



AuScope

Simulation & Modelling

February 2008
Newsletter No. 1



Collaborators



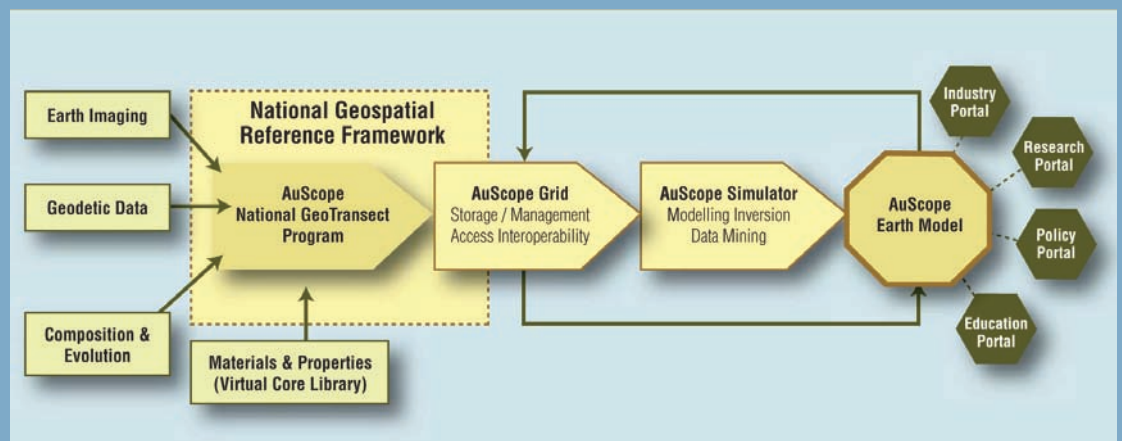
Introducing AuScope Simulation & Modelling Australia

Welcome from the AuScope simulation & modelling community. This is our first newsletter — we're introducing ourselves and the geological modelling capability we are building for the AuScope community. This is a very exciting time for us as we bring the knowledge and expertise of three computational geology initiatives together into a single, nationwide group. Auscope Simulation and Modelling grew out of the Australian Computational Earth Systems Simulator Major National Research Facility (ACcESS), the EarthByte Australian Research Council eResearch network, and the Predictive Mineral Discovery Cooperative Research Centre's computational geoscience programme. We have participating groups in

Canberra, Sydney, Brisbane, Perth and Melbourne located alongside concentrations of researchers and applied scientists who will use the modelling infrastructure. AuScope is building a National Earth Science Infrastructure Program as part of the federally funded National Collaborative Research Infrastructure Strategy (NCRIS) programme running from 2007 - 2011. The Simulation & Modelling component of this initiative is a nationwide effort to bring an integrated suite of advanced geological modelling software packages to the desktops of Australian geoscientists. Our goal is to create "dynamic images" of the Earth from surface to depth, spanning the billions of years of Earth's geological history, and crossing the range of geological scales - models

which bring the geological timescale to life. Modelling provides the linking element between the vastly different timescales and spatial scales in the processes and structures recorded by other components of AuScope - the tiny year-by-year movements seen by geodesy, the snapshot of Earth structure imaged by seismology and geophysics, the billions of years of chemical evolution sampled at the surface by geochemical techniques, the stress in the lithosphere revealed by seismicity and bore-holes. More information on our activities and those of AuScope in general can be found on the Auscope website at www.auscope.org.au

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For more information and the latest news,
visit <http://www.auscope.org.au>

New global digital grids of oceanic crustal data

Four companion digital models of the age, age uncertainty, spreading rates and spreading asymmetries of the world's ocean basins as geographic and Mercator grids with 2 minute resolution have been made available on the AuScope EarthByte web site:

<http://www.earthbyte.org/Resources/agegrid2008.html>
The grids include data from all the major ocean basins as well as detailed reconstructions of back-arc basins.

In addition we also use the age grid to compute new maps of global residual basement depth anomalies from the difference between observed oceanic basement depth and predicted depth using four alternative age-depth relationships.

These grids can also be downloaded from the

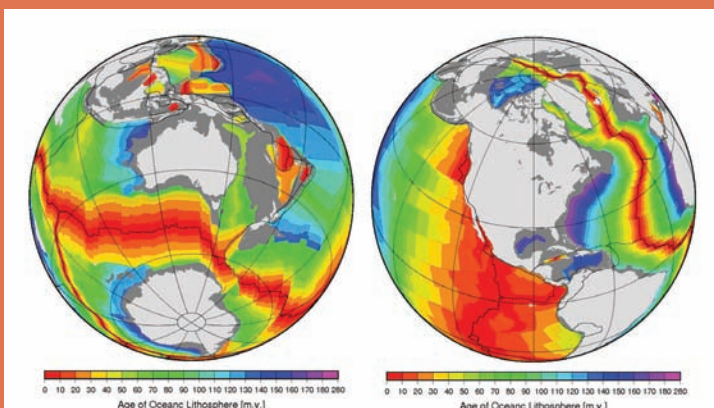
EarthByte site and may be of particular interest to geodynamicists because many of the regional depth anomalies they reveal reflect mantle processes – either deep mantle flow and/or asthenospheric flow.

Various geodynamic problems can potentially be investigated by combining these grids, together with our relative and absolute plate motion model (also posted on the EarthByte

site), with seismictomography and mantle convection model outputs. We recommend using Wessel and Smith's [1998] Generic Mapping Tools (GMT) to manipulate and plot the grids. The age, age uncertainty, spreading rate, and asymmetry grids are made available in 3 different ways: (a) 2 minute Mercator ".img" grids matching the recent Sandwell/Smith marine gravity and bathymetry

grids in geographic extent; (b) 2 minute geographic netcdf GMT short integer grids (".nc"); and (c) 6 min geographic netcdf GMT short integer grids (for those who don't need high resolution grids).

We use short integer files to reduce file size for quicker (and cheaper) downloading. The data sets are described in a paper in G-cubed [Müller, et al., in press].



Müller, R. D., et al. (in press), Age, spreading rates and spreading asymmetry of the world's ocean crust, *Geochemistry Geophysics and Geosystems*.

Wessel, P., and W. H. F. Smith (1998), New, improved version of Generic Mapping Tools released, *EOS Transactions, AGU*, 579.

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Staff News

AuScope Simulation & Modelling Victoria wish Pat Sunter all the best for his new career direction in Urban Planning/Modelling. Pat

recently resigned and moved interstate to complete a Graduate Diploma in this field at the University of South Australia. Pat has worked at

the Victorian Partnership in Advanced Computing since late 2002. Most recently, as Monash AuScope Project Manager, Pat successfully

saw the staff through the ACcESS/ AuScope transition and implemented practical and efficient management systems which will continue.

Cluster Corner: ESSCC upgrades supercomputing facility

Through funds provided by The University of Queensland the Earth Systems Science Computational Center will upgrade its parallel computing facility to a 5 Tflop Altix ICE system.

The new system will be operational before June 2008 and will replace the existing system which will be decommissioned by October 2008. The new machine will mainly serve the growing computational needs of the Auscope community. During the overlap period

ESSCC will give people assistance to move their applications over to the new system. The new server will have 128 quad-core Xeon processors running at 2.83 GHz.

A compute node is built from two processors sharing 4 Gbytes of memory. 64 of these nodes are linked through an 4 x bi-directional InfiniBand interconnect which creates a machine with 2 Tbytes of distributed main memory and 5Tflops theoretical peak performance.

Via InfiniBand interconnects the system is linked to an internal 15Tbytes disk system as well as to the QCIF data storage facility managed via a SGI DMF.

In order to meet the reliability requirements of the Auscope community the QCIF data storage facility is currently being upgraded with a redundant file manager through ARC and QCIF funds.

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Software Updates: Underworld 1.0

The main improvement in the capability of the Stg - Underworld framework over the last six months was a significant improvement to the decomposition algorithm for parallel simulations.

The meshes used for simulation can now be decomposed in three dimensional cubes instead of only one dimension slices.

What this means in practice is that the code will run more efficiently and gain a better parallel speedup for large models run on a parallel machine - especially when using the Multigrid solver in combination.

The restructuring necessary for this improvement caused problems with several other advanced features of the framework, such as periodic boundary conditions for material particles. With the delay till November of

the signing of the AuScope contract, it has taken longer than was hoped to find and fix these problems.

It is thus a high priority to improve the robustness of the code to a high level again. This will include restoring the testing and regression test suites to full operation. Once this is done, a patch release will be made and installed on supported supercomputers.

Work has already begun on the features considered important for the long-term ability of the code to tackle key problems in Geodynamics. Prototype versions of some of these features, such as Adaptive Mesh Refinement, will be ready to demonstrate at the Underworld Retreat in February 2008.

Pat Sunter
Monash AuScope

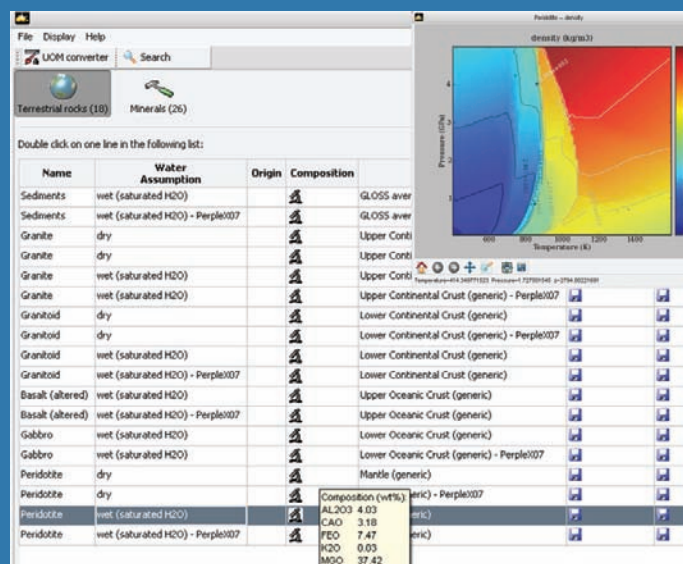
Software Updates: PreMDB

PreMDB, a thermodynamically consistent material database, will be a key tool for comparing geological, geodynamic and geotechnical calculations.

By coupling thermochemistry with rock mechanics, thermodynamic potential functions are used to calculate reversible material properties such as thermal expansion

coefficient, specific heat, elastic shear modulus, bulk modulus and density. Laboratory-derived transport properties, such as thermal conductivity (diffusivity) and melt viscosity are also included.

Klaus Regenauer-Lieb
UWA/ CSIRO Expl. & Mining



AuScope Grid News: A virtual rock laboratory

Building upon the ESyS_Particle software developed by ACCESS, QLD Simulation and Modelling personnel and AuScope Grid personnel aim to construct a virtual rock laboratory on the AuScope Grid.

The virtual rock laboratory will provide an intuitive platform for construction of numerical rock physics experiments, simulation on the AuScope Grid and post-analysis of results. In the initial stages the virtual rock laboratory will provide a suite of familiar tools for measuring rock properties: brazilian, tri-axial, Hopkinson bar and UCS tests. A simulation journal repository will be populated recording the input parameters, the virtual rock

sample, and the measured macroscopic properties of the virtual sample.

Ultimately, the meta-data stored in the simulation journal will become an online look-up table for selecting virtual rock samples with

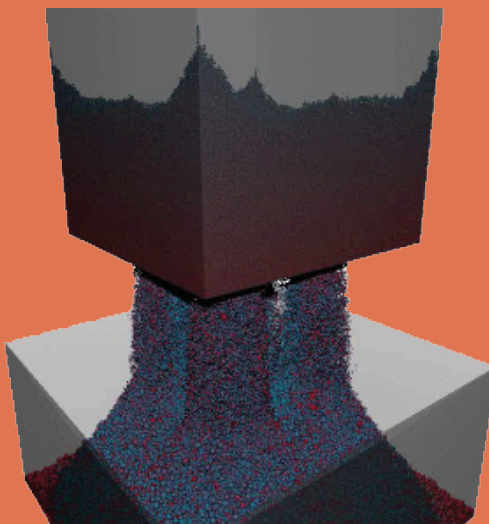
known elastic properties and to import these samples into progressively more detailed simulations of the meso- and macro-scale physics of brittle-elastic materials.

ESyS_Particle is a parallel Discrete Element Method

(DEM) simulator designed to model the mechanics of rock breakage and optimised for the ESSCC computing facility. The software has previously been applied to the study of the formation and evolution of fault gouge zones, dynamic earthquake rupture and wave propagation, rock breakage and comminution, slope failure, and most recently, full-scale simulations of block-caving flows.

Software developers intend to submit a new AuScope version of this software in July 2008, under the moniker of *esyS.lsm*.

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Underworld Retreat 2008

The Monash AuScope Simulation & Modelling group recently concentrated all their scientific and programming efforts at a four-day long Underworld Retreat in Melbourne.

The aim of the retreat was to discuss, design and prototype improvements to the modelling capabilities of the computational frameworks (Underworld) that the Monash AuScope group are co-developing.

The Retreat was strongly attended by Monash AuScope research staff and students, and VPAC software developers.

Three CIG collaborators from the USA were also able to attend the Retreat; Marc Spiegelman from Lamont -

Doherty Earth Observatory, Walter Landry from Computational Infrastructure for Geodynamics and Matt Knepley from Argonne National Laboratory.

A number of specialised geodynamical and numerical modelling issues were



addressed, such as Magma Migration (CIG Magma project).

The retreat concluded with a unique Tramcar Dinner around Melbourne.

Louis Moresi
Monash AuScope

AuScope Authors

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Goyette, S., Takatsuka, M., Clark, S., Müller, R.D., Rey, P. & Stegman, D., 2007. Increasing the Usability and Accessibility of Geodynamic Modelling Tools to the Geoscience Community: UnderworldGUI. *Visual Geosciences*, 1-12, DOI 10.1007/s10069-007-0006-3.

Schellart, W.P., Freeman, J., Stegman, D.R., Moresi, L. & May, D. 2007. Evolution and diversity of subduction zones controlled by slab width. *Nature*, **446**, 308-311, doi:10.1038/nature05615.

Siret, D., Poulet, T., Regenauer-Lieb, K and Connolly, J.A.D. (In Review). PREMDB, a thermodynamically consistent material database as a key to geodynamic modelling. *Geochemica Acta*.

Software Updates: *esys.escript*, a powerful tool for numerical modeling

The idea behind *esys.escript* is to give scientists an environment which allows quick implementation and running of new numerical models. It is built as an extension to the widely used and easy to use python language while all computational expensive tasks such as data manipulations, the solution of partial differential equations, mesh generation and visualization are implemented in C and

C++. The user describes models with a very high level of abstraction. Instead dealing with lower level concepts like meshes, matrices or arrays the user works with the concepts of partial differential equations and spatial functions.

This on one hand improves the productivity of computational scientists as they can focus on the development of their models and on the other hand produces very readable, reusable and portable code.

esys.escript has successfully been used in a variety of Auscope applications including mantle convection, plume formation, volcanoes, tsunamis, crustal fault system dynamics and reactive transport.

Version 1 of *esys.escript* is available now. It includes interfaces to the finite element library *finley*, the visualization tool *vtk*, and the mesh generator *gmsh*. It supports parallelization

for (virtual) shared memory computers via *OpenMP*. Support for *MPI* to run on clusters with distributed memory is expected to be released by April 2008.

For further information, visit: <https://shake200.esscc.uq.edu.au/twiki/bin/view/ESSCC/EsyUser>.

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Cluster Corner: Time to Tango

VPAC's new supercomputer (SC), Tango, using dual-core AMD chips and with a total of 368 CPU cores, is up and running, and available for use by Monash Underworld users.

Tango and Edda (VPAC's existing SC) both now use the Modules system to make using and keeping track of multiple centrally-installed

software packages easier. As of this writing, they both have Underworld 1.0.0 Release Candidate 3 installed, using stable version of MPICH and PETSc.

At Monash, the mini-supercomputer owned by Monash Geodynamics, Tako, is up and running and has proved very useful for modelling runs. Tako also uses the

Modules system above, and has stable versions of MPICH, PETSc and Underworld. In the future it will employ a scheduling system, but at present it doesn't - thus care is necessary when launching jobs. The Brecca SC has survived it's move to Monash, and has an Underworld stable release installed and available through the grid client

Grisu developed by Markus Binstener at VPAC, and demonstrated at APAC07 and SuperComputing07 recently. While there are still issues with the Monash firewall to be resolved, we hope this will be of use in future.

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