Progress Report (October 2013 to present)

Overview
NOTE: We ask the reviewers to note that some of this progress report is duplicated from the supplemental request since both cover the work done from October 2013.

Our current allocation for the period October 2013 to September 2014 is 1079619 service units on Stampede, 10000 service units on Maverick and 5000 service units on the visualization cluster Longhorn. These allocations are due to expire on September 29, 2014. As of July 10, 2014 we have used 84% of our allocation on Stampede. We are certain we will be using up the remainder of the allocation by September 30, 2014. An overview of the allocation usage and results are shown in the table below.

Category	Stampede SUs	Publications/Talks
Geodynamo Benchmarking	54,500	3
Geodynamo Science	370,000	5
Mantle convection	210,000	8
Code development	67,500	0
Total	702,000	16

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.

Geodynamo Development and Validation
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. 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 magneto hydrodynamics 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 examine the performance of Calypso on the MIC coprocessor boards. Calypso was also extended to use parallel HDF5 and XDMF to improve visualization and performance, and then tested on the Stampede system. 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.

After Calypso was tested and improved on Stampede, Dr. Hiroaki Matsui used it to perform high-resolution studies of core dynamo evolution. An example time slice of one simulation is shown below in Figure 1. The full movie of a simulation, showing the radial component of the magnetic field, is available at:

http://wiki.geodynamics.org/software:calypso:start

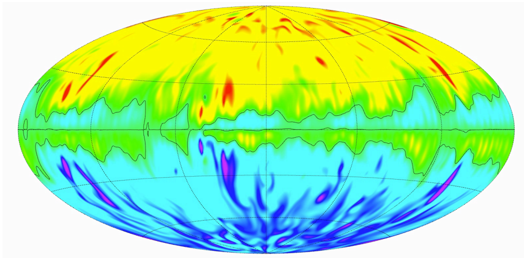

Figure Error! No sequence specified. **– Time slice of radial magnetic field from core dynamo simulation using Calypso, run on Stampede using 20 nodes (320 cores).**

Working with other researchers, Dr. Matsui has developed a set of benchmark tests to compare different geodynamo simulation codes for accuracy and performance. These benchmarks investigate the evolution of a dynamo to steady state using a variety of boundary conditions (magnetically/electrically insulated, vacuum, etc.). As of July 10, 2014, 12 research groups from institutions around the world have participated in this benchmark using approximately **54,000 SUs** on Stampede and resulting in a presentation at the AGU conference in December 2013. For a full list of participating groups and details regarding each code that was benchmarked, we refer readers to http://www.geodynamics.org/archive/community/workinggroups/geodyn/benchmark

We anticipate further publications from this work in the near future in a journal special edition. We will also 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.

CIG will be conducting a workshop in October 2014 to discuss the results from the geodynamo accuracy and performance benchmarks and to motivate the next generation of geodynamo codes.

CIG Code Development and Testing

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 Earth's mantle. Using the K20 GPGPU nodes on Stampede, an undergraduate student is studying the effectiveness of GPU based sparse matrix solvers. This work is ongoing, but preliminary results comparing sparse matrix-vector multiplication (ignoring transfer) are promising and are shown below in Figure 2 and Figure 3.

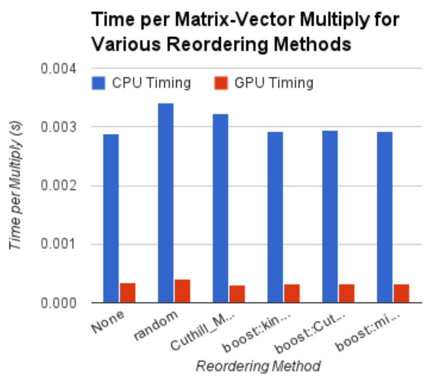

Figure 2 – Effect of node reordering on GPU and CPU sparse matrix-vector multiplication.

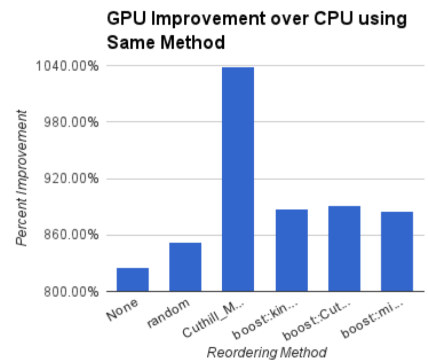

Figure 3 – Overall relative performance of sparse matrix-vector multiplication

Another undergraduate is using the Stampede resource to improve tracer particle integration methods in Aspect.

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

Max Rudolph, Xi Liu, and Prof. Shijie Zhong at the University of Colorado, Boulder, have used approximately 160,000 SUs to investigate different simulation regimes of mantle convection using the CitcomS code. These simulations use imposed velocity boundary conditions from plate reconstructions and to understand the thermochemical evolution of the mantle over the past 500 Myr. The simulations also involved a series of numerical experiments to simulate 3D spherical mantle convection, mainly degree 2 dominant, for both purely thermal and thermochemical cases. The researchers analyzed how the chemical piles influence the convective structure and the geoid. They conclude that while chemical piles don't do much to the convective structure, they influence the geoid. With chemical piles, the geoid is only contributed by the upper part of the mantle. The results of these studies contributed to four papers and presentations given over the past six months. Based on the experience from using the CIG allocation, these researchers are now in the process of applying for their own allocation in the near future.

Geodynamo Studies

CIG has worked with several researchers in geodynamo studies to support their research using small amounts of the allocation on Stampede. Dr. Adolfo Ribeiro at UCLA used roughly 150,000 SUs of the allocation to investigate turbulent convection in stellar interiors and planetary cores taking place in presence of strong magnetic and rotational forces. Little detailed information exists to describe magneto-hydrodynamic 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 AGU 2013 as well as submitted a paper to the Journal of Fluid Mechanics.

Dr. Hiroaki Matsui at CIG also investigated multi-scale convection and analysis of fluctuations in numerical geodynamo with the Stampede allocation, submitting this work to two journals.