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, both for large numbers of cores (Figure 1) and on the MIC coprocessor (Figure 2). Both of these show good scalability depending on the problem size, though the MIC coprocessor version needs further work to improve performance.

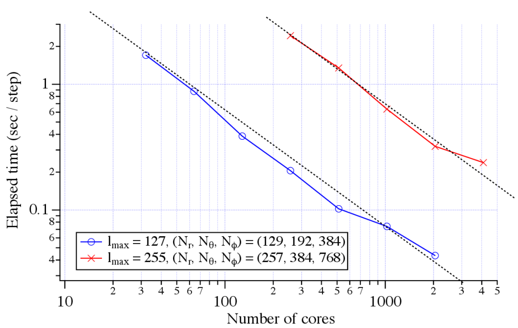

Figure 1 Calypso scaling on the TACC Stampede system for different sized simulations

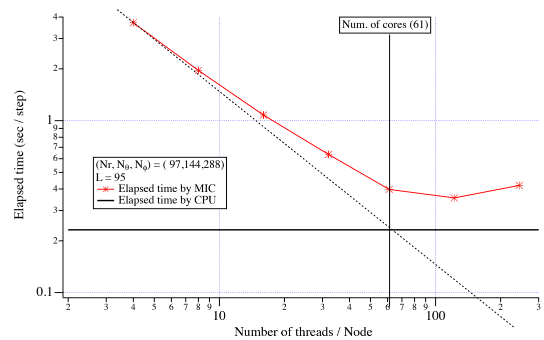

Figure 2 - Calypso scaling on the MIC processor

The largest scaling test above corresponds to roughly a 17 million elements and scales well up to 3000 cores.

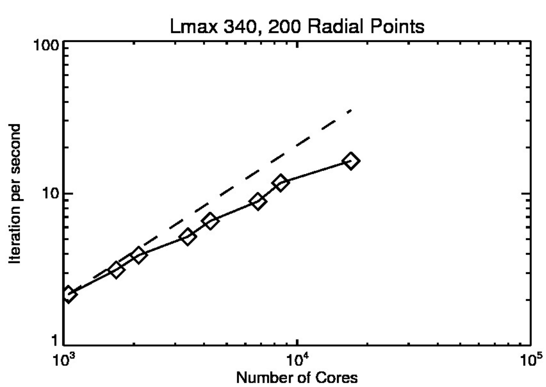

Figure 3 - Simulation scaling for approx. 512^3 solar dynamo simulation on Kraken

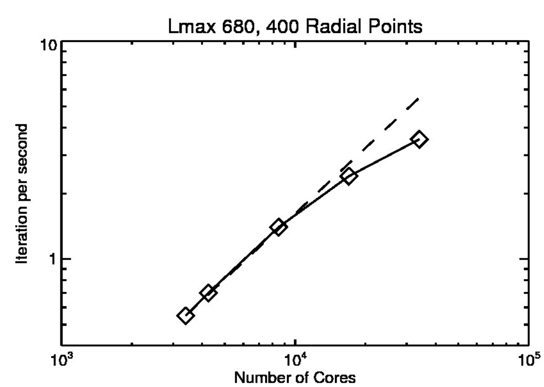

Figure 4 - Simulation scaling for approx. 1024^3 solar dynamo simulation on Kraken

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 previously implemented 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 and 4 show the recently measured scaling of ASH on the Kraken system. At a resolution of approximately 1024^3 (1e9 grid points) the simulation scales well up to nearly 20,000 cores.

Figure 5 shows the performance results for the Rayleigh code using upto 131,072 single-threaded cores on Mira. Figure 5(a) shows the parallel efficiency for the non-magnetic and magnetic runs at the 2048^3 problem size. Efficiency is defined as the ratio of the realized speedup to the ideal speedup. Ideal performance is taken relative to 16,384 cores, the minimum core count for this problem size. Figure 5(b) shows the strong scaling results for the same set of runs. Ideal scaling for each series is indicated by the dashed line.

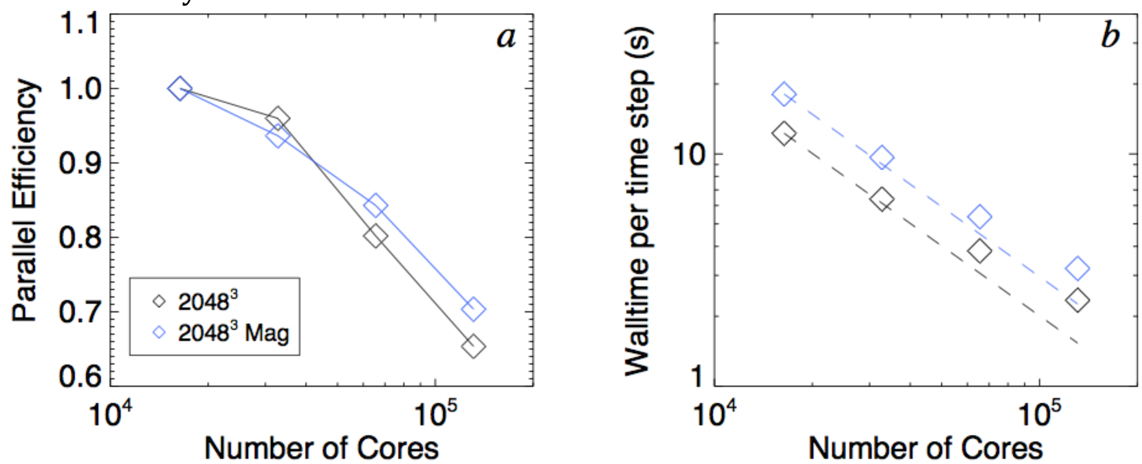

Figure 5 Scaling results for Rayleigh on Mira

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 6 and Figure 7 below. These demonstrate that this next-generation code scales well on problems up to tens of millions of elements and up to over 1000 processors.

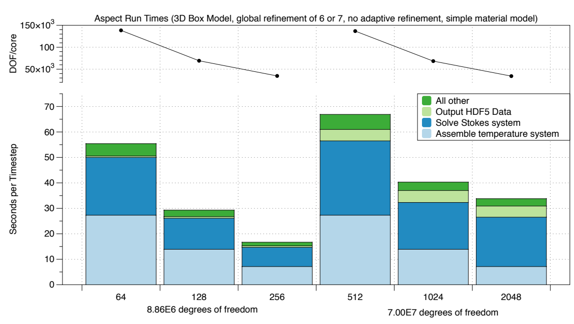

Figure 6 – Strong scalability of 3D box model (128^3 or 256^3 elements) on Stampede

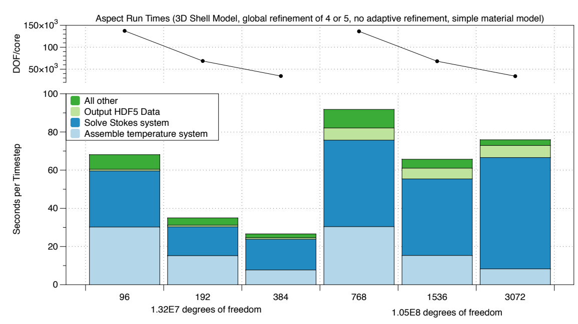

Figure 7 – Strong scalability results for 3D spherical shell model on Stampede

The weak and strong scalability of Aspect was also examined on a local cluster. The results are shown in Figure 8 ASPECT Weak Scaling Results Figure 9 ASPECT Strong Scaling Resultsbelow. These plots demonstrate good scalability up to several thousand processors for large problems.

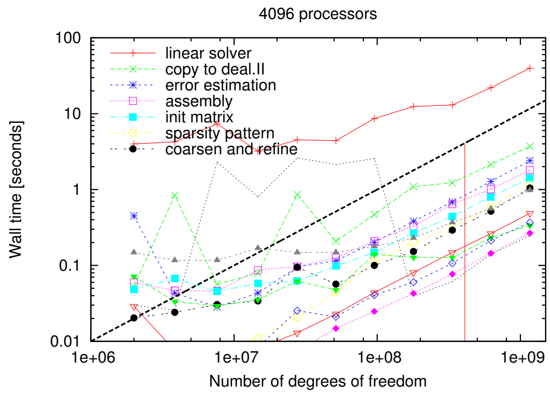

Figure 8 ASPECT Weak Scaling Results

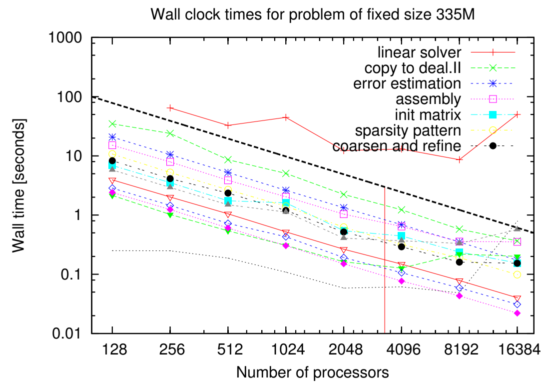

Figure 9 ASPECT Strong Scaling Results

CitcomS. CitcomS can use either conjugate gradient or multigrid solvers and has good scaling properties. On IBM Blue Gene/L, using 64 X 12 processors on a full spherical model, it has a computation efficiency of 65 percent, compared with the same problem using 12 processors [King et al., 2005]. Recent tests on TACC Lonestar show good scalability (> 0.6) for regional models with 6.4 million unknowns using up to 256 cores. Details regarding these results are shown in the figures below.

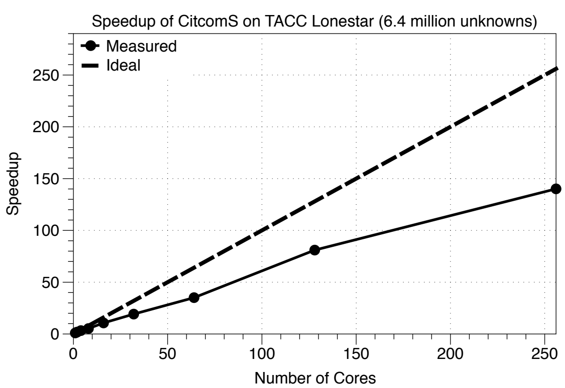

Figure 10 CitcomS speedup on Lonestar

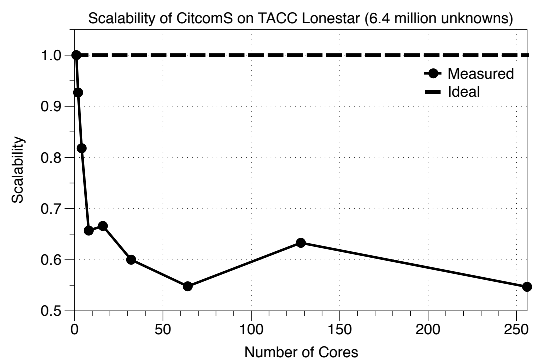

Figure 11 CitcomS scalability results