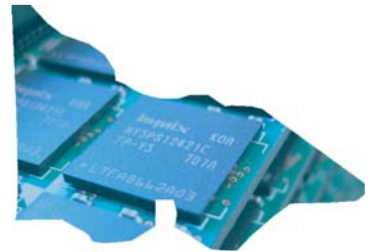




AuScope

Simulation & Modelling Victoria



Nov. 2007 Newsletter One

Project Principals



Louis Moresi
Monash University
Chair, AuScope
Simulation &
Modelling



Steve Quenette
VPAC
Manager, VPAC
Computational
Software
Development



Patrick Sunter
*VPAC/ Monash
University*
AuScope Monash
Project Manager



Mike Sandiford
Univ. of Melbourne
Research Leader,
Surface Process
Modelling

Introducing AuScope Simulation & Modelling Victoria.....

The merging of Geodynamics research and High Performance Computing infrastructure

Welcome to the first newsletter from the AuScope Simulation & Modelling Victoria project. AuScope is an organisation for a National Earth Science Infrastructure Program, as part of the federally funded National Collaborative Research Infrastructure Strategy (NCRIS) programme, and running from 2007 - 2011.

Simulation & Modelling Victoria is led and hosted by Monash University, under the direction of Associate Professor Louis Moresi. Monash will be undertaking the infrastructure development in partnership with the Victorian Partnership of Advanced Computing (VPAC), particularly VPAC's Manager

of Computational Software Development, Steve Quenette, and his team. Professor Mike Sandiford at the University of Melbourne will also be closely involved, and will contribute to the project's direction.

I am pleased to announce that Monash University have formally signed the Participants Agreement to become part of AuScope, so the project is now in full swing. Monash's collaboration with VPAC's CSD group, and Melbourne University's Geoscience department, will be maintained through a long-term subcontract for development services & expertise. The VPAC Computational Mechanics team are now permanently hosted

at Monash, as we move towards a dedicated AuScope facility there. The short story of our goals for Simulation & Modelling Victoria under AuScope is to improve and extend the software infrastructure collectively developed under ACCESS. Underworld, SPMModel, gLucifer, and all their underlying frameworks will become not only more reliable, but targeted to the long-term scientific research needs of the community of Geophysicists we support. Further details will be available from the Monash AuScope website shortly.

Patrick Sunter
Monash AuScope Project Manager
patrick@vpac.org

News & Events

Upcoming Underworld Retreat 29th - 31st January 2008

In the tradition of scientific and programming 'retreats' held by Monash Cluster Computing and VPAC, we are happy to announce the next event of this type will be an Underworld retreat. We will be inviting several international guests, primarily those collaborating in CIG from the United States.

AuScope Launch Day 1st February 2008

The final day of the retreat will be a science seminar day held at Monash, and will double as the official launch of the Monash AuScope Simulation & Modelling Victorian Node.

VPAC Summer Internships December 2007 - February 2008

The VPAC Summer Internship program is designed to allow VPAC's member universities and collaborators to explore and prototype new

applications/ models, especially those requiring High Performance Computing (HPC).

For the students, it provides those with an interest in applied computer science and related fields such as mathematical modelling to learn from VPAC's experienced staff, and gain practical skills on real projects.

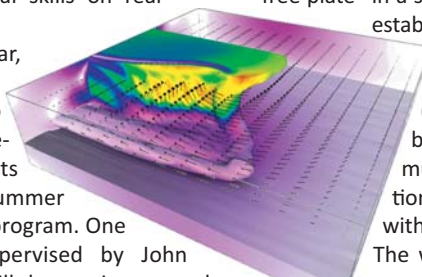
This year, there will be two AuScope related projects in VPAC's Summer Internship program. One project, supervised by John Spencer, will be to improve the multi-project collaboration systems used for AuScope, such as Trac.

The other will be a project to model re-cycling of the lithosphere and the geochemical evolution that is part of this process, to be supervised by Luke Hodkinson.

OzBench Workshop February 26th-28th 2007

Earlier this year, Dave Stegman (Monash) attended the first OzBench Workshop at the University of Western Australia.

Several research groups which have been investigating the dynamics of a "free plate" in a subduction system, established the Subduc-



tion Benchmarking Initiative (OzBench) to combine the range of multiscale computational tools available within Australia.

The workshop demonstrated that three codes with three different numerical methods, provided very similar results of a single application, of a wide subducting plate (i.e. 6000 km in lateral extent).

The results of the Ozbench Workshop are now the subject of

a manuscript (submitted in September 2007 to Physics of the Earth and Planetary Interiors).

SC07 Conference November 2007

SC07 is the International Conference for High Performance Computing, Networking, Storage and Analysis. It is the premiere conference on present and emergent technologies in high performance computing, the technology backbone to AuScope's Simulation and Modelling program. VPAC was one of over 300 exhibitors at the meeting held in Reno, USA, and demonstrated derivative research posters of the AuScope Simulation and Modelling Victoria group.

Steve Quenette attended, and will no doubt have lots of news and reviews about new technologies and techno-toys demonstrated there to share with us.

<http://sc07.supercomp.org/>

Staff Profile



Luke Hodkinson
Senior Computational Scientist

What is a Computational Scientist, as opposed to a Computer Scientist?

Wikipedia tells us they are "someone skilled in scientific computing... This person is usually a scientist, an engineer or an applied mathematician who applies high performance computers in different ways to advance the state-of-the-art in their respective applied disciplines in physics, chemistry or engineering". This is perhaps a bit better than my definition, which is a "computer

geek that's better at mucking around with maths than average". Either way, Luke is the highly esteemed Senior Computational Scientist of VPAC's Computational Mechanics group, and this is also his role on the Monash AuScope project. Luke has been with VPAC since 2003, initially through our summer internship program, but soon progressing to a full-time role developing the Stg-Underworld framework with MC².

One of the highlights of Luke's career at VPAC so far was his stint at Argonne National Laboratory in 2004, where he worked on advancements to PETSc under Matt Knepley's guidance - and incidentally became something of a darts-playing sensation. Luke has maintained a valuable collaboration with Matt and other U.S. leaders in the Computational Infrastructure for Geodynamics (CIG) community. He has even fixed bugs in PETSc, a feat far beyond most of us!

Luke's current interests and

projects in AuScope include Adaptive Mesh Refinement, and advanced geometries and topologies. Luke is also project leader of the MADDs magma migration project with CIG, under the direction of Marc Speigelman. His work has formed part of several recent publications by our community, and he recently presented a paper on Scalable 3D decomposition implementation for Finite elements at the APAC07 conference.

Outside his work with us, Luke is known for his keenness for motorbike riding, his periodic efforts to cut down his coffee intake, and his project to build a DIY pinball table at home. He can also be seen playing games on his new Uber laptop after knock-off time (it's so fast it has green trim on the monitor), and writing dissertations on the execrable games performance of Windows Vista.

Patrick Sunter
patrick@vpac.org

Milestones

October - December 2007

Membership of AuScope requires committing to milestones for the infrastructure development process. The milestones we are working towards for the current quarter ending in December are:

Underworld 1.1.0 Release:

Will include features developed over previous six months, e.g. SPR, and dual mesh for simplified refinement.

Underworld 2.0 Design and Preliminary Coding:

Outlines proposed design and algorithms for mesh refinement, and generalised constitutive framework;

Underworld 1.1.0 Manual Draft:

Draft version of offline, PDF manual including HOWTOs and tutorials;

gLucifer 2.0 Alpha Release:

New Analysis and Drawing Operator engine open to user trials.

SPModel 1.0.0 Release:

Stable release of existing SPModel functionality;

Improved unit test coverage, and updated documentation.

Regression Testing framework upgrade:

Regression testing framework on target architectures;

System can handle tags and branches.

Staff News

Kathleen Humble returns to part-time work with the team, after taking maternity leave for the birth of her healthy son, Edmund. Kath is initially working from home one day/week co-ordinating the work on an Underworld Manual.

Mirko Velic has become a full-time member of the AuScope team. Mirko's mathematical expertise will be important for the many ambitious numerical projects planned under AuScope.

Belinda May recently joined the AuScope team as a Computational

Software Developer, after having worked for several months at VPAC on the Kidneyome project in the field of computational medicine. Belinda has already shown considerable aptitude for working with the Stg-Underworld codebase.

Ewan Willis, who has been working on a prototype of an improved gLucifer part-time over the last year, recently landed his "dream job" at Tantalus, an independent Australian games development company. Ewan has started there already, but has kindly agreed to finish the gLucifer2

prototype this year. All the best in future Ewan.

Julian Giordani, who has been lead Underworld developer in 2007, is mid-way through his period of overseas leave, which began with a successful tutorial of Underworld to a French conference. Jules is apparently having a great time, and will be back in February 2008. Ciao from Melbourne Jules!

More positive staff news expected soon - stay tuned!

Software Update

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.

Unfortunately, the restructuring necessary for this improvement caused problems with several other advanced features of the framework, such as periodic bound-

ary 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. Once this is done, a patch release will be installed on supported supercomputers.

Underworld 2.0

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 January 2008.

Cluster Corner

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 - by Jay for her honours project especially! 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 Gris developed by Markus Binsteiner at VPAC, and demo'd 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.

John Spencer
VPAC and AuScope Monash
Systems Integrator
jspencer@vpac.org

