APS | DFD 16

Division of Fluid Dynamics
Portland, Oregon | November 20 -22

APS physics

Session A35:

Turbulence: General I

8:00am to 9:31am

Chair: Edward Smith, Imperial College London

Imperial College London

A Molecular Dynamics Simulation of the Turbulent Couette Minimal Flow Unit

APS 2016

8:00 AM–8:13PM

By
Edward Smith

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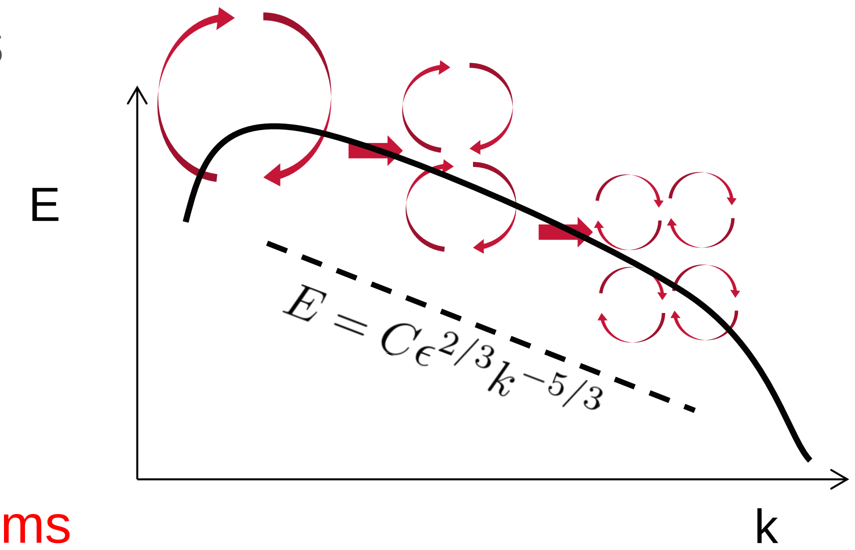
APS physics

EPSRC
Pioneering research and skills

What is Turbulence?

- Turbulent flow
  - Fluid flow which is spatially and temporally varying
  - Inertial effects dominate viscous
  - No clear order and not simply chaotic motions
- Some standard characteristics
  - Statistics are reproducible
  - The law of the wall
  - Range of scales
- Minimal Channel flow
  - Is it turbulence?
  - Insight into fundamental mechanisms
  - For molecular dynamics this is all we can do with current computers



The Minimum Flow Unit

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

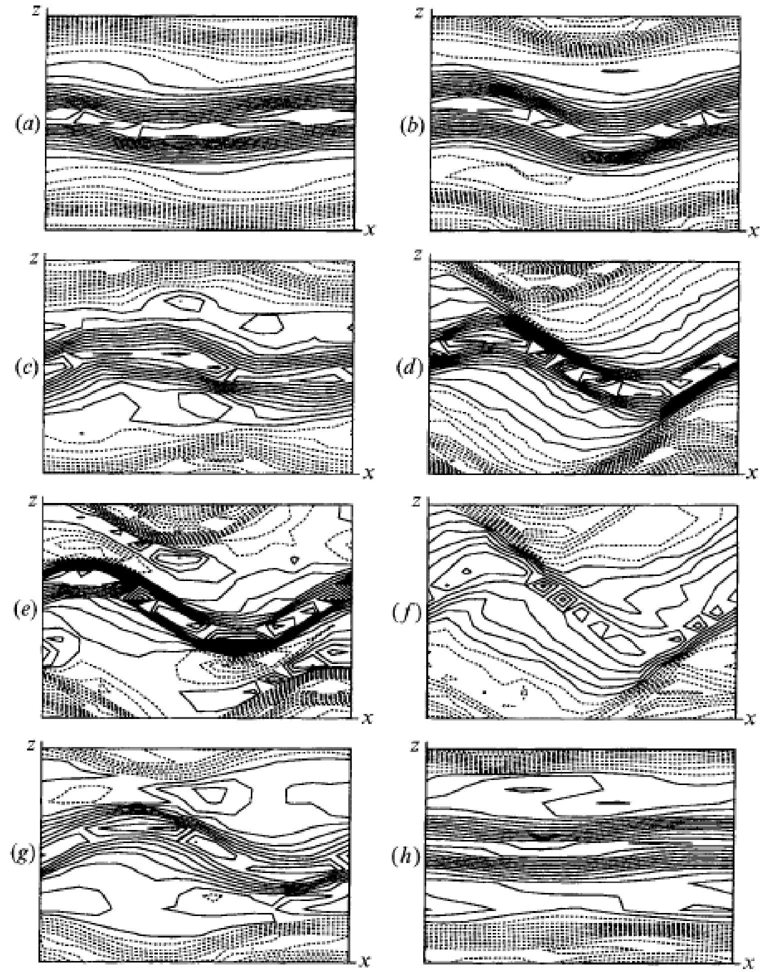
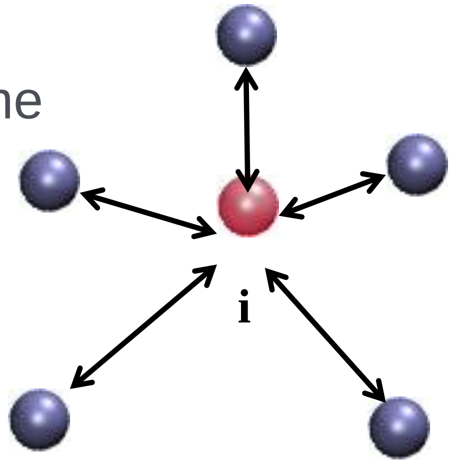


FIGURE 2. Iso-contours of u-velocity in the (x, z)-plane centred between the walls; solid contours positive, dashed contours negative. Contour interval 0.032. (a) $t = 757.5$, (b) $t = 764.8$, (c) $t = 772.0$, (d) $t = 777.8$, (e) $t = 783.0$, (f) $t = 794.1$, (g) $t = 808.2$, (h) $t = 830.2$.

Molecular Dynamics

Discrete molecules in continuous space

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

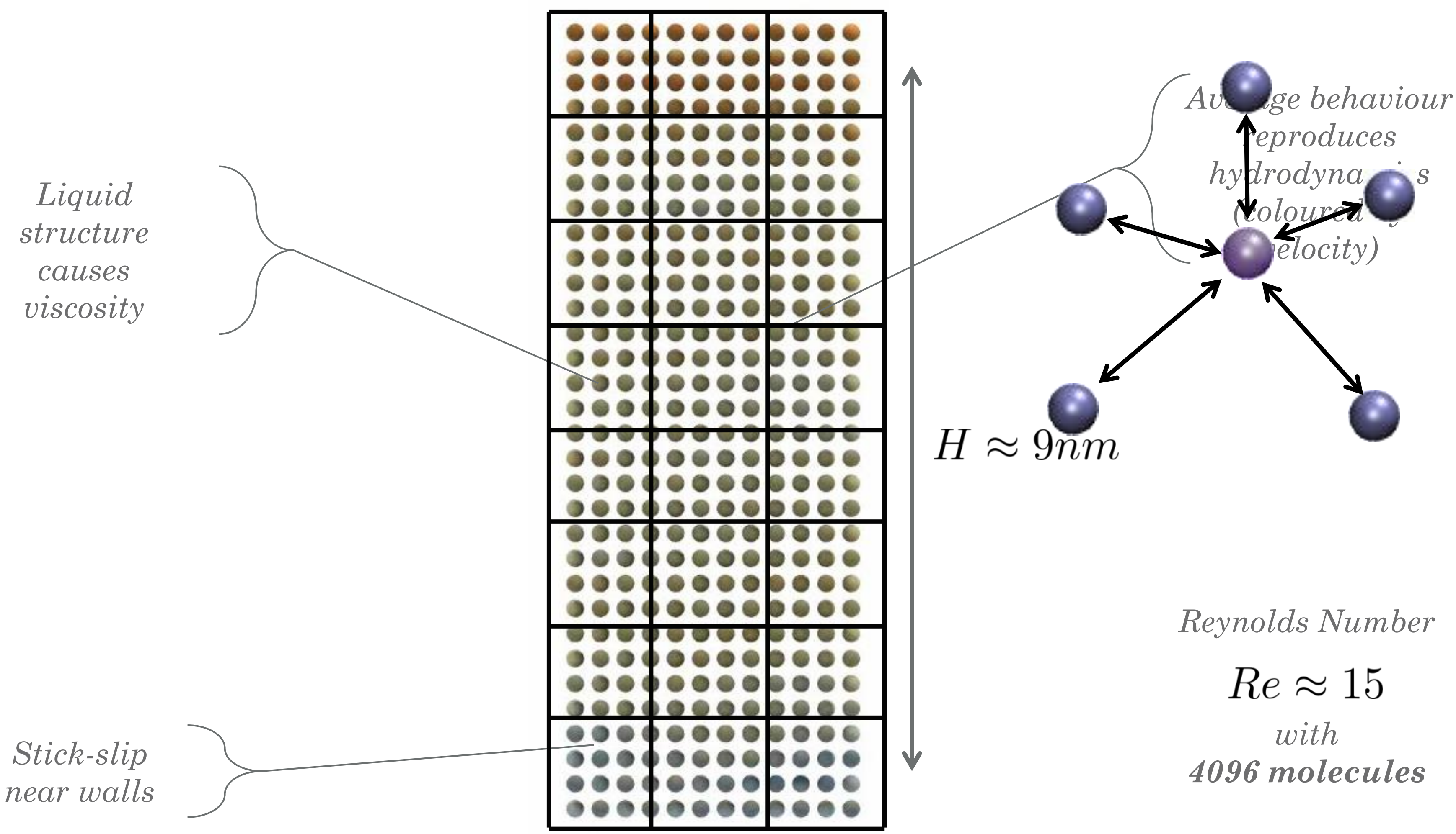


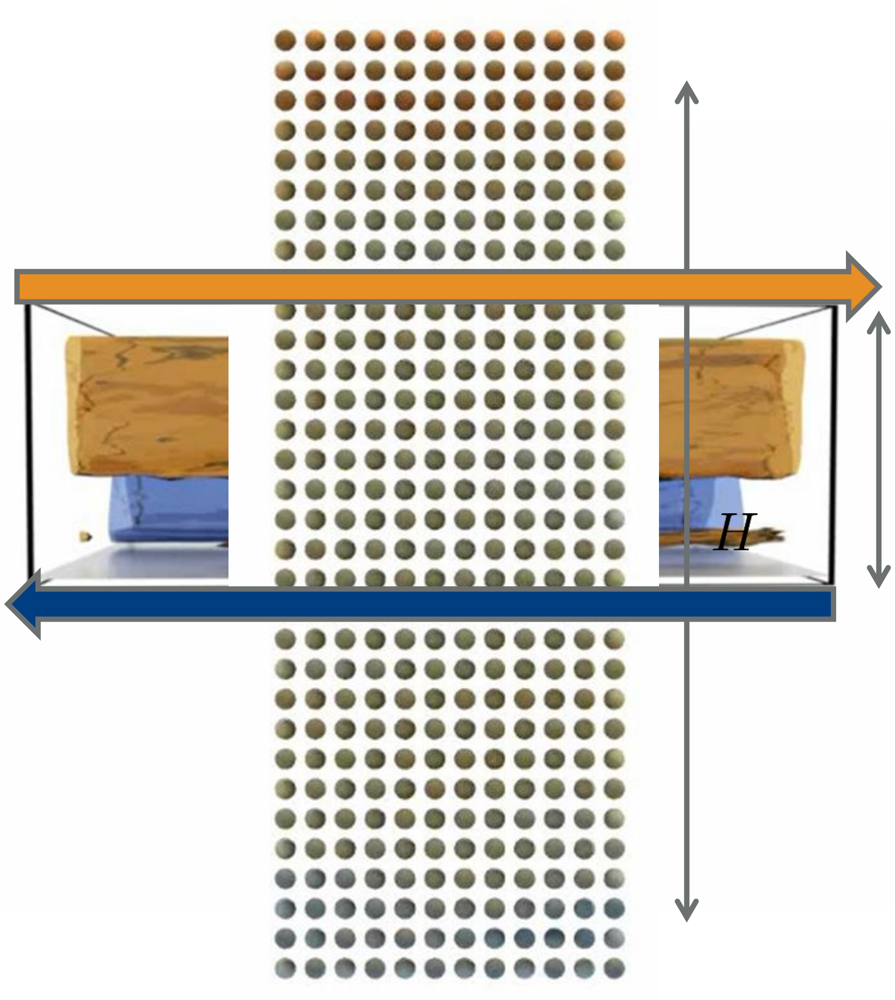
$$\ddot{\boldsymbol{r}}_i \rightarrow \dot{\boldsymbol{r}}_i$$
$$\dot{\boldsymbol{r}}_i \rightarrow \boldsymbol{r}_i(t)$$

Acceleration obtained from forces

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

$$m_i \ddot{\boldsymbol{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^{N} \boldsymbol{f}_{ij} \qquad \Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$


Liquid structure causes viscosity
Stick-slip near walls
$H \approx 9nm$
Av ge behaviour
reproduces
hydrodyna s
(coloured
elocity)
Reynolds Number
$Re \approx 15$
with
4096 molecules



Reynolds Number

$$Re \approx 100$$

with

4096 molecules

Minimal channel Couette flow

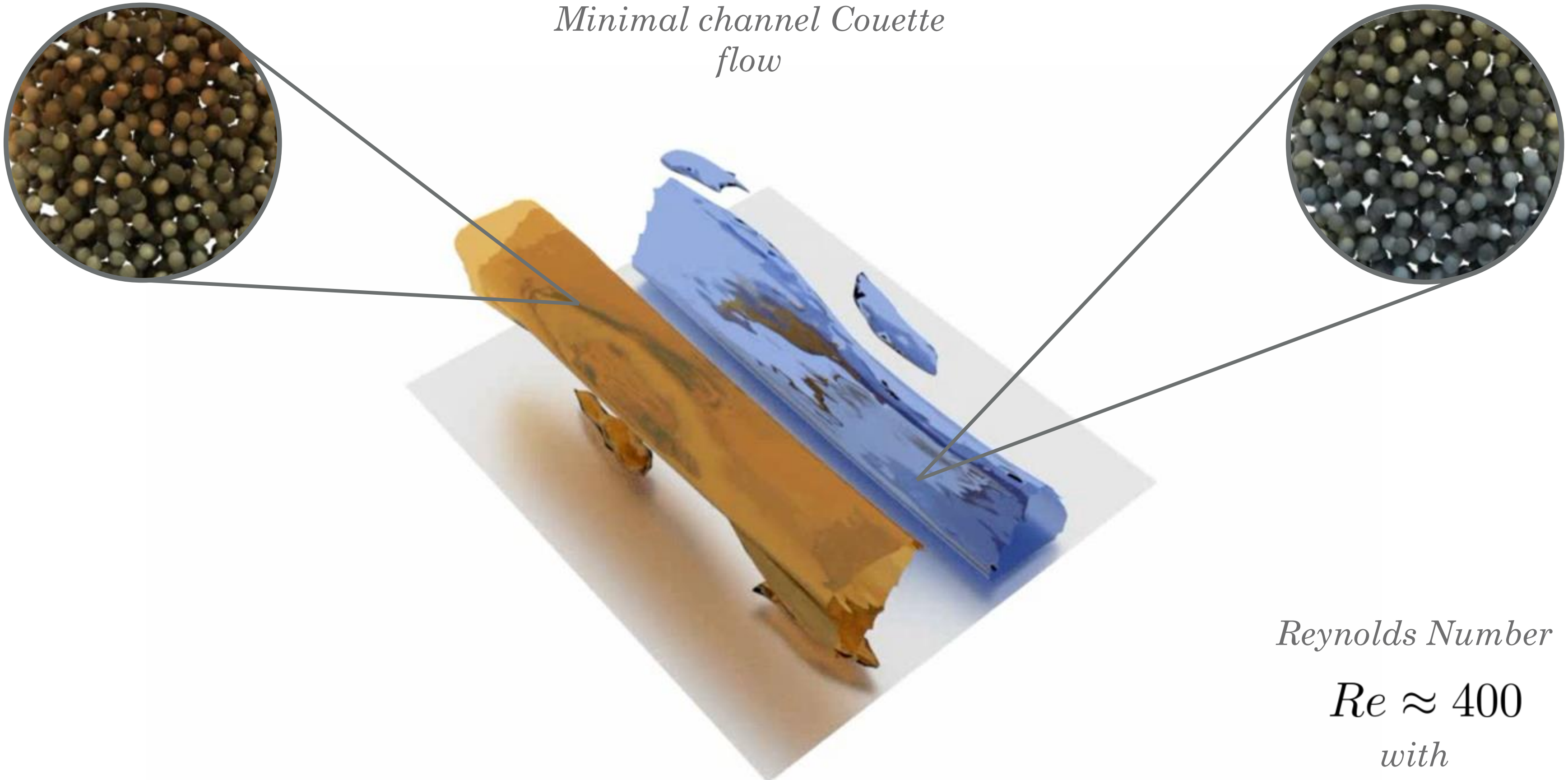
Reynolds Number

$Re \approx 400$

with

300 million molecules

Minimal channel Couette flow



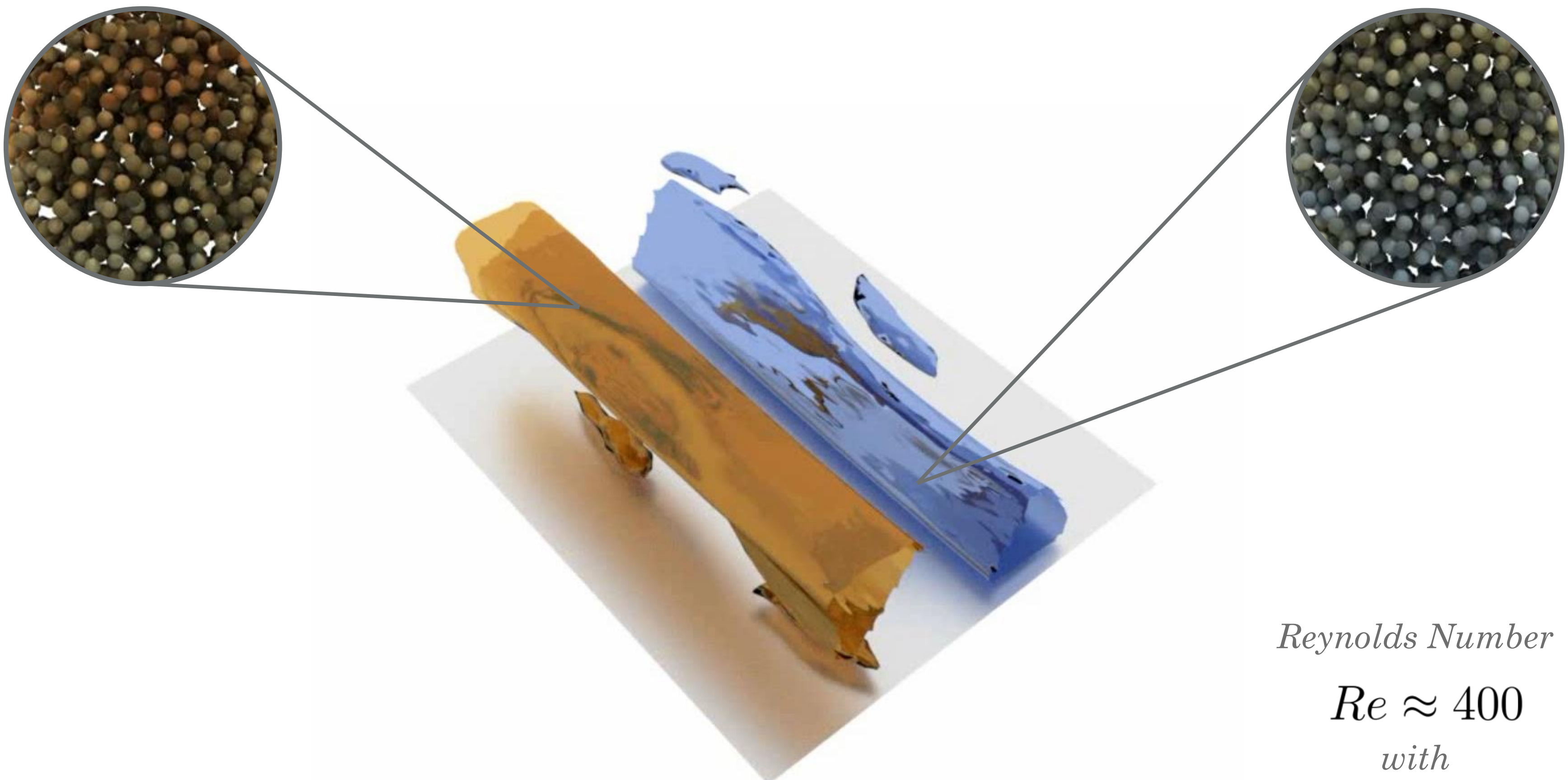
Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$$Re \approx 400$$

with

300 million molecules



Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$$Re \approx 400$$

with ***300 million molecules***

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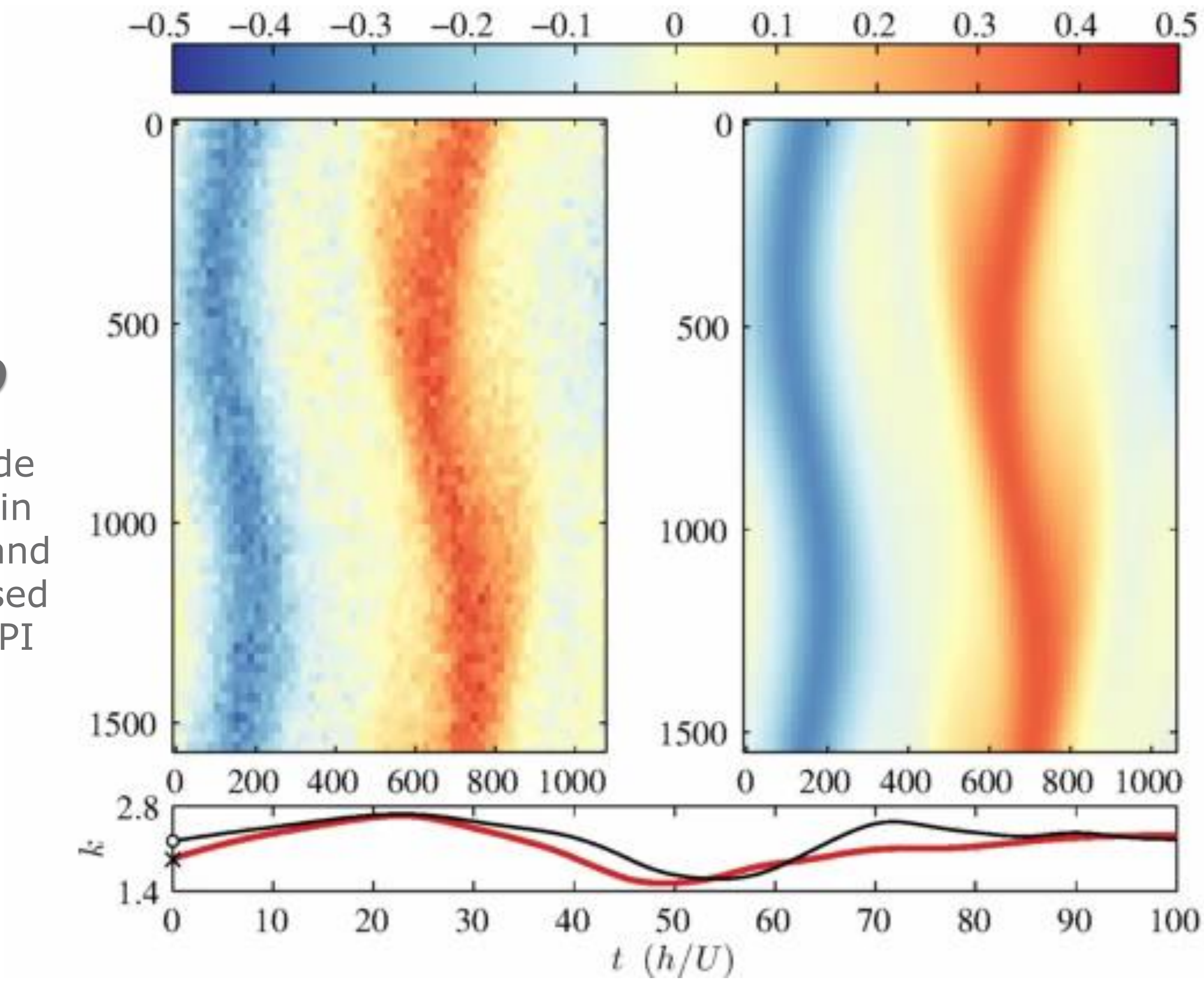
Centre slice velocity



MD

Own code written in Fortran and parallelised using MPI

CFD (Channelflow)

F. Gibson. Channelow: A spectral Navier-Stokes simulator in C++. Technical report, U. New Hampshire, 2012. Channelflow.org.

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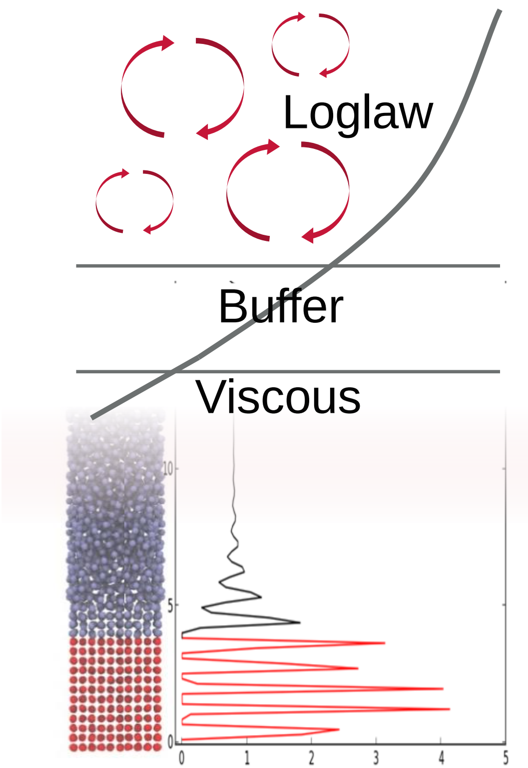
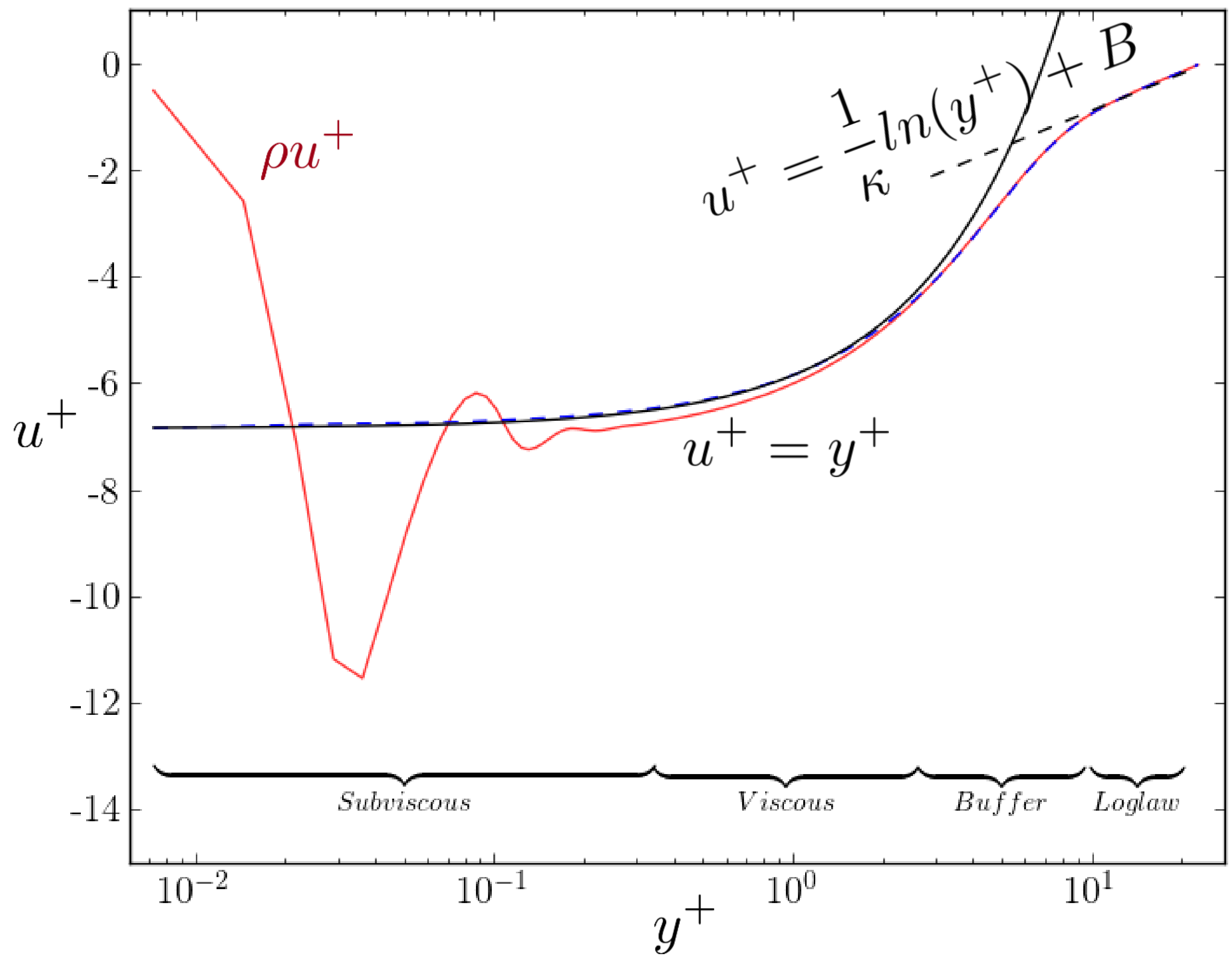
Law of the wall



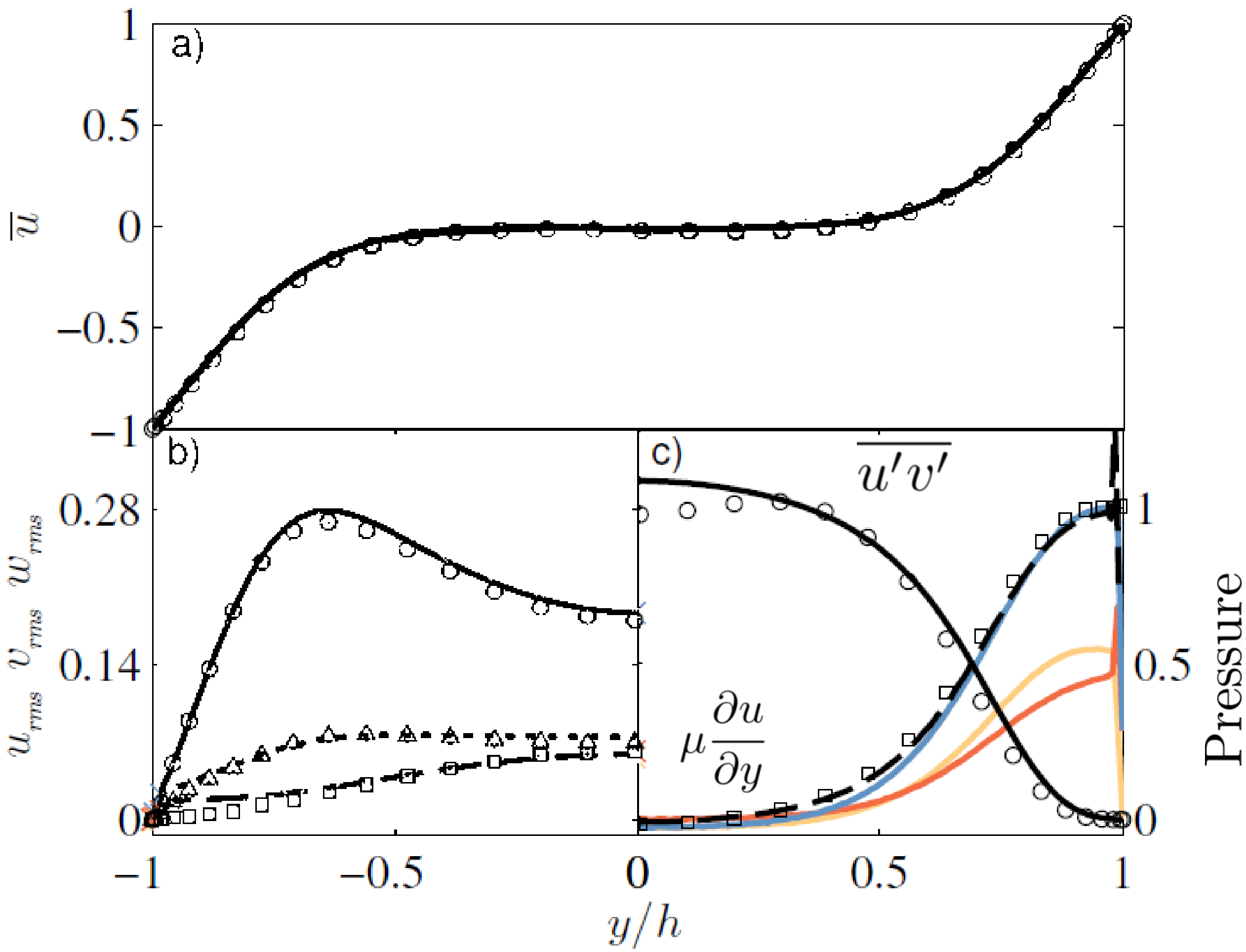
Subviscous? (MD)



Statistics

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

- Good agreement with literature
  - CFD (symbols)
  - MD (lines)
- Contributions from sub-grid scales
  - Total Pressure
  - Kinetic part
  - Configurational part



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Pressure and viscosity from an MD Simulation

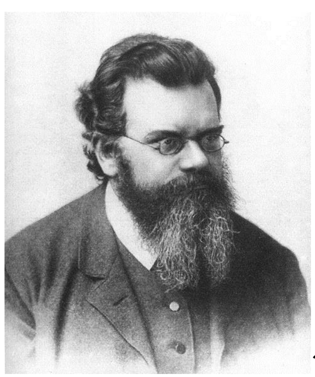
- Pressure includes kinetic and structural (configurational) component
  - Average over a control volume

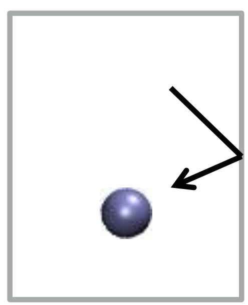
$$\oint_S \mathbf{\Pi} \cdot d\mathbf{S} = \underbrace{\sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i \boldsymbol{p}_i}{m_i} \cdot d\mathbf{S}_i \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij}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

- Autocorrelation of the shear pressure is the viscosity

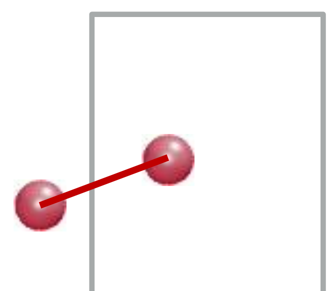
Kinetic theory part

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

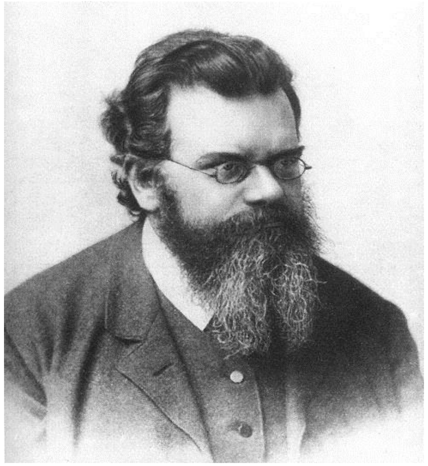
Same Concept, Different Scales

- Reynolds Decomposition

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

- Peculiar velocity

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

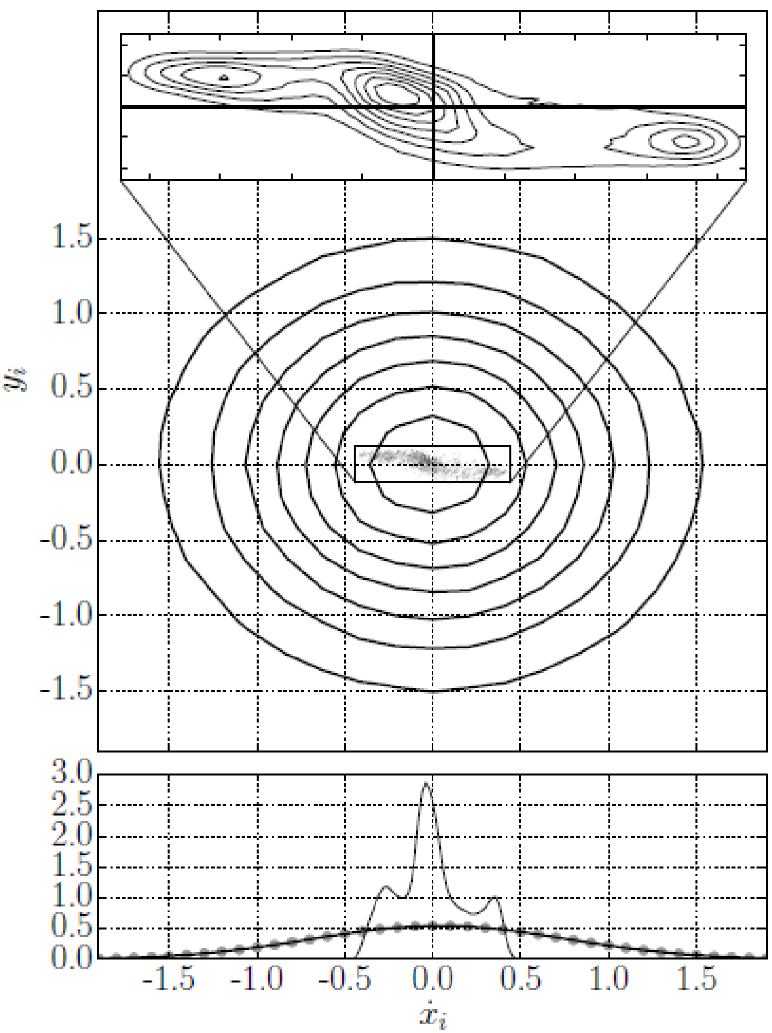


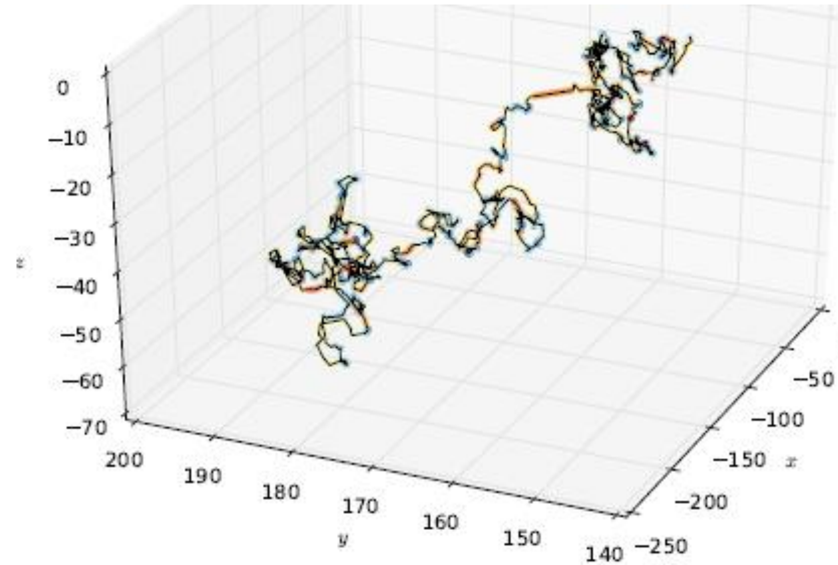
- Kinetic pressure and Reynolds stress are the same thing on different length/time scales

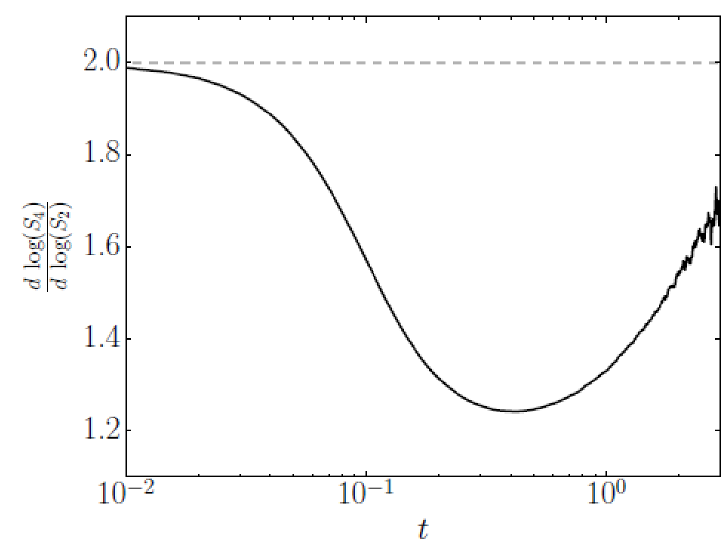
$$\overline{\sum \langle m_i \dot{\boldsymbol{r}}_i \dot{\boldsymbol{r}}_i \rangle} = \overline{\sum \langle \boldsymbol{p}_i \boldsymbol{p}_i / m_i \rangle} + \overline{\rho \boldsymbol{u}' \boldsymbol{u}'} + \overline{\rho \boldsymbol{u} \boldsymbol{u}}$$

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

Probability density functions, diffusion and structure factor







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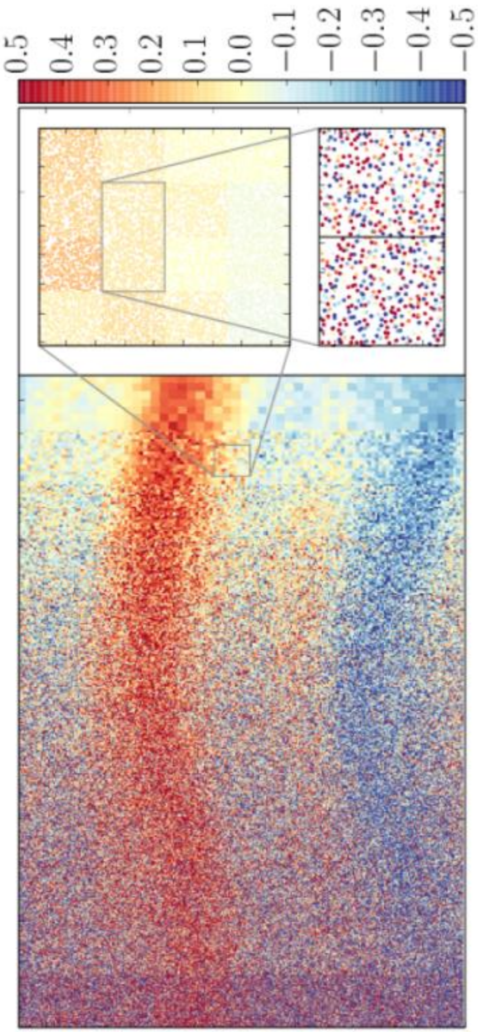
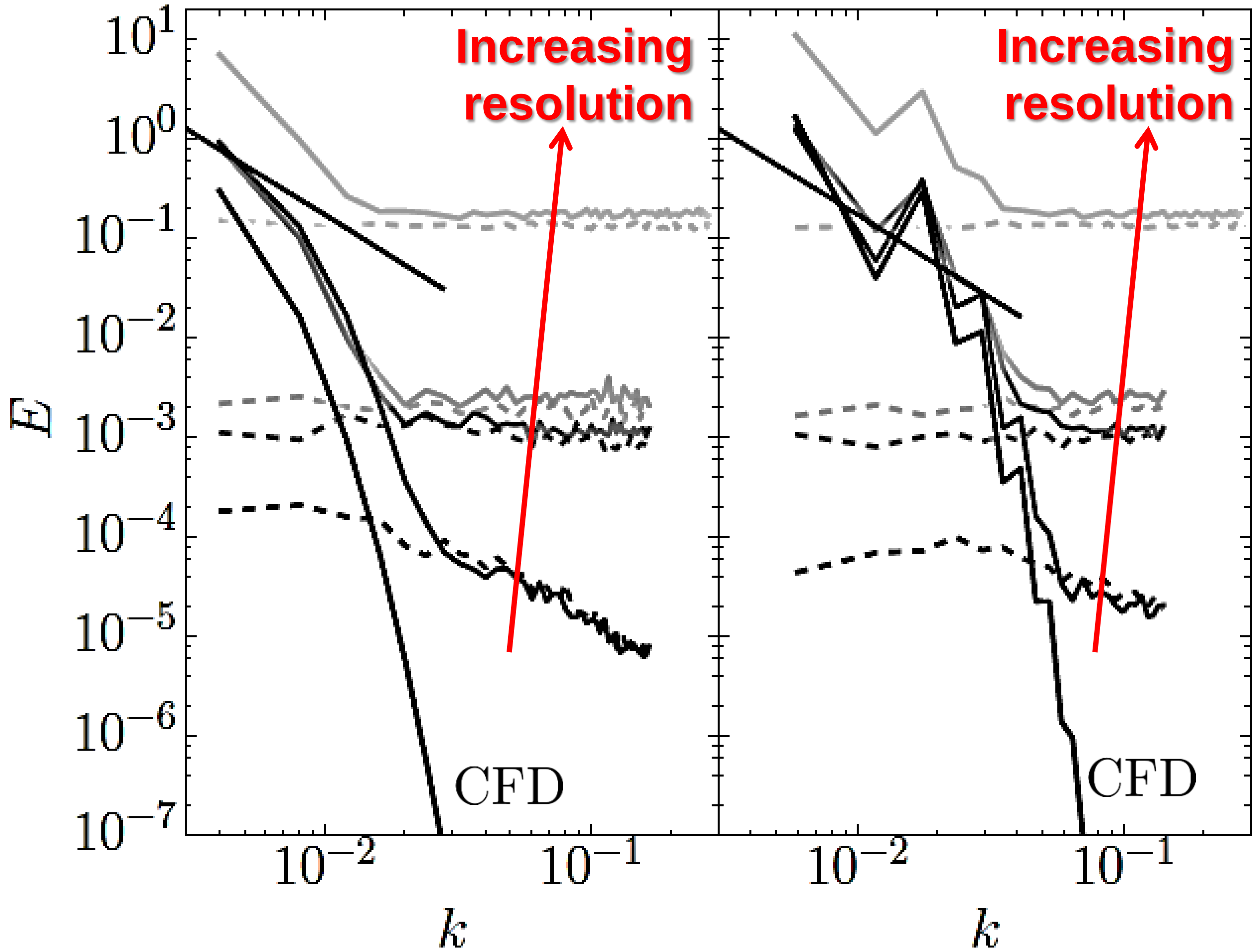
Spectra

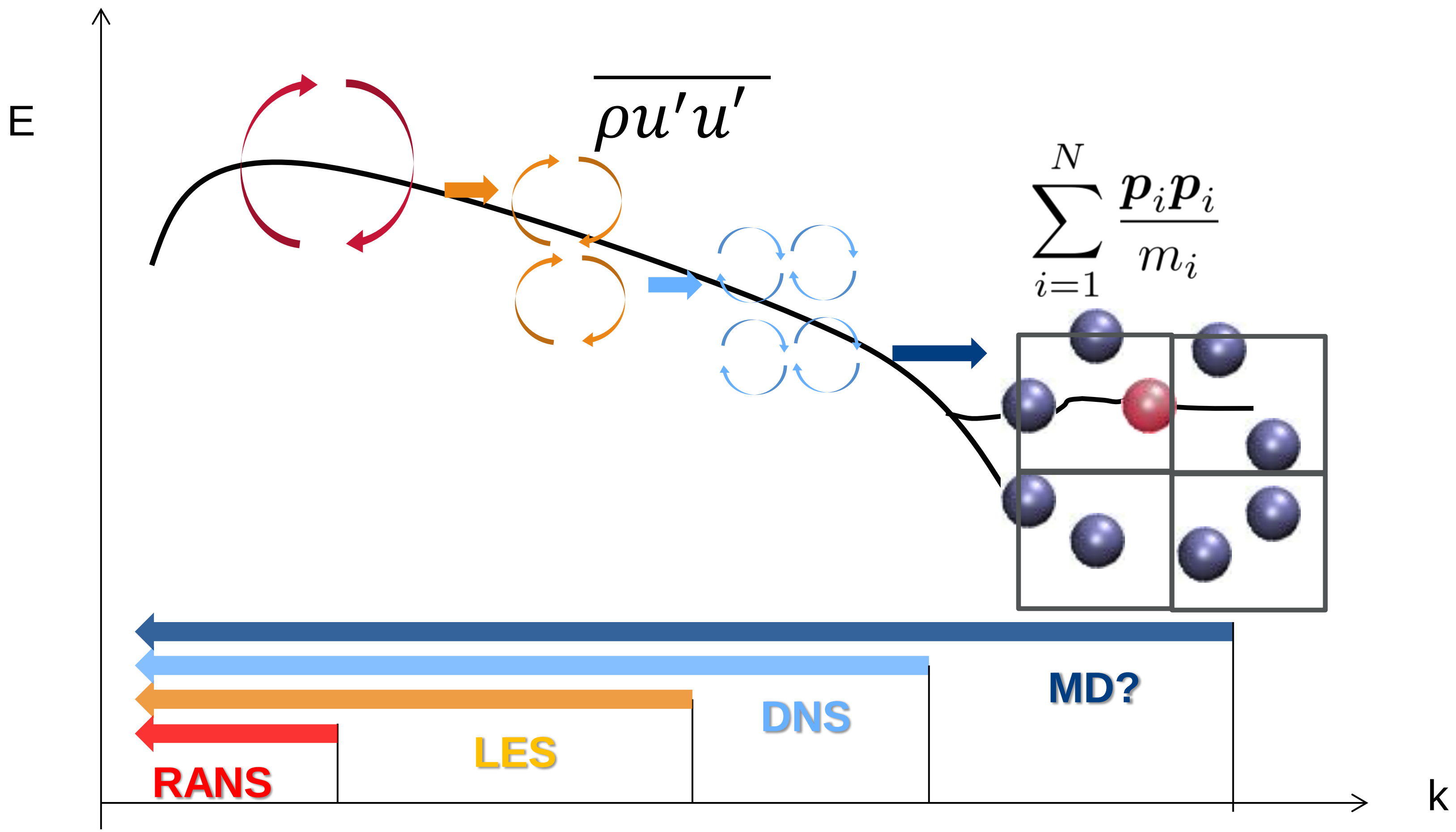




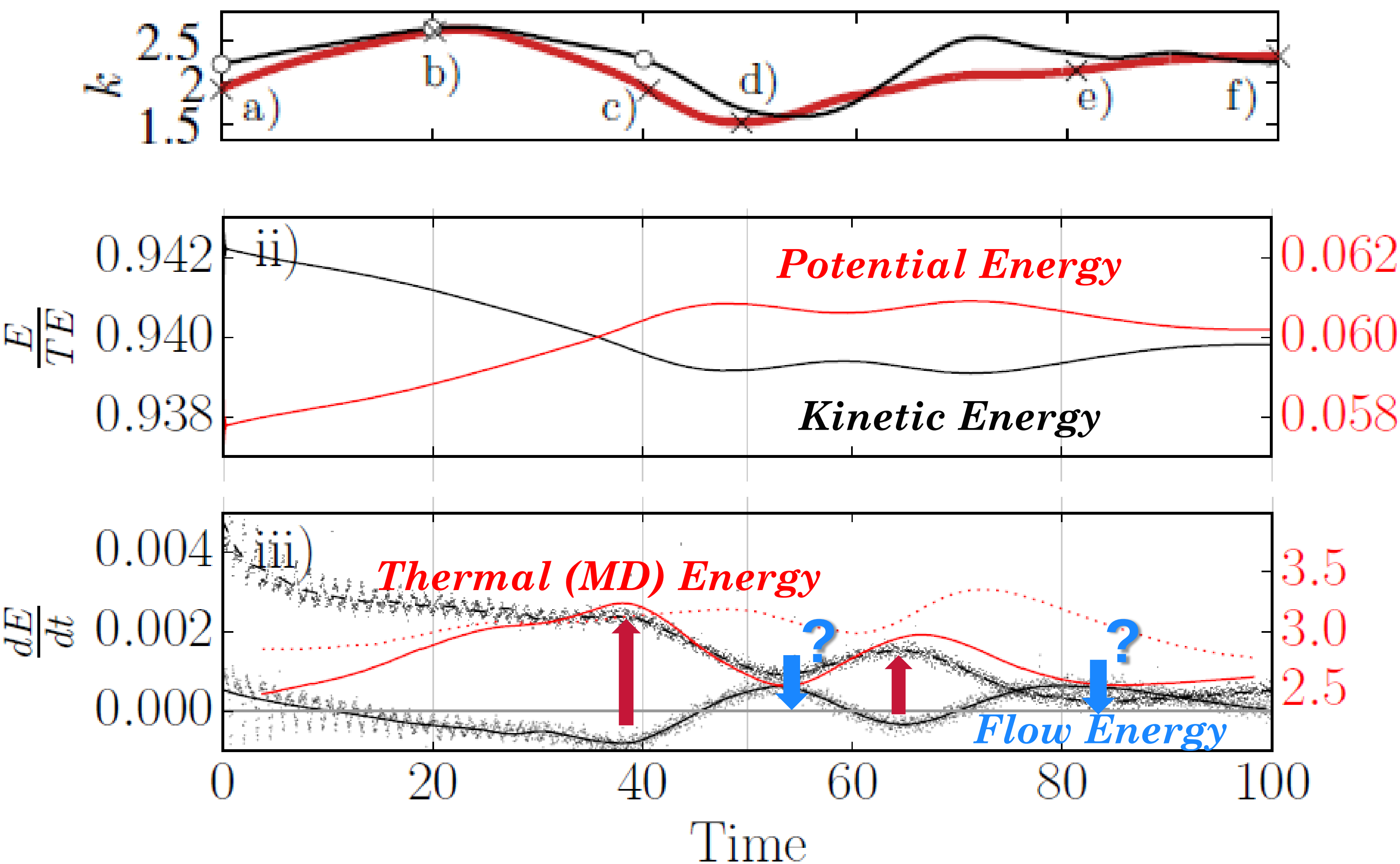
Dotted lines - laminar initial condition at same Re

Reynolds Stress to Kinetic Pressure

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



Energy is Conserved by Molecular Dynamics



Summary

- MD has turbulent like flow features (never seen before)
  - Statistics, law of the wall, spectra, PDFs, etc

- MD Reproduces More Physics and Full Range of Scales
  - Thermal motions and all classical sub-grid scales
  - Molecular liquid lattice has cages and molecules rotate
  - Average gives pressure and viscosity which inspires the Reynolds stress tensor and closure assumptions

- Minimal Channel looks promising
  - Although arguably not turbulence, reproduces a key mechanism
  - For molecular dynamics this ran on 256 cores but large HPC or GPUs could do far more