Project Overview

The Computational Infrastructure for Geodynamics (CIG), an NSF center, aims to enhance the capabilities of the geodynamics community through developing software that addresses many important unsolved problems in geophysics. CIG's strategy has been to

1) support the benchmarking and validation of its codes
2) develop new codes and ensure they achieve good performance and scalability
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.

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 evolution. Numerical simulation has a large role in understanding the fluid motion in the outer core of the Earth and the resulting geomagnetic field generation (the geodynamo). Although previous work [Glatzmaier, 1995] has successfully reproduced some spatial and temporal characteristics of the geomagnetic field, there is still a massive discrepancy between fully accurate numerical dynamo simulations and the actual core because of very low viscosity in the core from liquid iron. This low viscosity results in a wide range of length scales required for a comprehensive simulation, ranging from the outer core ($L \sim 1000$km) to 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 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. Progress on fundamental questions, such as the dynamic origin of plates, layering and stratification within the mantle, geochemical reservoirs, the thermal history of the Earth, the interpretation of tomography, 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 critical 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 Time-Scales. 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 a diversity of deformational mechanisms. Recently, deep seismic profiling, receiver function analysis, and magneto-telluric 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 simulation. The deep lithospheric mantle encompasses a differential temperature of up to 1,000° 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 geodetic monitoring of crustal deformation in real time using GPS and InSAR, 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 make possible quantitative predictions of how stress changes from fault interactions influence seismicity levels. 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. 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. Within the context of CIG, 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, used in the modeling of Earth structure, earthquake rupture, and aspects of wave propagation. CIG aids the community by making 3D codes that provide a more-accurate representation of Earth properties such as wave anisotropy and attenuation available to the community. 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 — which implies that 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 they need substantial infrastructure in order to be run. CIG has facilitated 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, core dynamics, seismology, and short/long time-scale tectonics.

Computational Experiments and Resource Requirements

Numerical Approaches

Calypso. Calypso is a newly developed code to perform magnetohydrodynamics simulations in a rotating spherical shell modeled on the Earth's outer core. Convection in this core is driven by the temperature difference between the outer and inner boundaries of the fluid shell. It uses a pseudo spectral method for discretization in the horizontal/vertical directions, and a finite difference method in the radial direction. Linear terms (e.g. diffusion, buoyancy, Coriolis force) are evaluated using spherical harmonics, while non-linear terms (advection, Lorentz force, magnetic induction) are evaluated in physical space. For time integration, Calypso uses a Crank-Nicolson scheme for the diffusion terms and second-order

Adams-Bashforth for the other terms.

Rayleigh. Rayleigh is designed to solve the anelastic MHD equations in a rotating sphere, in which compressibility associated with stratification is permitted but sound waves are filtered out. Rayleigh, like Calypso, is based on spectral methods, but has been specifically designed to minimize the all-to-all global communications. This improves the scalability of the Rayleigh code.

Aspect. Aspect is a recently developed code intended to solve the equations that describe thermally driven convection with a focus on doing so in the context of convection in the earth mantle. 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, viscosity and temperature models and tracer particles 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. 2011].

CitcomS. CitcomS is a finite element code designed to solve thermo-chemical convection problems relevant to the planetary mantle in a 3D spherical geometry [Moresi and Solomatov, 1995; Moresi and Gurnis, 1996, Zhong et al., 2000]. 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; Ramage and Wathen, 1994]. 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 Steamline 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 larger variations in discretization size and complex nonplanar fault geometry), implementation of a variety of finite-element types (e.g., higher order elements as well as conventional linear and parabolic tetrahedral and hexahedral elements), 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

Pau (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, Seriani and Oliveira, 2008]. The spectral element 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, Komatitsch et al., 2010a] as well as on clusters of GPU accelerating graphics cards [Komatitsch, 2010b].

Further details regarding each code and downloads of the source are available at the following addresses (Rayleigh is not publicly available yet).

Code Name	Website
Calypso	http://geodynamics.org/cig/software/calypso/
Rayleigh	https://www.youtube.com/watch?v=km0Bv6p2UO8, https://www.youtube.com/watch?v=6u0P-pyJsXo
Aspect	http://aspect.dealii.org
CitcomS	http://geodynamics.org/cig/software/citcoms/
PyLith	http://www.geodynamics.org/cig/software/pylith
SPECFEM3D_GLOBE	http://www.geodynamics.org/cig/software/specfem3d-globe

Resource Requirements

CIG researchers used up the prior year's allocation at a faster than anticipated rate, exhausting the allocation midway through the 2013-2014 period. In February 2014 CIG successfully applied for a supplemental allocation. We anticipate continued high computing requirements for the 2014-2015 year, due to the ongoing geodynamo benchmarking, development, testing and benchmarking of the new geodynamo code (Rayleigh), development of other next generation codes and various small scale studies.

CIG plans the following use of its proposed XSEDE resources during the period of October 1, 2014 to September 30, 2015 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, and PyLith.

- *Geodynamo accuracy and performance benchmarks.* Various researchers collaborating with CIG have already analyzed the accuracy of a dozen geodynamo codes. However, there are still several codes whose accuracy needs to be checked. The performance of each of the geodynamo code also needs to be checked for scaling and efficiency. This will require multiple short runs on a range of core counts for about fifteen different codes. Each evaluation involves three test cases (non-magnetic, insulated boundary, pseudo vacuum) with varying wall time and core requirements (8 hours x 64 cores, 16 hours x 256 cores, 36 hours x 1024 cores). In total this will require 15 x (512+4096+36864) = 622,000 SUs.

- *Geodynamo multi-scale convection modeling.* Dr. Hiroaki Matsui at CIG plans to investigate the dynamics of multi-scale convection 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 improving model scale and code performance. To establish the validity of this approach, it is necessary to do medium scale runs on Stampede. The code will also be developed further to improve support for accelerators.
- *ASPECT, Calypso and Rayleigh development.* The ASPECT mantle convection code and the Calypso and Rayleigh geodynamo codes need further development and scaling work. This will be primarily done by CIG researchers Prof. Timo Heister, Dr. Hiroaki Matsui, and Dr. Nick Featherstone, respectively. 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 4096 cores for brief periods
(1-4 hours) and estimate a total requirement of 50,000 SUs for this development.
- *High-Resolution Subduction Models.* Dr. Margarete Jadamec will be using CitcomCU (a variant of CitcomS) for continuing the research into high-resolution subduction models with multiple plates. Observational and experimental constraints indicate plate boundaries are inherently three-dimensional and are characterized by lateral strength variations. For example, a power law rheology (one that includes the effects of the dislocation creep) can explain both observations of seismic anisotropy and the decoupling of mantle flow from lithospheric plate motion, due to the dynamic reduction of mantle wedge viscosity (Jadamec and Billen, 2010, 2012). However, large viscosity variations occurring over short distances pose a challenge for computational codes, and models with complex 3D geometries require substantially greater numbers of elements, increasing the computational demands (Spera et al., 1982; Moresi and Solomatov, 1995; Moresi et al., 1996; Tackley, 1996; Zhong et al., 2000; May and Moresi, 2008; Geenen et al., 2009; Burstedde et al., 2009; Jadamec and Billen, 2010; Furuichi et al., 2011). Dr. Margarete Jadamec recently received Best Conference Paper and Science Track Paper awards for work on this topic at XSEDE12 (Jadamec et al., 2012). She is continuing this work in collaboration with computational scientists and as a part of (CIG). High-resolution subduction models with multiple plates are particularly computationally challenging, because the model domain contains numerous regions with large viscosity

contrasts and complex non-linear flow. In addition, the models incorporate a high level of geometric complexity due to the geophysical data incorporated to construct accurate geometries representative of actual plate boundaries. A large-scale computational resource, such as Stampede, is critical for these next generation models, as they require a minimum of 3000 CPUs per run. Lower resolution models (380-460 processors), have already been run on Lonestar, followed by the first testing phase of high-resolution models (3000+ processors) run on Stampede (Jadamec and Fischer, 2013). 500,000 SUs would enable both (a) a suite of high-resolution models testing solver parameters run on 3000 to 8000 CPUs for 1-3 hours with a usable computational result and (b) 2-3 high-resolution models with the optimized parameters run for 24 hours with a usable scientific result.

- *Von Karmann sodium experiment*. After performing the geodynamo benchmark on Stampede, Prof. Jean-Luc Guermond plans to perform initial tests in duplicating the Von Karmann sodium experiment on a computational platform. This initial work will confirm that the experiment can be replicated at lower resolutions, with the aim of using the results to apply for a larger allocation on Stampede at a later date
- *Geodynamo turbulence studies.* Dr. Adolfo Ribeiro has already used the CIG allocation to study turbulence in geodynamo systems and plans to continue this work with the aim of applying for a separate allocation in the near future.
- *Chemical piles, geoid mantle convection studies.* Xi Liu and Max Rudolph, working with Prof. Shijie Zhong, plan to finish work on their studies of chemical pile evolution and their influence on the geoid. The researchers plan to apply for a separate allocation shortly based on their successes so far
- *CitcomS and Aspect*: Several small-scale research projects are planned for CitcomS and Aspect in the upcoming year. First, to continue previous work in steady and unsteady mixing, we plan to extend the previous study of 3D unsteady mixing in a box to a spherical shell representing the Earth's mantle. We anticipate running 10 simulations at a resolution of 100km^3 elements for 10,000 time steps each. Based on the expected resolution requirements and run times shown in the code performance document, we anticipate resource requirements of 10 x (10000 steps x 30 seconds/step x 384 cores) = 320,000 SUs. Each simulation is expected to generate several terabytes of data and thus we will also require time (500 SUs) on the Longhorn visualization cluster to properly analyze and visualize the results.
- *Spherical Shell Stability Analysis.* Dr. Pierre-Andre Ariel, working with CIG, plans to continue work analyzing the stability of convective flow patterns in the ASPECT mantle convection code and CitcomS. Thermal advection simulations will quickly form a stable configuration of upwelling plumes forms for low Rayleigh numbers. However, it was recently discovered that a given configuration can spontaneously change to another stable configuration if the simulation is run for sufficiently long time periods. We intend to further investigate this using CitcomS and Aspect by running simulations at different Rayleigh numbers for extended periods. By using both codes we hope to better

understand whether this is a numerical artifact, a previously unknown property of such systems, or a combination of the two. We anticipating running 15 simulations for extended periods (48 hours) with 512 cores for a total resource requirement of 369,000 SUs.

Software	Purpose	Requested SUs
Calypso/Rayleigh	Validation/Testing	622,000
	Development	50,000
	Von Karmann sodium experiment simulation	122,000
	Geodynamo Turbulence studies	256,000
CitcomS	High-resolution subduction models with multiple plates	500,000
	Chemical Piles, geoid mantle convection studies	120,000
Aspect	Mixing Simulation	320,000
	Spherical Shell Stability Analysis	369,000
	Subduction zone models	82,000
	Development/Overshoot	30,000
Computation Total		**2,470,000**
ParaView/VisIt	Visualization	5,000
Visualization Total		**5,000**

In total, a yearly allocation of 2,500,000 SUs 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 5,000 SUs on a visualization oriented system such as Longhorn to assist in analyzing and visualizing large data sets resulting from benchmark or research runs.

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