Gale

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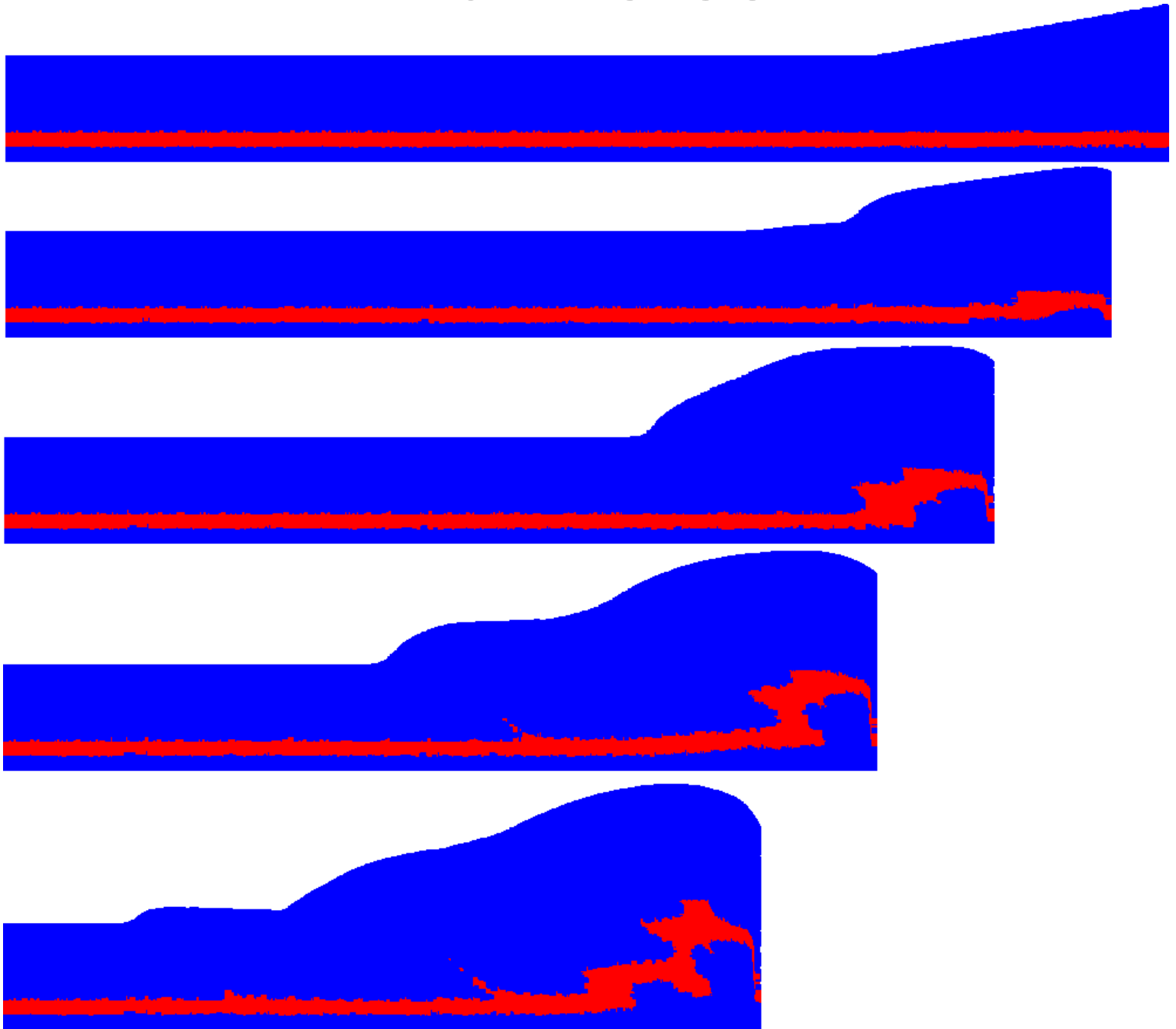
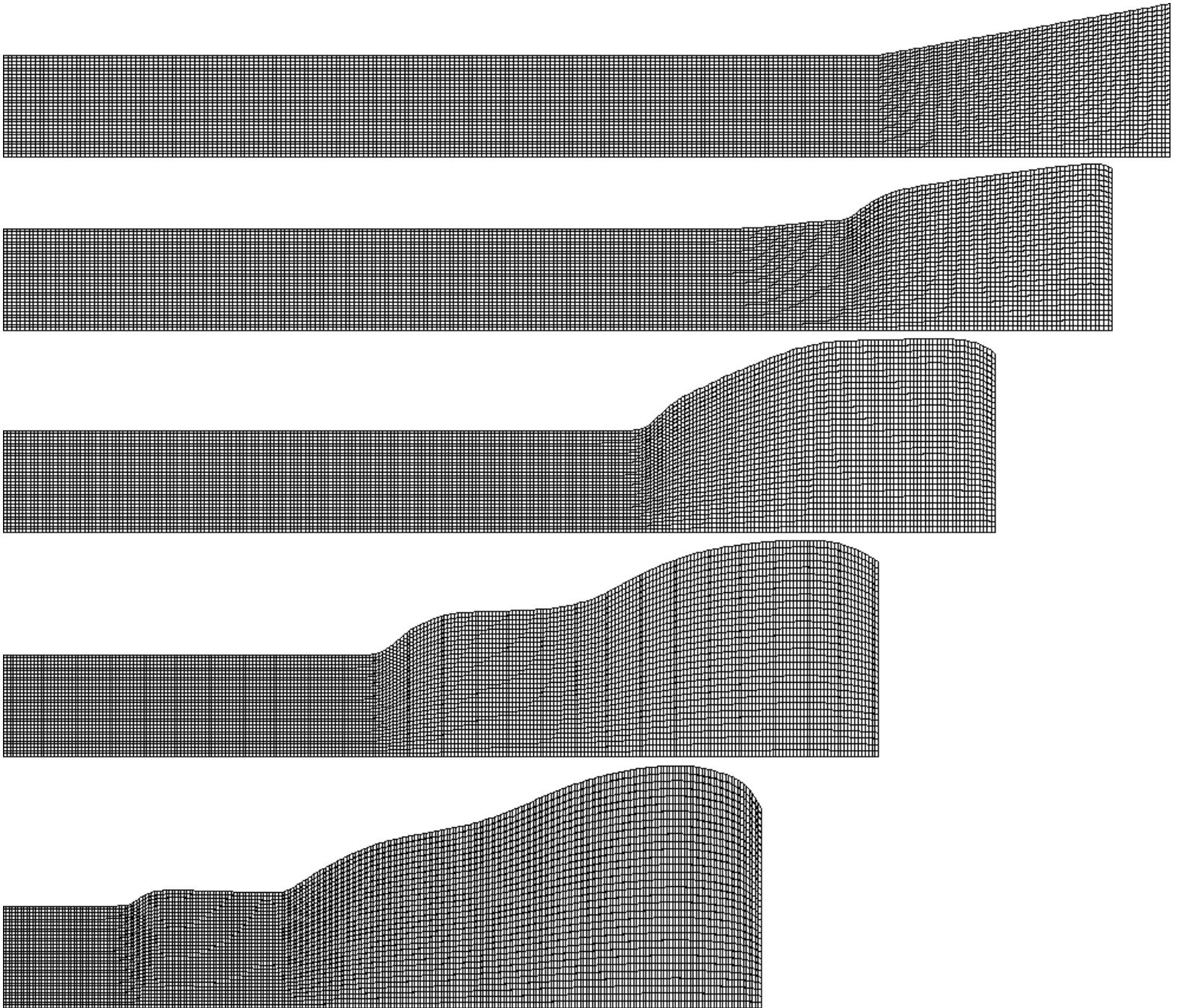
What is Gale

- A 2D/3D parallel code for Stokes and the energy equation
  - Accurately tracks material properties with particles
  - True free surface

Particles



True Free Surface



What is Gale

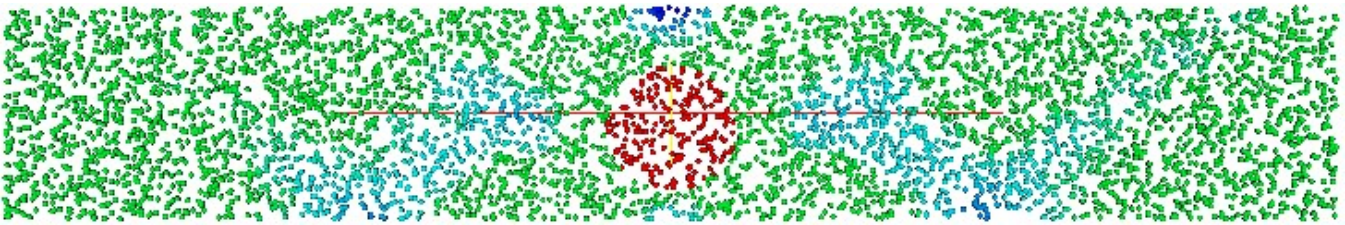
- Developed by CIG in response to a request from the long term tectonics community
- Built upon an existing code, Underworld, which was developed by the Victorian Partnership for Advanced Computing and Louis Moresi's group at Monash University

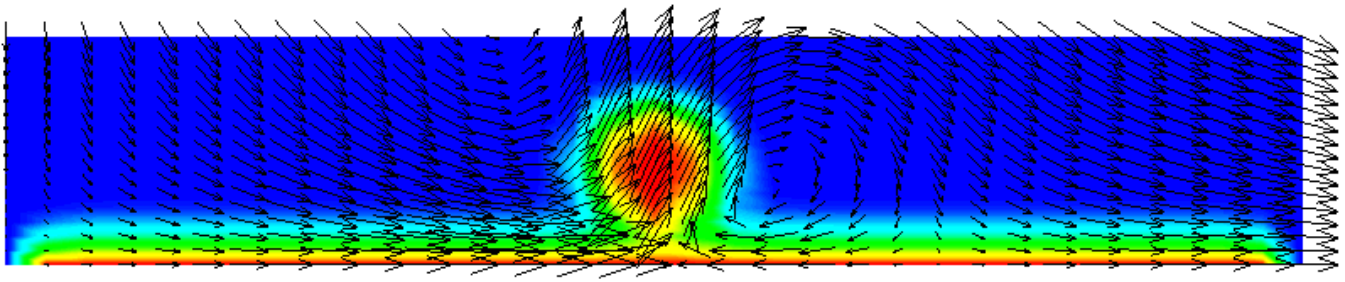
What is Gale

- Free Software
  - No paperwork
  - No license fees
  - No weird restrictions
    - Give it to your friends and enemies
    - Modify and redistribute. You can even try to compete with CIG (Good luck!)
    - Commercial and non-commercial use is fine
  - Just download and go

Extensive Documentation

- 100+ page manual
- 9 complete cookbook examples

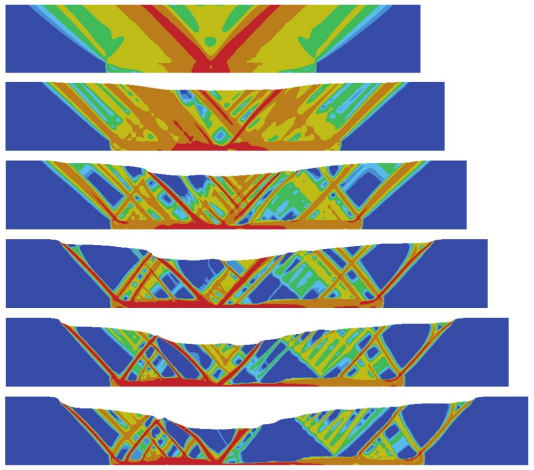




COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)
VICTORIA PARTNERSHIP FOR ADVANCED COMPUTING (VPAC)
MONASH UNIVERSITY

Gale

User Manual
Version 1.3



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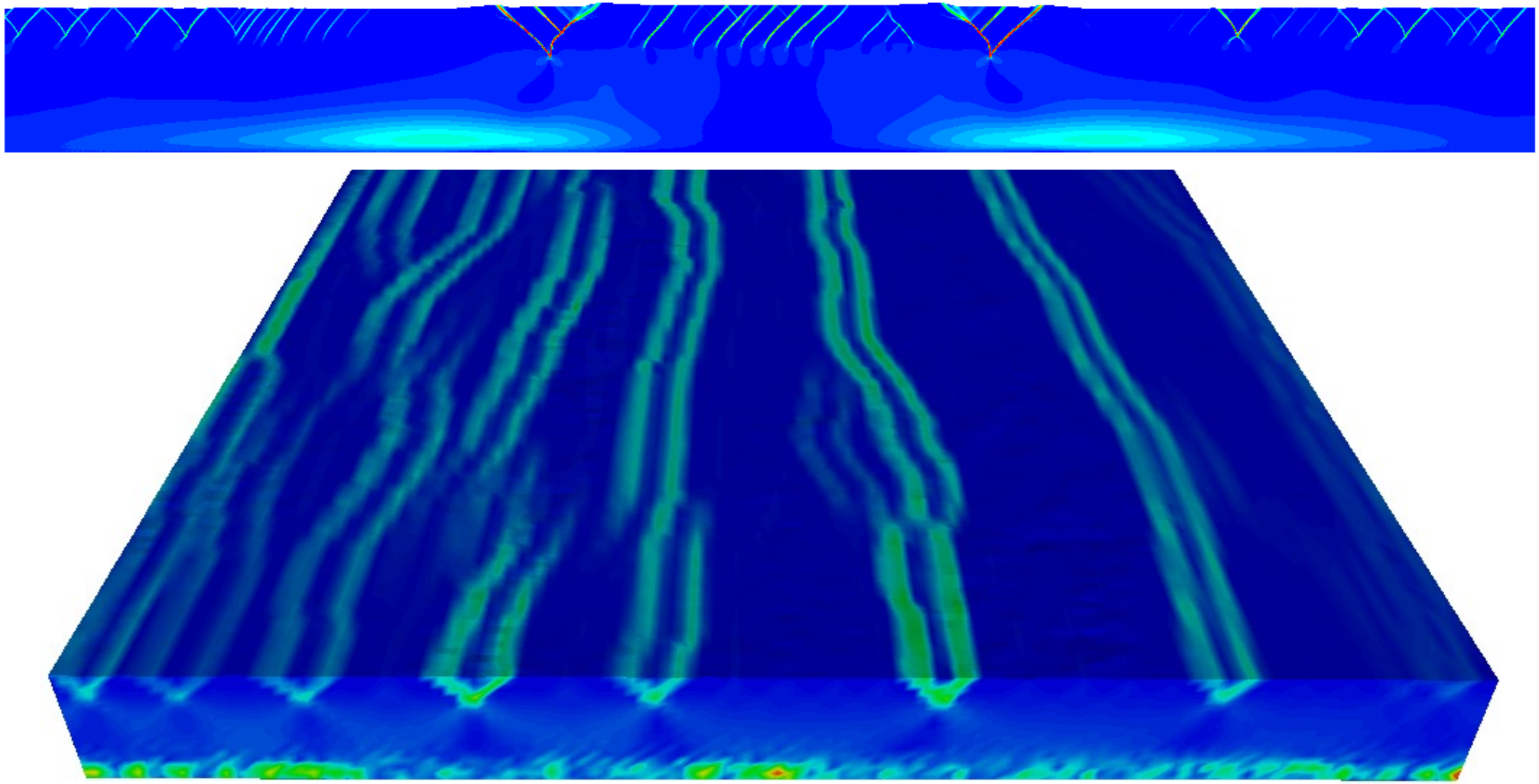
www.geodynamics.org

Geologic Example



Binaries

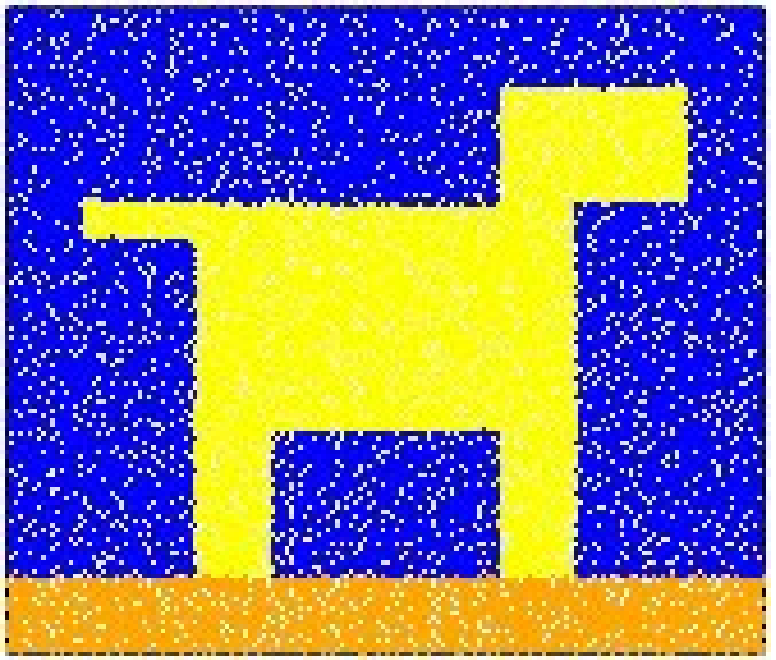
- Precompiled binaries are available for Linux x86, Linux AMD64, Mac PPC, Mac-Intel, Win32
- Gale is also installed on TACC Lonestar

Gale Capabilities

- Limited API for surface processes
- Many rheologies built in
  - Mohr-Coulomb
  - Drucker-Prager
  - Von Mises
  - Frank-Kamenetskii
  - Or make your own

Gale Capabilities

- Complex shapes which you mix and match just by changing the input file
  - Ellipsoid
  - Box
  - Half-plane
  - Polygon
  - Cylinder

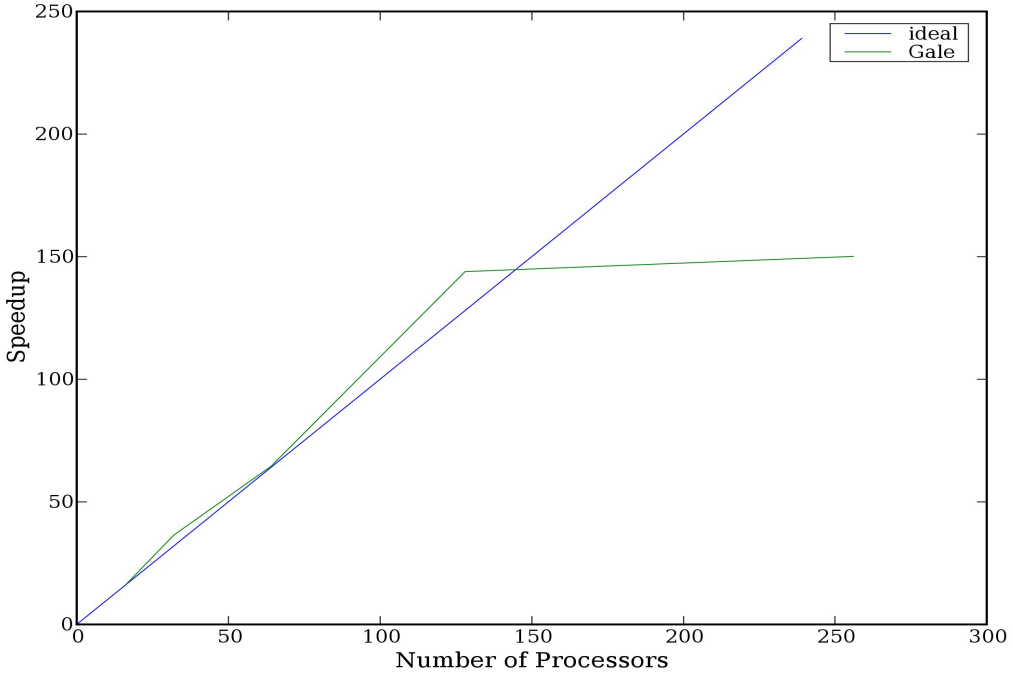


Gale Capabilities

- Many different boundary conditions
  - Fixed
  - Moving with a wide range of velocity profiles
  - Free slip
  - Stress: normal and tangential
  - Friction: static and kinetic
  - Inflow/Outflow

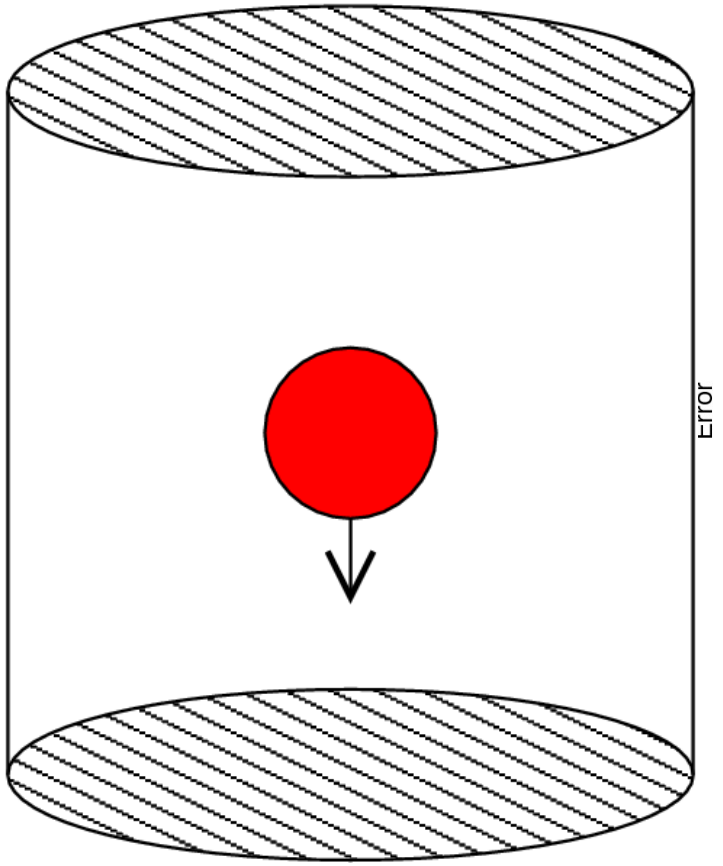
Gale Capabilities

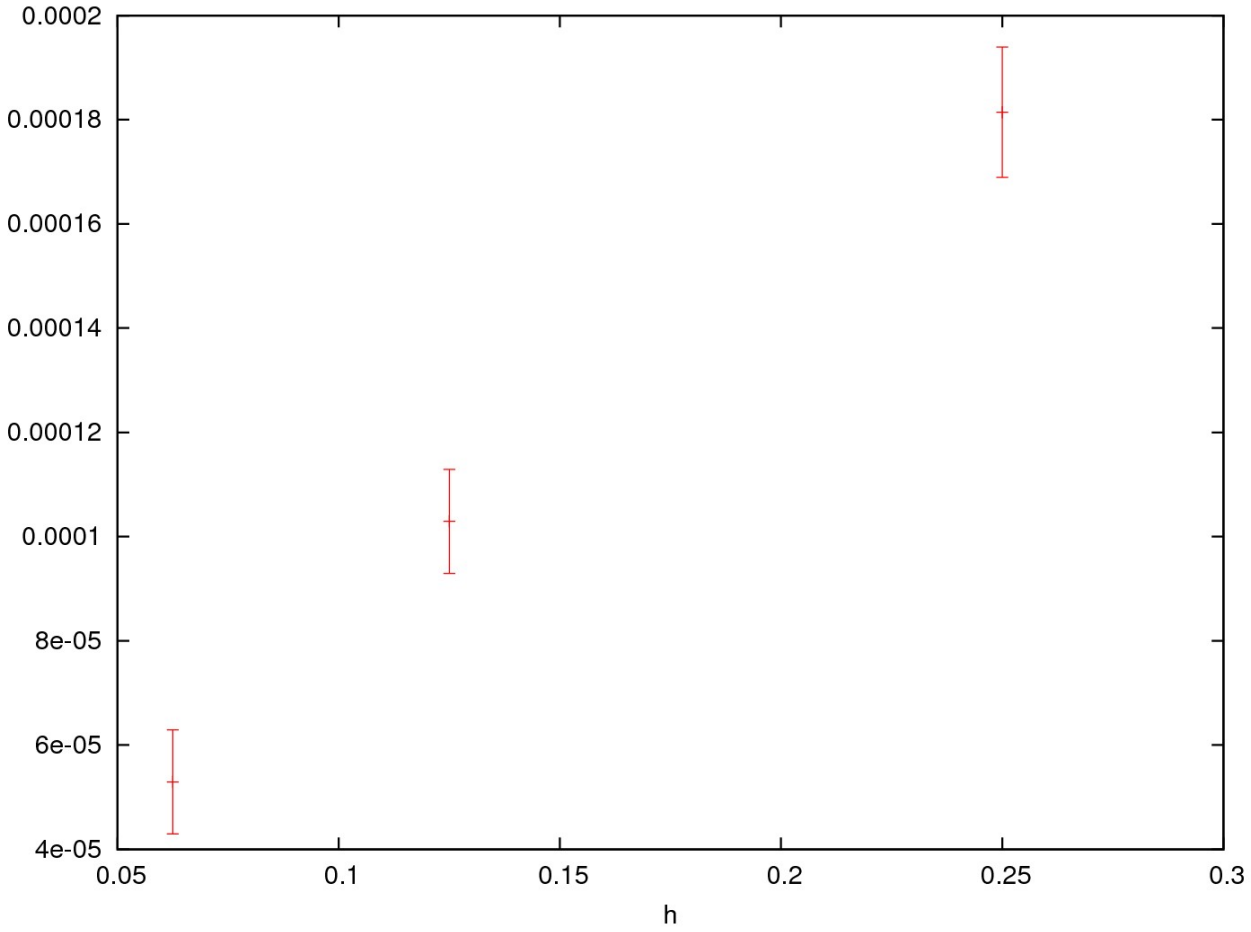
- Works in parallel
  - Linear scaling demonstrated from 16 to 128 processors for a small problem
  - No fundamental limit



Benchmarks

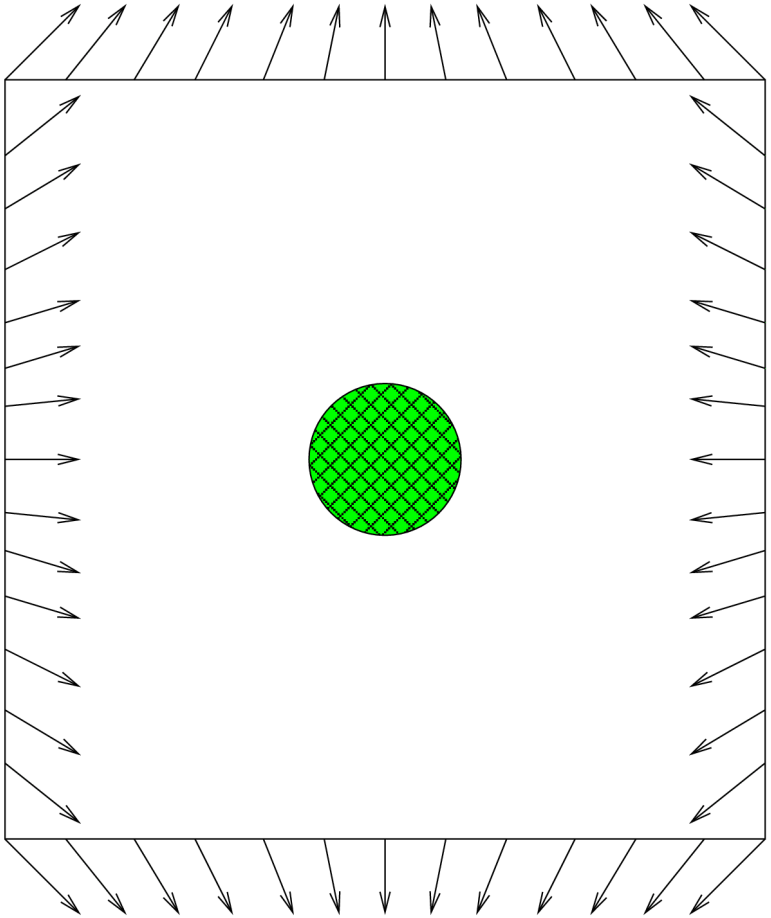
- Falling sphere in a cylinder

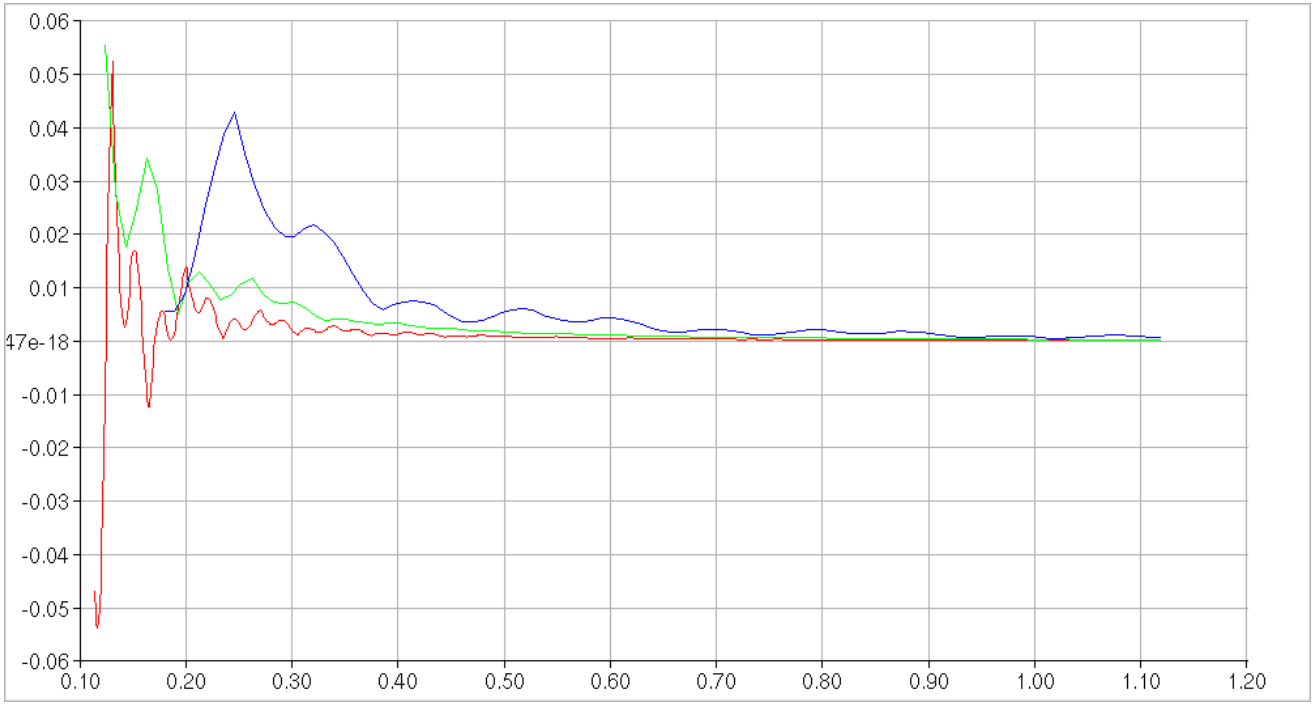




Benchmarks

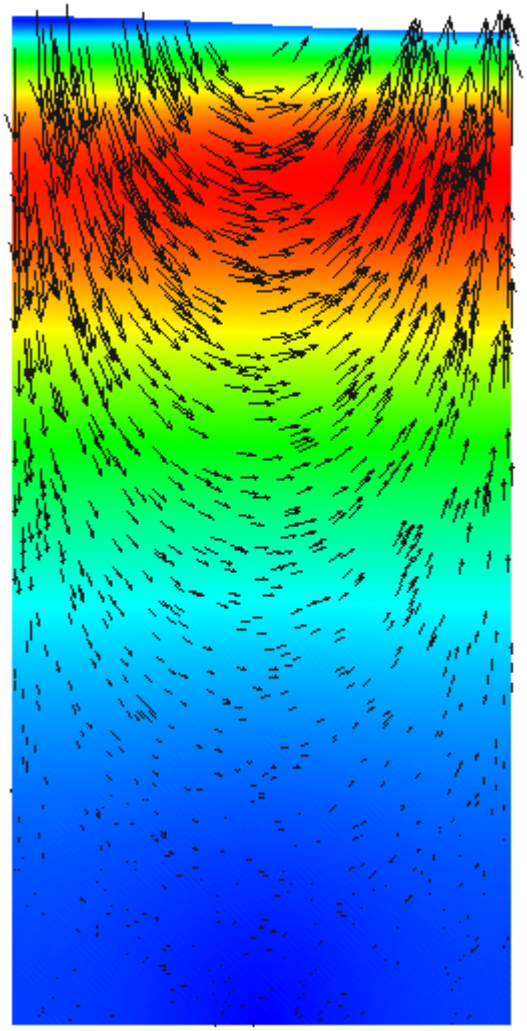
- Circular inclusion

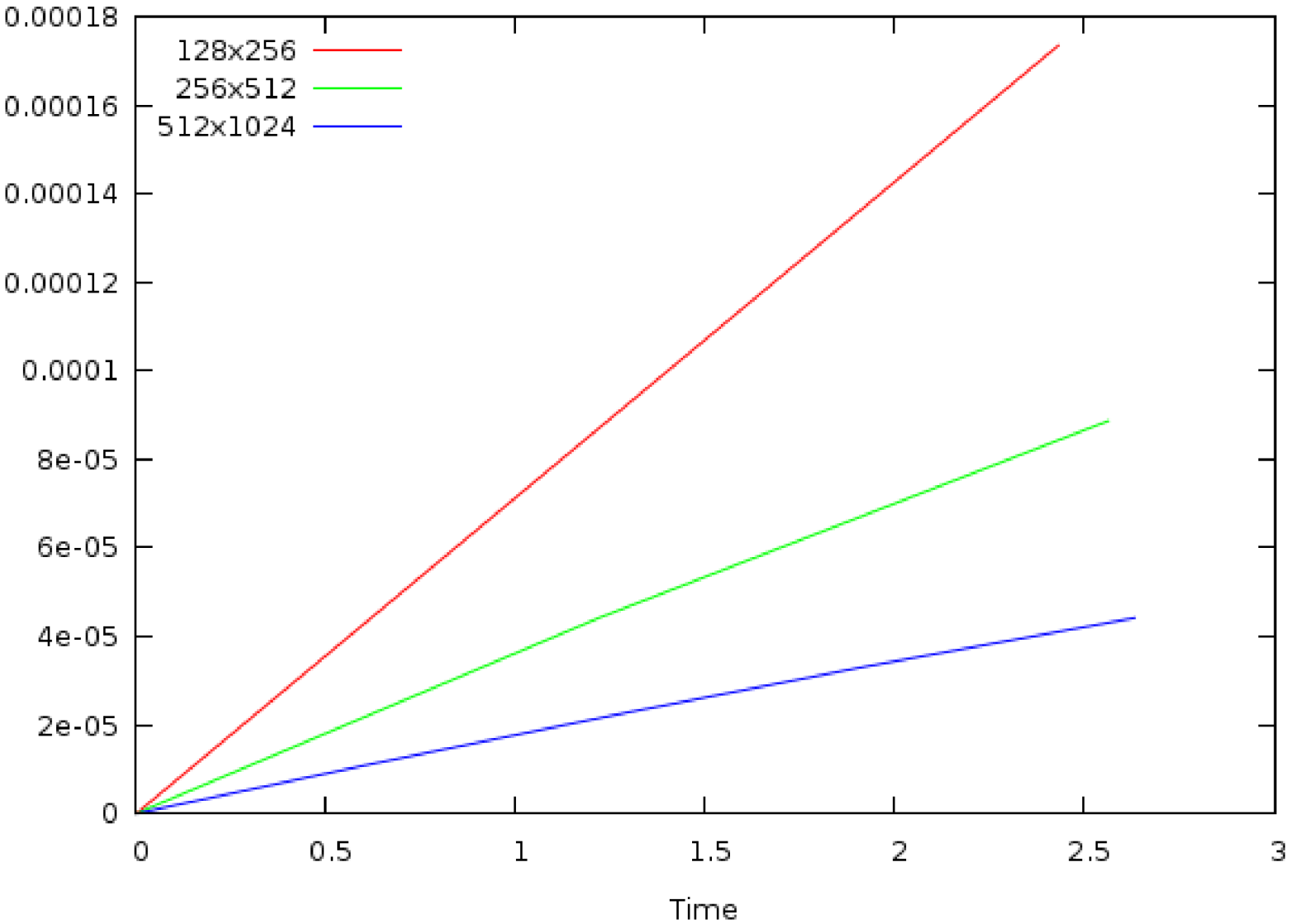




Benchmarks

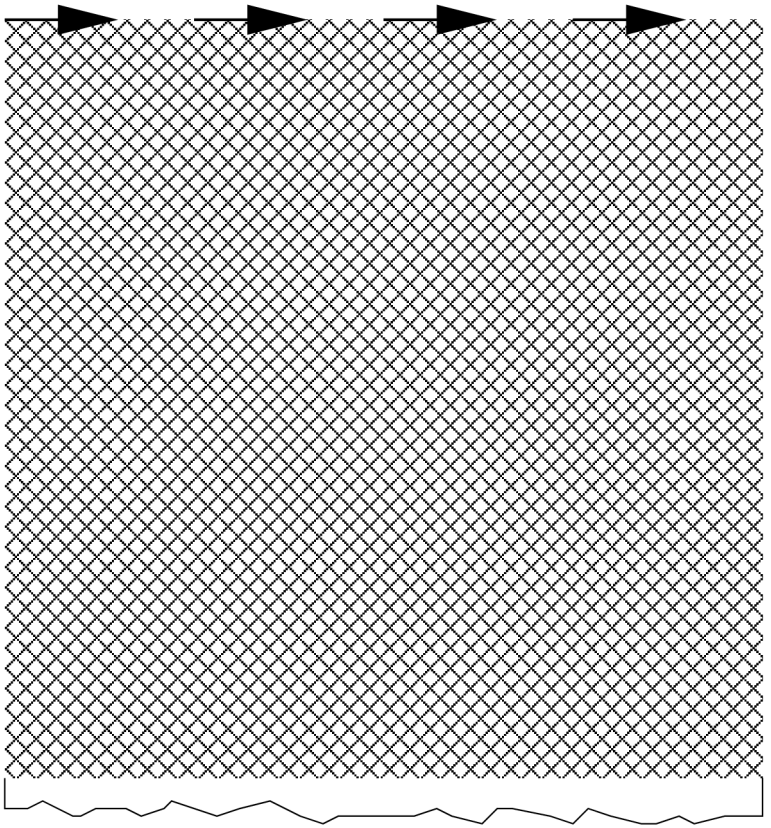
- Relaxation of topography





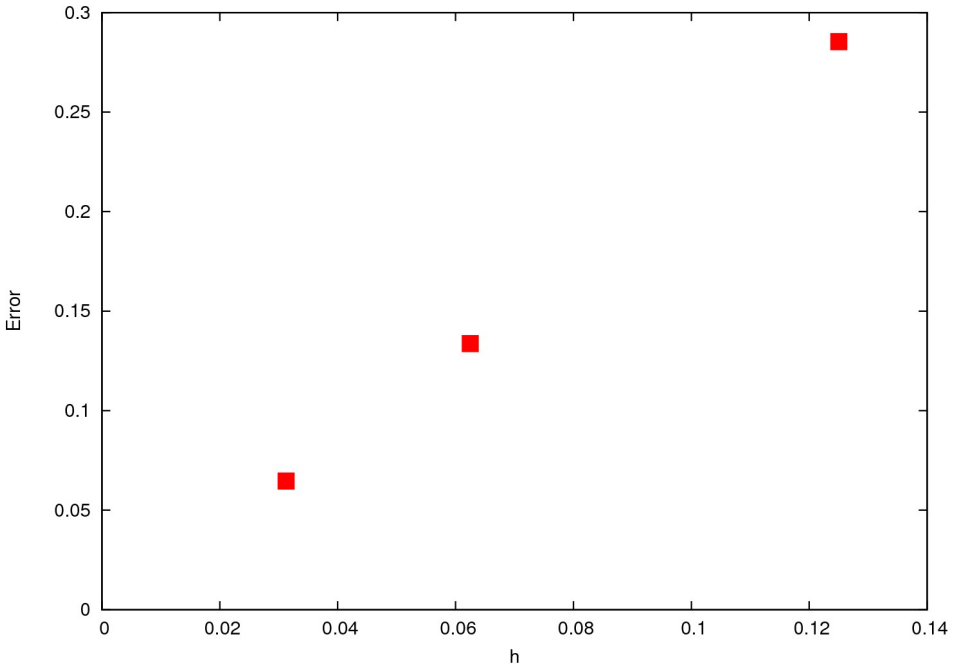
Benchmarks

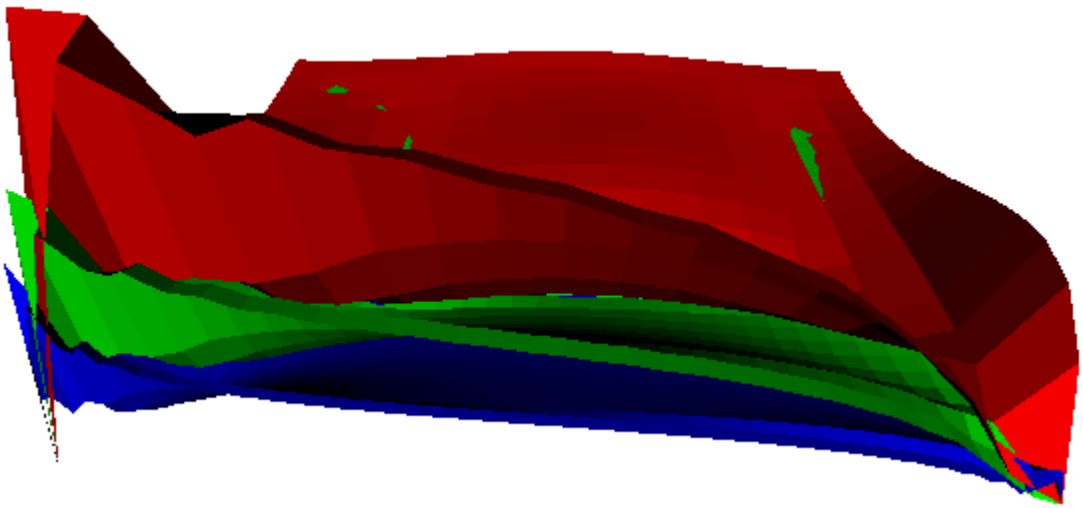
- Shear



Shear Benchmark

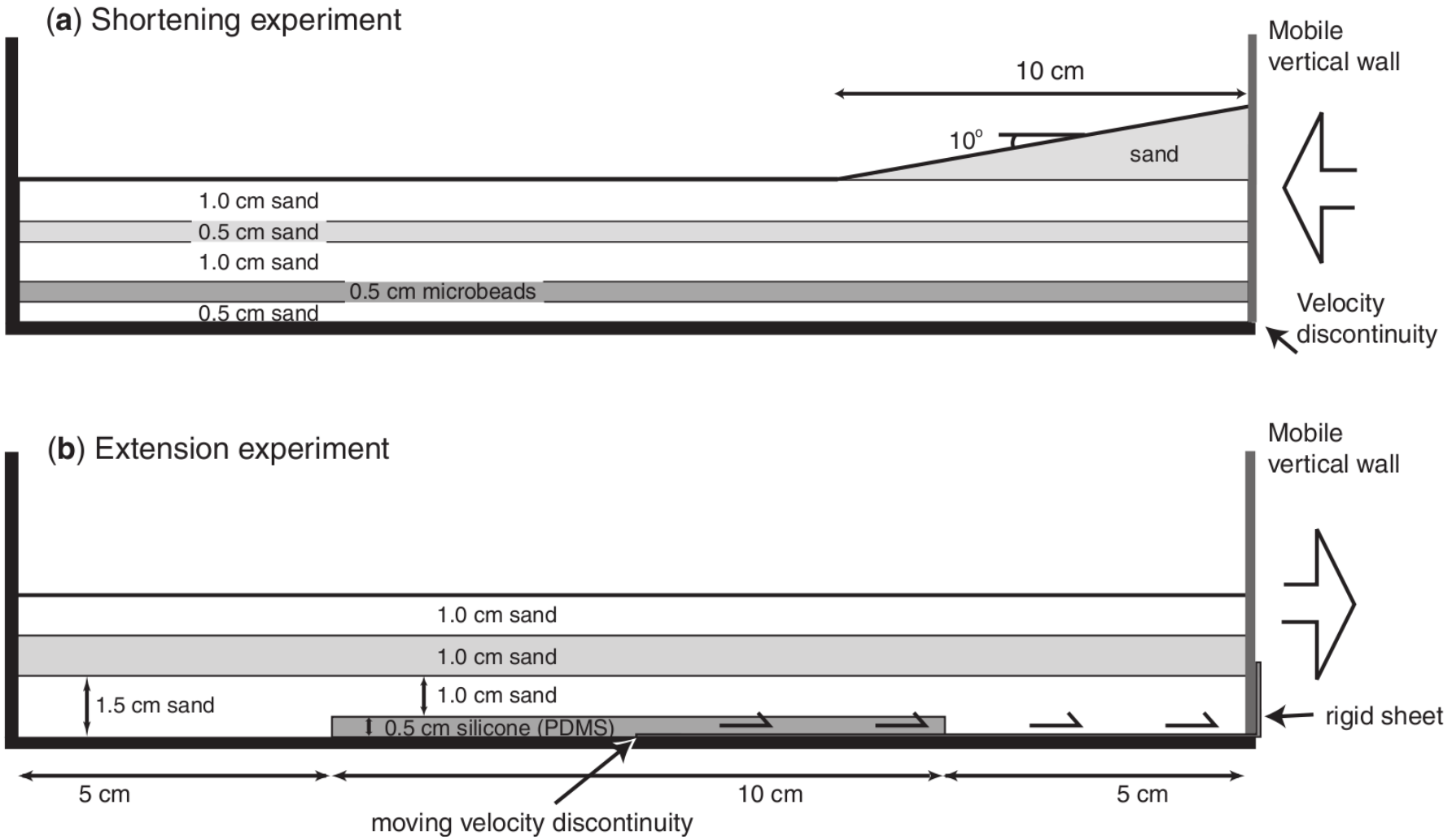
- Static Friction
- Kinetic Friction



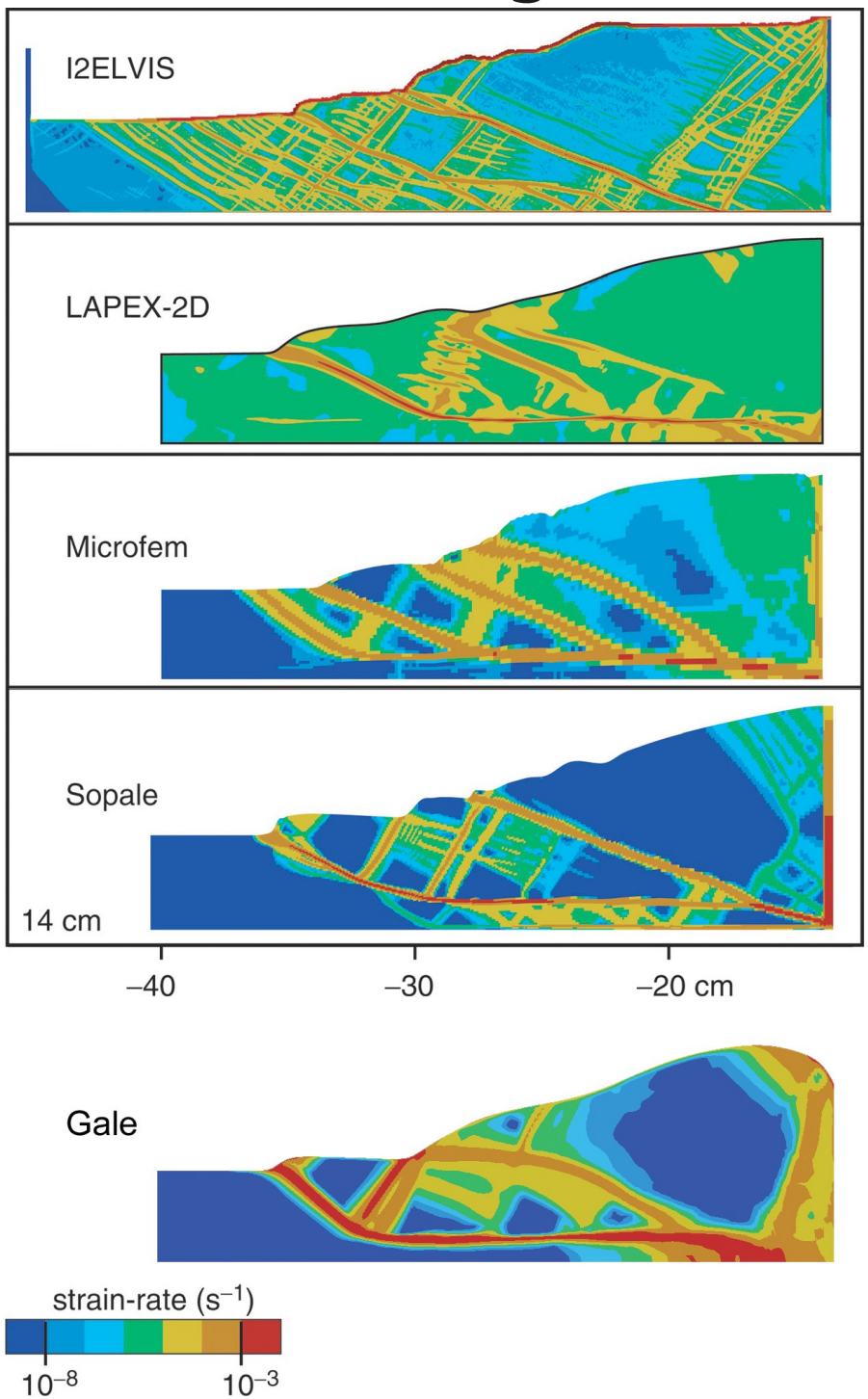


Benchmarks

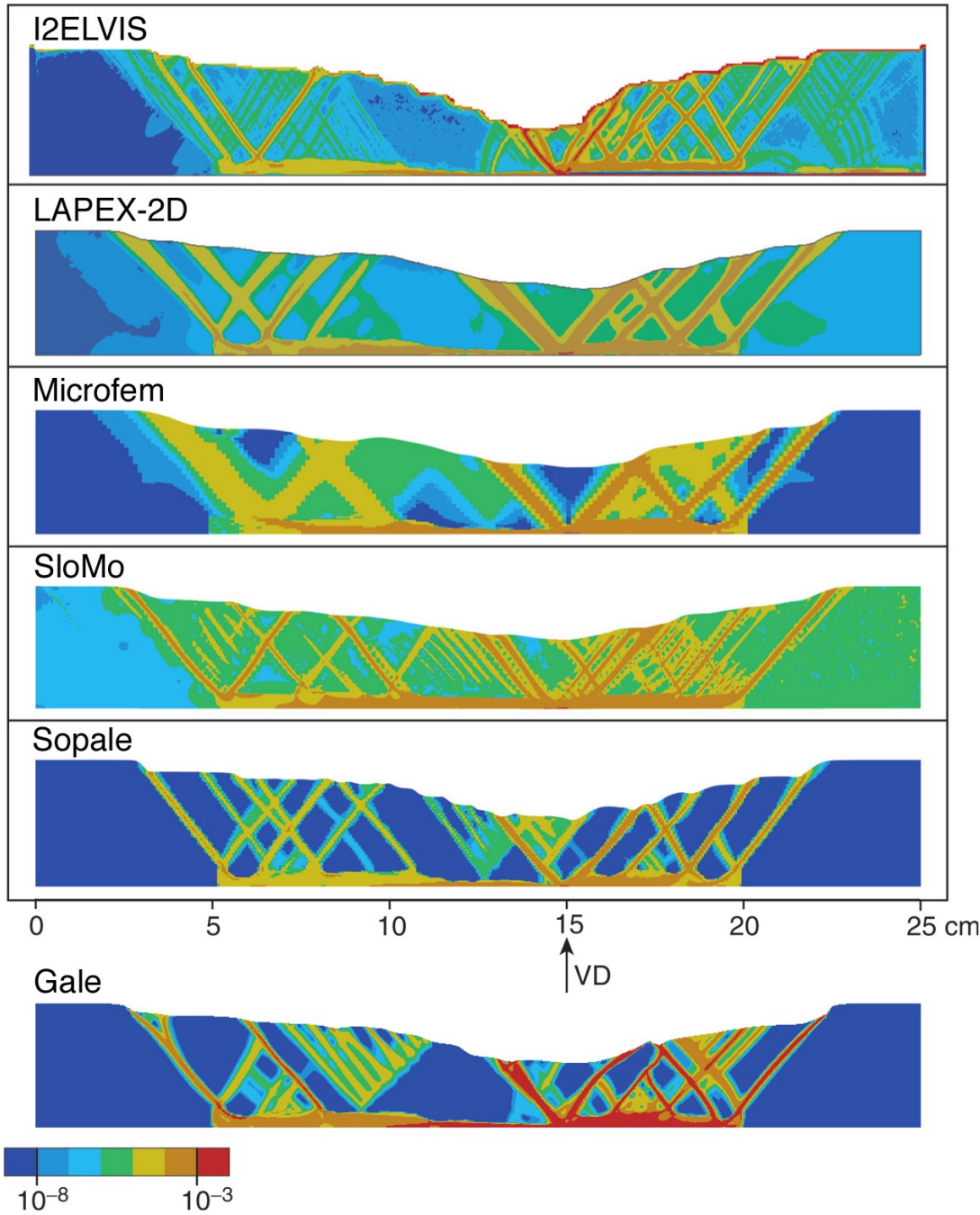
- Geomod 2004



- Shortening

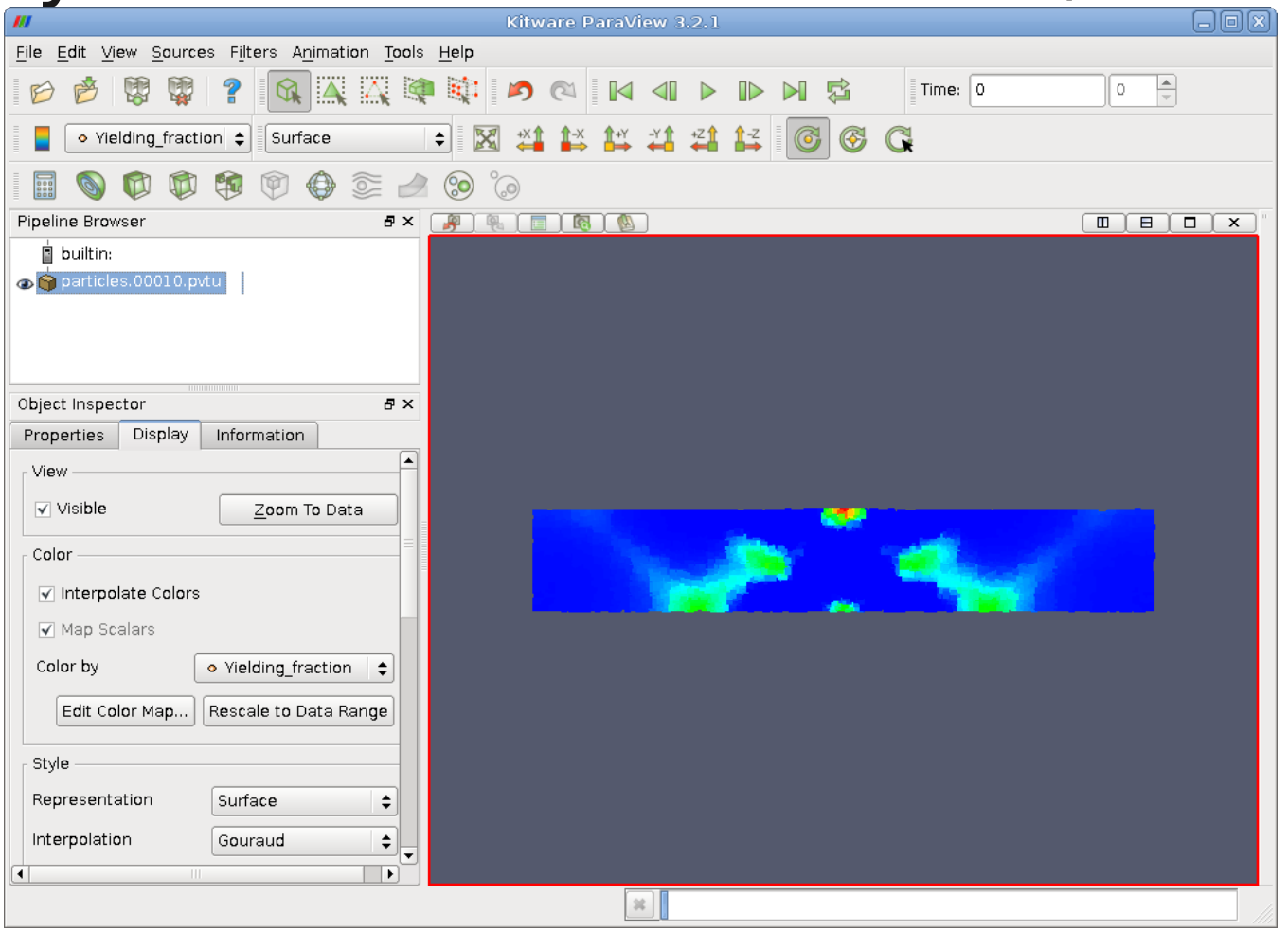


- Extension



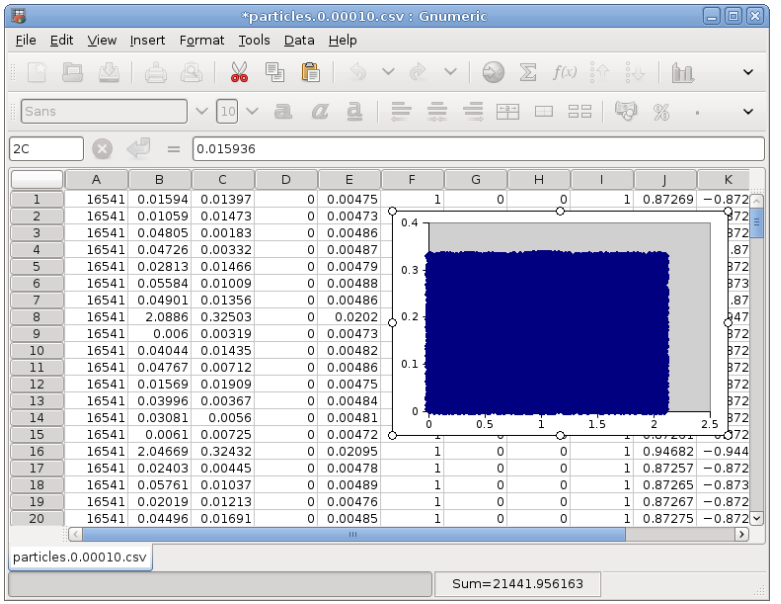
Visualization

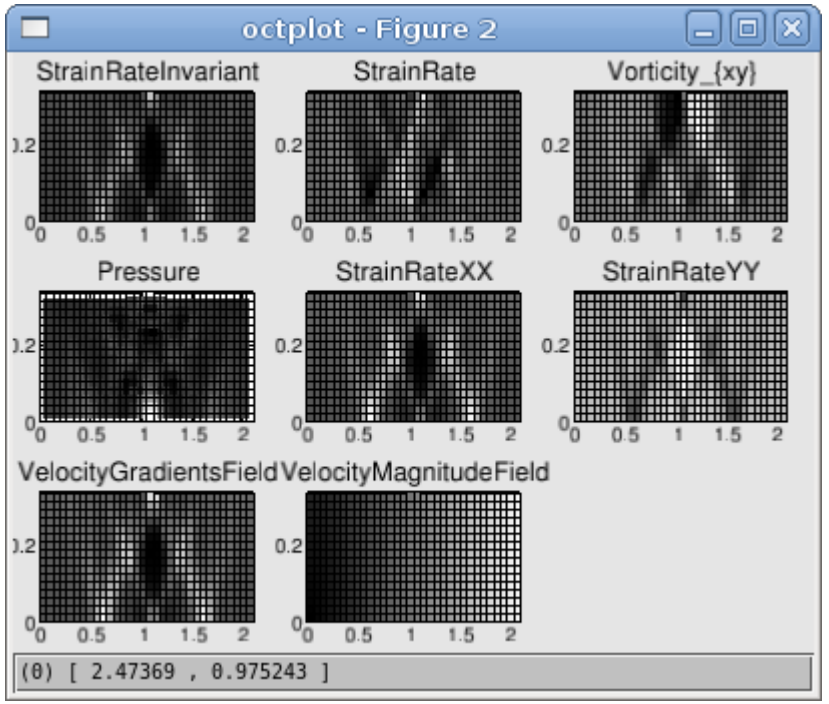
- Gale outputs in parallel VTK format, making it easy to visualize in Paraview, Mayavi, or Visit.

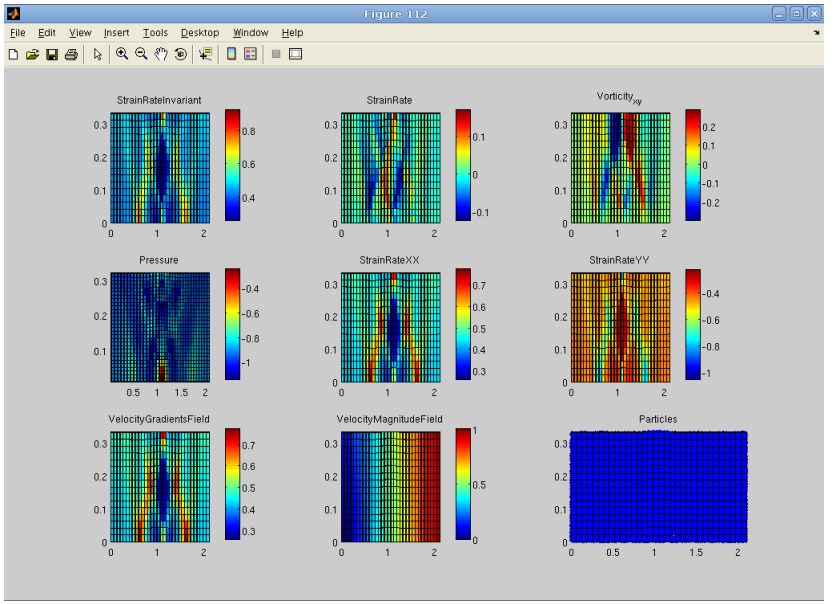


Visualization

- There are also scripts to visualize with Octave, Matlab, and Excel







Future Work

- Deformed lower boundaries
- Parallel surface processes
- Better normal stress boundary conditions
- Geomod 2008 benchmarks

Installation

- Easy: Use the binaries (even on TACC)
- Failing that, you will have to build it yourself.
- Gale requires
  - libxml2 (including development headers)
  - Petsc 2.3.2 (not 2.3.3)
  - mpi
- Generally, Petsc is the hardest part

Petsc Installation

- Get the 2.3.2 source tarball from
  - http://www-unix.mcs.anl.gov/petsc/ petsc-as/download/index.html
- Unpack it
  - tar -zxf petsc-2.3.2-p10.tar.gz
- cd petsc-2.3.2-p10

Petsc Configuration

- Try configuring it
  - config/configure.py
- If this works, you will have to set two environment variables
  - PETSC_ARCH
  - PETSC_DIR
- Then type “make all”

Petsc Troubleshooting

- Unfortunately, this often does not work.
- If configuration seems to hang forever, the problem could be that you have to submit all mpi jobs to the queue.
- Add the option –-with-batch=1
  - config/configure.py --with-batch=1

Petsc Troubleshooting

- Then petsc will ask you to submit a script “conftest” to the batch system.
- In practice, I have always been able to just run the script manually
- Then run “python reconfigure”

Petsc Troubleshooting

- Your mpi compiler may be in a non standard location
  - --with-mpi-dir=/opt/mpich/myrinet/intel
- Fortran binding may cause problems
  - --fc=0

Petsc Troubleshooting

- Petsc can not find a blas or lapack library.
  - If you are using the Intel compiler, then find out where mkl is and add the option --with-blas-lapack-dir=/path/to/mkl
  - Otherwise, use the option --download-c-blas-lapack=yes

Petsc Troubleshooting

- You can get a complete list of options to configure
  - config/configure.py --help

Petsc Optimized and Debug

- Petsc, by default, creates libraries with debugging information.
- To turn on optimization, add the option --with-debugging=0

Gale Installation

- Gale uses the same configuration mechanism as Petsc.
- So you will usually copy the compiler information from Petsc to Gale
  - PETSC: config/configure.py –with-mpi-dir=/opt/intel
  - GALE: ./configure --with-mpi-dir=/opt/intel

Gale Installation

- You do not have to copy any information about blas and lapack
- If you set the environment variable PETSC_ARCH and PETSC_DIR, then Gale will find and use that automatically.
- Otherwise, use the –with-petsc-arch and –with-petsc-dir options.

Gale Installation

- Once you are done configuring, type “make” and then “make install”.
- The executable will be in bin/Gale, and will have the same optimization/debug options as Petsc.

Running Serial Jobs

- Gale always needs an input file
  - ./Gale input/cookbook/yielding.xml
- If you do not give an input file, you will get an error
  - Error in _AbstractContext_New: The dictionary is empty, meaning no input parameters have been feed into your program. Perhaps you've forgot to pass any input files (or command-line arguments) in. Gale-debug: build/StGermain/Base/IO/src/Journal.c:603: Journal_Firewall: Assertion `expression' failed. p0_12616: p4_error: interrupt SIGx: 6

Running Serial Jobs

- If you give an input file that does not exist, you will get a different error
  - Error: File foo.xml doesn't exist, not readable, or not valid. Gale-debug: build/StGermain/Base/IO/src/Journal.c:603: Journal_Firewall: Assertion `expression' failed. p0_13533: p4_error: interrupt SIGx: 6

Running Serial Jobs

- Some MPI implementations change the current directory, so that Gale will not be able to find your input file.
- The workaround is to give the complete name of the input file
  - ./Gale /home/walter/gale/input/cookbook/yielding.xml

Running Serial Jobs

- Gale also accepts Petsc's command line options.
- For example, to use a direct LU solve instead of GMRES (Often much faster)
  - ./Gale input/extension.xml -pc_type lu -ksp_type preonly

Running Serial Jobs

- You can also override any parameter in the input file from the command line
  - ./Gale extension.xml –maxTimeSteps=10

Running Parallel Jobs

- If you have your own multi-cpu machine, then to use more than one processor, prepend mpirun or mpiexec to the whole command
  - mpirun -np 2 bin/Gale /home/walter/gale/input/extension.xml

Running Parallel Jobs

- On a shared facility such as the teragrid, you will have to submit a job to the queue.
- This varies from site to site. The site administrators should provide a sample script.

Using a Parallel Direct Solver

- If you have everything working, you can get a parallel direct solver working by configuring Petsc with
  --download-mumps=yes
  --download-blacs=yes
  --download-scalapack=yes
  --with-blacs=yes
  --with-scalapack=yes
- Then add to the command line
  -mat_type aijmumps -ksp_type preonly
  -pc_type lu

Writing Input Files

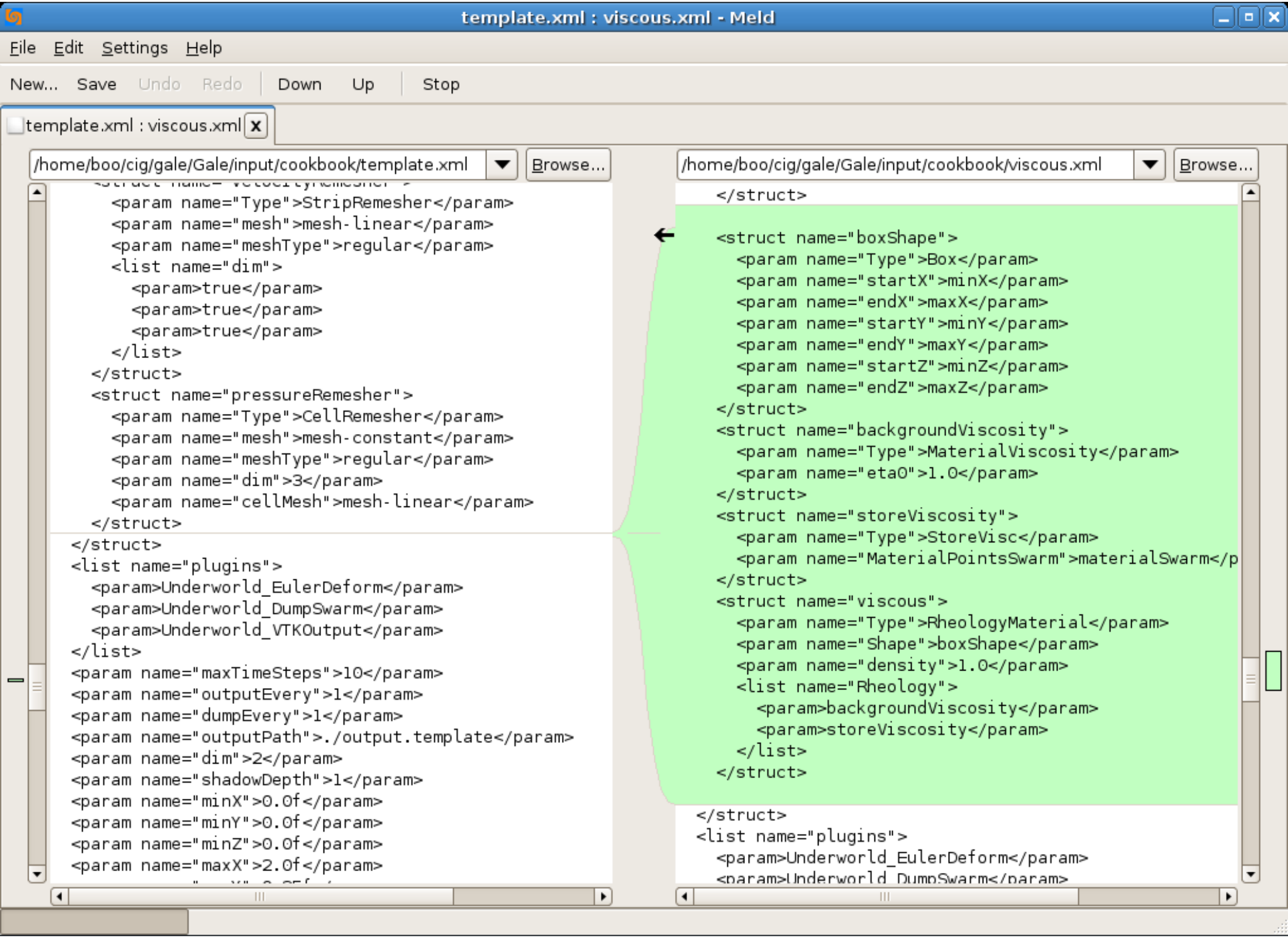
- Gale is based upon a generic library for scientific computing: StGermain
- So you must explicitly specify a number of things which are normally implicit (e.g. we are solving a Stokes flow problem)
- The input format (XML) is similarly generic and (unfortunately) wordy.

Writing Input Files

- So the input files tend to be rather large.
- Most of the parameters will not change. So you only need to copy in a template
  - input/cookbook/template.xml

Writing Input Files

- The manual leads you through the modification of this template to create different models.
- We will start with the first example, where we add a viscous material to the template.


template.xml : viscous.xml - Meld
File Edit Settings Help
New... Save Undo Redo Down Up Stop
template.xml : viscous.xml
/home/boo/cig/gale/Gale/input/cookbook/template.xml
Browse...
/home/boo/cig/gale/Gale/input/cookbook/viscous.xml
Browse...
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<param>true</param>
<param>true</param>
</list>
</struct>
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</struct>
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<param>Underworld_DumpSwarm</param>
<param>Underworld_VTKOutput</param>
</list>
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<param name="dumpEvery">1</param>
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<param name="shadowDepth">1</param>
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<param name="minY">0.0f</param>
<param name="minZ">0.0f</param>
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<param name="startY">minY</param>
<param name="endY">maxY</param>
<param name="startZ">minZ</param>
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</struct>
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</list>
</struct>
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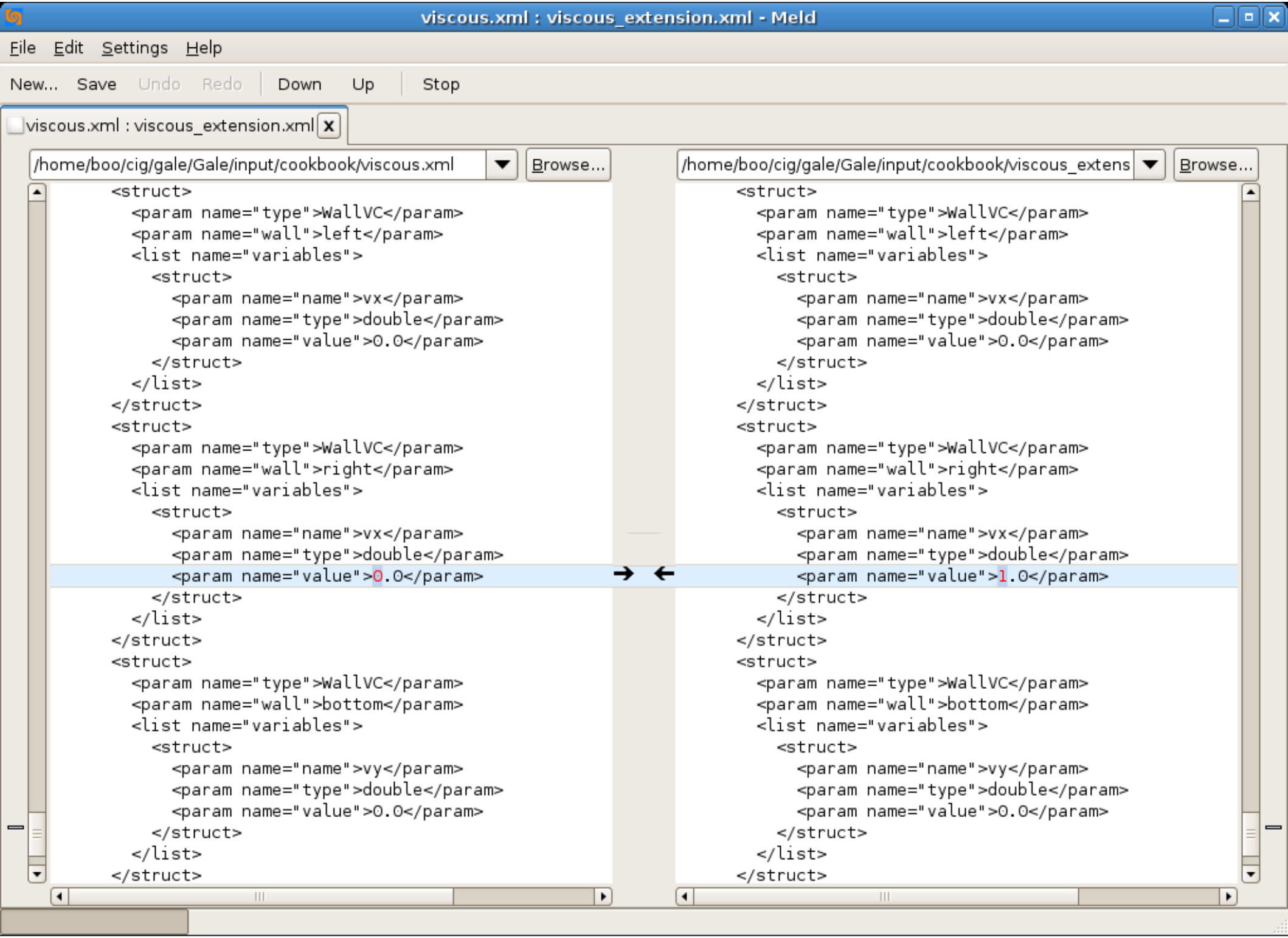
Writing Input Files

- Next, we add a moving boundary


viscous.xml : viscous_extension.xml - Meld
File Edit Settings Help
New... Save Undo Redo Down Up Stop
viscous.xml : viscous_extension.xml
/home/boo/cig/gale/Gale/input/cookbook/viscous.xml
Browse...
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Browse...
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</struct>
<struct>
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</struct>
<struct>
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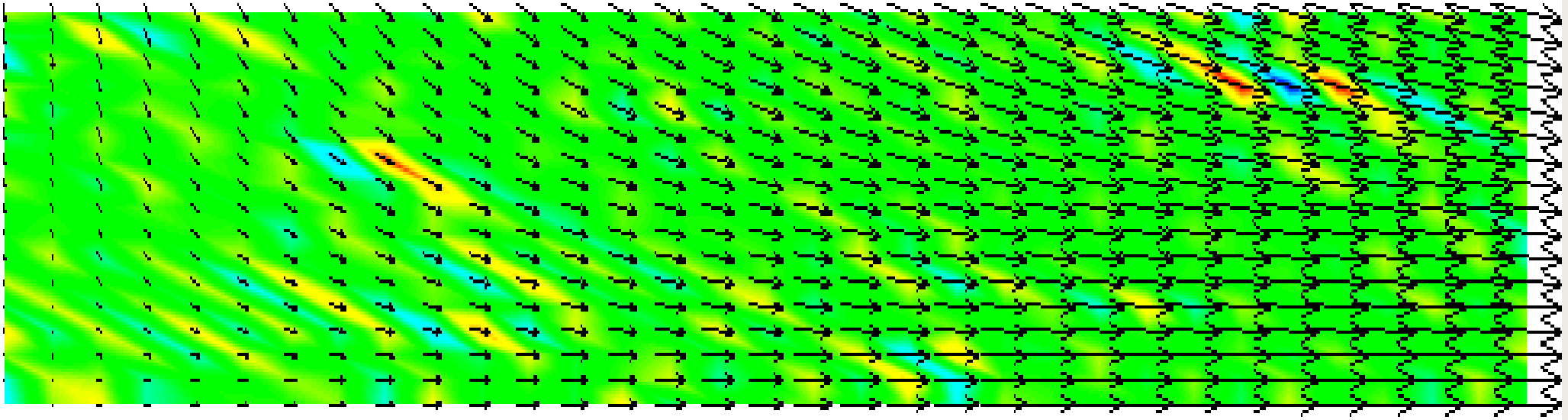
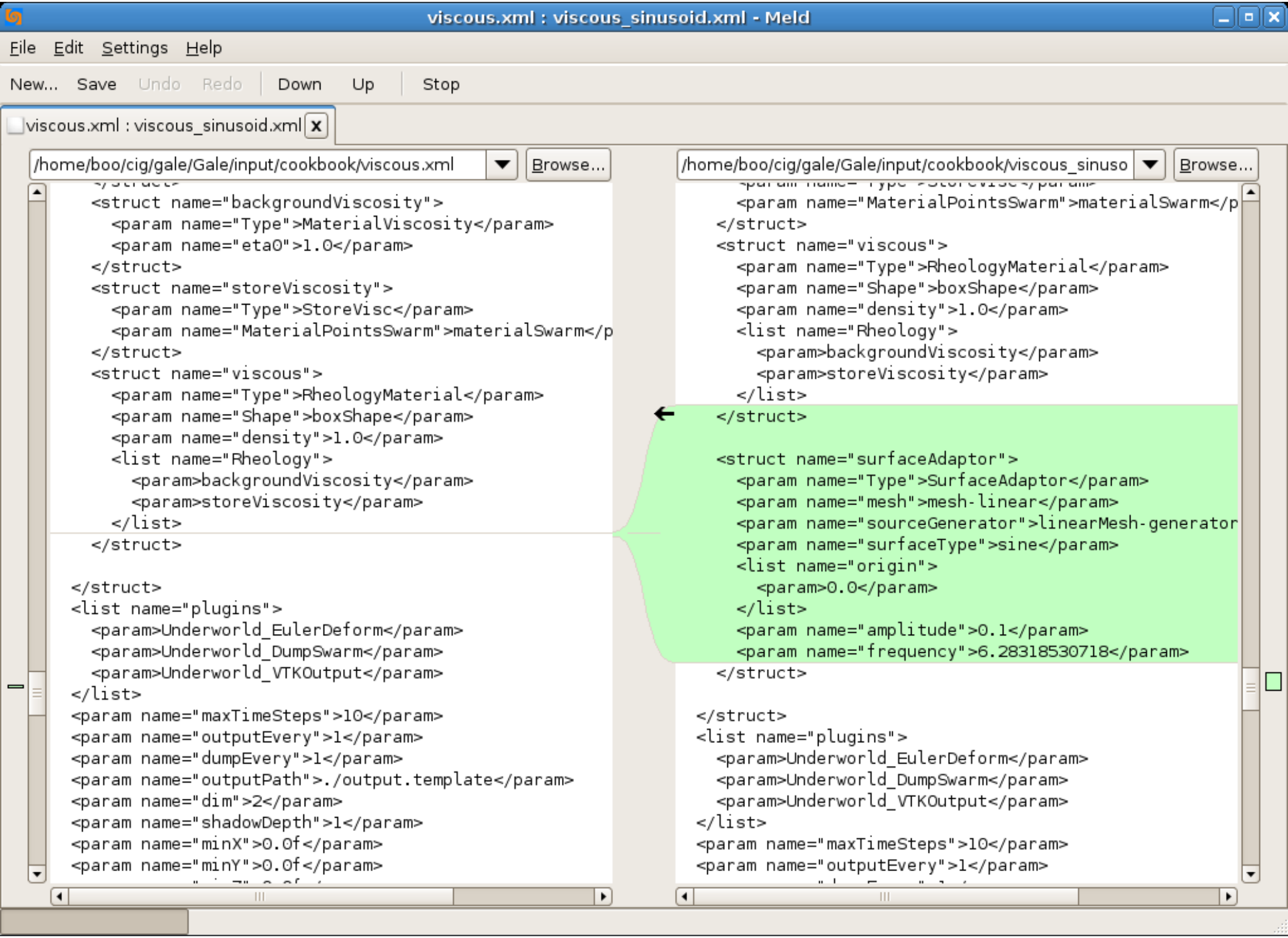
Visualization

- We can then visualize the results in Paraview



Visualization

- The banding is a numerical artifact. If we increase the number of particles per cell, then the effect decreases.
- For the other simulations, you will not see this banding, even though we have not changed the number of particles per cell.


viscous.xml : viscous_sinusoid.xml - Meld
File Edit Settings Help
New... Save Undo Redo Down Up Stop
viscous.xml : viscous_sinusoid.xml
/home/boo/cig/gale/Gale/input/cookbook/viscous.xml
Browse...
/home/boo/cig/gale/Gale/input/cookbook/viscous_sinuso
Browse...
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</struct>
<struct name="storeViscosity">
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<list name="plugins">
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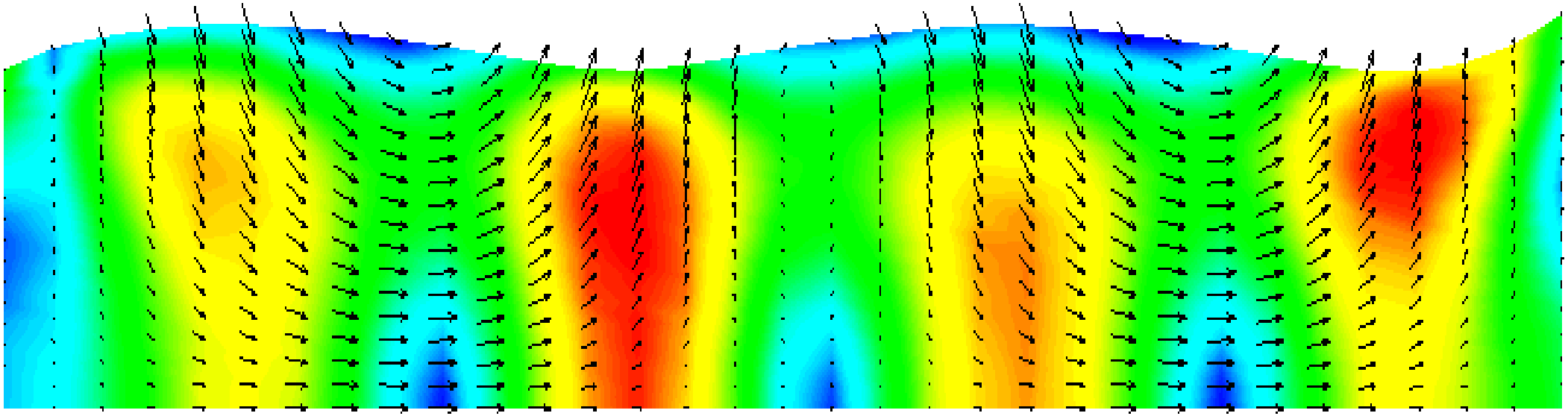

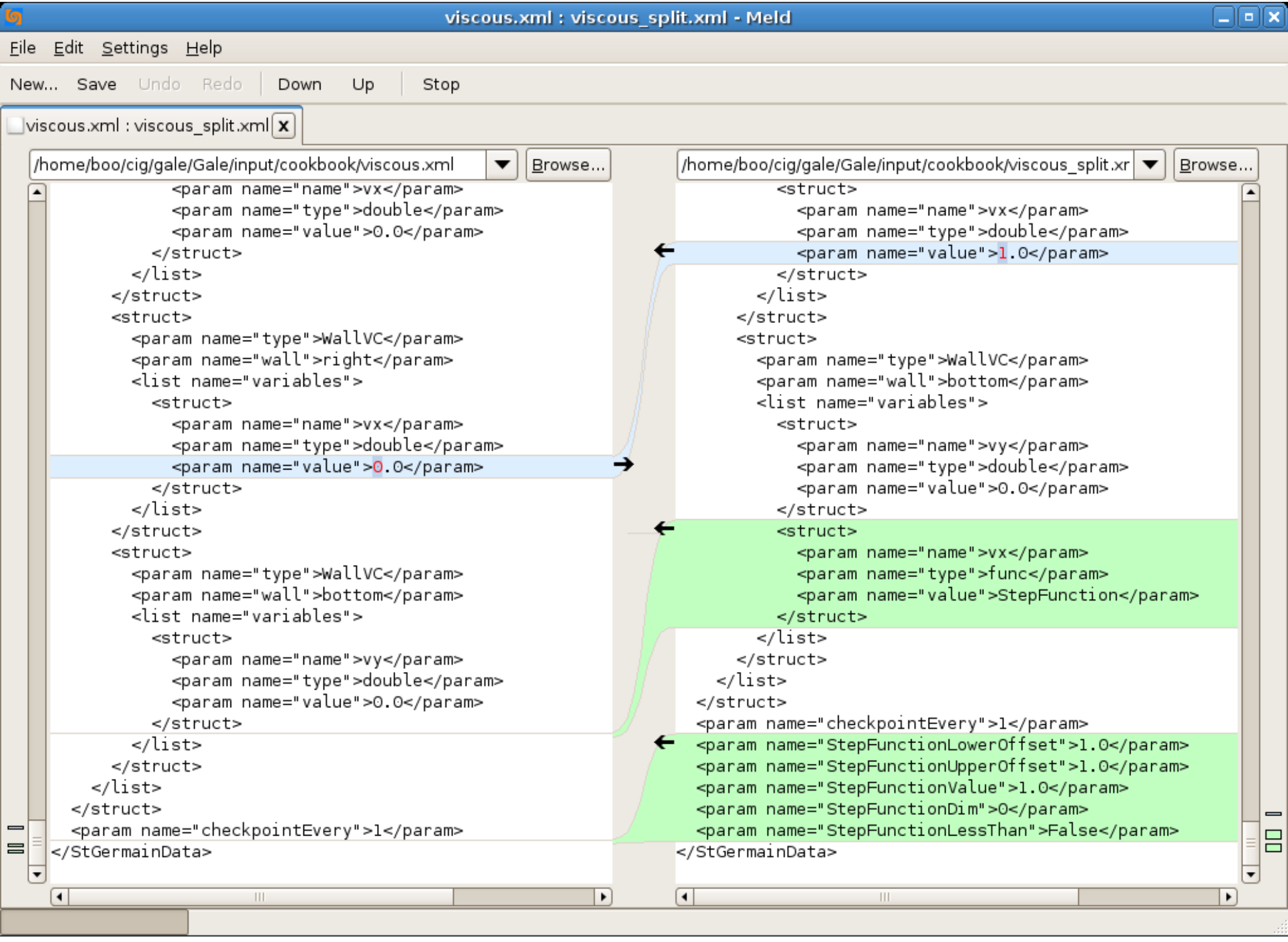
viscous.xml : viscous_split.xml - Meld
File Edit Settings Help
New... Save Undo Redo Down Up Stop
viscous.xml : viscous_split.xml
/home/boo/cig/gale/Gale/input/cookbook/viscous.xml
Browse...
/home/boo/cig/gale/Gale/input/cookbook/viscous_split.xr
Browse...
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<param name="type">double</param>
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</struct>
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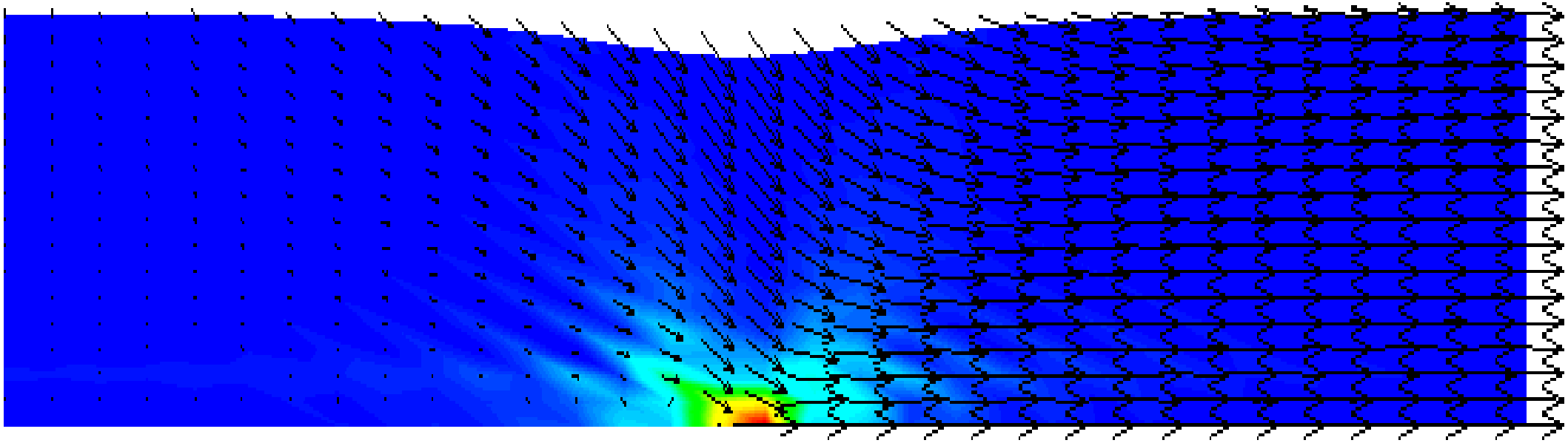

Evaluating Accuracy

- You must vary the accuracy parameters for every single publishable result.
  - Resolution
  - Number of particles/cell
  - Linear and nonlinear solution tolerance
  - size of the boundary region
  - size of the whole simulation (for some boundary conditions)