HIGH-ORDER METHODS FOR TURBULENT TRANSPORT IN ENGINEERING AND GEOSCIENCES

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EXECUTIVE SUMMARY

Turbulent flows are prevalent in both natural and engineered environments; understanding them provides insight into the transport and mixing processes in a variety of systems. Here, we describe two ongoing turbulence simulation projects based on the scalable open-source spectral element code Nek5000. The first study explores the effect of biofilms on turbulent transport of fine-scale particles. Using measured biofilm morphology and new particle-tracking capabilities, these simulations have indicated mechanisms through which the structure of the biofilms influence the transport of fine particles and nutrients. The second project develops a scalable overlapping mesh method for high-fidelity simulations of turbulence in complex industrial and natural systems. In the development of this new capability, we have simulated turbulence in several configurations involving complex static and moving meshes.

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, the combustion in automotive and aerospace applications, sediment and pollutant transport in rivers and oceans, and atherogenesis in arterial blood flow. Our objective is to develop robust algorithms that can address research questions through direct numerical and large-eddy simulation of turbulent flows 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., at high speeds).

As mentioned, the first project studies the 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 those studies, however, had the spatial and temporal resolution to unravel the interaction between the biofilm structure and the flow, or the 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, we developed new methods for generating the computational mesh.

The second project is geared toward developing a scalable overset mesh method for large-scale high-fidelity turbulent simulations in complex geometries. We have developed the methodology to address problems that either have complicated meshes, involve disparate spatial scales, or have moving boundaries that would require the remeshing of standard conforming meshes.

METHODS & CODES

The turbulence simulations were 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 [3]. 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. 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. We conducted for the first time spectrally accurate DNS simulations for a channel with complex natural roughness. This was possible because of the development of sophisticated mesh-smoothing algorithms for Nek5000 [4]. For the second project, we used a recently developed method known as NekNek that has proven the validity of the overset grid method in context of SEM [5]. This new algorithm has been further developed and tested at scale on Blue Waters for large complex industrial problems [6].

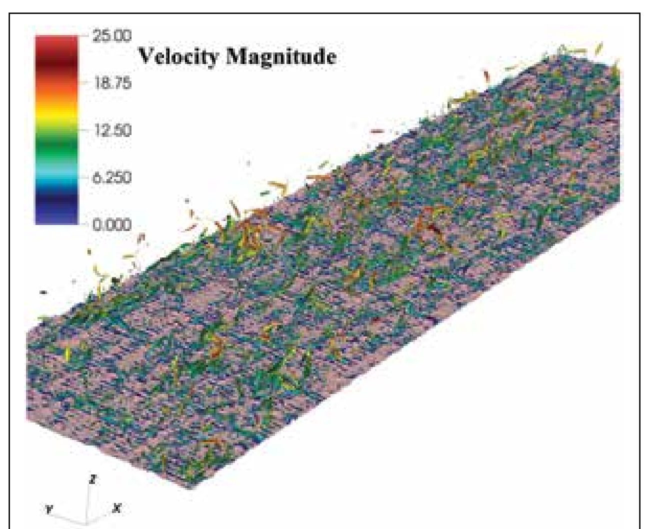

Figure 1: The image shows the coherent turbulent structures in the flow caused by the biofilm. Apart from the hairpin vortices, one may observe the vorticial tubes formed behind the roughness elements, which are absent in the case of the smooth bed. The vorticial structures have been colored using the magnitude of velocity.

RESULTS & IMPACT

We conducted simulations of the flow over biofilm with a bulk Reynolds number of 8,000 with mesh resolutions ranging from 20 million to 200 million grid points. The number of points depended on the details with which the biofilm morphology was captured. The results show the coherent turbulent structures in the flow caused by the biofilm (Fig. 1). Apart from the hairpin vortices, one may observe the vorticial tubes formed behind the roughness elements, which are absent in the case of a smooth bed. This vortex formation results in a relative increase in the turbulence kinetic energy near the bed. Applicability of the current study goes beyond biofilms, as the methodology developed to simulate the flow over the biofilms could be utilized for any kind of natural surface roughness encountered in industrial and aerospace engineering applications.

For the second study, we simulated several turbulent flows to test the applicability of NekNek to complex industrial problems. The cases reported here include a jet flowing into a tank (Fig. 2), which is an idealized version of a setup encountered across different industries. We can observe that the domain has been decomposed into two subdomains, orange and black, with orange accounting for the incoming jet and the black for the rest of the domain. The results showed appreciable agreement among simulations with Nek5000 and NekNek, with around 20% reduction in computation cost. Scaling studies with the new NekNek code indicate that it retains the good strong-scale capabilities of the native Nek5000 [6].

WHY BLUE WATERS

The two studies we have reported here not only have large-scale computation requirements, but they also require fast turnaround times for the simulations, especially for the second study, in which we are testing a range of setups. This requires access to a dedicated petascale high-performance computing system, and Blue Waters fits that bill perfectly. We have conducted simulations using up to 296 million computational points, with the code demonstrating linear speed-up for this problem out to 32,768 MPI ranks. Since visualization of fluid flow is important to understanding its mechanics, we also work with Blue Waters project staff to create animations of the phenomena using data from the simulations.

PUBLICATIONS & DATA SETS

Mittal, K., and P.F. Fischer, Mesh smoothing for spectral element method. *J. Scientific Computing*, accepted for publication (2018).

Mittal, K., S. Dutta, and P.F. Fischer, Nonconforming Schwarz–Spectral element methods for incompressible flow. *Parallel CFD2018* (Indianapolis, Ind., May 14–17, 2018).

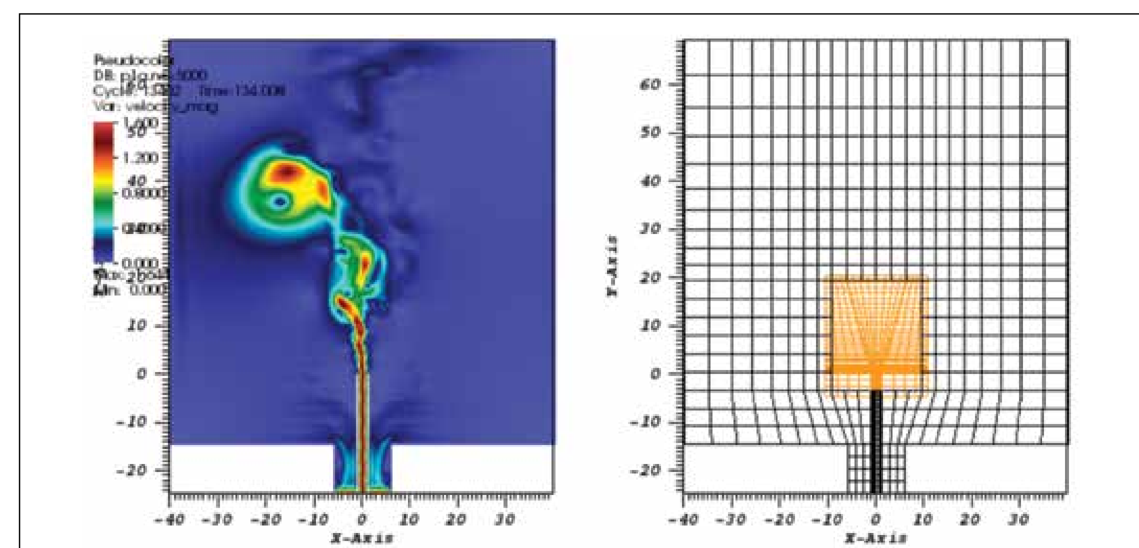

Figure 2: The figure shows velocity magnitude from a NekNek simulation of a turbulent jet entering a container. It also shows the two subdomains (orange and black) decomposed from the global domain. Adopting NekNek allows a reduction of the computational points required to simulate the problem.