CIG Science Gateway and Community Codes for the Geodynamics Community - MCA08X011

July 2023 ACCESS Allocation renewal - Maximize
Progress Report - October 2022 to present

Overview

Our current allocation for computation for the period from October 2022 to September 2023 is 85,890 Service Units (SUs) on Stampede2 and 2,215,340 SUs on Expanse. The allocation for the storage is 2048.0 GBs on SDSC Expanse Projects Storage and 10,000 GBs on TACC Long-term tape Archival Storage (Ranch).

As of June 30, 2023, we have used 55,635 SUs of our allocation on Stampede2, and 267,810 SUs on SDSC Expanse. We would like to renew our allocation as additional computations are planned for the next year on Stampede3 and SDSC Expanse. An overview of the allocation usage and results are shown in Table 1. We note that only publications for peer reviewed journal articles are listed, although the results have also been presented at numerous scientific workshops.

Table 1: Allocation usage as of July 13, 2023

Category	Stampede2 (SUs)	Expanse (SUs)	Publications/Talks
Geodynamo	22,810		1/4
Short-term Tectonics (PyLith)	4,738		0/0
Long-term Tectonics (ASPECT)	4,930		0/0
Mantle Convection (ASPECT/StagYY)	23,154	262,419	1/5
Stokes Solver (ASPECT)		5,382	1/2
Miscellaneous	7	9	
Total usage	55,635/85,890 (65%).	267,810/ 2,215,340 (12%)	

Geodynamo

Code Development and Simulation for the Past Earth

The Earth's inner core has solidified and grown with the cooling of the Earth in the last one billion years. Dr. Hiroaki Matsui (UCD) has performed dynamo simulations to investigate parameter ranges to sustain the intense magnetic field in the past Earth when the solid inner core was smaller than present day. He has and continues to investigate the dependency of the range of the amplitude needed for convection (Magnetic Reynolds number, Rm) to sustain the

dipolar magnetic field and its dependency on the inner core size. The results show that the lower limit of Rm increases with smaller inner core size, while there is almost no dependency of the upper limit of Rm to sustain the dipolar magnetic field [Nishida et al., submitted].

Dr. Matsui used 7,568.04 SUs on Stampede2 as of July 13, 2023 for this research.

Heterogeneous boundary conditions for geodynamo simulations

Dr. Daniele Thallner has used resources on Stampede2 to run 64 numerical geodynamo simulations using the LSD code. These simulations aim to explore the effects of spatially heterogeneous core-mantle boundary (CMB) heat flux on the long-term geomagnetic field. In the first model series, he ran several short simulations that explored how previously published simulations with homogenous CMB heat flux behaved when heterogenous boundary conditions were applied and if they would sustain geodynamo action. Based on these tests, further simulations were run with CMB heat flux boundary conditions depicting Earth's present-day state. The present-day state of CMB heat flux pattern was defined by two heat flux maps: one based on seismic tomography models, which has been used in previously published geodynamo simulations, and a second map based on high-resolution heat flux information from the output of plate-driven 3D global mantle convection models run with ASPECT. Preliminary data, presented at multiple conferences, suggests that simulations with the more detailed CMB heat flux patterns from ASPECT have generated more dipole-dominated geomagnetic fields that showed smaller degrees of secular variation and were less likely to reverse their polarities. The results are currently being prepared for publication.

In total, 15,241.91 SUs were used on Stampede2 as of July 13, 2023.

Code Testing - Stokes Solver Development

Dr. Marc Fehling (CSU) and Prof. Wolfgang Bangerth (CSU) developed general algorithms for parallel hp-adaptive finite element methods (FEM) that work for continuous and discontinuous elements. They ran weak and strong scaling experiments on Expanse which involved the solution of a Laplace problem in 2D with billions of unknowns and a Stokes problem in 3D. Results have been collected in the manuscript Fehling and Bangerth (2023).

They continue to improve the Stokes solver with the development of global coarsening multigrid methods for hp-FEM in a matrix free formulation. Dr. Fehling presented the first results of scaling experiments at the SIAM Conference on Computational Science and Engineering 2023 (CSE23) [Fehling and Bangerth, 2023].

In total, 5,382 SUs have been used on Expanse as of July 13, 2023.

Mantle Convection Studies

A. Adams (PhD student, UCSD) and R. Kepler (undergraduate researcher, UCSD), under the supervision of Prof. Dave Stegman (UCSD), used the StagYY code to investigate mantle convection on Venus. The project has three components. The first component comprises models investigating lithosphere instability and plume-lithosphere interaction on Venus. The models were 2D, with a spherical annulus geometry and filled in several parts of a tectonic regime diagram that were needed. The manuscript was submitted to JGR-Planets (Adams et al., 2023). The second component expanded similar models into a larger parameter space so they could be directly compared with those from other research groups. Although the same code was used, the results here are strikingly different in terms of the predicted planetary tectonic regimes - stagnant lid, global overturn, or regional instability. We identified all the differences in parameters and model design (about 10) and explored a few cases to test. We identified three

cases that we predict are most likely to be the cause of discrepancies between models. A suite of 27 models were run, investigating changes in the yield stress and amount of crustal buoyancy checking our grid resolution (2048x384) against the lower resolution that is typical for models by other groups (512x96) as well as an intermediate resolution (1024x192). This work is nearing completion and we anticipate writing the manuscript this summer and submitting it in late summer or fall. The third component is the development of a regional 3D model equivalent to our 2D models. This required first migrating to the newest branch of the code. We then reproduced a previous result from the older version used in our recent publications. We have thus far succeeded in building a low resolution, simplified regional 3D spherical model that will be used in future runs. See Adams et al. (submitted).

In total, 262,419.00 SUs have been used on Expanse as of July 13, 2023.

Prof. Juliane Dannberg, Dr. Arushi Saxena, Dr. Daniele Thallner, and Dr. Rene Gasmoeller ran ASPECT on Stampede2 to provide 'realistic' heterogeneous boundary conditions from mantle convection with prescribed plate motion models for geodynamo simulations. Model results constrain the spatial and temporal variations of Earth's core-mantle boundary heat flux throughout the supercontinent cycle. This is an important boundary condition for geodynamo simulations and can critically affect the magnetic field created by the geodynamo. We have started to use these boundary conditions in geodynamo simulations with the LSD code (Thallner), and will make our model output and the workflow of applying the boundary conditions to a geodynamo simulation available to the community.

In addition, these models tracked chemical composition over a model time of one billion years. providing a large-scale, realistic application test for the particle method implemented by Prof. Rene Gassmoeller. Tests showed that the accuracy of the newly implemented particle method is substantially improved. Publications for this project are currently in preparation, and the results have been presented at several conferences.

In total, 23,152.63 SUs have been used on Stampede2 as of July 13, 2023.

Long-Term Tectonics Simulations

In June 2023, Daniel Douglas (PhD student, NMT), under the supervision of Prof. John Naliboff (NMT), began conducting large 3D simulations of regional subduction along the Kermadec Trench using ASPECT on Stampede2. The goal is to test a range of new ASPECT features - matrix free solver, new rheological formulations, two-phase fluid transport, and crystal preferred orientation (CPO), in complex models. These models form the basis for future one-way coupling with global models using prescribed plate boundaries. The simulations run on approximately 30 nodes for 24-48 hours,

In total, 4,930.24 SUs have been used on Stampede2 as of July 13, 2023.