# Geodynamic benchmarking tests in HPC

Rebecca Farrington<sup>1</sup>, Louis Moresi<sup>1</sup>, Steve Quenette<sup>2</sup>, Robert Turnbull<sup>1</sup>, Patrick Sunter<sup>2</sup>

<sup>1</sup>School of Mathematical Sciences Monash University Clayton, VIC 3800, Australia

<sup>2</sup> Victorian Partnership for Advanced Computing, Carlton South, Victoria 3053, Australia

June 10, 2005

#### **Abstract**

The increase in large science focused computational frameworks has raised many issues involving the ability to maintain accurate scientific benchmarks throughout the ongoing evolution of the code. These science based tests allow not only developers access to the latest updates, but the science users aswell. It is these scientific tests required for geodynamic code benchmarking in a HPC environment that are investigated. The importance of benchmarking in computational science, for both quality assurance and reliability, is discussed and a case study for thermochemical convection modelling is presented. The implementation of automated testing for science units is described with particular attention to the problems arising from science tests compared to traditional computational tests.

**Keywords**: Benchmarking, High Performance Computing, Geodynamics

# 1 Introduction

Our research group is in the process of developing a general-purpose, parallel, solid-mechanics / fluid dynamics Lagrangian-Integration-Point finite element code primarily for use in geodynamics research. The project is multi-institutional and multi-disciplinary. It involves the simultaneous development of three codes: 1) a supporting framework code, 2) a generalized solver for handling governing mathematical equations, and 3) a code aimed towards modeling geological materials with complex constitutive behaviours. The codes are community-developed and have a tiered structure of dependency, so modifications made by developers at the low-level need to be seamlessly integrated by those working higher up at the science application level.

In a research environment the end-use-cases for the code are continually being refined as new models are run and new discoveries are made. We have adopted a very flexible approach to the code development with a short cycle of implementation, checking, release and redesign. The operation of the code is as modular as the inherent cross-coupling of the physical processes will allow. The code has to run within the environment of various parallel supercomputers which are far from homogeneous.

This leads to an interesting environment for testing the code. Firstly, the hierarchical nature of the system places a strong emphasis on reliability as no testing of the higher levels is possible until the underlying levels have passed appropriate tests. However, due to the continually evolving requirements at the scientific level, it is not possible to freeze the framework or solver code once it has been tested. Secondly, the scientific applications are written for an active research environment where the precise characteristics of the modeled phenomena are uncertain. At the mathematical level, the concept of a unit test corresponds to isolating a particular component of the system of equations which has a known analytic solution, correspondance to a documented experimental result, or well-established community benchmark. At the system level, it is commonly necessary to involve the research community in evaluating the code. We therefore allow system tests which try to distinguish between total failure, acceptable numerical error and "important" changes in behaviour even if they are within error. This last category of feedback is to signal changes which may cause concern to an experienced numerical analyst. Finally, in a grid-computing environment where the code is running as a web-service, the testing environment provides a capability audit of the installed system in a particular operating environment. Thus, in a situtation where not all the possible modules are supported, the code will know that it can offer a limited set of services.

At the scientific level, much of the testing environment necessarily involves human intervention. The role of the automated testing environment is then to provide a comprehensive overview of the system state, highlight problem areas, and highlight correlations between failures, changes in behaviour, and code updates. In this paper, we discuss these issues with reference to examples taken from computational geodynamics.

# 2 Problem Description

# 2.1 Geodynamics

In computational geodynamics we are concerned with the stresses and corresponding motions on the surface and within terrestrial planets. In order to model, for example, mantle dynamics we use the principles of conservation of mass, energy and momentum as well as assuming an incompressible, boussinesq fluid to model thermal convection. This leads to the governing equations

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = Q(T) + \kappa \nabla^2 T$$

$$\eta \nabla^2 \mathbf{v} = \nabla p + g\rho \hat{z}$$
(1)

where  $\mathbf{v}$  is the cartesian velocity vector, T is temperature, Q(t) the heat source,  $\kappa$  thermal diffusively,  $\eta$  viscosity, p pressure, q gravity and  $\rho$  density. It is usual to work with a non-dimensional system of equations to improve numerical accuracy as we solve for very small velocities (cm/yr) driven by very large stresses ( $10^8 - 10^9 Pa$ ) acting on fluids with very large viscosity ( $10^{19-23} Pas$ ). Once rescaled, the equations can then be solved efficiently using a particle-in-cell finite element method (7) (8).

# 2.2 Code Description

The code used for our geodynamic modeling is a parallel, particle-in-cell finite element code with a modular structure designed to encourage rapid prototyping of new scientific modeling concepts. A plugin infrastructure allows for highly complex mechanical models to be implemented efficiently (and safely from the point of view of other users of the code). This is achieved by the addition of either numerical or scientific applications at various entry points which are called during the code's execution. Modules cannot be firewalled from each other or prevented from interacting, as the physical process

which one module implements is often strongly physically coupled to processes implemented in other modules. Each plugin needs to work both in isolation and interacting as part of a larger system.

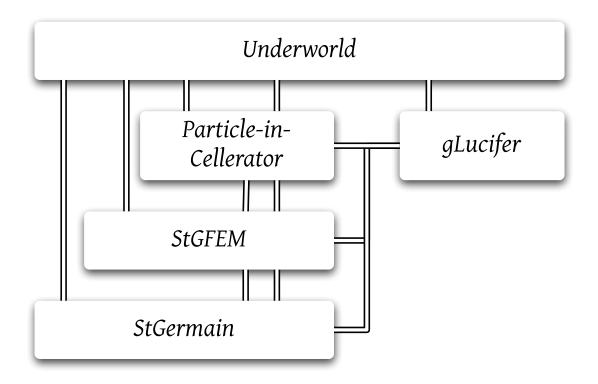


Figure 1: Structure of the geodynamics code. Each of the blocks in this diagram is a collection of modules with related functionality. The base layer, StGermain, provides low level parallel infrastructure for scientific computing; StgFEM provides specialization for dealing with distributed finite element problems; the Particle-in-Cellerator provides the Lagrangian integration and Lagrangian constitutive model frameworks. There is a hierarchy of dependencies between each of these blocks. gLucifer provides parallel visualization and the operators needed to construct new visual objects for all of these blocks. Underworld interacts most strongly with the highest level of the hierarchy, but may contain its own plugins for any of the deeper levels.

*Underworld* is the specialised part of our code aimed towards modelling geological materials with complex constitutive behaviours. It utilises the plugin environment to build upon a science-neutral finite element modelling framework. It describes, for example, the initial and boundary conditions, the material properties, and rheological laws specific to geodynamics.

The Particle-In-Cellerator (PICellerator) is a separate package that implements the Particle-In-Cell intergration schemes for the science neutral finite element framework. Underworld assumes this integration scheme in the implementation of its material-history-dependent rheological laws.

StgFEM is a framework for developing science netural finite element codes. It is broken into two sub-frameworks, one for creating finite element discretisations and one for creating systems of linear equations. It utilises the linear solver package PETSc.

StGermain is a fundamental supporting framework for developing extensible scientific codes and

frameworks. It provides the implementation for plugins and associated infrastructure.

gLucifer (10) is the visualisation framework used with and developed for StGermain. It provides interactive and background rendering for serial and parallel applications running on local and remote machines. Images and movies are created during run time, allowing for timely analysis of results. This visual output can be a key method for determining if the code output is valid.

### 2.3 Development Team

The development team consists of a broad range of loosely interacting scientist and programers across a number of organisations. The team has organised goals but is also encouraged to developed code in an organic fashion. This is particularly prevalent for the science applications. Each plugin is developed individually, to meet the needs of a specific researcher. The plugin is also available to the wider community, interacting with many other modules in configurations not anticipated by the original author.

It is important to ensure each developer is aware of this possibility when designing new applications, ensuring they are not only free from software bugs, but scientifically accurate as a stand alone product and as a dynamic, interacting piece of the larger framework. The plugins should be developed with an acknowledged robustness, enabling usage outside its original specifications.

### 2.4 Testing responsibility & requirements

The science tests for a given plugin should be the responsibility of the individual developer &/or team. The development of these test is a non trivial task, and should be considered an integral part in the development of scientific models.

To correctly assess the plugins effect on the system it must interact in a safe and predicable way. Each plugin, before it can be integrated into a stable release of the code, needs to be accompanied by a series of test-cases and the expected results. It should be possible to run in a "do nothing" mode by setting particular combinations of parameters. The plugin loads and executes all of its code, but the physical processes have no effect with this particular combination of settings. Where possible, parameter combinations which reproduce the behaviour of other plugins should be given. For example: a visco-elastic deformation module should be able to reproduce viscous behaviour if the elastic modulus is infinitely large.

# 3 Benchmarking

### 3.1 Why benchmark codes?

The classical way of verifying physical modeling codes is to compare results with simple analytic solutions, experimental observations, scaling results and other versions or codes. This process is known as benchmarking.

Carefully chosen, relatively simple benchmark problems allow us to gain confidence that the results of more complex problems are reliable. Benchmark problems are an important component of the peer review assessment of scientific work based upon modelling.

One of the challenges in developing benchmarking problems is to design simple tests with well-understood solutions which can be "incremented" to include new physical effects. A good example comes from convection: the linear diffusion equation can be solved analytically and therefore easily tested. Advection is harder to test in isolation and becomes a case requiring specialised advection schemes. Advection-diffusion as a coupled problem is easier to solve numerically and is therefore used to benchmark both diffusion and advection.

# 3.2 Bug detection versus error detection

It is important as a modeller to "know your code". It can only provide an approximate solution to the mathematics. Benchmarking helps in this characterisation, looking at whole sub-systems of the code. It is therefore only possible once at least one component of the system of equations can be solved.

Benchmarks are designed to detect inaccuracies in the implementation of the algorithm. Incompatibilities between plugins, (in)appropriate choices of discretisation resolution, and an (in)appropriate match between the chosen algorithm and the nature of the mathematics. Benchmarks are are designed to identify inaccuracies in the science, not to flush out bugs in the framework but are sensitive to their existence.

#### 3.3 Good Benchmarks

The classic benchmark is appropriate for relatively simple models, where analytical solutions exist, or those with only a small number of interacting components. The process becomes increasingly difficult with the complexity of models. The ideal benchmark problem should be fast, with deviations from expected results appearing within the system during early stages of testing and should try to isolate

one of the mathematical components of the full problem.

A benchmark problem should ideally be sensitive to algorithm change — for example by ensuring that it lies near a bifurcation between strongly different regimes. Small changes in the model may then push to the solution into another part of the phase space, through a period doubling, from a time-independent to time-dependent condition, or past a catastrophic transition. The overall model results may still be within acceptable accuracy limits as defined by a pass/fail test but the change in behaviour should always be documented.

Changes in model results should always be highlighted as part of a testing / benchmarking regime even if they indicate a reduction in error relative to simple models: reproducibility of model results is paramount. This change in behaviour, whether considered degrading or improving may also have significant effects on dependants or particular applications. For example, a method for tracking compositional interfaces(5) commonly used in geodynamics relies on correcting known properties of the chosen advection scheme to reduce numerical diffusion. A "helpful improvement" of the advection scheme to a more accurate, higher order scheme would immediately break this algorithm.

# 4 Case study: Thermochemical Convection

Thermochemical convection problems frequently arise in geodynamics including, for example, the behaviour of chemically buoyant continental crust overlying the mantle and the entrainment of the dense, low lying D" layer at the base of the mantle. The mathematical description of thermochemical convection is that of thermal convection outlined in equation 1 with the addition of a compositional buoyancy force and a compositional conservation equation (pure advection of material domains).

The non-dimensional equations governing thermochemical convection are therefore given by

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = Q(T) + \kappa \nabla^2 T$$

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = Q(C) + \kappa \nabla^2 C$$

$$\eta \nabla^2 \mathbf{v} = \nabla p + (RaT - RbC)\hat{z}$$

(2)

where

$$Ra = \frac{g\alpha\Delta\rho d^3}{\kappa\eta}, Rb = \frac{g\beta\Delta\rho d^3}{\kappa\eta}$$
 (3)

with C being composition, Q(C) the compositional buoyancy term and  $\beta$  compositional equivalent of the thermal expansivity.

For thermochemical convection, a strongly non-linear phenomenon, many individual plugins and modules within the code must be used: diffusion-advection schemes, particle transport and integration schemes, and momentum solvers. One difficulty surrounding these high-level problems lies in identifying unexpected emergent behaviour which results when the modules are combined. Positive outcomes for individual module tests will not necessary yield accurate benchmark results.

Automated testing of high-level simulations is not as straightforward as achieving a single number result within a specified accuracy. For these simulations there is no single solution which is widely considered to be 'correct', whether experimental or numerical. It is therefore often more important to reproduce scaling behaviour than a single number for comparison. It is these tests which can not only be complicated to develop, but time consuming to perform throughout development.

#### 4.1 Thermal advection-diffusion schemes

In order to solve for the energy equation used in infinite prandtl number, boussinesq fluid solutions we must implement an advection-diffusion solver. To test the accuracy of our implemented solver, results are benchmarked to the published numerical examples of a streamline upwind, petrov-galerkin formulation for convecting flows by of Brooks and Hughes (1982) (2).

These simulations solve the linear advection-diffusion equation for a range of problems, as detailed in section 3.4.2 of (2). These include skewed advection for homogenous, natural and essential, boundary conditions and the advection of a cosine hill in a rotating flow field. Test results for these simulations are shown in figure 2. The results are compared for each nodal value, with the deviation to the published figures tested to ensure accuracy.

#### 4.2 Momentum solver

The momentum solver is used for both the continuity and momentum equation, solving for stokes flow. To test the accuracy of the scheme, the common stokes flow problem of driven cavity flow is used, as outlined in Hughes (1987) (3). This simulation solves stokes flow within a box with free-slip boundary conditions,  $V_x = 0$ , along the bottom and sides, with  $V_x = 1$  along the upper boundary, as shown in

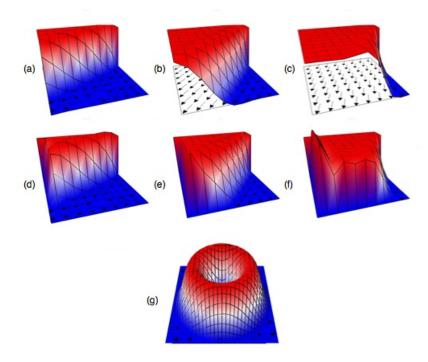


Figure 2: Results for the advection-diffusion scheme benchmark as detailed by (2). Advection skew to mesh with homogeneous natural outflow boundary condition  $vx = cos(\phi)$   $vy = sin(\phi)$  with (a)  $\phi = 22.5$ , (b)  $\phi = 45$  and (c)  $\phi = 67.5$ . Advection Skew to mesh with homogeneous essential outflow boundary condition  $vx = cos(\phi)$   $vy = sin(\phi)$  with (d)  $\phi = 22.5$ , (e)  $\phi = 45$  and (f)  $\phi = 67.5$ . Advection of a cosine hill (g).

#### figure 3.

The resulting Vrms trends for the implemented scheme can then be compared to those of previously calculated results.

#### 4.3 Thermal convection benchmarks

Thermal convection, with instabilities driven by thermal density gradients, requires both energy and momentum solvers, and thermal advection diffusion routines. The momentum equation must also be solved for a thermal buoyancy forcing term. The benchmark standard for isoviscous thermal convection codes is outlined in case 1 of Blankenbach et al (1989) (1).

Simulations are run for a range of Rayleigh numbers in a box of aspect ratio 1. The resulting steady state Nusselt number, the ratio of convective to diffusive heat transport, shown in figure 4, and Vrms values are used to determine accuracy.

**VelocityBox** 

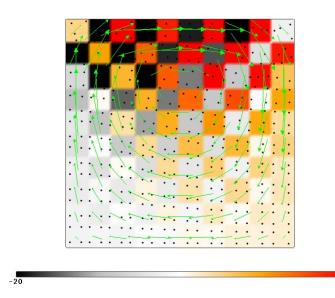


Figure 3: Benchmarking test results used for momentum solver as outlined in (3). Lid driven convection problem with free-slip bottom and side boundary conditions with an upper boundary condition of  $V_x = 1$  along the central nodes, and Vx = 0 along the 2 edge nodes on both sides. The velocity vectors are shown at time step 3.

#### 4.4 Particle advection schemes

In order to model materials with different properties particles are included in the simulation. These particles are assigned material properties, including density and viscosity. The particles are moved through the velocity field using advection schemes.

The accuracy of the particle advection scheme can be assessed by testing the tracing of passive markers (Appendix C of van Keken et al (1997) (4)). The accuracy is tested by the deviation in the particles position after one complete cycle of a steady state flow, as shown in figure 5.

The test available for the individual solution schemes are relatively straight forward. The momentum solvers, thermal advection diffusion and particle advection schemes can be tested accurately to ensure correct simulation results. Complexities arise when these schemes are brought together with particle integration methods to model geodynamic problems like that of Rayleigh-Taylor instabilities.

### 4.5 Rayleigh-Taylor convection and particle integration schemes

The instabilities within Rayleigh-Taylor convection are caused by compositional density variations, with the forcing term applied to the momentum equation being compositional buoyancy. The particle advection and integration schemes therefore need to be tested for accurate modelling.

There are many different integration schemes available to apply the weightings to specific particles

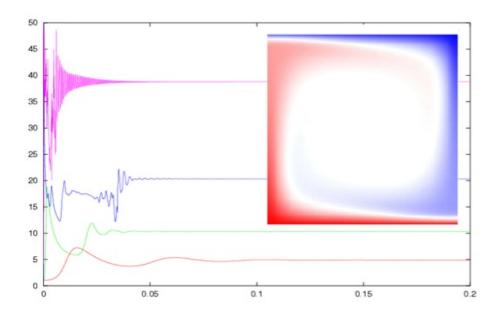


Figure 4: Nusselt number against dimensionless time for thermal convection as detailed in (1). Results are used to benchmark thermal convection, using one cell convection in a box with free-slip boundary conditions of dimension  $1\times1$  are allowed to evolve to a steady state (inset). The resulting steady state Nusselt number for Rayleigh numbers ranging from  $10^4$  to  $10^7$  are used as a benchmark, testing the advection diffusion, energy and momentum solvers for accuracy. The Nusselt number against time and the steady state temperature field are shown.

with respect to the local coordinates and material properties. The simulations shown in figure 6 are produced using approximately 20 particles per element which are initially spread uniformly throughout the domain.

The benchmark used to test the Rayleigh-Taylor simulations is outlined in van Keken et al (1997)(4), with our results shown in figure 6. The variations between these solutions, a result of differing resolution, grow with time. Hence, after a relatively short period the solutions diverge, with distinct instabilities within the boundary layers of figure 6(a) growing at a faster rate than those of figure 6(b).

#### 4.6 Thermochemical benchmarks

Modelling thermochemical convection requires an application incorporating all of the previously mentioned equations and solution methods. This introduces interdepencies at all levels, thereby increasing the complexity of the system remarkably.

The benchmark used for these simulations is again outlined in van Keken et al (1997) (4). Our simulation results shown in figure 7 match those published in figure 8 for t = 0.01 and figure 12a of (4). The entrainment rate of the dense fluid into the overlying fluid is also used as a measurable in this benchmark, however the published results to diverge within a short time.

Unlike thermal convection, that converges towards the single solution, the solutions diverge once

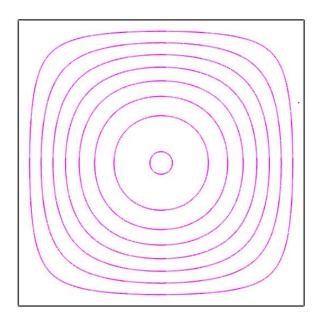


Figure 5: Benchmarking result for the particle advection scheme as detailed in (4). The advection of tracer particles through a constant velocity field by the stream function  $\psi = \psi_{max} sin(\pi x) sin(\pi y)$ , where  $\psi_{max} = \frac{250}{\pi}$ . The original position of the particle is  $(0.5, \frac{arcsin(0.05)}{\pi})$  and the particle should tracer around streamline  $\pi = 0.05$  until it finishes one revolution at time 0.2204.

particles are involved. We therefore have the complexity of models increasing with possible benchmark measurements decreasing. Quantifying individual routines for accuracy can be straight-forward, however measuring their interactions is not.

How do we then attempt to automate these benchmarkings into an ever evolving framework? Ensuring many different groups working on a range of geodynamic problems have access to the most up-to-date and accurate code.

# 5 Automated Testing of Benchmark Solutions

The aim of automated science tests is to achieve benchmarking of both interacting and isolated science components as unit tests. This is a shift from the current perception of benchmarking as an operation on a complete code to an action on a specific unit within the code. It requires seeming effortless test creation for the science implementer, a computational scientist not a programmer. It also requires the ability to break science into appropriately sized units, as demonstrated above.

To achieve a solution satisfactory to both scientists and programmers, benchmarking is implemented in three phases: the modular/unit-based code, the ability to have unit tests and finally the development of science testing tools.

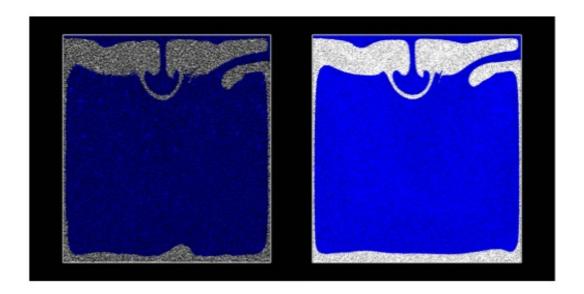


Figure 6: Benchmarking results for Rayleigh-Taylor convection as detailed in (4). The motion of an initially low, lying buoyant layer is tracked through time with the location of the initial maximum Vrms and Nusselt numbers used to measure accuracy. The particle field at dimensionless time t = 1200 for a resolution of (a)  $64 \times 64$ , (b)  $128 \times 128$  is shown.

### 5.1 Modular/Unit-based coding

Object oriented programming is typically shunned in scientific codes. In HPC environments there is a perceived loss of performance associated with the encapsulation of data and methods. Course-grain Object Orientation does not severely affect performance with respect to the ability to maintain code(9), and languages such as C can have interfaces created to enable the methodology.

StGermain enables the detangling the 'spaghetti' code once typical in scientific applications into course-grained ideas. It provides three mechanisms for describing objects: Classes, Components and Plugins. Classes suit the fine grain objects that have a role within the infrastructure, but typically not scientific concepts. Components are used to represent objects that can be configured to interact with others at run time. They are typically course-grain concepts, a mesh or a linear algebra solver.

These components and classes interact to form the system. Plugins are used to introduce new component types, change the configuration or behaviour of the system. The plugins are typical of scientific units. For example, a plugin used to modify rheology adds to the material properties and modifies the rheological law, but is not a class per se. Classes, components and plugins are then considered units and are subjected to unit tests.

In the case study we outlined the key science units needed for thermochemical convection.

The advection diffusion schemes and momentum solvers are special cases of a system of linear

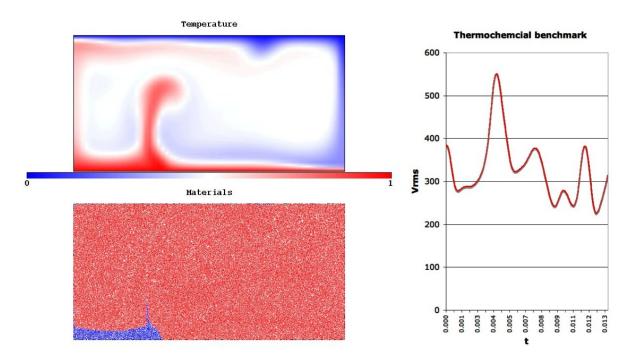


Figure 7: Benchmarking results for thermochemical convection as detailed in (4). The entrainment of a low, lying dense layer by thermal convection is evolved through time. The (a) temperature field (top left) (b) particle field (bottom left) and (c) Vrms trend against dimensionless time (right) are shown and used to access accuracy.

equations abstract component of StgFEM. The algorithms that implement these pieces of science have their own established benchmarks which is used as the unit test to that component.

The thermal convection benchmark is applicable to the system when both advection diffusion schemes and momentum solver components are in use. In this case the unit test is more like a system test or benchmark.

On the other hand, in the Rayleigh-Taylor instability model, the given particle integration and advection schemes are implemented via plugins. They customise the system into a particular configuration. With each configuration having their own unit tests for specific behaviour. The thermochemcial benchmark is a system test of the given configuration.

# 5.2 Enabling unit tests

The code's build system needs to be developed to support testing. There is a clear benefit in automatically building the tests with the code, and disabling any ability to switch this feature off. For the developer, this links ascertaining confidence in the supporting code with the development process. The computational scientist's work flow evolves from "changing the code, building the code and running the code" to "changing the code, developing tests, building the code and tests, optionally running the

tests, and then running the code".

Building the tests ensure that interface changes are trapped early, which in turn reduces the changes of code forks, replication of implementations and their tests. Where the development is done by a community of developers, then automation of the regression test becomes important.

Some infrastructure is required to build simple unit tests. StGermain provides an elementary set of features: selective printing, fire-walling and difference checking. Output streams are toggled on or off per unit at the user's discretion. A test may hardwire a unit's output to be on, where it would be otherwise disabled during production runs. Firewalls are effectively a print on assertion combination, thus simplifying the interface to a check of state within a unit. The build system itself is capable of comparing whether the output is identical to an expected outcome, enabling rapid testing without requiring any additional code.

Some of the initial science unit tests are already included in the testing suite, including the advection-diffusion schemes and momentum equation solvers. These regression tests are currently conducted automatically. We are left with the science tests, the benchmarks for Thermal, Rayleigh-Taylor, Thermochemical convection and the other geodynamic science tests as required by the user base.

# 5.3 Development of science level unit tests

At some point, the actual items within a unit being tested begin to have scientific meaning. For example, in thermochemical convection Nusselt number trends, temperature and particle fields may be subjected to comparison with an expected result. There are many reasons why these results may numerically differ but the scientific judgement considers them equivalent. One reason may be numerical accuracy of the hardware, another may be the use of another linear algebra solver.

Typically a scientist will subjectively assess the results via a visualisation in a suitable representation. In an automated system, this is not practical, and some mathematical operation is needed to reduce the judgement to one number within a tolerance. In simple cases convergence tests are suitable and implementation of convergence tests methods typically utilised by linear algebra solvers is possible. In the case of a high-level science test, these automated recursive testing becomes more complicated.

Testing the code manually using benchmarking problems is very accurate. We can easily ascertain the accuracy of many of the more complicated tests both visually and quantitatively through the Nusselt number or Vrms values. It is a combination of the quantitative results and the subjective visual appearance of the simulation at specific times which provides the benchmark. The visual check gives

us confidence in these global measurements. These visual checks are more difficult to automate than the calculated measures. This is particularly true when particles are involved. How do we measure the motion of individual plumes? To have a completely automated benchmarking test suite, we would need to implement some type of 'face' recognition software. A fix for this issue is to maintain the manual visual check through automated outputs which can be verified as required.

Simulations for thermal convection at high Rayleigh number or to resolve thermochemical convection require long periods of time to accurately produce results. Determining the resolution required for solutions to be resolved is also important. It is therefore preferable to run each science test for a range of resolutions and thus detail the required resolution as this may also change with the evolution of the code. These time increases are an important factor to consider during automation. The test will be produced frequently hence the cumulative time for these tests quickly becomes significant. It is also important to note that science tests should be run on a range of platforms. The resulting accuracy calculated, resolution required and visual checks also need to be published throughout the developer and user communities. Thus providing all parties with up-to-date information on the accuracy, resolution and versions required for the models.

In a grid computing environment we expect that the code will be providing a number of high-level science services. In our example, the code would provide both thermal and thermo-chemical convection solutions on request. As the code builds and installs, automated testing provides information on which of these services can be supported, and at what grid resolution successful results have been obtained (in serial and in parallel). This allows the code, built at different sites across the grid, to advertise the appropriate services with the additional information of which resolutions can be run on the local hardware, what level of parallelism is available, and, potentially, the likely performance.

### 6 Conclusion

The automation of science based testing within our framework will not only ensure that all members of the development and user community have access to the most accurate code at all times, it will also raise the importance of the science tests to the level of traditional system tests. It is no longer acceptable to simply have a working code, it must also be able to solve many, varied geodynamical problems at high resolution. While this has been possible for a long while, the short cycle of implementation and large base of end users has made it difficult to ensure all science aspects of the code are operational on demand. Implementing automated science testing will ensure all participants, both developers and

users, are aware of the status and version required for the end product which is, after all, the science.

# 7 Acknowledgements

We would like to acknowledge the support of the Australian Computational Earth Systems Simulator (ACcESS), the Australian Partnership for Advanced Computing (APAC), the Victorian Partnership for Advance Computing (VPAC) and Monash Cluster Computing (MC<sup>2</sup>).

Code documentation can be found at

- Underworld at http://www.mcc.monash.edu.au/twiki/view/Codes/UnderWorld
- PICellerator at https://csd.vpac.org/twiki/bin/view/PICellerator/WebHome
- StgFEM at https://csd.vpac.org/twiki/bin/view/CSD/StgFEM
- StGermain at https://csd.vpac.org/twiki/bin/view/Stgermain
- Snark at https://csd.vpac.org/twiki/bin/view//Snark.WebHome
- gLucifer http://www.mcc.monash.edu.au/twiki/view/Codes/Lucifer

# References

- [1] B. Blankenbach, F. Busse, U. Christensen, L. Crespes, D. Gunkel, U. Hansen, H. Harder, G. Jarvis, K. Koch, G. Marquart, P. Moore, D. andOlson, H. Schmeling, and T. Schnaubelt, *A benchmark comparison for mantle convection codes* Geophysical Journal International, 98:23-38, 1989.
- [2] A. Brooks & T. Hughes, Streamline upwind Petrov-Galerkin formulations for convection dominated flows with paricular emphasis on the incompressible Navier-Stokes equation, Comput. Methods Apll. Mech. Eng. 25, (1982) pp 199-259.
- [3] T. J. R. Hughes. *The Finite Element Method*, Prentice-Hall, Inc., Englewood Cliffs, NJ 07632, 1987.
- [4] van Keken, P. E. and King, S. D. and Schmeling, U. R. and Christensen, U. R. and Neumeister, D. and Doin, M.-P., *A comparison of methods for the modeling of thermochemical convection*, Journal of Geophysical Research **102**, October 1997, B10, pp 22477-22496
- [5] A. Lenardic and W.M. Kaula. A Numerical Treatment of Geodynamic Viscous Flow Problems Involving the Advection of Material Interfaces Journal of Geophysical Research, **98(B5)** pp 8243-8260, 1993.
- [6] L. Moresi and D. May and J. Freeman and B. Appelbe *Mantle convection modeling with viscoelastic/brittle lithosphere: Numerical and computational methodology* Computational Science Iccs 2003, Pt Iii, Proceedings **2659** pp 781-787, 2003.
- [7] L. Moresi, F. Dufour, and H. B. Muhlhaus. *Mantle convection modeling with viscoelastic/brittle lithosphere: Numerical methodology and plate tectonic modeling* Pure And Applied Geophysics, **159(10)** pp 2335-2356, August 2002.
- [8] L. Moresi, F. Dufour, and H. B. Muhlhaus. *A Lagrangian integration point finite element method for large deformation modeling of viscoelastic geomaterials* Journal Of Computational Physics, **184** pp 476-497, 2003.
- [9] S. M. Quenette, B. F. Appelbe, M. Gurnis, L. J. Hodkinson, L. Moresi, and P. D. Sunter *An investigation into design for code maintainability in HPC*, ANZIAM Journal (in review).
- [10] G. Watson and D.R. Stegman and C. Duboz and L. Moresi *gLucifer: Next-generation visualization framework* AGU 2004 Fall Meeting Abstracts, 2004.