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Exascale Advances with NekRS

Tuesday, July 30, 2024 9:10 AM (40 minutes)

We discuss results of recent Exascale studies with NekRS. Through numerous simulation examples, we illustrate that NekRS sustains 80% parallel efficiency for local problem sizes, n/P, ranging from 3M points per MPI rank on OLCF's Frontier (2 ranks per AMD MI250X) to 5M points per rank on ALCF's NVIDIA A100-based Polaris. On 72,000 ranks of Frontier, NekRS sustains 0.39 TFLOPS per rank or a total of 28 PFLOPS for thermal hydraulics simulations in a full reactor core. In addition to nuclear energy applications, we describe recent developments in SEM-based wall modeled LES for atmospheric boundary layer simulations relevant to wind energy applications. We also present several technical developments that are important to exascale workflows. These include meshing and mesh partitioning for large meshes having in excess of 1B spectral elements; in situ visualization advances that avoid writing multi-TB output files; and GPU-based interpolation utilities that essential for particle tracking and for support of overset grids. Performance scaling results are presented for each of these developments. NekRS development is supported by the US Department of Energy's Advanced Scientific Computing Research program.

Relevance for Nek [100 words max]

Argonne

Primary author: MIN, Misun (Argonne National Laboratory)

Presenter: MIN, Misun (Argonne National Laboratory)