ARCS Compute Grid Supporting Research Community Development: the Underworld Case Study

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INTRODUCTION

Collaboration between AuScope 'Simulation, Analysis, Modelling' Victoria and the Australian Research Collaboration Service (ARCS) has facilitated increased uptake of the Underworld [1, 2] Geoscience research code amongst the wider Australian Geoscience community. The Underworld job submission template developed for the Grisu Grid submission client graphical user interface allows novice users of Underworld, with no prior experience with compute clusters or the Linux command-line, to easily and quickly submit an Underworld input file to a cluster across the ARCS Compute Grid.

UNDERWORLD RELEASE MODULES

Underworld is a 3D-parallel geodynamic modelling framework under collaborative development by Monash University and the Victorian Partnership for Advanced Computing (VPAC), as part of the NCRIS AuScope capabilty in the 'Simulation, Analysis, Modelling' Victoria program. Underworld modules are installed across an increasing number of clusters at Platforms for Collaboration (PfC) (NCI National Facility and ARCS) High Performance Computing (HPC) facilities, for use directly at each site and across the ARCS Grid.

Underworld utilises a Lagrangian particle-in-cell finite element scheme (the prototype of which is the Ellipsis code), and is visualised using gLucifer. The Underworld source code is written in C in an Object Oriented style, following the methodology of design for change applied to computational codes implemented in StGermain, and uses PETSc (optimised numerical solvers) and MPI (parallelism) libraries. The Underworld to StGermain software stack is released under a mixture of BSD and LGPL licenses. Underworld supplies a set of template models which researchers can adapt to their own research, to investigate Geophysical settings such as mantle convention, lithospheric extension and tectonic plate subduction. AuScope provides assistance to researchers with adapting Underworld template models to their own research questions, on an individual and / or research group basis as required.

The Underworld release code is made available in a variety of forms for users of different operating environments and technical skillsets. The Underworld source code from each release can be downloaded from a Mercurial repository, as a tarball, or as a binary for supported environments. An Underworld module is also installed after each release at a range of HPC facilities, the details of which are then published via the NCI National Facility Software Map [3] to the Monitoring and Discovery Service (MDS) for acquisition by Grid submission clients such as Grisu. A copy of Underworld's user documentation, which caters to novice through to advanced users, is frozen at the time of each release and made available on the project's website for later reference.

GRISU GRID SUBMISSION CLIENT

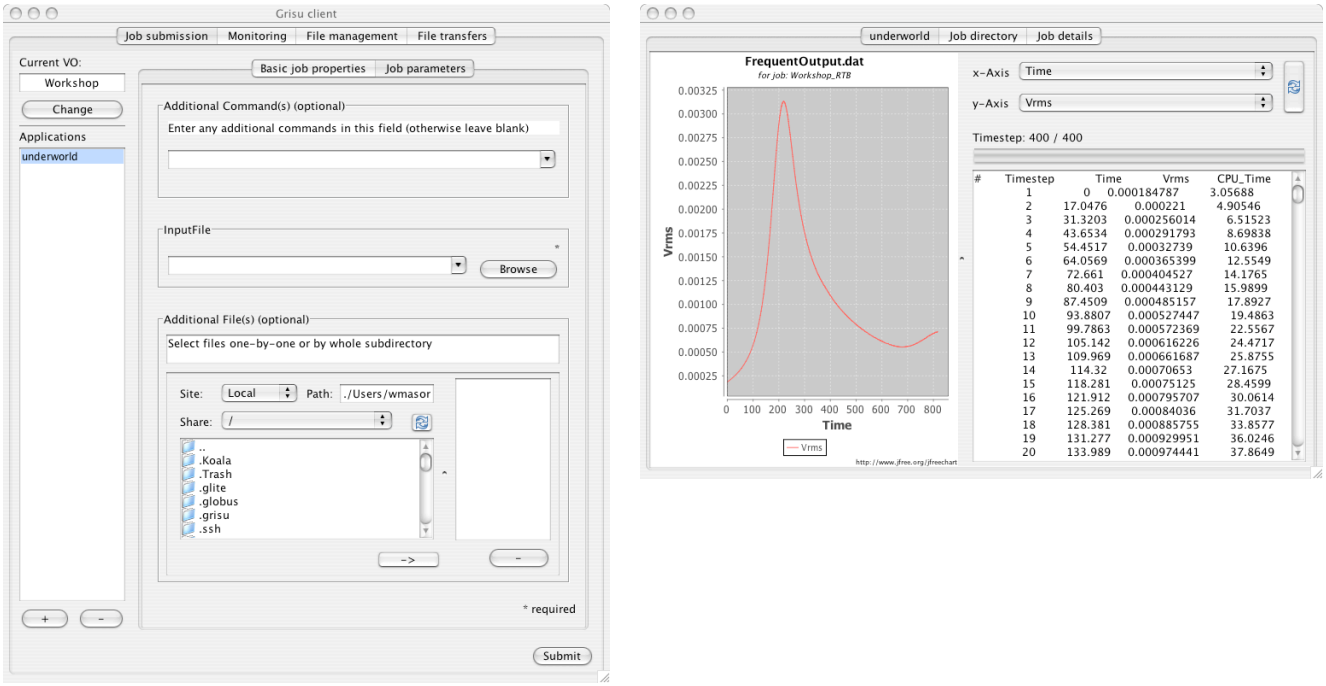
ARCS Compute Services [4] aims to provide Australian researchers with the necessary tools to utilise compute resources available at PfC HPC facilities on the ARCS Grid. Grisu, which is being developed by ARCS and was formally released on 30 April 2009, is a tool that enables users to submit remote compute jobs to a range of HPC facilities on the ARCS Grid with relative ease, giving them access to applications best suited to their needs regardless of geographical location. The Grisu Java Swing graphical user interface takes Job Submission Description Language (JSDL) documents that are marked with tags to render its appearance, accepting plugins customised to a particular code's requirements.

Figure 1 illustrates key aspects of a customised Underworld job submission and post-processing workflow, which utilises several of Grisu's generic capabilities. Key aspects of a sample Underworld job submission workflow [5] using Grisu include: login (Shibboleth, Standard or MyProxy); selection of the Underworld job submission template; selection of job parameters (job name, walltime, cpus, site and queue, email notification); Underworld input file selection (one or more files, individually or whole subdirectories, from local or remote accounts) and extra run-time commands (for more advanced users); staging-in of files and job submission in one step; job progress monitoring; and previewing, downloading and deletion of model output.

UNDERWORLD GRID WORKSHOP 2009

Following the Grisu release, we conducted an Underworld Grid Workshop at Monash University on 10 June 2009, with the support of AuScope, ARCS, the Monash e-Research Centre, VPAC and iVEC. Attendees included postgraduate students, academic and professional staff from several Victorian and interstate universities, Geoscience Victoria DPI and Geoscience Australia. Participants in the hands-on component used their own laptops, running Mac OSX, Linux and Windows operating systems, and logged into Grisu using Shibboleth with their ARCS Identity Provider (ARCS IdP) account details. The workshop provided a brief overview of the structure of Underworld input files, and demonstrated

sample workflows for running Underworld models, and previewing and retrieving the output, on different HPC facilities across the ARCS Grid using Grisu. Participants were guided through several exercises demonstrating a selection of Underworld and Grisu's key features, including restarting an Underworld job from participants' own checkpoint files generated during the workshop. Outcomes of the workshop included immediate Underworld uptake by additional members of the local Geoscience community, as well as new interest in the planned expansion of Underworld module installations at additional HPC facilities.



#	Timestep	Time	Vrms	CPU_Time
1	0	0.000184787	3.05688	
2	17.0476	0.000221	4.90546	
3	31.3203	0.000256014	6.51523	
4	43.6534	0.000291793	8.69838	
5	54.4517	0.00032739	10.6396	
6	64.0569	0.000365399	12.5549	
7	72.661	0.000404527	14.1765	
8	80.403	0.000443129	15.9899	
9	87.4509	0.000485157	17.8927	
10	93.8807	0.000527447	19.4863	
11	99.7863	0.000572369	22.5567	
12	105.142	0.000616226	24.4717	
13	109.969	0.000661687	25.8755	
14	114.32	0.00070653	27.1675	
15	118.281	0.00075125	28.4599	
16	121.912	0.000795707	30.0614	
17	125.269	0.00084036	31.7037	
18	128.381	0.000885755	33.8577	
19	131.277	0.000929951	36.0246	
20	133.989	0.000974441	37.8649	

Figure 1: Some custom features of an Underworld job submission workflow in Grisu.
Left: Job parameters panel of the "underworld" job submission template, featuring fields for selection of one or more input files (individually or whole subdirectories) to be staged in from local and / or remote accounts, as well as an optional command-line field for more experienced users to specify additional run-time commands.
Right: Underworld post-processing panel, illustrating preview and data plot from the output file FrequentOutput.dat, and status bar of number of timesteps run out of maximum timesteps set by the user in the input file.

CONCLUSIONS

Underworld module installations at HPC facilities on the ARCS Grid, together with the Underworld job submission template in Grisu, are bringing Underworld closer to a broader range of scientific researchers in the Australian Geoscience community.

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