Progress Report (December 2015 to present)

Overview

NOTE: We ask the reviewers to note that some of this progress report is duplicated from the renewal application since both cover the work done from April 2016.

Our current allocation for the period from April 2016 to March 2017 is 1040677 service units on Stampede, 15000 service units on Maverick and 7000 service units on the Ranch. These allocations are due to expire on March 31, 2017. As of Jan. 7, 2017 we have used 56% of our allocation on Stampede. We are certain we will be using up the remainder of the allocation by March 31, as Dr. Hiroaki Matsui and Dr. John Naliboff will be performing large 3-D development and scaling simulations through this date. An overview of the allocation usage and results are shown in the table 1.

Table 1: Allocation usage as of Jan. 8, 2017

Category	Stampede SUs	Publications/Talks
Geodynamo development	91,388	6
Geodynamo Science	116,324	9
Mantle convection	287,119	5
Techtonics	72,424	5
Total	571639	25

The main document of this proposal discusses CIG computational efforts on Stampede. These include: 1) development, validation and benchmarking of geodynamo codes; 2) development and testing of other CIG related codes; and 3) work with CIG related researchers for feasibility studies and small-scale research. Progress in these areas is discussed below along with resulting relevant publications included in the publication list.

Development, Validation, and Benchmarks for geodynamo simulation

In regards to the first area (development and validation of codes), CIG has used XSEDE resources to help develop and test a new geodynamo simulation code named Calypso. Calypso 1.1.1, the current version, was released in March 2014 and is available at http://geodynamics.org/cig/software/calypso/. Calypso performs magnetohydrodynamics simulations in a rotating spherical shell for geodynamo problems. The next version Calypso 1.2 is also developed and tested on Stampede with improvement of performance up to 16384 cores on Stampede (see report for code scaling). Furthermore, additional data output features (cross sectioning and isosurfacing) are implemented. A student, Harsha Lokavarapu is also developing and testing a GPGPU implementation using CUDA on Maverick. Calypso 1.2 will be released in early 2017.

CIG is also using the allocation to develop a next generation geodynamo code, named Rayleigh, which is capable of scaling to tens of thousands of cores. Rayleigh also keeps good scalings to 16386 cores on Stampede, and performs with 260,000 cores with good performance on ALCF Mira. Rayleigh will also be released in 2017.

Working with other researchers, Dr. Matsui has developed a set of benchmark tests to compare 15 geodynamo simulation codes for accuracy and performance. These benchmarks investigate accuracy and performance of a dynamo to quasi-steady state using a variety of boundary conditions. The benchmark results are published as a paper in Geochemistry, Geophysics, Geosystems in May, 2016.

We continue to work with researchers who participated to apply for their own allocation in order to do larger scale geodynamo studies with their codes tested on and tuned for Stampede.

As of Jan. 8, 2017, 91,388 SUs are used for these development and benchmarks of the geodynamo simulations on Stampede.

CIG Code Development and Testing for Mantle Convention and Long-Term Tectonics

CIG has also used XSEDE resources to continue development and testing of ASPECT (available at `http://dealii.org/aspect/`). This code is based on the deal.ii finite element library and uses adaptive mesh refinement to perform detailed 2D and 3D simulations of convection, particularly focused on the Earths mantle. We obtained good scaling to 1000 processor cores with both simple cubic domain and more realistic spherical shell domain (see report for code scaling).

Small Scale Studies

Finally, the third focus of the allocation is supporting researchers in small-scale studies. A large fraction of the allocation has been used for this purpose in cooperation with CIG researchers.

Mantle Convection Studies Throughout 2016, multiple researchers have modifed ASPECT to improve it's capabilites for modeling a wide variety of convective processes. Dr. Juliane Dannberg has investigated how the viscous rheology of the Earth's mantle and melt migration, through two-phase flow calculations, influence the mantle flow field and dynamics of plumes in the upper mantle. To provide more accurate tracking and resolution of thermal, viscous and compositional interfaces in the Earth's mantle, Dr. Ying He has applied the discrete Galerkin and Boundary Preserving Limiter methods to ASPECT.

Long-Term Tectonics Simulations Using a constitutive model that combines viscous flow with brittle failure, Dr. John Naliboff has applied ASPECT to long-term tectonics simulations of continental extension. Despite the highly non-linear material behavior, large and highly time-dependent 3-D simulations ($>$ 50 million degrees of freedom) show good scaling behavior across 1000's of CPUs and reveal complex deformation behavior commonly observed in nature. To date, Dr. Naliboff has used approximately 55,000 SUs on Stampede and will likely use an additional 100,000–200,000 SUs through the remainder of the allocation.

Marsian Mantle Convection Studies Robert Citeron *et al.* in UC Berkeley used 212,700 SUs to perform a mantle convection model for early Mars by CitcomS. From these simulations, they propose a model that current crustal North to south dichotomy of Mars is due to a mantle convection crust formation after a giant impact on the Mars.

Geodynamo Studies CIG has worked with several researchers in geodynamo studies to support their research using small amounts of the allocation on Stampede. Dr. Hiroaki Matsui at UC Davis and Dr. Takashi Nakagawa at JAMSTEC used approximately 116,000 SUs of the allocation to investigate the thermal structures of the inner core and dynamics in the stratified layer in the top of the outer core using Calypso.