CIG Science Gateway and Community Codes for the Geodynamics Community

January 12, 2018

Project Overview

The Computational Infrastructure for Geodynamics (CIG), an NSF cyber-infrastructure facility, aims to enhance the capabilities of the geodynamics community through developing scientific software that addresses many important unsolved problems in geophysics. CIG's strategy is to:

1. support the benchmarking and validation of its codes,
2. develop new codes and ensure they achieve good performance and scalability, and
3. assist new users by providing technical support, training, and small allocations of computation time.

These efforts have met with success, and the current CIG compute allocations on the XSEDE infrastructure have been used at a substantial rate to achieve these goals.

CIG supports the aforementioned efforts in the following areas of activity: geodynamo simulation, mantle dynamics, seismic wave propagation, and crustal and lithospheric dynamics on both million-year and earthquake time-scales.

In this proposal, we request support to continue these activities and to test next-generation, large-scale computational codes for use in geophysics. In the next section, we describe the major scientific questions and computing challenges that CIG focuses on. We then describe the codes and methodologies used and offer a justification of the requested resources.

Science Objectives

Core Dynamo and Dynamics. Numerical simulations have played a large role in elucidating fluid motion in the Earth's outer core and the resulting geomagnetic field generation (so called geodynamo). Although previous efforts (after Glatzmaier and Roberts, 1995) have successfully reproduced some spatial and temporal characteristics of the geomagnetic field, a large discrepancy still exists between the parameters used in geodynamo simulations and actual values associated with the outer core. This discrepancy reflects the extremely low viscosity of the liquid outer core. The low viscosity results in a vast range of length scales of the flow required for a comprehensive simulation, ranging from the geometry of the outer core ($L \sim 1000$km) to the thickness of the boundary layer ($L \sim 0.1$m). Computational resources are still insufficient to achieve this level of resolution, but the community is working to target a middle range ($L \sim 100$m) that can be achieved using the cutting edge numerical methods and high-end supercomputers available today.

Mantle Dynamics. Mantle convection is at the heart of understanding how the Earth works, but the process remains at best poorly understood because the mantle is not accessible to direct observation. Progress on fundamental questions, such as the dynamic origin of the tectonic plates that cover the surface, layering and stratification within the mantle, evolution of the thermal history of the Earth and its geochemical cycles, the interpretation of seismic tomographic models of Earth's interior structure, and the source of volcanic hotspots, all require an interdisciplinary approach. Numerical models of mantle convection must therefore assimilate information from a wide range of disciplines, including seismology, geochemistry, mineral and rock physics, geodesy, and tectonics.

The technical challenges associated with modeling mantle convection are substantial. Mantle convection is characterized by strongly variable (i.e., stress-, temperature-, and pressure-dependent) viscosities. The lithosphere exhibits processes such as fracture and shear zone deformation (strain localization) that are physically distinct from the viscous flow deeper in the mantle, and occur on fundamentally different (smaller) length scales. In addition, the mantle is chemically heterogeneous, is replete with silicate melts and volatiles, and has numerous pressure- and temperature-induced structural changes that affect its dynamics.

Crustal and Lithospheric Dynamics: Million Year Timescales. The lithosphere, with the embedded crust, represents the main thermal boundary layer of the Earth's heat engine and, as such, encompasses a wide range of pressure and temperature conditions with diverse deformation mechanisms. Recently, deep seismic profiling, receiver function analysis, and magnetotelluric sounding have greatly increased our understanding of crustal and lithospheric structure. Numerical modeling has become an essential step in the integration of these data into process-orientated models of mountain building, lithospheric stretching, sedimentary basin genesis, and plate boundary deformation.

Deformation of the lithosphere presents a number of challenges to numerical simulationsd. The deep lithospheric mantle encompasses a differential temperature of up to 1000°C and an effective viscosity contrast of many orders of magnitude. The complex physics of frictional materials is particularly challenging because it involves strain-localization, time- and rate-dependent yield strength and strain softening. Crustal deformation is a free-surface problem and sensitive to the complexities of the Earth's surface, including physical and chemical erosion, mass transport by rivers and ocean currents, and deposition of sediment. There are also broad implications for the feedback between erosion and tectonic uplift. Climate change during the late Cenozoic has influenced sediment (and thus geochemical) fluxes to the ocean and atmosphere, and the way in which crustal dynamics modulates the erosional response of the Earth to climate change remains an open question.

Crustal Dynamics: Earthquake time-scales. A rapidly advancing area of crustal geodynamics, one of great societal importance, is the problem of the physics of the earthquake cycle. Because of the recent development of the capability for high-accuracy measurement of deformation of the Earth's surface in real time, this field, long starved for data, is now a burgeoning observational science. Recent observations made with high precision space geodesy indicate that displacements caused by slow aseismic motions following earthquakes can be comparable to coseismic displacements, demonstrating substantial post-seismic evolution of strain and stress in addition to coseismic changes.

It has recently been recognized that relatively modest changes in stress can trigger earthquakes. Theoretical advances in rock mechanics have led to algorithms relating temporal variations in stress to changes in earthquake activity, and are beginning to enable quantitative predictions of how stress changes from fault interactions influence seismic cycles. For example, a 3D finite element model of the Coulomb stress has addressed whether the 1999 Hector Mine earthquake was triggered by the 1992 Landers earthquake. Although results from models such as these have been impressive, more definitive tests require an order of magnitude finer nodal spacing, meshes incorporating the actual elastic structure of the region, the interaction of many faults, and more realistic rheologies.

Seismic Wave Propagation. Seismology provides the means to image the three-dimensional structures within the Earth's interior that are responsible for geodynamic processes. The foundation of computational seismology is the generation of synthetic seismograms and adjoint methods, used in the modeling and inversion for Earth structure, earthquake rupture, and wave propagation effects. CIG aids the community by supporting 3D codes that provide a more-accurate representation of Earth properties such as anisotropy, attenuation and gravitational affects. Such 3D codes are now revolutionizing seismology, by allowing a direct investigation of countless geodynamic topics such as the fate of subducted lithosphere, existence of mantle plumes, lithospheric structure, and plate boundary zone complexity.

Infrastructure. Investigation into these vital Earth science issues has generally been hampered by lack of computational power to model or simulate Earth structures. Most geophysical processes are complex, coupled, and impossible to solve analytically or simulate in a laboratory, hence, a long-term, sustained effort in model building and large-scale simulation is needed. Geophysical models and codes have reached a level of maturity that allows and requires large-scale 3D coupled simulations, but require substantial computational resources and infrastructure. CIG facilitates solutions by developing open-source geodynamics software that addresses such problems, and by supporting workshops, training sessions, and conferences in the above sub-disciplines. However, even with investments by universities and institutions in small- to medium-sized clusters, a large number of problems in geodynamics still require more powerful capabilities. CIG intends to continue developing and benchmarking its codes, conducting training sessions on its applications, and encouraging new users to try XSEDE resources to see if they can be applied effectively to their research problem. This proposal details five major geodynamics software packages that CIG believes to be most important to the community performing research in mantle convection, planetary dynamos, seismology, and short/long time-scale tectonics.

Computational Experiments and Resource Requirements

Numerical Approaches

Calypso. Calypso is a code to perform magnetohydrodynamics (MHD) simulations in a rotating spherical shell modeled on the Earth's outer core. It uses a spherical harmonic transform method in the horizontal discretization and a finite difference method in the radial discretization. Linear terms (e.g. diffusion, buoyancy, Coriolis force) are evaluated in spherical space, while non-linear terms (advection, Lorentz force, magnetic induction) are evaluated in the physical space. For time integration, Calypso uses a Crank-Nicolson scheme for the diffusion terms and second-order Adams-Bashforth scheme for the other terms.

Rayleigh. Rayleigh is an open-source community dynamo code developed by Nicholas Featherstone (CU Boulder) with sponsorship by CIG. This code solves the three-dimensional, nonlinear, MHD equations of motion for a compressible fluid in a rotating spherical shell under the anelastic approximation. Rayleigh employs a pseudo-spectral algorithm with spherical harmonic basis functions and mixed explicit/implicit time-stepping (Adams-Bashforth/Crank-Nicolson). A poloidal/toroidal representation ensures that the mass flux and magnetic field remain solenoidal. Rayleigh is also used in a DOE INCITE project which was awarded 800 million core hours through 2015 to 2017. For 2018, the projected has been awarded 20 million core hours on ALCF Mira for finalizing the INCITE project.

ASPECT. ASPECT is a CIG developed code desinged to solve the equations that describe thermally driven convection in the Earth's mantle and tectonic deformation in the Earth's lithosphere. It allows for both 2D and 3D models of arbitrary shapes (generally focused on segments or whole mantle models), adaptive mesh refinement in locations of scientific interest, easy modification of material, gravity, rheology and temperature models, and tracers to model geochemistry and material transport. Recent work has started investigating the effectiveness of GPU or MIC coprocessors in ASPECT simulation. Further details are available in [Kronbichler et al. 2012, Heister et al. 2017].

CitcomS. CitcomS is a finite element code to solve thermo-chemical convection problems relevant to the planetary mantle in a 3D spherical geometry [since Moresi and Solomatov, 1995]. There are two forms of meshes and geometries for CitcomS, regional and spherical. CitcomS employs an Uzawa algorithm to solve the momentum equation coupled with the compressibility constraints [Moresi and Gurnis, 1996]. Nested inside the Uzawa algorithm, the code uses either a conjugate gradient solver or a multi-grid solver to solve the discretized matrix equations. The energy equation is discretized in the Streamline Upwind Petrov-Galerkin method [Brooks, 1981] and integrated with an explicit second-order predictor-corrector method.

PyLith. PyLith is a 2D and 3D finite-element code for modeling interseismic and seismic processes related to capturing the physics of earthquakes, including slow strain accumulation, sudden dynamic stress changes during earthquake rupture, and slow postseismic relaxation. Implicit time-stepping provides efficient time integration for quasi-static (interseismic deformation) problems, and explicit time-stepping provides efficient time integration for dynamic (rupture and wave propagation) problems. Key features of PyLith are its ability to accommodate unstructured meshes (which allows complex nonplanar fault geometry), implementation of a variety of finite-element types, and implementation of a variety of fault and bulk constitutive models appropriate for the Earth's lithosphere. The bulk constitutive models include linear and nonlinear viscoelastic models in addition to linear elastic models. PyLith uses PETSc [Balay et al., 1997, 2001, 2004] to achieve fast, efficient, parallel solution of the partial differential equation.

SPECFEM3D_GLOBE. In collaboration with Princeton, Caltech and the University of CNRS (France), CIG offers this software, which simulates global and regional (continental-scale) seismic wave propagation using the spectral-element method (SEM). The SEM is a continuous Galerkin technique, which can easily be made discontinuous; it is then close to a particular case of the discontinuous Galerkin technique, with optimized efficiency because of its tensorized basis functions. In particular, it can accurately handle very distorted mesh elements [Oliveira and Seriani, 2011].

SPECFEM3D_GLOBE has very good accuracy and convergence properties [De Basabe and Sen, 2007]. The SEM approach admits spectral rates of convergence and allows exploiting hp-convergence schemes. It is also very well suited to parallel implementation on very large supercomputers [Carrington et al., 2008] as well as on clusters of GPU accelerating graphics cards [Komatitsch, 2010].

Further details regarding each code and downloads of the source are available at the following URL in Table 1 (Rayleigh is currently not publicly available).

Table 1: List of Websites

Code	Website
Calypso	`https://geodynamics.org/cig/software/calypso/`
Rayleigh	`https://www.youtube.com/watch?v=km0Bv6p2UO8`
	`https://www.youtube.com/watch?v=6u0P-pyJsXo`
ASPECT	`https://geodynamics.org/cig/software/aspect/`
CitcomS	`https://geodynamics.org/cig/software/citcoms/`
PyLith	`https://geodynamics.org/cig/software/pylith/`
SPECFEM3D_GLOBE	`https://geodynamics.org/cig/software/specfem3d_globe/`

Resource Requirements

CIG researchers used a significant portion of the past period's allocation for studies of the geodynamo and mantle convection. In the upcoming period, we anticipate using SUs at higher rate than the previous period, due to the ongoing development, testing, and the ramp up of benchmarking and research use of CIG codes.

CIG plans the following use of its proposed XSEDE resources during the period of April 1st, 2018 to March 31, 2019 in support of (1) scalability testing and code validation, (2) development of new numerical methods for better code performance, (3) workshop training sessions, and (4) nurturing new geophysics users on XSEDE resources using Calypso, Rayleigh, ASPECT, CitcomS, PyLith and SPECFEM3D_GLOBE. New users anticipate million of core hours will be required to conduct their research in which CIG expects to support the feasibility testing and spin up which will enable researchers to apply for their own allocations. More details are provided below.

ASPECT, Calypso, Rayleigh, and SPECFEM3D_GLOBE development. THe mantle convection and lithospheric deformation code ASPECT is continuing development and scaling work lead by CIG researchers at UC Davis, Colorodo State University Fort Collins, and Clemson University. Calypso and Rayleigh geodynamo codes are also continuing development and scaling work by Dr. Hiroaki Matsui, and Dr. Nick Featherstone, respectively. SPECFEM3D_GLOBE is principally developed by Prof. Jeroen Tromp, Dr. Matthieu Lefebvre, amd Dr. Dimitri Komatitsch. The allocation will be used to establish the scaling performance and efficiency of each code, add functionality, and improve the support for Xeon Phi and/or GPGPU based computation. To perform simulations to ensure the validity of the codes and check their scalability and performance, we anticipate requiring up to 256 nodes for brief periods (10-20 hours) and estimate a total requirement of 5,000 SUs for each code (10,000SUs in total) on Stampede2 for this development. We also request 15,000 SUs on Comet GPU nodes for development of GPGPU based computation.

Geodynamo performance benchmarks Various researchers collaborating with CIG have already analyzed the accuracy of a dozen geodynamo codes. The performance of each of the geodynamo code also needs to be checked for scaling and efficiency. Dr. Hiroaki Matsui previously performed the performance benchmark on Stampede [Matsui, H. *et al.*, 2016]. We need to perform the benchmark again on the new supercomputer Stampede2. This will require multiple short runs on a various range of core counts for about fifteen different codes. This benchmark is performed with varying wall time and node up to 1024 nodes. This test will require 15(models) x 3(hour) x 512(nodes) = 23,040 SUs.

Geodynamo turbulence studies Dr. Hiroaki Matsui plans to investigate the dynamics of turbulence in a planetary dynamo using Calypso. Because the current model based on an accurate Earth core dynamo requires extremely high resolution (on the order of 10 million cores for 1000 hours), Dr. Matsui is currently working on application of sub-grid scale modeling for geodynamo simulations. To establish the validity of this approach, it is necessary to perform large scale simulation for reference and small scale simulations including SGS models on Stampede2. The large scale simulation requires 80 nodes for 240 hours, and 16 nodes times 120 hours will be required for the smal scale simulations with SGS model. In total, we request 21,120 SUs for the geodynamo turbulence studies.

High-Resolution 3D modeling of lithospheric deformation, mantle convection and fluid transport with ASPECT Dr.'s John Naliboff, Juliane Dannberg, Rene Gassmoeller, Gerry Puckett and Louise Kellogg are actively developing ASPECT to enable high-resolution modeling of processes that capture both solid deformation, fluid transport and thermodynamically consistent fluid-solid reactions. The underlying development efforts include increasing solver or particle tracing efficiency, implementing new physics (e.g., governing equations), coupling to external software packages and testing complex model designs based on the underlying software developments. At present, these developments efforts aim to address a wide range of geologic processes, including melt generation during plume-lithosphere interaction, global volatile cycling through the lithosphere and convecting mantle, subduction zone seismicity and coupling between surface processes and solid Earth deformation. In all cases, the simulations derived from these efforts include highly non-linear behavior and frequently involve high-resolution 3D simulations that require upwards of 50,000-100,000 SUs. Here, we a requesting 1,000,000 SUs on Comet to continue these development efforts and test preliminary high-resolution simulations that will form the basis of future XSEDE research allocations and proof of concept tests cases freely available to the Geodynamics community.

In total, a yearly allocation of 64,160 SUs on Stampede2, 1,000,000 SUs on Comet, and 15,000 Comet GPU nodes will enable CIG to continue offering support and training to users of these common geophysics codes. This will also allow extensive studies of code accuracy, performance and validation using high-resolution simulations. We also request 10,000 GB on the

Table 2: Summary of requested SUs

Software	Purpose	Requested SUs
Calypso	Development and optimization	5,000
	Geodynamo turbulence studies	21,120
Rayleigh	Development and optimization	5,000
Calypso/Rayleigh	Performance benchmark	23,040
ASPECT	Development and optimization	5,000
SPECFEM3D_GLOBE	Development and optimization	5,000
	Total for Stampede2	64,160
ASPECT	Mantle convection	1,000,000
	Total for Comet	1,000,000
Calypso	GPGPU development	15,000
	Total for Comet GPU	15,000

data storage system Ranch and 10,000 GB on the data storage system Data Oasis to assist in analyzing and visualizing simulation results and to develop GPGPU based computations.

References

Balay, S., K. Buschelman, W.D. Gropp, D. Kaushik, M.G. Knepley, L. Curfman McInnes, B.F. Smith, and H. Zhang, PETSc Web page, http://www.mcs.anl.gov/petsc/, 2001.

Balay, S., K. Buschelman, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L. Curfman McInnes, B.F. Smith, and H. Zhang, *PETSc Users Manual* , ANL-95/11 - Revision 2.1.5, Argonne National Laboratory, 2004.

Balay, S., W.D. Gropp, L. Curfman McInnes, and B.F. Smith, Efficient Management of Parallelism in Object Oriented Numerical Software Libraries, *Modern Software Tools in Scientific Computing*, Edited by A.M. Bruaset and H. P. Langtangen, 163–202, Birkhauser Press, 1997.

Brooks, A.N. A Petrov-Galerkin Finite Element Formulation for Convection Dominated Flows. Unpublished doctoral thesis, California Institute of Technology, Pasadena, CA, 1981.

Carrington, L., D. Komatitsch, M. Laurenzano, M. Tikir, D. Micha, N. Le Goff, A. Snavely, and J. Tromp. High-frequency simulations of global seismic wave propagation using SPECFEM3D_GLOBE on 62 thousand processor cores. *Proceedings of the ACM/IEEE Supercomputing SC2008 conference*, 1–11, doi: 10.1145/1413370.1413432. Article #60, Gordon Bell Prize finalist article, 2008.

De Basabe, J. D. and M. K. Sen. Grid dispersion and stability criteria of some common finite-element methods for acoustic and elastic wave equations.*Geophysics*, **72(6)**, T81–T95, doi: 10.1190/1.2785046, 2007.

Glatzmaier, G. A. and P. H. Roberts. A three-dimensional self-consistent computer simulation of a geomagnetic field reversal. *Nature*, **377**, 203-209, 1995.

Heister, T., Dannber, J., Gasmöeller, R., Bangerth, W. High accuracy mantle convection simulation through modern numerical methods II: realistic models and problems. *Geophys. J. Int.*, **210**, 833–851, doi: 10.1093/gji/ggx195, 2017.

Komatitsch, D., D. Göddeke, G. Erlebacher, and D. Micha. Modeling the propagation of elastic waves using spectral elements on a cluster of 192 GPUs. *Computer Science Research and Development*, **25(1-2)**, 75–82, doi: 10.1007/s00450-010-0109-1, 2010.

Kronbichler, M., T. Heister, W. Bangerth, High Accuracy Mantle Convection Simulation through Modern Numerical Methods. *Geophys. J. Int.*, **191**, 12–29, doi: 10.1111/j.1365-246X.2012.05609.x, 2012.

Matsui, H., E. Heien, J. Aubert, J.M. Aurnou, M. Avery, B. Brown, B.A. Buffett, F. Busse, U.R. Christensen, C.J. Davies, N. Featherstone, T. Gastine, G.A. Glatzmaier, D. Gubbins, J.-L. Guermond, Y.-Y. Hayashi, R. Hollerbach, L. J. Hwang, A. Jackson, C.A. Jones, W. Jiang, L.H. Kellogg, W. Kuang, M. Landeau, P. Marti, P. Olson, A. Ribeiro, Y. Sasaki, N. Schaeffer, R.D. Simitev, A. Sheyko, L. Silva, S. Stanley, F. Takahashi, S. Takehiro, J. Wicht, and A.P. Willis, Performance benchmarks for a next generation numerical dynamo model, *Geochem. Geophys. Geosys*, **17**, DUI:10.1002/2015GC006159, 2016.

Moresi, L.N., and V.S. Solomatov, Numerical investigation of 2D convection with extremely large viscosity variations, *Phys. Fluid*, **7**, 2154–2162, 1995.

Moresi, L., S. Zhong, and M. Gurnis, The accuracy of finite element solutions of Stokes flow with strongly varying viscosity, *Physics of the Earth and Planetary Interiors*, **97**, 83–94, 1996.

Oliveira, S. P. and G. Seriani. Effect of element distortion on the numerical dispersion of spectral element methods. *Communications in Computational Physics*, **9(4)**, 937–958, 2011.