HIGH-ORDER METHODS FOR TURBULENT TRANSPORT IN ENGINEERING AND GEOSCIENCES

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EXECUTIVE SUMMARY:

We describe simulation of two cases of turbulent flows. The first addresses sediment transport in bifurcating rivers and channels. The second provides input to system design codes for energy co-generation in industrial plants. The simulations are based on the scalable open-source code Nek5000, which employs minimally dispersive spectral element discretization. Results to date shed light on the physics of observed sediment deposition behavior in bifurcating channels.

INTRODUCTION

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 (formation of fatty deposits on arterial walls) in arterial blood flow. Our objective is to address these questions through direct numerical and large-eddy simulation of turbulent flow by solving the governing Navier–Stokes and associated transport equations. The open problems are as varied as the associated geometries and are challenging because of the range of scales present in turbulent flows at high Reynolds numbers (i.e. high speeds).

This project focuses on two topics from civil and mechanical engineering. The first project addresses sediment transport in bifurcating rivers. It has been observed that when a stream divides between a main branch and a side channel, a disproportionate amount of the near-bed sediment is often directed into the side channel, which can ultimately alter the flow dynamics and cause blockage of the side channel. Experiments investigating this effect date back almost a century, but the dynamics of the process have yet to be clearly identified.

The second project aims to construct fundamental building blocks for analysis of turbulent flow losses in energy co-generation systems. Patera's group at MIT developed reduced-order models for thermal-fluids systems with provable error bounds. These models reduce complex nonlinear partial differential equations to low-dimensional ordinary differential equations that can be solved on a laptop or a phone. The models, however, require high-fidelity baseline computations at a few points in the originating state space. Industrial co-generation systems involve many piping components (e.g., orifices, junctions, and elbows) and are of such complexity as to be intractable, even on the world's fastest computers. Fortunately, low-dimensional models permit assembly of the simulation results for individual piping components, each of which is within our grasp on platforms such as Blue Waters. Using a map of the response of each component, coupled with rigorous reduced-order models, it will be possible to design complex systems with confidence at low cost.

METHODS & RESULTS

Our turbulence simulations were based on the open-source spectral element code Nek5000 [1]. 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 was recognized with a Gordon Bell prize in HPC [2] and has scaled beyond one million MPI ranks.

For the sediment transport simulations, we built a sequence of meshes that followed the original experimental investigations [3] and commenced with a parameter study examining a range of flow splits and Reynolds numbers. In addition to turbulent flows, we analyze laminar cases in order to understand secondary flow mechanisms (boundary layer flows driven by external pressure gradients) that might dictate near-bed transport. Our first set of simulations investigated the effects of the channel flow split distribution (e.g., 85% in the main branch, 15% in the side) on the flow patterns downstream of a 90° bifurcation at Reynolds number Re=7,000. Fig. 1 shows the low-speed sections in the flow (blue) that yielded longer particle residence times and greater likelihood for bed deposition. The sediment transport problem requires sophisticated tracking algorithms to capture the physics of low-density particulate transport. We developed a parallel particle tracking routine that is stable for all Stokes numbers. It uses hash tables and fast generalized all-to-all exchanges to rapidly migrate particles to their host processors. We are currently testing the particulate physics on canonical problems that yield known particle distributions.

For the co-generation project, we will simulate flow through a pipe section with a hole in the side. The initial computational domain will consist of 60,000 elements of order 10, corresponding to 60 million gridpoints and 240 million degrees of freedom to be determined at every time step. The run time for each data point in the parameter space will be approximately 30 hours on 8,192 cores. In the target device, the pipe acts as a plenum for low-speed distribution of product into a large mixing tank. The first set of computations will yield pressure and flow relationships over a range of inlet/outlet pressure pairings. We will also investigate the sensitivity of the results to hole shape (taper, chamfer, etc.).

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.

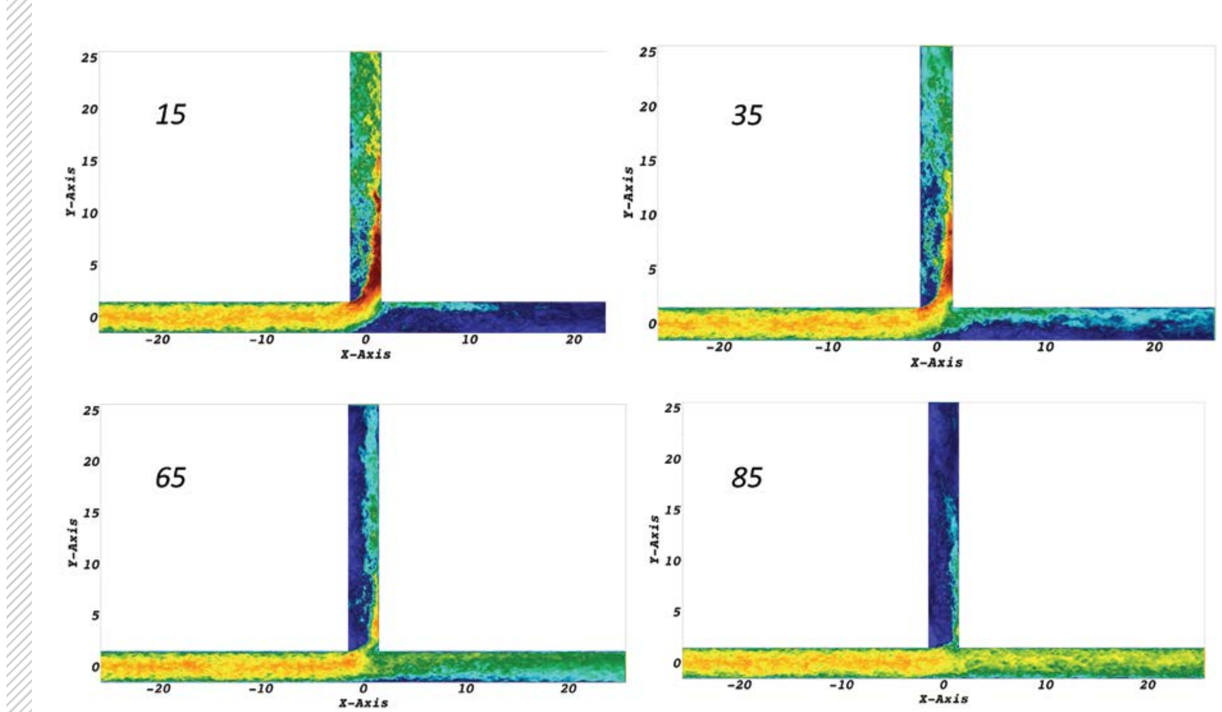

FIGURE 1: Nek5000 simulations of turbulent flow patterns at z=.05 H, Reynolds number 7,000, for main-channel flow percentages ranging from 15% to 85%, with low velocities in blue and high velocities in red. Biased velocity distributions are evident in both the main and side channels. [Simulation by Som Dutta]