

# High-Order Methods for Turbulent Transport in Engineering and Geosciences.

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## Executive Summary

We describe two ongoing turbulence simulation projects. The first addresses sediment transport in bifurcating rivers and channels. The second is about building capacity to conduct large-scale high-fidelity turbulent simulation for complex industrial systems, with a minimum turnaround time. The simulations are based on the scalable open-source code, Nek5000, which employs minimally-dispersive spectral element discretizations. For the first project, the results to date have shed light on the physics of observed sediment deposition behavior in bifurcating channels. As part of the second project, methodologies have been developed that have lowered the pre-processing time required for conducting high-fidelity turbulent simulations under complex geometrical settings.

## 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 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. The open problems are as varied as the associated geometries and are challenging because of the range in scales present in turbulent flows at high Reynolds numbers (i.e., high speeds).

Our current Blue Waters simulations are focused 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, it is often the case that a disproportionate amount of the near-bed sediment is 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 [1], but the dynamics of the process have yet to be clearly

identified. For this project we have also developed a semi-implicit Lagrangian particle algorithm, that could be used for efficiently modeling transport of poly-disperse particles.

The second project aims to build fundamental building blocks in order to reduce the pre-processing time for analysis of turbulent flow under complex geometrical settings. Currently the work is being done in collaboration with GE, and is geared towards analysis of complex turbulent flow through gas turbines, like the one used in the airplanes. The prime motivation for reducing the pre-processing time is to make high-resolution turbulent simulations more amenable to industrial co-design projects. Accurate simulation of turbulent flows in complex geometries require high-quality computational meshes that require time to build. Though, often the design process of a component (e.g. turbine blade) involves multiple changes, before the final version is approved. This massively increases the pre-processing time on the computational fluid dynamics (CFD) analysis front. The tools being developed for this project will help reduce the pre-processing time substantially. The additional goal of this work was to understand incompressible flow phenomenon over low-pressure turbine blades. The aforementioned analysis will eventually serve as the basis for other sophisticated analysis in the future, such as the compressible turbulent flow.

## Methods and Results

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.

For the sediment transport simulations, we have built a sequence of meshes that follow the original experimental investigations [1] and commenced with a parameter study examining a range of flow splits and Reynolds numbers. In addition to turbulent flows, we are looking at laminar cases in order to understand secondary flow mechanisms (boundary layer flows driven by external pressure gradients) that might dictate near-bed transport. Simulations investigate the effects of the channel flow split distribution (e.g., 65 percent in the main branch, 35 percent in the side) on the flow patterns downstream of a 90 deg. bifurcation for a range of Reynolds number 10 – 25000, and also for different diversion angles for Reynolds number of 25000. The accompanying figure (see fig. 1) shows velocity magnitude at a height 5 percent from the bottom for two different diversion angles (30 and 150 deg.) at Reynolds no. of 25000.

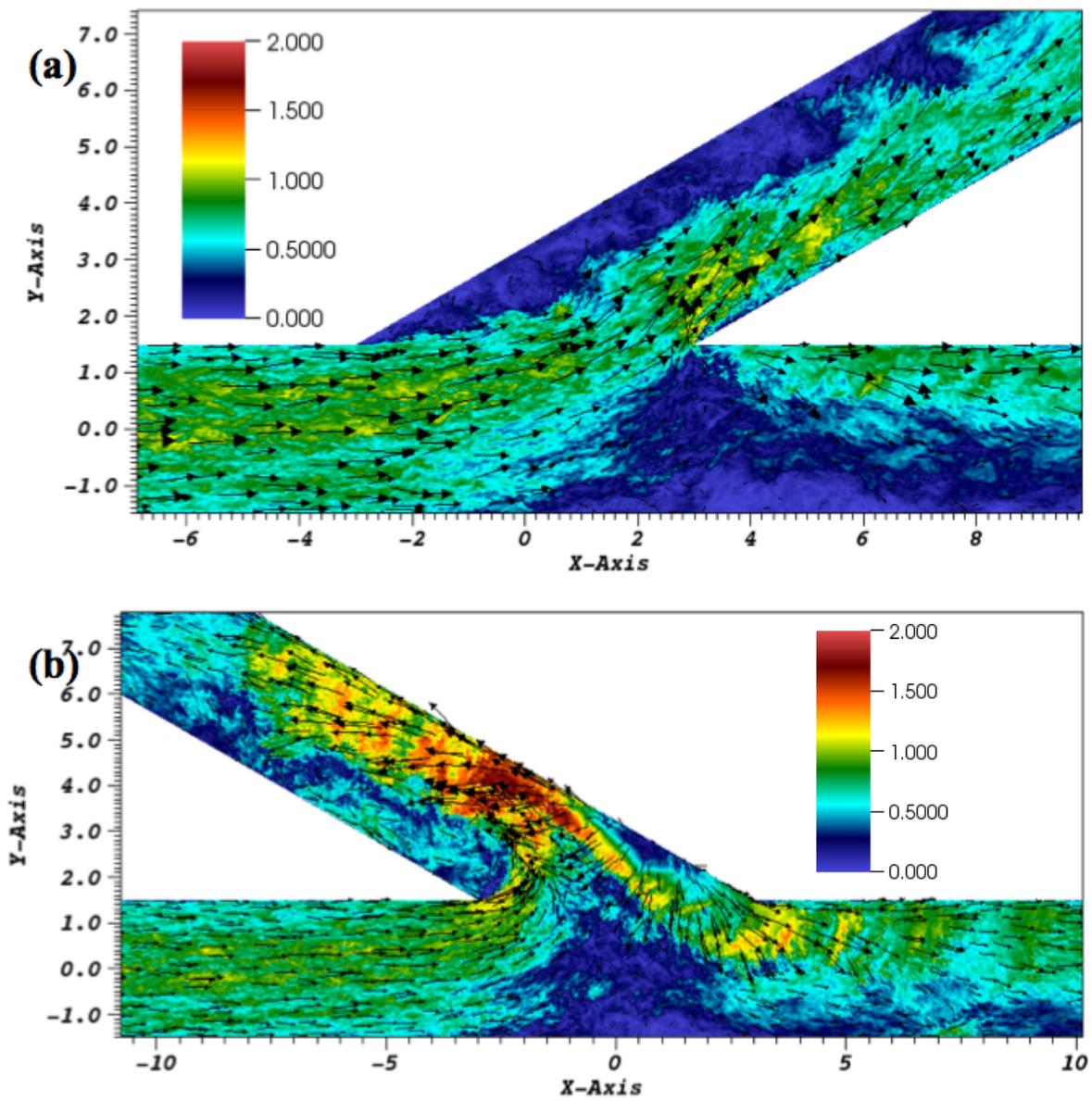


Figure 1: Velocity-magnitude of the turbulent flow at  $z = .05H$ , Reynolds number 25000, for diversion angle of (a) 30-degree and (b) 150-degree. Total flow is equally divided between the two channels after diversion. (Simulation by Som Dutta, UIUC.)

It shows that even though the total flow is almost equally divided between the two branches of the bifurcation, near the bottom most of the flow enters the lateral-channel. This pattern shows up irrespective of the angle of diversion, and causes most of the sediment traveling near the bed to enter the lateral channel [4]. The computational points used for the cases with Reynolds no. 25000 is around 250 million, which were simulated on upto 32768 mpi ranks; making these simulations computationally intractable for anything but petascale HPC platforms like Blue Waters. The sediment transport part of the simulations requires sophisticated tracking algorithms to capture the physics of low-density particulate transport. We have developed a parallel particle tracking routine that is stable for all Stokes numbers [5]. It uses hash tables and fast generalized all-to-all exchanges to rapidly migrate particles to their host processors. Currently the algorithm has been used to simulate upto 200,000 particles, and ongoing developments would allow simulation of millions of particles efficiently.

For the simulations related to the low-pressure turbine blades. Tools have been developed, that have reduced the pre-processing (mesh-building) time substantially for complex meshes. Apart from building the mesh, the tools developed carryout functions like, mesh-smoothing, mesh skinning (for adding boundary-layer elements) etc. One of the first component simulated was the Low Pressure Turbine blade LPT-106, in a doubly periodic domain discretized into 23 million computational points. Fig. 2 shows the velocity magnitude contours for the flow at Reynolds number of 60,000. The obtained data was time and spatially averaged to determine the pressure distribution and shear stress at the blade surface, and wake loss behind the blade.

Calculations were also done to study how cooling effectiveness at the trailing edge of turbine blades is affected by the lip thickness of the trailing edge cutback. These calculations were performed on a pseudo three dimensional domain discretized into 17 million computational points.

## 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.

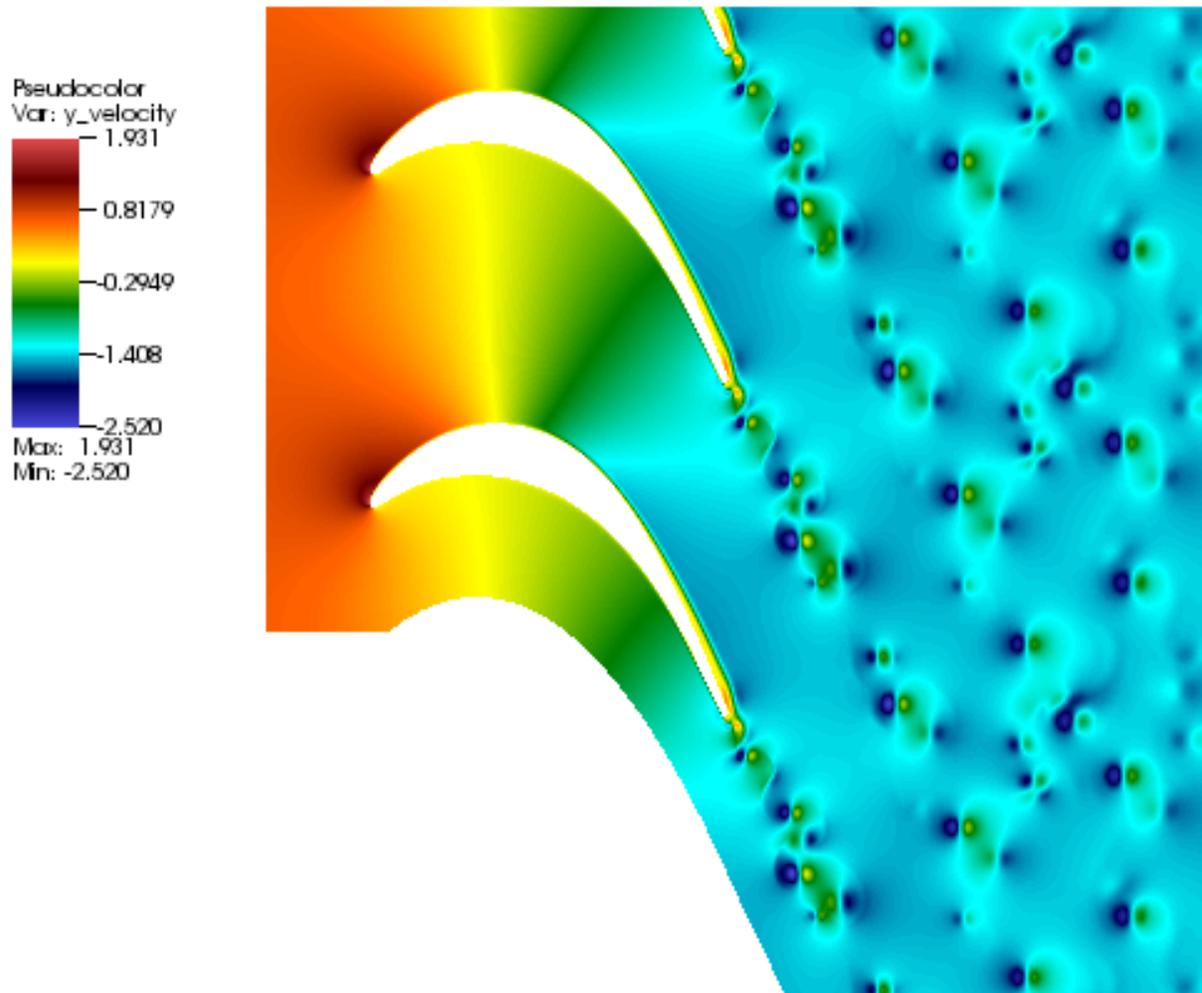


Figure 2: This plot shows the velocity magnitude contours for incompressible flow at Reynolds number of 60,000 over a low pressure turbine blade (LPT-106). The domain was discretized into 23 million computational points. In the current figure, the planar-averaged vertical (wall-normal) component of velocity has been plotted. (Simulation by Ketan Mittal, UIUC.)

## References:

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