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 Stampede2 up to 256 nodes (see Figure 1). We also tested Calypso using CUDA on Maverick and MIC coprocessors on Stampede (see Figure 2). The scaling result on Stampede shows good scalability depending on the problem size, and further work is required for CUDA and MIC versions to improve performance.

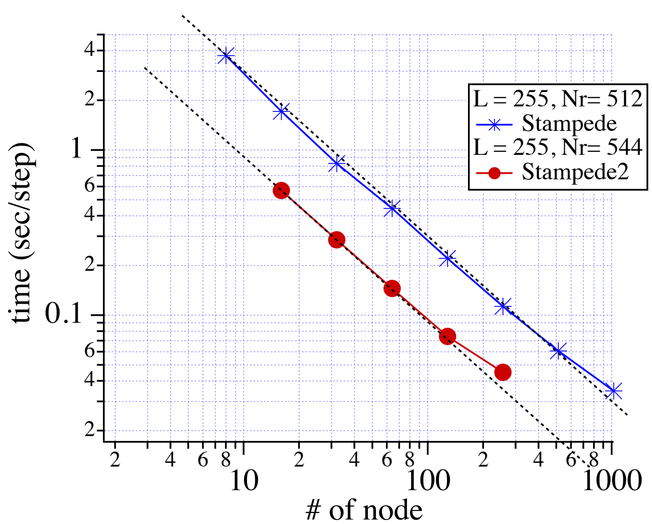

Figure 1: Comparison of Calypso's strong scaling on the TACC Stampede and Stampede 2. Ideal scaling is plotted by a dotted line.

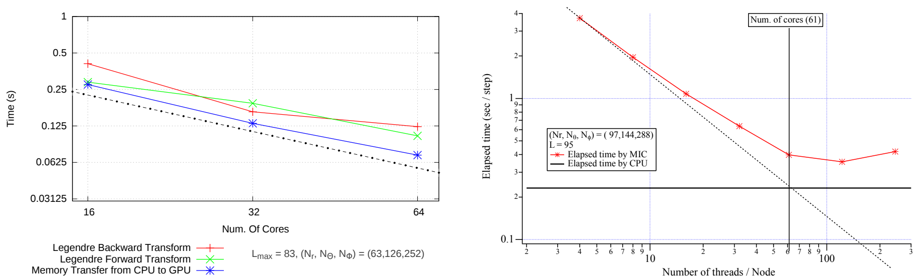

Figure 2: Strong scaling of Legendre transform by Calypso using CUDA on TACC Maverick (left) and scaling using MIC processor on TACC Stampede (right). Ideal scaling is plotted by a dotted line.

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 3 show the recently measured scaling of Rayleigh code on TACC stampede.

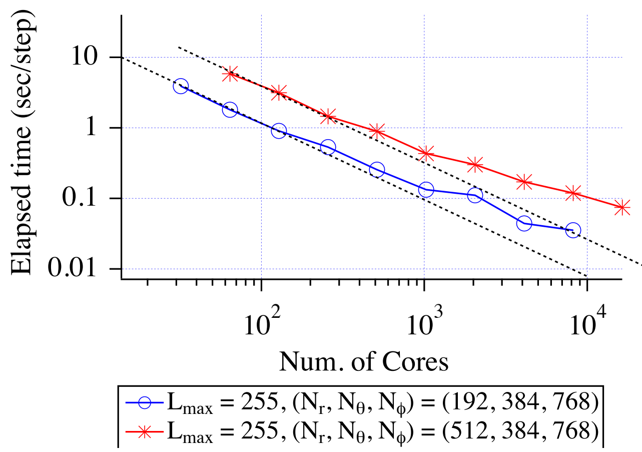

Figure 3: Rayleigh's strong scaling on the TACC Stampede system for different sized simulations. Ideal scaling is plotted by a dotted line.

ASPECT

Aspect performs mantle convection 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 Stampede are shown in Figure 4 for a 3D box model and Figure 5 for a spherical shell model. These demonstrate that this next-generation code scales well on problems up to tens of millions of elements and up to over 1000 processors.

ASPECT also has the capability to advect tracer particles for the purpose of tracking distinct properties that in some cases can be used to modify the simulations (Particle-In-Cell Method). The scaling for the passive particle tracing also demonstrates good scaling up to 10000 cores as shown in Figure 6.

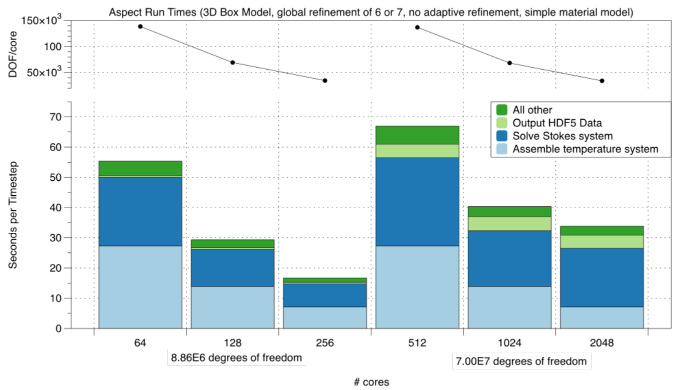

Figure 4: Strong scalability of 3D box model (128^3 or 256^3 elements) on Stampede.

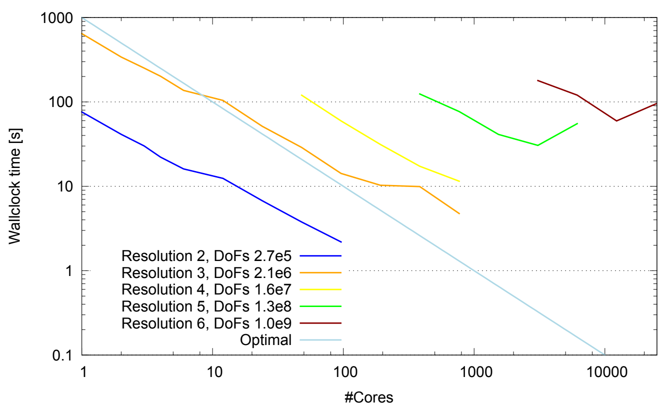

Figure 5: Strong scaling of ASPECT's spherical shell model. The wall clock time for one time step is measured by a mantle convection model including temperature dependent viscosity and composition perturbation in a spherical shell.

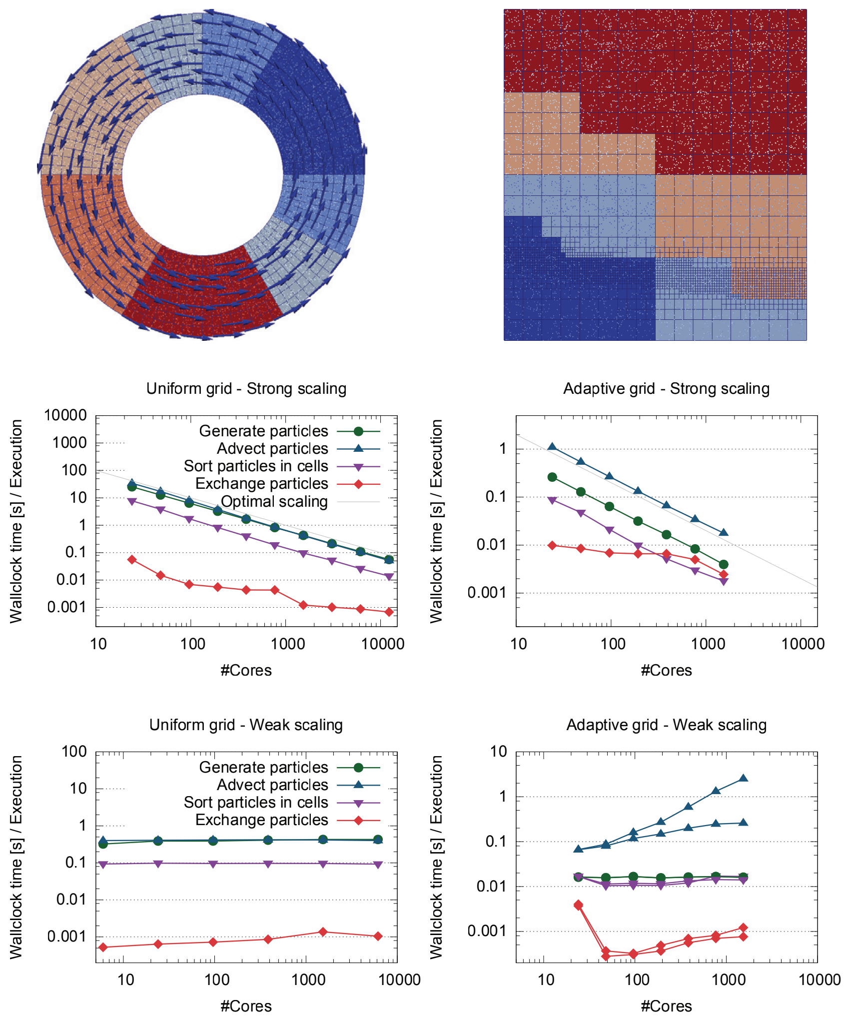

Figure 6: Scaling results for particle tracer for ASPECT. Results for a uniformly refined mesh are shown in the left column, and results for an adaptively refined mesh are shown in the right. Model geometry and partition among processes (also velocity vectors) are shown in the top row. Strong scaling for a constant number of cells and particles and variable number of processes is plotted in the middle. Weak scaling where the numbers of cells and particles per process is kept constant is shown in the bottom row. The bottom right panel contains data without load balancing techniques (dashed lines), and with balanced repartitioning (solid lines).