Code Performance and Scaling

CIG plans to primarily use five 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 being developed for magnetohydrodynamics based geodynamo studies. It uses a pseudo spectral method for toroidal 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 (see Figure 1). The largest scaling test above corresponds to roughly 17 million DOFs for one scalar and scales well up to 34,304 cores. The scaling result on Stampede2 shows good scalability for the both KNL and Skylake (XEON) nodes. Comparisons between the KNL processor and XEON processor on Stampede2 show the strong scaling on both processors are very similar.

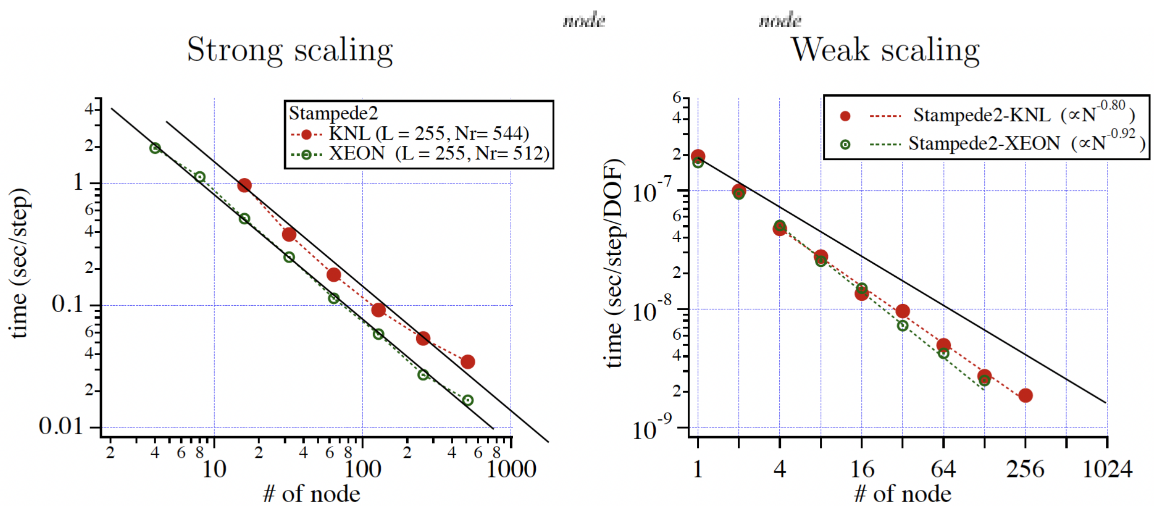

Figure 1: Comparison of Calypso's scaling on the TACC Stampede2. Strong scaling results are shown in the left panel, and weak scaling results are shown in the right panel. Ideal scaling O(N_{node}^{-1}) and O($N_{node}^{-2/3}$) for the strong and weak scaling, respectively, is plotted by solid lines.

SPECFEM3D GLOBE

In collaboration with Princeton and CNRS (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. Scaling of SPECFEM3D GLOBE on TACC Stampede2 is shown in see Figure 2.

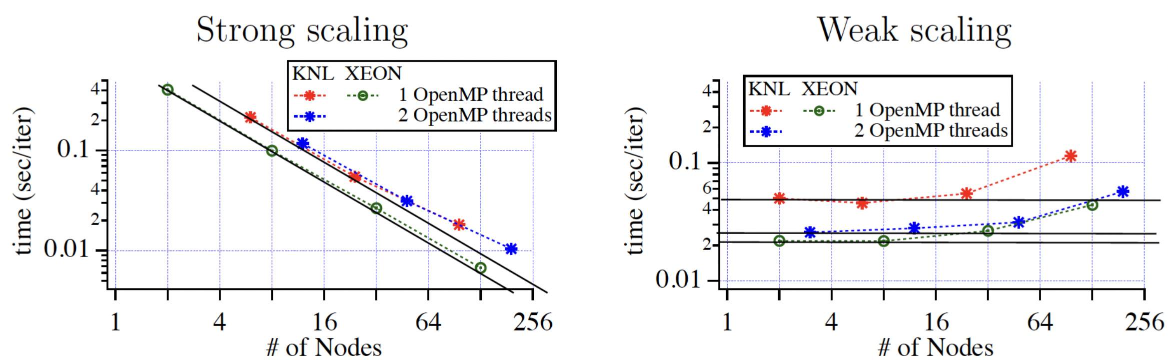

Figure 2: SPECFEM3D globe scaling on the TACC Stampede2. Strong scaling results are shown on the left, and weak scaling results are shown on the right. Ideal scaling, O(N_{node}^{-1}) and constant for the strong and weak scaling, respectively, is plotted by solid lines. In the scaling tests for the KNL 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 method. ASPECT utilizes the Trilinos library for linear solvers and their preconditioners. Scaling capabilities of the stable ASPECT version for large-scale 3D mantle convection simulations on Stampede2 are shown in Figure 3 (left panel) for a spherical shell model. Scaling tests on Frontera shown in Figure 3 (right panel) have shown that our solver scales beyond the resources available on XSEDE. We do not anticipate limitations by scaling for the proposed models.

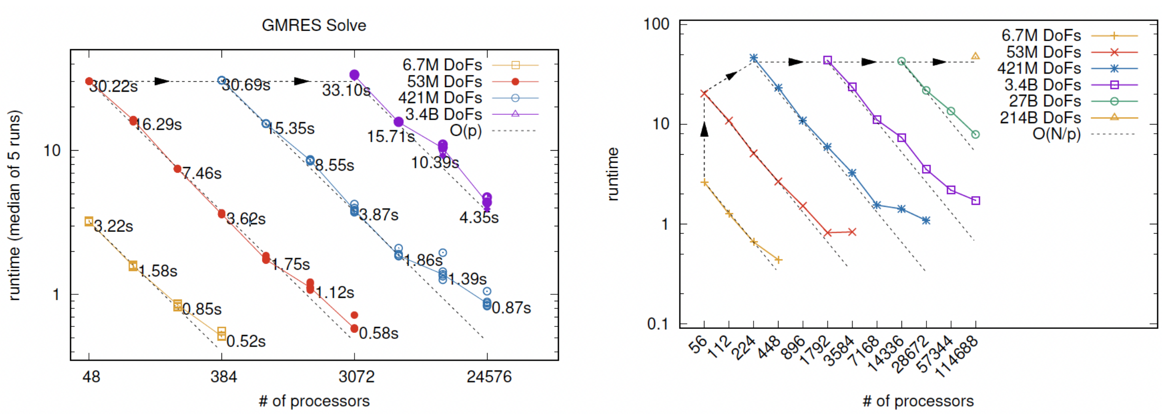

Figure 3: Left: Elapsed time for a globally refined Stokes problem of various refinements and varying number of processors. The solver uses a block Schur complement preconditioner where we estimate the inversion of the velocity block of the Stokes system with one GMG V-cycle. We plot 5 separate runs and the solid lines connect the median of the 5 runs. We see good scaling to between 17K-34K DOFs per processor. Right: Strong and weak scaling results for ASPECT on Frontera. Depicted is the time for a Stokes solve using the matrix-free geometric Multigrid preconditioner developed as part of the previous XSEDE allocations.

LSD

Leeds Spherical Dynamo (LSD). LSD solves the Boussinesq dynamo equations by representing velocity, and magnetic field, as poloidal and toroidal scalars. It is pseudo-spectral; the variations in a sphere are expanded in spherical harmonics, and radial variations are discretized by finite differences with a non equidistant grid using Chebyshev zeros as grid points. The nonlinear terms are evaluated by the transform method. Time stepping uses a predictor-corrector method and the time step is controlled using a CFL condition and error information from the corrector step. The LSD code is parallelized using MPI in both radial and in θ (meridional) directions.

LSD will be used in a one-way coupled model together with ASPECT. ASPECT output will be used as (time-independent) boundary condition for LSD. LSD was previously shown to scale well up to thousands of cores on Stampede1 (Figure 4, left). We have verified that the performance of LSD is still very close to the previously reported numbers, and have repeated the scaling tests for LSD on Stampede2 for model sizes we expect for this project (Figure 4, right). We expect to run the models on 96 cores with a parallel efficiency of 92% or 192 cores with a parallel efficiency of 75%.

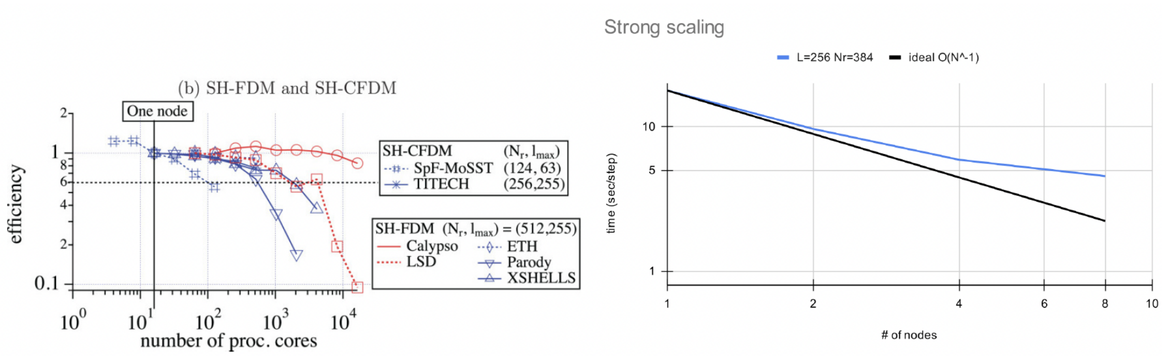

Figure 4: Left: Strong scaling results for LSD from Matsui et al. (2016) on Stampede1 (red dotted line). Right: Strong scaling results for LSD on Stampede2. We have limited this scaling test to the number of nodes expected for this project.

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