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: dynamo 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 Dynamics and Dynamos. It is widely accepted that the Earth's outer core consists of liquid iron alloy and that the geomagnetic field is sustained by its convection (so called geodynamo). Numerical simulations have played a large role in elucidating the fluid motion in the Earth's outer core and geodynamo processes. 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 due to the small viscosity. 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 and Lithospheric Dynamics. Mantle convection and lithospheric dynamics is at the heart of understanding how plate tectonics on Earth works. However, the processes governing plate tectonics remain poorly understood due the lack of direct observations from the deep part of the Earth and the highly non-linear nature of solid Earth deformation. Progress on fundamental questions, such as the dynamic origin of the tectonic plates that cover the surface, coupling between lithospheric deformation and convection deep inside the mantle, feedbacks between erosion and tectonic uplift, the drivers and dynamics of observed magmatism and volatile transport, and the evolution of plate boundary systems all require an interdisciplinary approach. Numerical models of mantle convection and lithospheric dynamics must therefore assimilate information from a wide range of disciplines, including seismology, geochemistry, mineral and rock physics, geodesy, and diverse geologic data sets.

The technical challenges associated with modeling mantle convection and lithospheric dynamics are substantial. They are characterized by strongly variable (i.e., stress-, temperature-, and pressure-dependent) viscosities. The lithosphere exhibits processes such as elastic flexure and brittle 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 and lithosphere are chemically heterogeneous, replete with silicate melts and volatiles, and have numerous pressure- and temperature-induced structural changes that affect its dynamics.

While substantial progress has been made in recent years in large part to due to improved numerical methods, scaling for massive 3D simulations, and new techniques for assimilating geophysical data sets, significant challenges remain across a wide range of topics. Here, we propose to develop and test new numerical methods in computationally expensive 2D and 3D simulations towards the following scientific goals:

1. Stabilization and accurate decomposition of non-linear viscoelastic-plastic deformation, which governs deformation within the lithosphere

2. Development of new nonlinear solvers for models using matrix-free preconditioners (Geometric Multigrid) and two-phase flow (see below).

3. Assessing the accuracy and efficiency of particles versus composistional fields for tracking viscoelastic stresses.

4. Testing of various new features for simulating lithospheric dynamics

5. Improved methods for calculating crystal preferred orientations (CPOs) during dynamic simulations

6. Further integration with external software packages that provide a platform for geologic data assimilation and assembly of complex initial conditions.

7. Developing a new generation of high-resolution global mantle flow models incorporating plate boundary databases and a wider range of input data, in particular improving the rheological profiles, density and temperature scaling relations with seismic tomography, including a grain-size dependent rheology. These models will be used to examine the relative importance of the contributing factors on predicting the observed surface velocities and strain rates.

   To further expand on point 2 above, based on the optimization and development work enabled by the usage of Stampede2 and Frontera over the last 12 months, we were able to dramatically improve scaling and performance of the linear solvers in ASPECT (see the progress report for more details). This work is not done as the new solver is currently restricted to a small subset of the possible simulations.

   In this next period we plan to:

   - Continue the development and testing of the matrix-free Multigrid solver and generalize it (to be able to use other physics, boundary conditions, etc.).
   - Work on improving large scale IO (loading of large datasets, MPI combined with large amount of input data, faster graphical output, generic intermediate exchange format).
   - Investigation of new visualization technology.

   All of these items require access to medium to large allocations on different machines.

The details of these topics and associated work plans are outlined within the Resource Requirements section.

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 inbetween and 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 and fluid injection 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 evidence of 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 source, and wave propagation effects. CIG aids the community by supporting 3D codes that provide a more-accurate representation of Earth's structure and properties including 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, the nature of ULVZ's, lithospheric structure, and plate boundary zone complexity.

Infrastructure. An important role of CIG for the geoscience community lies in the maintenance of geodynamics software packages and in training and supporting the computational needs of their users. The XSEDE allocations enabled part of this work that pertains to large scale computations in two ways: First, running on the various leading edge systems allowed us to improve the software packages and their underlying software stack to run on XSEDE resources. Second, we developed installation and usage guides on XSEDE resources that allows users to get started quickly and without requiring extensive knowledge and research into the machine in question. See https://github.com/geodynamics/aspect/wiki for some examples.

Our work has enabled many scientists to be able to evaluate and use XSEDE resources who otherwise would not have been able to do so.

To that end we plan to:

- Port and tune the software to new XSEDE machines/compilers.
- Continuously maintain the whole software stack and report and fix bugs that appear.
- Perform performance tests and tuning of the codes.
- Create installation and usage guides.

Computational Experiments and Resource Requirements

Numerical Approaches

Calypso. Calypso is a code for magnetohydrodynamics (MHD) simulations in a rotating spherical shell to solve the geodynamo processes. 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, and 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. We were awarded 27,000 node*hours for TACC Frontera Pathway allocataion from July 2020 to July. 2021 for both ASPECT and Calypso. For Calypso, we optimized its visualization module for the new Frontera system.

Rayleigh. Rayleigh is an open-source community dynamo code developed through CIG (NSF support). It solves the fully nonlinear MHD equations of motion for a compressible fluid in a rotating spherical shell under the anelastic approximation and 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. This code has been performance tested extensively on XSEDE's Stampede2, NASA's SGI Pleiades system and Argonne's Blue Gene/Q system, Mira. Rayleigh demonstrates strong scaling with 80% of ideal efficiency up to 131,072 cores for 2048^3 problem sizes using pure MPI. An OpenMP/MPI hybrid mode of this code has allowed an additional factor of 2 in scalability on the Mira supercomputer for the larger problem sizes. Rayleigh was also used in a DOE INCITE project which was awarded 820 million core hours through 2015 to 2018.

ASPECT. ASPECT is a CIG-developed code designed 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 geometry (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]. We were awarded 27,000 node hours for early access of TACC Frontera from May 2019 to Jan. 2020 for both ASPECT and Calypso. For ASPECT, we optimized the GMG solver and visualization modules for the new Frontera system.

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].

Table 1: List of Websites

Code	Website
Calypso	`https://geodynamics.org/cig/software/calypso/`
Rayleigh	`https://geodynamics.org/cig/software/rayleigh/`
ASPECT	`https://geodynamics.org/cig/software/aspect/`
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, lithospheric deformation, and mantle convection.

CIG plans the following use of its proposed XSEDE resources during the period of April 1st, 2021 to March 31th, 2022 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, PyLith and SPECFEM3D_GLOBE. New users anticipate million of core hours will require additional SUs 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.

Rayleigh Development: Enabling the use of GPUs. Rayleigh geodynamo code is presently parallelized by using MPI and OpenMP. We have recently begun to explore how

GPUs might be used to accelerate some of its mathematical computations. The bulk of Rayleigh's computational time is spent performing two mathematical operations. The first is the Legendre transform, required to carry out the transformation between a physical-space representation and one based on Spherical Harmonic basis functions.

We are now working to accelerate both the Legendre transform and the linear solve through the use of GPUs. At present, we have a beta version of the Legendre transform that employs OpenACC and cuBLAS to offload a portion of the matrix multiplies to the GPU. We are now exploring how the MAGMA linear algebra library can be used to similarly accelerate the linear solve. These developmental algorithms rely on a combination of MPI, OpenMP, CUDA, and OpenACC. For the present development, we are requesting 15,000 core hours on the PSC Bridges to use the NVIDIA Tesla P100 Pascal nodes to optimize and performance test our GPU version of Rayleigh on up to 1024 cores.

Calypso Development: Improving visualization modules. Calypso and its visualization modules are parallelized by MPI and OpenMP. Visualization can be performed concurrently to output visualized images in short time increments without the need to output large datasets. We request 5,000 SUs for development and optimization of the parallel domain re-partitioning module is included in request below.

PyLith, Calypso, and SPECFEM3D_GLOBE development. The short-term tectonic finite element code PyLith is continuing development and scaling work lead by Brad Aagard (USGS), Matt Knepley (University of Buffalo), and Charles Williams (GNS). Calypso and Rayleigh geodynamo codes are also continuing development and scaling work by Dr. Hiroaki Matsui (UC Davis), and Dr. Nicholas Featherstone (SWRI), respectively. SPECFEM3D_GLOBE is principally developed by Prof. Jeroen Tromp (Princeton), Dr. Matthieu Lefebvre, and Dr. Daniel Peter. The allocation will be used to establish the scaling performance and efficiency of each code, add functionality, and improve the support for many-core architectures. 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 (15,000 SUs in total) on Stampede2 for this development.

Data analysis and visualization of large scale dynamo simulation by Rayleigh. To understand dynamics and dynamo processes under the highly turbulent convection which is expected in the planetary cores, we performed large scale dynamo simulation using the Rayleigh code for the Earth and Jupiter under the support of DOE INCITE project. Because the data consists of approximately 10 billion grids, parallel computing is also required for its visualization and data analysis. Dr. Hiroaki Matsui and Dr. Nicholas Featherstone will perform visualization and data analysis of these data on Stampede2. We will request 200(times) x 0.2(hours) x 512(nodes) = 20,480 SUs for this study.

Investigation of geomagnetic reversal through dynamo simulations. Dr. Hiroaki Matsui and Graduate student Takumi Kera, Tohoku University, are investigating triggering of dipolar reversals of the geomagnetic field through dynamo simulations using Calypso. To represent the dipolar reversal with the Earth-like magnetic field, approximately 40 million steps are required to complete several reversals. Each case is expected to need 240 hours with 32 nodes of Stampede2. we plan to perform three cases and are requesting 23,040 SUs for the geomagnetic reversal study.

Mantle Convection and Lithosphere Dynamics Modeling with ASPECT. Below, we outline distinct projects using ASPECT that will require resources on Stampede2 and Expanse.

New matrix-free solver development. Prof. Timo Heister will continue his work on improving the performance of matrix-free solvers in ASPECT. While the jobs required for this work may require using the maximum number of nodes, runs are typically limited to a few hours. Here, we conservatively request 5,000 SUs on Stampede2 and 89,662 SUs on Expanse (equivalent number to Stampede2) to continue this development work. The results of new scaling and examples will be contributed directly to the ASPECT repository.

Tracking of viscoelastic material properties. Prof. John Naliboff will continue his work on the viscoelasticity implementation in ASPECT by testing the relative efficiency and accuracy of using particles versus compositional fields to track the viscoelastic stress tensor components in high-resolution 3D simulations. While related development work for a range of analytical benchmarks has occurred in 2D, the trade-offs between efficiency and accuracy are likely to be different in high-resolution 3D simulations. Here, we conservatively request 5,000 SUs on Stampede2 for this proposed work.

Global Models with Prescribed Plate Boundaries Dr. Arushi Saxena, Prof. Juliane Dannberg, and Prof. Rene Gassmoeller, will extend their work on global mantle convection models with prescribed plate boundaries. Examples of this type of model have been widely requested by the ASPECT user community, and this work will provide the basis for multiple groups to do related research projects. Here, the goal is to work out various techniques and issues for diverse data assimilation, solver stability, adaptive mesh refinement techniques, and highly non-linear material properties.

Our preliminary global mantle model includes the input seismic global tomography model, constant grain size, laterally varying lithospheric depths, and a composition defining the plate boundaries. The model uses an adaptive mesh with a minimum resolution of $\sim$100 km to match the 1° global tomography model resolution, and a maximum resolution of 25 km at plate boundaries and the core-mantle boundary. This model simulation solves for a total of $\sim$58 million degrees of freedom and runs for about 27 hours on 64 CPU cores (1700 core hours, equivalent to 36 SUs on Stampede2).

Our current model resolution is not sufficient to accurately represent the input tomography model, realistic fault thicknesses, slab geometries, and crustal thickness variations. The desired model resolution would require adaptive mesh refinement at locations of plate boundaries ($\sim$1 km scale), and intermediate resolutions in other regions of interest. In addition to the mesh refinement, the models will be more complex, including a variable grain size influenced by mantle flow and mesh deformation due to a prescribed topography. We anticipate that we will need several of these models with varying input parameters to analyze the misfit between the observed and the modeled surface velocities, strain rates, and maximum compressive stress directions.

Given this resolution we expect the final models to require ∼1 billion DOFs. As our scaling results show, our wallclock time scales linearly with DOFs up to 110,000 processors and 30 billion DOFs on NSFs Frontera (an earlier models on Stampede2 scaled equally well). We expect a cost of 34,000 core hours per model run (20 × 1,700 core hours). To complete our parameter study described above, we expect to run 50 models requiring 1.5 M core hours = 36,000 SUs on Stampede2.

New Features for Lithospheric Dynamics. Prof. John Naliboff, Dr. Bob Myhill, Prof. Cedric Thieulot, and Dr. Jonathan Perry-Houts will extend their work on lithospheric dynamics to test a number of new features that will be of significant use to the ASPECT user community. This work will include testing new features for plasticity stabilization, viscoelastic-plastic deformation, coupling to surface processes (ex: sedimentation), and composite rheological formulations. While the majority of development work for these topics will be completed using small simulations on local resources, the resources requested here will be used for limited proof-of-concept production models that will be highlighted in the ASPECT repository. Although the size and required run times of lithospheric dynamics simulations vary dramatically, we have found a reasonable average for high-resolution simulations on Stampede2 is 15 nodes used over 48 hours (720 SUs). Here, we request resources to conduct the equivalent of 10 simulations (7,200 SUs).

Integration and extension of CPO calculations. Dr. Menno Fraters will extend his work on integrating crystal/lattice preferred orientation (CPO/LPO) in ASPECT. This work will include more testing of the current implementation of the modified D-Rex CPO model in ASPECT, test better integration with the Geodynamic World builder which can create CPO initial conditions, and explore the addition of water models and CPO mobility models into the CPO implementation in ASPECT. We expect to use 6 nodes for 48 hours per model (288 SUs). Here we request resources on Stampede2 to conduct the equivalent of 40 simulations plus some overhead (12,000 SUs).

Table 2: Summary of requested SUs for Stampede2

Software	Purpose	Requested SUs
Calypso	Development and optimization	5,000
	Geodynamo turbulence studies	21,120
Rayleigh	Data analysis and visualization	20,480
SPECFEM3D_GLOBE	Development and Optimization	5,000
PyLith	Development and Optimization	5,000
ASPECT	Stokes Solver	5,000
	Tracking Stress	5,000
	Plate Boundaries	36,000
	Lithospheric Dynamics	7,200
	CPO Calculations	12,000
	Total for Stampede2	121,800

Table 3: Summary of requested SUs for Expanse

Software	Purpose	Requested SUs
ASPECT	Stokes Solver	89,662

Table 4: Summary of requested SUs for PSU Bridges

Software	Purpose	Requested SUs
Rayleigh	GPGPU optimization	15,000

Summary In total, a yearly allocation of 121,800 SUs on Stampede2, 89,662 SUs on Expanse, and 15,000 SUs on PSU Bridges will enable CIG to continue offering feature development, 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 data storage system Ranch.