Progress Report (October 2014 to present)

Overview

NOTE: Some of this report duplicates our renewal application both which cover the period of October 2014 - current.

Our current allocation for the period October 2014 to March 2016 is 1,886,789 service units on Stampede, 5000 service units on Maverick and 10,500 service units on the Ranch. These allocations are due to expire on March 31, 2016. As of January 12, 2016 we have used 60% of our allocation on Stampede, 99% on Maverick and 50% on Ranch. We are anticipating the remainder of the allocation to be used by March 31, 2016. An overview of the allocation usage on Stampede and research outcomes are shown in Table 1.

Table 1: Allocation usage as of January. 8, 2016

Category	Stampede SUs	Publications/Talks
Mantle Convection	261,366	6
Geodynamo Benchmarking	465,366	3
Geodynamo Science	358,242	9
Code Development	38,236	5
Total	1,123,210	23

The main document of this proposal discusses the Computational Infrastructure for Geodynamics' (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 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.

Geodynamo Development and Validation

We used XSEDE resources to help develop and test a new geodynamo simulation code named Calypso. The initial version of Calypso was released in September 2013. 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 (MHD) simulations in a rotating spherical shell for geodynamo problems. CIG has used XSEDE resources to test weak and strong scaling of Calypso on Stampede (described in the Code Scaling document), and to examine the performance of Calypso on the MIC coprocessor boards. Development and testing of the next version, Calypso 1.2, has led to an improvement of performance for up to 16,384 cores on Stampede (see allocation request for code scaling). Additional data output features such as cross sectioning have also been implemented. The project supported undergraduate student Mr. Lokavarapu (UC Davis) to develop and test a GPGPU implementation using CUDA on Maverick (Lokavarapu, 2015).

CIG is also using the allocation to develop a next generation geodynamo code, Rayleigh, which is capable of scaling to tens of thousands of cores. Rayleigh also scales well to 16,386 cores on Stampede, and shows good performance on up to 130,000 cores on ALCF Mira. Rayleigh is currently in beta release; it will have its first version release in June 2016.

Community Geodynamo Benchmarks

Working with other researchers, we developed and defined a set of benchmarks 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. As of January 2016, 15 research groups from institutions around the world have participated in this benchmark exercise using approximately 465,000 SUs on Stampede.

CIG conducted a workshop in February 2015 at NCAR, Golden, Colorado; 33 participants gathered to discuss the benchmark results from the geodynamo accuracy and performance benchmarks and to motivate the next generation of geodynamo codes. The benchmark results were submitted as a paper to the journal *Geochemistry, Geophysics, Geosystems* in November, 2015 [Matsui *et al.*, 2015]. For a full list of participating groups and details regarding each benchmarked code, we refer readers to
`http://www.geodynamics.org/archive/community/workinggroups/geodyn/benchmark`

CIG also worked with researchers Dr. Marti (CU Boulder), Prof. Takehiro (Kyoto U.), Dr. Sasaki (Kyoto U.), and Dr. Schaeffer (U. de Grenoble)) who participated in the benchmark exercise, to apply for their own allocation in order to perform larger-scale geodynamo studies with their codes now tested on and tuned for Stampede.

CIG Code Development and Testing for Mantle Convention

We 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 Earth's mantle. We obtained good scaling to 1000 processor cores with both a simple cubic domain and a more realistic spherical shell domain (see report for code scaling). An undergraduate student studied the effectiveness of GPU based sparse matrix solvers using the K20 GPGPU nodes on Stampede. This work is ongoing; preliminary results comparing sparse matrix-vector multiplication (ignoring transfer) are promising and are shown in Figure 1.

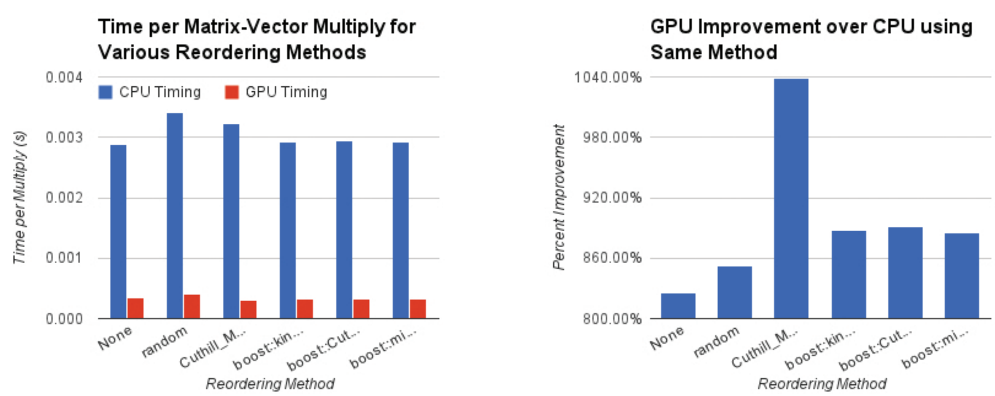

Figure 1: Effect of node reordering on GPU and CPU sparse matrix-vector multiplication (left) and overall relative performance of sparse matrix-vector multiplication (right) on Stampede.

Tracking of active or passive fields with distinct compositional, geochemical or rheologic properties is important for incorporating physical realism into mantle convection simulations, and for investigating the long term mixing processes in the mantle. Numerically advecting fields are difficult since they are non-diffusive and have sharp boundaries, and therefore require different methods than usually used for temperature. Dr. He (UC Davis) developed a new solver using the Local Discontinuous Galerkin algorithm to solve the advection-diffusion equation. The new solver was applied to two established mantle convection benchmarks [He *et al.*, 2015].

Small Scale Studies

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.

Allocation Development Using this allocation to conduct scaling tests, researcher Robert Citron successfully applied for his own allocation, "Simulations of Mantle Convection on Mars". Prof. Jadamec (U. of Houston) also plans to submit a request based on research conducted under this allocation. See also above section *Community Geodynamo Benchmarks*.

Mantle Convection Studies Ms. Liu (CU Boulder) and Prof. Zhong (CU Boulder) studied the Earth's long-wavelength geoid anomaly. The Earth's long-wavelength geoid anomalies have long been used to constrain the dynamics and viscosity structure of the mantle in an isochemical, whole mantle convection model. In their study, they formulated dynamically self-consistent 3-D spherical mantle convection models to investigate how chemically distinct and dense piles above the core-mantle boundary may influence the geoid. Their results help constrain and interpret the large-scale thermochemical structure of the mantle using surface observations of the geoid and topography, as well as seismic models of the mantle [Liu and Zhong, 2015].

Ms. Haynie and Prof. Jadamec (U. of Houston) continued studies on subduction zone modeling. To understand the dynamics of subduction of plateaus in the oceanic plate in Alaska, they have a run a series of 2D and 3D models. These studies aim to help further explain uplift and deformation in the overriding continental plate [Haynie and Jadamec, 2015].

Prof. Stamp (MIT) contributed to the development of ASPECT by developing new tutorials and cookbooks. The added features allowed her to pursue further research in rift margins especially as applied to the East African Rift System [Stamps *et al.*, 2014; Stamps *et al.*, 2015a, b, c].

Geodynamo Studies Dr. Matsui (UC Davis) investigated the effects of the thermal boundary condition at the core mantle boundary (CMB) on the dynamics and dynamo action in the outer core using Calypso [Matsui *et al.*, 2015]. Prof. Buffett (UC Berkeley) also investigated a response of the fluid motion due to change of temperature heterogeneity at the inner core boundary using Calypso [Buffett and Matsui, 2015].

Dr. Ribeiro (UCLA) used roughly 350,000 SUs of the allocation to investigate turbulent convection in stellar interiors and planetary cores taking place in the presence of strong magnetic and rotational forces. Little detailed information exists to describe MHD turbulence in geo- and astrophysical contexts. To address this deficit, Dr. Ribeiro has developed a state-of-the-art, mixed laboratory-numerical experimental platform using Stampede resources and presented the state of his work at the American Geophysical Union annual meeting [Ribeiro, 2015] as well as published a paper in *Metals* [Ribeiro *et al.*, 2015].

Dr. Nore and Prof. Guermond (TAMU) performed kinematic and MHD dynamo simulations in a cylindrical geometry to represent results of Von Karmann sodium (VKS) dynamo experiment, which is the first experiment with a working dynamo. She finds a similar magnetic field pattern to the observed magnetic field in the experiment and in the mean field kinematic dynamo models, and predicts dynamo action in a cylinder for the DREsden sodium facility for DYNamo and thermo-hydraulic studies (DRESDYN) by MHD simulatios [Nore *et al.*, 2015a, 2015b].