MONASH University
Monash Cluster Computing

Introducing Underworld: The code from down under

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thanks to D. Stegman, L. Moresi, D. May, P. Sunter, L. Hodgekinson, S Quenette

VPAC
VICTORIAN PARTNERSHIP FOR ADVANCED COMPUTING

Underworld Facts

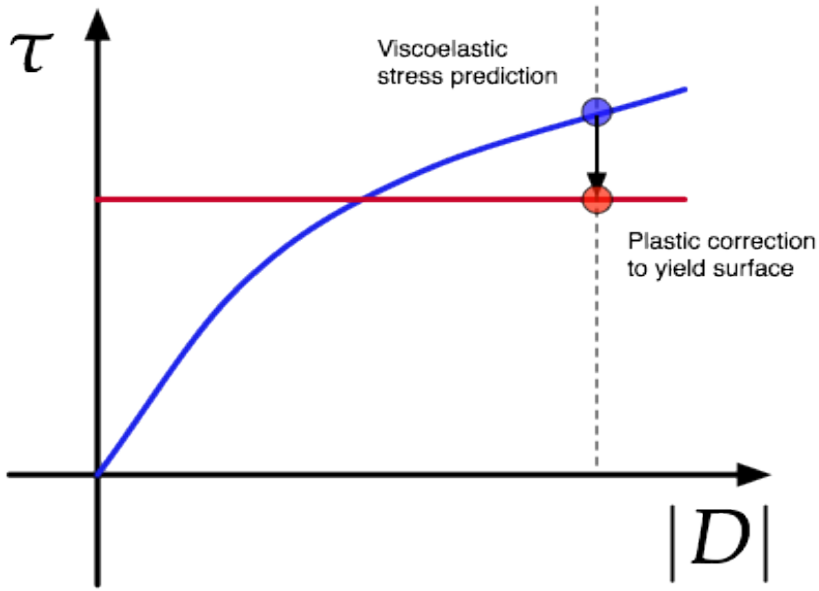
- A 3D Parallel, **Community based** Geodynamics Code. Capable of Convection and Deformation modelling.
- Has it's own visualisation software, called gLucifer.
- Written in C, but in an Object Oriented style.
- Uses PETSc libraries for optimised numerical solvers.
- Uses MPICH libraries for parallelism.
- Australian made, in Melbourne.

Equations in Underworld

$$\tau_{ij,j} - p_{,i} = \rho(T, C, \ldots) g_i - f_{,i}^{\Delta T}$$

$$u_{i,i} = 0$$

Momentum and Mass conservation



Scheme for plastic correction

$$\frac{\overset{\nabla}{\tau}_{ij}}{\mu} + \frac{\tau_{ij}}{\eta} + \alpha \Lambda_{ijkl} \tau_{kl} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}$$

Constitutive rule

$$T_{,t} + u_i T_{,i} = (\kappa T_{,i})_{,i} + Q$$

Energy conservation

$$C_{,t} + u_i C_{,i} = 0$$

Advection of materials

Underworld History

Underworld originally started as a re-write of Ellipsis

- 3D Hybrid Particle-In-Cell Finite Element Method code which solved Stokes Flow Problems.
- Well suited for modeling mantel convection and lithospheric deformations via Lagrangian material properties

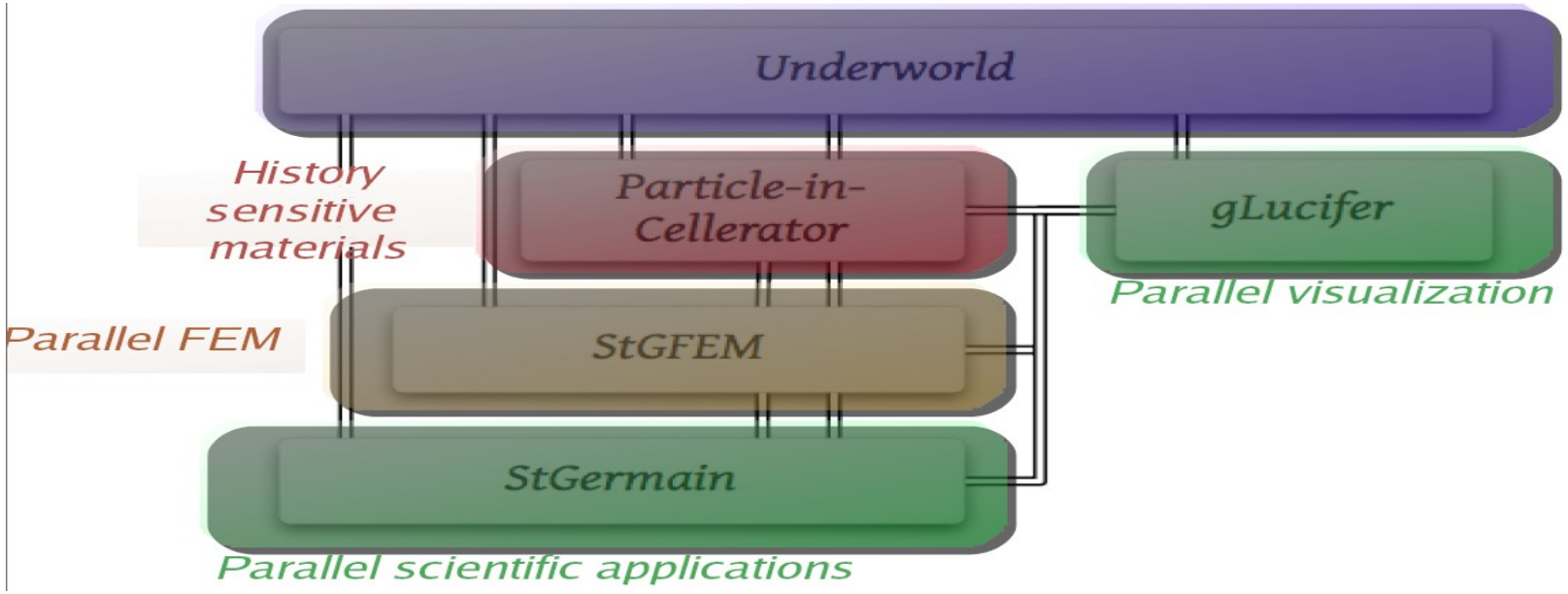
(for details L.Moresi et al. *"A Lagrangian integration point finite element method for large deformation modeling of viscoelastic geomaterials*", J. of Comp. Phys, 184, 2003)

Underworld's initial purpose was to extend Ellipsis

- Enable parallelism
- Enhance the extensibility of the code
- Develop an open source, Geodynamic code for the scientific community to use and develop

The Underworld Framework Family

- To enable those ideas the code was broken into “frameworks”



- Underworld is actually a geodynamics framework build on other more generic frameworks.

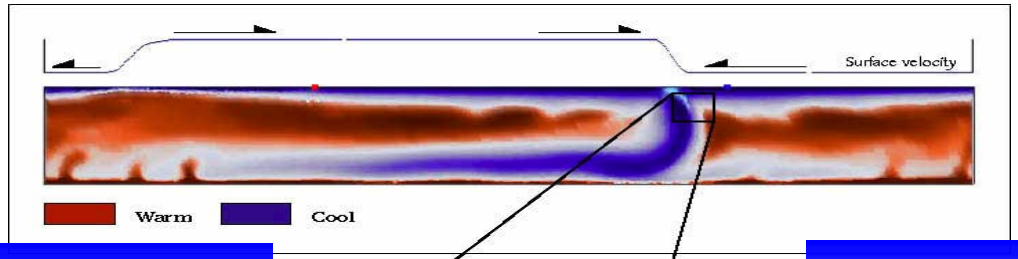
- Other frameworks provide:
  - Parallel FEM implementations (StgFEM)
  - Parallel PIC implementations (PICellerator)
  - Parallel 4D visualisation package. (gLucifer)

Workflow through frameworks

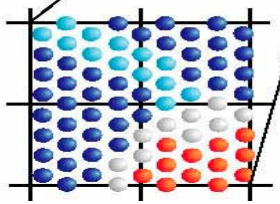
Builds SLEs with a Geodynamic interpretation, via rheological rules

StgFEM
Solves System of Linear Equation (SLE)

Solve for a Velocity and Pressure field on Eulerian Meshes



Underworld
Constitutive Relationships and data analysis



PICellerator
Handles Particle

Advects particles per timestep and maintains particle data structures

Main Community:

- Mcc (Monash Cluster Computing)

  Members: Scientist, PhD Students and me. ~10 people.

  Activities: Scientific usage. Geodynamics and Numerics expertise. Lead development of the Underworld framework.

- VPAC (Victorian Partnership of Advanced Computing)

  Members: Software engineers and computer scientist. ~7 people

  Activities: Software engineering practices and framework design. Development for lower level frameworks. Maintain hardware.

- CIG

  Members: Maintaining geodynamic code

  Activities: Support for Geodynamics codes and development of GALE. see

  http://www.geodynamics.org/cig/software/packages/long/gale

Community Development

The Underworld project has a **distributed** developer and user community.

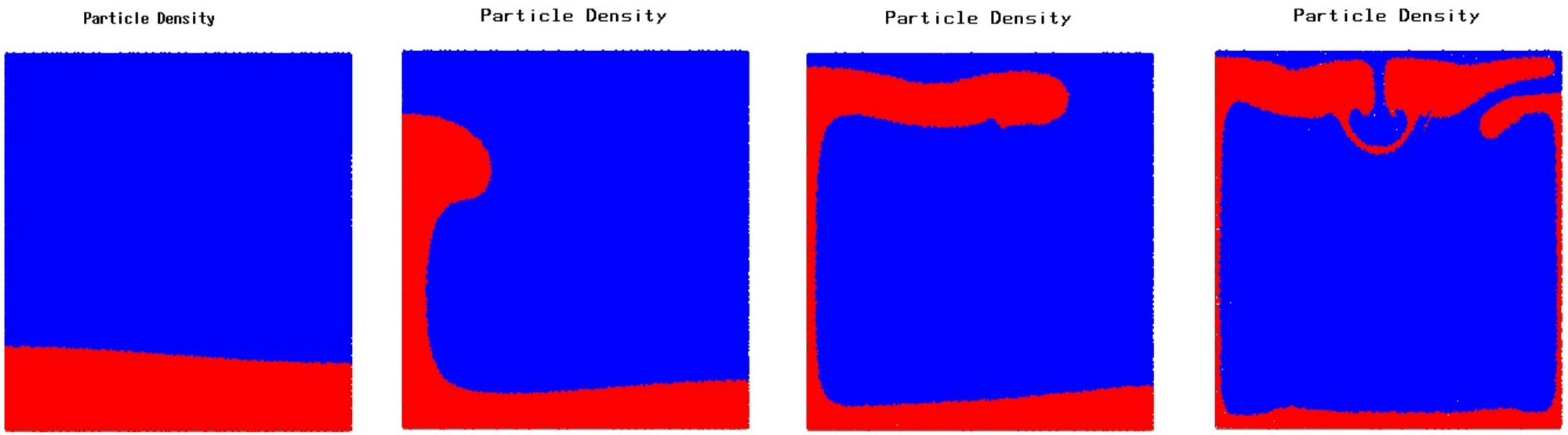
To keep track of Underworld's status we use several tools.

- **wiki**. Public information on Mcc + Underworld. User documentation.
  http://www.mcc.monash.edu.au/Main
- **svn** repositories. Revision history for the code.
  https://www.mcc.monash.edu.au/stgUnderworld/trunk
- **trac**. Bug and issue tracking.
  http://csd.vpac.org/trac/CM/AuScope/Underworld
- **email lists**. For users and developers
  underworld-users@vpac.org
- **Testing suit**.
  - Automated unit test, compiled & run every night.
  - Benchmark tests (system integration test)
  - Analytical solution to test code against.

Benchmarking Underworld

Two benchmarks we regularly hit are, both from P.E van Keken et al, 1997

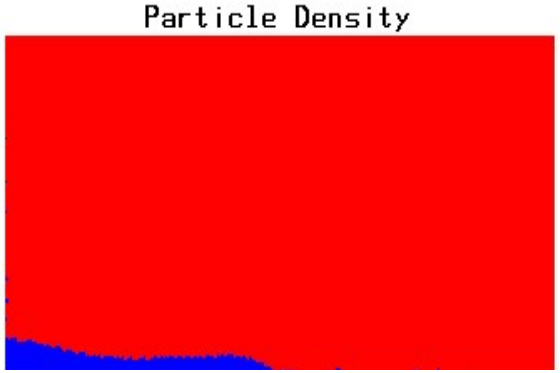
1) Isoviscous Rayleigh-Taylor instability

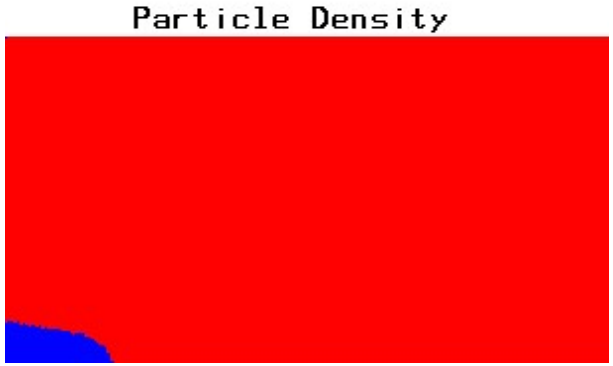


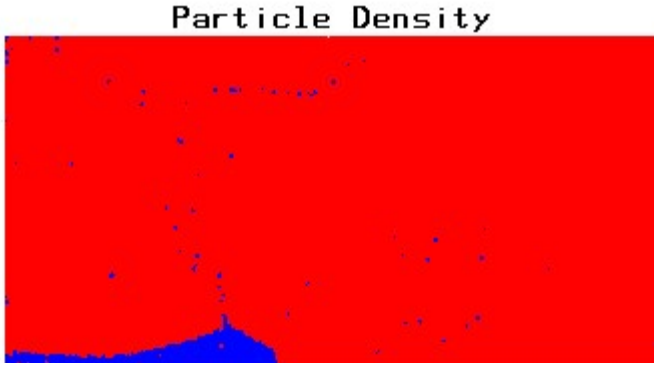
Good agreement in Vrms peaks and flow behaviour

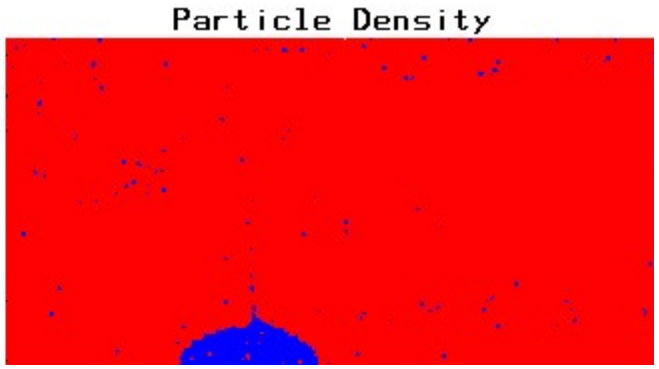
Benchmarking Underworld

ThermoChemical Entrainment (van Keken et al. 1997)

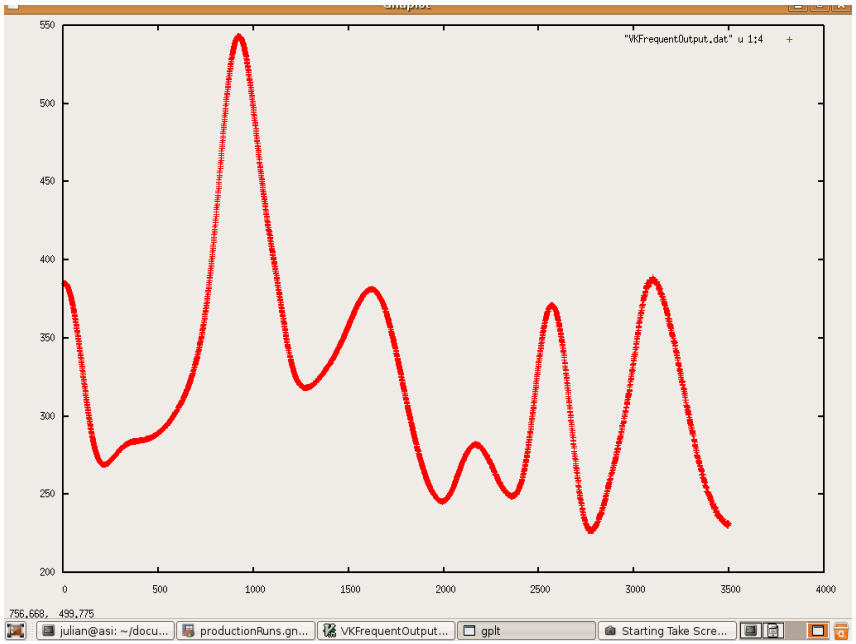








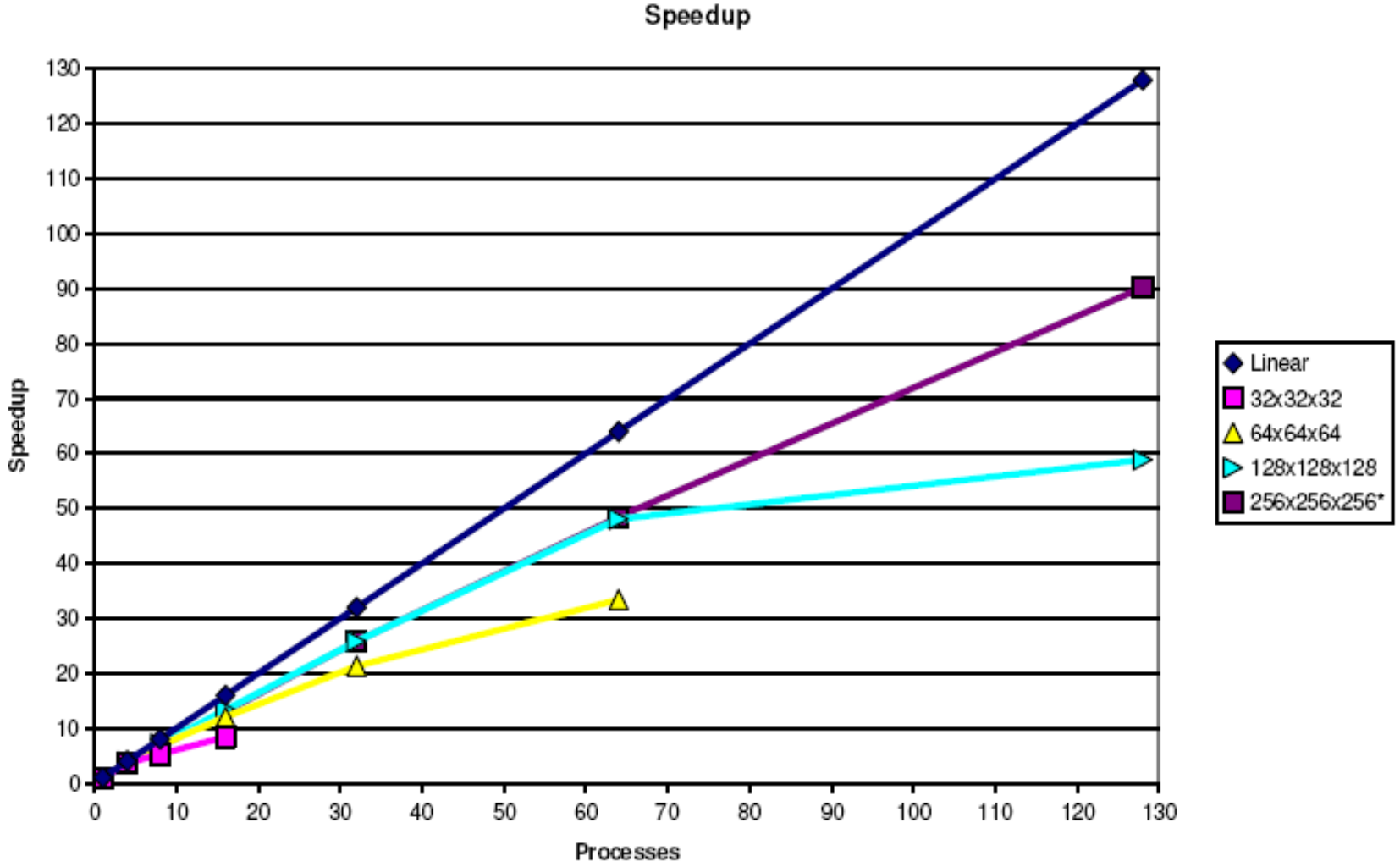
Good agreement in Vrms peaks and flow behaviour



Parallel Benchmarking

Recently our code parallel algorithm was upgraded from a 1-D decomposition to 3-D composition. Improving parallelism

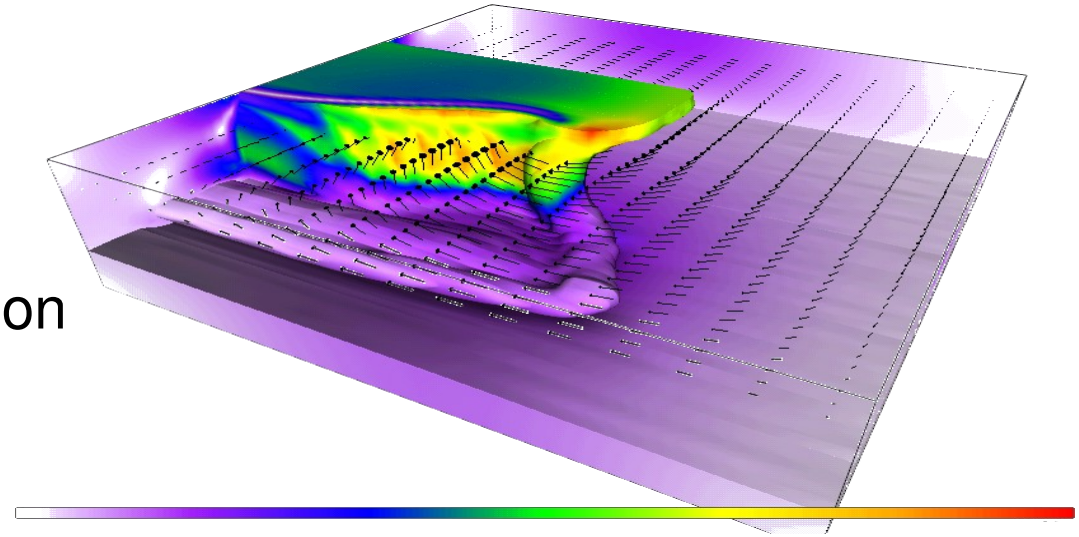
Speedup for non linear viscoplastic problem



Underworld Science

The Underworld project is maturing into a valuable tool for Geodynamic investigations and other closely related disciplines. Examples include:

- W.P. Schellart et al. (2007) investigate the 3D nature of slab subduction evolution. With particular emphasis on the affect of slab width on subduction zones.



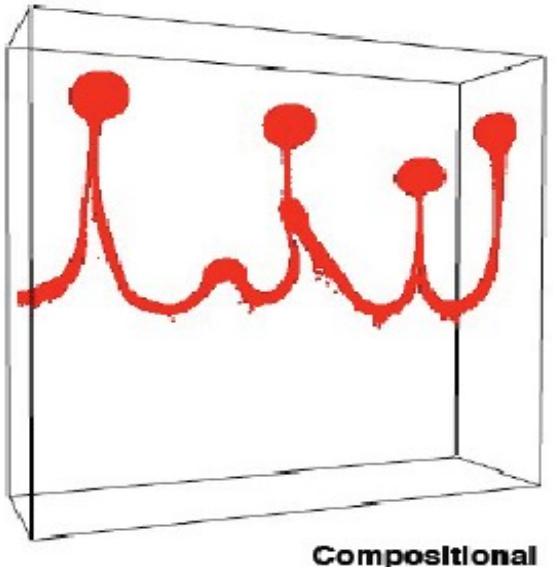
Generated by D. Stegman

W.P. Schellart et al.,“Evolution and diversity of subduction zones controlled by slab width”, *Nature, 7133(446):308-311, 2007.*

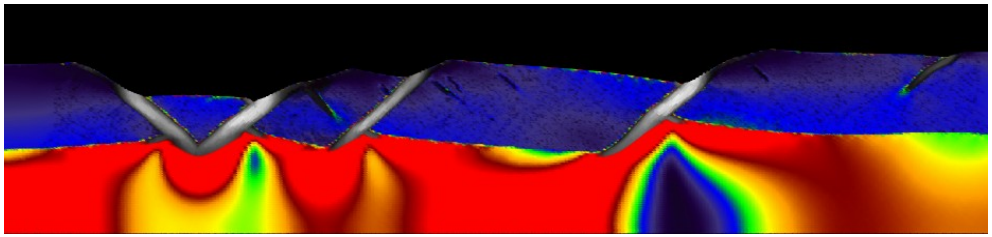
Underworld Science (cont.)

Generated by C. Mériaux

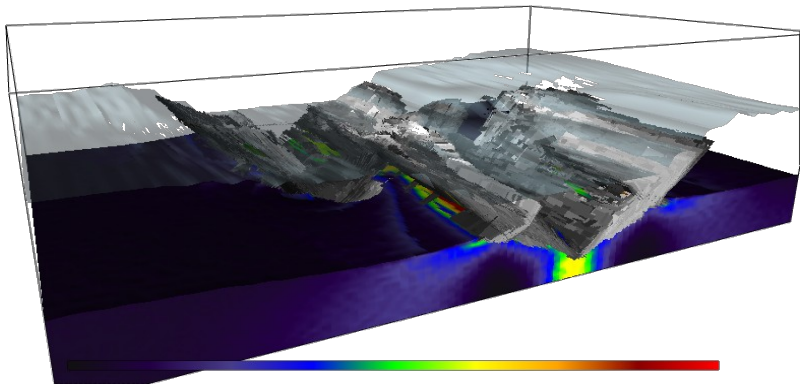
- L. Moresi et al. “Computational approaches to studying non-linear dynamics of the crust and mantel”, *Physics of the Earth and Planetary Interiors*, 163:69-82, 2007.



- L. Moresi, H.-B. Mühlaus. “Anisotropic viscous models of large-deformation Mohr-Coulomb failure”, *Philo. Magazine*, 86:3287-3305, 2006



Generated by L. Moresi



Becoming Involved

The Underworld Project is seeking to further it's scientific scope and community base.

Project plans for future development include:

- Improved numerical scheme, solver methods
- Inclusion of “real world” data into models
- Adaptive Mesh Refinement (AMR)

As such, collaborations into development efforts and scientific investigation are welcome. If you'd like to know more please

Email:

underworld-users@vpac.org

Louis.Moresi@sci.monash.edu.au

Visit:

http://www.mcc.monash.edu.au/Software/UnderWorld

Or.... try the LiveCD

... The Underworld LiveCD

This LiveCD contains:

- A stripped down version of Underworld-1.0
- Facilitated by an custom made Ubuntu 7.04 LiveCD distribution
- Relevant documentation of Underworld which can be found on our wiki
  http://www.mcc.monash.edu.au/Software/UnderWorld

It is a temporary environment:

Everything you do using this LiveCD will only effect the RAM of your machine, **not the hard disk** (includes any output files). A usb drive can be used to record data from the tutorial environment.

To get the LiveCD working:

- Make sure the BIOS is set to “Boot of CD” first. (Hold 'c' mac users)
- Insert CD and reboot your computer

Utilities

Basic tools from the command line:

- gedit or vim ..... the default editor
- evince ..... the default pdf viewer
- gthumb or eog ..... the default image viewer
- vlc ..... the default movie viewer
- Underworld ..... commandline executable of Underworld-1.0

Or you can use the 'nautilus' file manager.

XML 101

- Input files are in XML
- Open the file ExampleXML/ExampleInputFile.xml.
- Things of interest:

<include>Underworld/BaseApps/ThermalConvection.xml</include>

XML files are used hierarchically

<list name="plugins" mergeType="merge">

Plugins list usually related to output

<struct name="components" mergeType="merge">

Components list, “Objects” used in simulation

Running Underworld

To run code type:

:~$ Underworld ExampleXML/ExampleInputFile.xml

(<Crtl> + c , to stop simulation)

notice the output directory created.

:~$ ls output, to view

- images, .png
- movie, .mpeg
- FrequentOutput.dat
- Full time-stamped version of the XML file used

XML 102

Majority of the XML files you will call hierarchically are located in
/usr/local/Underworld-1.0.0/lib/StGermain/

Includes:

- Visualisation definitions – see Viewports directory
- Initial and Boundary Conditions definitions – see VariableConditions directory

Comments in XML: <!-- Bonjour le monde-->

Concatenate all xml files your simulation use with the **FlattenXML** command.

:~$ FlattenXML myInputFile.xml

Material Definitions

```
<struct name="components" mergeType="merge">
    <struct name="temperatureDependence">
        <param name="Type">Arrhenius</param>
        <param name="TemperatureField">TemperatureField</param>
        <param name="eta0">1.0e-6</param>
        <param name="activationEnergy">27.63102112</param>
    </struct>
    <struct name="shape">
        <param name="Type">Everywhere</param>
    </struct>
    <struct name=”material”>
      <param name=”Type”>RheologyMaterial</param>
      <param name=”Shape”>shape</param>
      <param name=”Rheology”>temperatureDependence</param>
    </struct>
</struct>
```

Class type

User defined name

Simply input parameters

See *Codex* for input parameter help

Codex

- Location: www.mcc.monash.edu.au/codex/web.html

- Explains input parameters required for Components
  - *Parameters* are simple inputs i.e numbers, booleans
  - *Dependencies* are other Components

- It's experimental and incomplete (so be patient)

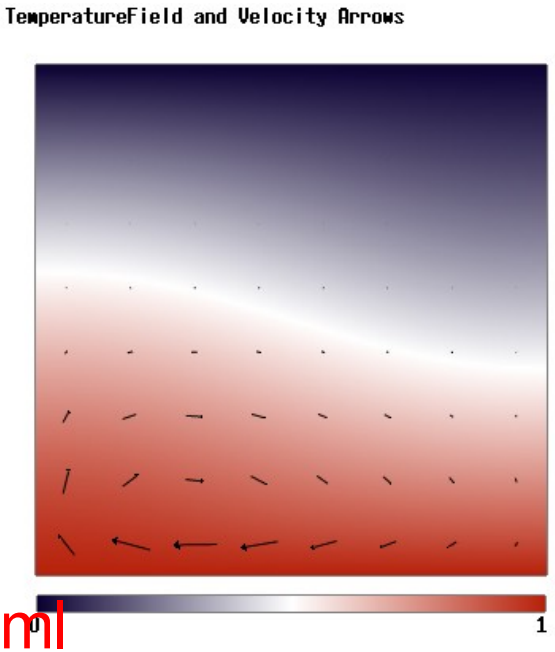
- Preserves object oriented structure

- Best used with browsers “find” command

Example 1

Straight thermal convection. FEM only

See ~/ExampleXML/FrankKamenetskii.xml



Run with

:~$ Underworld ExampleXML/FrankKamenetskii.xml

Examine output in output directory.

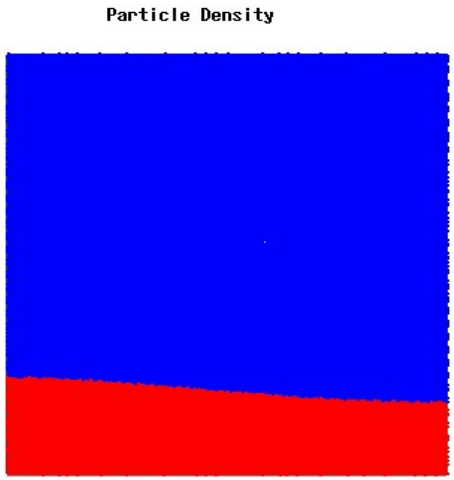
Modify the # timesteps and output directory.

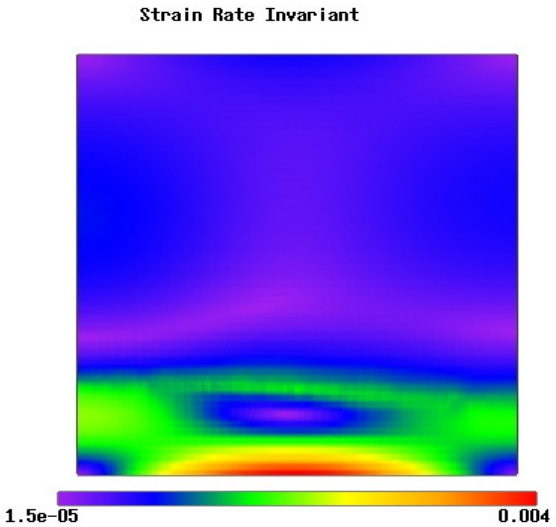
Add another visualisation viewport

Example 2

Straight Chemical convection. FEM + PIC

See ~/ExampleXML/RayleighTaylorBenchmark.xml





Modify the geometry of the lighter fluid

see the “Codex” in the Underworld Documentation for help on shape geometries

Now modify the density contrast between the materials

Try 3D job at low resolution.

Further Features

Checkpointing / Restart

Checkpointing – is a snap shot of the fields and swarm

Can be used to restart simulations from previous runs.

FrequentOutput.dat

Information from your run. Most plugins alter output into this File.

PerformanceTests directory

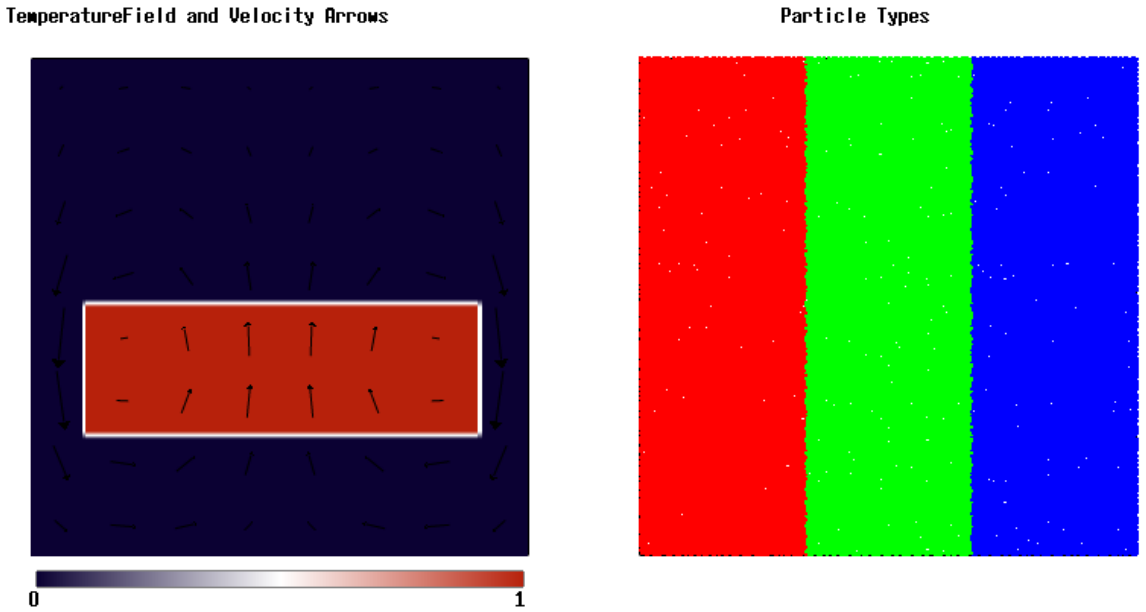
Contains some analytical solutions which we test against and the setups we have for Benchmarks.

Analytical solutions are described in a pdf documents all_solns.pdf

Example 3

Thermal Convection, multiple materials. FEM + PIC

See ~/ExampleXML/MultiThermalDiffusivity.xml



Change the shape of the initial thermal patch.

Alter Diffusivity values

Change Rayleigh number.

The End

Thank you for listening

Underworld wiki page
http://www.mcc.monash.edu.au/Software/UnderWorld

Codex (Documentation)
http://www.mcc.monash.edu.au/codex/web.html

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or me (I'll be away until the end of the year)
Julian.Giordani@sci.monash.edu.au