GranularSim Installation Guide

Version Version 18 .2

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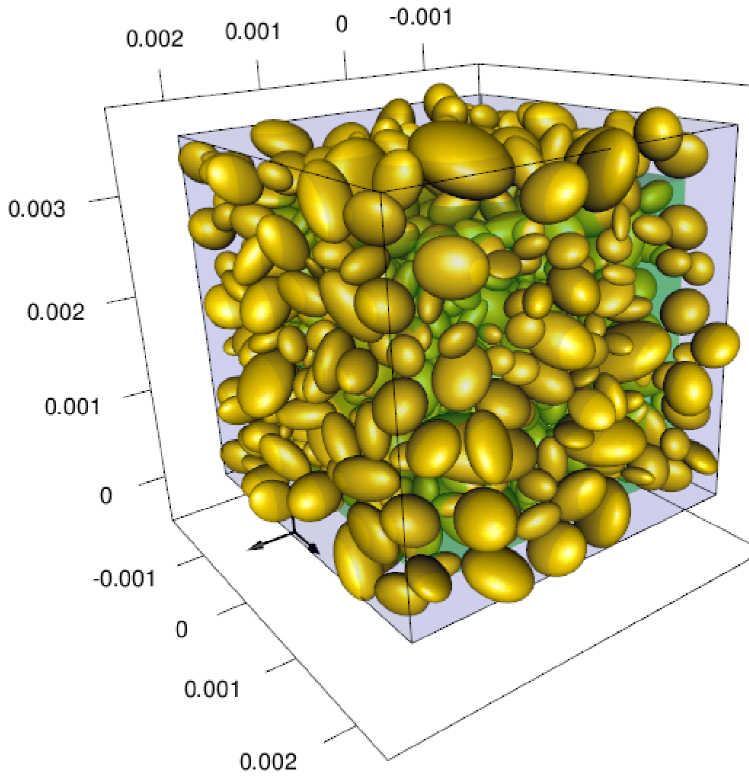

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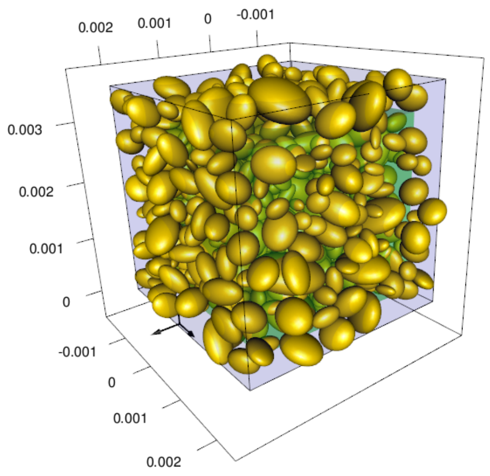

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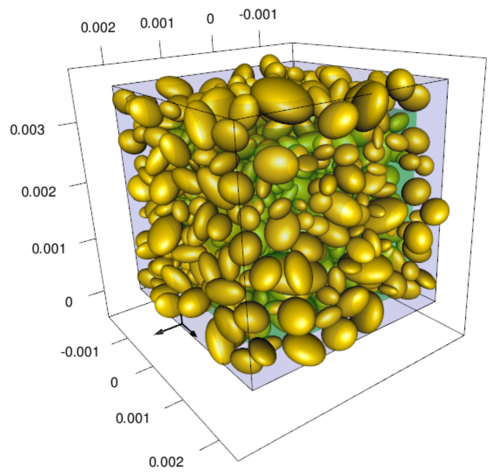


1 — Overview of GranularSim

GranularSim is a rewritten and updated version of the parallel discrete element code ParaEllip3D developed at the University of Colorado at Boulder, with the intent of having a more general code that can be improved and appended to more easily. The primary use case is the simulation of soils and other granular materials.

The main components of GranularSim include a discrete element (DEM) code that can handle ellipsoidal particles, a peridynamics (PD) code that couples to DEM particles, and a smoothed particle hydrodynamics (SPH) code that also couples to DEM particles. In addition, the code is able to handle special boundary conditions that are needed for hierarchical upscaling.

GranularSim provides outputs in VTK format and results can be visualized either with ParaView or with VisIt (https://wci.llnl.gov/simulation/computer-codes/visit/).

1.1 Obtaining the Code

GranularSim can be obtained either as a zipped archive (approx. 550 Mb) from

```
https://github.com/bbanerjee/ParSim/archive/master.zip
```

or cloned from Github using either HTTP

```
git clone --recursive https://github.com/bbanerjee/ParSim.git
```

or SSH

```
git clone --recursive git@github.com:bbanerjee/ParSim.git
```

The above commands check out the ParSim source tree and installs it into a directory called ParSim in the user's home directory. The ParSim code contains several research codes. The main GranularSim code can be found in the ParSim/GranularSim/src directory. Manuals for GranularSim are in ParSim/GranularSim/Manuals .

You may also need to install git on your machine if you want to clone the repository from Github :

```
sudo apt-get install git-core
```

The –recursive flag is needed in order to make sure that the submodules googletest , cppcodec , and qhull are also populated during the download process.

1.2 Developer version

If you are a developer, we will suggest that you use the following longer process.

1. Create a GitHub account

   ```
     https://github.com/signup/free
   ```

2. Install git on your machine

   ```
     sudo apt-get install git-core
   ```

3. Setup git configuration

   ```
     git config --global user.email "your_email@your_address.com"
     git config --global user.name "your_github_username"
   ```

4. Email your github username to the owner of ParSim .
5. Create a clone of the ParSim repository

   ```
     git clone https://github.com/bbanerjee/ParSim
   ```

6. Check branches/master

   ```
   git branch -a
   ```

7. Configure ssh for secure access (if needed)

   ```
   cd ~/.ssh
   mkdir backup
   cp * backup/
   rm id_rsa*
   ssh-keygen -t rsa -C "your_email@your_address.com"
   sudo apt-get install xclip
   cd ~/ParSim/
   xclip -sel clip < ~/.ssh/id_rsa.pub
   ssh -T git@github.com
   ssh-add
   ssh -T git@github.com
   ```

8. For password-less access with ssh , use

   ```
   git remote set-url origin git@github.com:bbanerjee/ParSim.git
   ```

9. To change the default message editor, do

   ```
   git config --global core.editor "vim"
   ```

If you are new to GranularSim , we strongly suggest that you fork the code from GitHub and submit your changes via pull requests.

1.2.1 Getting the latest version, adding files etc.

1. Check status

   ```
   git status
   git diff origin/master
   ```

2. Update local repository

   ```
   git pull
   ```

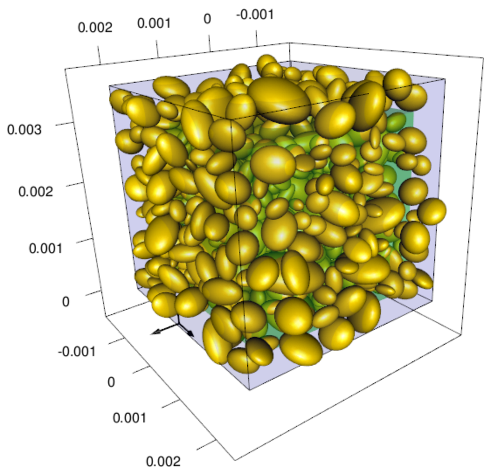
3. Add file to your local repository

   ```
   git add README
   git commit -m 'Added README file for git'
   ```

4. Update main repository with your changes

   ```
   git push origin master
   ```

If you are new to GranularSim , we strongly suggest that you fork the code from GitHub and submit your changes via pull requests.



2 — Prerequisites and library dependencies

GranularSim depends on several tools and libraries that are commonly available or easily installed on various Linux or Unix like OS distributions.

The following instructions are tailored for installations on Ubuntu/Debian-like systems.

2.1 Using a package manager

If you are using a package manager to install the prerequisites, follow the instructions in this section. Otherwise, go to section 2.2.

2.1.1 Compilers

You will need a C++ compiler, either g++ or clang :

```
sudo apt-get install g++
```

```
sudo apt-get install clang-3.8
```

You will also need a C Compiler such as gcc :

```
sudo apt-get install gcc
```

2.1.2 Cmake

You will probably need to install Cmake to control the software compilation process. To do that:

```
     sudo apt-get install cmake
```

2.1.3 Boost

You will need Boost for parts of the code (and also some of the unit tests) to compile. GranularSim uses the boost MPI and serialization libraries. It's easiest to install everything from Boost.

```
sudo apt-get install libboost-all-dev
```

2.1.4 MPI libraries

Install the OpenMPI libraries:

```
sudo apt-get install mpi-default-dev
```

2.1.5 OpenMP libraries

For threaded simulations you will need the OpenMP library. This library is included with both gcc and clang . All GranularSim programs are compiled with OpenMP enabled.

2.1.6 Eigen3 library

Some parts of GranularSim use the Eigen3 library. You will have to install this library if you don't have it in your system:

```
sudo apt-get install libeigen3-dev
```

2.1.7 XML libraries

If you are reading data in Vaango format into GranularSim , yo will need the libxml2 library:

```
sudo apt-get install libxml2
sudo apt-get install libxml2-dev
```

GranularSim reads and writes data in Ellip3D format. You will need zenxml to read that data. This header-only library is included with the source code.

2.1.8 JSON libraries

The json header-only library is also cloned into the repository when you use the –recursive flag. You don't need any further installation.

2.1.9 Zlib compression library

You will also need to install the development version of zlib .

```
sudo apt-get install zlib1g zlib1g-dev
```

2.1.10 GoogleTest library

The googletest libraries are cloned into the repository when you use the –recursive flag. You don't need any further installation.

2.1.11 VTK libraries

In order for output to be written in VTK format, you will also need the VTK libraries. Use

```
sudo apt-get install libvtk5-dev
sudo apt-get install python-vtk tcl-vtk libvtk-java libvtk5-qt4-dev
```

2.1.12 Qhull library

You will have to compile Qhull before you can compile GranularSim .

The Qhull source code is a submodule of the repository. For gcc builds, do the following to compile Qhull :

```
cd ParSim/GranularSim/src/qhull/build
cmake ..
make
```

If you want to compile with clang , use

```
cd ParSim/GranularSim/src/qhull
mkdir build_clang
cd build_clang
CC=/usr/local/bin/clang CXX=/usr/local/bin/clang++ cmake ..
make
```

The actual paths to the clang compilers may vary depending on your system setup.

2.2 Building from source

Building on desktop is easier if you use a package manager. However, in some situations you may have to build from source. We will discuss an example of building the code on a Cray machine below.

We have been successful in building on a Cray with the gcc compiler but failed with clang because the C++11 headers were not available on that machine. Our experience is discussed below but yours may differ.

2.2.1 Check what is already installed

Sometimes the head node and the compile node may have different versions of the gcc libraries.

To check the modules that are available on the compilation node, log into that node using a command such as

```
  ssh scompile@machine.domain
```

and then run

```
  module avail
```

In this example we will assume that gcc 6.1.0 , cmake , git , and zlib are already installed and available as the default option. We will load those modules using

```
  module load gcc/6.1.0
  module load cmake/3.6.2
  module load git
  module load zlib
```

2.2.2 Building VTK

Typically, you will not find VTK installed on the machine and will have to build the associated libraries. We have found that VTK-7.1.1 can be built with gcc-6.1.0 while older versions do not build properly.

To download the VTK source code use

```
mkdir VTK-7.1.1
cd VTK-7.1.1
wget https://gitlab.kitware.com/vtk/vtk/repository/v7.1.1/archive.tar.gz
tar xvfz archive.tar.gz
```

To build the code, created a build directory and run

```
mkdir build
cd build
ccmake ../vtk-v7.1.1-b86da7eef93f75c4a7f524b3644523ae6b651bc4/
```

We suggest that you adjust the build flags in the ccmake graphical interface so that the build script downloads all the necessary libraries. Also specify that the build be an optimized build and that no tests are to be run. You will also need to specify the install prefix to be a local vtk directory.

To run the build script use:

```
make -j8
make install
```

2.2.3 Building Boost

We have been able to successfully build boost-1.65.1 .

To build the Boost mpi libraries, you may have to create the file /home/user/user-config.jam containing the single line using mpi ; before you do the bootstrap procedure.

The process is quite straightfoward:

```
wget https://dl.bintray.com/boostorg/release/1.65.1/source/boost_1_65_1.tar.gz
tar xvfz boost_1_65_1.tar.gz
cd boost_1_65_1/
./bootstrap.sh --prefix=../boost --with-libraries=mpi,serialization --show-libraries
./b2  link=shared install
```

One problem that we ran into with modern compilers is that some preprocessor directives are not understand by the compiler. If you run into that problem, locate the file

```
boost/include/boost/archive/detail/iserializer.hpp
```

and replace

```
#ifndef BOOST_MSVC
    #define DONT_USE_HAS_NEW_OPERATOR (                     \
           BOOST_WORKAROUND(__IBMCPP__, < 1210)             \
        || defined(__SUNPRO_CC) && (__SUNPRO_CC < 0x590)    \
    )
#else
    #define DONT_USE_HAS_NEW_OPERATOR 0
#endif
```

with

```
#ifndef BOOST_MSVC
        #if BOOST_WORKAROUND(__IBMCPP__, < 1210)               \
            || defined(__SUNPRO_CC) && (__SUNPRO_CC < 0x590)
                #define DONT_USE_HAS_NEW_OPERATOR 1
        #else
                #define DONT_USE_HAS_NEW_OPERATOR 0
        #endif
#else
    #define DONT_USE_HAS_NEW_OPERATOR 0
#endif
```

2.2.4 Building libxml2

Building libxml2 is straightforward. Just follow the sequence of steps below:

```
wget ftp://xmlsoft.org/libxml2/libxml2-2.9.7.tar.gz
tar xvfz libxml2-2.9.7.tar.gz
module load zlib
module unload python
./configure --prefix=<home-directory>/libxml2 --enable-shared --without-python
make -j4
make install
```

2.2.5 Building eigen3

The eigen3 build is also straightforward:

```
wget http://bitbucket.org/eigen/eigen/get/3.3.4.tar.gz
tar xvfz 3.3.4.tar.gz
```

```
mkdir eigen-build
cd eigen-build
cmake ../eigen-eigen-5a0156e40feb/ -DCMAKE_INSTALL_PREFIX=../eigen3
make install
```

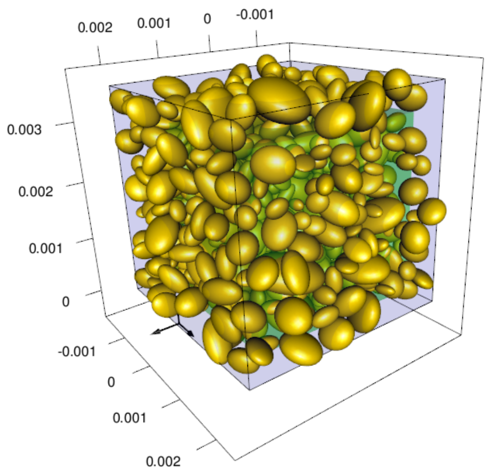
2.2.6 Building qhull

The qhull source is downloaded as a submodule of the ParSim source code. Building qhull is done in-source:

```
cd ParSim/GranularSim/src/qhull
cd build
cmake .. -DCMAKE_INSTALL_PREFIX=.
make
make install
```

2.2.7 Building googletests and zenxml

Googletests are built automatically while building GranularSim while zenxml is a header-only file that requires C++14 capabilities in the compiler. Both are downloaded when the ParSim repository is cloned.



3 — Configuring and Building GranularSim

3.1 Basic instructions

Once you are sure that all the prerequisites have been installed, you can build GranularSim .

3.1.1 The GranularSim repository

After you get the code from GitHub, follow these steps:

- Go to the GranularSim directory:

```
cd ParSim/GranularSim
```

- The source code is in the directory src .

3.1.2 Out-of-source optimized build

- For the optimized build, create a new directory called opt under GranularSim :

```
mkdir opt
```

- followed by:

```
cd opt
```

- To create the make files do:

```
cmake ../src
```

3.1.3 Out-of-source debug build

- For the debug build, create a directory dbg under GranularSim :

```
mkdir dbg
cd dbg
```

- To create the makefiles for the debug build, use

```
cmake -DCMAKE_BUILD_TYPE=Debug ../src
```

3.1.4 Clang compiler:

If you want to used the clang compiler instead of gcc :

```
cmake ../src -DUSE_CLANG=1
```

3.2 Compiling the code:

Next you need to compile the files from src . So go to the opt directory and then type :

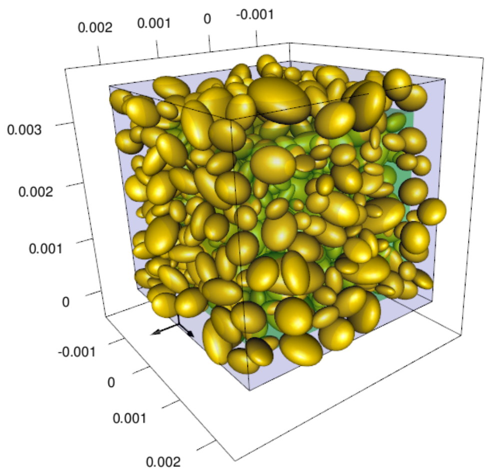
```
make -j4
```

After this compilation you have all the executable files in your opt directory. The same process can be used for the debug build.

3.3 Building GranularSim with compiled libraries

When you have built your own libraries the build procedure for GranularSim is slightly different. For example, for the optimized build, do the following:

```
module load gcc
module load zlib
module load openmpi
git clone --recursive https://github.com/bbanerjee/ParSim.git
cd ParSim/GranularSim/
mkdir opt
cd opt
CC=gcc CXX=g++ \
cmake -DCMAKE_BUILD_TYPE=Release \
      -DBOOST_ROOT=/projects/user_name/boost \
      -DVTK_DIR=/projects/user_name/vtk/lib/cmake/vtk-7.1/ -DWITH_VTK7=1 \
      -DEIGEN3_INCLUDE_DIR=/projects/user_name/eigen3/include/eigen3 \
      ../src
make -j4
```



4 — Installing VisIt

Visualization of GRANULARSIM data is currently possible using VISIT . The VISIT package from LLNL is general purpose visualization software that offers all of the usual capabilities for rendering scientific data. It is still developed and maintained by LLNL staff, and its interface to GRANULARSIM data is supported by the VTK team.

4.1 Directory structure

The following directory structure is suggested for building VisIt:

```
/myPath/VisIt
/myPath/VisIt/thirdparty
/myPath/VisIt/2.10.2
```

4.2 Using the VisIt install script

Download the build script from
http://portal.nersc.gov/project/visit/releases/2.10.2/visit-install2_10_2. Follow the instructions at http://portal.nersc.gov/project/visit/releases/2.10.2/INSTALL_NOTES. GRANULARSIM writes its output in the VTK file format. If VISIT does not recognize the VTK file format, you may have to follow the detailed instructions below.

4.3 Using the VisIt build script

1. Get the build_visit script from http://portal.nersc.gov/project/visit/releases/2.10.2/build_visit2_10_2.
2. Set the MPI compiler to be used (must be the same version used to build VTK):

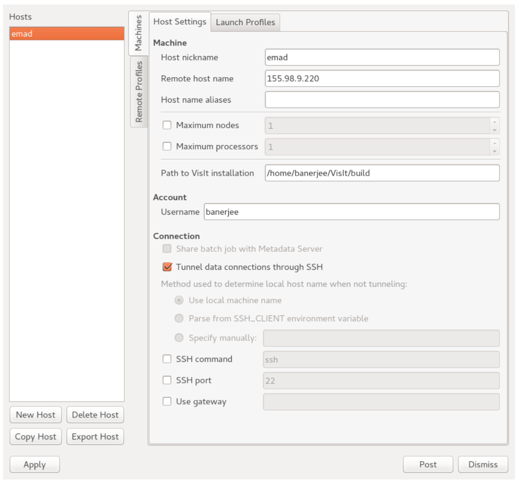
```
export PAR_COMPILER=‘which mpic++‘
export PAR_COMPILER_CXX=‘which mpicxx‘
export PAR_INCLUDE ="-I/usr/lib/openmpi/include/"
```

3. Use the build_visit script to download, build, and install the thirdparty libraries required by VisIt.
4. Go the the VISIT thirdparty directory:

```
cd /mypath/VisIt/thirdparty
```

5. Run build_visit :

```
/myPath/VisIt/2.10.2/build_visit --console --thirdparty-path /myPath/VisIt/
    thirdparty --no-visit --parallel --fortran --uintah
```


Hosts: emad
Machines | Remote Profiles
Host Settings | Launch Profiles

Machine
Host nickname: emad
Remote host name: 155.98.9.220
Host name aliases:
☐ Maximum nodes: 1
☐ Maximum processors: 1
Path to VisIt installation: /home/banerjee/VisIt/build

Account
Username: banerjee

Connection
☐ Share batch job with Metadata Server
☑ Tunnel data connections through SSH
Method used to determine local host name when not tunneling:
● Use local machine name
○ Parse from SSH_CLIENT environment variable
○ Specify manually:
☐ SSH command: ssh
☐ SSH port: 22
☐ Use gateway

Figure 4.1: Setting up Host Profile

> To add additional libraries to enable other database readers using the build_visit script you will have to add the appropriate flags when you run build_visit .

6. The build_visit script will take a while to finish. After the script finishes it will produce a machine specific cmake file called <your_machine_name >.cmake . This file will be used when compiling visit.
7. Move the <your_machine_name >.cmake file to the VisIt source config-site directory:

```
mv <your_machine_name>.cmake /myPath/VisIt/2.10.2/src/config-site
```

8. Go to the VisIt source directory:

```
cd /myPath/VisIt/2.10.2/src
```

9. Run cmake using the cmake that was built by the build_visit script

```
/myPath/VisIt/thirdparty/cmake/<version>/<OS-gcc_version>bin/cmake .
```

10. Finally make VisIt :

```
make -j 8
```

One can install VisIt or run it directly from the bin directory.

4.3.1 Remote visualization

In order to read data on a remote machine, you will need to have a version of VisIt and the VTK data format reader plugin installed on that machine. You will also need to make sure that the VisIt executable is in your path. You may need to edit your .<shell>rc file so that the path to VisIt is included in your shell's PATH variable.

> The version of VisIt installed on your local desktop and the remote machine should be the same.

4.3.2 Host Profile

Next you will want to set up a Host Profile for your remote machine. Select Host Profiles from the Options menu and set up a new profile as shown in figure 4.1.

After filling in the remote machine information, check the Tunnel data connections through SSH option. Click on Apply and then do a Save Settings in the Options menu.

For the remote visualization option to work, you must have ports 5600 - 5609 open. You can try this by running the following on your local desktop (on Linux distributions),

```
traceroute -p 560[0-9] <remote machine>
```

If the tunneling option does not work, try the Use local machine name option.

Now you should be able select Open from the VisIt File menu. After selecting your host from the host entry list, you will be prompted for a password on the remote machine (unless you have set up password-less ssh access).

Once the ssh login has completed, you should see the directory listing. You can then change directories to your data directory and load the data.