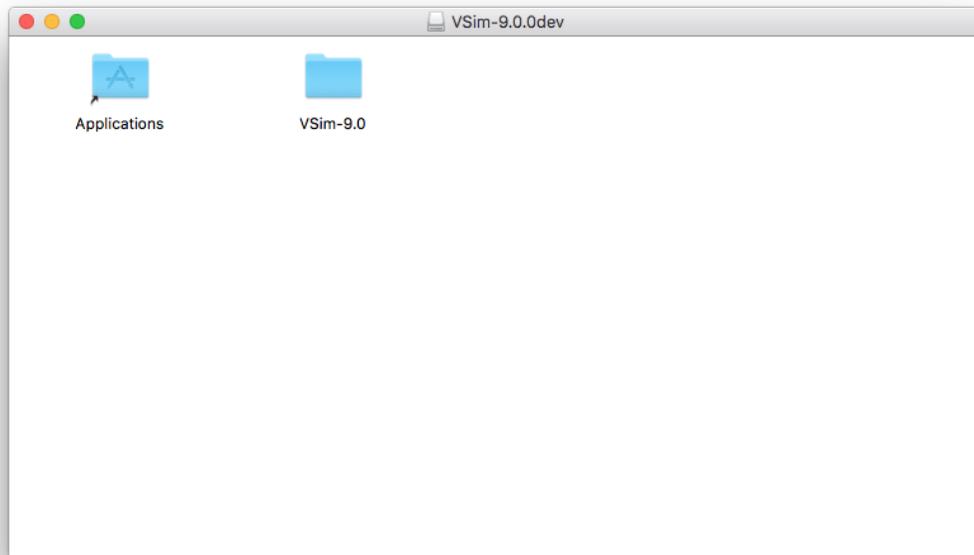


Fig. 2.2: Dialog for the Mac installer

MacOS El Capitan and later Users:

As of El Capitan, Apple instituted GateKeeper, which by default prevents one from executing an unsigned application. The symptom can range from inability to install a license to being told the application is damaged as shown in [Fig. 2.3](#).

If you get to this point, you must start over:

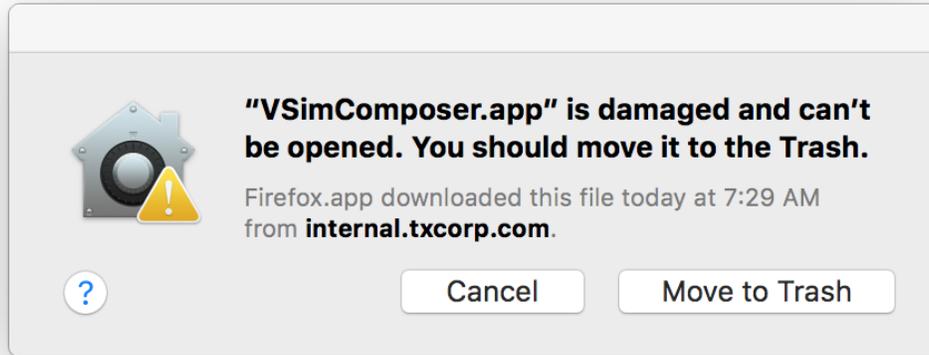


Fig. 2.3: Warning that VSImComposer is damaged, put up by GateKeeper.

Enabling just VSImComposer (works for 9.0.0)

- Make sure you have deleted ALL instances of the version of VSIm that you are about to install, including desktop icons.
- Unmount any VSIm installer disk image.
- Double click on the VSIm installer disk image to mount it.
- A window should open up that shows your Application folder and a VSIm-9.0 folder.
- Drag the VSIm-9.0 folder into the Applications folder.
- In a terminal window, run:

```
sudo spctl --add /Applications/VSIm-9.0/VSImComposer.app
```

- Run VSImComposer from inside the Applications folder.
- You should now be able to add a VSIm license.

Disabling GateKeeper, installing, then re-enabling GateKeeper (works for 9.0.1)

- Make sure you have deleted ALL instances of the version of VSIm that you are about to install, including desktop icons.
- Unmount any VSIm installer disk image.
- Disable GateKeeper

```
sudo spctl --master-disable
```

- Go to System Preferences → Security & Privacy, and make sure that *Anywhere* is selected under *Allow apps downloaded from:*. If it is not, unlock (bottom left corner button) and select it.
- Double click on the VSIm installer disk image to mount it.
- A window should open up that shows your Application folder and a VSIm-9.0 folder.

- Drag the VSIm-9.0 folder into the Applications folder.
- Run VSImComposer from inside the Applications folder.
- You should now see [Fig. 2.4](#).

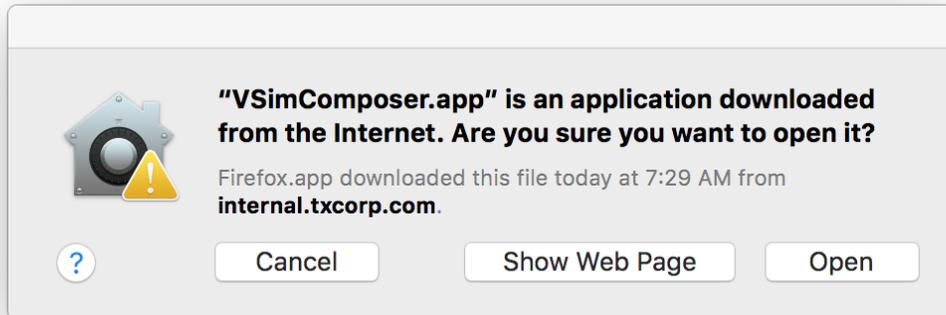


Fig. 2.4: Warning that VSImComposer was downloaded from the internet, put up by GateKeeper.

- Press *Open*.
- You should now be able to add a VSIm license.
- Re-enable GateKeeper

```
sudo spctl --master-enable
```

Errors

If you open VSIm and get a message saying “License File Not Found”, make sure that the path for your license starts with:

```
/Applications/VSIm-9.0/...
```

If not, start over.

If you are still not allowed to open VSImComposer.app, you may be able to fix this by going to System Preferences → Security & Privacy, unlocking, and if you see “VSImComposer.app was blocked ...”. Press *Open Anyway*.

2.4 VSIm Documentation

In addition to this PDF version of the VSIm documentation, all of the documentation is accessible from within the VSImComposer interface, as well as online at the Tech-X web site, [VSImDocumentation](#).

2.4.1 VSIm Installation

VSIm Installation Instructions guides the user through the installation process for VSIm. Release notes are also provided in this document.

2.4.2 VSIm User Guide

VSIm User Guide contains comprehensive VSIm documentation, including directions for running VSIm from the command line support resources. When you are ready to create your own simulation, consult this document for in-depth information about VSIm features.

2.4.3 VSIm Examples

VSIm Examples provides numerous tutorials for both beginning and advanced VSIm users.

2.4.4 VSIm Customization

VSIm Customization discusses macros and analyzers in further detail, for users who would like a higher degree of customization in their simulations and postprocessing.

2.4.5 VSIm Reference

VSIm Reference is a quick-reference manual for VSIm users to look up specific VSIm features and code block syntax for use in editing a VSIm input file.

2.4.6 Searching the Documentation

All documentation is available through the VSImComposer itself by clicking on the **Help** icon on the far left or by going to the top menu bar and selecting *Help* → *Help Contents*.

The *Search* field in particular is a fast way to find terms and examples, and supports the following options:

- Wildcard search

Use an asterisk * to represent a sequence of characters such that the term you entered can either be the whole or a part of the results displayed. For example:

- Searching for “process*” will display “process” as well as results like “processes”, “processing”, etc.
- Searching for “*process” will display “process” as well as results like “postprocess”, “preprocess”, etc.
- Searching for “**process*” will display “process” as well as results like “preprocessed”, “postprocessing”, etc.

- Omit words You can omit words in your search by putting a minus - sign in front of the word to omit. For example, typing “cylindrical -coordinates” would omit results that contain the word “coordinates”, so your results would only include terms like “cylindrical capacitor”, etc.

All searches are case insensitive.

2.5 VSIm Release Notes

The release notes describe new features for the VSIm computational engine (Vorpal) and the VSImComposer graphical user interface. Deprecated features and bug fixes are also noted within the release notes.

2.5.1 New and Updated VSim 9.0 Features

VSim Computational Engine (Vorpal)

A new reaction framework that has more and faster reactions was implemented. The speed of the new reaction framework comes from implementing the no-time-counter algorithm.

Previous reactions implemented with this new capability are

- elastic collisions
- charge exchange collisions electron ionization
- impact ionization
- field ionization
- recombination (e.g., $H^+ + e^- \rightarrow H$)
- 3-body recombination (e.g., $H^+ + e^- + e^- \rightarrow H + e^-$)
- electron impact dissociation (e.g., $H_2 + e^- \rightarrow H + H + e^-$)
- excitation (e.g., $H + H/e^- \rightarrow H^* + H/e^-$)
- dissociation (e.g., $H_2 + H/e^- \rightarrow H + H + H/e^-$)
- electron attachment (e.g., $H + e^- \rightarrow H^-$)
- negative ion detachment (e.g., $H^- + H/e^- \rightarrow H + e^- + H/e^-$)

New reactions are

- dissociative ionization (e.g., $H_2 + e^- \rightarrow H^+ + H + e^-$)
- dissociative recombination (e.g., $H_3^+ + e^- \rightarrow H_2 + H$)
- general inelastic binary reaction with 2 reactants \rightarrow 2 products, momentum conserved, and a specified energy lost. (e.g., $H_2 + H_2^+ \rightarrow H_3^+ + H$)

In addition, field ionization removes the ionization energy from the field.

One can now specify the species in fluid and particle blocks by element name, which sets the mass, charge, ionization energy, and excitation energy. Once a predefined species has been set, it is ready to be used within the rxn framework. In addition, these properties can be defined for a custom species with (species=custom) in the ptcl/fluid block. Further, one can still override the values for any species, e.g., select Hydrogen but set its ionization energy to be different from 13.8 eV.

The secondary emission process was generalized so that the impact of any species on a wall can lead to the emission of itself or any other species. (In the prior implementation, the allowance of secondary emission was determined by the order of appearance in the input file.) The user now has some control over secondary particles, including customizable weighting and tagging, as well as correlated secondary emission of multiple species.

Memory usage was reduced for electromagnetic simulations.

The computation of surface fields at boundaries was improved, making the motion of particles more accurate, even in cells that overlap the boundary.

Slab histories with reduced communication and memory usages were developed, enabling larger simulations on multi-core CPUs.

The methodology for second-order dielectric updaters with conformal boundaries and dispersion was developed and implemented.

Restarts were enabled for simulations with grid boundaries having cuts at domain boundaries.

All random processes can be controlled by a seed.

There are now emitter diagnostics that record individual particle data of emitted particles as well as sums and averages over all particles emitted in each time step.

More robust cut-cell absorption with optional diagnostics recording the absorption location, the surface normal at that location, and the exact time of absorption.

For variable weight particles, collisions now demonstrate the correct collision frequency based on the supplied cross-section (with version 9.0.1)

VSim Analyzers

All analyzers updated to a common interface to reduce the need to look up certain individual properties.

Custom analyzer development was simplified through restructuring so that basic services (file reading, options) flow automatically.

New analyzers:

- S Parameters from History (computeSPParamsFromHists.py)
- S Parameters from Overlap Integral Calculation (computeSPParamsViaOverlapIntegral.py)
- Compute Geometry Cavity Merit Factor G (computeCavityG.py)
- Extract Modes via Operator (extractModesViaOperator.py)
- Compute Accelerating Voltage and Transit Time of a Cavity Mode (computeTransitTimeFactor.py)
- Create Field Data on an Unstructured Mesh Representing Surface Geometry (putFieldOnSurfaceMesh.py)
- Annotate fieldOnLine history files (annotateFieldOnLine.py) (added back in 9.0.2)
- Generates particle number density, and associated fields based on particles stored in history data files (annotateSpeciesAbsPtclData2.py) (added back in 9.0.2)
- Sum a history, for example to get a total charge from a current measurement (computeCumulativeSumHistory.py) (added back in 9.0.2)
- Computes the emittance as a bunch travels through the simulation (computeEmittanceFromDump.py) (new in 9.0.2)
- Computes the emittance as a bunch travels through the simulation on a plane (computeEmittanceOnPlane.py) (new in 9.0.2)
- Computes history output containing maximum and minimum particle coordinates for each timestep (computePtclLimits.py) (added back in 9.0.2)
- Computes spectrograms from time-series data in history files (computeSpectrogram.py) (added back in 9.0.2)
- Converts XYZ particle data around the x axis to cylindrical components (convertPtclComponentsCartToCylX.py) (added back in 9.0.2)
- Converts XYZ particle data around the z axis to cylindrical components (convertPtclComponentsCartToCylZ.py) (added back in 9.0.2)
- Creates data files with containing particle paths over time (createParticleTracks.py) (added back in 9.0.2)
- Reads in a single H5 file for a particle species and exports it as a text file or as a sequence of text files (exportSpecies.py) (added back in 9.0.2)
- Performs arithmetic operations on two histories from the same simulation and writing to a third history (performTwoHistoryArithmetic.py) (added back in 9.0.2)

The following analyzers were removed:

- addPtclComponentKEeVx.py
- addPtclComponentKEeVy.py
- addPtclComponentKEeVz.py
- calculateEmittance.py
- calculateFieldMaxAmplitude.py
- computeFarFieldFourierComponent.py
- computeFieldCrossProduct.py
- computeLineIntegral.py
- computeSurfaceFlux.py
- getFieldComponentsOnPlane.py

VSimComposer

The input file is now generated more quickly. Status messages have been expanded to give more detail. The Run Panel was restructured to allow all parameters to be visible at once, and to show the VSim recommendation for certain parameters, such as the time step. The Analyze Panel was restructured to allow several analyzers to be open at once, with separate output windows for each.

Visual Setup generalized to allow easier specification of many simulation parameters:

Basic Settings

- Phase shift boundary conditions
- Easier switching between 2D and 3D simulations
- Decomposition direction specification
- Dump in groups (for use by extract modes by operator)
- Suppress dumps of certain fields

Fields

- Expanded options for Linear Solver
- 2nd order dielectrics, up to 9 dielectrics
- Feedback driven ports
- Import external VSim and function defined fields

Particles

- Charge accumulation particle boundaries
- Partial transmitter particle boundary
- Diffuse reflector particle boundary

- Monte Carlo interactions
- Particle load From file

Collisions

- Background gas can be a fluid
- Specification of Charged Particles by species name as an option
- Managed weight particles weight setting

Histories

- Accelerating Voltage and Field Slab History

Space Time Functions

- Feedback SpaceTimeFunctions can now use absorbed particle current histories as the feedback history. (with version 9.0.1)

VSIM Documentation

The documentation was rewritten and expanded. There are now five manuals, VSIM Installation, VSIM User Guide, VSIM Examples, VSIM Customization, and VSIM Reference. The User Guide contains an extensive section on the basic concepts of simulation.

VSIM Examples

VSIM examples contains many new examples, in particular concerning photonics and plasma discharges. In detail:

- a6Magnetron1Modes.sdf
- a6Magnetron2Power.sdf
- arrayedWaveguideGrating.sdf
- cylFiber.sdf
- cylindricalWaveguide.sdf
- dielectricWaveguide.sdf
- dielectricWaveguideMode.sdf
- dipoleOnConductingPlane.sdf
- microringResonator.sdf
- microringResonatorMode.sdf
- pillboxCavity.sdf
- singleParticleCircularMotion.sdf
- antennaOnHand.sdf (new in 9.0.2)

One example was removed (advancedDipoleAboveConductingPlane.sdf).

VSim Distribution and Licensing

Installers and installations reduced in size.

2.5.2 VSim 9.0 Bug Fixes

VSim Computational Engine (Vorpal) Bug Fixes

- Collisions between a single species were occurring at a factor of 2 too often, this has been fixed and the reactions have been validated (with version 9.0.1)
- Accuracy of reaction rate improved for nearly mono-energetic collisions (with version 9.0.2)
- Power law and exponential polynomial cross-sections have improved documentation and performance (with version 9.0.2)
- Bug fix in reactions using fluids with moving window (mainly laser ionization) for parallel artifacts (with version 9.0.2)
- Reactions of fluids with or resulting in variable weight particles now have more accurate results and flexibility by introducing new attribute to fluids - numMacroPPCRxns - that determines how many equivalent macro particles per cell are used for the fluids within reactions. For variable weight, this determines the maximum number of macroparticles that could result from the reaction in each time step. (with version 9.0.2)

Visual Setup Bug Fixes

- Corrected potential bug in update period specification for reactions framework (with version 9.0.1)
- Improved partial pre-processing for reactions and monte carlo interactions (with version 9.0.1)
- Corrected improper warning message with MAL boundaries (with version 9.0.1)
- Allowed assignment of non-expression space time functions for relative density particle loaders (with version 9.0.1)
- Automated interpolation for proper particle loading on cylindrical grids (with version 9.0.1)
- Enabled right click assignment of constants and parameters to strings when the default value is a string (with version 9.0.1)
- Removed unused menu item (with version 9.0.1)
- Fixed bug where external help window would block composer window (with version 9.0.1)
- Fixed bug where Analyzer lost focus when set to default (with version 9.0.1)
- Fixed name of starting run log file (with version 9.0.1)
- Fixed bug where removed stfuncs would still be listed (with version 9.0.1)
- Fixed bug where stfuncs could be removed while being referenced (with version 9.0.1)
- Fixed composer freezing if translator could not be found (with version 9.0.1)
- Improved speed of loading SDF files (with version 9.0.2)
- Fixed issues with “Abort Setup” button (with version 9.0.2)
- Prevented crash when changing the name of variable to pre-existing variable name (with version 9.0.2)
- Improved usability of long item lists in the right click context menu of the setup properties (with version 9.0.2)
- Improved usability of save dialog (with version 9.0.2)

- Fixed issue with new setup tree items having the same name as a previous item (with version 9.0.2)
- Fixed bug in certain analyzers on Windows (with version 9.0.2)
- Added more time logging when opening files (with version 9.0.2)
- Made importing STP files faster (with version 9.0.2)
- Fixed bug where unselected shapes were not made invisible (with version 9.0.2)
- Centered default values of lineout intercepts (with version 9.0.2)
- Fixed bug so that window title bar updates when shortDescription is changed in a text-based simulation (with version 9.0.2)
- Ensured user chosen histories are respected when reloading data (with version 9.0.2)
- Fixed bug where variable names inside expressions in setup were not updated when the variable name was changed (with version 9.0.2)
- Allowed user setting of temporary directory (TMPDIR) to address issues when the default directory is too long (with version 9.0.2)
- Fixed bug with disable of “Save and Setup” button when a run is canceled (with version 9.0.2)
- Fixed issue with loading sdf files with arrays of constructive solid geometry in them (with version 9.0.2)
- Fixed bug with pseudo potential and accelerating voltage histories in electrostatics (with version 9.0.2)
- Added verification that dielectric materials are not used in electrostatic simulations (with version 9.0.2)
- Enabled field imports for 2D simulations (with version 9.0.2)
- Bug fix to include cylindrical axis only if necessary (with version 9.0.2)
- Bug fix for partial Neumann boundary conditions had wrong offset in some situations (with version 9.0.2)
- Added of PEC Normal Basic Setting to select the normal of PEC materials. This feature is useful for CAD imports that may have a reversed normal from expectation. (with version 9.0.2)
- Added option to include effects of unmodeled photons in decay reactions (with version 9.0.2)
- Allowed binary combination histories to be used in feedback functions (with version 9.0.2)
- Changed default parameters of electrostatic solvers to more commonly used values (with version 9.0.2)
- Clarified basic setting of how a Perfect Electric Conductor is assigned to a shape (with version 9.0.2)

2.5.3 New and Updated VSim 8.2 Features

The following features are new or have been updated for the 8.2.0 release.

VSim Computational Engine (Vorpal)

- Added a new Monte-Carlo elastic collision algorithm with threshold energy functionality
- Removed assumption in elastic collisions of first incoming particle being light compared with second incoming particle with the result being energy conservation in the collisions of particles of similar masses.
- Fixed memory leaks with some histories on long runs

VSim Graphical User Interface (VSimComposer)

- Removed gstreamer-0.10 requirement on Linux

VSim Macros and Translator

- Capitalization fix in embcs.mac

Other

- Improved general robustness of license management
- Made cluster and node-locked license tokenfile behavior consistent between Vorpai and VSimComposer

2.5.4 Known Issues in VSim 8.2

- Remote VSimComposer does not work * Windows Cluster support was lost with upgrade to MPI on windows needed for certain simulations. * EM Cylindrical not implemented for visual setup * Occasionally, for parallel runs, the stl reader can spuriously set some regions outside of objects to being inside. When this happens, it is manifest in the visualization of the corresponding geometry field in Data Overview. In all cases observed so far, this has been fixed by offsetting the grid a small amount, changing the number of cells, and/or changing the number of parallel processes.

2.5.5 New and Updated VSim 8.1 Features

The following features are new or have been updated for the 8.1 release.

VSim Computational Engine (Vorpai)

- Scattering processes added for antimony (Sb), including electron-electron scattering
- Added transport and emission from antimony (Sb) using the density of states
- Added model to specify percentage of specular and diffusive emissions
- Added Species kind “bandSpeciesES” to the VSimSD license
- Fixed issues with several command-line arguments including -h and -help
- Improved warnings when improper values are given for simulation parameters
- Fixed issue with line dumping without a name
- Fixed issue where all 3 components of deltaAtBreaks were not checked to determine if the grid is uniform

VSim Examples

These examples now have Visual Setup:

- A Loop Antenna created from a coaxial cable (VSimEM)
- Horn Antenna (VSimEM)
- Patch Antenna Far Field (VSimEM)

- Rectangular Waveguide (VSimEM)
- Electron Gun (VSimMD)
- Gyrotron Mode (VSimMD)
- Helix Traveling Wave Tube 1: Dispersion (VSimMD)
- Helix Traveling Wave Tube 2: Impedance and Attenuation (VSimMD)
- Helix Traveling Wave Tube 3: Power Run (VSimMD)
- 2D Magnetron (VSimMD)
- Multipacting Resonance in Waveguide (VSimMD)
- Multistage Collector (VSimMD)
- 3D Stripline Multipacting (VSimMD)

Other example features include:

- Updated examples to take advantage of new macro functionality
- Added the numerical Cerenkov filter option to EM examples
- Improved Photonic Crystal examples

VSim Macros and Translator

- New macro to allow numerical Cerenkov filters in Visual Setup as a parameter of the field solver
- New macro, stfuncs.mac, to handle built-in Space-Time functions including Python file import and feedback
- Added support to set localVelocity parameter off of shape emitters
- Updated the reflecting particle boundary macros to handle rails and corners
- Added history to let user set pseudoPotential by coordinates in addition to via grid index
- Added support for secondary emitters to test particles
- Added support to simplify creation of rectangular and coaxial waveguides
- Added pipe primitive
- Fixed issue with HalfWave Dipole Antenna failing on GPU
- Fixed several issues dealing with handling of cylindrical coordinates
- Improved performance of filters macro
- Improved embcs.mac and VSimEm.mac for a faster implement of MAL boundaries
- Improved particles.mac (support for particle species loader with repeat loading)
- Removed unused macros, unnecessary parameters, and cleaned up referenced inside macros
- Fixed several issues with histories.mac for logging of ptclQty and speciesAbsPtclData
- Fixed issue with parallel restarts on Win10 with CAD geometries
- Fixed issue with specifying name of external magnetic fields
- Better handling of global variables in macros

VSIM Analyzers

- Improvements to data analysis executables
- New analyzer, `exportSpecies.py`, that exports a particle species to a text file or sequence of text files
- New analyzer, `getFieldComponentsOnPlane.py`, to get field components on a plane
- Updated the `computePtcNumDensity.py` analyzer to perform spatial averaging
- Improved `addPtcComponentKEeV.py`, fixing a bug involving mismatched components after multiple runs, adding check on restart, executing dump files in numerical order, better specifying of `KEeV`, `KEeVx`, `KEeVy`, or `KEeVz`, all in one script

VSIM Graphical User Interface (VSIMComposer)

- Improvements to tree-based/visual setup
- Fixed issue in visual setup of current sources, changing field specified from E-Field to a proper J-Field
- Better handling of Space-Time functions in Visual Setup tree
- Added support for Field Scaling Electrons
- Improved Constructive Solid Geometry tessellation and meshing for geometry primitives
- Improved speed of Visual Setup rendering
- Added support for geometries described by Python functions
- Improved expression handling in Visual Setup tree
- Fixed issues with certain plots incorrectly displaying in Visualization Tab
- Fixed automatic scrolling issues in Run and Analyze Tabs
- Added support for scaling and translation of STL files
- Added support for all macro changes above in Visual Setup tree
- Fixes issues with resizing of the grid
- Improved usability and robustness of Visual Setup tree interface
- Improved wildcard searching in Documentation/Help
- Improved searching with omitting terms with minus sign in Documentation/Help
- Reduced the verbosity of search results in Documentation/Help
- Added instructions on searching in Documentation/Help
- Improved navigation in sidebar contents in Documentation/Help
- Fixed issue with equation rendering speed in Documentation/Help.
- Improved appearance of overall Documentation/Help formatting
- Improved documentation of Visual Setup

Other

- Over 50 use issues fixed.

2.5.6 Known Issues in VSim 8.1

- Remote VSimComposer does not work
- Windows Cluster support was lost with upgrade to MPI on windows needed for certain simulations.
- EM Cylindrical not implemented for visual setup
- Occasionally, for parallel runs, the stl reader can spuriously set some regions outside of objects to being inside. When this happens, it is manifest in the visualization of the corresponding geometry field in Data Overview. In all cases observed so far, this has been fixed by offsetting the grid a small amount, changing the number of cells, and/or changing the number of parallel processes.

2.5.7 New and Updated VSim 8.0 Features

The following features are new or have been updated for the 8.0 release.

VSim Computational Engine (Vorpal)

- New package: VSim for Semiconductor Devices for modeling electron transport in diamond or Gallium Arsenide
- Fast dielectric algorithm can take multiple dielectrics assigned to multiple shapes
- Windows Cluster Support with graceful shutdown of job
- Automatic detection of GPU acceleration
- Ability to use cross-section data files from a user definable location
- 17+ new simulation object kinds (including Species, Particle Sources/Sinks, Emission Models, Histories, Field Updaters, Grids, Grid Boundaries, and Domains)
- Improved reliability of fast electrostatic solves on Linux

VSim Examples

- Charge Carrier Dynamics in Diamond (VSimSD)
- Electron Transport in GaAs (VSimSD)
- MESFET Device (VSimSD)
- Metal Schottky Contact and Transport in Diamond (VSimSD)
- Transport and Emission in Diamond (VSimSD)
- Electron Emission in GaAs (VSimSD)
- Langmuir Probe (VSimPD)
- Turner Plasma Discharge, Case 2 (VSimPD)
- Electron Gun (VSimMD)
- Half-Wave Dipole in Free Space (VSimEM)
- Linear Phased Scanning Array (VSimEM)
- Gaussian Laser Beam and Photonic Crystal Cavity (VSimEM)
- Dipole Source and Photonic Crystal Cavity (VSimEM)

- Scattering off Multiple Objects (VSImEM)
- Drude-Lorentz Metal-Insulator-Metal Waveguide (VSImEM)
- Spherical Lens (VSImEM)
- Halfwave Antenna (VSImBase)
- Cylindrical Capacitor (VSImBase)

VSIm Macros

- Macros standardized and simplified
- Ability to use macros from a user definable location.

VSIm Analyzers

- VSIm now comes with more than 30 data analysis executables.
- Standardization of all analyzers so that user defined input will show up as entry boxes.

VSIm Graphical User Interface (VSImComposer)

- Easy, configurable tree-based/visual setup for many problems
- Ability to import materials from a file.
- Easily switch between different simulation types (electrostatic, electromagnetic, with or without particles) with GUI adapting to the selection.
- Import CAD objects from multiple formats (step, stl, ply, vtk) and set materials of those objects
- Multiple Geometry shapes can be visually added to simulation.
- Ability to define parts through constructive solid geometry.
- Ability to define expressions and parameters and use those in defining the simulation.
- Ability to assign materials to parts, regardless of how they were imported or constructed.
- Minimize data reloading during visualization.
- Uniformization of output across all platforms.
- Multiple simulations can be saved to one directory.

Other

- Over 373 use issues fixed.

2.5.8 Known Issues in VSIm 8.0

- Remote VSImComposer does not work
- EM Cylindrical not implemented for visual setup

- Occasionally, for parallel runs, the stl reader can spuriously set some regions outside of objects to being inside. When this happens, it is manifest in the visualization of the corresponding geometry field in Data Overview. In all cases observed so far, this has been fixed by offsetting the grid a small amount, changing the number of cells, and/or changing the number of parallel processes.

2.5.9 Deprecated Features for VSim 8.0

VSim Computational Engine (Vorpai)

The following engine features are deprecated as of the VSim 8.0.0 release and may no longer be supported in future releases of VSim:

Attributes Deprecated in Version 8.0

- The kinds *bitRevDensSrc*, *bitRevDensSrcVW*, *gaussDensSrc*, *gridDenSrcVW*, and *planarPtclEmitter* of the *ParticleSource* block have been deprecated. Please use the *xvLoaderEmitter* kind instead.
- *kind* is deprecated for the *Decomp* block. The regular decomposition is the only one available and therefore this attribute is not needed at all. Please simply omit “*kind =*” from the *Decomp* block
- *stCadRgn* kind of *STRgn* block has been deprecated. Please use *gridRgnBndry* kind of *GridBoundary* block instead. The *gridRgnBndry* is a much faster method for importing STL geometries.
- *cell* kind of *Species* block has been deprecated.

Features Deprecated in Version 8.0

- Chinese is no longer supported for VSimComposer

2.5.10 Attributes Deprecated in Version 7.0

- The attributes *GridDenSrc*, *CoordProdGridPosGen*, *CoordProdGridDenSrcVW* of the *ParticleSource* block have been deprecated. Please use *gridPosGen* of the *xvLoaderEmitter* kind instead.
- The attribute *numPhysCells* of the *Grid* block has been deprecated. Please use *numCells* instead.

2.5.11 Deprecated in Version 6.0

Attributes

- The attributes *kind=yeeEmField* and *kind=exp24EmField* of the *EmField* block have been deprecated. Use *MultiField* block instead
- The attributes *kind=block*, *kind=cosSqPulse*, *kind=expPeak*, *kind=gaussianGrad*, *kind=gaussianLapl*, *kind=linearRamp*, *kind=mask*, *kind=muWaveMode*, *kind=periodicSTFunc*, *kind=qFormPolyn*, *kind=radSymFunc*, *kind=sawtoothWave*, *kind=strap* and *kind=waveguide* of the *STFunc* block have been deprecated. Use *kind=expression* and specify desired functional expression instead
- The attributes *kind=smoothWide1D* and *kind=spaceScalarFieldFuncUpdater* of the *FieldUpdater* block have been deprecated. Use *kind=smooth1D* instead
- The *Component* sub block of the *EmField* of *kind=funcEmField* has been deprecated. The components are now set using *STFunc* blocks with the names E0,E1,E2,B1,B2 and B3.

VorpalView

- VorpalView, an IDL-based visualization tool, is a deprecated feature as of VSim 6.0.0.

2.5.12 Deprecated in Version 5.2

- The *STFunc* block with the name *loadProb*, which is a sub-block of the *ParticleSource* block, which is, in turn, a sub-block of the *Species* block, has been renamed to an *STFunc* block with the name *macroDensFunc*.
- The attribute *loadInGuardCellFlag* of the *ParticleSource* block with *kind=ptclEmitter*, which is a sub-block of the *Species* block, has been renamed *loadInGuardCell*.
- The attributes *kind=speciesTrackTagInternals*, *kind=speciesTrackTagTraj*, *kind=speciesTrackTraj*, and *kind=speciesTracVel* have been deprecated. Use *kind=speciesTrackTag* instead. We are now only supporting history tracking if the user uses tagged particles.

2.5.13 Deprecated in Version 5.0

Attributes

- The *components* attribute in the *FieldUpdater* blocks of *kind=gpuSTFuncUpdater*, *kind=STFuncUpdater*, and *kind=unaryFieldOpUpdater* has been renamed *writeComponents*.
- The attributes *kind=nonRelESCell* and *kind=2ndOrderRelBorisCell* of the *Species* block have been deprecated. The same models can be accessed with *kind=cell* and *pusher=nonRelEs* for *kind=nonRelESCell* and *kind=cell*, *pusher=relBoris* and *stencil=spline2ndOrder* for *kind=2ndOrderRelBorisCell*.

Blocks

- *Collision*
- *ImpactCollider*
- *Ionizer*. Use the Monte-Carlo framework (i.e., the *MonteCarloInteractions* blocks) in place of using the above deprecated blocks.

2.5.14 Attributes Deprecated in Version 4.2

- The attribute *function* of the *BoundaryCondition* block and the *EmField* blocks of *kind=yeeStaticElecField*, *kind=funcEmField*, and *kind=yeeStaticElecFieldTrillinos*, has been replaced with an *STFunc* block with the name *function*.
- The *UserFunc* block now requires specific names. Arbitrary names for this block have been deprecated.

2.5.15 Attributes Deprecated in Version 4.0

- The attribute *periodicityDirs* of the *Decomp* block has been renamed *periodicDirs*.
- The attribute *indices* of the *BoundaryCondition* and *InitialCondition* blocks has been replaced with the attribute *components*.
- The attribute *function* of the *STFunc* block has been replaced by the attribute *kind*.

- The attribute *singleEmission* of the *ParticleSource* block, which is a sub-block of the *Species* block, has been deprecated. The option *singleEmission=true* has been replaced by the option *ptclCountType=noCounting*, while the default setting is equivalent to the option *singleEmission=false*.

2.5.16 Attribute Deprecated in Version 2.0

- The attribute *xtendUpdate* of the *FieldUpdater* block has been replaced by the attributes *cellsToUpdateAboveDomain* and *cellsToUpdateBelowDomain*.

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