High-Order Methods for Turbulent Transport in Science and Engineering.

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Executive Summary

Our research focuses on development and deployment of advanced numerical algorithms for the simulation of turbulence in science and engineering. The principal vehicle for this work is the open-source code, Nek5000, developed by the PIs, which employs high-order spectral element discretizations and which strong scales to millions of cores. Nek5000 is used by hundreds of researchers around the world on leading edge HPC platforms. Current projects at UIUC include multiphase compressible turblence, dispersal of pollutants in the ocean, sediment transport in bifurcating streams, film cooling in turbines, turbulent combustion in IC engines, thermal transport in particle accelerators, and wind- and wave-driven energy production.

Blue Waters simulations in 2015-2016 will be driven by UIUC graduate students Pedro Bello-Maldonado, Som Dutta, Anne Goering, Li Lu, and Ketan Mittal. A rough breakdown of time requirements (in node hours) for each project and researcher is given below.

Pedro Bello-Maldonado	Scalable solvers	10,000
Som Dutta	Sediment transport	50,000
Paul Fischer	Application development and support	30,000
Anne Goering	Enhanced thermal transport	60,000
Li Lu	Compressible multiphase turbulence	30,000
Ketan Mittal	Free-surface turbulence	60,000

Proposed Simulations

Turbulent transport is the principal driver for many processes in physics, engineering, geosciences, and biology. Examples include the in-fall of matter into black holes, combustion in automotive and aerospace applications, sediment and pollutant transport in rivers and oceans, and atherogenesis in arterial blood flow. Our objective is to address these questions through direct numerical (DNS) and large-eddy (LES) simulation of turbulent flow by solving the governing Navier-Stokes and associated transport equations. Current simulations within our group are addressing a variety of questions relating to turbulent transport in engineering sciences.

The first project is analyzing mechanisms for sediment transport in bifurcating rivers. Experimental evidence indicates that a disproportionate amount of near-bed sediment is directed into side channels when streams bifurcate, which ultimately alters the flow dynamics and leads to potential blockage of the side channel. Investigations into this effect date back almost a century, but the dynamics of the process have yet to be clearly identified.

A second project is looking at heat transfer enhancement in cooling passages by using wire coil inserts. Experiments and simulations have indicated that up to a four-fold increase in the heat transfer coefficient for optimally-sized inserts. Our objective is to understand the fundamental enhancement mechanisms in order to aid in the design process and to predict off-design behavior.

We are also investigating compressible multiphase turbulence for a variety of applications in turbine and internal-combustion engines. This work entails significant development efforts in Nek5000 and we do not anticipate many full production runs on Blue Waters for this project until the end of the year.

Free-surface turbulence is another question of interest. One of the applications is in the sediment transport case described above. Near-bed sediment transport is driven by secondary flows that are governed by far-field pressure gradients. The pressure distribution for open channels differs significantly from closed channels, so support for free-surface turbulence is of primary importance.

Methods

Our turbulence simulations are based on the open-source spectral element code, Nek5000 [2]. The spectral element method (SEM) is a domain-decomposition approach in which the solution is represented by tensor-product polynomials on individual bricks that are assembled to cover the entire domain. The bricks are typically curvilinear, which allows accurate representation of the geometry. The local tensor-product structure allows low-cost and low-storage matrix-matrix product-based operator evaluation so that high-order polynomials may be used with almost no overhead. The SEM thus yields minimal numerical dissipation and dispersion at low cost, which is ideal for simulation of turbulent flows in complex domains. Nek5000 has been recognized with a Gordon Bell prize in HPC [3] and has scaled beyond a million MPI ranks.

Why Blue Waters

Blue Waters provides the computational power and the relatively short queue times to quickly turn around large-scale turbulence simulations. This capability is critical, particularly in the early development stages of the project when we first start to explore resolution requirements and mesh sensitivity. The process is interactive and would be significantly hampered by slow turn-around times.

References:

[1] Fischer, P., J. Kruse, J. Mullen, H. Tufo, J. Lottes, and S. Kerkemeier, (2008), NEK5000: Open source spectral element CFD solver, https://nek5000.mcs.anl.gov/index.php/MainPage

[2] H. M. Tufo and P. F. Fischer, "Terascale Spectral Element Algorithms and Implementations" Gordon Bell Prize paper, Proc. of the ACM/IEEE SC99 Conf. on High Performance Networking and Computing. IEEE Computer Soc., CDROM (1999).