Computational Infrastructure for a MARGINS Successor Program

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Computational infrastructure has played a significant role in MARGINS research and we believe that its potential as a tool for integrative studies will grow significantly in a successor program. A MARGINS successor program could benefit by strengthening linkages and interaction with existing efforts both within the geosciences and those that exist more broadly. Here, we describe the NSF supported Computational Infrastructure for Geodynamics (CIG), the lessons learned, and the opportunities that will unfold. The Computational Infrastructure for Geodynamics (CIG) is a facility that NSF supports for software development and maintenance in the geosciences. The resources provided by CIG are particularly useful for the MARGINS community given the goal of enhancing our understanding of plate margin processes through an interdisciplinary approach. As a community-governed organization, CIG has a small team of software engineers who provide software services to the community in terms of programming, documentation, training, and support. Guidance for the programmers comes from a Science Steering Committee. CIG commenced in 2004 with much of the software team housed at Caltech. In our currently pending with NSF, CIG will move to the University of California, Davis, while continuing to provide broad support to the community.

With a high level of community participation, CIG has leveraged the state of the art in scientific computing into a suite of open-source tools and codes. Many of the problems addressed generally in geodynamics are computationally challenging, often involving processes occurring over a wide range of time and spatial scales. Since existing solution methods are often not sufficiently robust to solve these problems, CIG has pursued a strategy of partnering with the larger world of computational science. In some cases, scalable, robust methods have yet to be discovered and new research is needed while in other cases methods can be imported from allied disciplines. CIG software is being developed collaboratively with investigators from national labs, software companies, and academics in applied mathematics.

The software is developed and maintained for problems ranging widely from mantle dynamics, crustal and earthquake dynamics, magma migration, seismology, and related topics, important components of the Seize, RCL, and SubFac initiatives. CIG has been able to introduce a number of important stand alone codes that has been used widely in margins-related research, such as *CitcomS* for thermal-chemical convection, *PyLith* for the entire earthquake cycle from tectonic loading and unloading to dynamic rupture, or *Gale* for the spontaneous initiation and evolution of faulted rift and compressional margins. In all cases, we have attempted to balance the needs of respecting the three-dimensional geometry of the geological environment and the strong variations in material properties that occur in tectonic problems, with the need to scale efficiently from desktops to the most massively parallel supercomputers available. In other cases, CIG has opted not to pursue the development of single stand-alone codes, such as in magma migration because the community has not been able to agree on the equations governing the underlying physics. In the case of magma migration, we have developed benchmarks and developed a test suite of codes for solving them.

One of the underlying computational challenges spanning nearly all of geodynamics is the need to resolve fine-scale features (such as faults or the sharp boundary of a rising mantle plume) embedded in a larger domain (such as a plate or the mantle). The computational challenge is the need to resolve the fine features as they form, evolve and entirely disappear. Often, the fine scale features are associated with strong jumps in materials properties (such as jumps in viscosity over many orders of magnitude) making the problems highly ill conditioned. CIG has pursued a multiple approach to bring useful software to the geoscience community. The first is a collaboration with the developers of *deal.II*, a finite element library with a wide range of functionality in Adaptive Mesh Refinement (AMR), through the creation of a geodynamics, AMR test suite. We currently have tutorials for Stokes flow and mantle convection but will soon release examples in magma migration and visco-elastic deformation. We have also pursued a research strategy with the Institute of Computational Science and Engineering (ICES) at the University of Texas, Austin through which we have recently demonstrated global mantle convection problems having resolutions as fine as 1 km while scaling on tens of thousands of computational cores (processors). In terms of resolution and scalability, the applications are far reaching for all of geodynamics.

An entirely different strategy that CIG has pursued for the community has been the development and maintenance of Science Gateways to allow users to initiate and monitor simulations on the TeraGrid (the current incarnation of the NSF supercomputer centers and a powerful resource that is under utilized by the geosciences community). One portal applicable to the MARGINS community is CIG's computational seismology gateway in which users can simulate seismic wave propagation in fully three-dimensional earth models using the versatile *Specfem3D* code. On the web, users can select the seismic sources and stations (with the data automatically retrieved), select the earth model, start the simulation on a remote parallel computer, and later download the results in the popular SAC format. The Gateway allows users to upload their own 3D earth model or to import the results of a global model of mantle convection.

The CIG vision for the future is on one of interoperable software that allows users to seamlessly move from data to dynamic models and back to data using computational models that are able to handle the extreme variations in material processes and multi-physics, while respecting the complex geometry of geological processes (Fig. 1). Strengthening the linkages between the MARGINS community and CIG is a clear route to expanding the use of computational models in a MARGINS successor program.

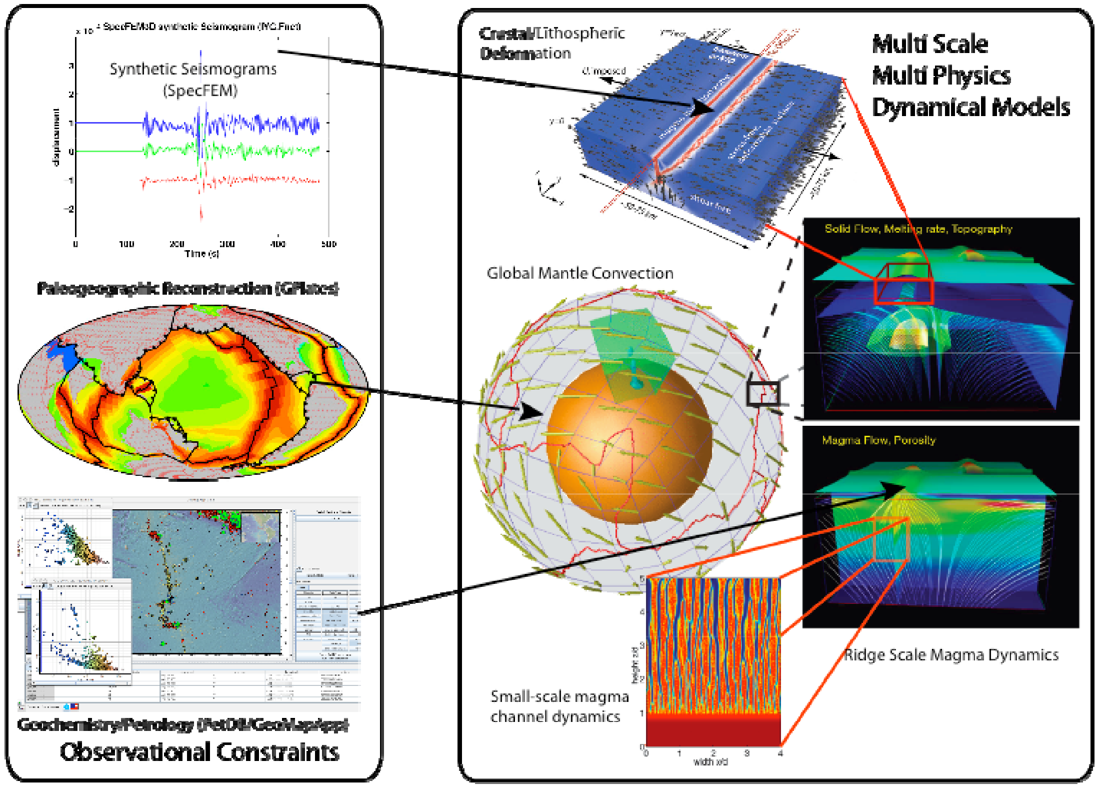

Figure 1: Examples of computations and data available to help us understand solid earth dynamics at a range of scales as envisioned in the next phase of CIG. In this case, the dynamics of plate boundary processes and their interaction with global mantle flow. RIGHT PANEL: Example output of computational codes for global mantle convection (*CitcomS*), midocean ridge flow with melting and melt transport, crustal scale magma injection and faulting (*Gale*), and small scale reactive melt channel formation. Each model was designed to consider a particular scale or set of processes. The challenge is how to permit users to combine these models, as needed, to explore the dynamics of the coupled interactions and use them to make inferences from geophysical and geochemical data. LEFT PANEL: Example data used to test and drive models, including seismic waveforms (*SPECFEM*), plate reconstructions (*GPlates*), and geochemistry (*PetDB*).

Additional information on CIG can be found at:
http://www.geodynamics.org/

The CIG-II proposal and the comprehensive document “Expanding Computational Infrastructure: The First Five Years of CIG” can be found at
http://www.geodynamics.org/cig/proposalsndocs/blogs/cig2-proposal/index_html