GSim Installation and Release Notes

Release 1.0.0rc1

Tech-X Corporation

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CONTENTS

CHAPTER

ONE

OVERVIEW

This guide shows how to customize GSim, the arbitrary dimensional, electromagnetics and plasma simulation code, to add macros and analyzers.

GSim is an arbitrary dimensional, electromagnetics and plasma simulation code consisting of two major components:

- GSimComposer, the graphical user interface.
- Vorpal [NC04], the GSim Computational Engine.

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

CHAPTER

TWO

INSTALLATION DETAILS

2.1 What is Installed with GSim?

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

2.1.1 GSimComposer

GSimComposer is a graphical user interface for

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

The GSimComposer 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 GSimComposer. New GSim users can use these examples as templates. Advanced GSim users can use GSimComposer to validate the syntax of their own input files, whether their files have been created using GSimComposer or by using a text editor.

The GSimComposer Run pane invokes the GSim 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 GSim.

GSimComposer now allows selection of analysis programs, either supplied with GSim or user written.

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

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

2.1.2 GSim Computational Engine

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

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/).

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

GSim 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 GSimComposer.

More Information

More information about GSim can be found at the GSim Product Website (https://www.txcorp.com/gsim). Send questions about installing or running GSim to Tech-X Customer Support at support@txcorp.com.

Extensive assistance in the use of GSim 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 GSim System Requirements

2.2.1 Operating System

GSim 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 10 or Windows Server 2022 or later
- Linux distributions with glibc 2.28 or later (Verified on Rocky Linux 8, Ubuntu 22.04.3 LTS)
- MacOSX Monterey (12.7.1) or later
- Cray XC30

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

2.2.2 Memory

Usage of RAM varies with the computational problem size, but with a minimum of 16 GB will run most all examples as described in the documentation. Examples like the Smith Purcell examples will use more than 16 GB, so a more liberal estimate would be 32 GB, but of course any heavy computation could require more.

2.2.3 Graphics Rendering

The visualization in GSim uses OpenGL and requires optimal graphics drivers that support OpenGL 3.2. 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.

Note: There is a known visualization issue on certain Linux laptops, when Desktop Scaling is set to non-integer scaling values. For example 100% & 200% are ok, but fractional values like 175% (scaling of 1.75) can cause display artifacts in the visualize tab.

Note: There is a known Windows-OpenGL issue when using GSim over a Microsoft Remote Desktop connection where the application window appears blank on some Windows machines with some graphics cards or some drivers. We provide a RemoteGSimComposer.bat script to work around this issue. It disconnects the remote session and starts GSim while disconnected, so that when the user reconnects, GSim works properly. If you see this issue, launch this script by right-clicking on RemoteGSimComposer.bat and choose "Run as administrator".

On Windows systems using high resolution screens that high DPI (dots-per-inch), poor sizing can occur where fonts are small or panels are cut off. This can be remedied by overriding the scaling behavoir performed by the system. The figure belows shows how to override this scaling by setting a properties of the Composer executable.

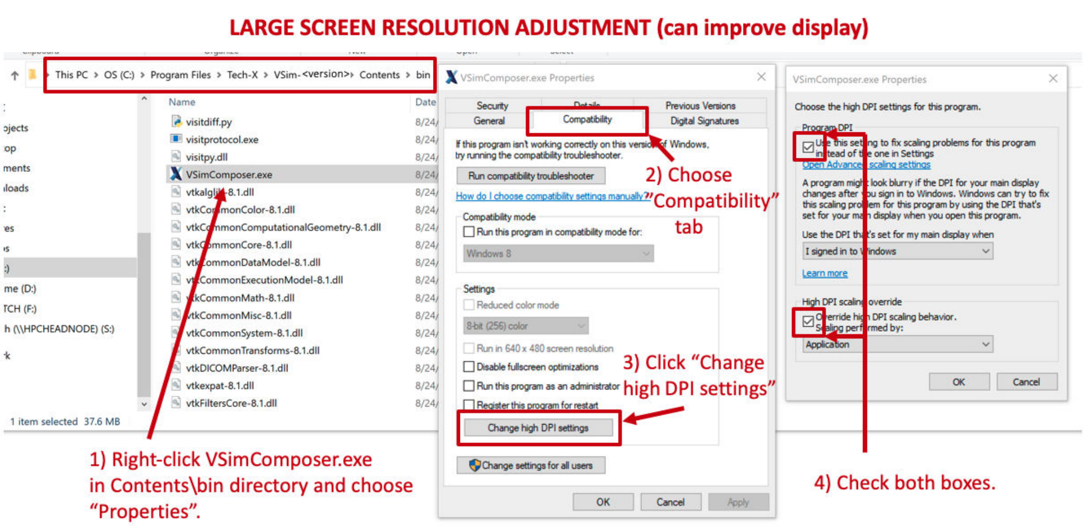

Fig. 2.1: How to override system high DPI scaling on Windows.

On Windows systems with 2 graphics cards, it is sometimes necessary to force the system to use the better card that supports the OpenGL functions needed. In this case, there is a operating system setting to force which graphics processor is used for Composer. On Windows 11, navigate to the System settings and then to Display > Graphics as shown below.

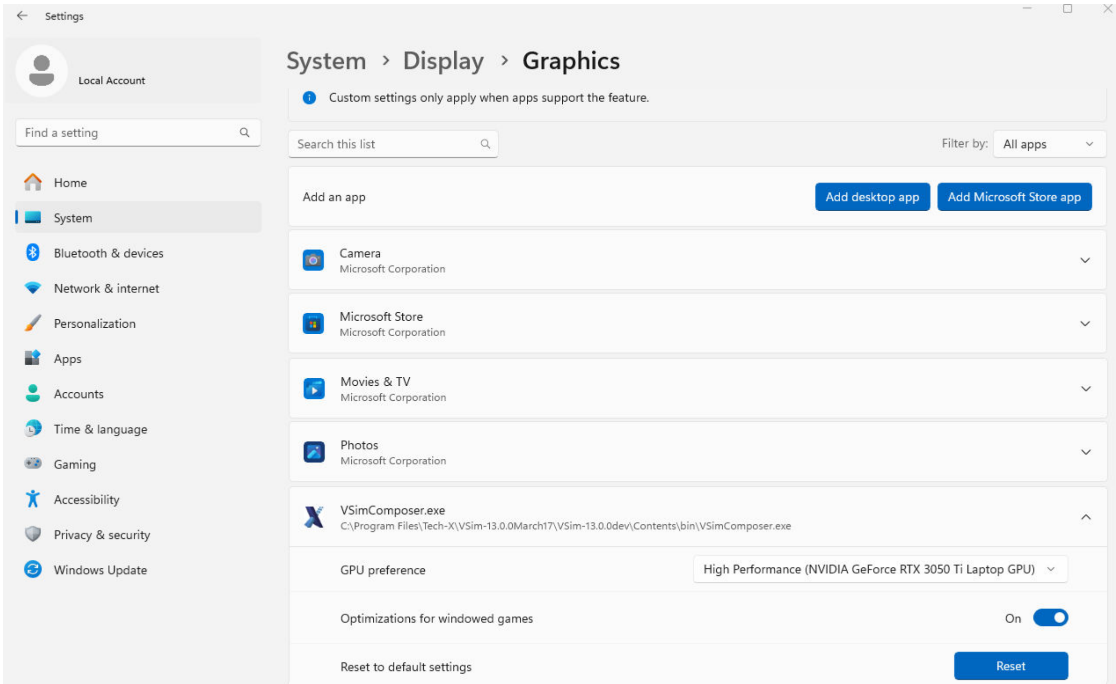

Fig. 2.2: How to force the system to use a particular graphics card for Composer on Windows.

2.2.4 Graphics Acceleration

GPU acceleration requires a CUDA capable graphics card and a NVidia video driver that supports CUDA 12.3. If you see the error message `CUDA error 222 (cudaErrorUnsupportedPtxVersion) the provided PTX was compiled with an unsupported toolchain.` then this indicates that you should try upgrading the driver for your CUDA card. The drivers need are NVIDIA Linux Driver 545.23.08 or NVIDIA Windows Driver 546.12.

Each CUDA card model will have a certain amount of memory and one must ensure that the problem size fits into that memory. On Windows, total CUDA memory is managed by the Windows Display Driver Model (WDDM) which functions differently than other operating systems, in that the WDDM subsystem handles GPU compute memory allocation and scheduling, rather than being handled by the CUDA runtime as on other platforms. Thus, the Windows GPU memory virtualization functionality is a property of Windows rather than CUDA and will endup being larger than the card's physical memory. We suggest, however, you keep the problem size within the card's physical memory so that optimal performance is maintained.

2.2.5 Disk Space

The GSim-1.0 Windows installer is around 536MB, and requires around 1.5GB of disk space to install. The Linux installer is 992MB due to the inclusion of additional system packages, and unpacks into around 3.3GB. Please ensure you have enough additional space to run your simulations.

2.2.6 Windows Performance

GSim performance on Windows compared to Linux can be significantly limited by power settings. If the power setting was on "balanced," which is the default even on a desktop or server, Windows will limit CPU utilization when GSim is running, i.e. Windows will not allow GSim to take all the CPU resource. To overcome the limitation, change the power settings under "Control Panel -> System and Security -> Power Options -> Preferred plans" to "High performance."

2.2.7 Large Scale And Accelerated Computing

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

GSim 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.

GSim 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 GSim desktop users may explore how the files work by running them in 2D. Some microwave device examples, such as the Smith Purcell Radiation example, 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.

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

Note: The Andrew File System (AFS) is not recommended to run GSim 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 GSim.

For installation instructions see: *GSim Installation Instructions*

2.3 GSim Installation Instructions

These are instructions on installing the GSim product. Please see the *GSim System Requirements* first to make sure your system meets the requirements.

2.3.1 Windows GSim Software Installation

The GSim 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\GSim-1.0 (Windows 64-bit)`

which includes the major & minor version of your software. To open the GSim software, go to the Start Menu, click on the Tech-X folder, click on GSim-1.0, then click on GSimComposer. See Fig. 2.3.

Workaround for some Windows App Blocking

Some Windows Operating Systems are configured to only allow installation of applications acquired through the Windows store. If you find this to be the case right click the installer , select properties and check the **Unblock** box

Alternatively if Applications not from the Windows Store are blocked take the following steps.

1. Open Settings and click Apps
2. Select the option to allow Windows 10 to **Allow apps from anywhere**

2.3.2 Windows GSim Software Installation on a Network Share

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

To start, ensure that you have the shared network location that you want to install to. It is easy to find instructions on how to set up network file sharing on Windows, but the quick steps for Windows 10 are:

1. Open Windows File Explorer.
2. Navigate to the folder you wish to share.
3. Right-click the item and choose Properties.
4. In the Properties dialog click the Sharing tab.
5. Click the Share button.
6. In the Network access dialog, choose the people on your network to share the folder with and click the Share button.
7. In the next frame of the Network access dialog, note the names in the Individual Items list. There will be the name you assigned it in step (6) and the UNC (Unified Naming Convention) Path of the shared directory, which will have the form `\MACHINEpathtoshareddirectory`.
8. Click the Done button in the Network access dialog.
9. At this point you can change the UNC Path to a single string by clicking the Advanced Sharing… button and then clicking the Share checkbox and typing a string.
10. Click Close in the Properties dialog.

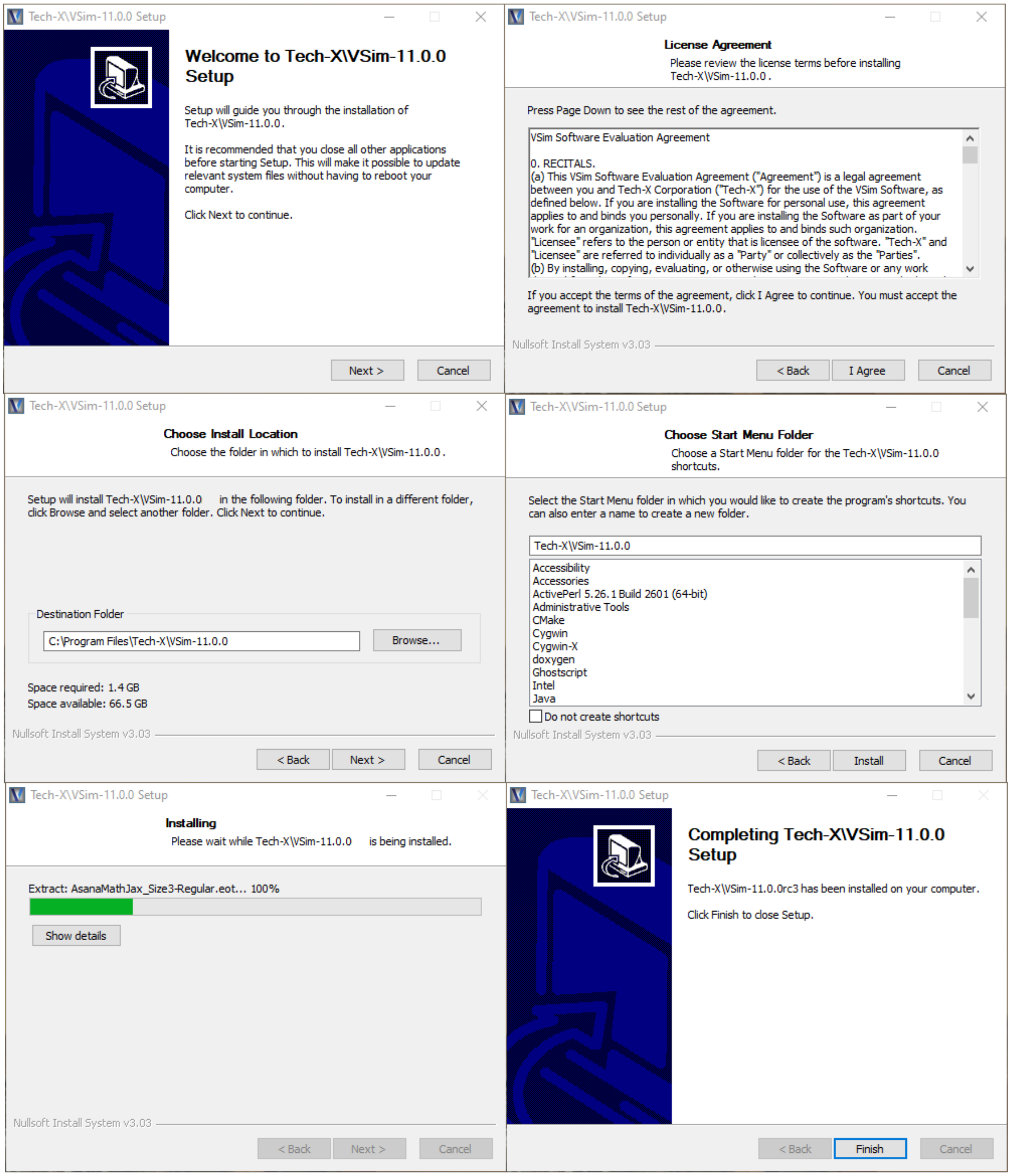

Fig. 2.3: Dialogs for Windows installation

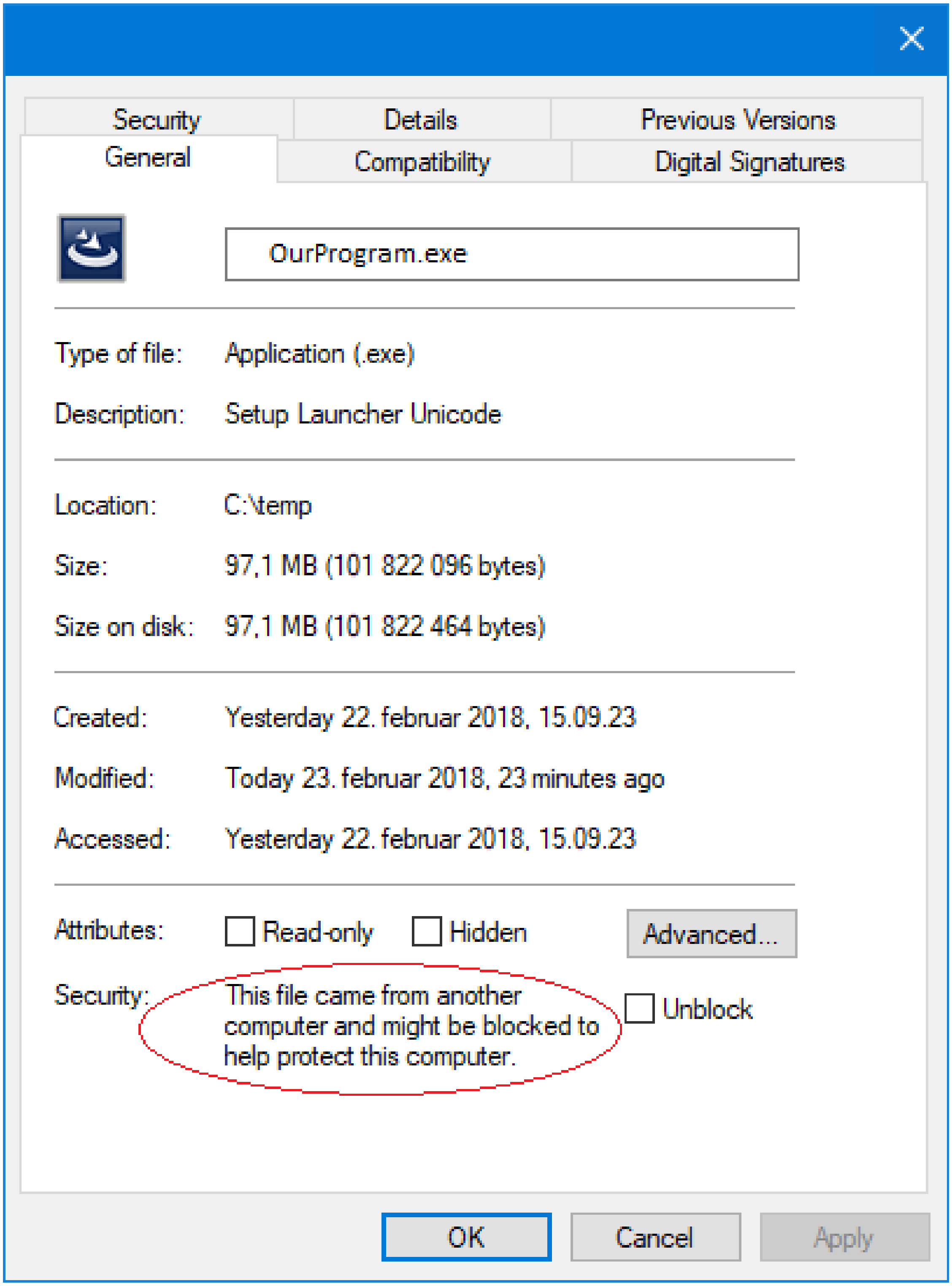

Fig. 2.4: Windows app unblocking

Now that this folder is accessible, install to the folder by following the Windows Installation instructions above. When you get to the "Choose Install Location" step, type in the shared location as your installation location or click the Browse button and navigate to it. Note that you first go to the Network machine in the left pane (not This PC) and then you navigate down in directories according to the UNC Shared Path. One can install GSim from the machine where the folder is shared from, or from another machine that has access to the shared folder.

When running GSim from a network location, one can map the UNC Shared Path to a network drive on any machine that has access to the path. To do this from Windows Explorer on the machine where GSim will be run, navigate to the second to last folder in the UNC Shared Path, right-click on the icon for the last folder, and select the Map Network Drive menu item. At this time you will be prompted to select a drive letter and can change a couple settings. After making your choices press Finish.

For a concrete example, say we have the follow values:

```
- Installation Computer Name = JANESCOMPUTER
- Shared Folder = C:\Users\jane\Documents\myshare
  (shared on JACKSCOMPUTER)
- Folder UNC Shared Path = \\JANESCOMPUTER\jane  (note here Jane
  has chosen the advanced option of a single name "jane" to represent
  the full path of \Users\jane\Documents\myshare)
- GSim installation Folder = C:\Users\jane\Documents\myshare\GSim
- Mapped Network Drive on JACKSCOMPUTER = S:\
```

So, for this example, the drive `S:\` will show up on `JACKSCOMPUTER` and is mapped to `\JANESCOMPUTER\jane` which is a share name for `C:\Users\jane\Documents\myshare` on `JANESCOMPUTER`. So, Jack should see `S:\GSim` as the installation location for GSim and he can conveniently run GSimComposer by double-clicking

```
S:\GSim\Contents\bin\GSimComposer.exe
```

Finally, to ensure all users have access to the license, the license should be copied to the `Contents\engine\bin` subdirectory next to the Vorpal engine. So, in our example, this would be on JANESCOMPUTER at the location:

```
C:\Users\jane\Documents\myshare\GSim\Contents\engine\bin\license.txt
```

inside the original installation of GSim. This is best done by using Windows Explorer rather than adding the license using the GSimComposer settings.

2.3.3 Windows Cluster GSim Software Installation

There are a few extra steps when installing on a Windows Cluster and we detail them here. GSim will work on a Windows cluster that uses Microsoft HPC Pack (Version 2012 R2 or later is required).

First, install GSim on the cluster headnode using the instructions above in the *Network Share Section*. The cluster license file will need to be copied into the correct location as described above and it will need to refer to the correct shared directory – normally a good choice for this directory would be a subdirectory of the UNC Shared Path alongside the GSim installation.

For operation on a Windows Cluster it is crucial to use the MPI that comes with Microsft HPC Pack. So, we must set aside the MPI that is distributed with GSim. Using the exmaple from the *Network Share Section* above, one would open a Command Prompt and execute the following commands:

```
S:\>cd GSim\Contents\engine\bin
S:\GSim\Contents\engine\bin>move mpiexec.exe mpiexecOFF.exe
      1 file(s) moved.
S:\GSim\Contents\engine\bin>move msmpi.dll msmpiOFF.dll
      1 file(s) moved.
```

This will ensure that the mpiexec.exe in the PATH variable will be the one on the system. This can be verified by the following:

```
S:\GSim\Contents\engine\bin>where mpiexec.exe
C:\Program Files\Microsoft MPI\Bin\mpiexec.exe
```

This completes the installation and now it can be tested using the "Running Vorpal on a Windows HPC Cluster" section of the User Guide.

Now (also following the exmaple in the *Network Share Section* above), Jack can use GSimComposer to create a simulation directory (say `mysim`) in the shared folder, for example:

S:\jack\simulations\mysim

This directory and, therefore, the simulation input will then be available to all the nodes on the cluster when a job is submitted.

2.3.4 Linux GSim Software Installation

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

`/usr/local/GSim-1.0`

The unzip and untar command is

```
$ cd /usr/local
$ tar xf GSim-1.0-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 "GSim-11.0.0-Linux64-offscreen.tar.gz. After untarring, the user interface is started with the command:

```
$ cd GSim-1.0
$ ./GSimComposer.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/GSim-1.0/GSimComposer.sh
<execute engine, analyzers, etc.>
```

See the "Running Vorpal from the Command Line" section in the User Guide for more instructions. on command-line operations.

2.3.5 Mac OS X GSim Software Installation

Unpacking the DMG file:

The GSim distribution package for Mac OS X is a .dmg installer. Invoke the installer by double clicking on it. Drag the GSim-1.0 folder into your Applications folder (visible in the installer window). From the Application folder, double click on the GSimComposer icon in the GSim-1.0 folder. See Fig. 2.5. This default installation path is:

`/Applications/GSim-1.0`

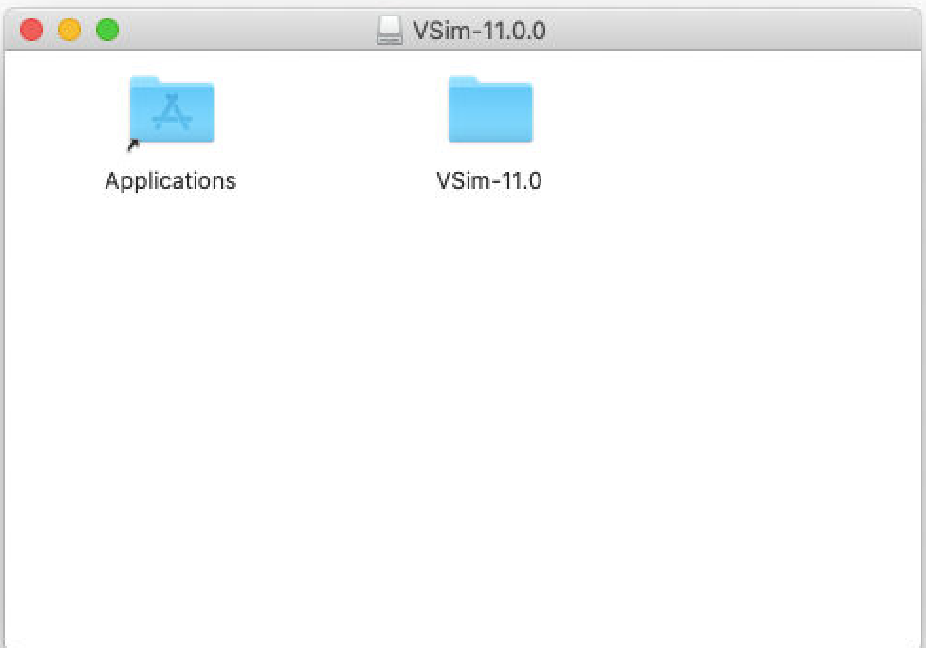

Fig. 2.5: Dialog for the Mac installer

Workaround for signing issues:

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. 2.6.

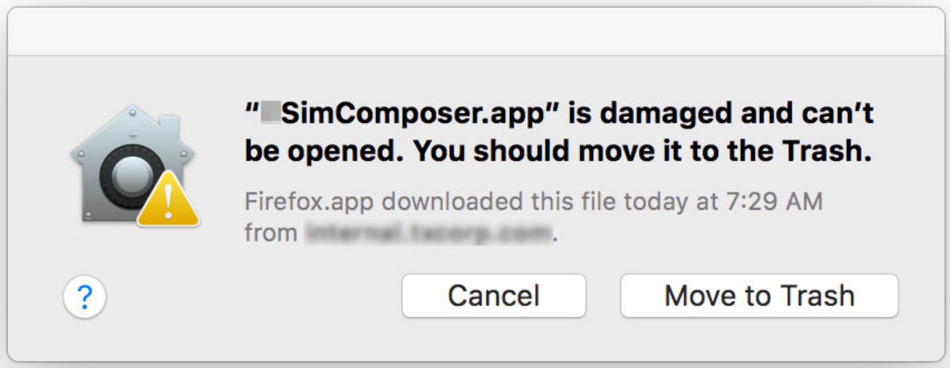

Fig. 2.6: Warning that GSimComposer is damaged, put up by GateKeeper when code signing is not properly recognized.

If you are experiencing this, then close GSimComposer and open an XTerm and run the commands:

```
$ cd /Applications    # or wherever one has installed GSim-1.0
$ xattr -rd com.apple.quarantine GSim-1.0
```

Then reopen GSimComposer – the message should be gone.

2.4 GSim Documentation

In addition to this PDF version of the GSim documentation, all of the documentation is accessible from within the GSimComposer interface, as well as online at the Tech-X web site, GSimDocumentation.

2.4.1 GSim Installation

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

2.4.2 GSim User Guide

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

2.4.3 GSim Examples

The "Example" manual provides numerous tutorials for both beginning and advanced GSim users.

2.4.4 GSim Customizaton

The "Customization" manual discusses macros and analyzers in futher detail, for users who would like a higher degree of customization in their simulations and postprocessing.

2.4.5 GSim Reference

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

2.4.6 Searching the Documentation

All documentation is available through the GSimComposer 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 Making your data web accessible

If your simulation files are stored on a workstation with a web server, you can make your files web accessible, as discussed here.

Requirements

- Working OpenLdap directory server
- Must have ssl support on port 636
- Available credentials to connect to openldap server. Anonymous binds not supported
- User accounts in the LDAP directory must have the homeDirectory attribute set

Procedure:

1) Install Apache Httpd web server, php and the php ldap library

$ dnf install httpd mod_ssl php php-ldap
$ systemctl start httpd
$ systemctl enable httpd

2) Edit index.php and set appropriate values for the following variables

$ldap_server_uri = 'ldaps://ldapserver.example.com';
$search_scope = 'ou=users,dc=example,dc=com';
$proxy_dn = 'ldapserver_bind_dn';
$proxy_pass = 'ldapserver_bind_password';

3) Copy index.php, display.php, and logout.php into the Apache Httpd web server's DocumentRoot directory. On Redhat based machines e.g Fedora, Centos, the default DocumentRoot is /var/www/html.

4) Go to https://localhost , log in and verify that you are able to see your files.

2.6 Software Licensing

GSim uses several open source packages and here we provide grateful acknowledgement and a list of these licenses

2.6.1 Trilinos

Trilinos, used by the Vorpal computational engine, is comprised of packages that are either BSD or LGPL compatible (See https://trilinos.github.io/license.html).

BSD compatible packages (such as Amesos2, AztecOO, Belos, Epetra, EpetraExt, Galeri, Ifpack, Ifpack2, Intrepid, Kokkos, Komplex, Shards, Teuchos, Tpetra, TriUtils, Xpetra, and Zoltan) in Trilinos licensed by Sandia contains the following notice:

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```

Both Vorpal Computational Engine and Composer use HDF5 (see Hdf5 license at https://raw.githubusercontent.com/HDFGroup/hdf5/develop/COPYING).

The notice for HDF5 is:

```
(Begin notice)

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-----------------------------------------------------------------------------

(End notice)
```

Composer uses OpenSSL (http://www.openssl.org/source/license.html).

The notice for OpenSSL is:

```
/* ====================================================================
 * Copyright (c) 1998-2011 The OpenSSL Project.  All rights reserved.
 *
 * Redistribution and use in source and binary forms, with or without
 * modification, are permitted provided that the following conditions
 * are met:
 *
 * 1. Redistributions of source code must retain the above copyright
 *    notice, this list of conditions and the following disclaimer.
 *
 * 2. Redistributions in binary form must reproduce the above copyright
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 *    software must display the following acknowledgment:
 *    "This product includes software developed by the OpenSSL Project
 *    for use in the OpenSSL Toolkit. (http://www.openssl.org/)"
 *
```

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Composer also uses libssh (https://www.libssh.org/development/).

The notice for libssh is:

```
libssh Developer's Certificate of Origin. Version 1.0

By making a contribution to this project, I certify that:

(a) The contribution was created in whole or in part by me and I
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```

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```
    Discusses bugs,  as well  as engine internals,  design issues,
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Our home page can be found at

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2.7 GSim Release Notes

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

2.7.1 New and Updated 1.0 Features

GSim Computational Engine (Vorpal)

- A new Global Model.

GSim Examples

- Initially release wit the following examples:
  - GSimPPlasma -> Simple Gases -> Argon Plasma
- Improved

GSim Macros and Translator

- Initially release iwth macros and translators needed to pre process the exmaples above.

GSim Analyzers

- The following analyzers are initially available in GSim:

GSim Graphical User Interface (GSimComposer)

CHAPTER

THREE

SPECIAL TYPES OF INSTALLATIONS

3.1 GSim on a Private Cloud Installation Instructions

These instructions are for setting up GSim to run on a single server as a "private cloud" serving any user that is able to log onto the Linux machine.

First, install GSim onto the Linux server. Here we assume that GSim is installed in the location

```
/usr/local/\ |PRODUCT_VER|\ /
```

You will want to make sure all user have execute permissions on the GSimComposer.sh script in this directory.

Next, install no machine from rpm. There is an automatic 30 day license, but a license will need to be purchased for production use. This command with install from the rpm:

```
rpm -Uvh nomachine*rpm
```

Edit the /usr/NX/etc/server.cfg file and set the following keys:

```
EnableWebMenuTutorial 0
EnableWebPreconfiguration 1
```

Copy the default nxweb custom config file to a new file that has the .nxs extension with the following command:

```
cp /usr/NX/share/config/default.nxs.sample /usr/NX/share/config/default.nxs
```

Edit /usr/NX/share/config/default.nxs and add the following to the end of the "General" section

```
<option key="Session" value="unix" />
<option key="Desktop" value="console" />
<option key="Custom Unix Desktop" value="application" />
<option key="Command line" value="/usr/local/\ |PRODUCT_VER|\ /\ |COMPOSER|\ .sh --
↪topLeft --maxSize" />
```

Verify that /usr/NX/share/config/default.nxs is owned by nxhtd and permission is set to 700

If you chose to use a commercial SSL certificate, set SSLCertificateFile and SSLCertificateKeyFile to the path of certificate and key in /usr/NX/etc/htd.cfg

Start, Stop, or Restart the NoMachine server as follows:

```
systemctl start nxserver
systemctl stop nxserver
systemctl restart nxserver
```

In a web browser, go to https://hostname:4443 and verify that a user can login and that GSim loads automatically.