Code Performance

CIG plans to primarily use four codes on XSEDE for research and further develop these codes to improve their performance and scalability. The scalability and performance of these codes measured on XSEDE resources is presented below.

Calypso

Calypso is a recently developed code for magnetohydrodynamics based geodynamo studies. It uses a pseudo spectral method for solenoidal and poloidal components in combination with a finite difference method for radial components. We tested the scalability and performance of Calypso on Stampede up to 16384 cores (se Figure 1). The largest scaling test above corresponds to roughly a 17 million DOFs for one scalar and scales well up to 17408 cores. The scaling result on Stampede2 shows good scalability, but a little bit worse than the scaling on the Stampede. The Stampede2's performance of each node is approximately two times of Stampede's performance. Comparing between KNL processor and XEON processor on Stampede2, the performance of the both processors are very similar.

Rayleigh

CIG is also currently developing Rayleigh, a state of the art code for dynamo simulations in collaboration with Dr. Nick Featherstone (JILA, University of Colorado Boulder). Dr. Featherstone develops Rayleigh based on a solar dynamo code (ASH Anelastic Spherical Harmonic). He has developed techniques to scale this code efficiently to more than 10,000 cores and we expect these techniques to also be applicable to geodynamo simulations. Figures 2 show the recently measured scaling of Rayleigh code on TACC Stampede2. As in the Calypso's case, the performance of the both KNL and XEON processors are very similar.

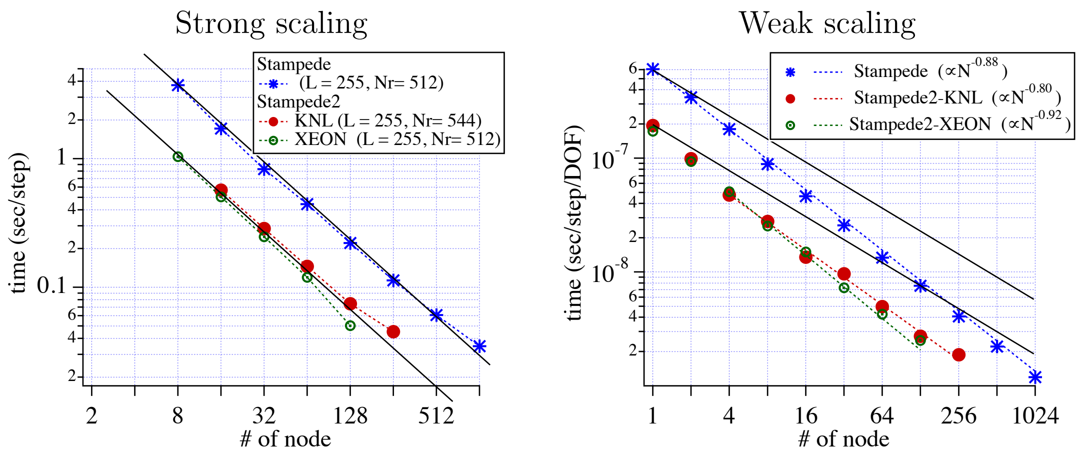

Figure 1: Comparison of Calypso's scaling on the TACC Stampede and Stampede 2. Strong scaling results is shown in the left panel, and weak scaling results are shown in the right panel. Ideal scaling ($O(N_{node}^{-1})$ and $O(N_{node}^{-2/3})$ for the strong and weak scaling, respectively) is plotted by solid lines.

SPECFEM3D_GLOBE

In collaboration with Princeton, Caltech and the University of Pau (France), CIG offers this software, which simulates global and regional (continental-scale) seismic wave propagation using the spectral-element method (SEM). The SEM is a continuous Galerkin technique, which can easily be made discontinuous; it is then close to a particular case of the discontinuous Galerkin technique, with optimized efficiency because of its tensorized basis functions. Dr. Hiroaki Matsui recently measured scaling of SPECFEM3D_GLOBE on TACC Stampede2 (see Figure 3).

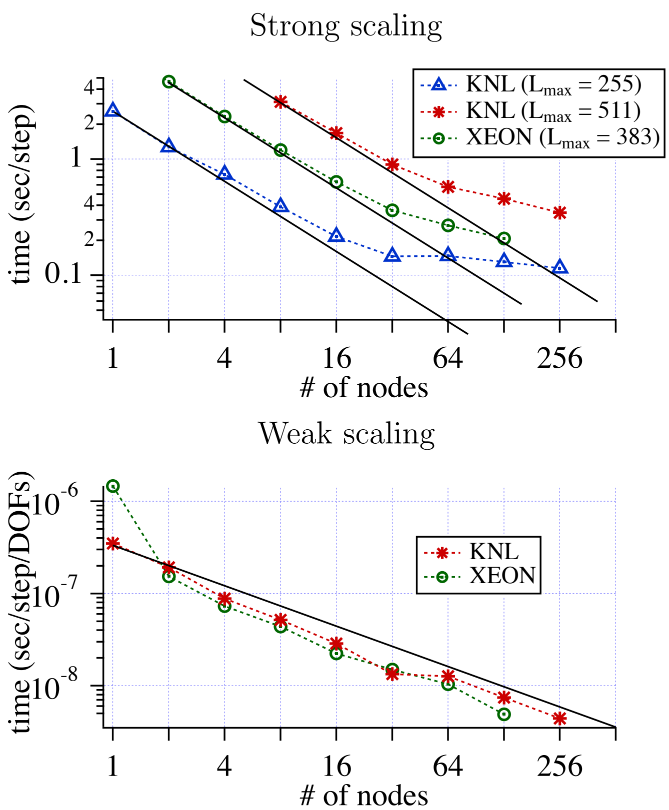

Figure 2: Rayleigh's scaling on the TACC Stampede 2. Strong scaling results is shown in the top panel, and weak scaling results are shown in the bottom panel. Ideal scaling ($O(N_{node}^{-1})$ and $O(N_{node}^{-2/3})$ for the strong and weak scaling, respectively) is plotted by solid lines. Rayleigh only uses MPI parallelization, and 64 of 68 processor cores are used in the each KNL node.

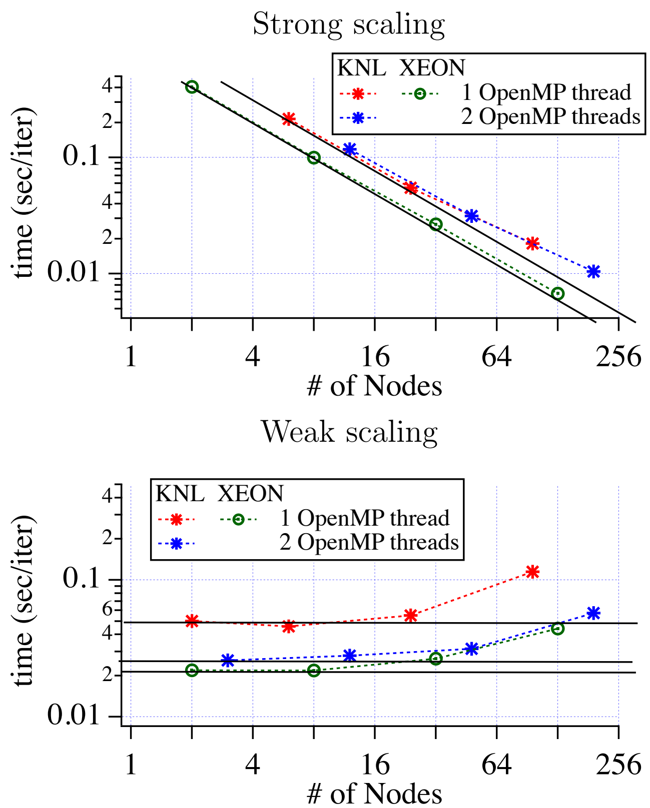

Figure 3: SPECFEM3D_globe scaling on the TACC Stampede2. Strong scaling results is shown in the top panel, and weak scaling results are shown in the bottom panel. Ideal scaling ($O(N_{node}^{-1})$ and constant for the strong and weak scaling, respectively) is plotted by solid lines. In the scaling tests for the KNL nodes, 64 of 68 processor cores are used and 1 or 2 OpenMP threads cases are tested.

ASPECT

ASPECT performs mantle convection and lithospheric deformation simulations using a finite element model and utilizes the Trilinos library for preconditioner and solver support (support for the PETSc library is under development). The scaling capabilities of ASPECT for large-scale 3D mantle convection simulations on Comet are shown in Figure 4 for a spherical shell model. These demonstrate that this next-generation code scales well on problems up to 1.8×10^8 DOFs and up to over 1000 processes.

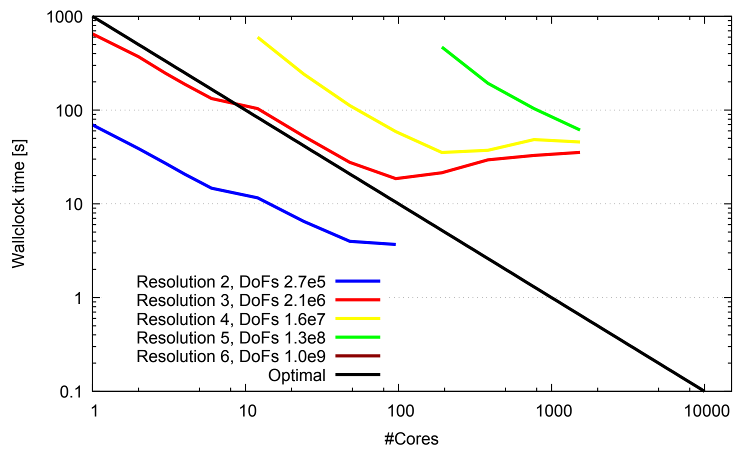

Figure 4: Legend: Strong-scaling results for ASPECT on the XSEDE cluster COMET. The scaling is derived from the wall-clock time of a thermal-mechanical model run for two time steps.