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Nek5000 Applications Pave the Way to Petascale

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Summary

Petascale computing platforms, featuring $P=10^4$-10^5 processors are soon to be available to the Nation's science programs. Current developments in the transport code, Nek5000, are focusing on $P > 10^6$ to prepare for the next generation of computers and beyond. Several recent applications of Nek5000 illustrate the scientific potential of state-of-the-art solvers at the petascale.

Nek5000 is a spectral element based code for the simulation of fluid flow, convective heat and species transport, and magneto-hydrodynamics (MHD) in general 2D and 3D domains. A singular feature of Nek5000 is its ability to scale to the large processor counts that characterize Petascale computing platforms, such as the parallel computers soon to be deployed at Argonne and Oak Ridge National Laboratories.

Several features of Nek5000 make it highly suitable for Petascale science. The spectral element (SE) method, on which the code is based, yields rapid numerical convergence, which implies that simulations of small scale features transported over long times and distances incur minimal numerical dissipation and dispersion. In effect, accuracy per gridpoint is maximized. The code also features SE multigrid and has a parallel coarse-grid solver that scales to P > 10,000. Over the past year, several challenging applications have extended the computational and scientific scopes of Nek5000.

Magnetorotational Instabilities. A joint effort with University of Chicago astrophysicists to study magnetorotational instabilities (MRIs), believed to trigger some of the most energetic events in the universe, was chosen as the first external science application on the BG/L platform at IBM Watson. Our results indicate the existence of the MRI as well as, for the first time, the

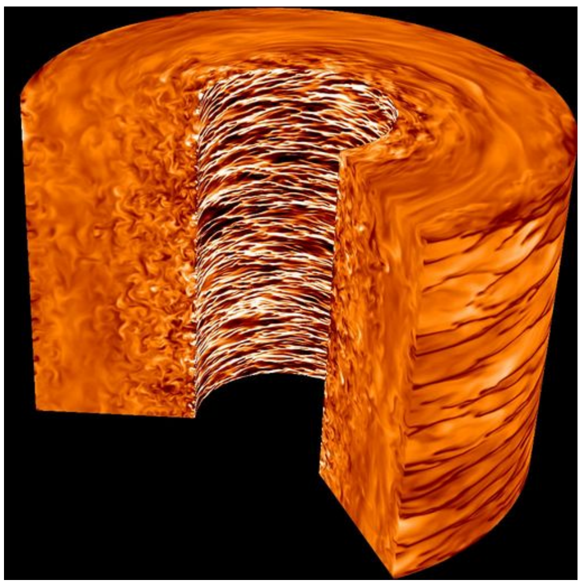

Fig. 1. Anglular momentum deviation in turbulent Taylor-Couette flow destabilized by the MRI. Simulation by Aleks Obabko, Paul Fischer, and Fausto Cattaneo.

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development of a turbulence-induced mean magnetic field capable of sustaining the MRI (Fig. 1).

Running the MRI simulations on 16K and 32K processors allowed us to explore the scalability of our approach and to identify critical areas to be addressed in the advance to Petascale. A particular achievement was the success the SE multigrid, which required only 6-8 iterations to compute pressure fields on 10^7 gridpoints. An important area requiring attention is post-simulation analysis, where parallel tools are clearly required. LLNL's VisIt code looks promising in this respect.

Reactor Thermal-Hydraulics. We have been using Nek5000 to study flow past wire-wrapped fuel pins in liquid-metal-cooled reactors. These simulations are a first step to the development of advanced computational fluid dynamics capabilities for thermal analysis of future reactors. Applied mathematics research is essential to realizing this vision, which aims to provide comprehensive analysis tools spanning from desktop to exaflop. Our initial simulations, supported through a 2007 INCITE award, have focused on large-eddy simulations of turbulent mixing in single-pin periodic arrays and bounded 7-pin bundles (Fig. 2). These results are being compared to existing experimental data. Petascale simulations at realistic pin-counts will be undertaken in 2008-09 and, properly validated, will serve to extend design data beyond the scope of past experiments.

Other Applications. Nek5000 has been successfully applied in a variety of applications by several university and laboratory groups outside of ANL. A series of recent computations by Vladimirova and Chertkov at LANL probed questions of self-similarity and universality in Rayleigh-Taylor turbulence. These computations are notable in that, at 340 million gridpoints, they are the largest Nek5000 simulations to date. Nek5000 has also been used extensively by the group of Loth at the University of Illinois, Chicago, to study transition to turbulence in vascular flows. Results of this collaboration were featured in the electronic edition of the NY Times (http://www.nytimes.com/packages/html/health/20070527_STROKEB_FEATURE/blocker.html) and will appear in the 2008 edition of *The Annual Review of Fluid Mechanics.*

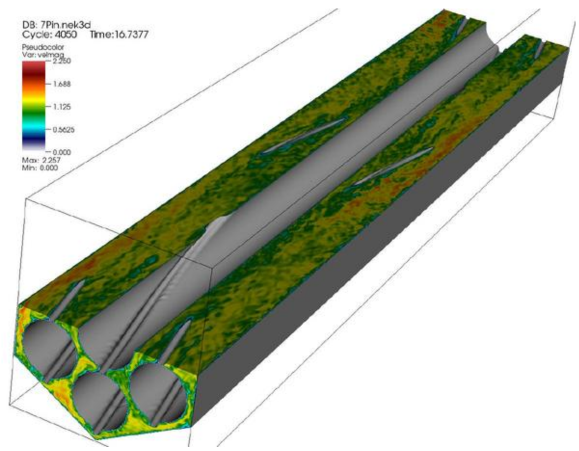

Fig. 2. Turbulent velocity field in a 7-pin bundle with wire-wrap spacers computed on ANL's BG/L using 132,000 elements of order N=7.

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