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Molecular Simulation of Turbulent Couette Flow

By Edward Smith

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Overview

- Introduction
  - What is Turbulence?
  - Computational Fluid Dynamics (CFD)
  - The Minimal Couette Channel
- Molecular dynamics
  - Non Equilibrium Molecular Dynamics (NEMD)
  - Computational Developments
  - Simulation Details
- Turbulent Simulation
  - Statistics and verification
  - The law of the wall
  - Reynolds stress and the molecular pressure tensor

Section 1

INTRODUCTION

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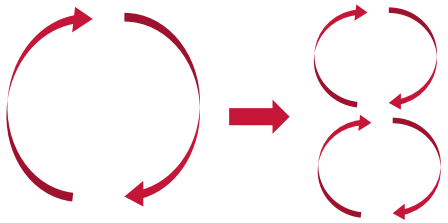
What is Turbulence?

- Turbulent flow
  - Observed in almost any fluid flow -- spatial and temporally varying
  - Apparently random (chaotic) motion
  - Described by deterministic non-linear equations
- Some standard characteristics
  - Statistics are reproducible
  - The law of the wall
  - A cascade of eddies with vortex breakdown and reformation

Big whirls have little whirls that feed on their velocity,
and little whirls have lesser whirls and so on to viscosity.
Lewis Fry Richardson



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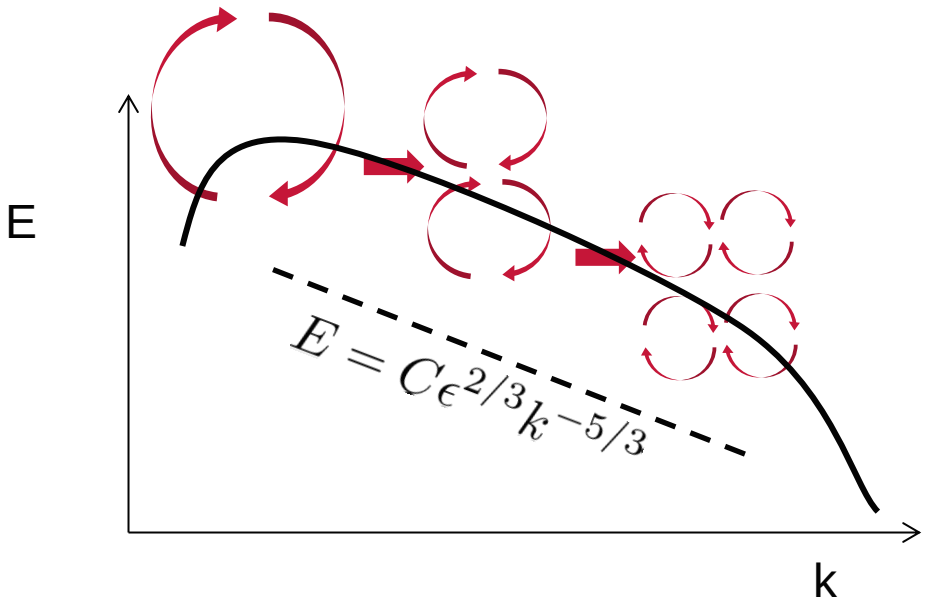
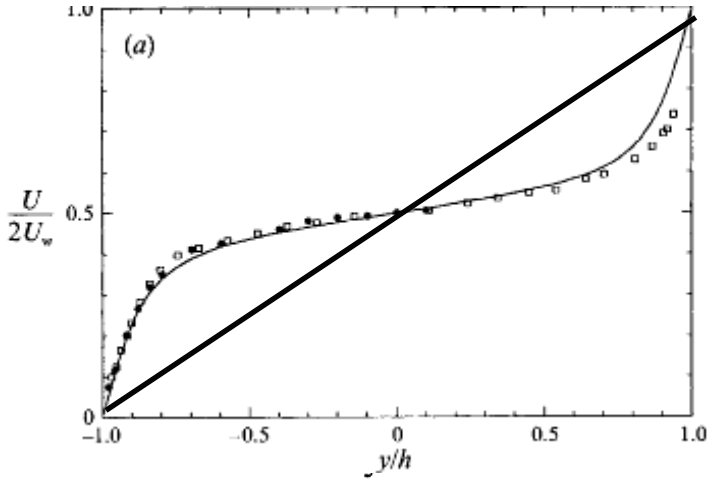
What is Turbulence?

- Standard characteristics
  - Statistics are reproducible
  - Law of the wall
  - Energy spectrum and cascade





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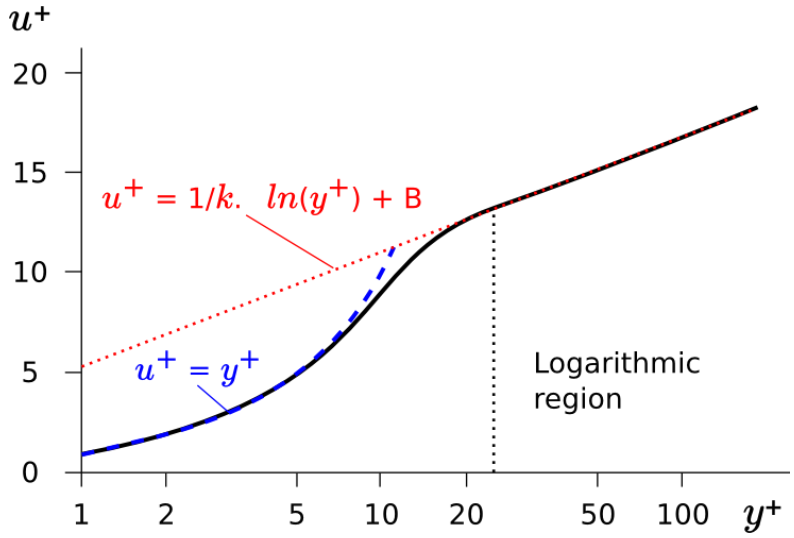

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Why is Turbulence Important?

- The central problem of fluid mechanics
  - Improved understanding would revolutionise many areas of engineering
    - Aerospace
    - Vehicle aerodynamics
    - Fluid transport
    - Power generation
    - Weather prediction

- Turbulence result in fluid mixing, heat transfer and drag
  - Should be promoted in some cases and reduced in others
    - Heating fins
    - Dimples on a golf ball
    - Active control of surfaces
    - Surface coatings

Computational Fluid Dynamics

- Assumed continuous at every point in space
  - Mass Conservation

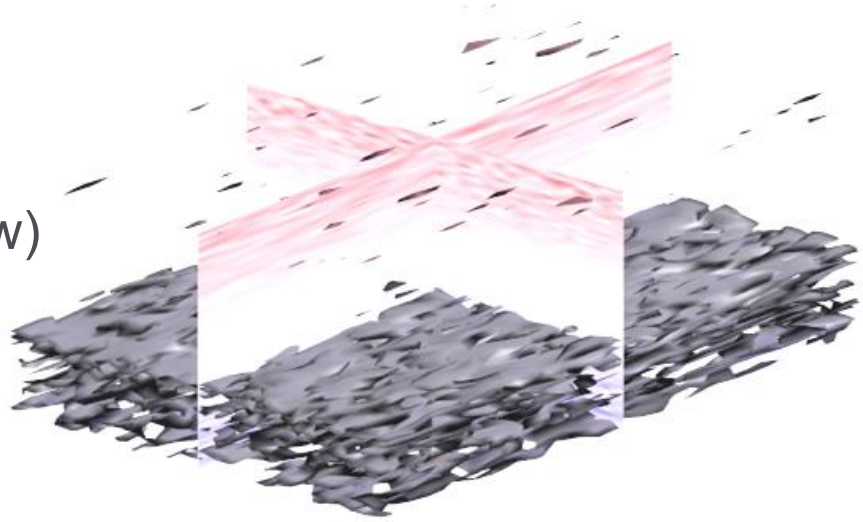
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - Momentum Balance (Newton's Law)

$$\frac{\partial}{\partial t} \rho \boldsymbol{u} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u} \boldsymbol{u} = \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}$$

  - Energy Conservation

$$\frac{\partial}{\partial t} \rho \mathcal{E} dV = -\boldsymbol{\nabla} \cdot [\rho \mathcal{E} \boldsymbol{u} + \boldsymbol{\Pi} \cdot \boldsymbol{u} + \mathbf{q}]$$



Direct Numerical Simulation of
Turbulent Couette Flow

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Computational Fluid Dynamics

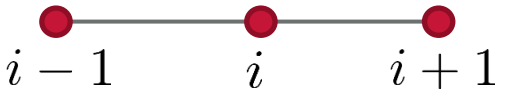
- The Navier-Stokes Equation

$$\frac{\partial}{\partial t}\rho \boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} \quad = \quad -\boldsymbol{\nabla}\cdot\Pi$$

$$\boldsymbol{\Pi} = P\boldsymbol{I} - \mu\boldsymbol{\nabla}\boldsymbol{u}$$

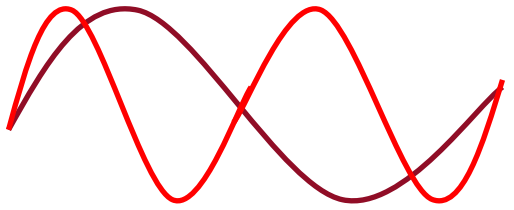
- Finite Difference Method

$$\frac{\partial u_i}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{\Delta x}$$



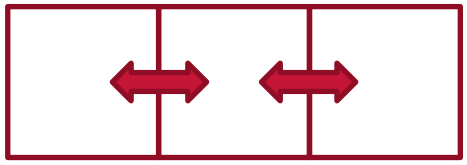
- Spectral Methods

$$u(x) = \sum_{n=1}^{X-1} \tilde{u}_n \overline{T}_n(y) e^{2\pi i(k_x x/L_x + k_z z/L_z)}$$



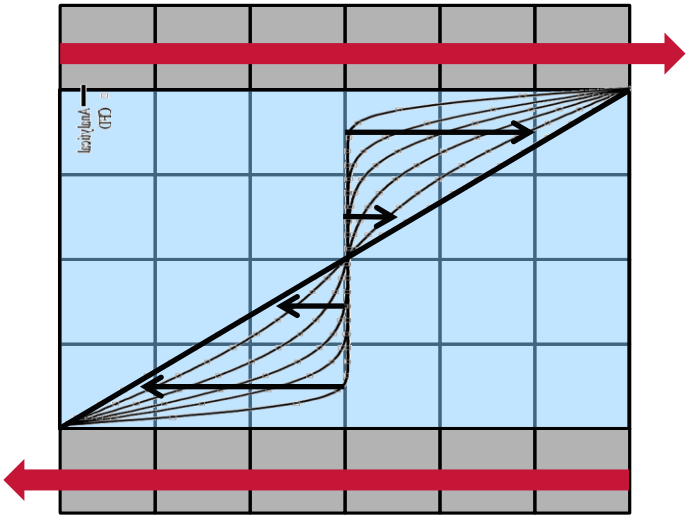
- Finite Volume Method

$$\frac{\partial}{\partial t}\int_V \rho\boldsymbol{u}dV = -\oint_S \rho\boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S} - \oint_S \boldsymbol{\Pi}\cdot d\boldsymbol{S}$$



Computational Fluid Dynamics

- Domain split into a number of volumes
  - Solved at every point in space before next time step
  - Boundary conditions must be specified



- Wall driven or Couette flow
  - Two infinite plates with fluid in between
  - A good model for many industrial cases of interest

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Computational Fluid Dynamics

- The Incompressible Navier-Stokes Equation

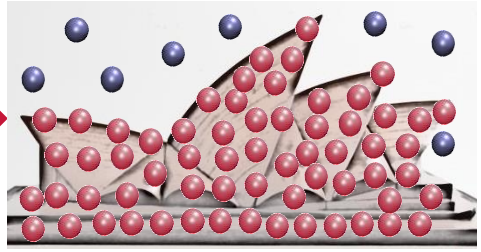
$$\frac{\partial}{\partial t}\rho \boldsymbol{u} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u}\boldsymbol{u} = -\boldsymbol{\nabla} P + \mu \nabla^2 \boldsymbol{u} \qquad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

- Non dimensional form

$$\frac{\partial}{\partial t}\boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} P + \frac{1}{Re}\nabla^2 \boldsymbol{u} \qquad Re = \frac{\rho U L}{\mu}$$

- Reynolds number
  - Ratio of convection to diffusion
  - Scaling argument applied to any scale -- is there a minimum?

Arup wind tunnel model



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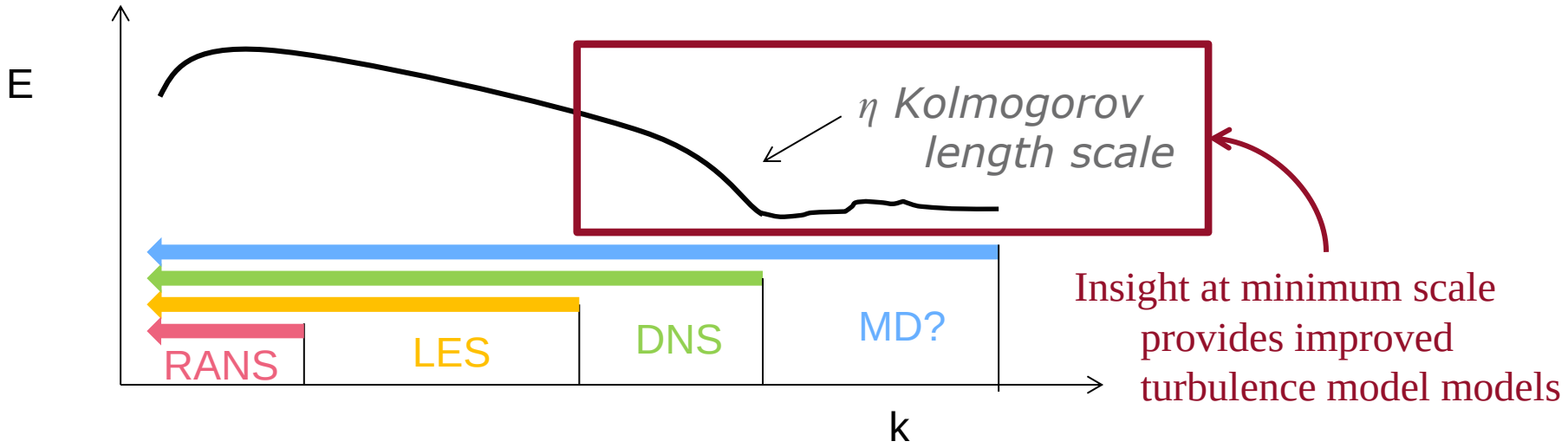
The Minimum Scale of Turbulence

- Kolmogorov scaling arguments suggest a minimum scale
  - Based on dimensional analysis $\eta \sim Re^{-3/4}$
- Used to determine the minimum scale required in a CFD simulation and the number of grid cells
  - Direct Numerical Simulation (DNS) solves the full range
  - Large Eddy Simulation (LES) models part of the spectrum
  - Reynolds Averaged Navier-Stokes (RANS) simulates time average



The Minimum Scale of Turbulence

- The minimum domain size required to sustain turbulent flow

Poiseuille flow, Re ≈ 2000

Couette Flow Re ≈ 400

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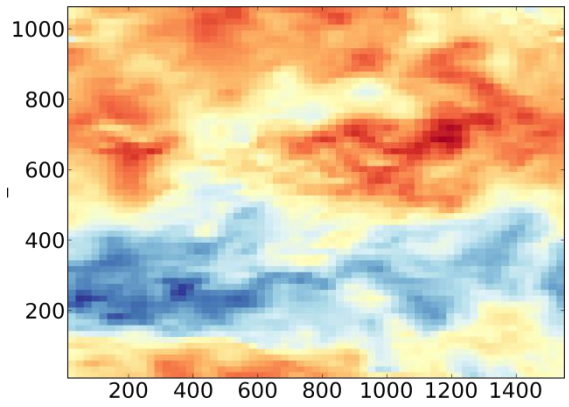
Three plots of decreasing Reynolds Number

$$Re = \frac{\rho U L}{\mu}$$

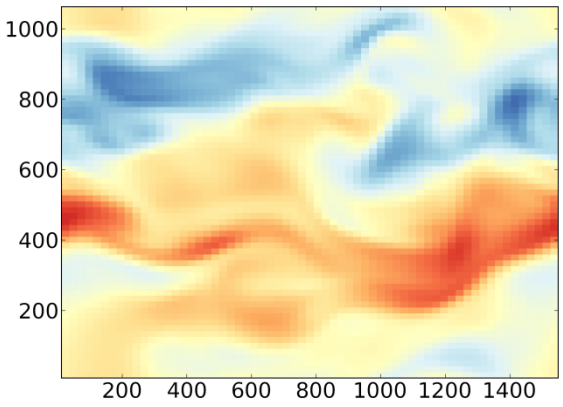
- From Jimenez and Moin (1991):

  At these Reynolds numbers, […] any sustained turbulence is subcritical. Under these circumstances the question of initial conditions may become important […] The very first run was initiated as an essentially random finite amplitude perturbation […] at a fairly large Reynolds number and subsequent runs were started incrementally from the results of that simulation.

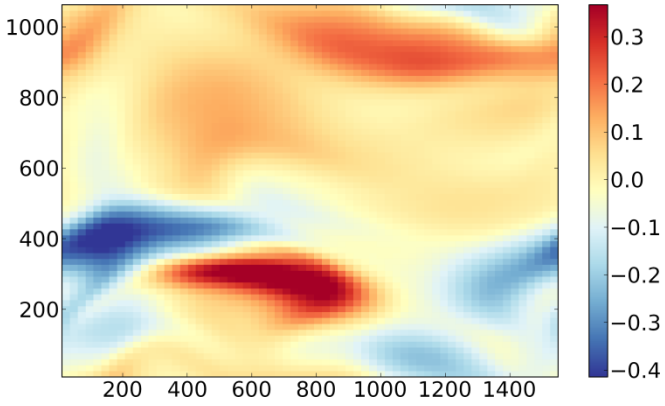
Re ≈ 4000



Re ≈ 1000



Re ≈ 400



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Literature On the Minimum Flow Unit

- From Hamilton et al (1995)
  - Turbulent structures observed
  - The u (stream-wise) velocity at the y centreline
  - One regeneration cycle (**100** flow through times)
- The minimal unit of turbulent flow
  - Turbulent Streak like structures become wavy
  - Break down into smaller turbulent structures
  - Reform into straight streaks
- Key to the fundamental mechanism of turbulence

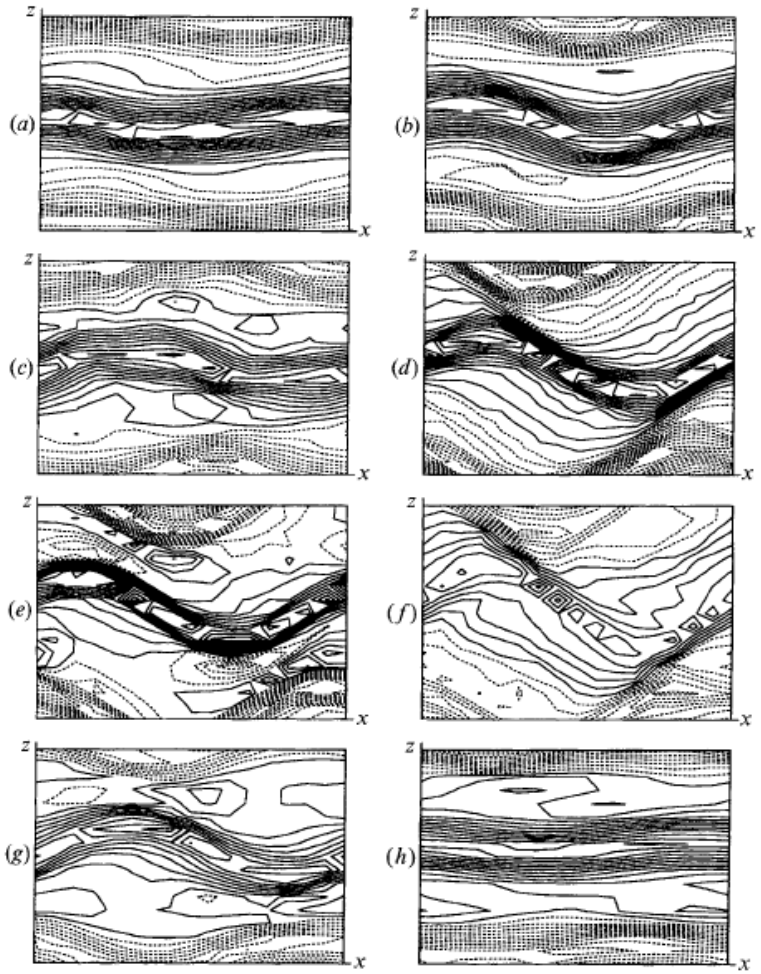

FIGURE 2. Iso-contours of u-velocity in the (x, z)-plane centred between the walls; solid contours positive, dashed contours negative. Contour interval 0.032. (*a*) $t = 757.5$, (*b*) $t = 764.8$, (*c*) $t = 772.0$, (*d*) $t = 777.8$, (*e*) $t = 783.0$, (*f*) $t = 794.1$, (*g*) $t = 808.2$, (*h*) $t = 830.2$.

Section 2

MOLECULAR DYNAMICS

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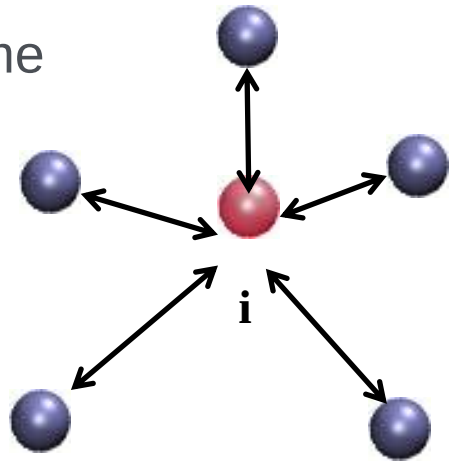
Molecular Dynamics

Discrete molecules in continuous space

- Molecular position evolves continuously in time
- Position and velocity from acceleration

$$\ddot{\boldsymbol{r}}_i \rightarrow \dot{\boldsymbol{r}}_i$$
$$\dot{\boldsymbol{r}}_i \rightarrow \boldsymbol{r}_i(t)$$



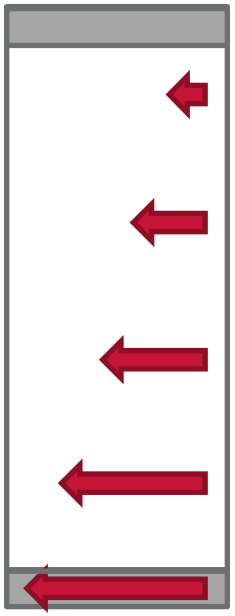
Acceleration obtained from forces

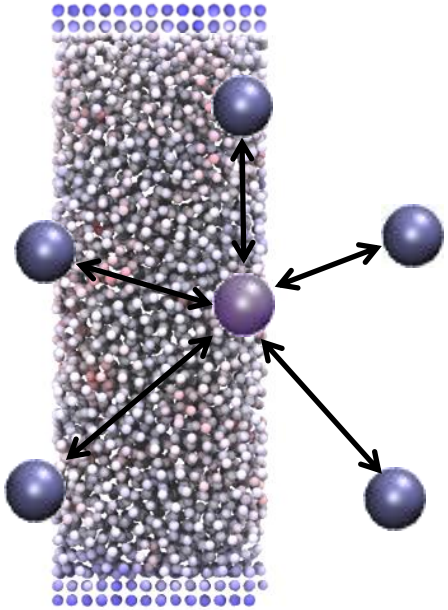
- Governed by Newton's law for an N-body system
- Point particles with pairwise interactions only

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^{N} \boldsymbol{f}_{ij}$$

$$\Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

Non-Equilibrium Molecular Dynamics



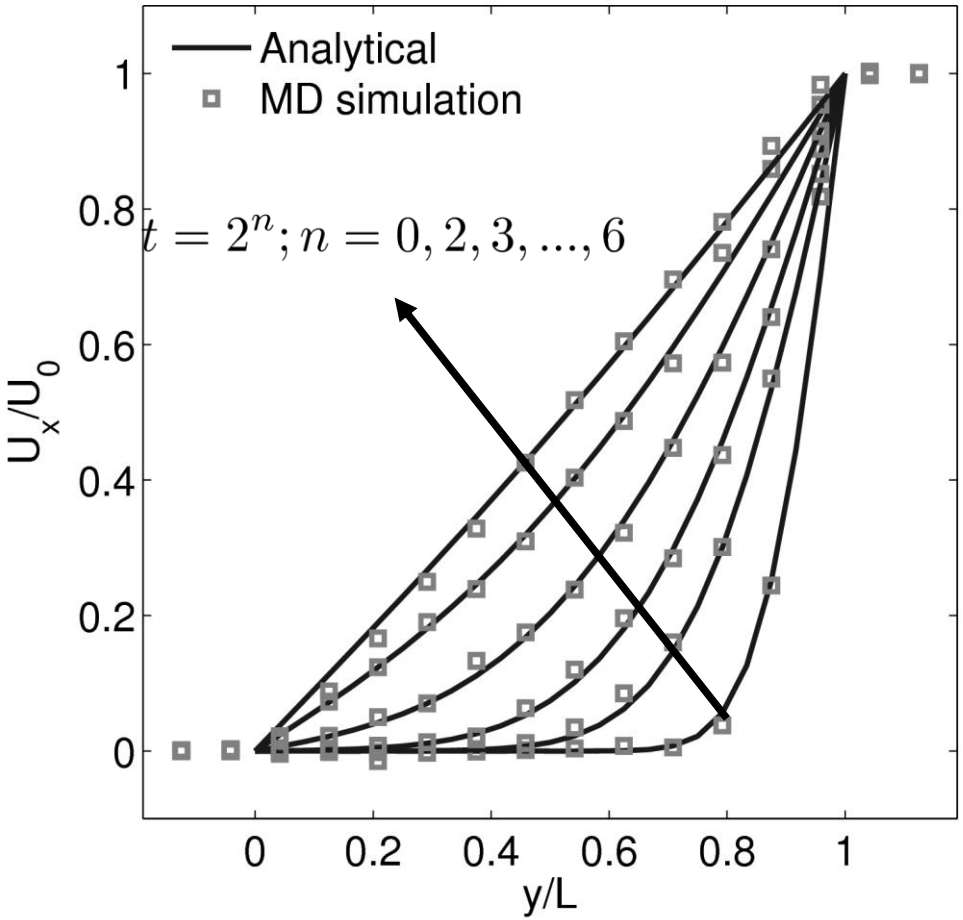


Molecular Dynamics Simulation of Couette Flow

- *Sliding walls are made by tethering molecules to lattice sliding sites at top and bottom*
- *Periodic boundaries in x and z directions*
- *Nose Hoover thermostat removes heat from the walls*

Non-Equilibrium Molecular Dynamics

- MD Simulation of Laminar Couette Flow
  - Matches the laminar evolution in the continuum model



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The Smallest Domain for the Minimum Reynolds Number

- Obtain viscosity from a range of 660 simulations for the WCA potential

$$Re = \frac{\rho U L}{\mu}$$

$$U = \pm 1$$

- The target value

$$Re > 400$$

$$\rho/\mu > 1.4$$

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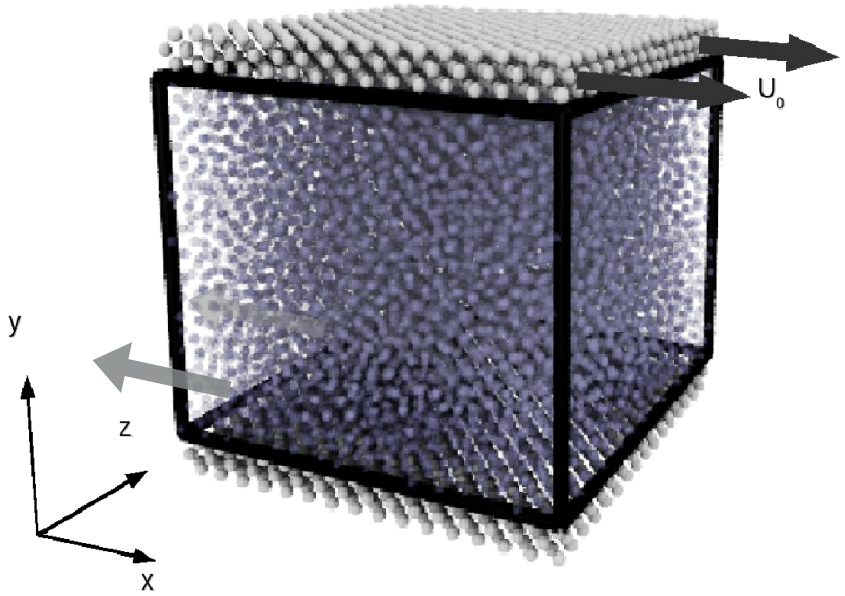
Domain Overview

- Simulation Setup
  - Sliding top and bottom walls in y with u = ± 1
  - Periodic in x and z directions
  - Walls are tethered, sliding molecules with NH thermostat



- Domain in reduced units: x = 1560.4, y = 566.7, z = 1069.9 at a density of 0.3 – about 300 million molecules

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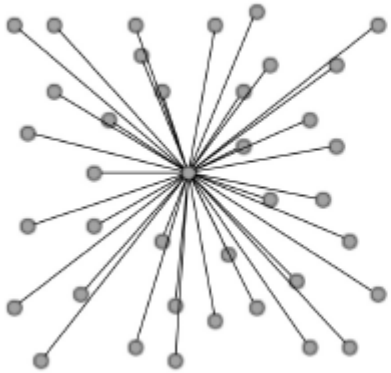
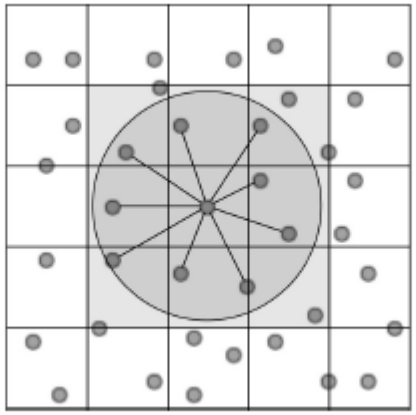
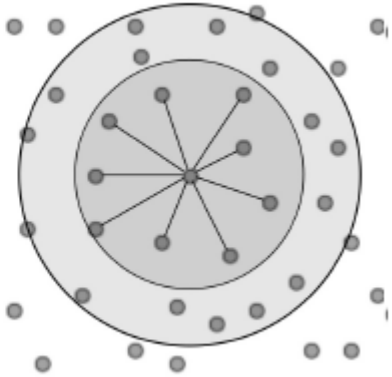
MD Computing – Serial optimisations

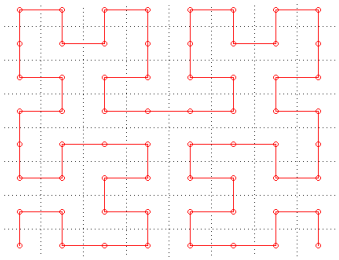
- Molecular Dynamics code developed for NEMD style problems and large systems
  - Highly optimised for simple point particles
  - All pairs simulation uses local cell and neighbour lists to reduce the N^2 calculation to order N



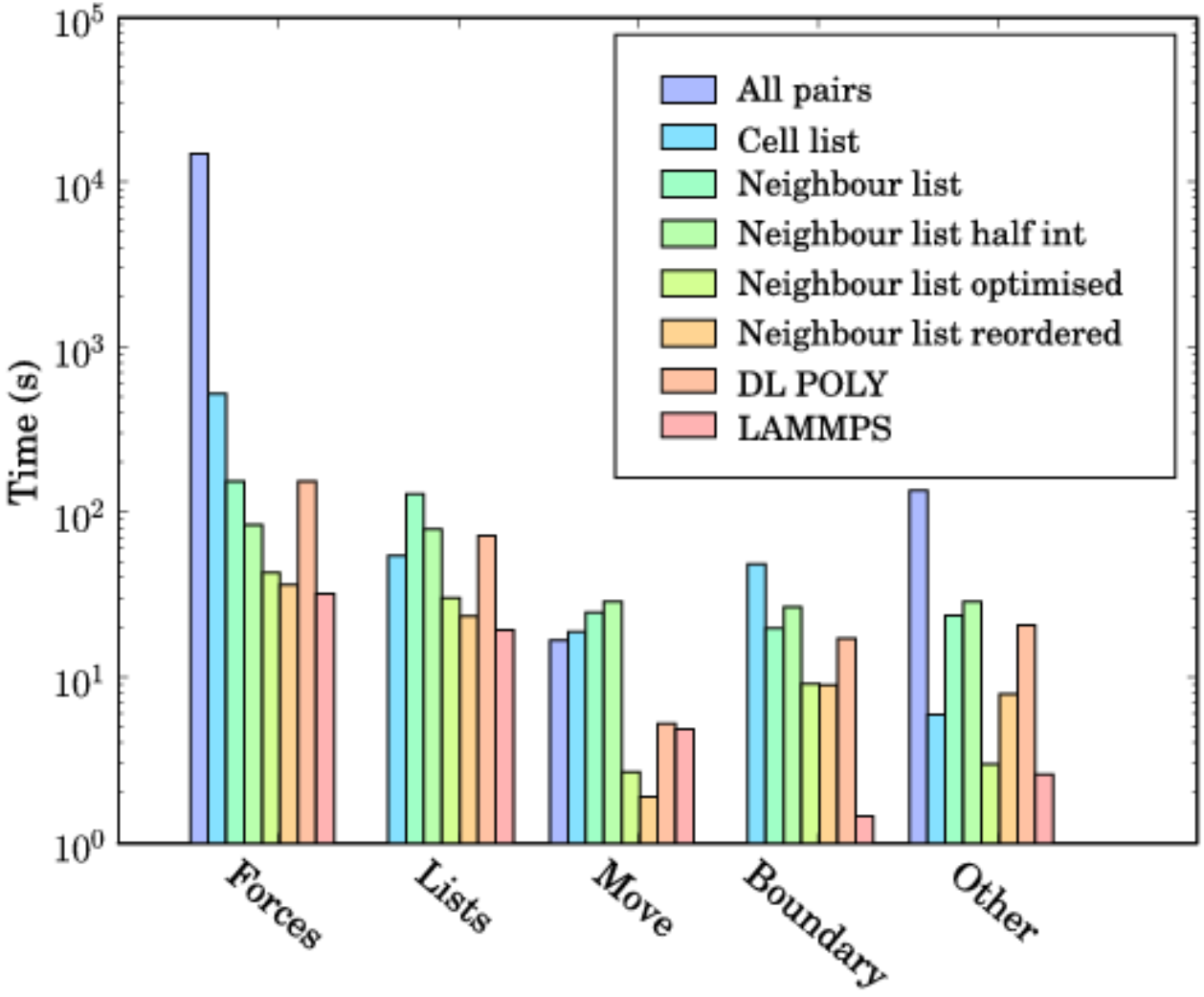




- Hilbert curve sorting improves cache efficiency of operations
  - Improvement becomes important on large systems



MD Computing – Serial optimisations



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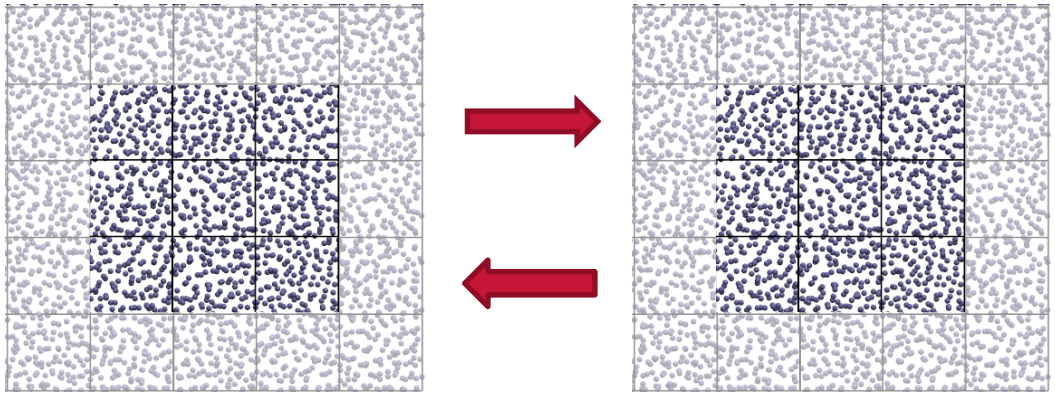
MD Computing – Parallel optimisations

Localisations lends itself to parallel computing using MPI

- Spatial decomposition employed
- Halo cells (ghost molecules) are used to link adjacent regions



Halo exchange of variable amounts of data

- MPI_Send, MPI_Probe and MPI_Recv employed

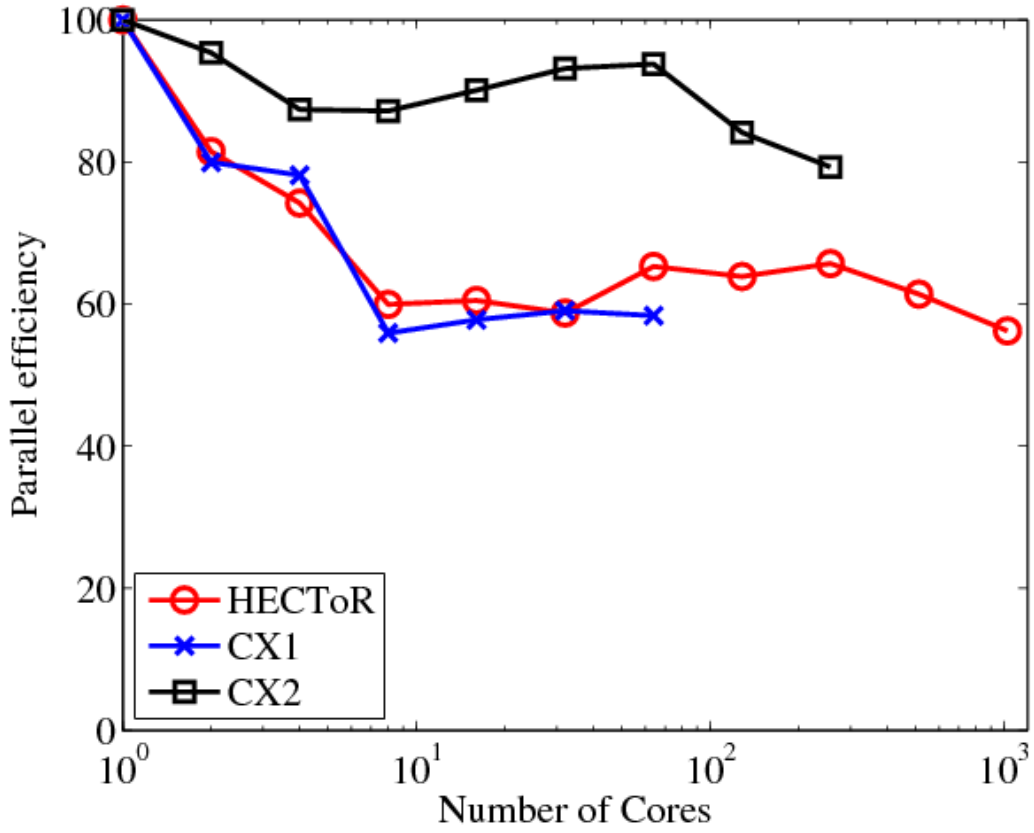
CUDA implementation developed but found to be too inflexible to justify the speedup (especially in parallel)

- 30x speedup reported if entire code on GPU (Anderson et al 2008)
- Speedup negated by transfer, multi-GPU implementation challenging

MD Computing – Parallel optimisations

Strong scaling vs 1 core with 3,322,336 molecules

- On HECToR and Imperial's supercomputers CX1/CX2
- Efficiency of 90% when comparing 1024 cores to 8 cores



Section 3

TURBULENT SIMULATION

Molecular Turbulent Couette Flow

- We have the system parameters for Re=400, an optimised code and now we need an initial condition
  - Initial velocity is obtained by a series of CFD runs at Re=4000, 2000, 1000, 700, 500 and then 400 in stages
  - A very long run at Re=400 to wash out any artefacts

- Equivalent continuum and molecular simulation using the same initial condition
  - Velocity field is enforced on the MD system using cell by cell rescaling which keeps the initial molecular fluctuations
  - Channelflow spectral code used for CFD
  - Both allowed to evolve naturally for 28,000 time units (100 flow through times or one regeneration cycle)

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Molecular Turbulent Couette Flow

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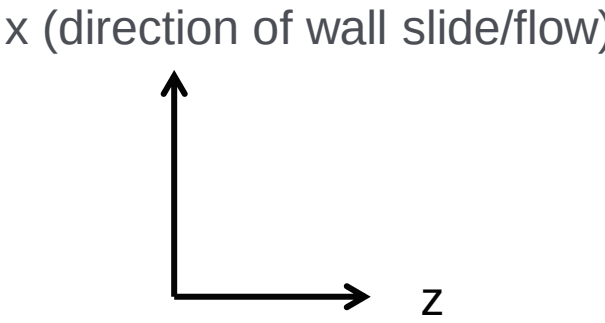
Time Evolving Results

Structures observed at the channel centreline in y

Velocity, u, in the x direction



Turbulent kinetic energy

$$k = \sqrt{u'^2 + v'^2 + w'^2}$$

Like a continuum temperature…

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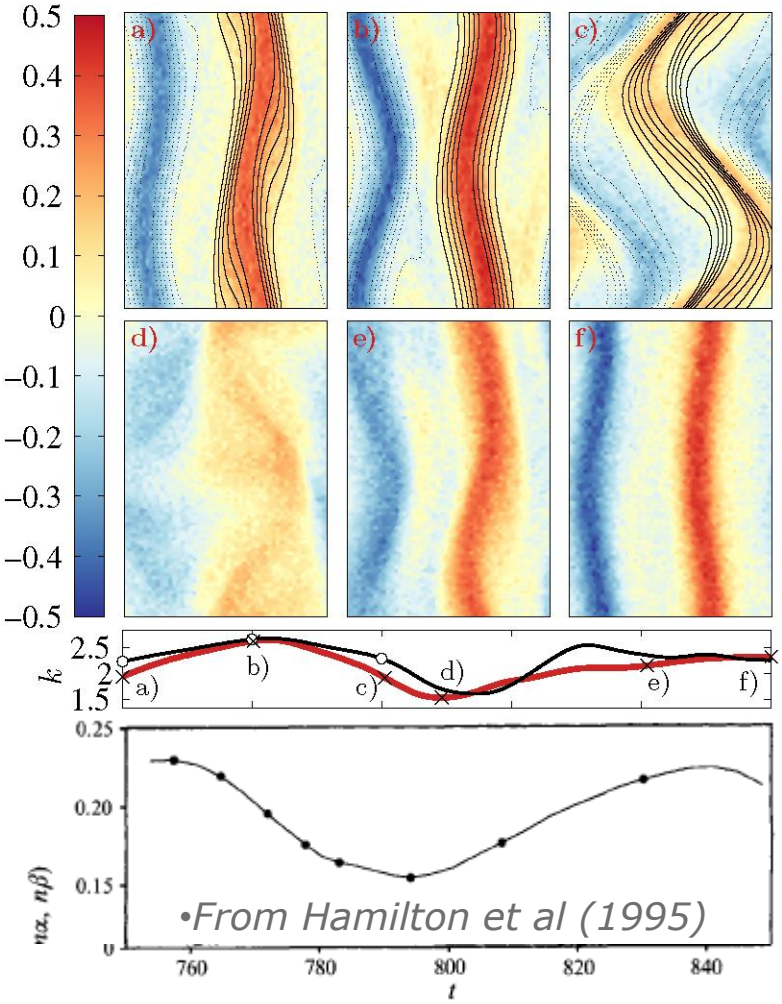
Time Evolving Results

- Structures observed at the centreline
  - Same in continuum and molecular system
  - Breakdown and regeneration
  - Two solutions diverge over sufficient time
- Turbulent kinetic energy
  - Defined by fluctuation in time average quantities:

    $k = \sqrt{u'^2 + v'^2 + w'^2}$
  - Identical to concept of peculiar momentum and temperature



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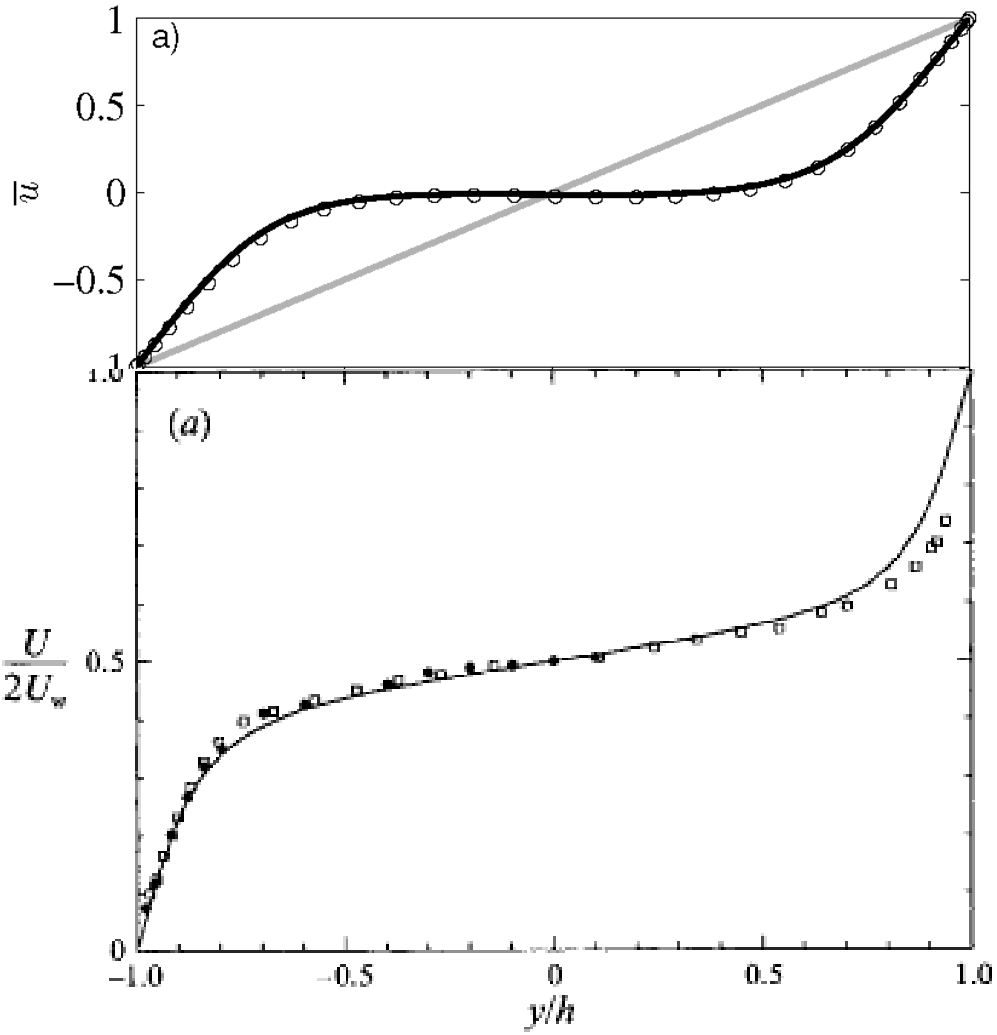
Statistical Results

- Averaged velocity profile
  - Taking average velocity in x and z
  - Over all time (28,000 time units)
- No longer Laminar profile across domain
  - Turbulent promotes mixing, increasing velocity near the walls
- Good agreement with literature
  - Numerical continuum studies
  - Experimental results from turbulent simulations



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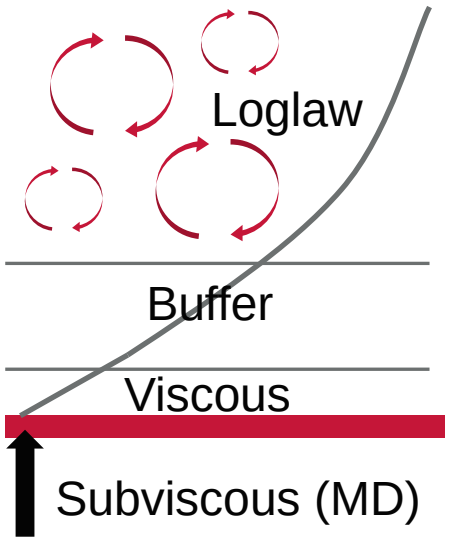
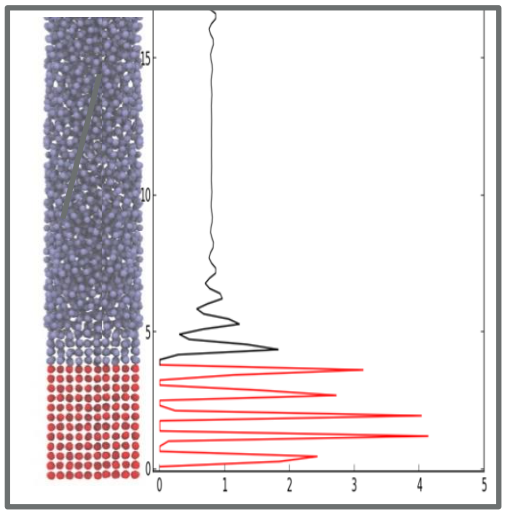
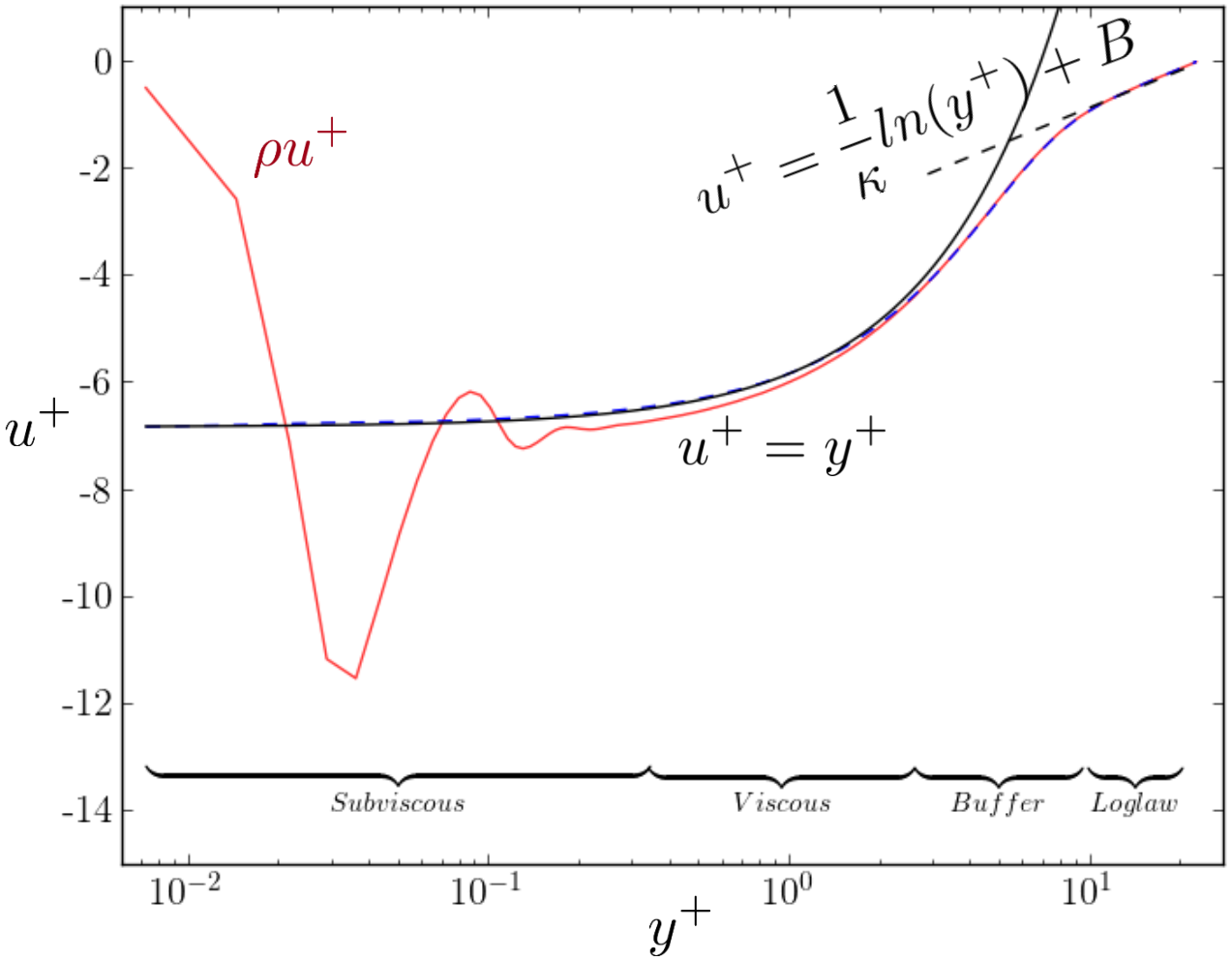
Law of the wall







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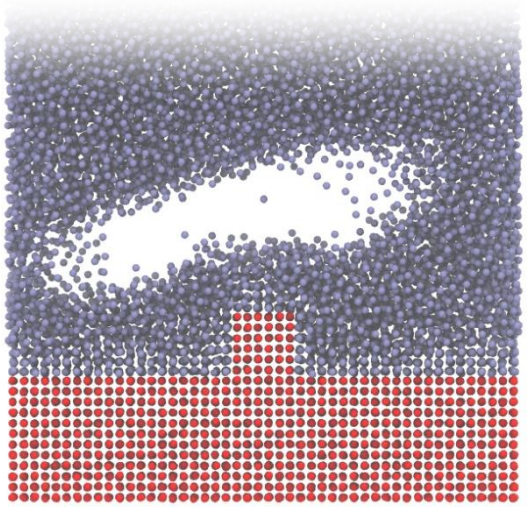
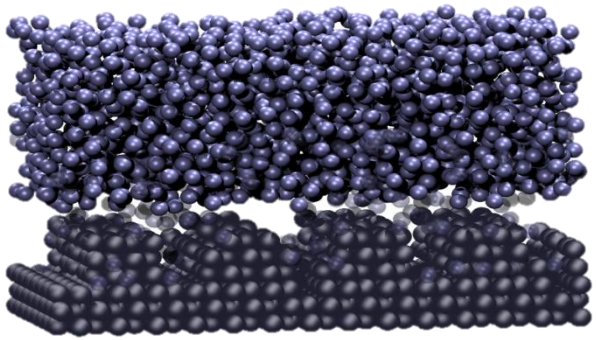
Molecular Surface Texture and Coatings





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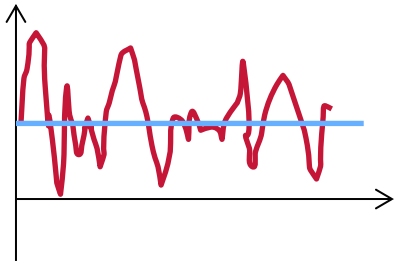
Reynolds Decomposition

- Split the motion into time average and fluctuating part



$$u = \overline{u} - u'$$

- Rewrite the Navier-Stokes using this and time average to get the Reynold Averaged Navier-Stokes (RANS)
  - Reynolds stress tensor doesn't disappear
  - Approximating this is central to most industrial CFD

$$\frac{\partial}{\partial t}\overline{\boldsymbol{u}} + \overline{\boldsymbol{u}} \cdot \boldsymbol{\nabla}\overline{\boldsymbol{u}} = -\boldsymbol{\nabla}\overline{P} + \frac{1}{Re}\nabla^2\overline{\boldsymbol{u}} + \overline{\boldsymbol{u}'\boldsymbol{u}'} \quad \Rightarrow \quad \overline{\boldsymbol{u}'\boldsymbol{u}'} \approx \mu_\tau \boldsymbol{\nabla}\boldsymbol{u}$$

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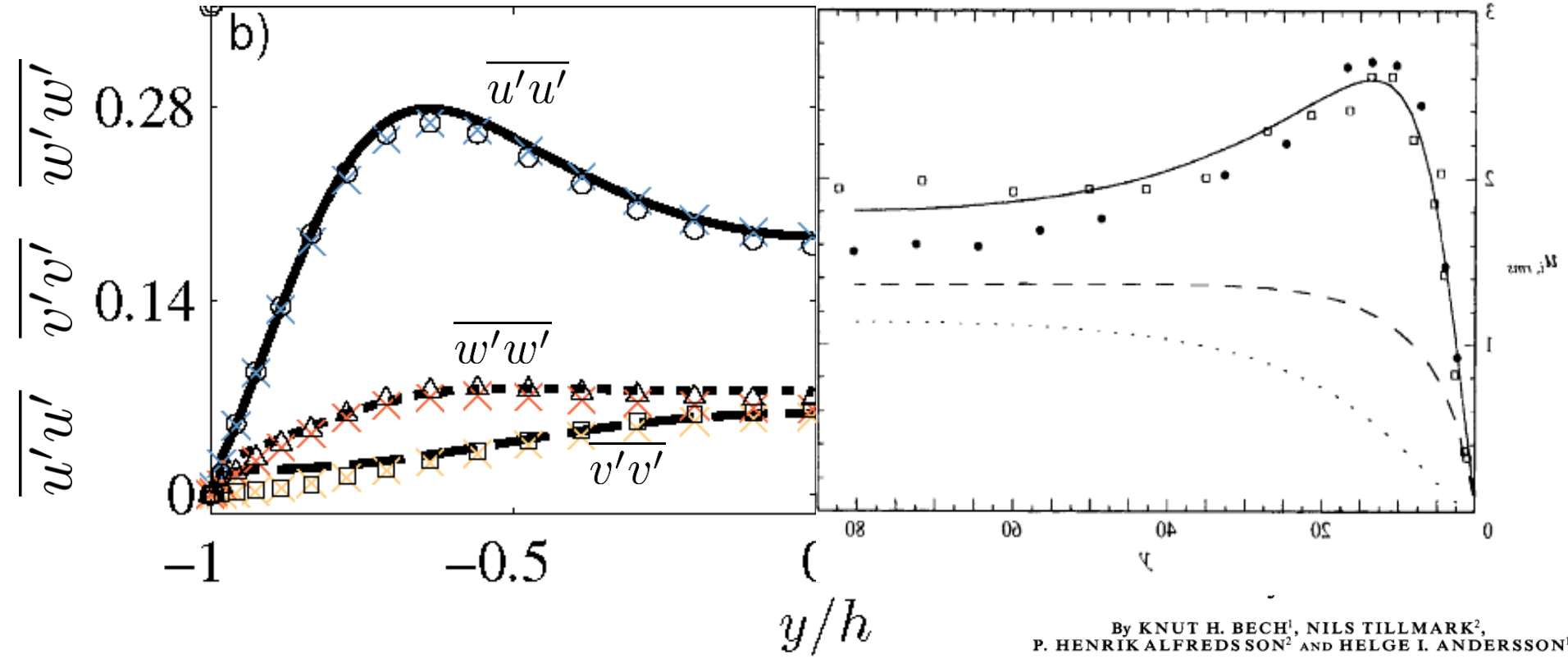
Statistical Results

- Observed velocity profiles match literature
  - Numerical results match very well
  - General profile is consistent with experimental data



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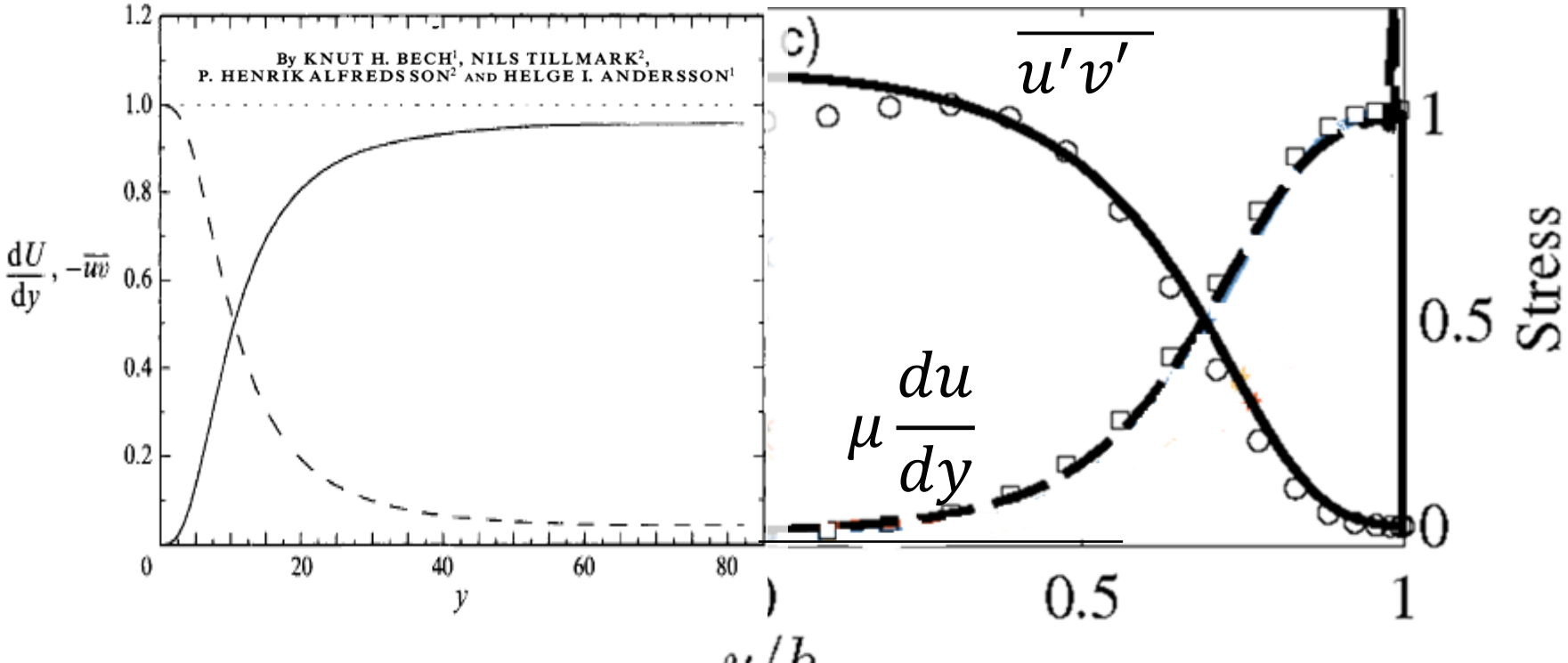
Turbulent Stresses or Molecular Stresses

- Observed stress/pressure profiles match literature
  - Continuum averaged properties agree



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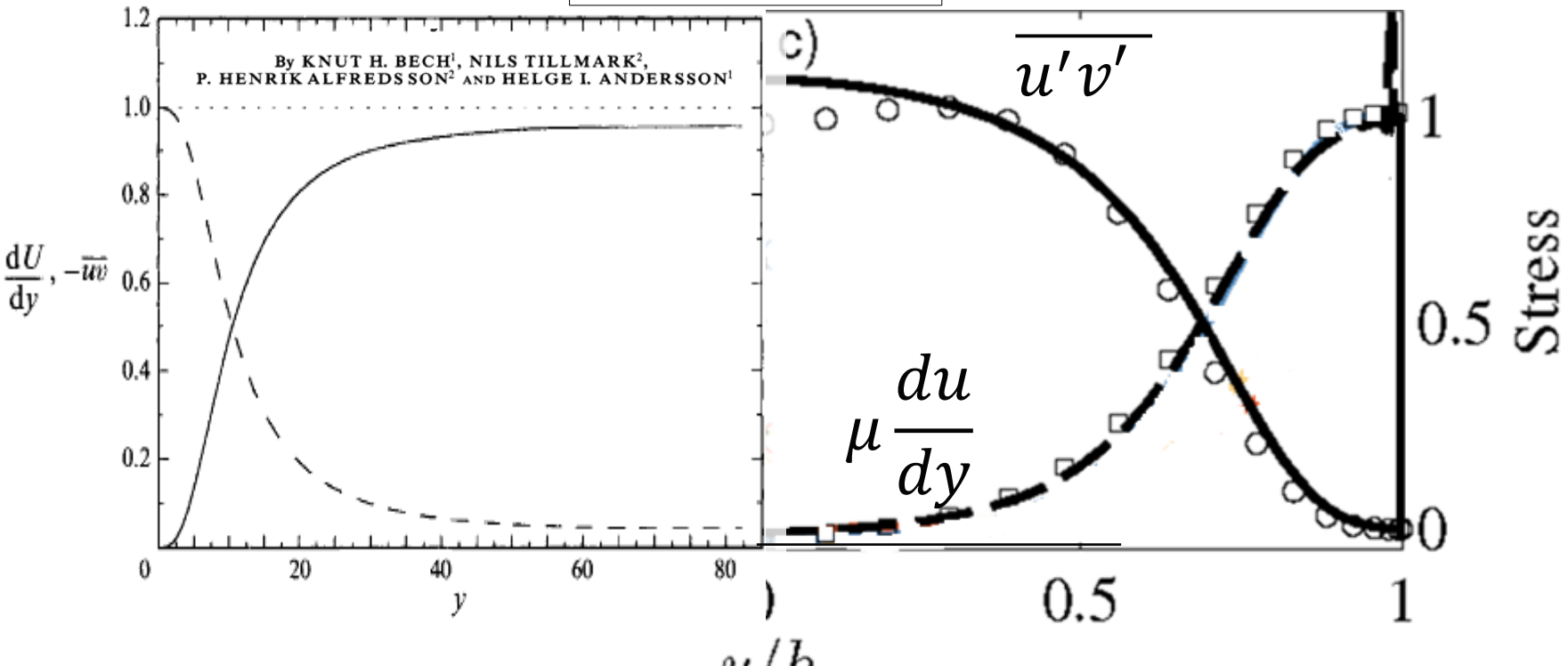
Turbulent Stresses or Molecular Stresses

- Observed stress/pressure profiles match literature
  - Continuum averaged properties agree
  - The molecular pressure provides insight not possible with CFD

Reynolds shear stress

Viscous shear stress



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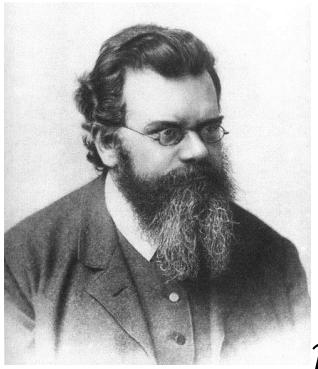
Pressure Tensor in an MD Simulation

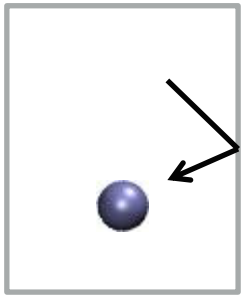
- Pressure definition in a dense molecular system has a long history
  - Virial form given by Rudolf Clausius in 1870
  - Irving and Kirkwood (1950) gave a full localised description,
  - Expressed as forces/fluxes over a plane (Todd, Evans and Daivis,1995)

$$\oint_S \boldsymbol{\Pi} \cdot d\mathbf{S} = \underbrace{\sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i \boldsymbol{p}_i}{m_i} \cdot d\mathbf{S}_i \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij} \right\rangle}_{\text{Configurational}}$$

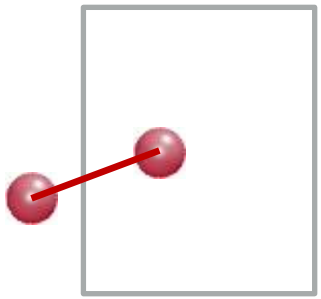
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





$$\dot{r}_i = \frac{p_i}{m_i} + u$$



Configurational part

Inter-molecular bonds act like the stress in a stretched spring

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Same Concept, Different Scales

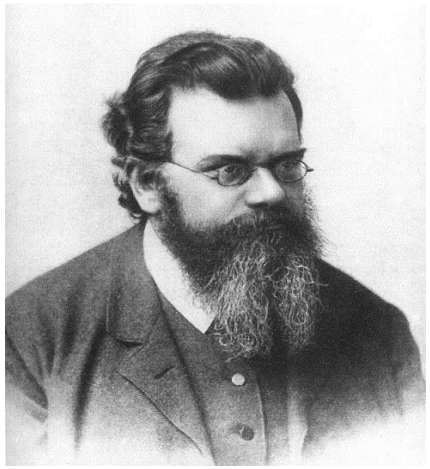
- Reynolds Decomposition

$$u = \bar{u} + u'$$

- Peculiar velocity

$$\dot{r}_i = \frac{p_i}{m_i} + u$$

$$u = \langle \dot{r}_i \rangle$$



- Kinetic part of the pressure tensor and Reynolds stress appear to be the same thing on different length/time scales

$$\overline{\sum \langle m_i \dot{\boldsymbol{r}}_i \dot{\boldsymbol{r}}_i \rangle} = \overline{\sum \langle \boldsymbol{p}_i \boldsymbol{p}_i / m_i \rangle} + \overline{\boldsymbol{u}\boldsymbol{u}} + \overline{\boldsymbol{u}'\boldsymbol{u}'}$$

Molecular average times $\langle \dots \rangle$ Continuum average time $\overline{\dots}$

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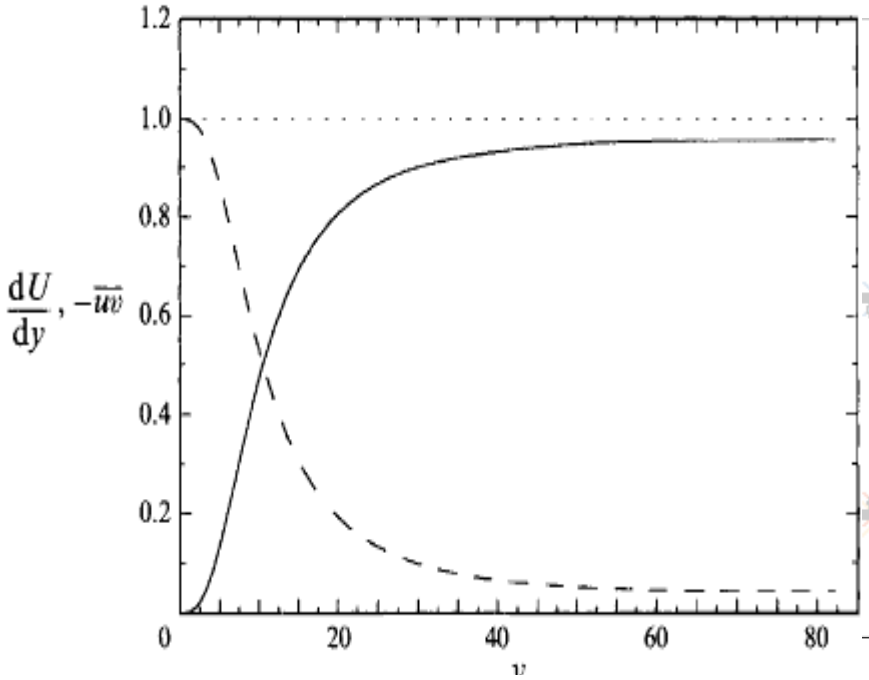
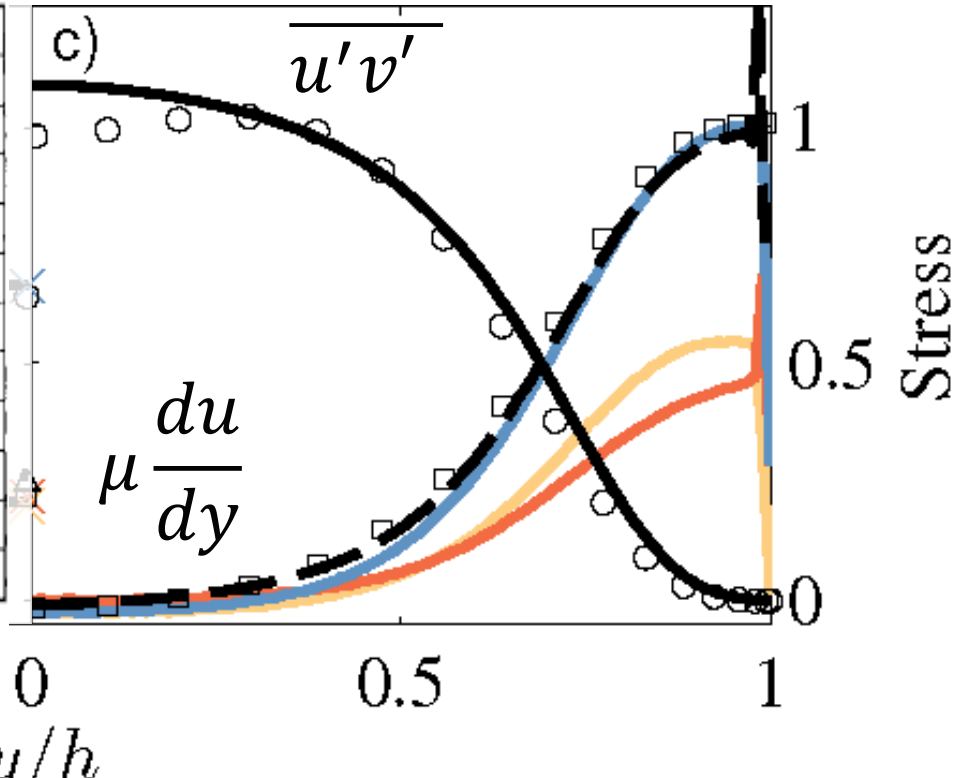
Turbulent Stresses or Molecular Stresses

$$\overline{u'v'} \approx \mu \frac{\partial u}{\partial y} \approx \oint_S \Pi_{xy} \cdot dS_y = \underbrace{\sum_{i=1}^{N} \left\langle \frac{p_{xi} p_{yi}}{m_i} \cdot dS_{yi} \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle f_{xij} dS_{yij} \right\rangle}_{\text{Configurational}}$$



An investigation of turbulent plane Couette flow at low Reynolds numbers

By KNUT H. BECH[1], NILS TILLMARK[2],



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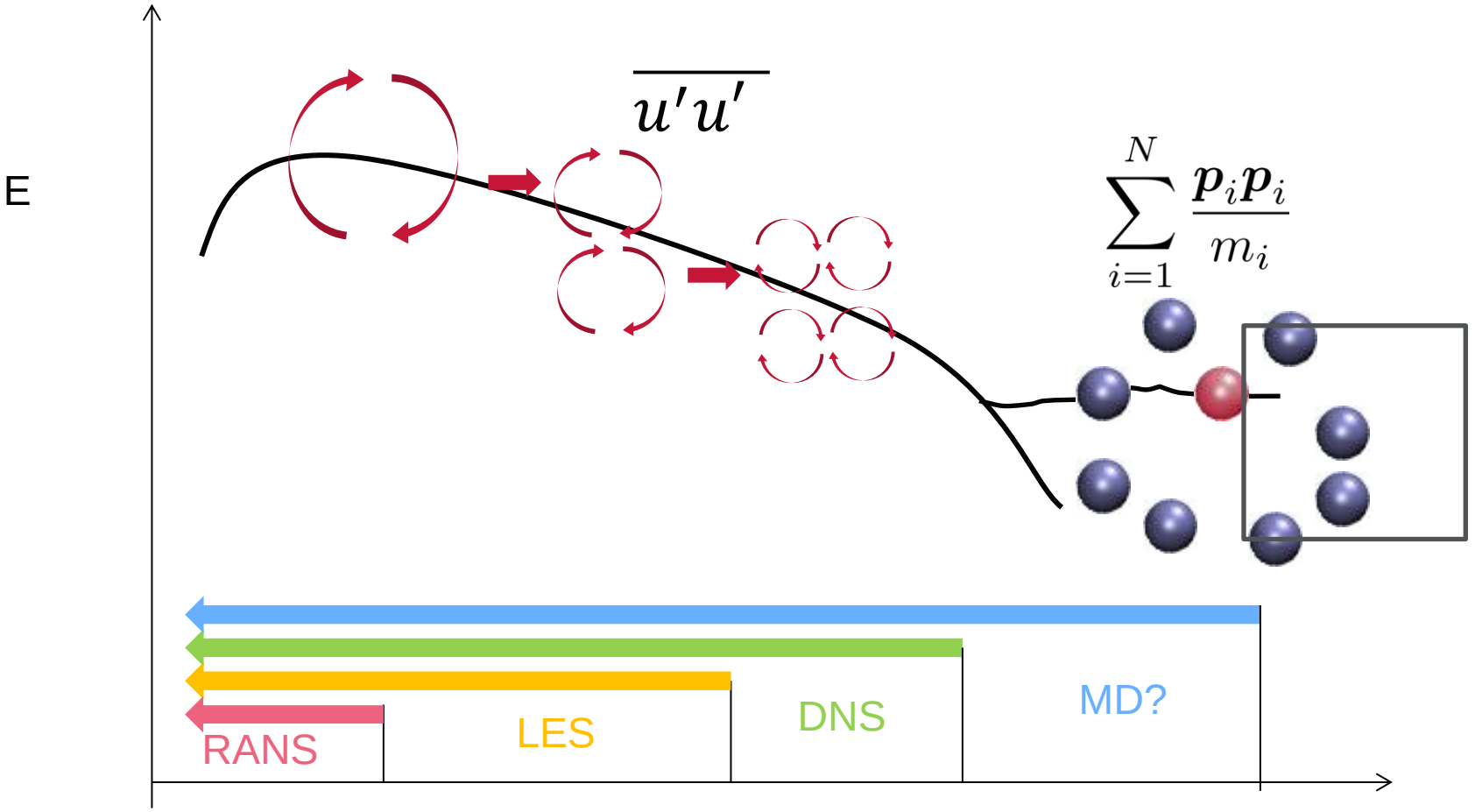
Is Reynolds Stress just Kinetic Pressure?

Big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to ~~viscosity~~ MD



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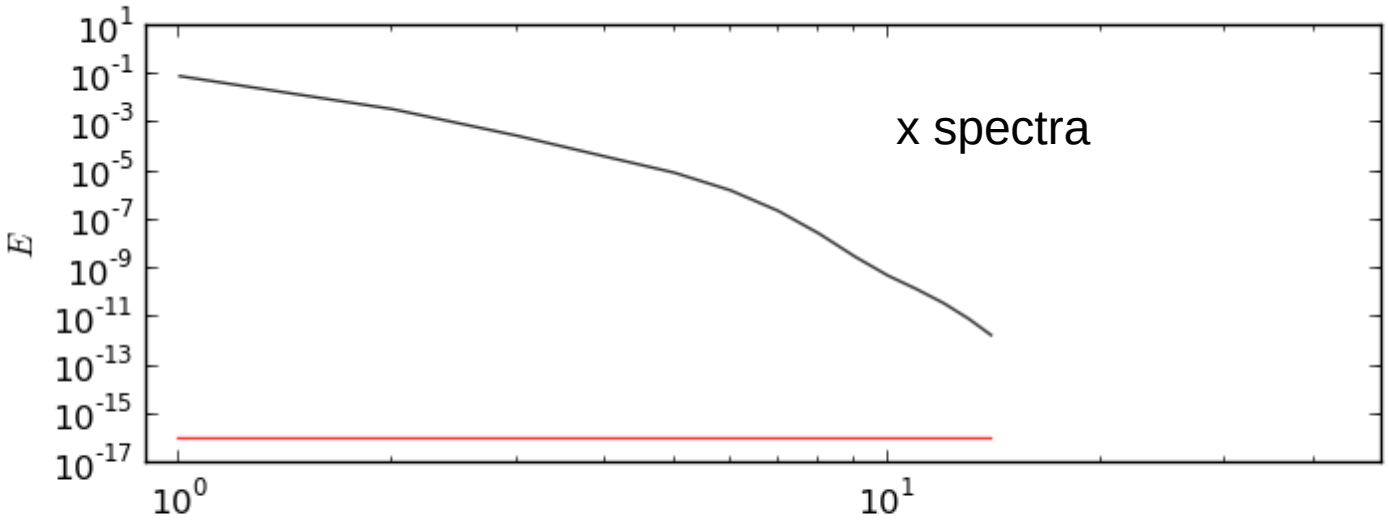
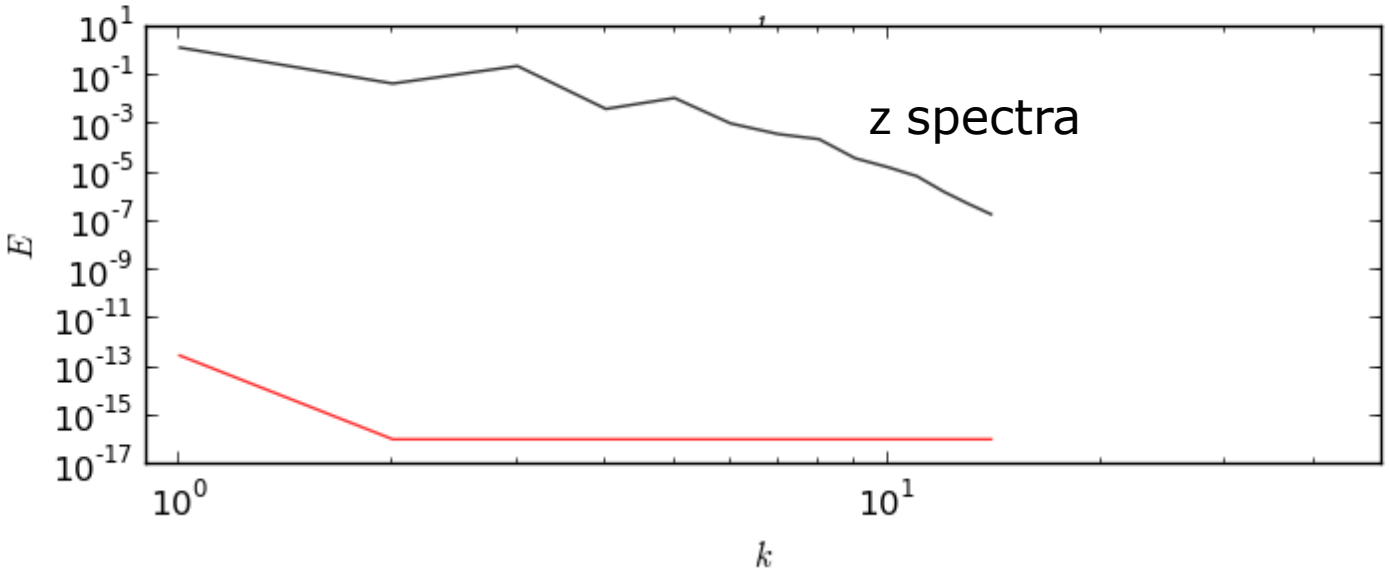
Velocity Spectra





Black Lines
Turbulent CFD Flow

— 1 Record

Red Lines
Laminar CFD Flow

— 1 Record

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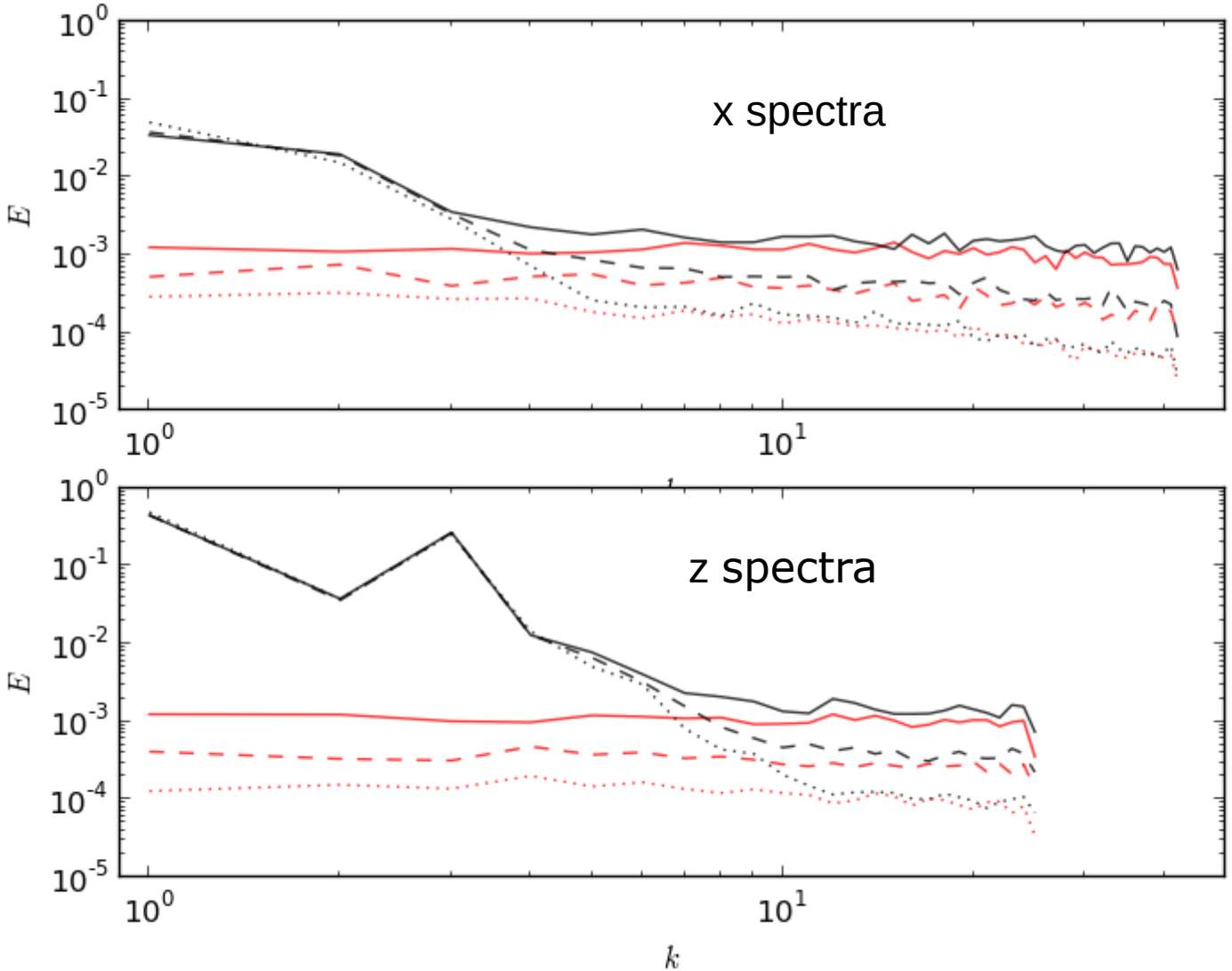
Velocity Spectra



Black Lines
Turbulent MD Flow
Averaged over
— 64 Record
– – 640 Records
---· 3,200 Records

Red Lines
Laminar MD Flow
Averaged over
— 64 Record
– – 640 Records
---· 3,200 Records

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Overview

- Introduction
  - What is Turbulence?
  - Computational Fluid Dynamics (CFD)
  - The Minimal Couette Channel
- Molecular dynamics
  - Non Equilibrium Molecular Dynamics (NEMD)
  - Computational Developments
  - Simulation Details
- Turbulent Simulation
  - Statistics and verification
  - The law of the wall
  - Reynolds stress and the molecular pressure tensor

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Thank you for listening

Any Questions

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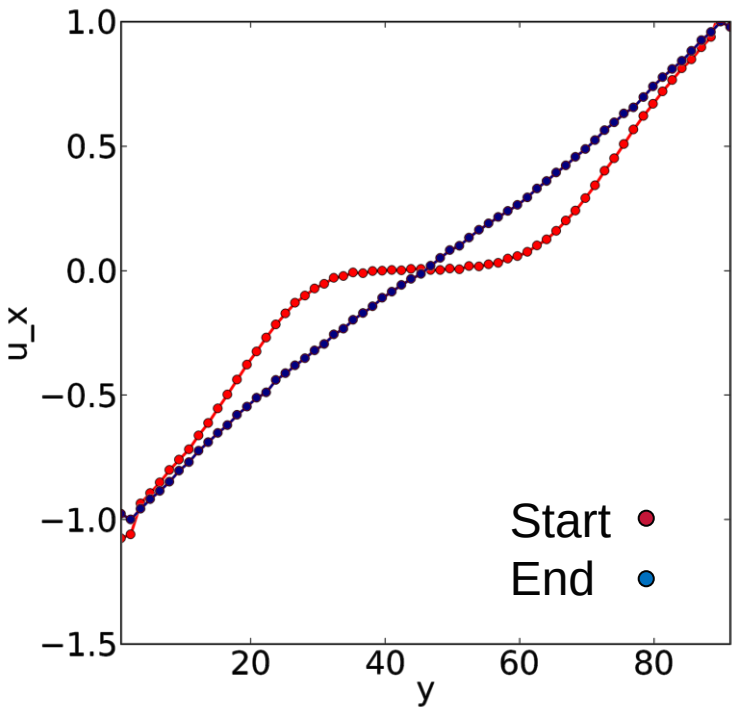
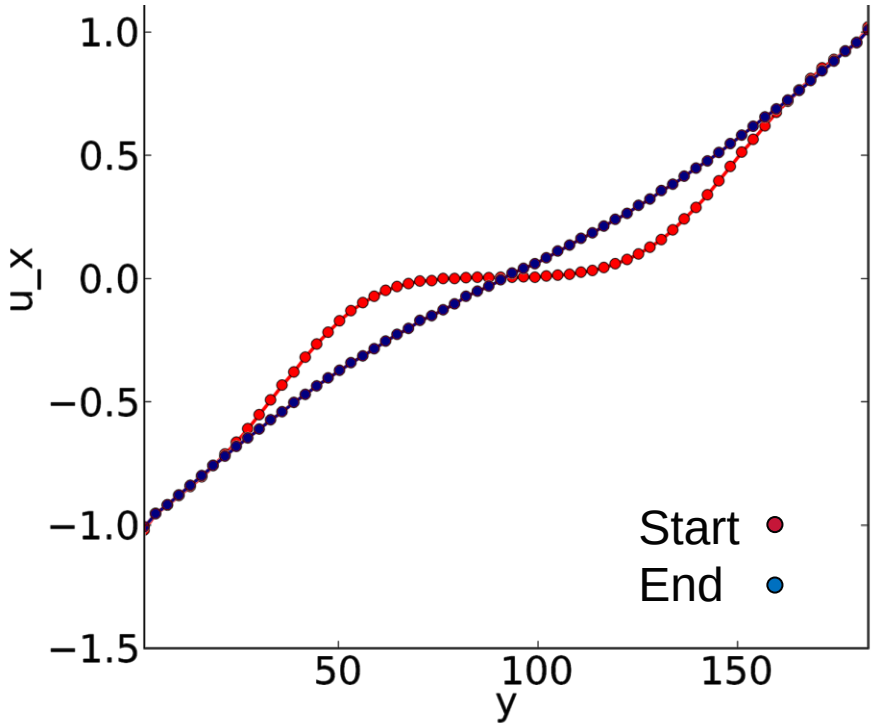
MD Lower Reynolds Number Cases

- Re = 43.5



Molecules = *2,000,000*

Re = 96.0



Molecules =*12,000,000*

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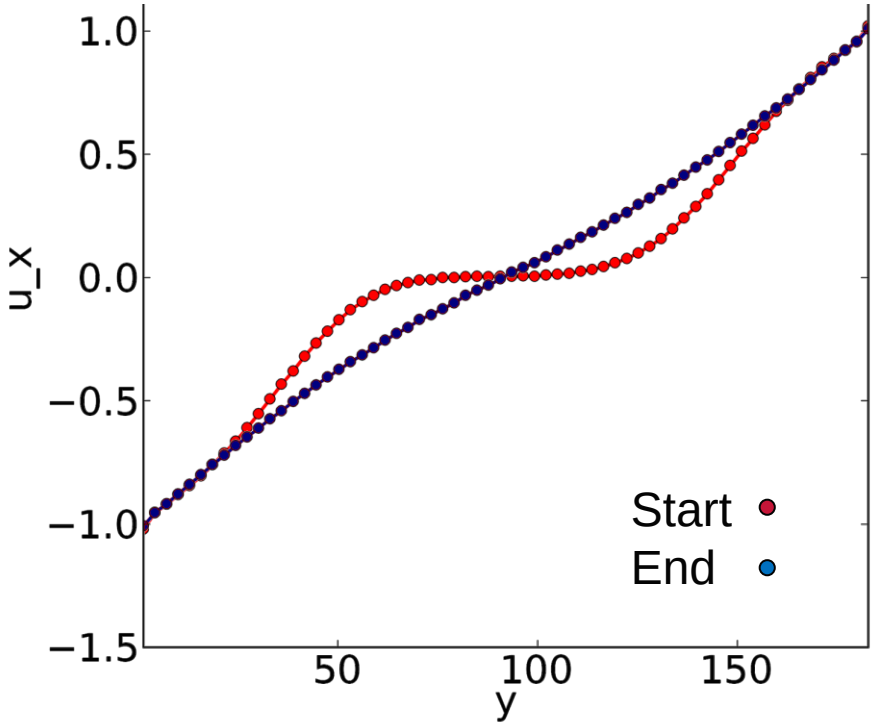
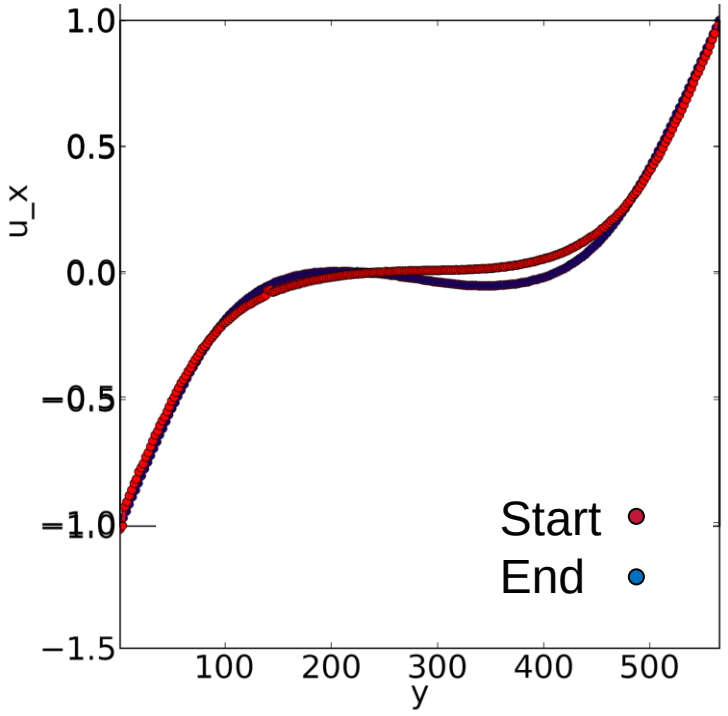
MD Lower Reynolds Number Cases

- Re = 96.0



Molecules =*12,000,000*

Re = 400.0



Molecules =300,000,000

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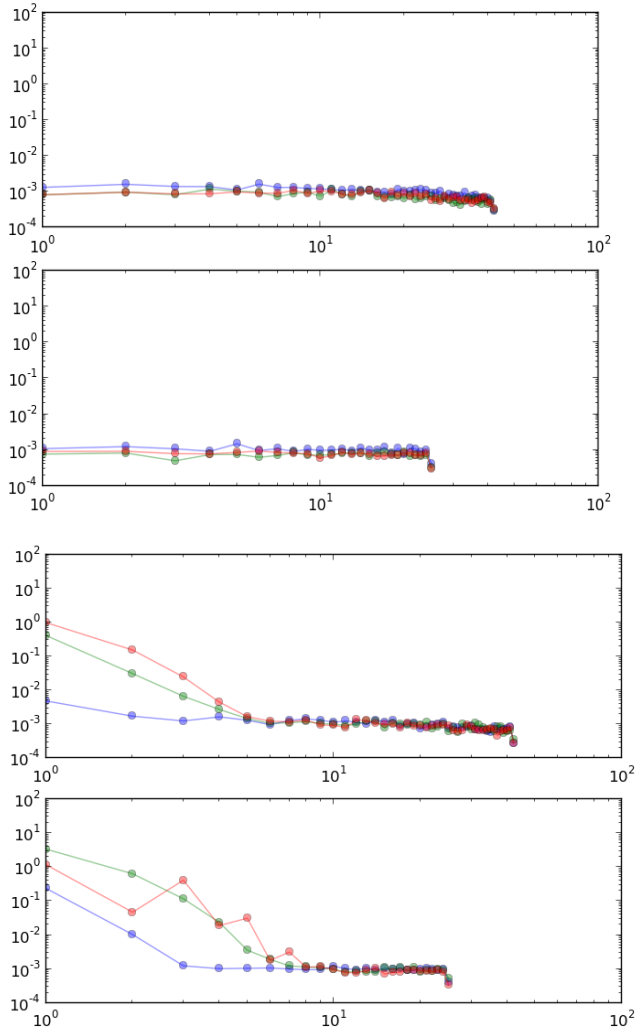
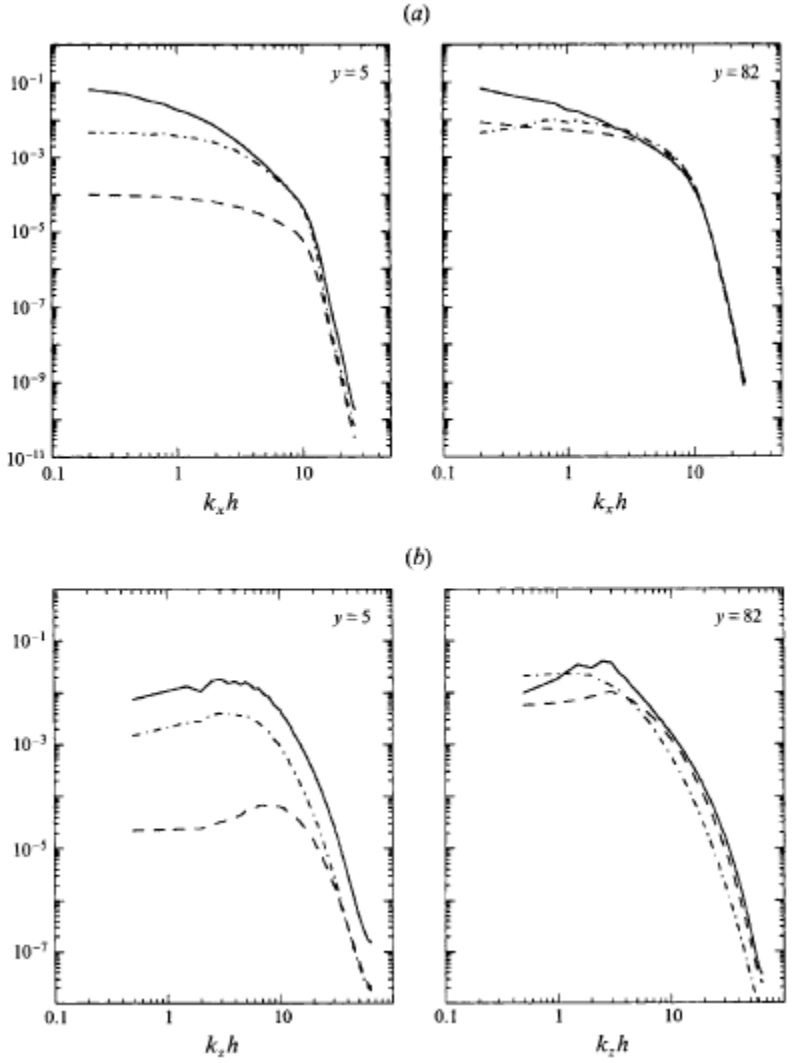
Velocity Spectra





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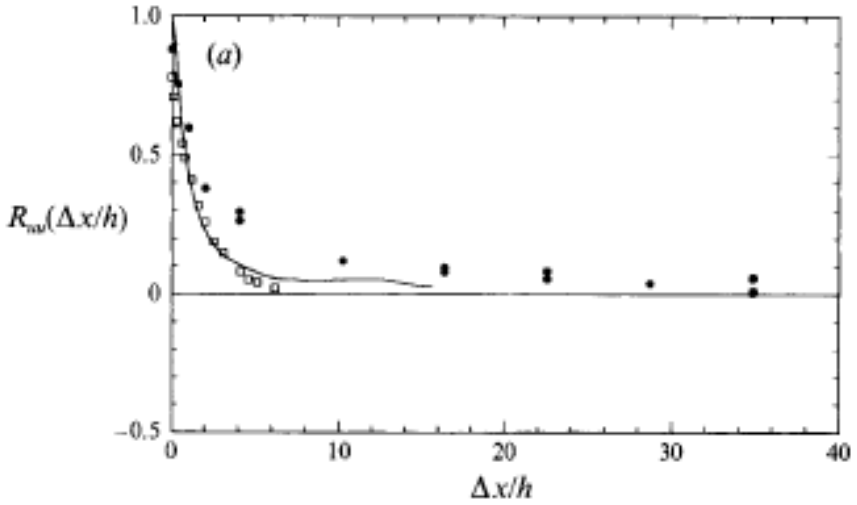
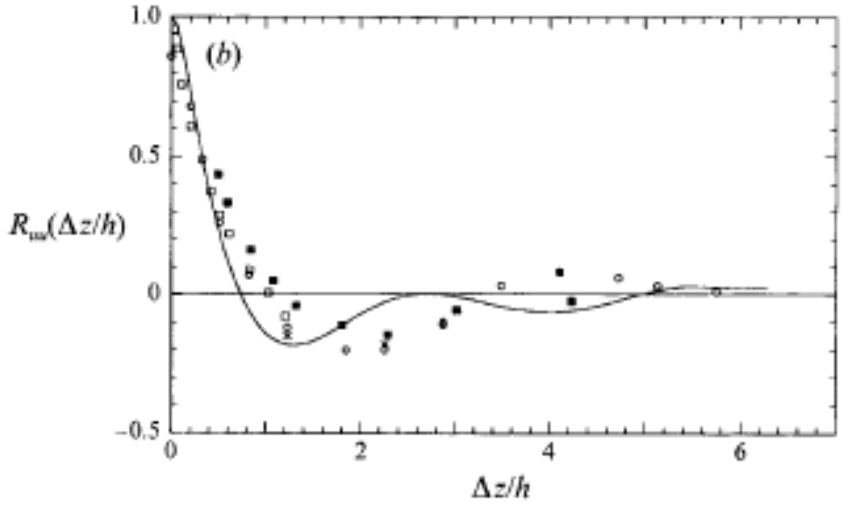
Spatial or Temporal Correlations

FIGURE 8. Correlation coefficient at the centreline. (*a*) Streamwise correlation: —, DNS; •, LDV. (*b*) Spanwise correlation: —, DNS; ○, LDV (unblocked channel); ×, LDV (blocked channel); ■, hot-film; □, Robertson & Johnson (1970), $Re = 11\,800$ (hot wire).





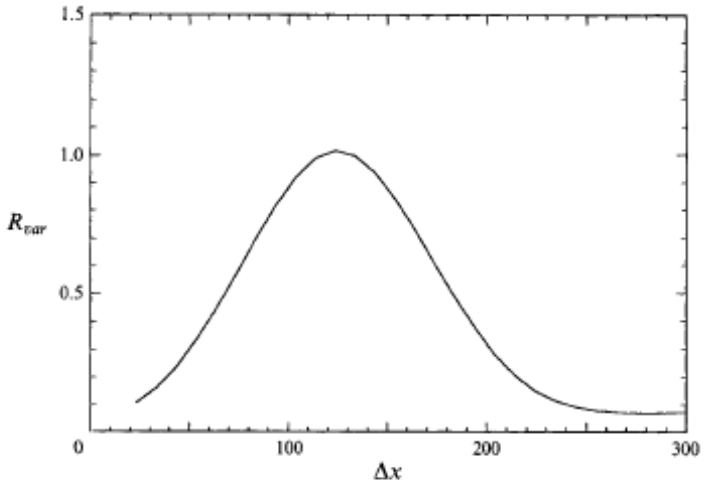


FIGURE 10. Space–time correlation ($\Delta T = 12$) of $var_u(x, z, t; L)$ from the DNS at $y = 13$. Integration length $L = 170$.

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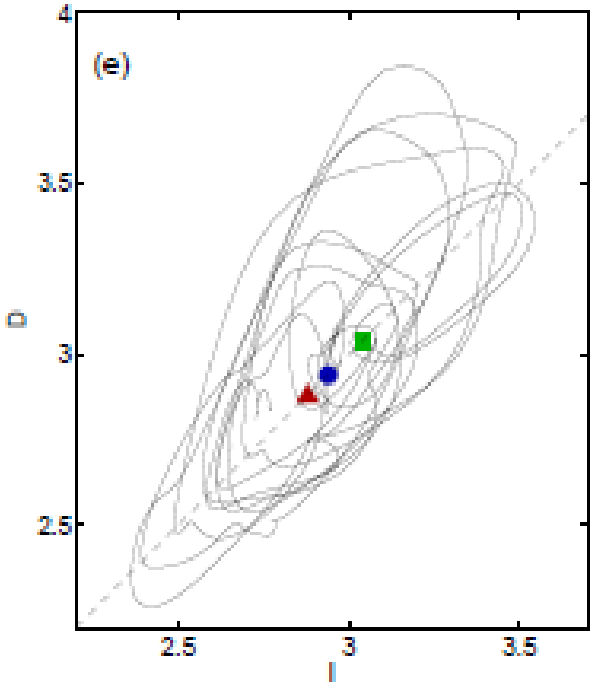
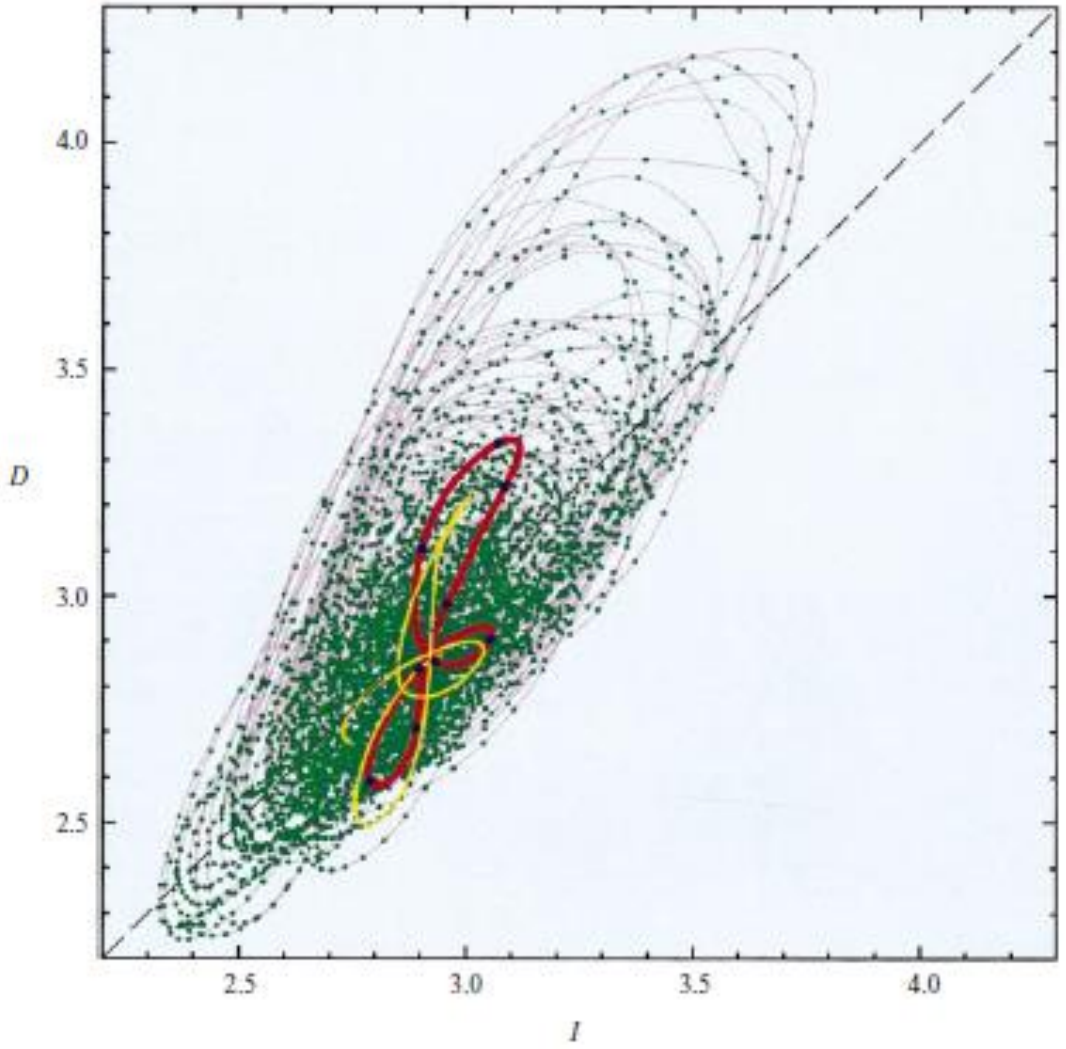
Periodic Orbit

$$E(t) = \frac{1}{V}\int_\Omega d\mathbf{x}\,\frac{1}{2}|\mathbf{u} + y\,\hat{\mathbf{x}}|^2$$

$$D(t) = \frac{1}{V}\int_\Omega d\mathbf{x}\,|\boldsymbol{\nabla}\times(\mathbf{u} + y\,\hat{\mathbf{x}})|^2$$

$$I(t) = 1 + \frac{1}{2A}\int_A dx\,dz\,\left(\frac{\partial u}{\partial y}\Big|_{y=1} + \frac{\partial u}{\partial y}\Big|_{y=-1}\right),$$





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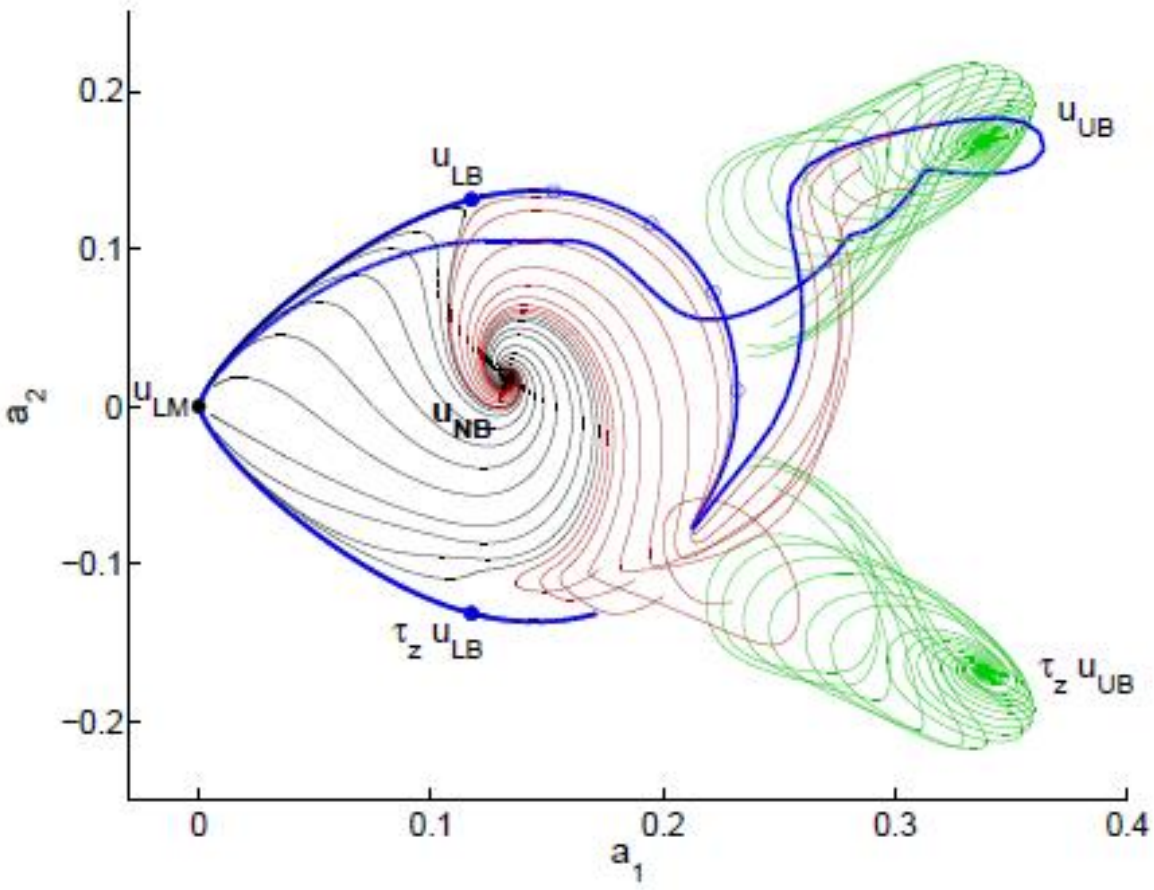
Phase Space Projection

- Using the minimal channel equilibrium solutions to build a basis set and take the dot product with the existing flow field



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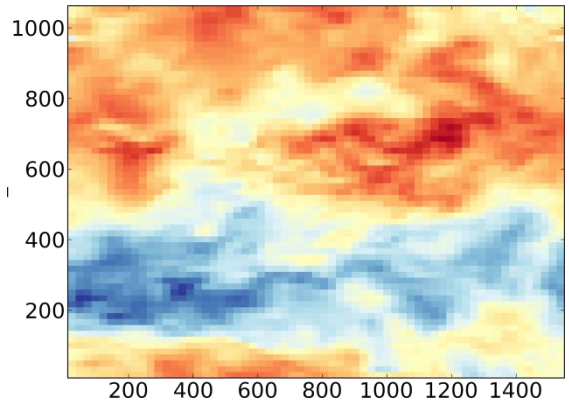
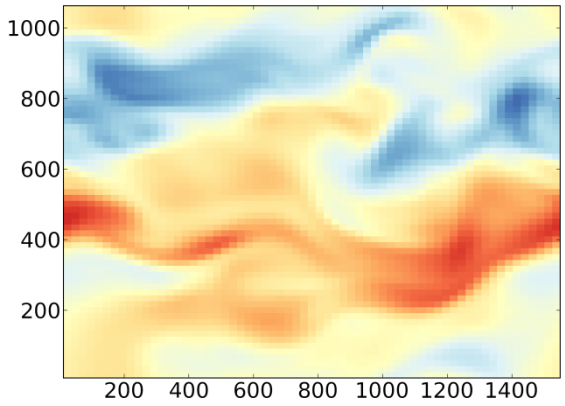
Three plots of decreasing Reynolds Number

$$Re = \frac{\rho U L}{\mu}$$

Re ≈ 4000



Re ≈ 1000



Re ≈ 400