CIG Science Gateway and Community Codes for the Geodynamics Community

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Project Overview

The Computational Infrastructure for Geodynamics (CIG), an NSF cyberinfrastructure 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 deformational 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 simulation. 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 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 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 making 3D codes that provide a more-accurate representation of Earth properties such as anisotropy, attenuation and gravitational affects 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, 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 need substantial infrastructure in order to be run. 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.

ASPECT. ASPECT is a CIG 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 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. 2011].

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 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]. 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 not publicly available yet).

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 geodynamo and mantle convections.. 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, 2017 to March 31, 2018 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 SUs 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 and Rayleigh development. ASPECT mantle convection code and the Calypso and Rayleigh geodynamo codes are continuing development and scaling work. This will be primarily done by CIG researchers at TAMU, 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 Stampede 2 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 each code (150,000 in total) on Stampede for this development. We also request 10,000 SUs on Maverick for development of GPGPU based computation.

Geodynamo multi-scale convection modeling. 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 improving model scale, code performance and sophisticated turbulence modeling. 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. We request to run with (384,288,576) grids for 5,000,000 time steps using 1024 cores. It will require (1024 x 384) = 344,064 SUs.

Present-Day Global Deformation Models of the Lithosphere and Convecting Mantle. The observed velocity and deformation of Earth's tectonics plate reflects forces arising from density variations in both the convecting mantle and lithosphere. Modeling global or regional deformation arising from these density variations thus requires interfaces to translate geophysical models of Earth's density variations to initial conditions within a forward modeling simulation. At present, ASPECT has interfaces to density models of the deep convecting mantle and Dr. John Naliboff has implemented a preliminary interface to density models of the shallow crust and lithosphere. Over the following year Dr. Naliboff will continue testing and modifying ASPECT to resolve the deformation patterns arising from these shallow Earth density variations, which often exhibit sharp gradients on scales of hundreds of meters to tens of kilometers. Given that the 3-D models incorporating these density variations are often global or continent-scale, resolving sharp density gradients at much smaller spatial scales requires both high-order interpolation methods and specific conditions for adaptive refinement of the finite-element mesh. Testing and development will focus on the accuracy of distinct interpolation and adaptive refinement methods, which will provide a basis for the broader geodynamics community to use ASPECT's interface to lithospheric density models for targeted research and proposals. The 3-D simulations associated from this work will likely range in size from millions to hundreds of millions degrees of freedom. Given this range, we request 100,000 SUs in order to test our modifications to ASPECT on a representative suite of models sizes.

High-Resolution Long-Term Tectonic Models. Dr. John Naliboff will continue developing ASPECT to examine 3-D long-term tectonic processes at high-resolutions. To date, ASPECT has been applied to long-term tectonic simulations of continental extension, with preliminary high-resolution 3-D simulations showing promising scaling behavior. For example, time-dependent and highly non-linear simulations with approximately 39 and 78 millions DOF ran in under 12 hours on STAMPEDE using 640 and 1920 CPUS, respectively. In addition to showing promising run times for large 3-D simulations, the continental extension simulations show very similar behavior to other well established long-term tectonics code for a test case designed as a long-term tectonics community benchmark (Naliboff et al., 2016). Over the course of the next allocation, ASPECT will be modified to include additional non-linear rheologies and tested for cases representing a wide range of long-term tectonic processes and environments. While the majority of testing will be conducted in 2-D, we request 200,000 SUs to perform additional testing in 3-D. Based on the preliminar results above, we estimate that this will provide sufficient computing time to run 20-40 high-resolution simulations (40-80 million DOF) over the course of the year. As noted above, these simulations and corresponding computing time will be applied to a wide range of problems largely based on the requests of the broader long-term tectonics community.

High-Resolution Subduction Models. Prof. Magali Billen will use ASPECT to develop high-resolution 3-D models of subduction that aim to understand how seismological observations of shear-wave splitting can be properly interpreted to determine the pattern and speed of mantle flow around subducting plates (current NSF-Geophysics grant). The numerical models will simulate both the subduction process and alignment (or mis-alignment) of grains within rocks arising from the highly non-linear viscous flow. The non-linearity of the material viscosity proves challenging for most non-linear solvers and requires a very small element size to limit the gradient in viscosity across individual elements (Billen and Hirth, 2007). Consquently, the AMR-capabilities of ASPECT are of the utmost importance in being able to adequately solve the flow problem (element sizes on the order of < 1 km) while modeling one quarter, one half or all of the earth's mantle (circular annulus with a depth of 2890 km and circumference of up to 40,000 km). The models being developed are on the same scale and complexity as those explored with the code Rhea (Stadler et al., 2010) but unlike these previous models, which determined the flow for a single time, our models will run for $>$10–100 million years (with time-steps on the order of 10,000 years). Here, we request an allocation of 200,000 SUs to develop preliminary models that will only be run for 1–2 million years. The aim of these models is to demonstrate efficient scaling for time-dependent simulations, examine distinct AMR routines and test new features in ASPECT for calculating grain alignment and shear-wave splitting. Based on extensive work with high-resolution 3-D subduction simulations in CitCom (Burkett and Billen, 2010; Jadamec and Billen, 2010; and Taramón et al., 2015), we estimate that 200,000 SUs will provide sufficient time to examine 10-20 high-resoltuion simulations of similar size to the largest models in the aforementioned references.

Numerical studies of 3D simulations with DG-BP method Dr. Ying He will run 3D computations using the Discontinuous Galerkin method with a Bound Preserving limiter (DG-BP), which has been recently implemented in ASPECT. However, we have only studied the numerical performance of the proposed numerical method in 2-D (Y. He, E. Puckett, and M. Billen, 2016) by running several simplified 2-D geodynamics model problems such including an advection falling box problem, a temperature advection-diffusion rising box/bubbles benchmark and thermal-chemical convection simulations in a compositionally stratified fluid. While the DG method with different limiting techniques is considered a state-of-the art numerical method (Shu, 2016), it is critical to test the capability, stability, scalability and and efficiency of our DG-BP implementation in ASPECT through high-resolution 3-D simulations . In order to do perform these tests and analysis, we need to perform resolution tests for each benchmark case on a sequence of 3-D computation grids ranging from very low to very high resolutions. The the number of degree freedoms of each computation will thus likely range from thousands to hundreds of millions degree of freedoms. Given the size of these simulations, we request 100,000 SUs to perform these computational tests that will provide a basis for the broader geodynamics to confidently utilize these features in high-resolution 3-D simulations.

Benchmarking Particle-in-Cell Methods for 3D Models Dr.'s R. Gassmoeller, E. Heien, E. G. Puckett, and W. Bangerth have developed flexible and scalable particle-in-cell (PIC) methods for massively parallel computational modeling in ASPECT. PIC in ASPECT contains several algorithms including generation of particles, time integration (Euler, Runga-Kutta 2, Runga-Kutta 4), interpolation of properties (cell average, bi-linear, bi-quadratic least squares), and visualization output. Dr. E. G. Puckett and Dr. C. Thieulot will utilize the highly scalable and efficient PIC methods to benchmark PIC methods for a manufactured solution to the Stokes equations in 3-D. We plan to investigate the influence of number of particles per cell in highly resolved meshes for different finite elements using different algorithms for the time integration as well as the interpolation of particle properties. The study will require numerous runs ranging from low resolved grids with little memory utilization and computationally inexpensive to highly resolved grids with tens of millions of particles proving to be both memory intensive and computationally expensive. We request 100,000 SUs to perform initial scaling tests for our 3-D PIC simulations that will be used as the basis for an XSEDE research proposal and also provide key information for the broader geodynamics community that plans to use the PIC features within ASPECT.

Melt Impact on Mantle Flow and Plume Generation Dr.'s Juliane Dannberg and Rene Gassmoeller will combine high-resolution 3D regional plume models and simulations of global mantle convection to study the interaction of subducted slabs with dense thermo-chemical piles. Due to the lower-mantle flow induced by slabs, the ascent of plumes from the edges of these piles is triggered, and this process can lead to bilaterally asymmetric zonation in plumes, which could explain observed geochemical trends at different ocean islands such as Hawaii. High-resolution numerical models are required to accurately quantify entrainment of material into plumes, and to characterize zoning as concentric (as predicted by traditional models) or bilaterally asymmetric (as inferred from observations). Related to the requirements of these earth-like high-resolution, highly non-linear models, they strive to improve ASPECTS's scaling to a higher number of processors, also studying the effect of spatially varying viscosity on the performance, and including cases with and without melt migration. Moreover, they plan to improve the numerical techniques used for the advection equations in ASPECT, comparing a newly implemented particle-in-cell technique with the available mesh-based approach. In particular, they will investigate the scalability of both methods to massively parallel computations and the use of appropriate load-balancing schemes.

Previous research runs on similar resources showed that a:

- 3D global mantle convection models with a resolution of 25 km (100 million DOFs) and a model runtime of 250 million years, took 90k SUs, running on 768 processors.
- two-phase flow models, a 3D model of a single mantle plume (600 x 600 x 300 km, 200 million DOFs, highest resolution of 0.5 km) and a model runtime of 200 thousand years running took 90k SUs with 1536 MPI processes
- regional mantle convection models with a resolution of 10 km (650 million DOFs) and a model runtime of 250 million years, took 660k SUs, running on 3072 processors.

In total, a yearly allocation of 1,694,064 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 15,000 SUs on a visualization oriented system such as Maverick to assist in analyzing and visualizing simulation results and to develop GPGPU based computations.

Table 2: Summary of requested SUs

Software	Purpose	Requested SUs
Calypso/Rayleigh	Development	100,000
	Geodynamo Turbulence studies	344,064
ASPECT	Development/Overshoot	50,000
	Present-Day Global Deformation Models	100,000
	High-Resolution Long-Term Tectonic Models	200,000
	High-Resolution Subduction Zone Models	200,000
	3-D Simulations with DG-BP Methods	100,000
	Benchmarking Particle-In-Cell Methods	100,000
	Mantle Mixing and Melt Transport	500,000
	Total for Stampede	1,694,064
ParaView/VisIt	Visualization	5,000
CUDA Calypso	Development	10,000
	Total for Maverick	15,000

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