Progress Report (October 2019 to present)

Overview

NOTE TO REVIEWERS: Some of this progress report is duplicative from the renewal application. Both reports cover the work done for the entire allocation period beginning in October 2019 to date.

Our current allocation for the period from Oct. 2019 to Oct. 2020 is 10,000 service units on Ranch, 68,657 service units on Stampede2. We extended the allocation period to Apr. 2021 and have also transferred 5,000 SUs from Stampede2 to 89,662 SUs to SDSC Expanse on Dec. 18, 2020 where an additional 10,000 SUs of storage were also allocated. As of Jan. 12, 2021, we have used 29,782 SUs of our allocation on Stampede2, and 327 SUs on SDSC Expanse. We will be using the remaining allocation by March 31, as Dr. Hiroaki Matsui, Prof. John Naliboff, Prof. Juliane Dannberg, and Prof. Rene Gassmoeller have planned additional computations during this period on Stampede2 and SDSC Expanse. An overview of the allocation usage and results are shown in the Table 1. We also note that for studies using ASPECT, only publications for journal articles are listed, although the results have also been presented at numerous scientific workshops.

Table 1: Allocation usage as of July 12, 2019

Category	Stampede2 SUs SUs	Publications/Talks
Geodynamo	786	8
Stokes Solver	1,621	1
Interface Tracking	3,294	1
Mantle Convection	6,310	0
Long-Term Tectonics	17,472	2
Additional Usage	299	0
Total	29,782	11

Code Development and Testing for Geodynamo

Dr. Hiroaki Matsui has migrated the line integral convolution (LIC) module which has been developed with Yangguang Liao into Calypso. The LIC module works in a massively parallel environment in order to visualize computations during the simulation (real time). Performance results suggest that data re-partitioning from the simulation is required to obtain maximum performance. Dr. Hioaki Matsui is developing a parallel domain re-partitioning modules to migrate into the Calypso and will be further testing this on Stampede2. We used 786 SUs for this development.

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

Stokes Solver Development Prof. Timo Heister used 1621.027 SUs on Stampede2 towards development and testing of a new matrix-free multigrid solver. In short, this new solver provides approximately a 3x improvement in Stokes run-time performance, used 10x less memory, and scales up to 100x larger problem sizes. Scaling results for this solver on both Stampede2 on Frontera are available on the CIG website, and have also been presented in a recent publication (Clevenger et al., 2020). Multiple examples of how to use the new solver are also provided within the ASPECT repository.

Interface Tracking Development Dr. Jonathan Robey and Prof. Gerry Puckett used 3294.216 SUs on Stampede2 towards testing of a new volume of fluid (VOF) interface tracking within ASPECT. In detail, the majority of the SUs were used for high-resolution simulations of subduction that tested the accuracy of the VOF method against a range of other interface tracking methods. The results of this work is summarized in Robey (2020).

Mantle Convection Studies Prof. Juliane Dannberg, and Prof. Rene Gassmoeller have used resources on Stampede2 for two separate projects. The first project modeled the development and evolution of melt at the important core-mantle boundary interface and its links to seismologically observed features the so called Ultra-Low-Velocity-Zones. These two-phase flow models require high-resolution and present complex challenges for the solver, which makes them expensive to run. Secondly, they developed an alternative to the common temperature-formulation used to model energy conservation in geodynamic computations. Instead of temperature they solved an entropy equation, which allows for a much more accurate and resolution independent modeling of phase transitions. This project required extensive code development, testing, and benchmarking against the (expensive) temperature method, which was facilitated by comparing model runs on Stampede2. Publications for both projects are currently in preparation. In total, 6310 SUs were used towards these projects.

Long-Term Tectonics Simulations Prof. John Naliboff has applied ASPECT to high-resolution, 3D simulations of long-term lithospheric dynamics. In detail, these simulations provided the first tests and production-quality examples of how to efficiently use compositional fields for accurately tracking lithologic layers and finite strain after the lithosphere has experienced significant amounts of deformation. In total, Prof. Naliboff used 17472.063 SUs on Stampede2, with the vast majority of this time being used for high-resolution 3D simulations that required between 5-20 nodes. The results of these simulations have produced two distinct publications (Naliboff et al., 2020; Gouiza and Naliboff, In Review), with the various files and software required to reproduce the simulations provided in multiple open-access repositories.

Additional Development and Testing Dr. Tahiry Rajaonarison (287.587 SUs), Dr. Robert Myhill (4.003 SUs), and Dr. Arushi Sexna (7.396 SUs) performed additional test-

ing towards, respectively, new methods for simulating short-term tectonic deformation, viscoelastic-plastic deformation, and global data assimilation. The results of this work have been contributed to the ASPECT repository or are in preparation for contributions.