Progress Report (April 2018 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 2018.

Our current allocation for the period from April 2018 to July 2019 are 10,000 service units on Ranch, 64,160 service units on Stampede2, and 500,000 service units on Comet. As of July 12, we used 135,150 SUs on Comet, and extended the allocation period to September 2019. Consequently, the total allocation for Stampede2 is 103,323 SUs. As of July 12, 2019, we have used 41% of our allocation on Stampede2. We are certain that we will be using up the remaining allocation by September 31, as Dr. Hiroaki Matsui, Dr. John Naliboff, Dr. Juliane Dannberg, and Dr. Rene Gassmoeller will be performing more calculations Stampede2 through this date. An overview of the allocation usage and results are shown in the Table 1.

Table 1: Allocation usage as of July 12, 2019

Category	Stampede2 SUs	Comet SUs	Publications/Talks
Long-Term Tectonics	6,460.102	3,218	3
Geodynamo	23,866.3	84,713	8
Mantle convection	12,547.943	47,219	14
Total	42,874	135,150	25

The main document of this proposal discusses CIG computational efforts on Stampede2. These include development, validation, and related research using geodynamo codes and 2) using mantle convection codes. 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-situ visualization of vector fields for geodynamo simulations. Graduate student Yangguang Liao is developing line integral convolution (LIC) modules for Calypso. The LIC module works in a massively parallel environment in order to visualize during simulations. While the LIC module works successfully in a parallel environment, results suggest that data repartitioning from the simulation is required to obtain maximum performance. To date, Liao used approximately 2,260 SUs for this study.

Geodynamo Multi-scale Convection Modeling Dr. Hiroaki Matsui is constructing a sub-grid scale (SGS) 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 84,713 SUs on Comet and 21,195 SUs on Stampede2.

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

Mantle Convection Studies Throughout 2018 and 2019, multiple researchers have used and modified ASPECT on Stampede2 to improve it's capabilities for modeling a wide variety of convective processes. Dr. Juliane Dannberg, Prof. Timo Heister and Dr. Rene Gassmoeller have implemented a new formulation of the two-phase flow equations for coupled magma and mantle dynamics, allowing it to efficiently and accurately compute large-scale 3-D simulations of melting and magma transport in the Earth's mantle. Furthermore, Dr. Juliane Dannberg and Dr. Rene Gassmoeller have used high-resolution 3D geodynamic models to investigate how geochemical trends observed in ocean islands may originate from chemical reservoirs present in the lowermost mantle. Additionally, Dr. Rene Gassmoeller, Dr. Juliane Dannberg, Prof. Timo Heister, and Prof. Wolfgang Bangerth have used ASPECT on Stampede2 to investigate the influence of more accurate compressibility approximations on mantle convection and long-term tectonic simulations. The results of this study are currently under review and the algorithms have been included in ASPECT for future applications.

Recently, Prof. Timo Heister and Thomas Clevenger have implemented a new experimental Geometrical Multigrid (GMG) solver into ASPECT and

performed strong scaling tests on Skylake nodes of Stampede2. The new solver that will be increasingly utilized during the next phase of XSEDE improves ASPECT's scalability up to 24576 cores (512 nodes) for a model with 3.4 billion degree of freedoms and will be utilized and further extended during the next phase of funding.

Finally, ongoing research on providing more accurate tracking and better resolution of thermal, viscous and compositional interfaces in the Earth's mantle has continued. Dr. Rene Gassmoeller, Prof. Gerry Puckett and Graduate student Harsha Lokavarapu developed more accurate Particle-in-Cell Methods for ASPECT on Stampede2 and implemented these techniques for future applications. Dr. Juliane Dannberg implemented equations that allow it to track the fractionation of iron isotopes under the presence of temperature gradients in the mantle. Both of these studies are currently under review.

Long-Term Tectonics Simulations Dr. John Naliboff has applied ASPECT to long-term tectonics simulations of lithospheric dynamics. To date, Dr. Naliboff has used approximately 6,406.194 SUs on Stampede2 and 3,218 SUs on Comet. These resources were primarily used for testing of new rheological models in ASPECT for a range of lithospheric dynamics model sizes (up to 50e6 DOF) and run times. A small number of SUs were used by Michael Berry (3.4780) and Prof. Magali Billen (50.430) for development and scaling in preparation for individual XSEDE research proposals.