

S3D Direct Numerical Simulation – Preparations for the 10-100PF era Ray Grout (NREL)

The evolution of supercomputing into the mid-petaflop era has been typified by heterogeneous compute nodes with the majority of the compute capability delivered by a large number of lightweight cores. In order to prepare for the extension of this trend, the DNS code S3D has been retooled in anticipation of a target architecture offering 10s of thousands of heterogeneous nodes containing many X86 cores as well as GPU derived accelerators. Movement of outer loops to the highest level in the code facilitates hybrid MPI-OpenMP performance and an elegant path to accelerated kernels using OpenACC. It is anticipated that relevant scientific simulations at this scale will have a per-node footprint that can be contained entirely on the accelerator, so provision is made to maintain primary solution variables in accelerator memory with specific regions moved to the CPU for inter-node communication and workload balancing. With the current performance it is estimated that the new code will make it possible to meet early science goals with the full build-out of the anticipated Titan system as well as provide a platform to transition into the exascale software research space.