Suppilmental allocatin for CIG Science Gateway and Community Codes for the Geodynamics Community

October 31, 2017

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.

In this supplement 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 objectives for the present supplemental allocation. We then describe the codes and methodologies used and offer a justification of the requested resources.

Science Objectives

Core Dynamo and Dynamics. After Glatzmaier and Roberts (1995), a number of groups have successfully reproduced some spatial and temporal characteristics of the geomagnetic field. However, it is expected that flow in the outer core has a vast range of length scales due to its small diffusivities. Consequently, massively parallel simulations is required to approach the actual Earth's parameters in the geodynamo simulations.

Mantle and Lithosphere Dynamics. Mantle convection and lithospheric deformation is at the heart of understanding how the solid Earth behaves on tectonic time scales, but the processes remains at best poorly understood because the interior of tectonic plates and deep mantle are not accessible to direct observation. Numerical models of these processes 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 and lithospheric deformation 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.

Code descrepsion

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 (diffusion, buoyancy, Coriolis force) are evaluated in spherical space, while non-linear terms (advection, Lorentz force, magnetic induction) are evaluated in the physical space. Calypso uses a Crank-Nicolson scheme for the diffusion terms and Adams-Bashforth scheme for the other terms for time stepping.

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. Further details are available in [Kronbichler, et al. 2012, Heister et al. 2017].

Table 1: List of Websites

Code	Website
Calypso	`https://geodynamics.org/cig/software/calypso/`
ASPECT	`https://geodynamics.org/cig/software/aspect/`

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, the ramp up of benchmarking, and research use of CIG codes. CIG plans the following use of its proposed XSEDE supplement resources to March 31, 2018.

ASPECT and Calypso development. ASPECT and the Calypso are continuing development and scaling work. This will be primarily done by CIG researchers at CSU Fort Collins, Dr. John Naliboff, Dr. Hiroaki Matsui, Prof. Magali Billen and Prof. Gerry Puckett at UC Davis. The allocation will be used to establish the scaling performance and efficiency of each code, add and test functionality, and improve the support for Stampede 2. To perform simulations to ensure the validity of the codes and check their scalability and performance, we anticipate requiring up to 256 nodes of Stampede 2 for brief periods (10-40 hours in total) and estimate a total requirement of 10,000 SUs and 5,000 SUs for ASPECT and Calypso, respectively.

High-Resolution Long-Term Tectonic Models. Dr. John Naliboff continues developing ASPECT to examine 3-D long-term tectonic processes at high-resolution. 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. While the majority of testing will be conducted in 2-D, we request 6,400 SUs to perform additional testing in 3-D on Stampede2. Based on the preliminary results above and additional testing on local clusters, we estimate that this will provide sufficient computing time to run 5-10 high-resolution simulations (40-80 million DOFs).

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. The numerical models will simulate both the subduction process and alignment (or misalignment) of grains within rocks arising from the highly non-linear viscous flow. 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). Based on previous 3-D subduction simulations by CitCom (Burkett and Billen, 2010; Jadamec and Billen, 2010; and Taramón et al., 2015), we request 6,400 SUs on Stampede 2 to perform 10-20 high-resoltuion simulations of similar size to the largest models in the aforementioned references.

Benchmarking Particle-in-Cell Methods for 3D Models. Dr. R. Gassmoeller, and Prof.'s E. G. Puckett, and W. Bangerth have developed flexible and scalable particle-in-cell (PIC) methods for massively parallel computational modeling in ASPECT. Prof.'s Puckett and Cedric 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 request 3,200 SUs for Stampede 2 to perform initial scaling tests for our 3-D PIC simulations.

In total, a supplemental allocation of 24,600 SUs for Stampede 2 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.

Table 2: Summary of requested SUs

Software	Purpose	Requested SUs
Calypso	Development and optimization	5,000
ASPECT	Development and optimization	10,000
	High-Resolution Long-Term Tectonic Models	6,400
	High-Resolution Subduction Zone Models	6,400
	Benchmarking Particle-In-Cell Methods	3,200
	Total for Stampede2	24,600

References

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