# Progress Report (April 2017 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 2017

Our current allocation for the period from April 2017 to March 2018 are 15000 service units on Maverick and 10000 service units on Ranch, and 26470 service units on Stampede2 which was transferred from Stampede on June. We also awarded a supplemental allocation on November, 2017, the total allocation for Stampede2 is 51,070.0 SUs. As of Jan. 9, 2018, we have used 85% of our allocation on Stampede2. We are certain that we will be using up the remaining allocation by March 31, as Dr. Hiroaki Matsui and Dr. John Naliboff will be performing more scaling tests and optimization for Stampede2 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 |
|---|---|---|
| Long-Term Tectonics | 1538 | 3 |
| Geodynamo development | 36,080 | 2 |
| Geodynamo Science | 5,616 | 8 |
| Mantle convection | 210 | 5 |
| Total | 43,444 | 18 |

The main document of this proposal discusses CIG computational efforts on Stampede2. 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 1.2, the current version, was released in July 2017 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 2.0 is currently being developed and tested on Stampede2 and demonstrates performance improvements for up to 256 nodes (17408 cores) on Stampede2 (see report for code scaling). Additional data output features (cross sectioning and isosurfacing) are also implemented. Calypso 2.0 will be released in 2018.

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 maintains good scalings to 16384 cores on Stampede2. Rayleigh version 0.9 will be released in early 2018.

orking 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 in the benchmarking study to apply for their own allocation in order to do larger scale geodynamo studies with their codes tested on and tuned for Stampede2.

As of Jan. 9, 2018, 36,080 SUs were used for development of and benchmarks for geodynamo simulations on Stampede2.

## 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 `https://github.com/geodynamics/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 mantle convection and lithospheric deformation.

## 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.

**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. Graduate student Harsha Lokavarapu also tested Particle-in-Cell Methods for ASPECT on Stampede.

**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 1,538 SUs on Stampede2.

**Geodynamo Multi-scale Convection Modeling** Dr. Hiroaki Matsui is constructing a sub-gird scale model for the geodynamo simulations. He performs large eddy dynamo simulations including the dynamic SGS model using Calypso. To date, Dr. Matsui has used approximately 5,616 SUs on Stampede2.