Petascale Direct Numerical Simulations of Turbulent Channel Flow

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Contents

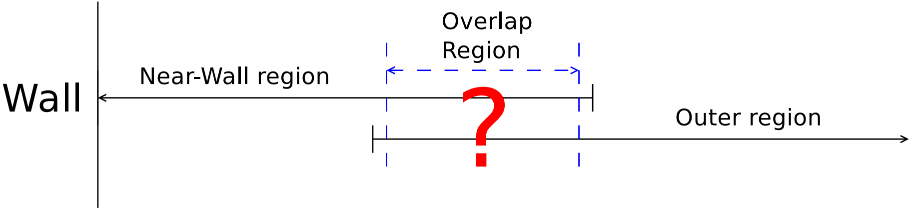
Project Overview

- Project Title
  - Petascale Direct Numerical Simulations of Turbulent Channel Flow
- Goal
  - Expanding our understand of wall-bounded turbulence
- Personnel
  - P.I. : Robert Moser
  - Primary Developer : M.K.Lee
  - Software Engineering Support : Nicholas Malaya
  - Catalyst : Ramesh Balakrishnan

Turbulent Flow

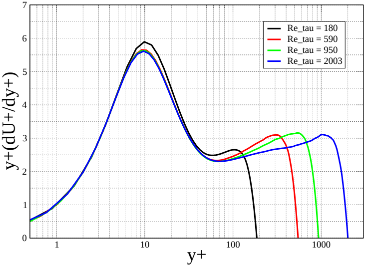
- We are living with turbulent flows.
  - Atmosphere
  - Transportation (Automobile, Airplane)
  - Blood flow in the heart
- Directly related with energy loss by drag of fluid motion
- Deterministic Chaos
  - Governing equation : Navier-Stokes equation
  - Analytic solution is unknown
  - Highly nonlinear / Unpredictable
  - Requires statistical approach
- "The most important unsolved problem of classical physics" by *Richard Feynman*

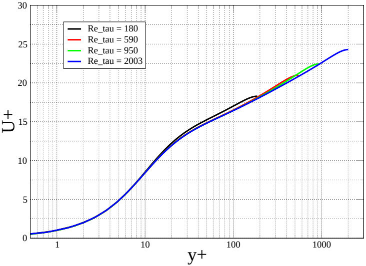
Overlap Region



- Connection between near-wall region and outer region
- Not understood as well as near-wall region

History



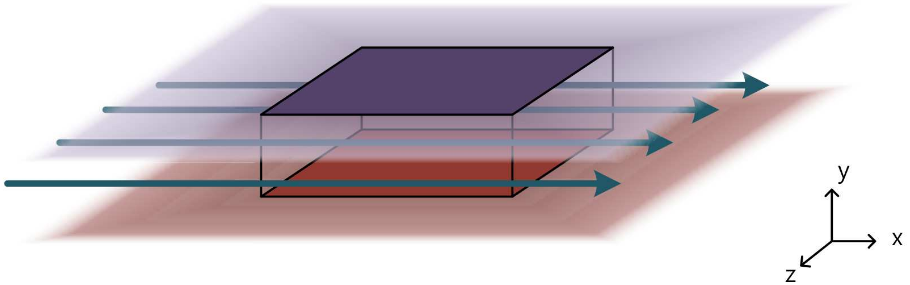


- $Re_\tau = 180$: Kim, Moin & Moser, 1987
- $Re_\tau = 590$: Moser, Kim & Mansour, 1999
- $Re_\tau = 940$: Del Álamo, Jiménez, Zandonade & Moser, 2004
- $Re_\tau = 2003$: Hoya & Jiménez, 2006

Computation of Overlap Region

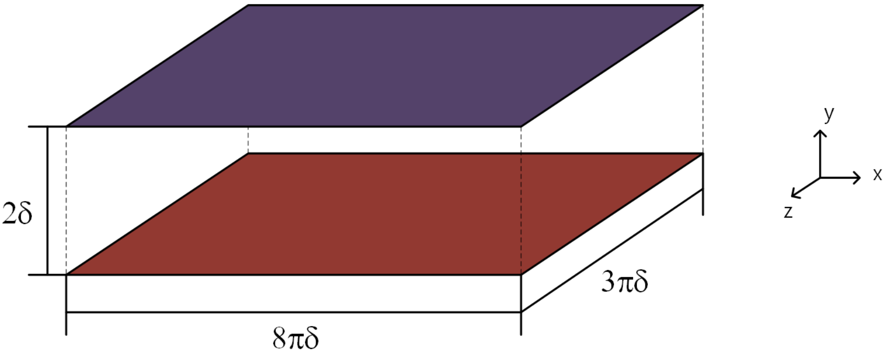
- High Reynolds(Re) number is required to obtain logarithmic layer.
- Even with existing channel flow DNS data at the high Re, $Re_\tau \approx 2000$, the region of log layer is small.
- To expand our understanding of log layer, DNS data at $Re_\tau > 4000 \sim 5000$ is required.
- Cost scales with Re^4
- Simulation at high *Re* is limited by computational power.
- **BG/Q enables us to simulate such a high *Re* flow**

Simulation Geometry



- Flow between two infinite parallel plates
- **$\mathrm{Re}_\tau \approx 5000$**
- Periodic boundary condition in streamwise / spanwise directions
- No slip, no mass flux boundary conditions at wall

Simulation Geometry



- Nx = 10,240 (Uniform) - DFT
- Ny = 1,536 (Stretched, denser near wall) - B-Spline
- Nz = 7,680 (Uniform) - DFT
- 242 Billion D.O.F.

Incompressible Navier-Stokes Equation

$$\frac{\partial u_i}{\partial t} = -\frac{\partial P}{\partial x_i} + H_i + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \qquad \frac{\partial u_j}{\partial x_j} = 0$$

where

$$H_1 = -\left(\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z}\right)$$

$$H_2 = -\left(\frac{\partial uv}{\partial x} + \frac{\partial v^2}{\partial y} + \frac{\partial vw}{\partial z}\right)$$

$$H_3 = -\left(\frac{\partial uw}{\partial x} + \frac{\partial vw}{\partial y} + \frac{\partial w^2}{\partial z}\right)$$

Formulation (Kim, Moin & Moser, 1987)

Applying Laplacian and Curl operator

$$\frac{\partial \omega_y}{\partial t} = h_g + \nu \nabla^2 \omega_y$$
$$\frac{\partial \phi}{\partial t} = h_v + \nu \nabla^2 \phi$$

where

$$\phi = \nabla^2 v, \qquad \text{At wall} \quad \omega_y = 0, \quad v = \frac{\partial v}{\partial y} = 0$$

$$h_g = \frac{\partial H_1}{\partial z} - \frac{\partial H_3}{\partial x}, \quad h_v = \frac{\partial^2 H_2}{\partial x^2} + \frac{\partial^2 H_2}{\partial z^2} - \frac{\partial^2 H_1}{\partial x \partial y} - \frac{\partial^2 H_3}{\partial y \partial z}$$

- Two equations in the same form
- No pressure term!!

Formulation (Spalart, Moser, & Rogers, 1991)

Time discretization : Low-Storage RK3 method

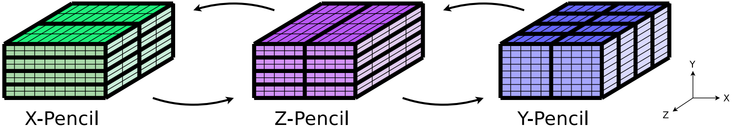
$$\begin{aligned}
\mathbf{u}' &= \mathbf{u}_n + \Delta t \left[L \left(\alpha_1 \mathbf{u}_n + \beta_1 \mathbf{u}' \right) + \gamma_1 N_n \right] \\
\mathbf{u}'' &= \mathbf{u}' + \Delta t \left[L \left(\alpha_2 \mathbf{u}' + \beta_2 \mathbf{u}'' \right) + \gamma_2 N' + \zeta_2 N_n \right] \\
\mathbf{u}_{n+1} &= \mathbf{u}'' + \Delta t \left[L \left(\alpha_3 \mathbf{u}'' + \beta_3 \mathbf{u}_{n+1} \right) + \gamma_3 N'' + \zeta_3 N' \right]
\end{aligned}$$

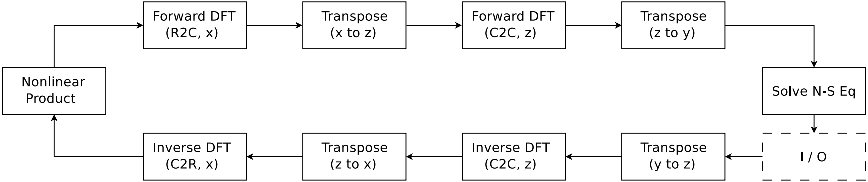
- Need only two additional fields
- L : Linear operator (Laplacian) $\rightarrow$ Implicit + Explicit
- N : Nonlinear Terms (h_g ,h_v) $\rightarrow$ Explicit

Simulation Process

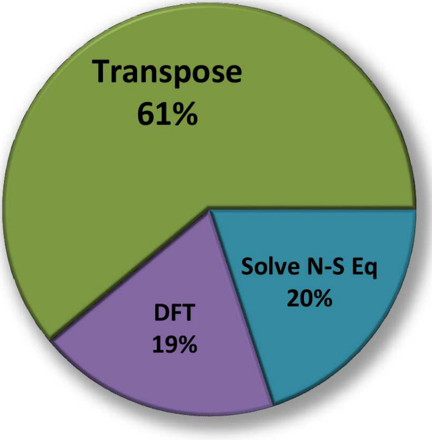
- Periodic boundary condtion in X-dir and Z-dir
  - Fourier Transform
  - $\partial/\partial x \rightarrow ik_x, \quad \partial/\partial z \rightarrow ik_z$
  - Ordinary differential equations in time
- h_g, h_v : Quadratic nonlinear terms
  - Computed in realspace
  - Dealiasing : require 1/2 additional grid points

Simulation Process - Pencil Decomposition





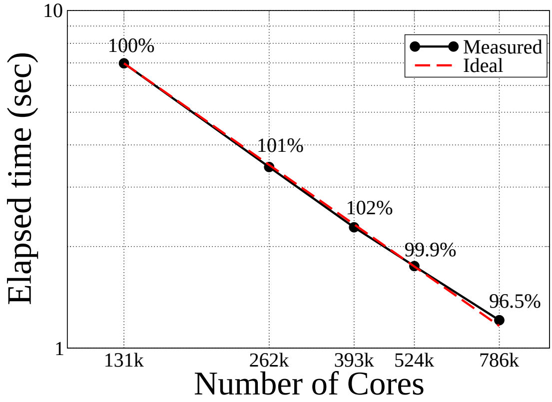
For one time step



* 8 Racks, 1 MPI task/node

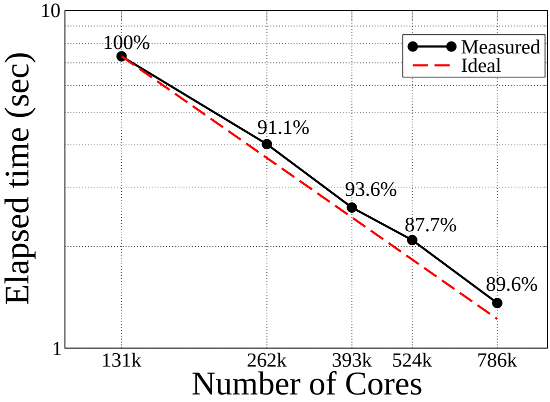
Solving Navier-Stokes Equation

- B-Spline for y dir derivatives
- $N_x = 18432, N_y = 1536, N_z = 12288$



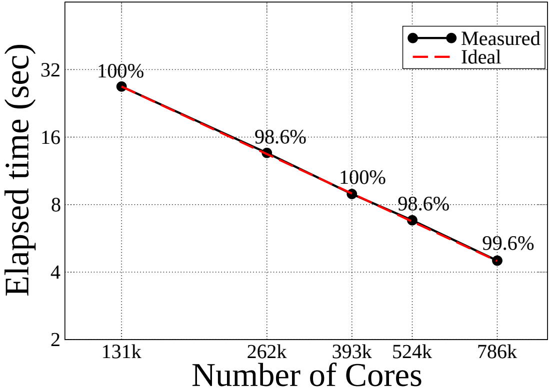
Discrete Fourier Transform

- FFTW 3.3
- $N_x = 18432, N_y = 1536, N_z = 12288$



Data Transpose

- FFTW 3.3 - MPI
- $N_x = 18432, N_y = 1536, N_z = 12288$



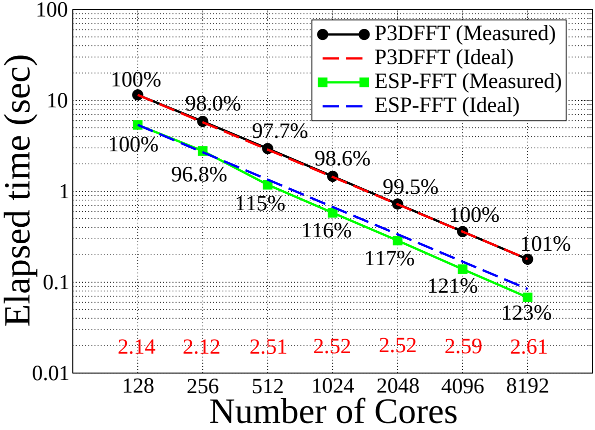
Comparison with P3DFFT

- parallel 3D FFT : Data transpose + FFT
- ESP-FFT
- P3DFFT 2.5.1
  - Most popular parallel 3D FFT library
  - Pencil decomposition
- Differences (P3DFFT / ESP-FFT)
  - Communication Pattern : Fixed / Various
  - Odd-Ball wavenumber : Stored / Removed
  - (Buffer) Memory requirement : $3\times$ / $1\times$
  - Threading capability : None / OpenMP (Data rearrangement, FFT)

* For benchmark, data is Fourier transformed in only x and z dir.

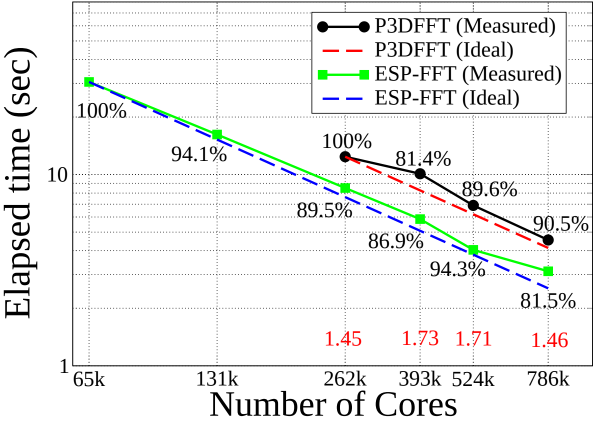
Comparison with P3DFFT (Small size)

- $N_x = 2048, N_y = 1024, N_z = 1024$



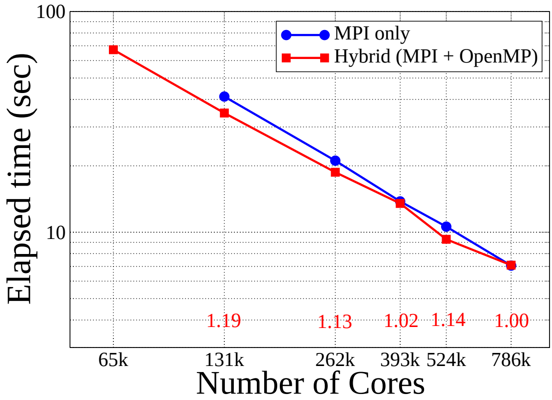
Comparison with P3DFFT (Large size)

- $N_x = 18432$, $N_y = 12288$, $N_z = 12288$

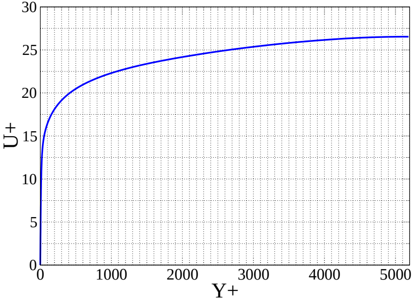


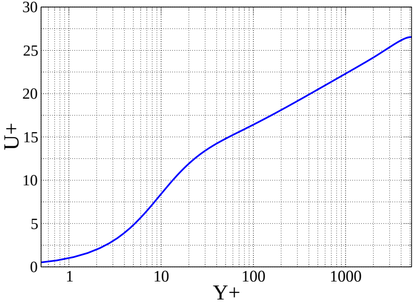
One full timestep

- $N_x = 18432, N_y = 1536, N_z = 12288$

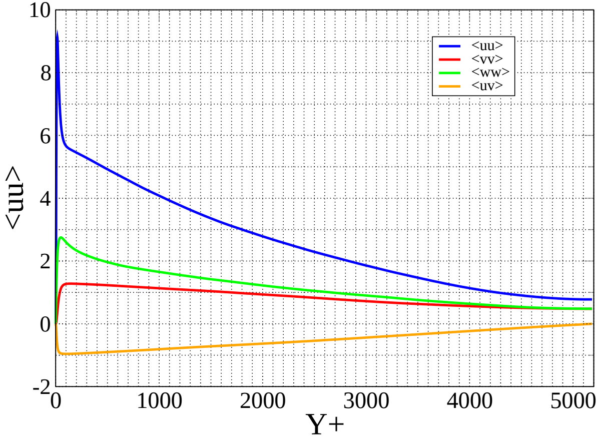


Mean Velocity Profile

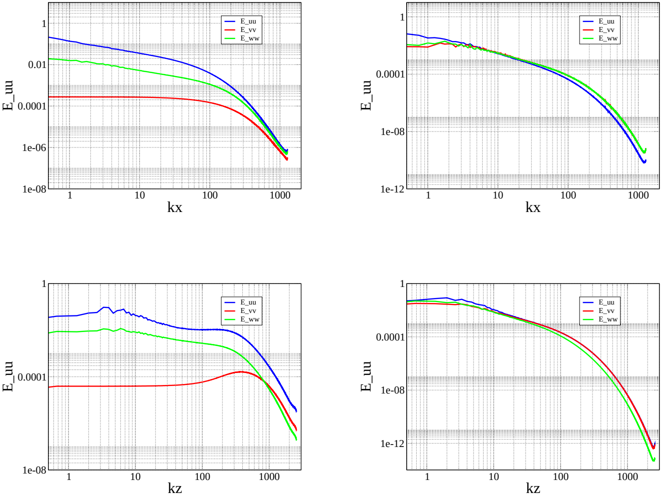




Variance & covariance of velocity components

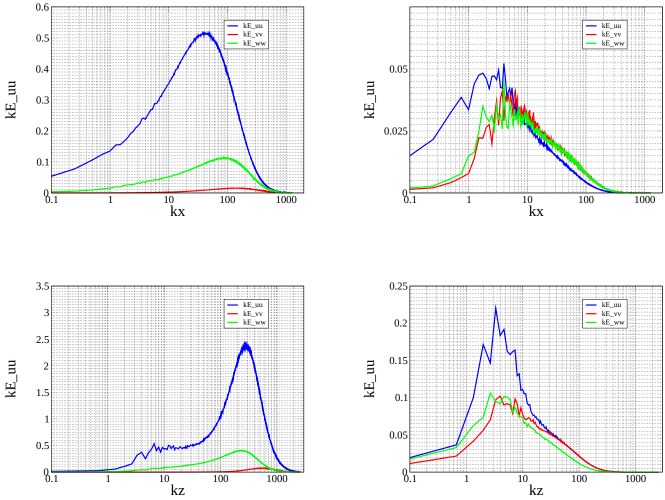


Energy Spectra



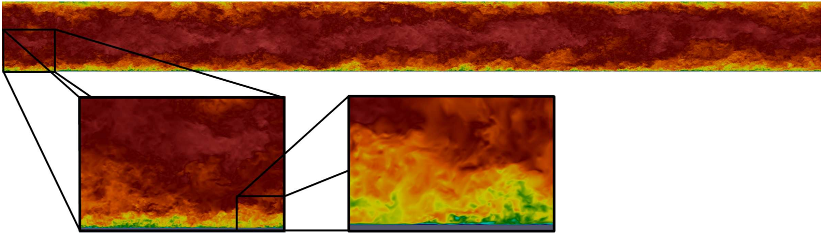
* Left : $Y^+ = 10.5$ / Right : $Y^+ = 4800$

Energy Spectra (wavenumber multiplied)

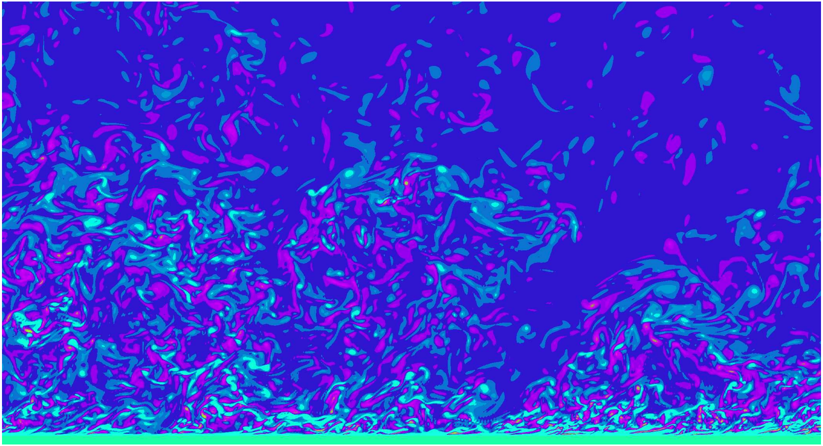


* Left : $Y^+ = 10.5$ / Right : $Y^+ = 4800$

Streamwise Velocity



Spanwise Vorticity



Summary and future work

- Summary
  - High *Re* DNS is required to expand our understanding of wall bounded turbulent flow
  - Excellent scalability is achieved
  - Preliminary results are demonstrated
- Future Work
  - Gathering more data until statistically converged
  - Investigating the multi-scale dynamics that governs the interaction of the inner and outer turbulence
  - Upon completion of simulation, simulation data will be publicly available at
    - http://turbulence.ices.utexas.edu

THANK YOU!!

Questions?

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