

Bringing Underworld to the Grid

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Computational Geodynamics: the Stg-Underworld Framework

StGermain-to-Underworld is a layered framework for modelling geodynamic systems, with an emphasis on achieving scalability on high performance computing (HPC) clusters. While the lower layers of the framework such as StGermain are quite abstract, Underworld itself is designed to support the particular needs of key problems in contemporary geodynamics, such as subduction of tectonic plates, thermal and thermo-chemical evolution of the Earth's mantle, and basin extension.

See www.mcc.monash.edu.au/Software/Underworld and www.stgermainproject.org for further information about the framework.

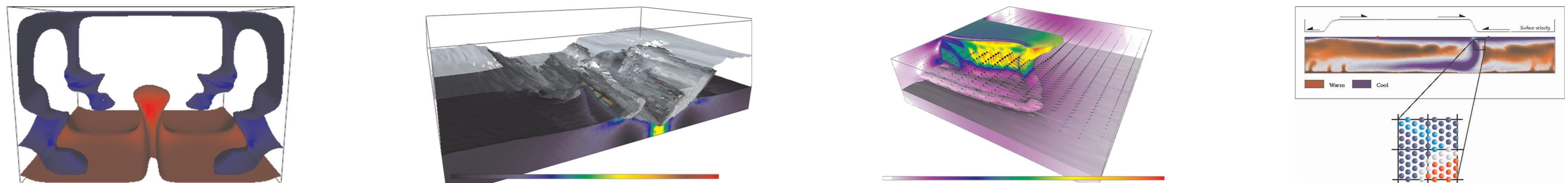


Figure 1: Example Underworld model output images.

What can the Grid do for Underworld?

Running simulations of the above-mentioned models is an expensive process. Current generation models require solving systems of several million unknowns over 100+ timesteps. This necessitates running large parallel jobs - using 64 processors, a medium-large model run takes in excess of ten hours. But as well as this compute-time expense, there is the time spent setting up, monitoring, and post-processing batch jobs on supercomputers.

Grid computing offers the potential to launch, monitor, and post-process many compute jobs simultaneously, all from a graphical user interface or web portal. Clearly, Underworld researchers could benefit from these capabilities. Specifically, the core needs for an Underworld grid service can be described as:

- submitting Underworld jobs to the grid
- staging input files from either the desktop, or remote sources such as the shared directory of a user's VO
- monitoring and managing running jobs - including viewing intermediate results
- staging output files to the desktop/home directory of a user's site/shared directories of their VO(s)

Grisu

Grisu (<http://grisu.vpac.org>) is a grid job submission client that, very much like a web portal, enables the user to submit jobs to the grid. Like other grid clients, it supports and implements a generic, application-independent workflow like the one illustrated in Figure 2.

Some of its features:

- communicates via web services to avoid firewall problems
- uses MyProxy credentials (username/password) to connect to the grid
- has multiple client implementations (Java Swing, command line)
- uses an XML templating system to support multiple applications. Grid administrators, developers and users can add the application/submission type they need with ease
- extendable via Java plugins to improve the support for specific applications
- comes with rudimentary file management support to enable the user to stage/move files outside the job submission workflow
- can be used as a library to add grid job submission/file staging features to existing (Java) applications

Lessons Learnt

Over the past year we have found the following are important foundations for setting up a grid service for Underworld:

- developing good communications between the grid application/middleware and scientific application developers. For example, as a result of discussions with the CSIRO APAC Grid Geoscience Support Project team, Underworld's input file system was streamlined to remove the need for multiple input files with absolute links between them
- developing a clear naming convention and roadmap for our releases, and liaising with APAC to keep the central registry of installed releases updated
- working closely with supercomputer system administrators to keep the latest release successfully installed as a module. This includes providing system tests to allow testing installation quickly and reliably
- beta-testing Grid clients over university networks, to ensure firewalls and proxies can be successfully navigated
- involving the scientific application's users in the process. For example, the APAC Grid Geosciences Project Roadshow acted as a catalyst for several users to commence beta-testing of grid clients with Underworld
- providing online documentation to assist users in connecting to the grid - see <http://www.mcc.monash.edu.au/Software/UnderWorldOnAPACGrid>.

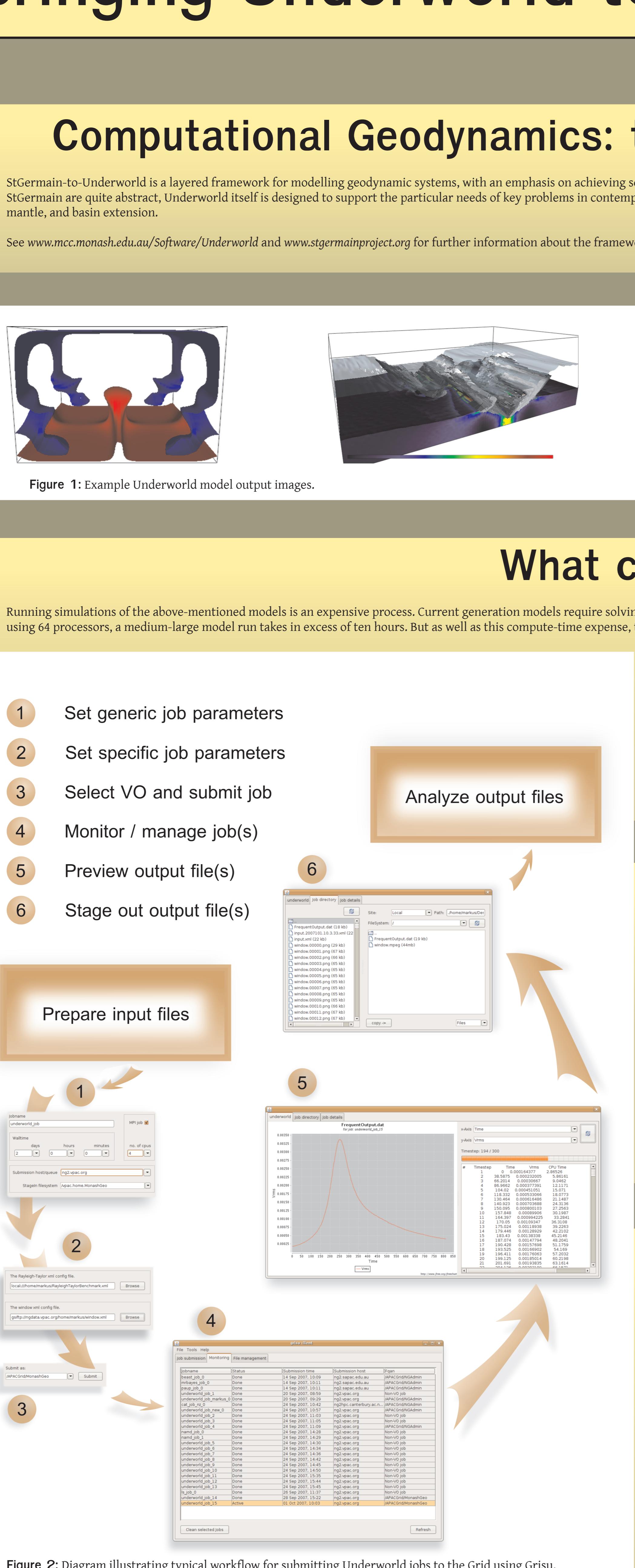


Figure 2: Diagram illustrating typical workflow for submitting Underworld jobs to the Grid using Grisu.

Acknowledgements:

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- all the Grisu beta-testers, especially Jay Stafford, Julian Giordani (Monash University) and Daniel Cox (SAPAC)
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- Monash University Science Faculty IT staff who have helped deal with firewall issues, in particular Paul Blaich.