CIG Geodynamics Software: Modeling Tools for the Earth Science Community

Computational Infrastructure for Geodynamics (CIG) is a membership-governed organization that supports and promotes Earth science by providing state-of-the-art tools for computational geophysics using modern software development practices. CIG continues to develop successful applications like CitComS, a finite element parallel code for modeling thermochemical convection in a 3D domain (e.g., within the Earth's mantle), now at version 3.0 which includes spherical compressible enhancements. CIG has also pursued improvements in Gale, a 2D/3D parallel code for long-term tectonics problems in orogenesis, rifting, and subduction. CIG has also committed to providing solutions for the magma community and is supporting development of a new code, the Magma Dynamics Demonstration Suite (MADDS) which will aim to prove the feasibility of including magma dynamics in more general software. All CIG software can be found via the CIG website. Geophysics researchers are encouraged to participate in the CIG community, CIG-supported workshops and training sessions, and to visit our website, http://geodynamics.org, to sign up for various mailing lists.

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CitComS 3.0 Features Compressible Convection

CitComS is a finite element code designed to solve thermal convection problems relevant to earth's mantle.

Parallel Code Written in C, the code runs on a variety of parallel processing computers, including shared and distributed memory platforms. In an effort to increase the functionality of CitComS to include greater control during simulations on large parallel systems, the software has been reengineered from previous versions of CitComS to work with a Python-based modeling framework called Pyre. With Pyre, CitComS can be dynamically coupled with other CitComS simulations or with other codes such as SNAC, which solves crustal and lithospheric problems.

Full Spherical or Restricted Region Options CitComS offers two variants, CitcomSFull and CitcomSRegional; the first solves for problems within a full spherical domain, and the second, for a restricted domain of a full sphere. Although the code is capable of solving many different kinds of convection problems using the flexibility of finite elements, there are aspects of CitComS which make it well-suited for solving problems in which the plate tectonic history is incorporated. You easily access either geometry by simply changing command line options.

Now at Version 3.0 New features include (1) two implementations of compressible convection; (2) the ability to resume computation from previous checkpoints; (3) multi-component chemical convection; (4) compressed ASCII output; (5) reading in initial temperature and tracer location from GRD files; and (6) an exchanger package for solver coupling.

Three CitComS Cookbooks

1. Subduction Model with Trench Rollback

The Problem: A common issue to address is the problem arising when the position of the oceanic trench is not constant in time (trench rollback) for a subduction zone. In addition, the trench rollback speed may vary in time, which can be caused, for example, by a rotation pole jump.

Proposed Scenario: Given two plates centered along the equator, with two different Euler poles, initially both plates have Euler poles situated far apart, so the velocities are approximately constant (about 5 cm/yr for the left plate and about 2 cm/yr for the right plate). After 30 Ma, a pole jump occurred for the right slab only, so the Euler pole moved closer.

The Result: The results for this problem are presented in Figure 1. Since the two Euler poles are kept fixed for the first 30 Ma, the shape of the subducting slab will be the same along the trench. At 25 Ma, the Euler pole for the right plate jumps toward the plate. Therefore, the velocity along the trench varies from about 1 cm/yr to about 2.5 cm/yr. This will produce in time a flat slab at one side of the model, and a steep slab at the other side.

Discussion: Seismic anisotropy of varying orientation in the mantle wedge is observed at various subduction zones. Trench-parallel flow is often invoked as the cause of the varying anisotropy. In the presented model, the subduction process is 3D and time-varying, which is necessary for the trench-parallel flow. The presented model is simplistic, but a more complicated/realistic trench geometry and subduction history can be constructed for a specific subduction zone.

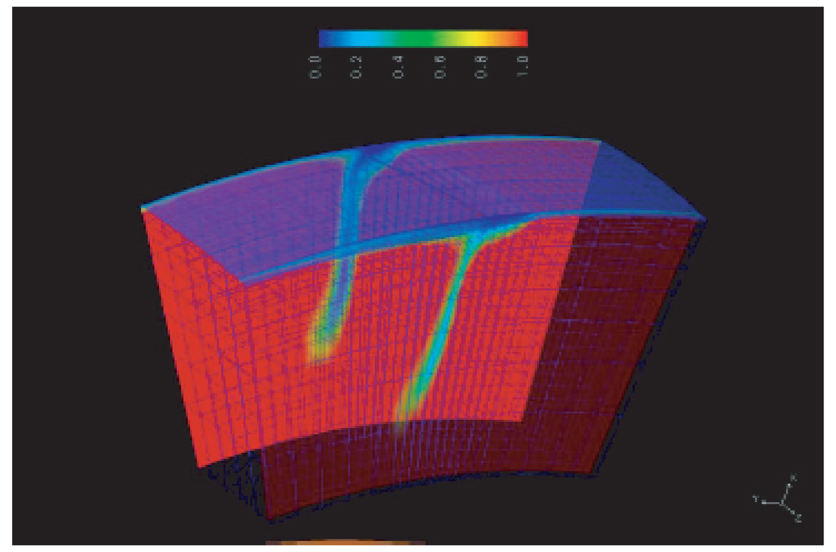


Figure 1. Result of Subduction Models with Trench Rollback The pole jump after 30 Ma produced a flat slab on one side (fore side) and a steep slab on the other side (back side).

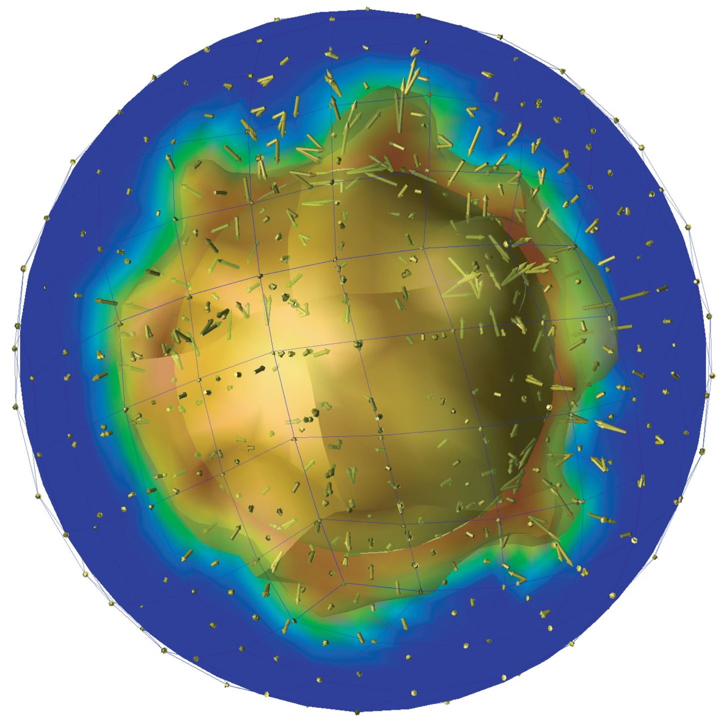


Figure 2. Result of Thermo-Chemical Convection The composition and velocity field at the 20th step. The arrows are the velocity vectors. The composition field is shown in an isosurface of 0.7 and in a cross section.

2. Thermo-Chemical Convection

The Problem: This example solves for thermo-chemical convection within a full spherical shell domain. Composition heterogeneity exists in the Earth mantle. The density anomalies due to the composition heterogeneity, as well as due to the thermal heterogeneity, drive the convection flow.

Proposed Scenario: The mantle is initially layered. The bottom layer is compositionally distinct and is denser with a buoyancy number of 0.4. The model is purely bottom heated with a Rayleigh number 10^7. The boundary conditions are constant temperature and free-slip.

The Result: The results for this problem are presented in Figure 2. The buoyancy ratio in this model is too low to stabilize the chemical layer. A few thermo-chemical plumes are rising from the lower mantle, especially the ones at 4, 11, and 12 o'clock directions. The resolution of this model is fairly low. The composition isosurface is slightly discontinuous across the cap boundary. A model of higher resolution will not have this kind of artifact.

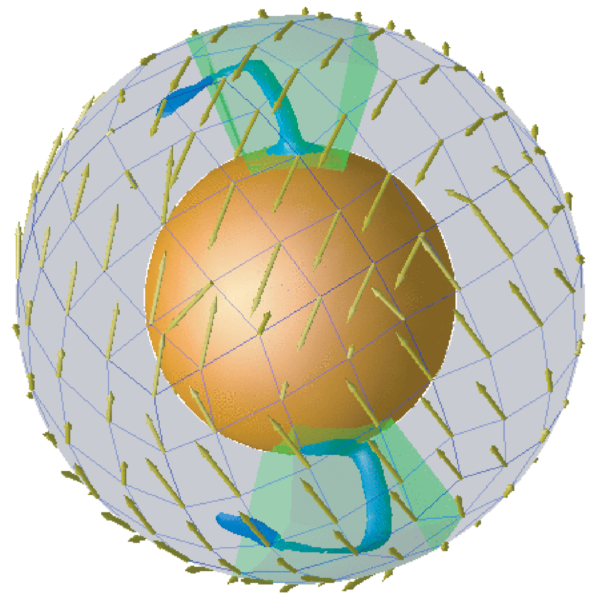


Figure 3. Interaction between two plumes under the global mantle flow.

3. Coupled Multi-Resolution Model

The Problem: Geological processes encompass a broad spectrum of length and timescales, often with different physical processes dominating at either different locations or scales. A challenging mantle convection problem is the tilting of a plume conduit in large-scale mantle flow. Hot material rising from a hot thermal boundary layer forms a low viscosity plume conduit. The tilting of a plume conduit has a substantial influence on the location of a hot spot. Numerical calculation of whole mantle flow with sufficient resolution to resolve a plume conduit remains beyond the capability of the most powerful computers, while numerical calculation of regional models is inadequate because of the missing large-scale flow.

Proposed Scenario: The motion of Hawaii and Reunion hot spots are modeled. A global solver (the containing solver) computes the global mantle flow driven by prescribed plate motion, with a grid spacing of 190 km. There are two regional solvers (the embedded solvers) which reside in the domain of the containing solver. The embedded solvers obtain their time-dependent, flow-through boundary conditions from the containing solver. The embedded solver for the Hawaii plume has a grid spacing of 56 km. The embedded solver for the Reunion plume has a grid spacing of 56 km.

The Result: The plate motion (yellow arrows) and two plumes (isosurface of T=0.08) are shown. The green boxes are the domains of the embedded solvers. The result of this simulation shows the interaction between two plumes under the global mantle flow.

Gale Adapts to the Terrain

Gale is a parallel 2D and 3D finite element code developed jointly by CIG, Victoria Partnership for Advanced Computing (VPAC), and Monash University.

Flexibilty Gale solves the Stokes and heat transport equations with a large selection of viscous and plastic rheologies. Material properties are tracked using particles, allowing Gale to accurately track interfaces and simulate large deformations. In addition, Gale has a true free surface and supports a wide variety of boundary conditions, including inflow/outflow, fixed, and stress. Thus, while Gale's original focus was on orogenesis, rifting, and subduction, it is flexible enough to be applied to such diverse problems as coronae formation on Venus and 3D evolution of crustal fault systems.

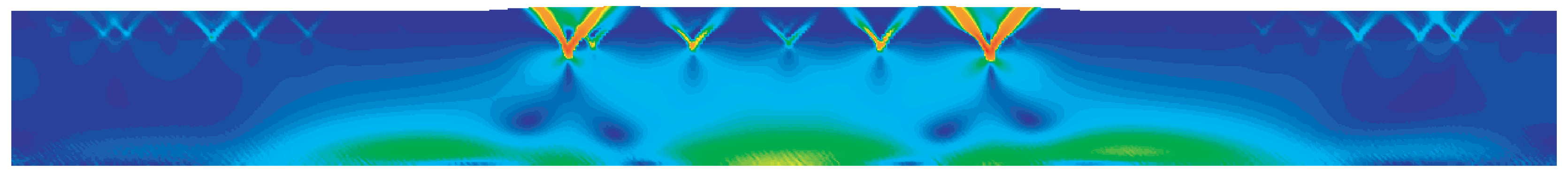
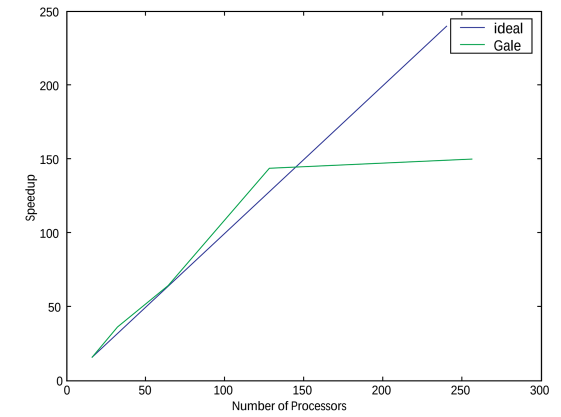
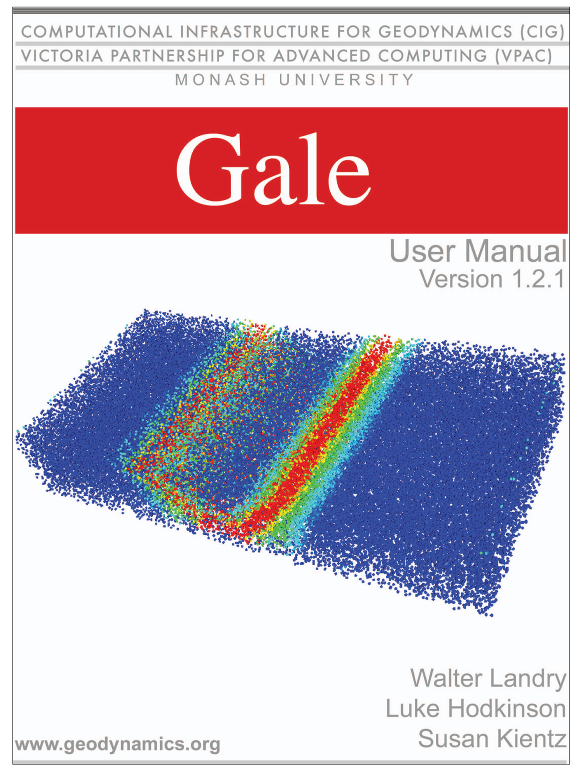


Figure 4. Strain rate of tibetan-scale (1000 km x 100 km) plateaus under extension.

Scalability Gale has been run on everything from laptops to 1000+ processor clusters.



Usability Gale is exhaustively documented with a 80+ page manual. Cookbook examples demonstrating how to use every major feature coupled with prebuilt serial binaries for Linux, Mac, and Windows make it easy to get started with small problems. For larger problems on parallel machines, there is thorough documentation on how to install and run the code on a variety of platforms. Results can be output in a simple ASCII format for further data analysis, or directly output in the standard VTK format for easy visualization with ParaView, MayaVI, or Visit.



Future Directions Gale continues to be developed, with the next release, slated for October 2007, implementing frictional boundary conditions, a simple API for plugging in custom surface process models, and easier visualization of large parallel runs.

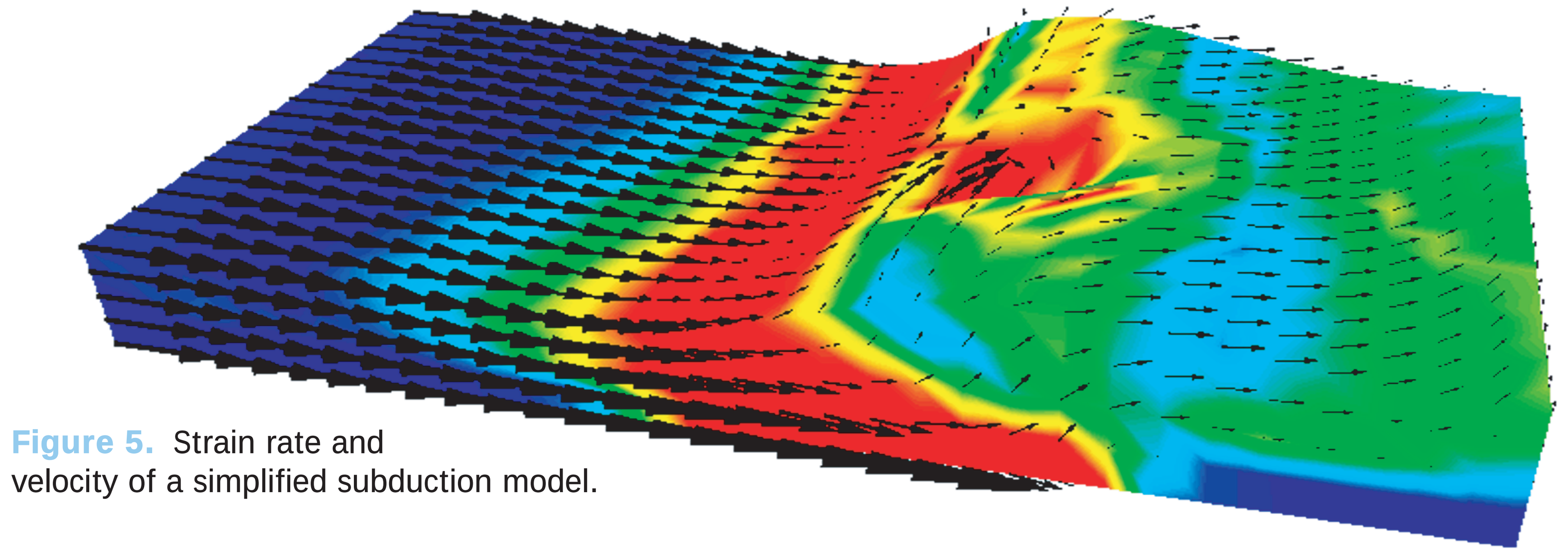


Figure 5. Strain rate and velocity of a simplified subduction model.

In Development: Magma Dynamics Demonstration Suite (MADDS)

Developed in Response to Community Need In a CIG-supported workshop (Columbia University, August 2006), the magma dynamics community expressed the need for generally available, documented, open-source software to explore how magma dynamics interacts with mantle convection and/or long-term tectonics and for developing a better integration of regional and global geodynamics and geochemical evolution of the Earth.

Benchmarks Identified The initial software suite focuses on implementing algorithms for coupled fluid-solid dynamics in deformable porous media. A systematic sequence of benchmark exercises includes (1) tests for accurate dynamic pressures in existing solid deformation codes; (2) flow within a column with forced melting; (3) magmatic solitary waves; (4) shear bands developed through the coupling with shear flow in 2D; (5) 2D ridge models driven by either buoyancy or shear flow in 2D, including forced adiabatic melting; (6) imposed velocity field; (7) self-consistent velocity fields; (8) coupling with temperature solvers; and (9) 3D ridge models with boundary conditions from global mantle flow model.

Pressure Solvers Reliability is First Step Because fluid flow is directly proportional to pressure gradients, it is essential that the pressure fields from solid-flow solvers are accurate. We have nearly completed the initial task of estimating the reliability of pressure solvers in existing software (i.e., StGermain Stokes solvers) and have implemented quadratic elements with both continuous and discontinuous pressure (i.e., Q2-Q1 and Q2-P1) along with Recovery by Equilibrium in Patches (REP) pressure smoothing. The current best elements for integration with magma-dynamics appear to be Q2-Q1 (Taylor-Hood) elements.

Project Draws on Many in Magma Field Marc Spiegelman (Columbia) is providing guidance to VPAC on the implementation of Madds. He also shared a spectral 2D and 3D mid-ocean ridge flow code (SPECRIDGE) and is developing with Richard Katz a PETSc-based solver for MADDS, starting with treatment of solitary waves. Other working group members are implementing MADDS in other general software platforms (e.g., Comsol Multiphysics). Laurent Montesi (WHOI) shared a pressure-velocity corner flow benchmark using power law rheology (NNcorner). These MADDS-related examples and others that will be developed are gathered in a Mercurial software repository at CIG.

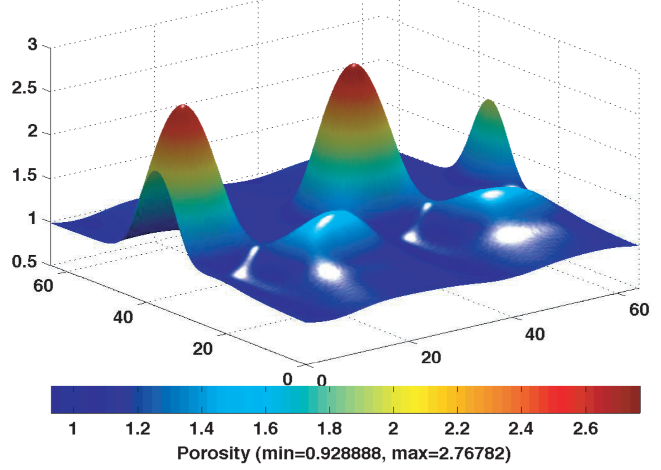


Figure 6. Time-dependent solution of magmatic solitary waves in 2D using a new Parallel Solitary Wave benchmark code.

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