NUMERICAL METHODS AND SOFTWARE FOR COMPUTATIONAL FLUID DYNAMICS, NEK5000

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EXECUTIVE SUMMARY

Complex turbulent flows are one of the most important types of flows and are prevalent in both natural and built environments. We describe here simulations of two cases of turbulent flows under complex boundary conditions. The first addresses flow over biofilms and similar natural wall roughness. The second simulates sediment transport in bifurcating rivers and channels. These simulations are based on the scalable open source code Nek5000, which employs minimally dispersive spectral element discretization. Results from the biofilm simulations shed light on the interaction of the biofilm with the flow. Results from the flow at the bifurcation shed light on the dynamics of the flow near the bottom of a channel.

RESEARCH CHALLENGE

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 our research 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).

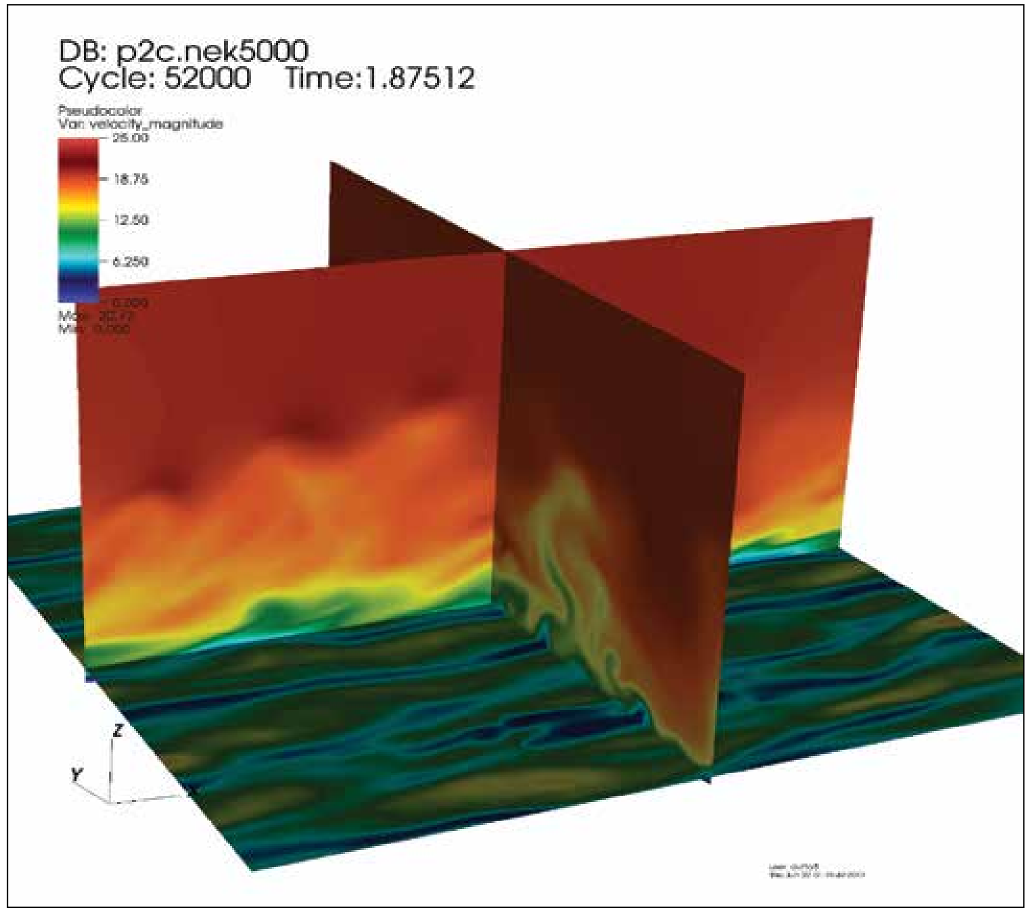

Figure 1: Instantaneous velocity magnitude at three orthogonal planes. The plane near the bottom of the channel shows the interaction of the flow with the biofilm patches, resulting in higher number of regions of low-velocity magnitude (streaks). One can also observe the effect of the biofilm on the flow, with relative increase in vortex shedding in the wall-normal direction.

The first project studies flow and fine particle transport over biofilms. Biofilms, in the form of microbial communities, serve as a key component in controlling carbon and nutrient cycling in freshwater systems. These microbial communities function as the coupling between physical and biological processes. They have a significant impact on a stream's hydrodynamics and influence the amount and lability of carbon exported downstream. Most research efforts to date have relied on the use of experimental analysis to understand how biofilm growth affects the flow hydrodynamics and fine particle transport [1]. None of the studies, however, had the spatial and temporal resolution to unravel the interaction between the biofilm structure and the flow, and its effect on fine particle transport. Thus, we conducted Direct Numerical Simulation (DNS) of the flow over biofilms, with the structure of the biofilm provided by experiments that measured the benthic biofilm using an Optical Coherence Tomography microscope. Due to the highly irregular structure of the biofilm bathymetry, new methods for generating the computational mesh were developed.

The second project addresses 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 [2,3]. High-resolution Large Eddy Simulations were conducted for flow and sediment transport at idealized experimental scale bifurcations.

METHODS & CODES

The turbulence simulations were based on the open-source spectral element code Nek5000 [4]. 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 [5]. 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. In the simulations with sediment (or fine particle) transport, the particles have been modeled as Lagrangian point particles using a novel semi-implicit timestepping scheme developed to simulate polydisperse particles accurately [6]. For the biofilm problem, the measured biofilm bathymetry data were smoothed while keeping the general structure intact, which was then used to generate the computational mesh. For the first time, spectrally accurate DNS simulations were conducted for a channel with complex natural roughness, and this was possible due to development of sophisticated mesh smoothing algorithms for Nek5000 [7].

RESULTS & IMPACT

DNS of the flow over the biofilm, with a bulk Reynolds number of 8,000, was conducted using about 200 million computational points. Initial results show the interaction of the flow with the biofilm patches, resulting in a higher number of regions of low-velocity magnitude (streaks—see Fig. 1). One can also observe the effect of the biofilm on the flow, with a relative increase in vortex shedding in the wall-normal direction. As we are conducting the study with "real roughness," the results will also have an impact on the study of flow over different kinds of roughness, which is important for mechanical and aerospace engineering applications.

The channel bifurcation cases have been simulated with about 250 million computational points; the Reynolds number of the flow is 25,000. One can observe that most of the flow near the bottom enters the side channel even though the total flow is equally divided between the two channels. This clearly hints at the mechanism for the sediment near the bottom to preferentially enter the side channel.

WHY BLUE WATERS

The study of flow in environmental fluid mechanics requires computational resources with sustained computing power at an unprecedented scale. Simulations have been conducted for up to 296 million computational points, with the code scaling strongly up to 32,768 MPI (message passing interface) ranks. Without access to Blue Waters, completing the study within a realistic timeframe would be impossible. In addition, since visualization of a phenomenon is an effective way to understand and explain its mechanics, we will work with Blue Waters project staff to create animations of the phenomena using data from the simulations.

PUBLICATIONS AND DATA SETS

Dutta, S., P. Fischer, M.H. Garcia, Large Eddy Simulation (LES) of flow and bedload transport at an idealized 90-degree diversion: insight into Bulle-Effect in *River Flow 2016,* CRC Press (2016).