ANL/ALCF/ESP-13/12

Petascale Direct Numerical Simulations of Turbulent Channel Flow

ALCF-2 Early Science Program Technical Report

Argonne Leadership Computing Facility

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prepared by
MyoungKyu Lee, Nicholas Malaya, and Robert D. Moser
University of Texas, Austin

May 7, 2013

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Project: Petascale Direct Numerical Simulations of Turbulent Channel Flow
Catalyst: Ramesh Balakrishnan

1 Executive Summary

This project is focused on utilizing the Petascale computing power of Mira to perform direct numerical simulations (DNS) of high Reynolds number turbulent wall-bounded flow in a channel. This DNS is aimed at developing a nearly complete understanding of the phenomena dominating wall-bounded turbulence, which is central to the energy losses inherent in transportation. The impact of such a development will likely be profound. Approximately 28% of US energy consumption is expended on transportation. This energy expenditure is due to the interaction between solid surfaces (of vehicles or pipes) and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. Since much of the drag in these flows is due to turbulent skin friction, much of this energy consumption is caused by wall-bounded turbulent shear layers.

Engineering developments to reduce drag and energy consumption are greatly impeded by the lack of accurate models of the turbulence phenomena involved. DNS at the Reynolds numbers proposed here and the subsequent analysis of the resulting data can provide the insights needed to develop such models, as well as new concepts for manipulating wall-bounded turbulence.

The central emphasis of this research is on reaching a sufficiently high Reynolds number to explore the physics that arise in the overlap region. The overlap region is where the viscous near-wall turbulence interacts with the outer-layer turbulences. This interaction is key to understanding high Reynolds number turbulent wall layers. To investigate this interaction, it is necessary that the Reynolds number be sufficiently high so that there is a substantial disparity in scale between the inner and outer layers. The results can then be extrapolated to arbitrary Reynolds numbers. Analysis of recent DNS of channel flow at $Re_\tau = 1000$ and 2000 indicated that $Re_\tau \approx 4000$ on a $12288 \times 1024 \times 9216$ grid might yield sufficient scale separation. Due to the substantial power of Mira, as well as software performance increases attained during this Early Science Project, the channel will be run at $Re_\tau \approx 5000$ on a $15360 \times 1536 \times 11520$ mesh. Given the mesh size, this is the largest scientific DNS ever conducted.

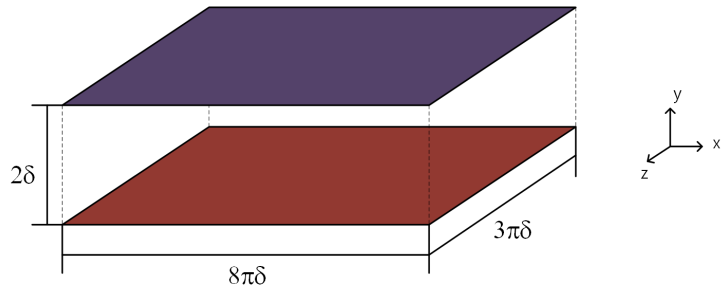

Figure 1: Diagram of the Channel DNS Geometry

2 Numerical Method

$$\frac{\partial u_i}{\partial t} = -\frac{\partial P}{\partial x_i} + H_i + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{1}$$

The incompressible 3D Navier-Stokes equations (**??**) are solved using the formulation of Kim, Moin and Moser. Their technique involves integrating evolution equations for the wall-normal vorticity ω_y and the Laplacian of the vertical velocity $\nabla^2 v$. Periodic boundary conditions are imposed in the streamwise and spanwise directions, while in the wall normal direction, no slip conditions are imposed at the walls. Fig. **??** details the system geometry. A semi-implicit, third-order Runge–Kutta/Crank–Nicholson scheme is used for the time discretization (Spalart *et al* 1991) The flow is driven by a uniform pressure gradient which is adjusted continuously to maintain a constant mass flux. In space, a Fourier spectral representation is used in the streamwise and spanwise directions. A B-spline collocation representation is used in the wall-normal direction to accommodate the non-uniform grid requirements while providing spectral-like resolution (Kwok 2001). The B-spline breakpoints (y_i) are stretched across the interval [-1,1] per

$$y_i = \sin\left(\frac{\alpha\pi}{2}\frac{(-1+2i)}{n-1}\right) / \sin(\frac{\alpha\pi}{2}). \tag{2}$$

Here, α is a stretching parameter (set to 0.97 to provide an appropriate near-wall resolution), and n is the number of breakpoints. The collocation-based differential operators are formed using the Greville abscissae, also called the Marsden–Schoenberg points, implied by these breakpoints.

The code is written in Fortran2003 and uses hybrid MPI/OpenMP parallelism. Fourier transforms are performed one direction at a time, using FFTW3. In addition, we utilize the new FFTW3.3 MPI API to accomplish the distributed memory transposes necessary at each step. Hand-made libraries are used for linear algebra, and B-splines of arbitrary order are generated with the GNU Scientific Library which uses the recursive relationship of de Boor. This code has

been ported and run on various large-scale machines on various architectures (TACC's Lonestar, Blue Waters, NCSA's Kraken, ALCF's Intrepid and Mira), and scales well on each system.

3 Technical Results

Analysis of recent DNS of channel flow at $Re_\tau = 1000$ and 2000 indicated that $Re_\tau \approx 4000$ on a $12288 \times 1024 \times 9216$ grid might yield sufficient scale separation. Due to the substantial power of Mira, as well as software performance increases attained during this Early Science Project, the channel will be run at $Re_\tau \approx 5000$ on a $15360 \times 1536 \times 11520$ mesh.

3.1 Spin-up

To increase the rate at which the large scale run reaches a statistically stationary state, we performed "spin-up" runs to step our simulation through higher resolution grids, until all essential scales are resolved. These spin-up runs are summarized in Table **??**.

Table 1: Parameters of channel DNS spin-up runs. N_x and N_z are numbers of Fourier modes, and N_y is number of collocation points. Δx^+ and Δz^+ resolutions are in terms of Fourier modes; Δy^+_{wall} and Δy^+_{CL} are the breakpoint spacings at the wall and centerline, respectively. T is the time span used to compute statistics. U_b is the bulk velocity, and L_x and h are the domain length in the streamwise direction and the channel half-height, respectively.

Name	N_x	N_z	N_y	Δx^+	Δz^+	Δy^+_{wall}	Δy^+_{CL}	TU_b/L_x
Coarsest	4096	3092	1024	30.68	15.24	0.104	14.91	≈ 0.88
Coarse	8192	4096	1536	15.34	11.50	0.068	9.94	≈ 0.53
Target	15360	11520	1536	8.18	4.09	0.068	9.94	≈ 10

3.2 Scaling

The code performs extremely well at scale. The communication benchmarks shown in Fig. **??** have been performed on as large as 32 racks. For our chosen problem size (8 racks), the parallel efficiency for a strong scaling problem is very nearly ideal, but even larger problem sizes have performed extremely well on Mira's interconnect.

Finally, benchmarks for a timestep of the entire codebase is shown in Fig. **??**. The codebase demonstrates excellent strong scaling across a large portion of the entire machine (32 racks). A more detailed discussion of these results will be presented at MiraCon2013.

3.3 I/O

In order to attain portable, high throughput I/O with rich metadata support, we use HDF5 for our restart needs. We have found that I/O is such a common task in turbulence simuations, and therefore have developed a higher level API for common restart requirements. This library, entitled , ExaScale IO (ESIO),

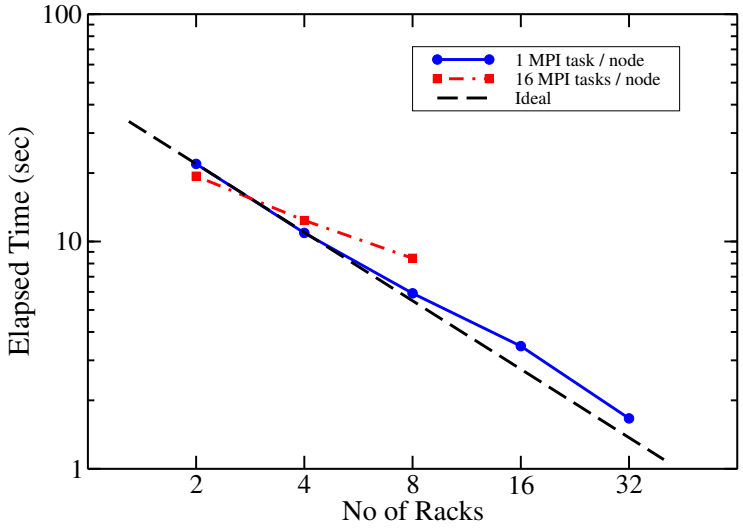

Figure 2: Strong scaling of the communication for the full problem size.

provides simple, high throughput input and output of structured data sets using parallel HDF5. ESIO is designed to support reading and writing turbulence simulation restart files but it may be useful in other contexts. The library is written in C99 and may be used by C89 or C++ applications. A Fortran API built atop the F2003 standard ISO_C_BINDING is also available.

For our DNS runs on Mira, ESIO is writing 1.8 TB in 444 seconds, at full scale (8 racks). This is a resonable write speed of approximately 4 GB/s, especially given the expected contention of at eight racks (1024 nodes$\times$16 tasks$*$ 8 racks $= 131,072$ writers) for the file system.

A restart must be written at least every 1000 steps, or about every three hours of simulation time. There will be at least of 250 restart files saved over the entire simulation. We allocated (as a safety factor) for the time required to read/write restart files to be approximately 5-10% of the total execution time, and in this case it is much less than this.

Nevertheless, we have observed far higher I/O write speeds in testing (peaks of 40 GB/s). As a result, we expect that significantly higher throughput can be attained, and expect to collaborate with ALCF Staff on this at MiraCon2013.

In addition, in late December and early January, during the porting of ESIO to Mira, we found several compiler compatibility issues between the ISO_C_BINDING standards and what was provided by IBM. Working with the ALCF staff identified a probable cause of this internal compiler error, namely that inappropriate fortran compiler scoping was at fault. In particular, an identically named (although different call pattern) function interface 'impl' using the iso_c bindings is producing the ICE. A workaround was demonstrated on a small piece of example code, by which renaming 'impl' to a unique string for

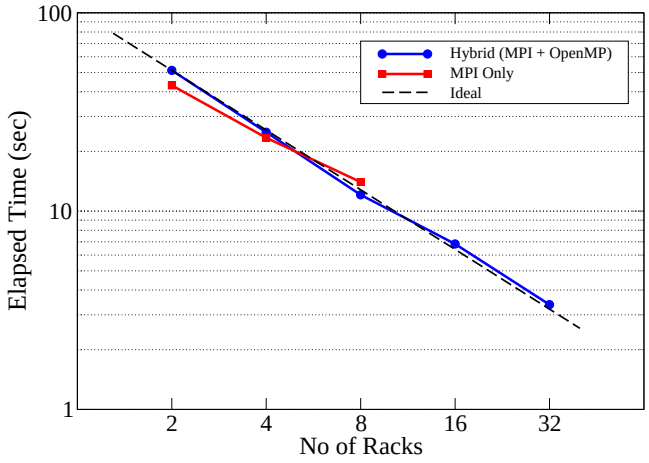

Figure 3: Strong scaling of a full timestep on Mira

every subfunction appeared to avoid the ICE. Thus, production runs were capable of utilizing this workaround, while simultaneously, on January 10th, 2013 PMR 57031,122,000 "XLF ICE on esio.F90" was submitted and confirmed by IBM.

3.4 Future Work

Future work will focus on automating job submission to maximize the time the application spends running. Additional work will focus on developing post-processing for the statistical quantities of interest. These can be developed in parallel with full production runs, and are not anticipated to delay the full project.

Estimating the convergence of statistics from the resulting simulation is critical to building confidence in the correctness of the codebase as well as the outputs of the simulation. However, turbulent velocity fields are correlated in time, so typical statistical sample estimates that rely on independent trials are biased. For this reason, we have developed methods that calculate the "effective sample size" of the statistics. This will be implemented in the codebase and provide an automated estimate of the remaining required runtime. The results of this work, accomplished using ALCF resources, will be the subject of an upcoming Physics of Fluids publication.

This project will transition to an INCITE2013 allocation in April. The process is expected to be continuous, with full scale production runs continuing

unabated.

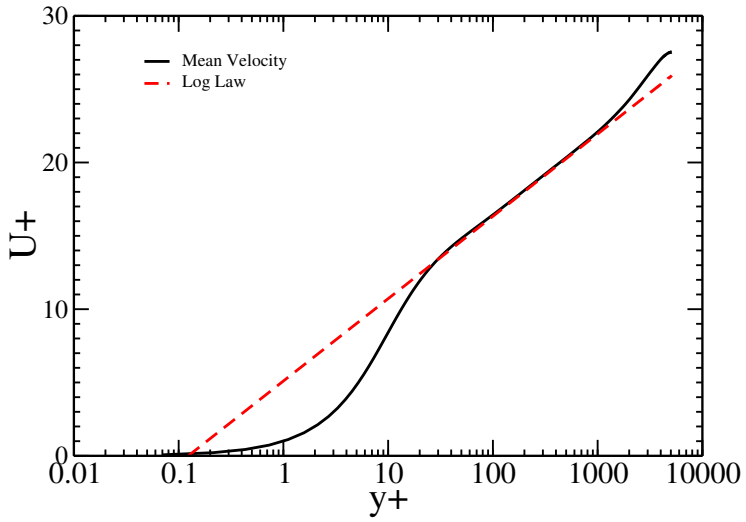

Figure 4: Mean velocity profile for $\mathrm{Re}_\tau \approx 5000$

4 Preliminary Scientific Results

Given the mesh size, this simulation is significantly larger than the 4096^3 homogeneous turbulence simulation (by a factor of ≈ 1.76). As a result, this simulation will be, to our knowledge, the highest resolution DNS ever conducted for scientific purposes.

However, the large scale simulation has not yet come to steady state. Therefore, the the simulation is not yet producing valuable statistical data. As a result, all observations about the field are extremely preliminary.

The mean velocity profile can be seen in Figure **??**. This plot demonstrates that the velocity profile does appear to be demonstrating logarithmic scaling with distance from the wall, as anticipated by theory. This is an early verification that the field is behaving as expected.

Given the wall-normal resolution, this simulation will provide an unsurpassed estimate for the Von Karman constant. Fig. **??** demonstrates a profile that appears to be flattening in the logarithmic region. While preliminary, the value appears to be converging upon a value of 1/.41. In statistically steady state, we have every reason to believe that this is the most precise calculation of the Von Karman constant ever conducted, either experimentally or via simulation.

4.1 Future Work

During the production runs, statistical estimators of various quantities of interest will be provided at `http://turbulence.ices.utexas.edu/`. This will already be of great value to the turbulence community. Furthermore, it must

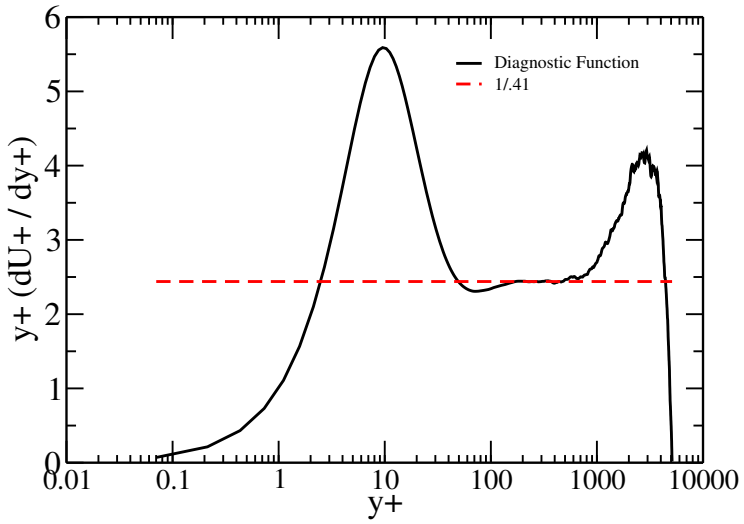

Figure 5: Karman constant estimate

be stressed that even after the completion of production runs, a great body of scientific work remains to be done. Once the simulations have been performed, the fields they generated can be used like an experimental facility to "measure" most any diagnostic quantity of interest. Scientific advances will come from repeated analysis of the simulation data to answer new questions and test hypotheses, by a number of researchers over a period of years. The most complete sequence of cases is for turbulent channels in the friction-Reynolds-number range $Re_\tau = 180 - 2000$, which now constitute the standard reference data set in the field and receive about 30-40 citations per year. As we supplementing these data with $Re_\tau = 5000$, we expect this will establish a reference data set that will remain useful for the turbulence research community for many years.

5 Work with ALCF Staff

During the course of this Early Science Project, we have worked with several members of the ALCF staff. Of particular note, we have dealt with Ramesh Balakrishnan extensively for both technical consulting on the codebase as well programmatic work. We also appreciate the help of Jeff Hammond for his assistance with the ICE Bug detailed in section **??**, and Kevin Harms for work related to disk space quotas and I/O in general.

Argonne Leadership Computing Facility
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 240
Argonne, IL 60439

www.anl.gov