Brunel University London

Molecular Fluid Dynamics

By

Edward Smith

05/03/19

The University of Melbourne

Summary

- Introduction
- Molecular Dynamics
- The Minimal Channel

Brunel University London

Section 0

INTRODUCTION

Computational Fluid Dynamics

- Fields assumed to be continuous at every point in space
  - Mass Conservation

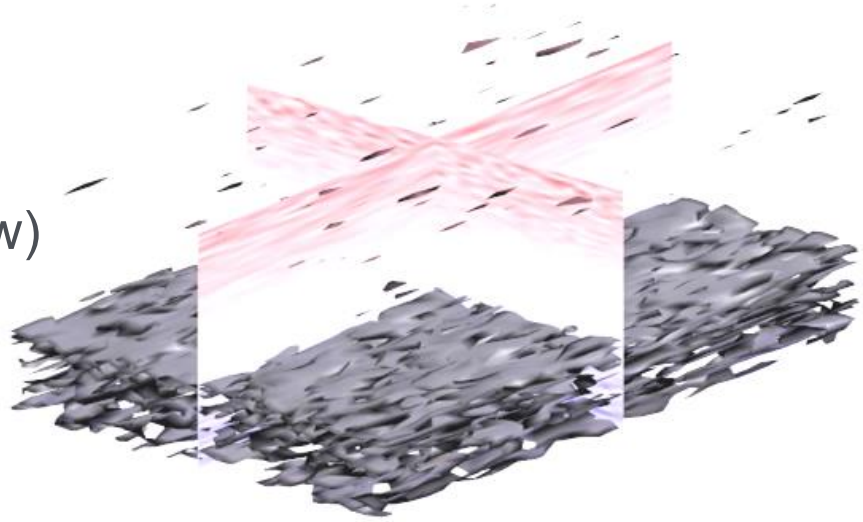
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - 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

Computational Fluid Dynamics

- The Incompressible Navier-Stokes Equation

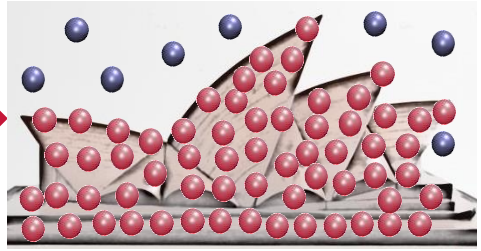
$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = -\boldsymbol{\nabla}P + \mu\nabla^2\boldsymbol{u} \qquad \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$$

- 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



Computational Fluid Dynamics

Brunel University London

- The Incompressible Navier-Stokes Equation

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

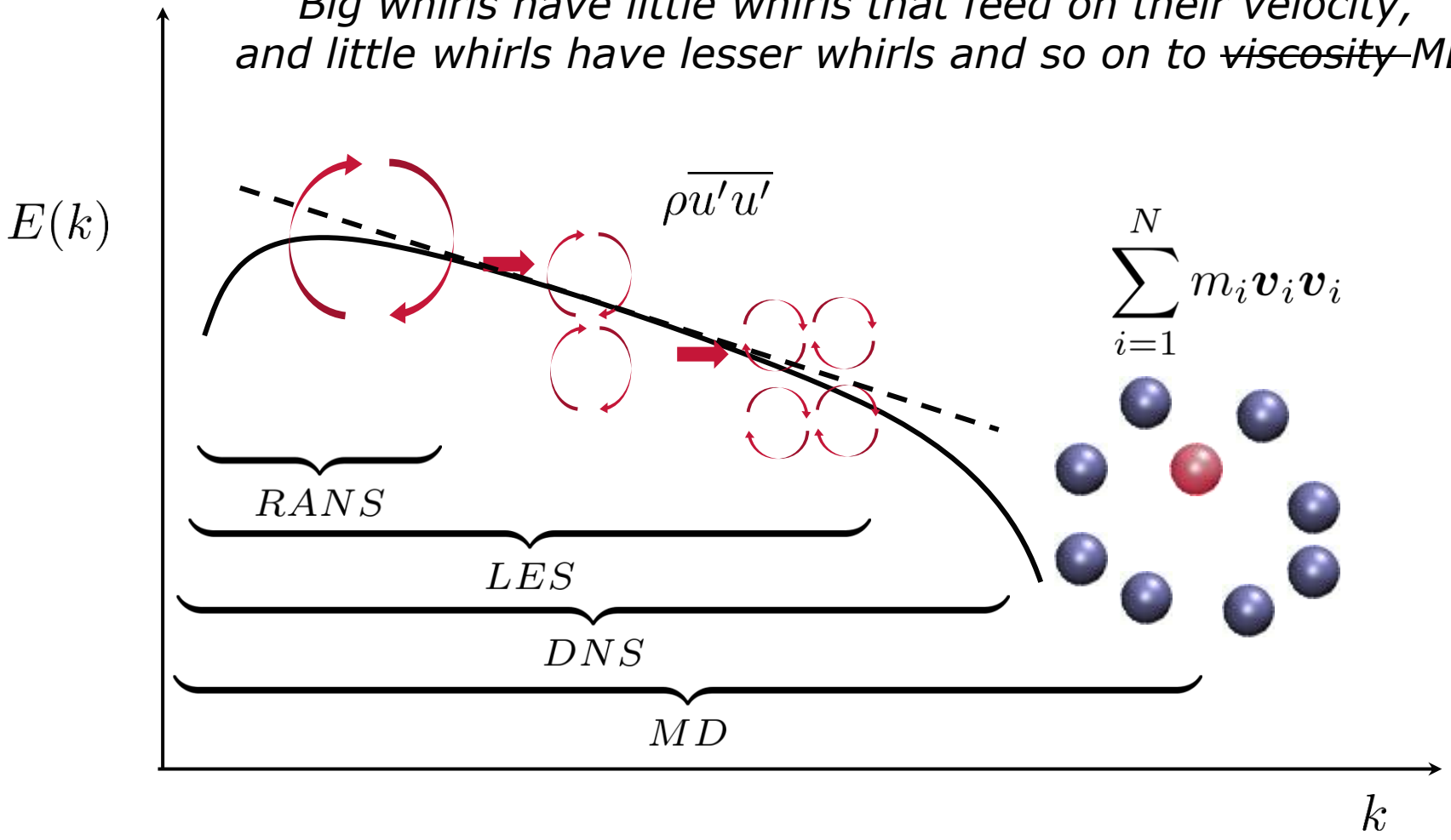
- Non dimensional form

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

- Reynolds number
  - Scaling argument applied to any scale
- Is there a minimum?
  - Travis et al (1997) single phase valid down to nanometers
  - Local thermodynamic equilibrium vs. hydrodynamic scales
  - Knudsen Number fairly useless for dense fluids

Molecular Dynamics – Beyond The Continuum

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



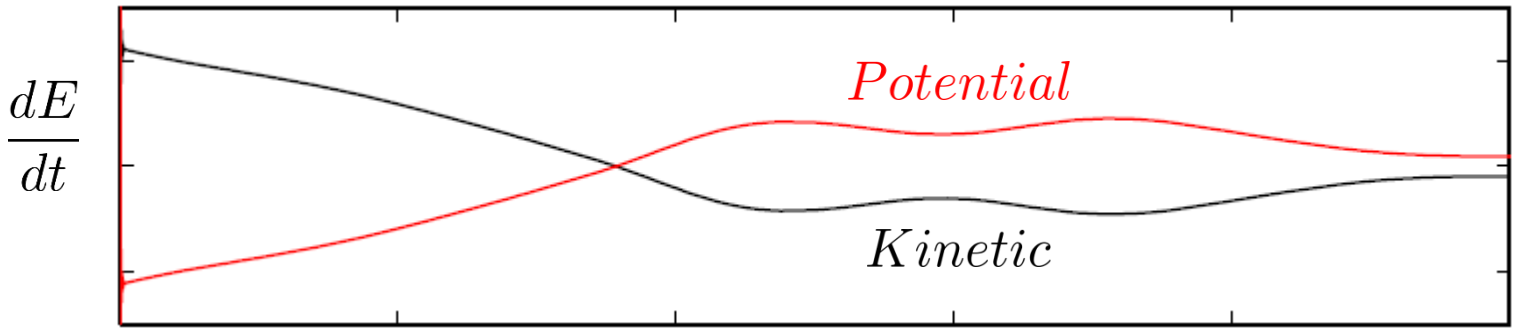
Brunel University London

Section 1

MOLECULAR DYNAMICS

Molecular Dynamics

- Solving just Newton's law
  - Energy is automatically conserved → total = kinetic + potential



  - Pressure, viscosity, heat flux and surface tension do not need to be specified and, are in fact, all outputs of the simulation
  - Phase change (evaporation, condensation) occur with no additional models needed
  - Solid-liquid surface constructed with molecular roughness
  - Can model complex molecules, water, polymers, biomolecules

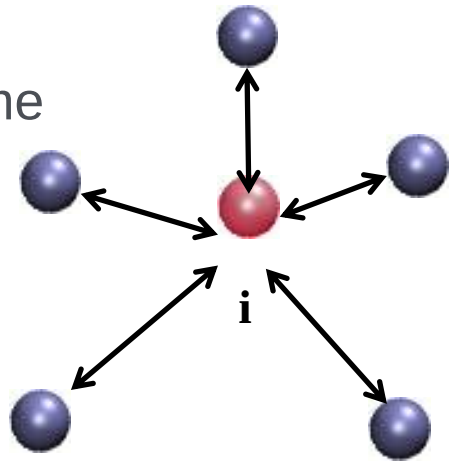
Molecular Dynamics

Brunel University London

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

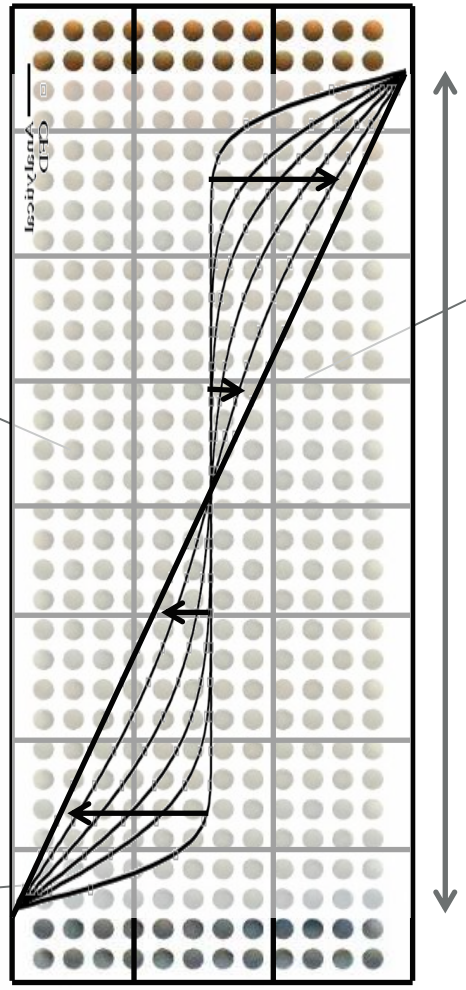
- Governed by Newton's law for an N-body system
- Point particles with pairwise interactions only

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

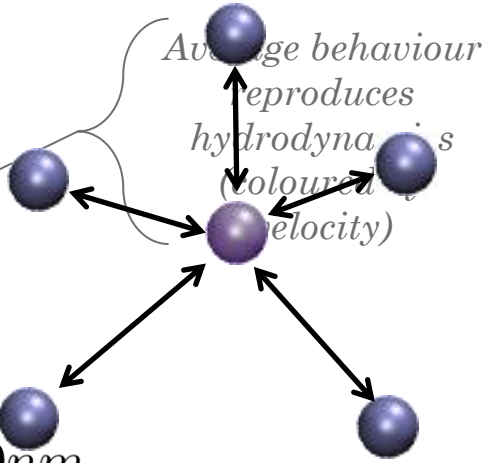
$$\Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

Molecular Dynamics

Liquid structure causes viscosity



Stick-slip near walls



$H \approx 9nm$

Reynolds Number

$Re \approx 15$

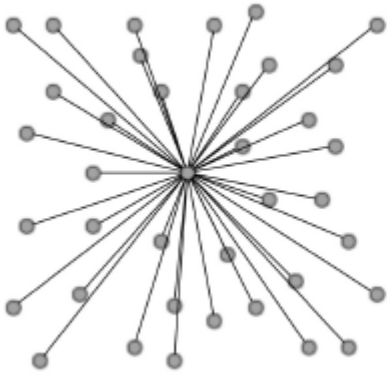
with

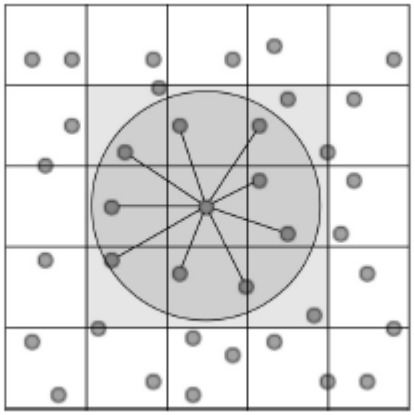
4096 molecules

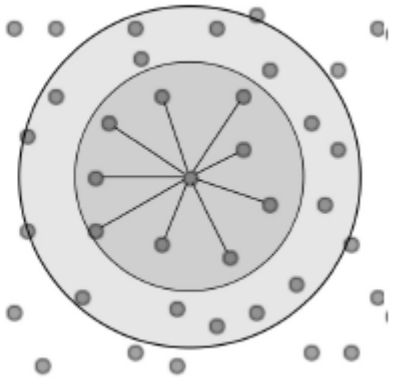
MD Computing

- Force Calculation
  - All pairs simulation uses local cell and neighbour lists to reduce the N^2 calculation to order N

$$F_i = \sum_{j \neq i}^{N} f_{ij}$$







- Move particles (leapfrog in time)

$$m_i \frac{dv_i}{dt} \approx m_i \frac{v_i(t + \Delta t/2) - v_i(t - \Delta t/2)}{\Delta t} = F_i$$

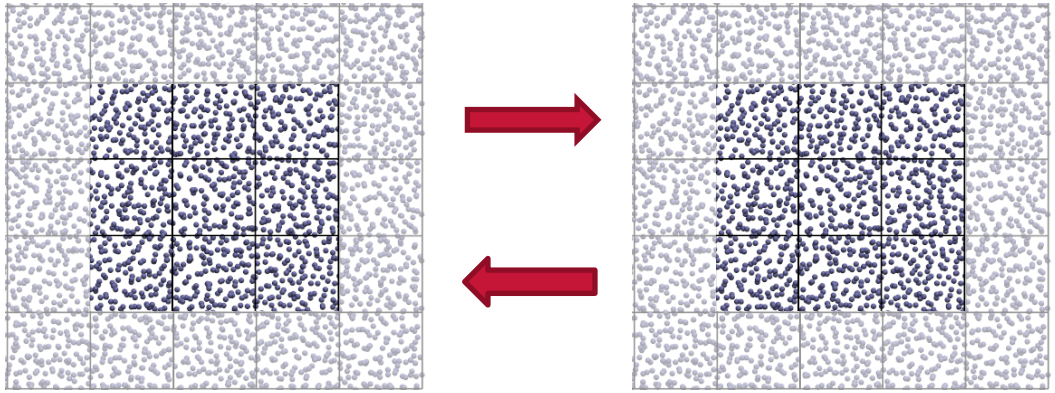
$$\frac{dr_i}{dt} \approx \frac{r_i(t + \Delta t) - r_i(t)}{\Delta t}$$

MD Computing – Parallel optimisations

Brunel University London

Localisations lends itself to parallel computing using MPI

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

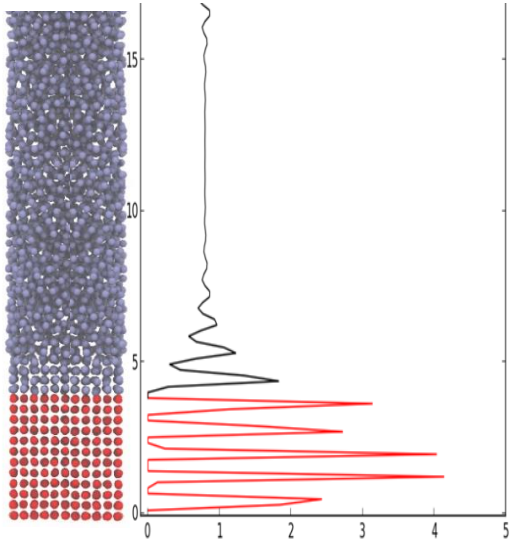


Halo exchange of variable amounts of data

- MPI_Send
- MPI_Probe and MPI_Recv

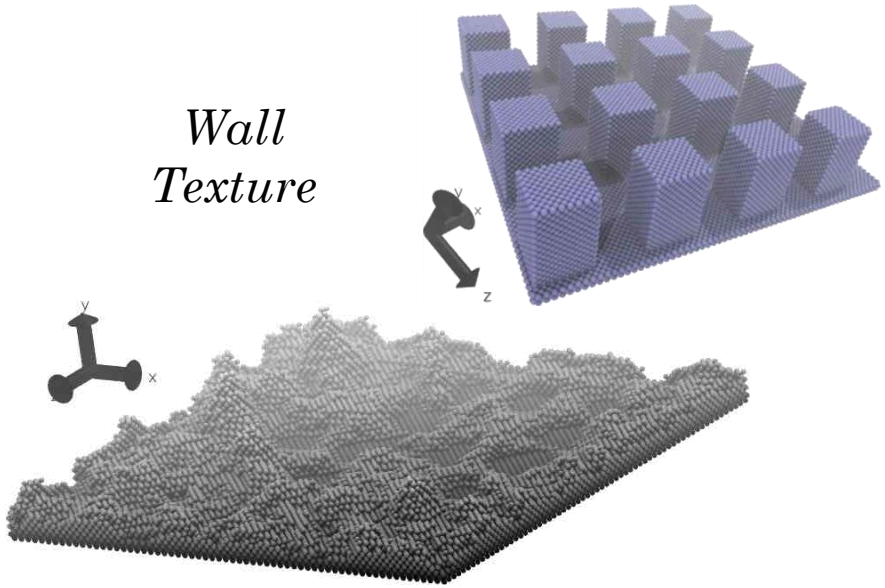
Molecular Dynamics – Complex Walls and Fluids

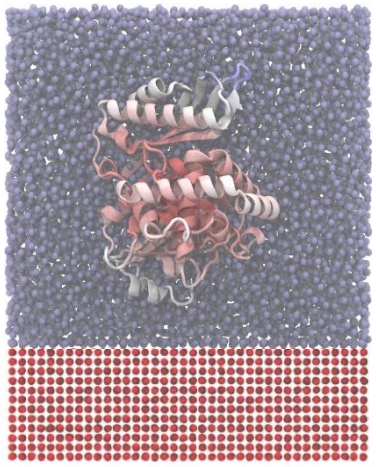
Liquid structure causes viscosity



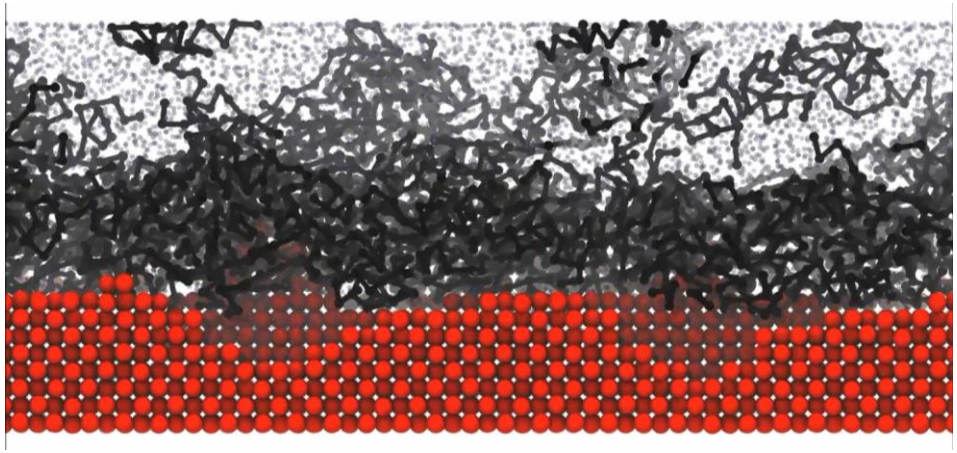
Stick-slip near walls

Wall Texture





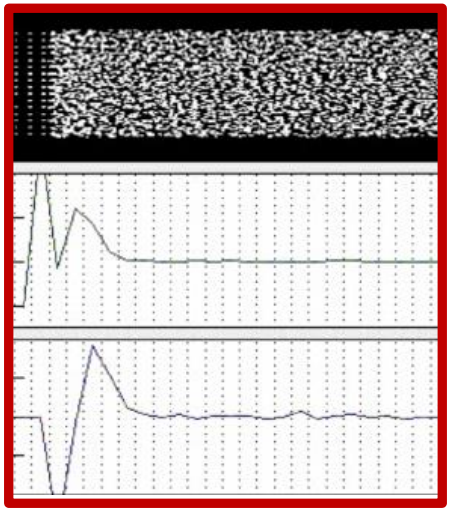
Molecules of arbitrary complexity



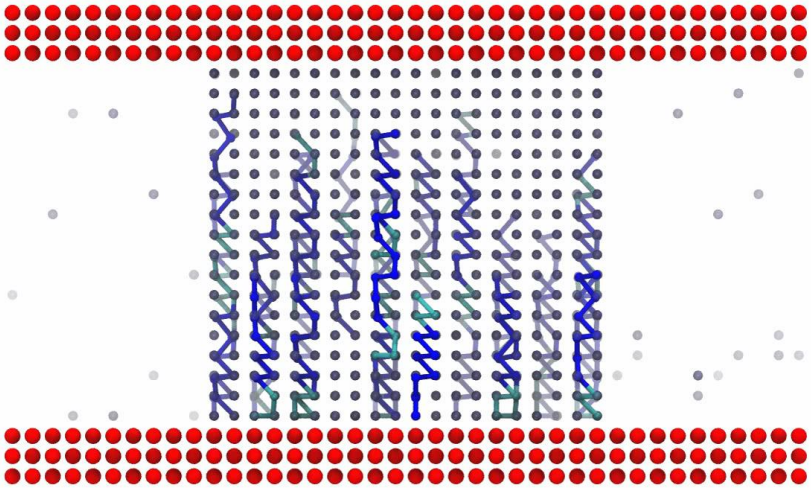
Oil, water and textured surface

Molecular Dynamics – Shocks and Multi-Phase

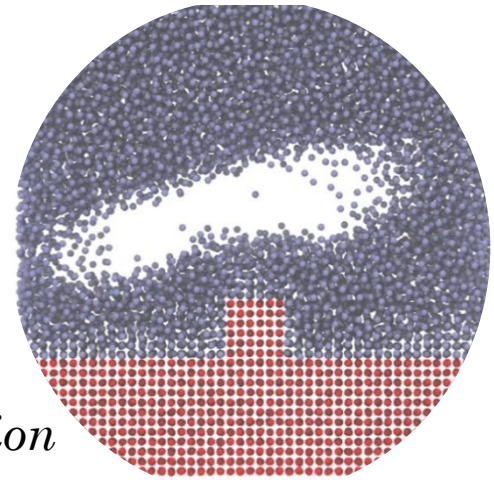
Shockwave



Droplet Formation

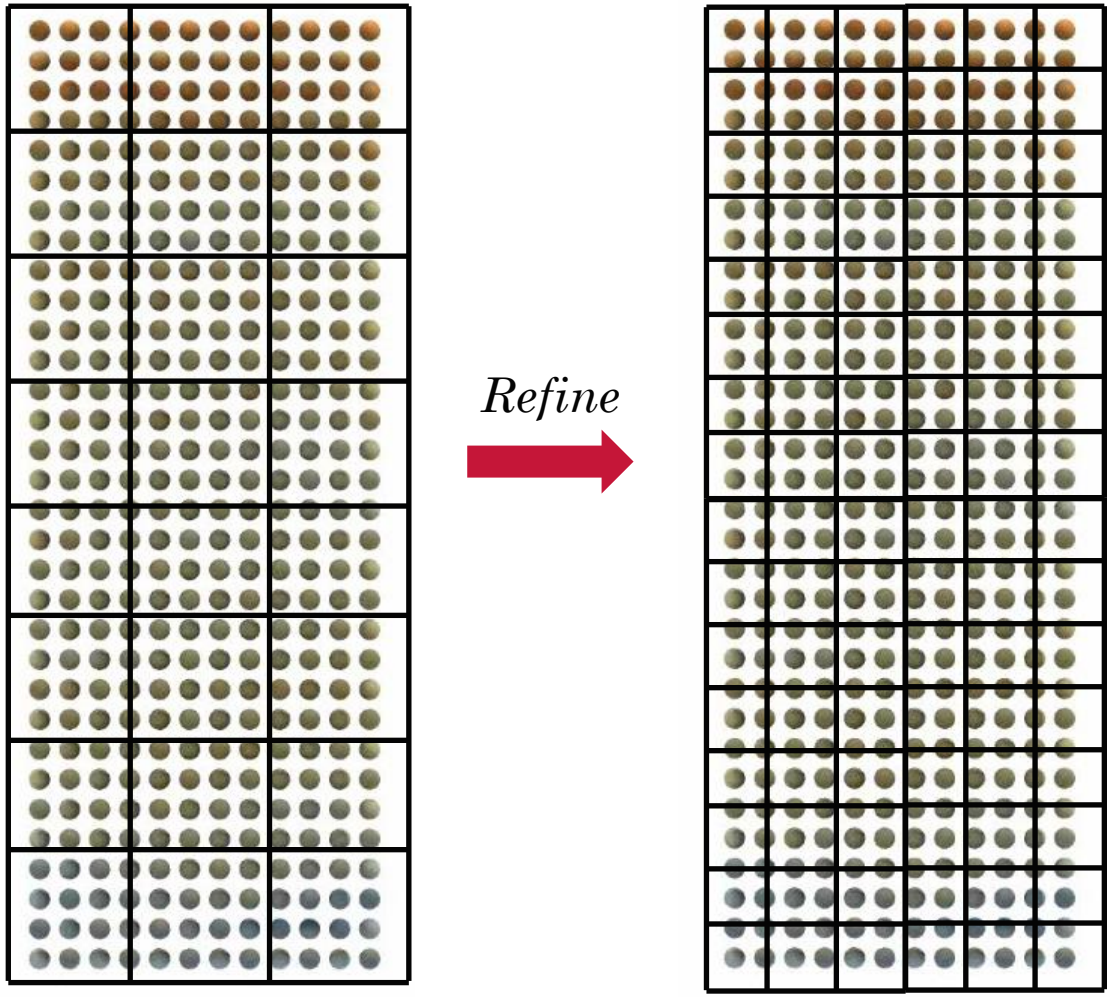


Contact line



Nucleation

Molecular Dynamics - Averaging



- Density in a cell

$$\rho = \frac{1}{V}\sum_{i=1}^{N}\langle m_i \rangle$$

- Momentum in a cell

$$\rho \boldsymbol{u} = \frac{1}{V}\sum_{i=1}^{N}\langle m_i \boldsymbol{v}_i \rangle$$

- Temperature in a cell

$$T = \frac{1}{3N}\sum_{i=1}^{N}\langle \boldsymbol{v}_i^2 \rangle$$

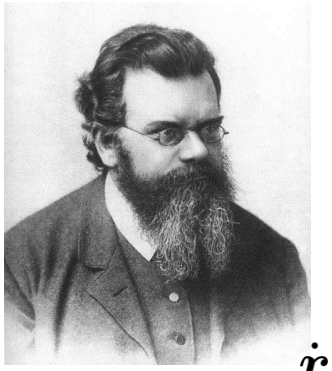
Pressure (stress) in an MD Simulation

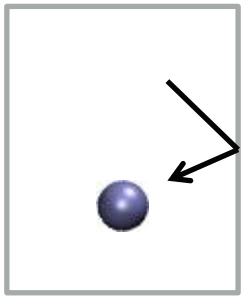
- Pressure definition in a dense molecular system
  - Kinetic part due to fluctuations
  - Configurational part due to liquid structure

$$\oint_S \Pi_{xy} \cdot dS_y = \underbrace{\sum_{i=1}^{N} \left\langle m_i v_{xi} v_{yi} dS_{yi} \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} \left\langle f_{xij} dS_{yij} \right\rangle}_{\text{Configurational}}$$

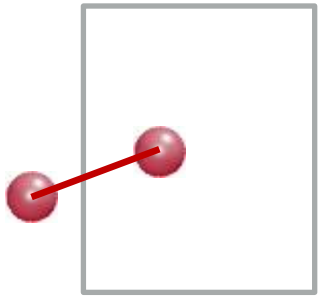
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





$$\dot{\boldsymbol{r}}_i = m_i \boldsymbol{v}_i + \boldsymbol{u}$$



Configurational part

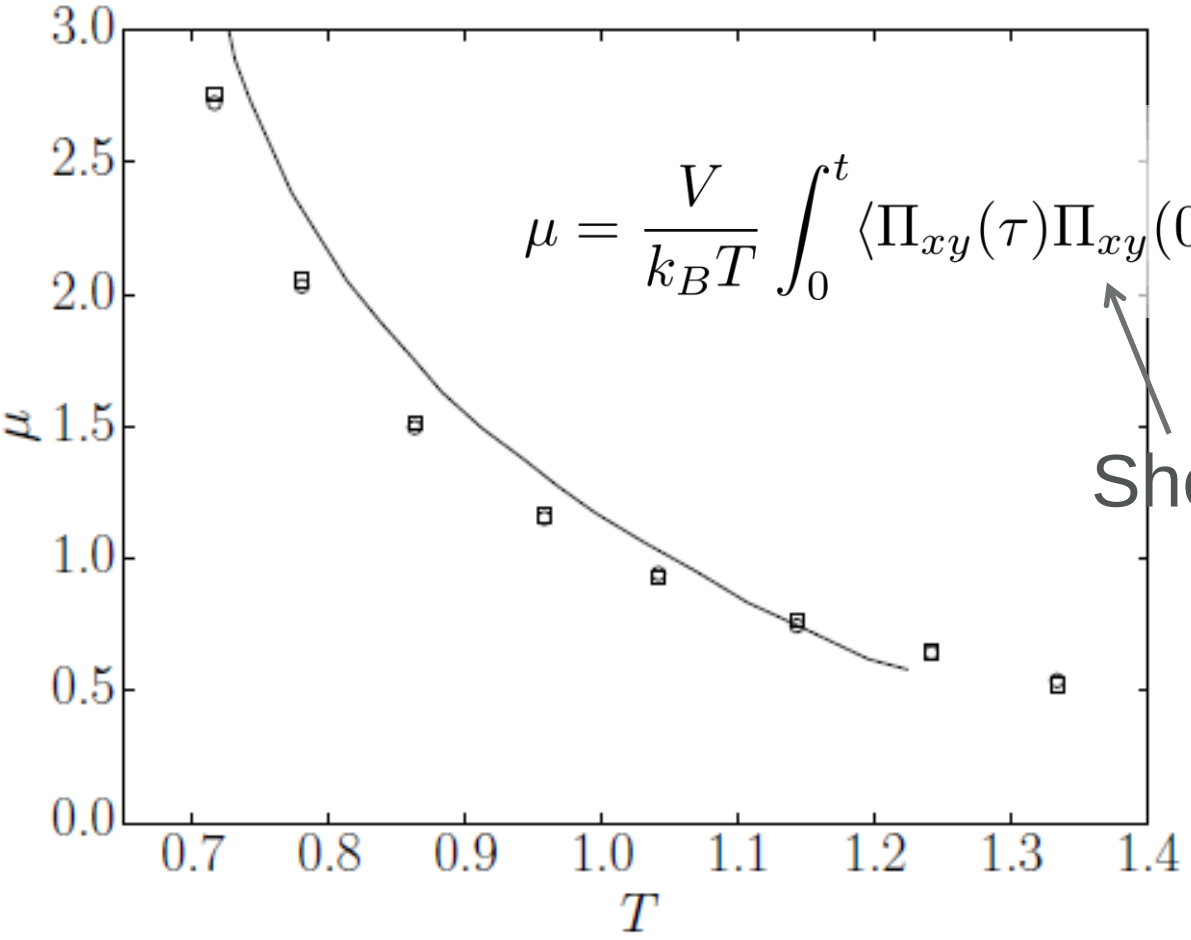
Inter-molecular bonds act like the stress in a stretched spring

Work with David Heyes and Daniele Dini

Brunel University London

Viscosity

- Good agreement with experiments



$$\mu = \frac{V}{k_B T} \int_0^t \langle \Pi_{xy}(\tau) \Pi_{xy}(0) \rangle d\tau$$

Shear stress

Work with Billy Todd and Peter Daivis

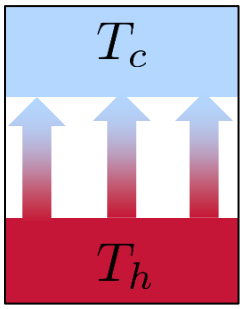
Brunel University London

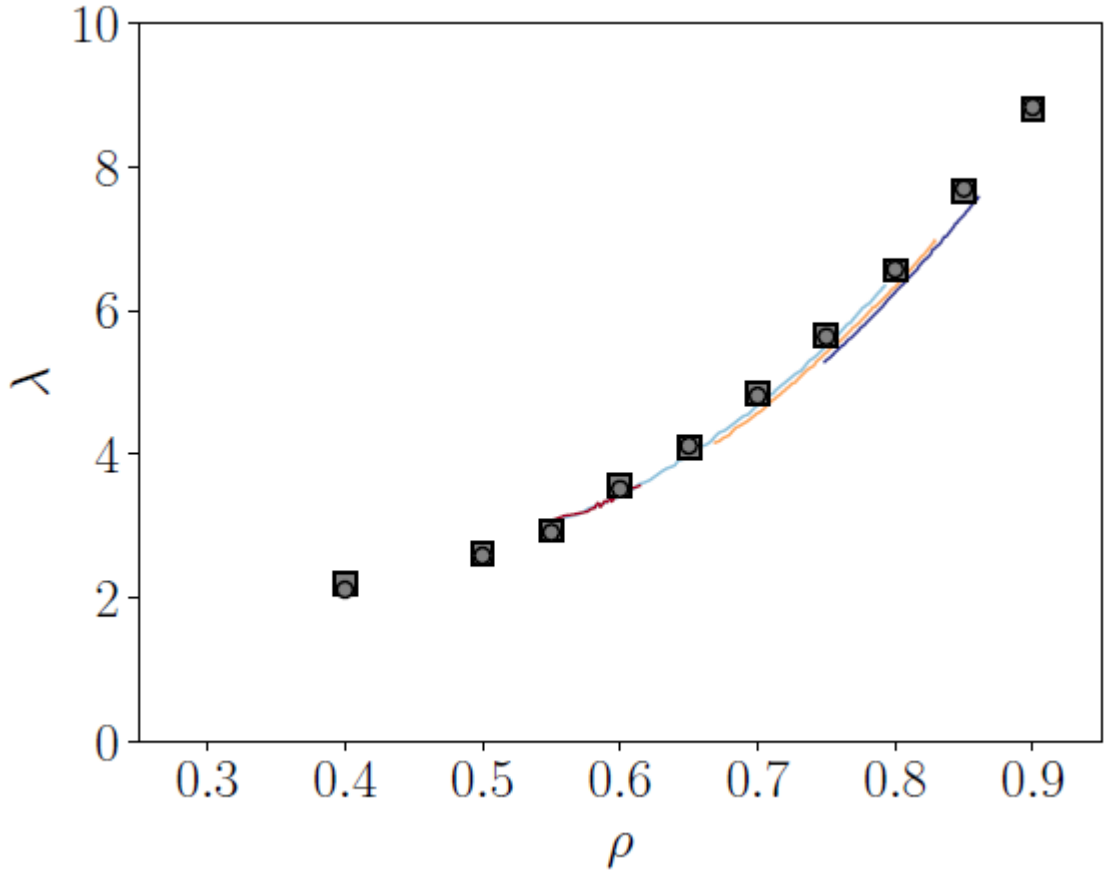
Fourier's law of heat conduction

- Good agreement with experiments

Talk about this
15th April
at Swinburne

$$q_y = -\lambda \frac{\partial T}{\partial y}$$

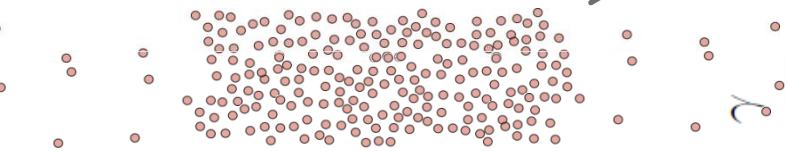




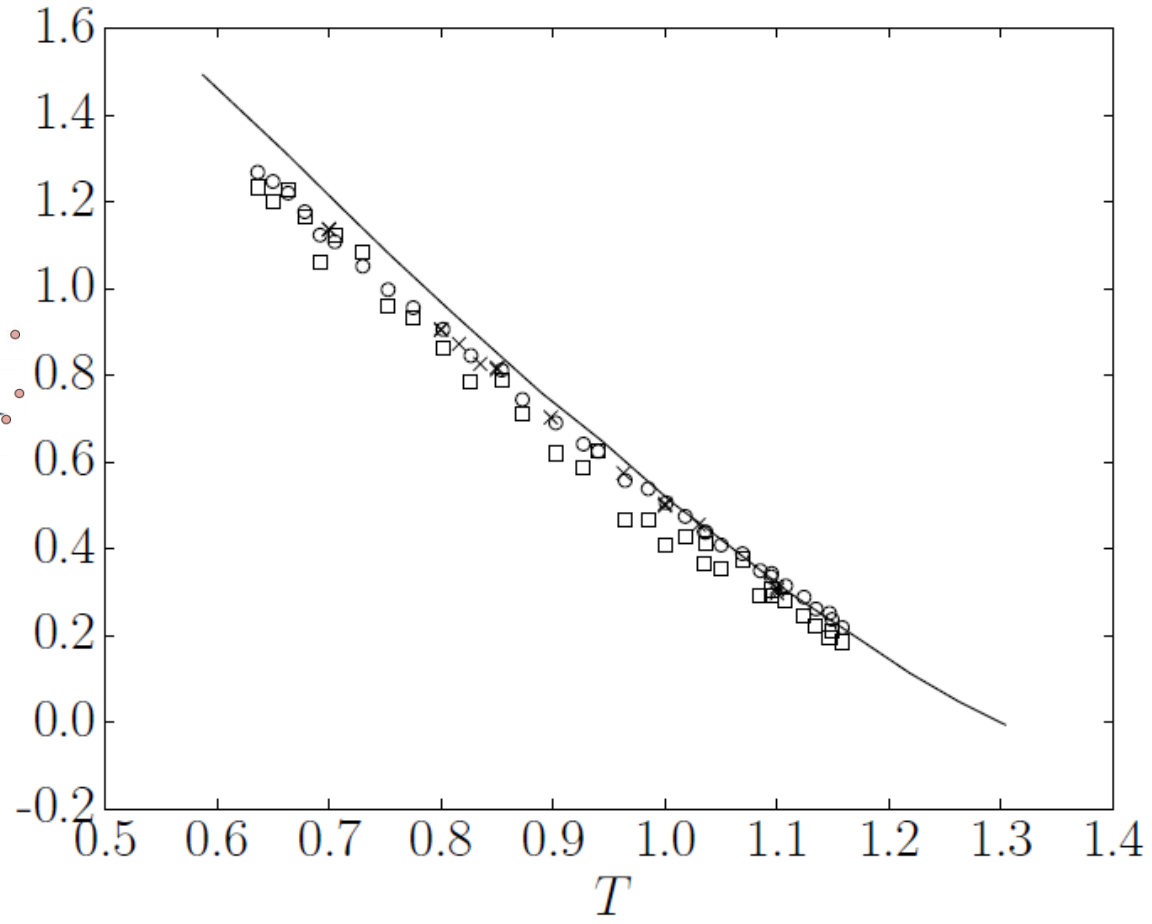
Results for Surface Tension

- Good agreement with experiments

$$\gamma = \int_{-\infty}^{x} [\Pi_N - \Pi_T]\, dx$$

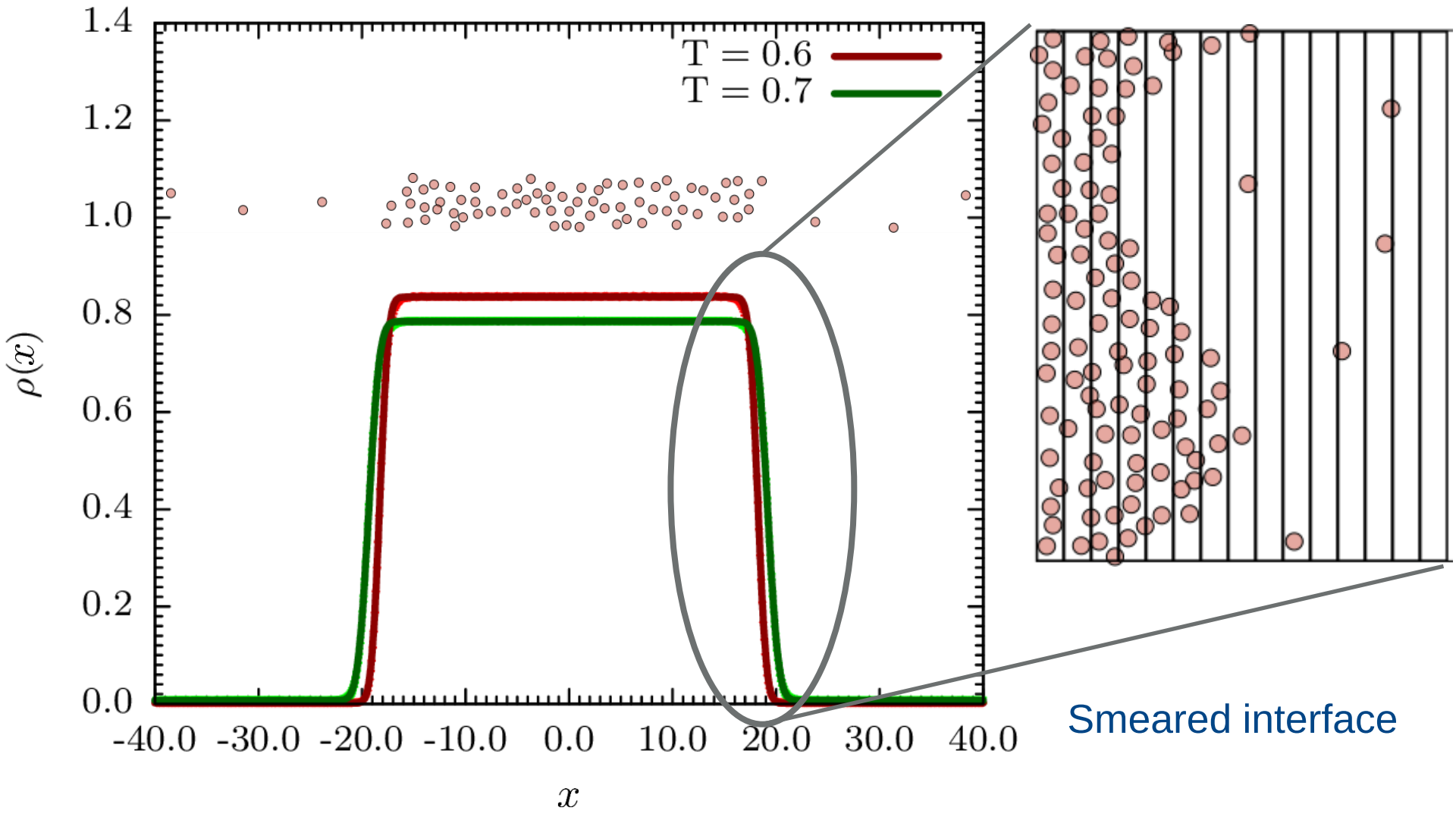


Integrate over Liquid Vapour interface(s)



Brunel University London

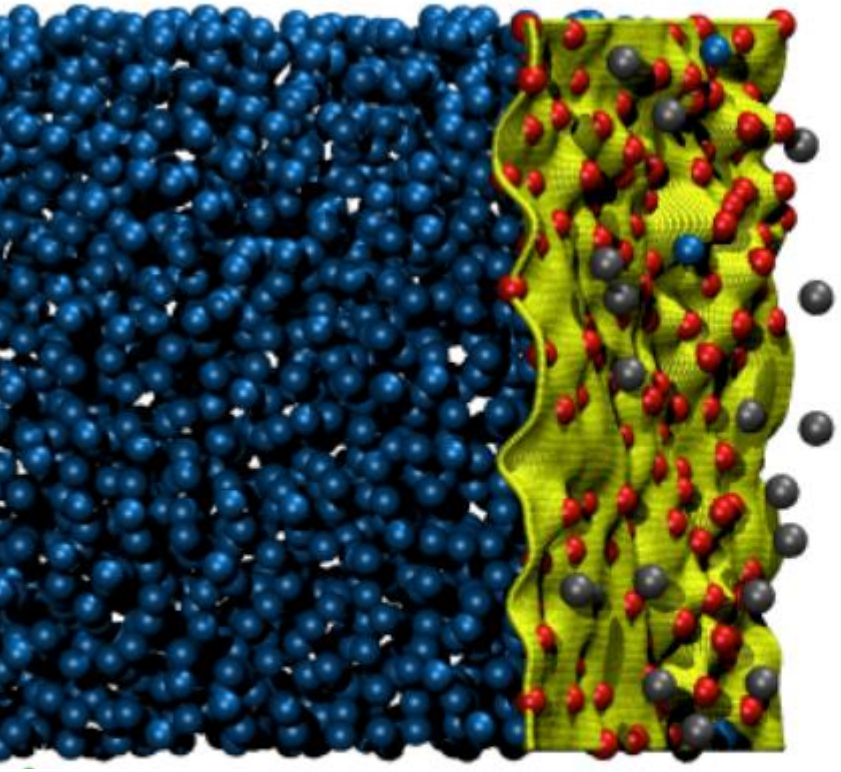
Surface Tension



Brunel University London

Intrinsic surface

- Intrinsic Surface by minimising a penalty function



$$W = \frac{1}{2}\sum_{i=1}^{N_s}\left(x_i - \xi(y,z)\right)^2 + \lambda C$$

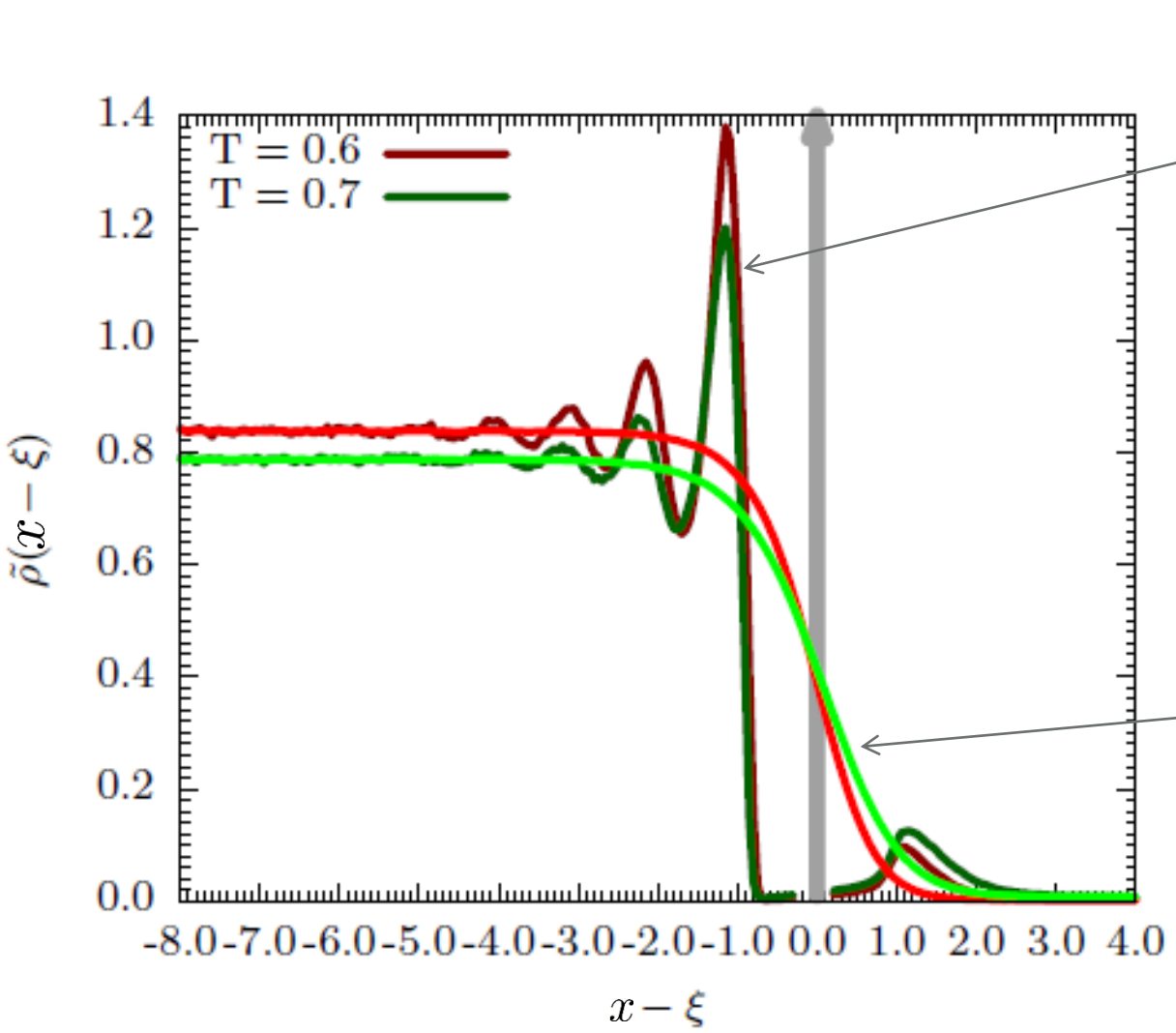
$$\xi(y,z) = \sum_{\mu,\nu} a_{\mu\nu} f_\mu(x) f_\nu(y)$$

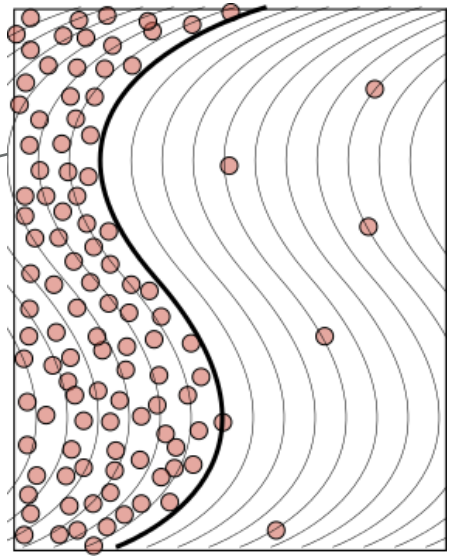
Function of sines and cosines

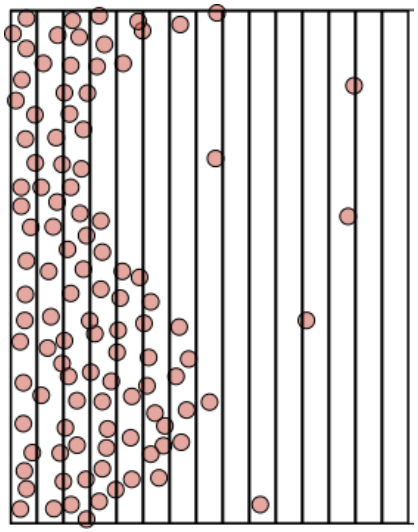
Chacon & Tarazona (2003) PRL 91, 166103

Brunel University London

Results for Density

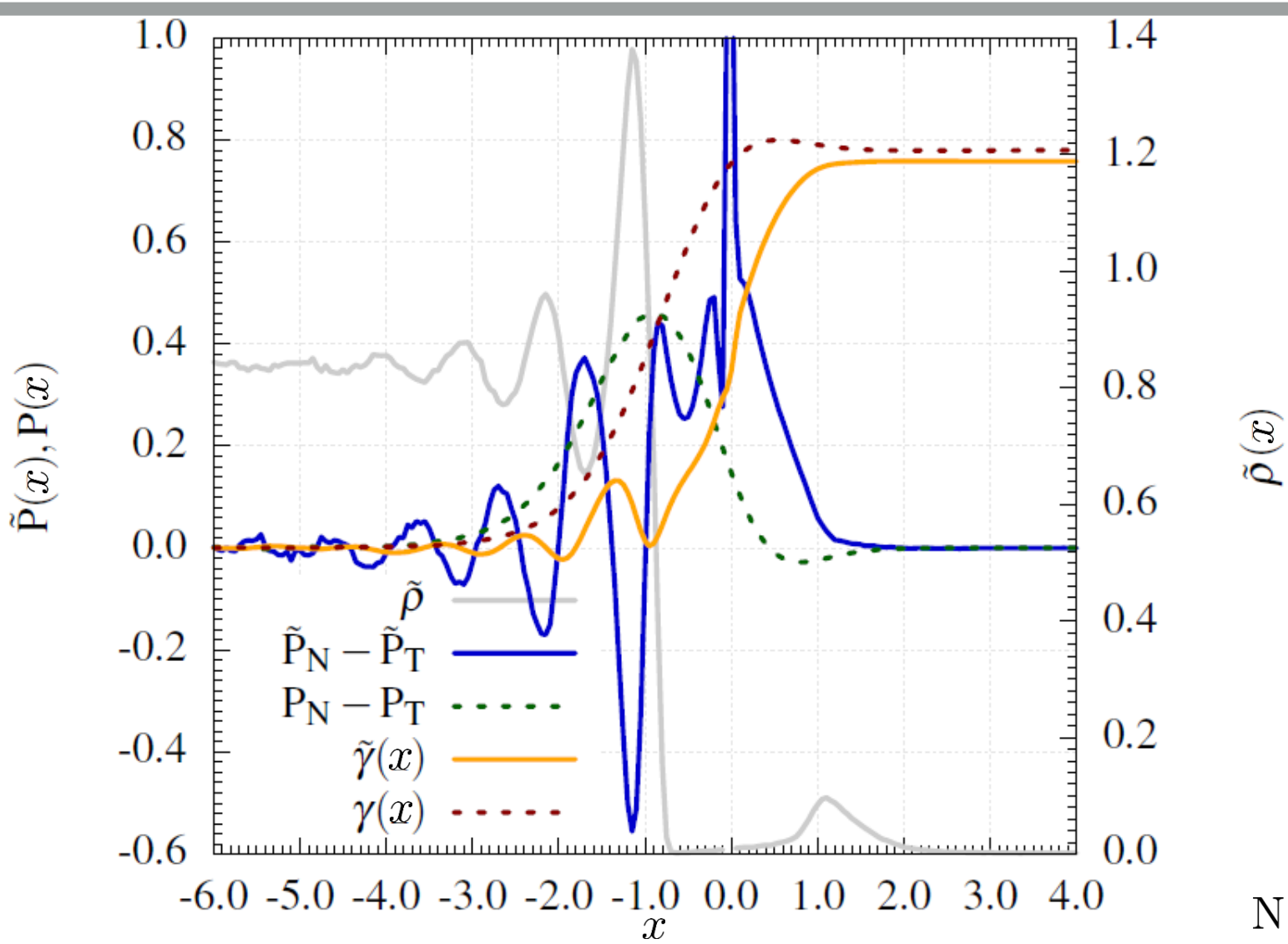






Brunel University London

Results for Pressure

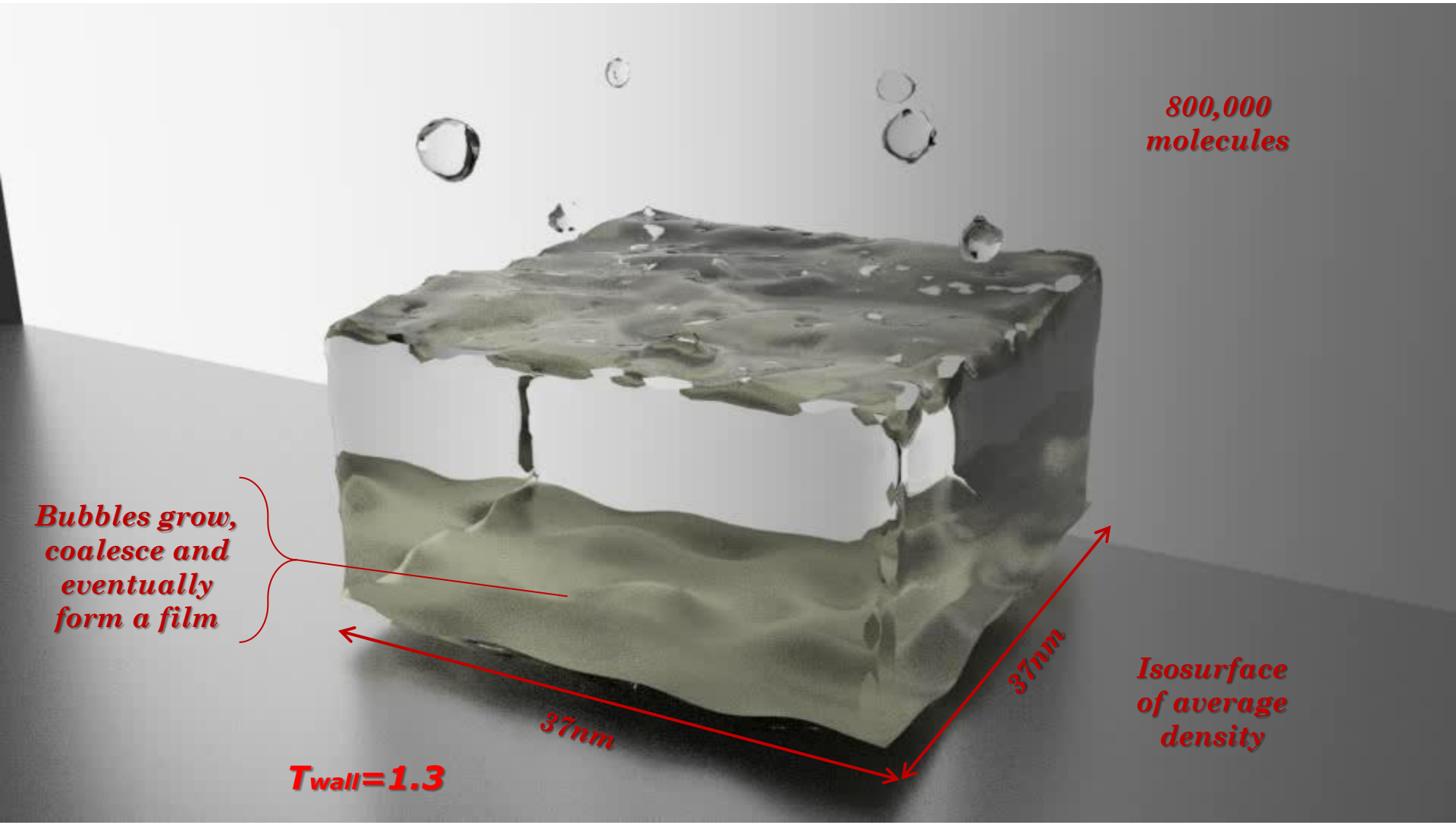


N.B. $\Pi \equiv P$

Molecular Dynamics simulation of Nucleation

Wall w
mo
rou

Isosurface of Density



Coupling – Using MD with CFD

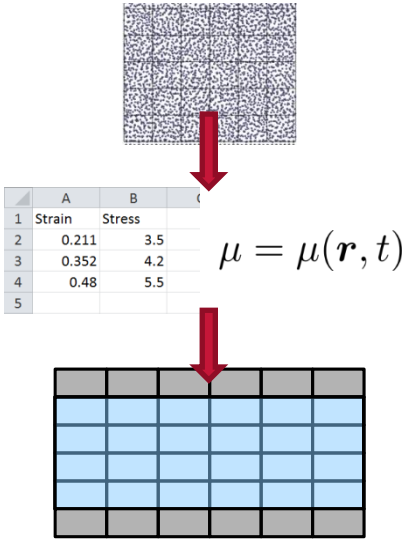
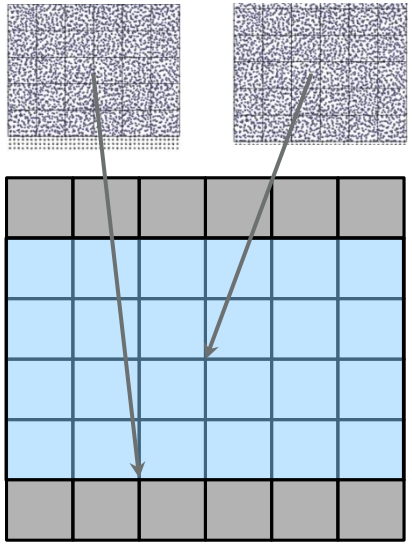


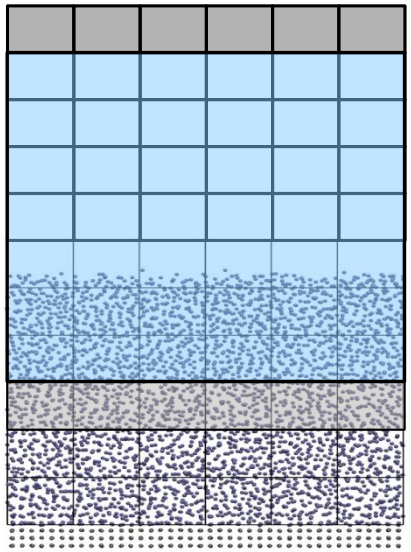
Table Lookup or Coefficients

MD parameter study stored in table and CFD uses data



Embedded Models (HMM)

MD – embedded in a CFD simulation [1)]

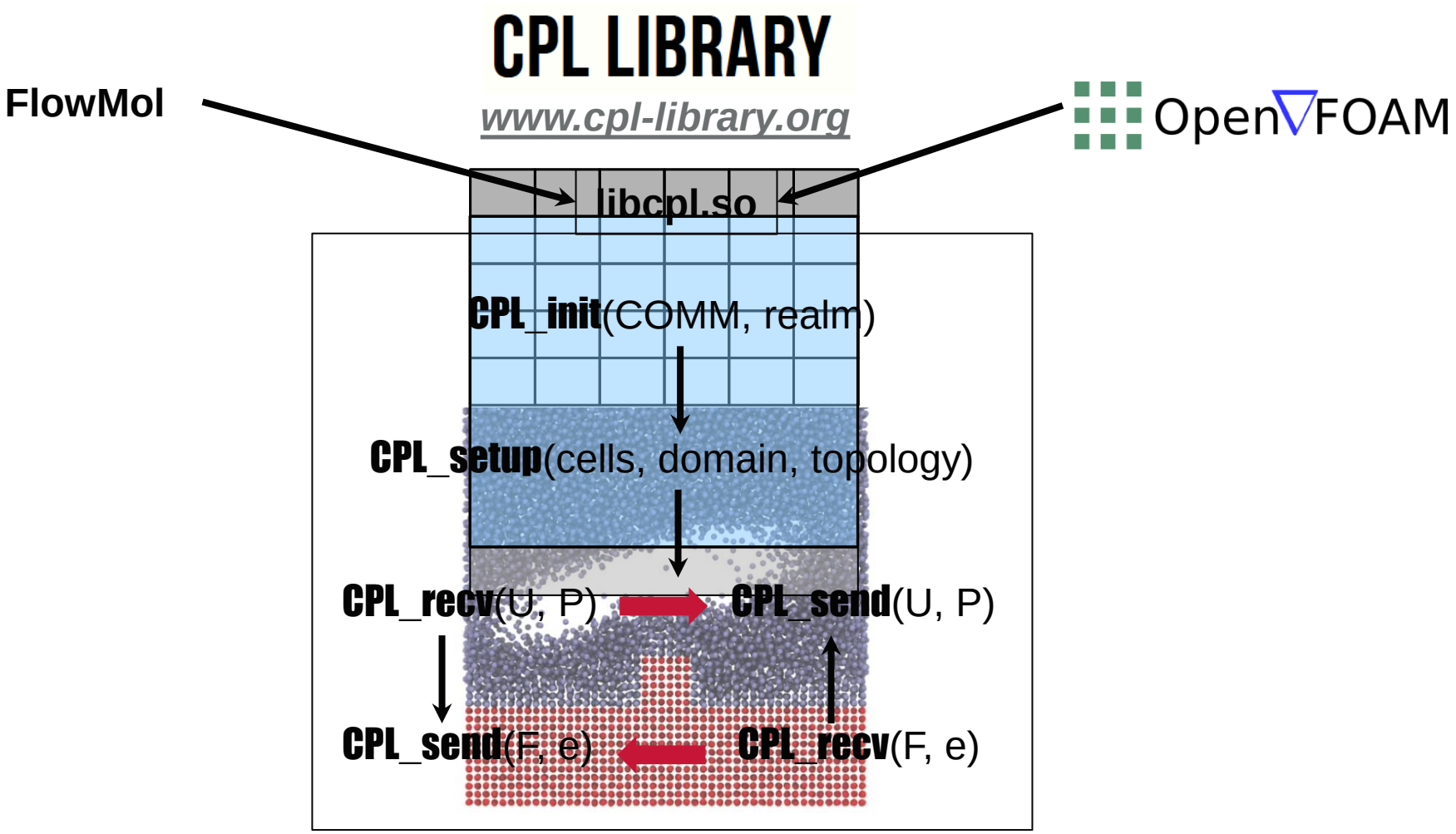


Domain Decomposition

MD –CFD linked along an interface [2)]

1) Ren (2007), E et al (2003), Borg et al (2013) 2) O'Connell and Thompson (1995), Flekkøy at al (2000), Nie et al (2004), Hadjiconstantinou et al (1999), Delgado-Buscalioni & Coveney, (2003), Mohamed & Mohamad, (2009)

Coupled Simulation Software

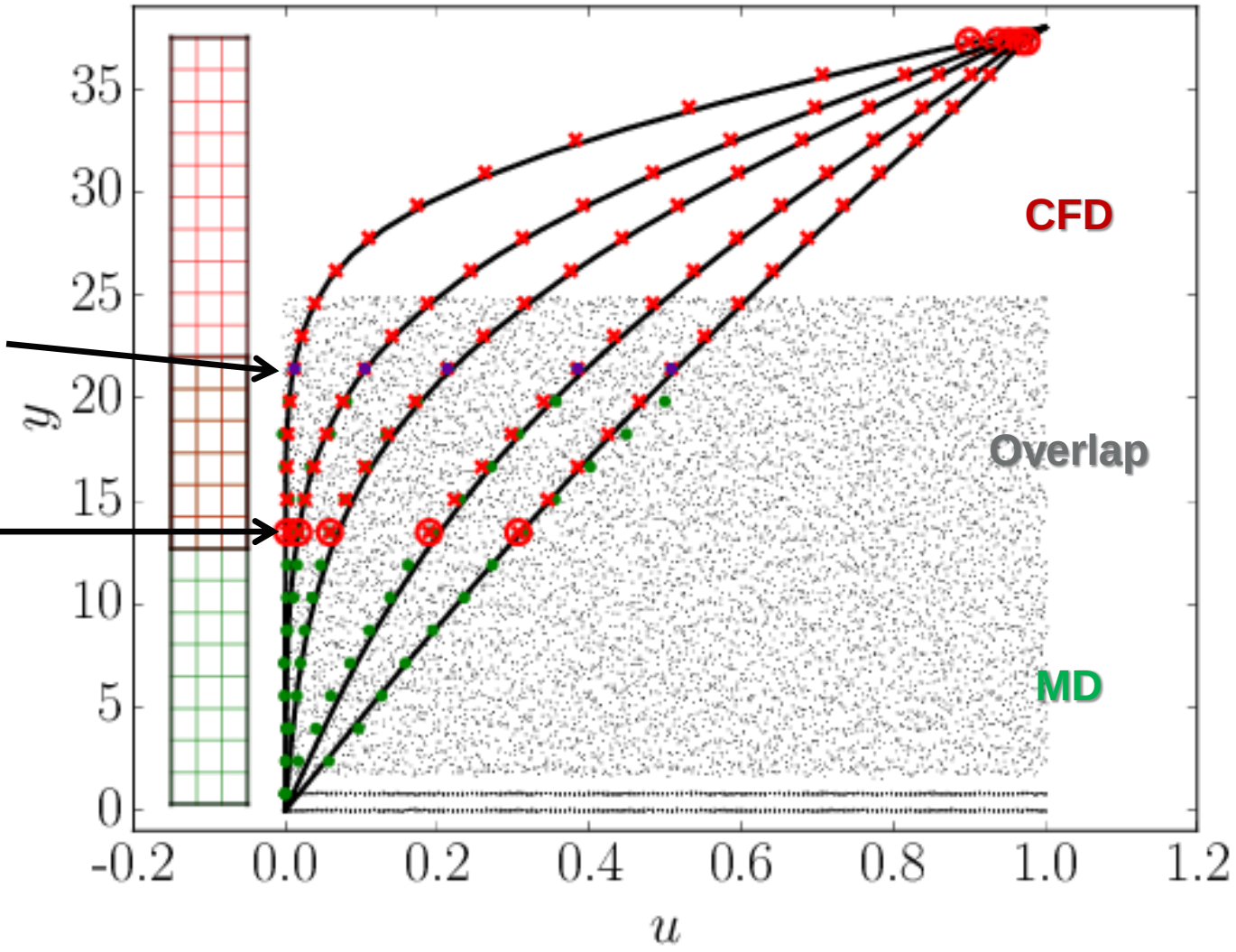


Coupling Results – Couette Flow

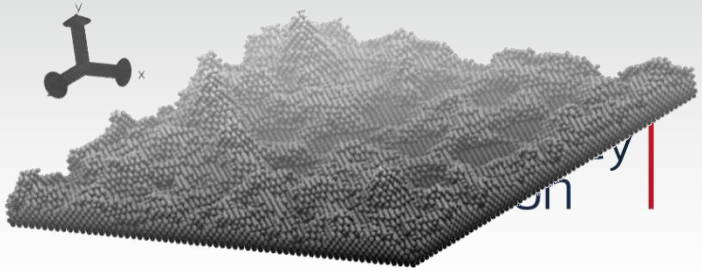
Brunel University London

Constraint

CFD Boundary



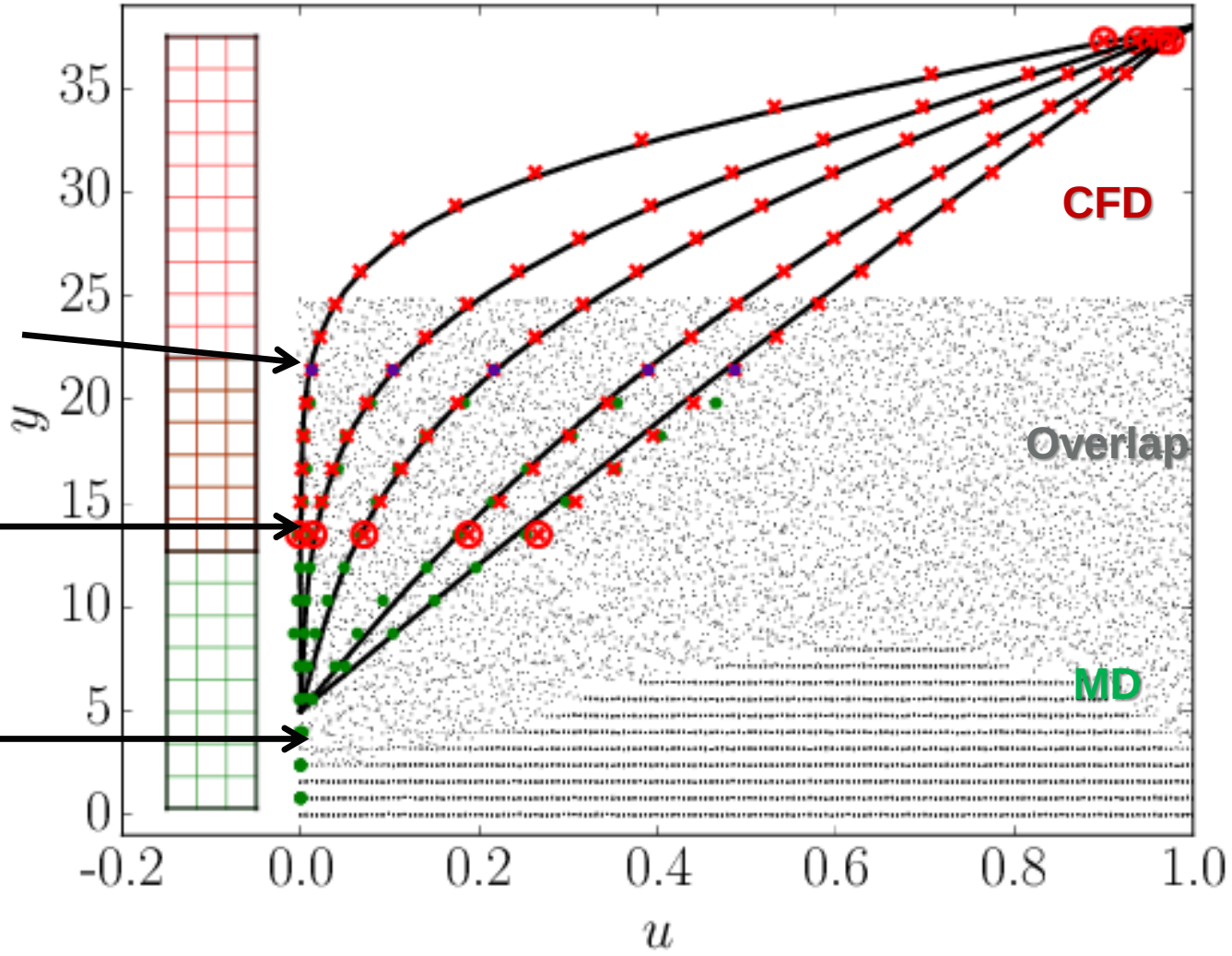
Coupling Results – Couette Flow



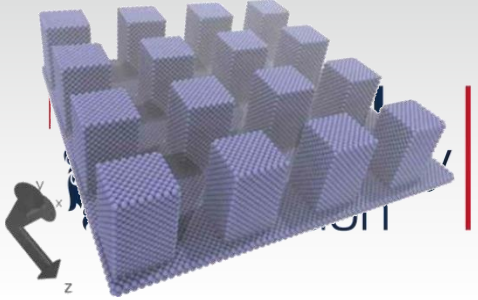
Constraint

CFD Boundary

Rough wall shifts zero velocity location



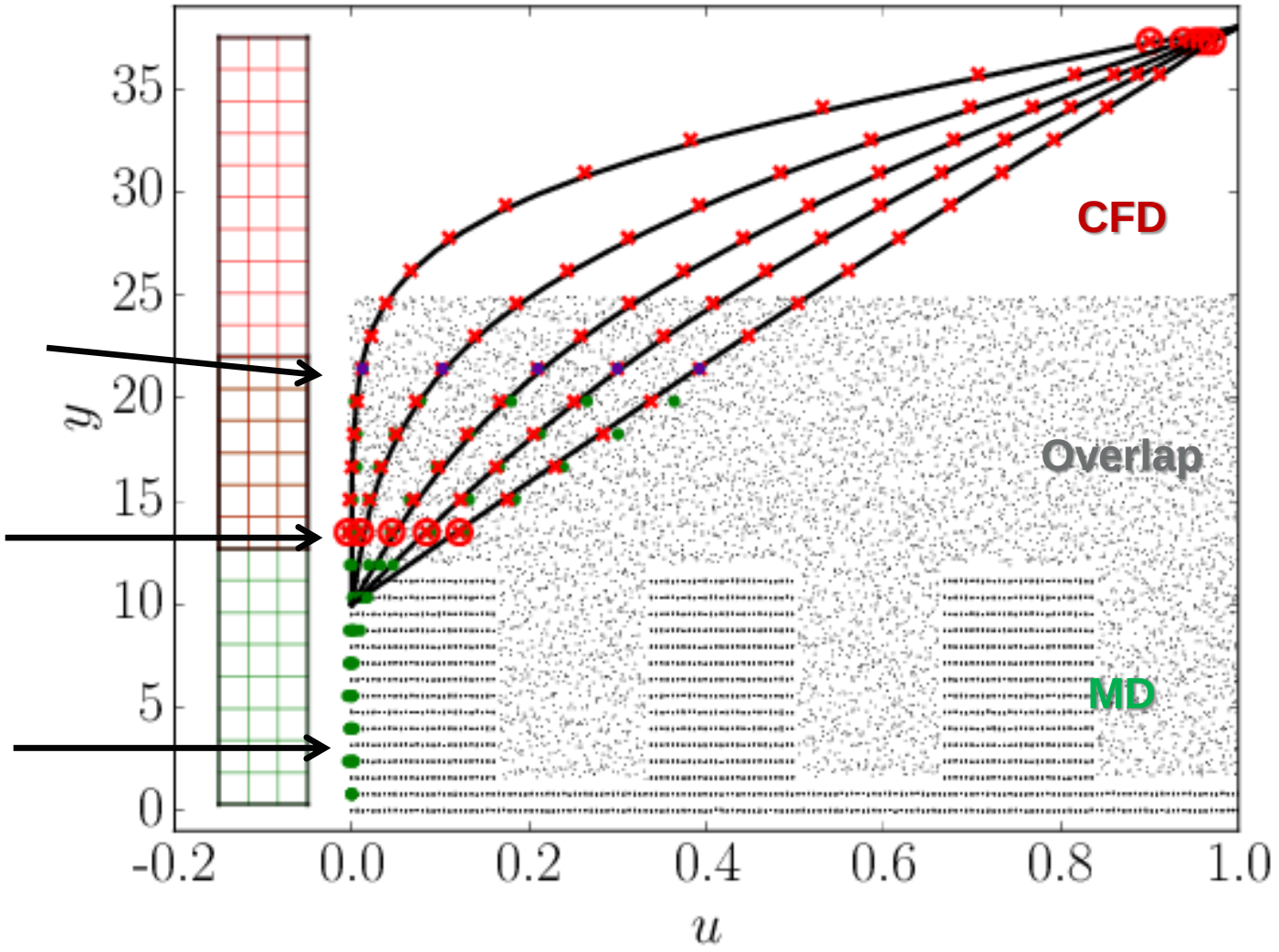
Coupling Results – Couette Flow



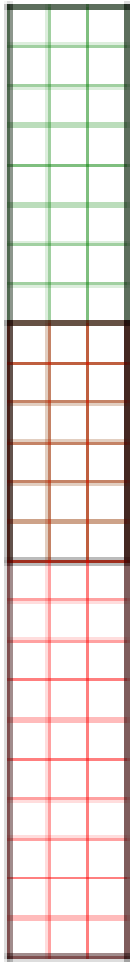
Constraint

CFD Boundary

Posts shifts zero velocity location



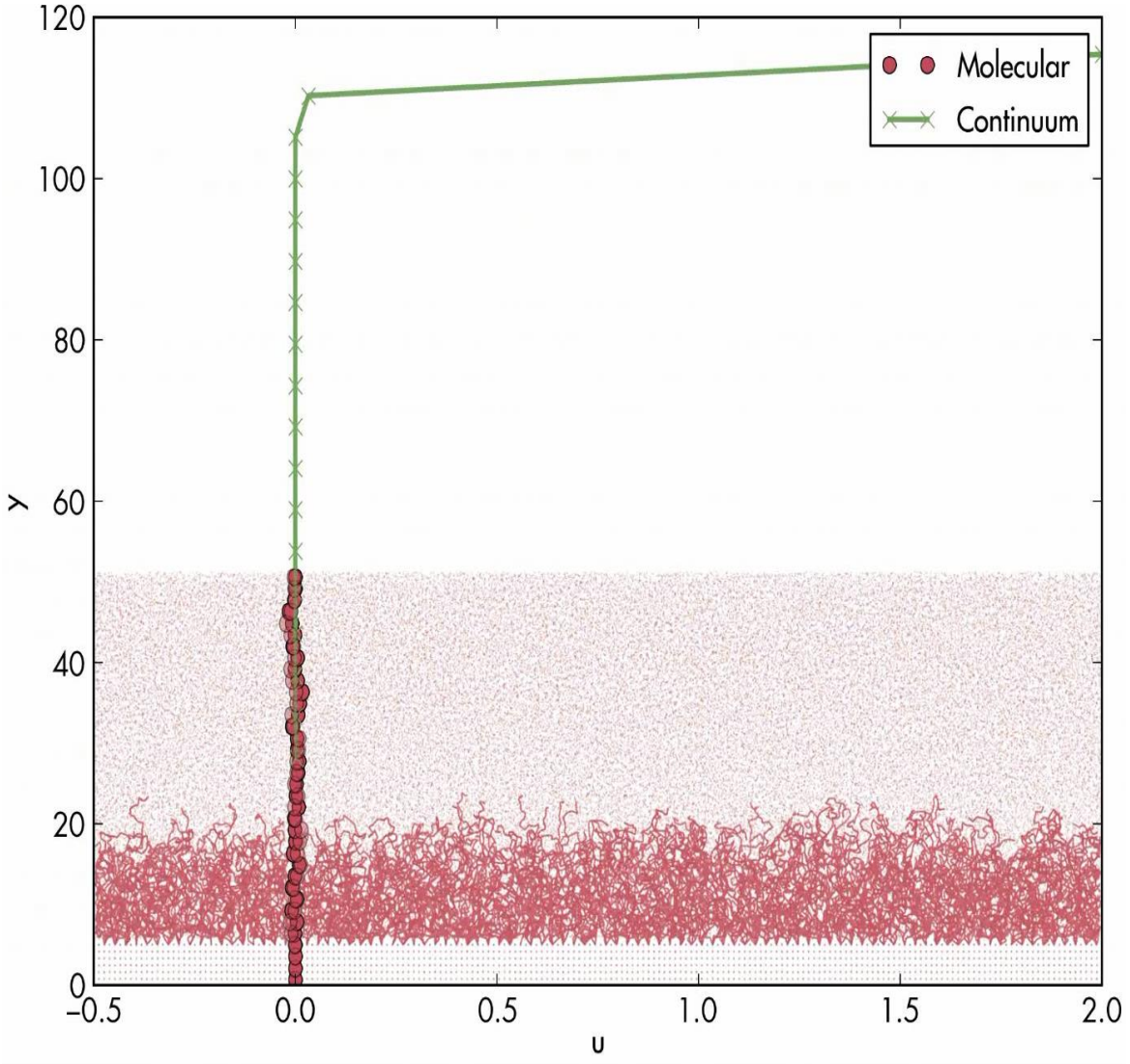
Coupling Results – Polymer Brushes



CFD Region

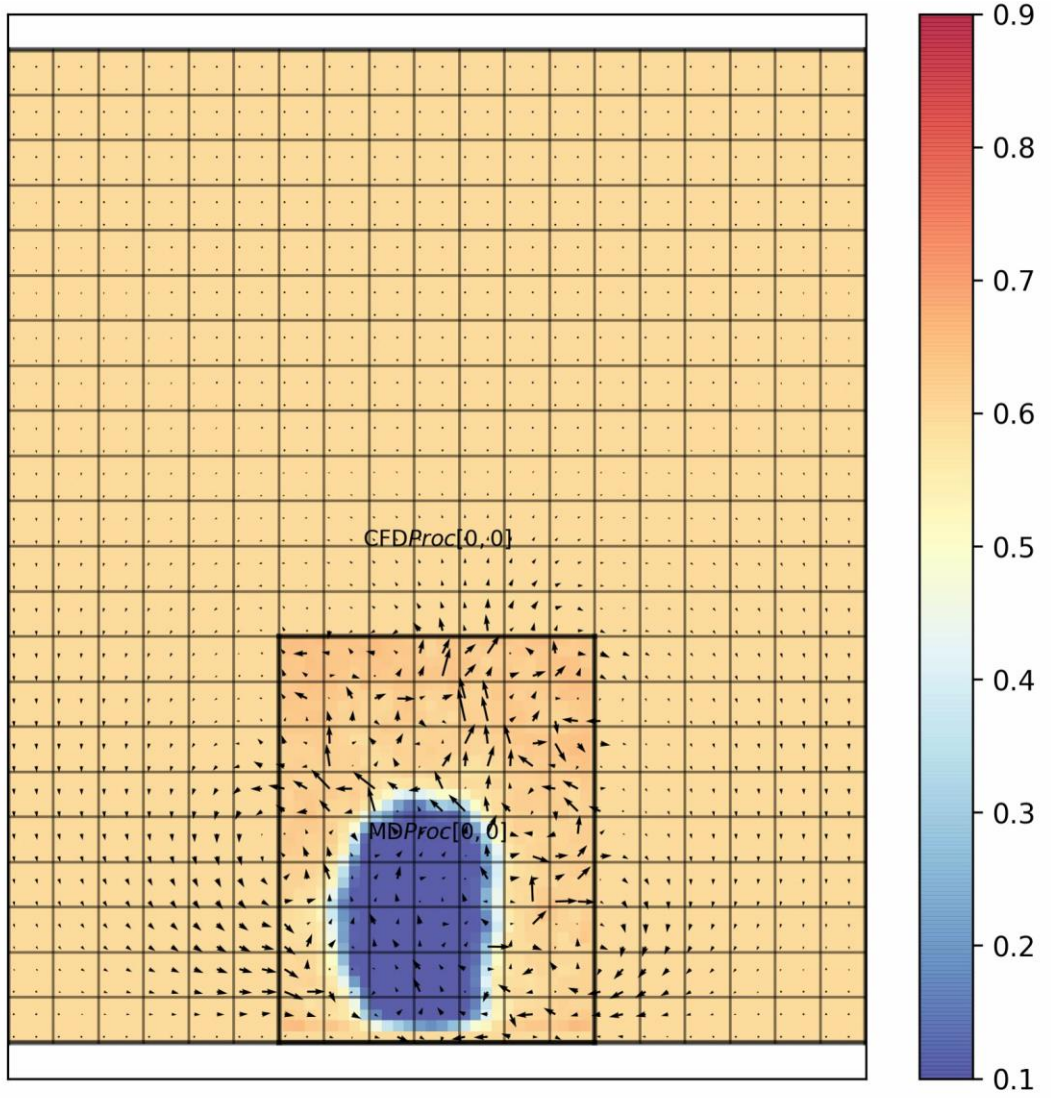
Overlap Region

MD Region



Coupled Simulation of Boiling

- Bubble nucleation occurs naturally in MD
- Density, velocity and temperature passed as boundary conditions



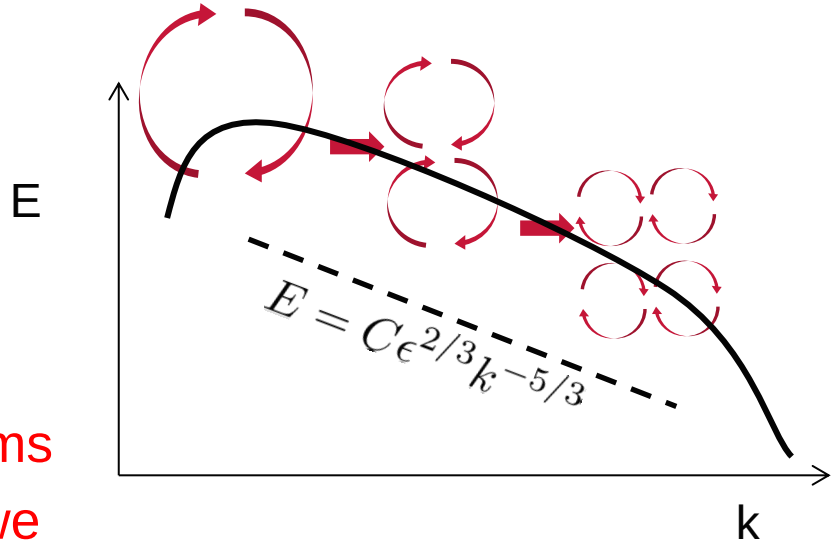
Brunel University London

Section 2

THE MINIMAL CHANNEL

Molecular Simulation of 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
  - Insight into fundamental mechanisms
  - For molecular dynamics this is all we can do with current computers



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
- Insight into the fundamental mechanism of near-wall turbulence

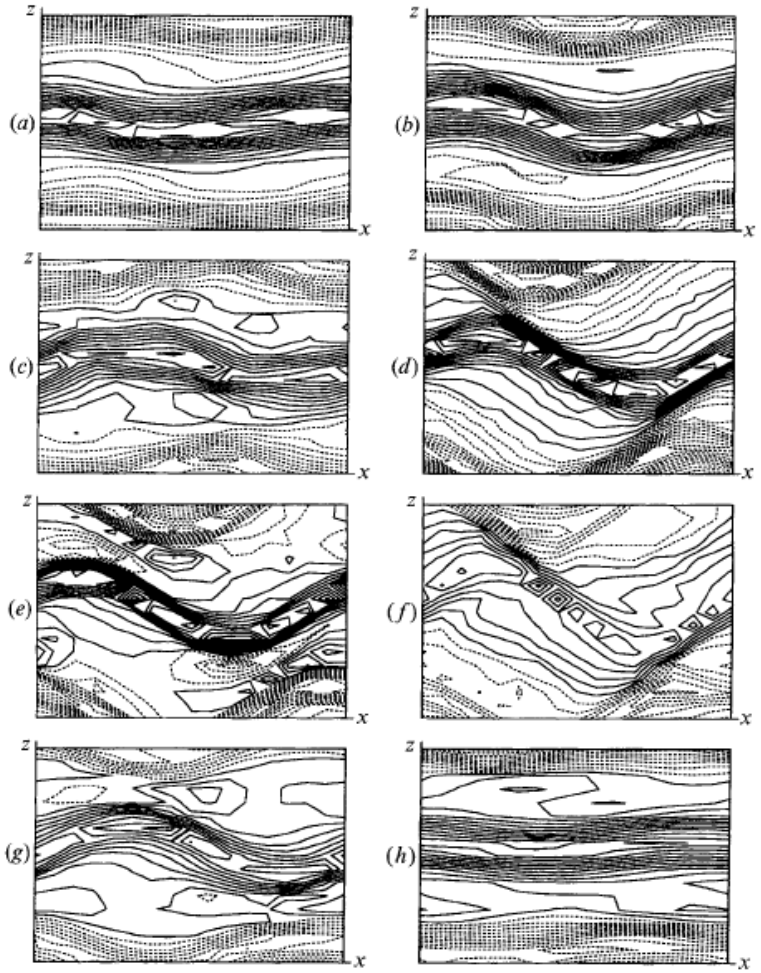
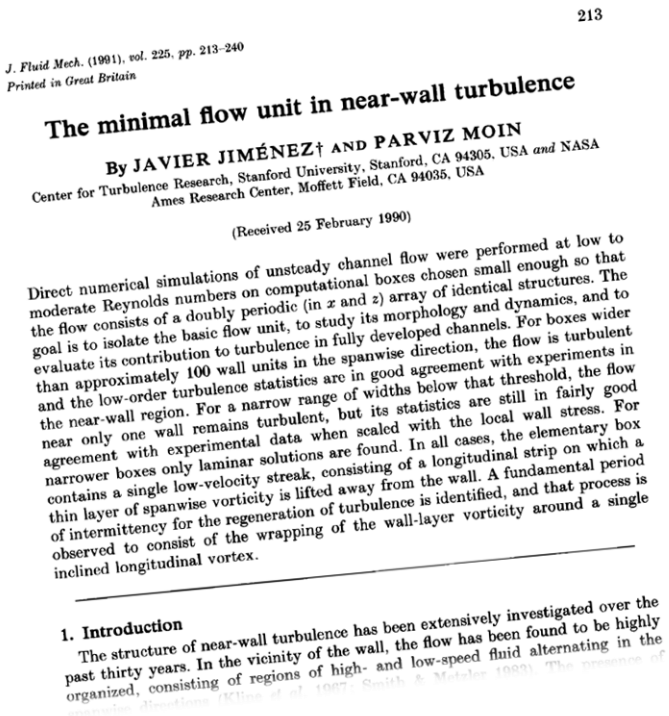


FIGURE 2. Iso-contours of u-velocity in the (x, z)-plane centred between the walls; solid contours positive, dashed contours negative. Contour interval 0.032. (*a*) $t = 757.5$, (*b*) $t = 764.8$, (*c*) $t = 772.0$, (*d*) $t = 777.8$, (*e*) $t = 783.0$, (*f*) $t = 794.1$, (*g*) $t = 808.2$, (*h*) $t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

Molecular Simulation of Turbulence

- The minimum domain size required to sustain turbulent flow

Poiseuille flow, Re ≈ 2000



213

J. Fluid Mech. (1991), vol. 225, pp. 213–240
Printed in Great Britain

The minimal flow unit in near-wall turbulence

By JAVIER JIMÉNEZ† AND PARVIZ MOIN
Center for Turbulence Research, Stanford University, Stanford, CA 94305, USA and NASA Ames Research Center, Moffett Field, CA 94035, USA

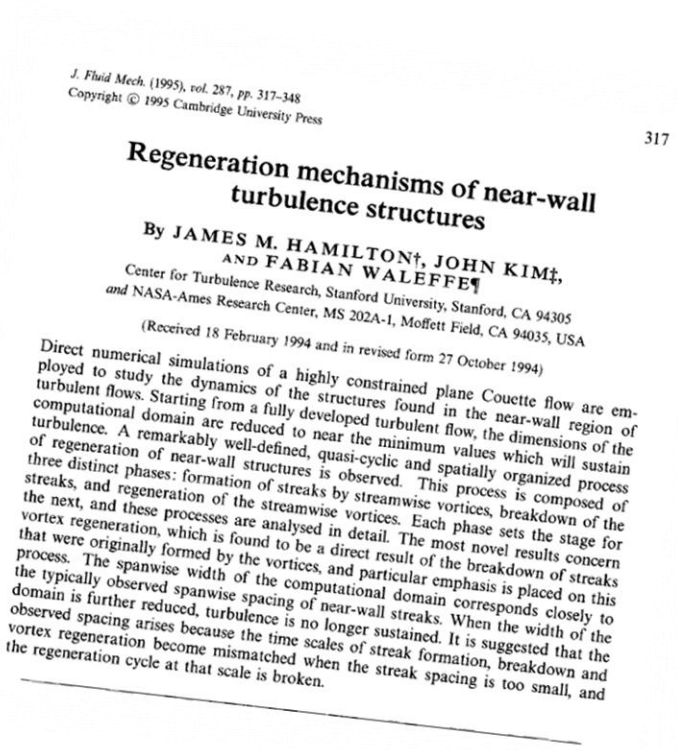
(Received 25 February 1990)

Direct numerical simulations of unsteady channel flow were performed at low to moderate Reynolds numbers on computational boxes chosen small enough so that the flow consists of a doubly periodic (in x and z) array of identical structures. The goal is to isolate the basic flow unit, to study its morphology and dynamics, and to evaluate its contribution to turbulence in fully developed channels. For boxes wider than approximately 100 wall units in the spanwise direction, the flow is turbulent and the low-order turbulence statistics are in good agreement with experiments in the near-wall region. For a narrow range of widths below that threshold, the flow near only one wall remains turbulent, but its statistics are still in fairly good agreement with experimental data when scaled with the local wall stress. For narrower boxes only laminar solutions are found. In all cases, the elementary box contains a single low-velocity streak, consisting of a longitudinal strip on which a thin layer of spanwise vorticity is lifted away from the wall. A fundamental period of intermittency for the regeneration of turbulence is identified, and that process is observed to consist of the wrapping of the wall-layer vorticity around a single inclined longitudinal vortex.

1. Introduction

The structure of near-wall turbulence has been extensively investigated over the past thirty years. In the vicinity of the wall, the flow has been found to be highly organized, consisting of regions of high- and low-speed fluid alternating in the

Couette Flow Re ≈ 400



J. Fluid Mech. (1995), vol. 287, pp. 317–348

317

Regeneration mechanisms of near-wall turbulence structures

By JAMES M. HAMILTON†, JOHN KIM‡, AND FABIAN WALEFFE¶
Center for Turbulence Research, Stanford University, Stanford, CA 94305 and NASA-Ames Research Center, MS 202A-1, Moffett Field, CA 94035, USA

(Received 18 February 1994 and in revised form 27 October 1994)

Direct numerical simulations of a highly constrained plane Couette flow are employed to study the dynamics of the structures found in the near-wall region of turbulent flows. Starting from a fully developed turbulent flow, the dimensions of the computational domain are reduced to near the minimum values which will sustain turbulence. A remarkably well-defined, quasi-cyclic and spatially organized process of regeneration of near-wall structures is observed. This process is composed of three distinct phases: formation of streaks by streamwise vortices, breakdown of the streaks, and regeneration of the streamwise vortices. Each phase sets the stage for the next, and these processes are analysed in detail. The most novel results concern vortex regeneration, which is found to be a direct result of the breakdown of the streaks that were originally formed by the vortices, and particular emphasis is placed on this process. The spanwise width of the computational domain corresponds closely to the typically observed spanwise spacing of near-wall streaks. When the width of the domain is further reduced, turbulence is no longer sustained. It is suggested that the observed spacing arises because the time scales of streak formation, breakdown and vortex regeneration become mismatched when the streak spacing is too small, and the regeneration cycle at that scale is broken.

The Smallest Domain For This Reynolds Number

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

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

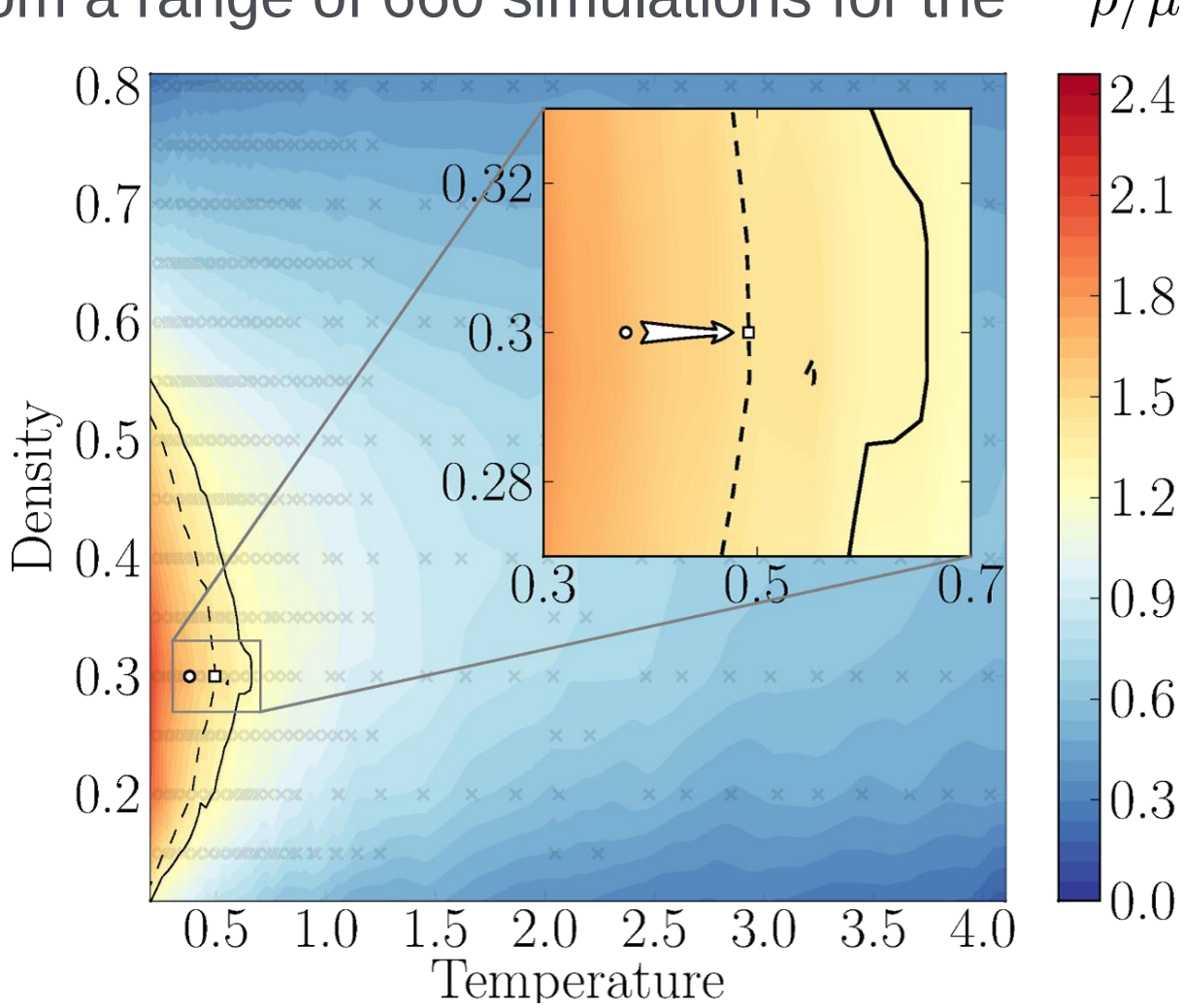
$$Re > 400$$

- The target value

$$u = \pm 1$$

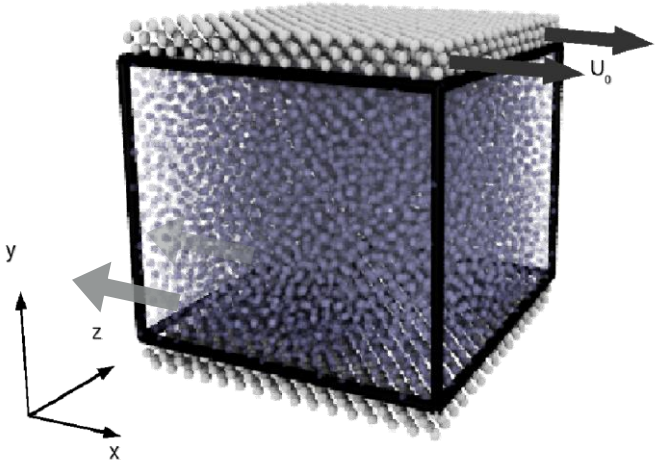
$$\rho/\mu > 1.4$$

$$L = 560$$



Domain Overview

- Simulation Setup
  - All Molecular Dynamics
  - Sliding top and bottom walls at y=0 and y=L with $u_x = \pm 1$
  - Periodic in x and z directions
  - Walls are tethered, sliding molecules with Nosé Hoover thermostat at T=0.4



- Domain in reduced units: x = 1560.4, y = 566.7, z = 1069.9 at density=0.3, ~300 million molecules on 256+ processors

Three plots of decreasing Reynolds Number

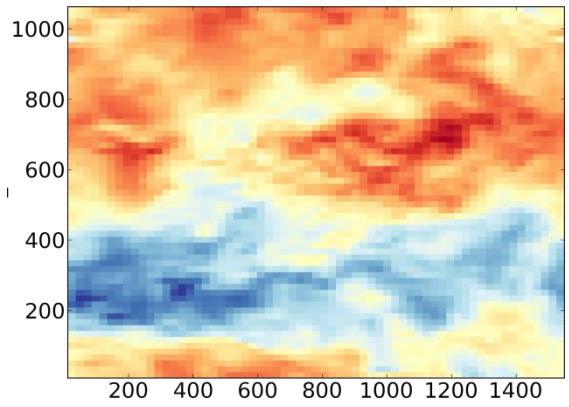
Brunel University London

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

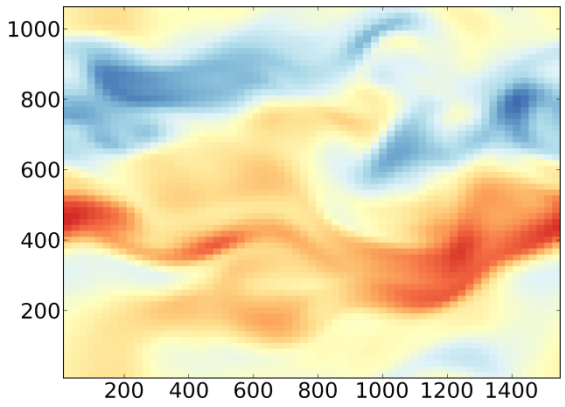
- From Jimenez and Moin (1991):

  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.

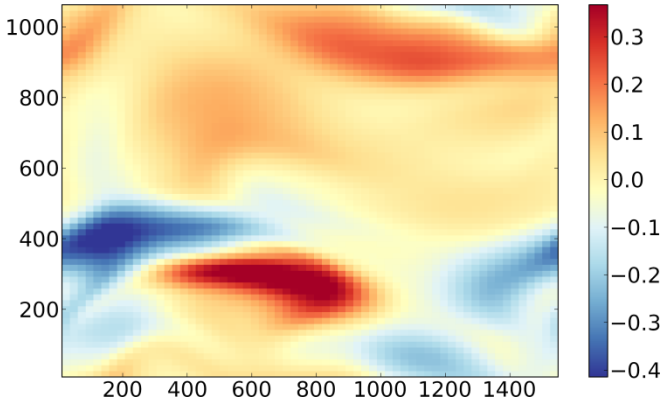
Re ≈ 4000



Re ≈ 1000



Re ≈ 400

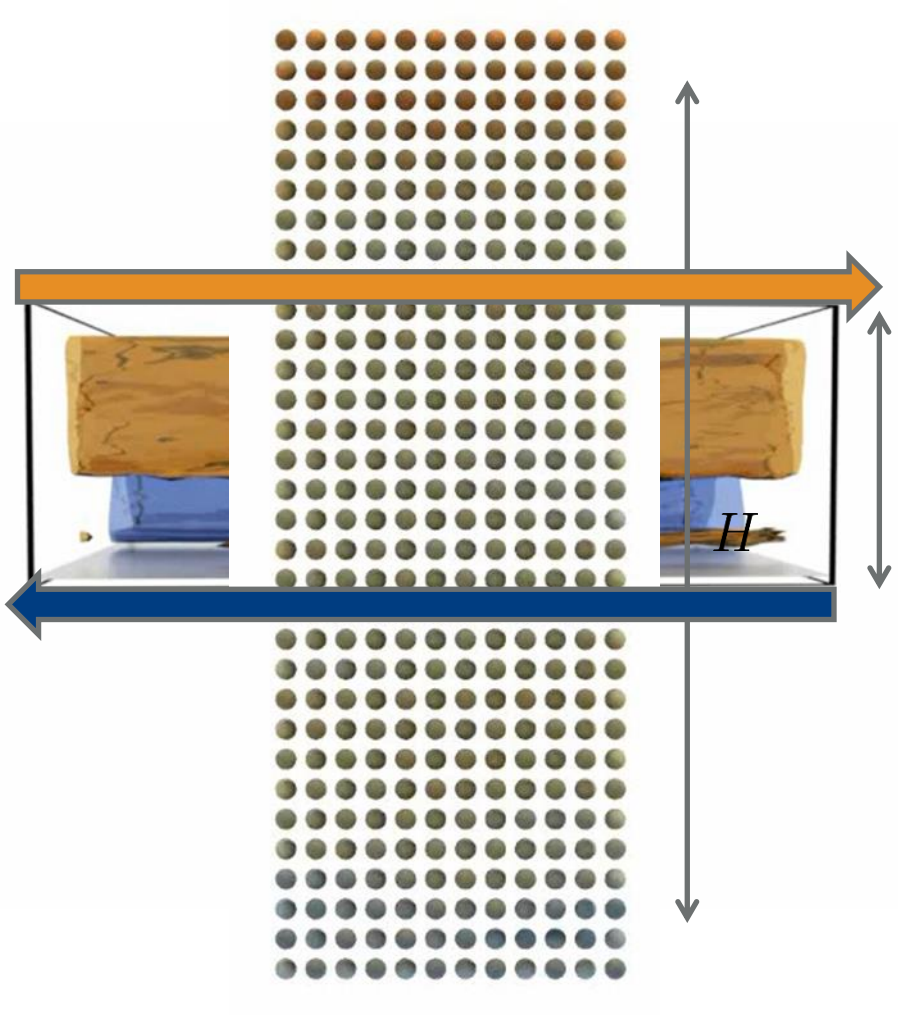


Molecular Simulation of Turbulence

Brunel University London

Molecular Simulation of Turbulence

Brunel University London



Reynolds Number

$Re \approx 400$

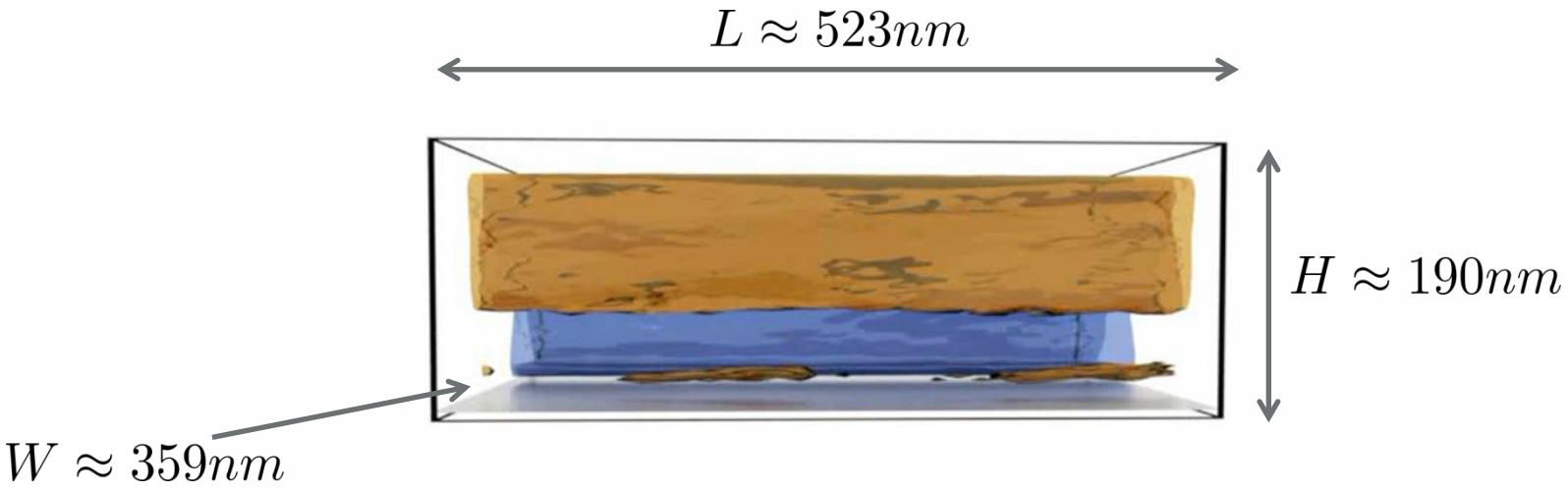
with

300 million molecules

Molecular Simulation of Turbulence

Brunel University London

Minimal channel Couette flow



Reynolds Number

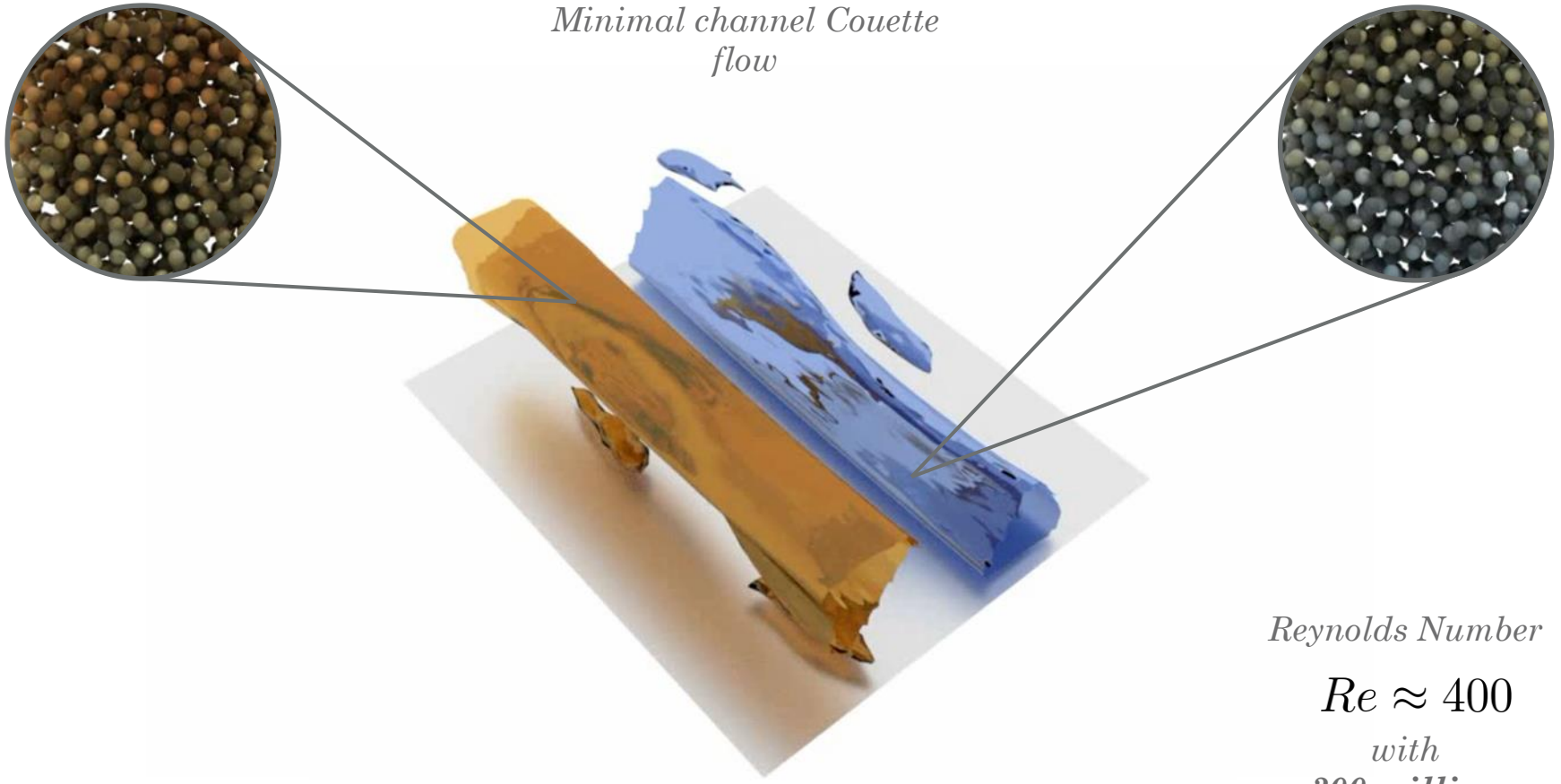
$Re \approx 400$

with
300 million molecules

Molecular Simulation of Turbulence

Brunel University London

Minimal channel Couette flow



Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

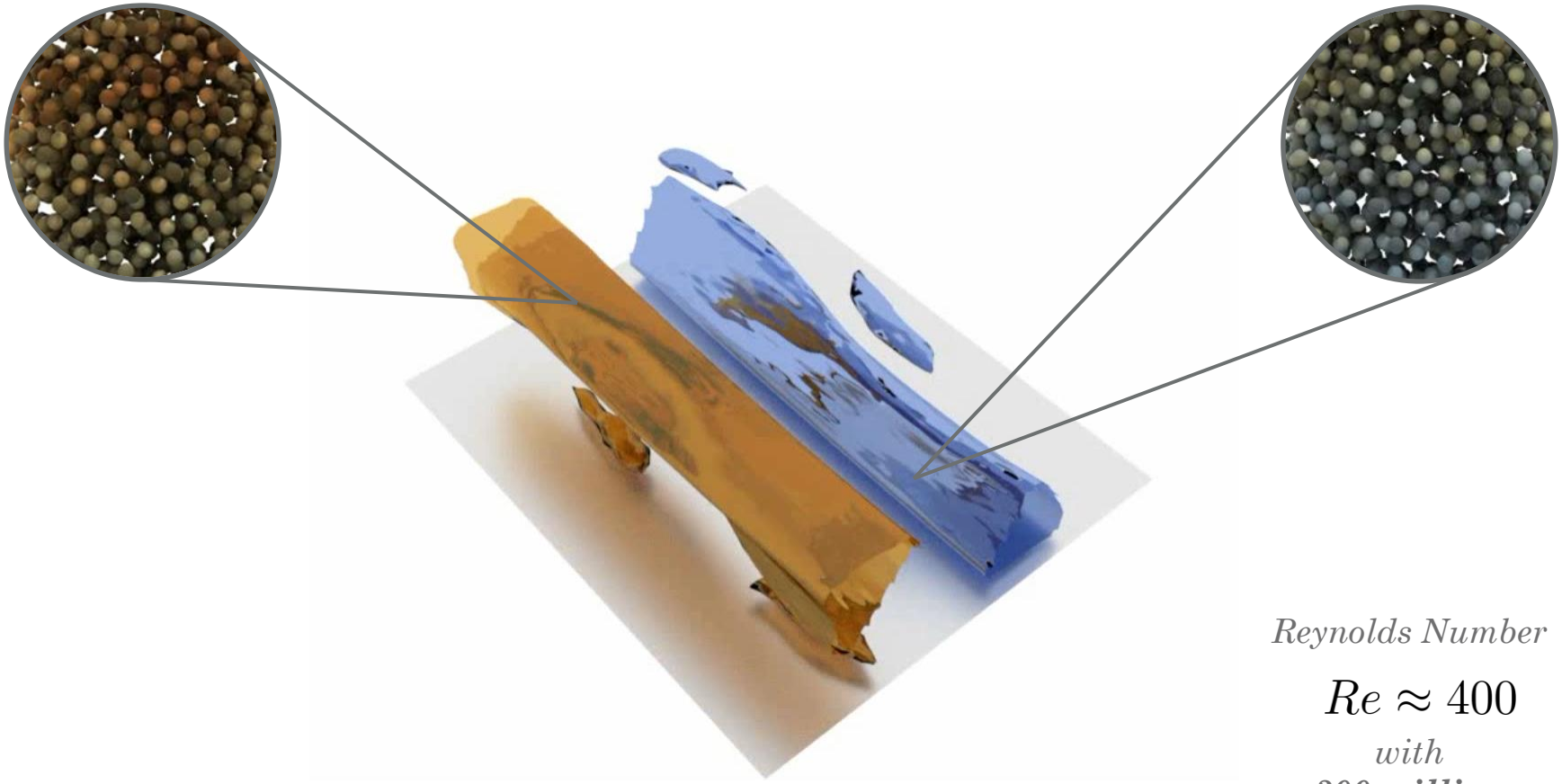
$Re \approx 400$

with

300 million molecules

Molecular Simulation of Turbulence

Brunel University London



Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

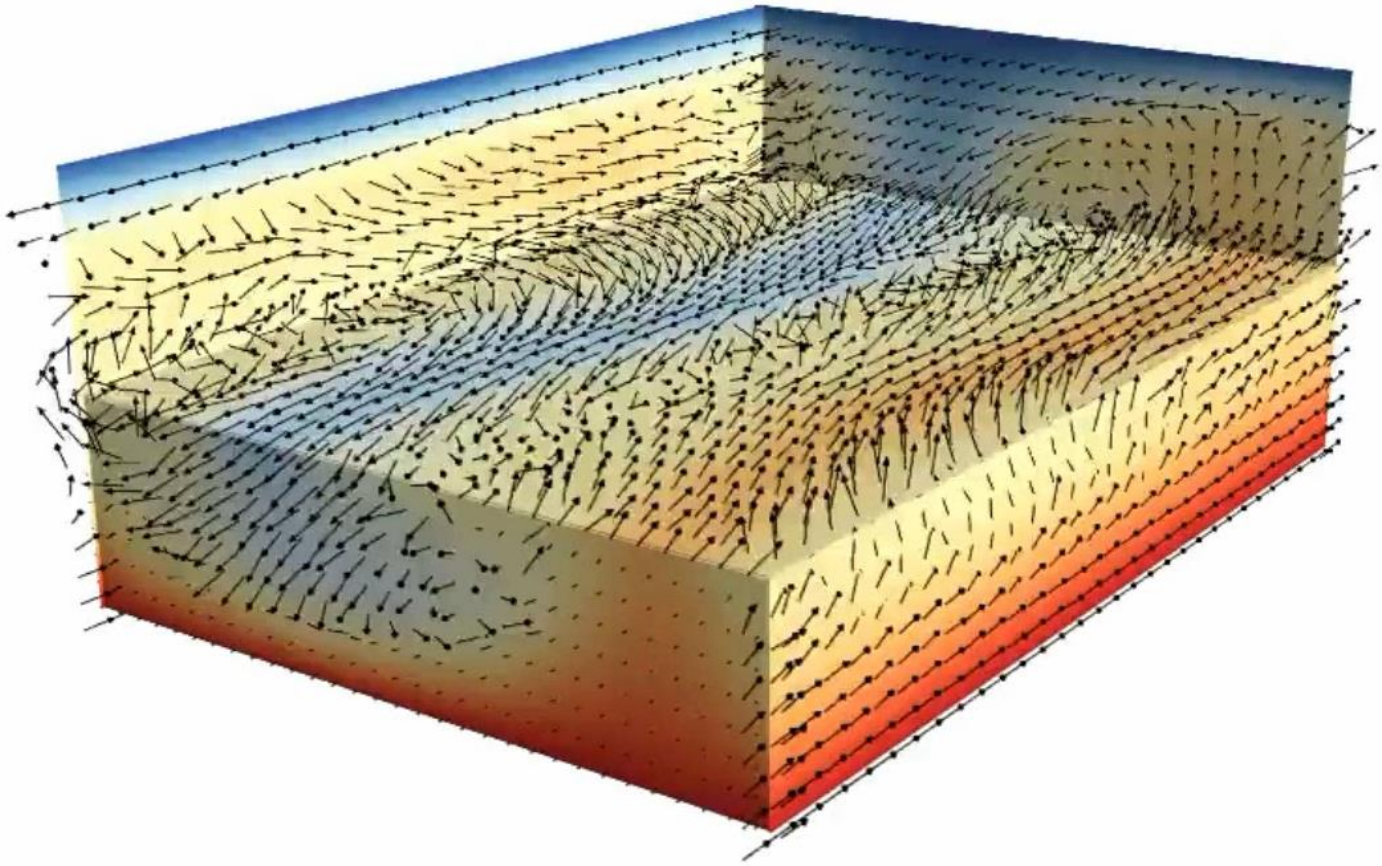
$Re \approx 400$

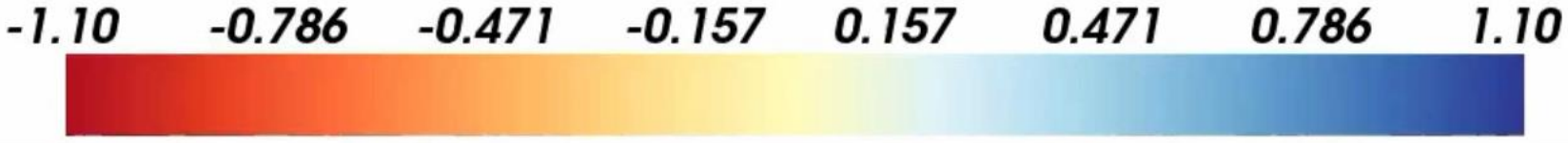
with

300 million molecules

Molecular Turbulent Couette Flow

Brunel University London

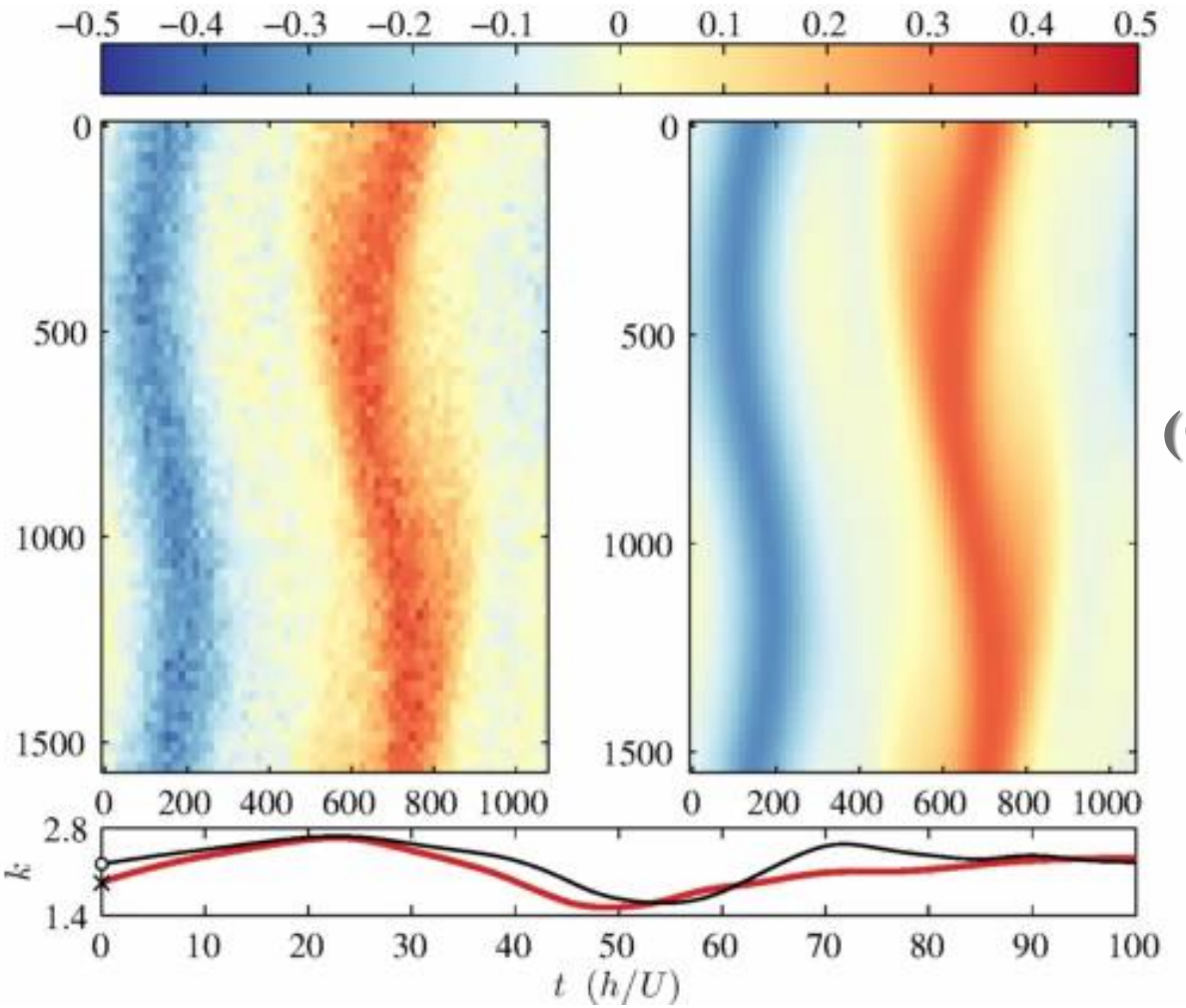




Molecular Simulation of Turbulence

Brunel University London

Centre slice velocity



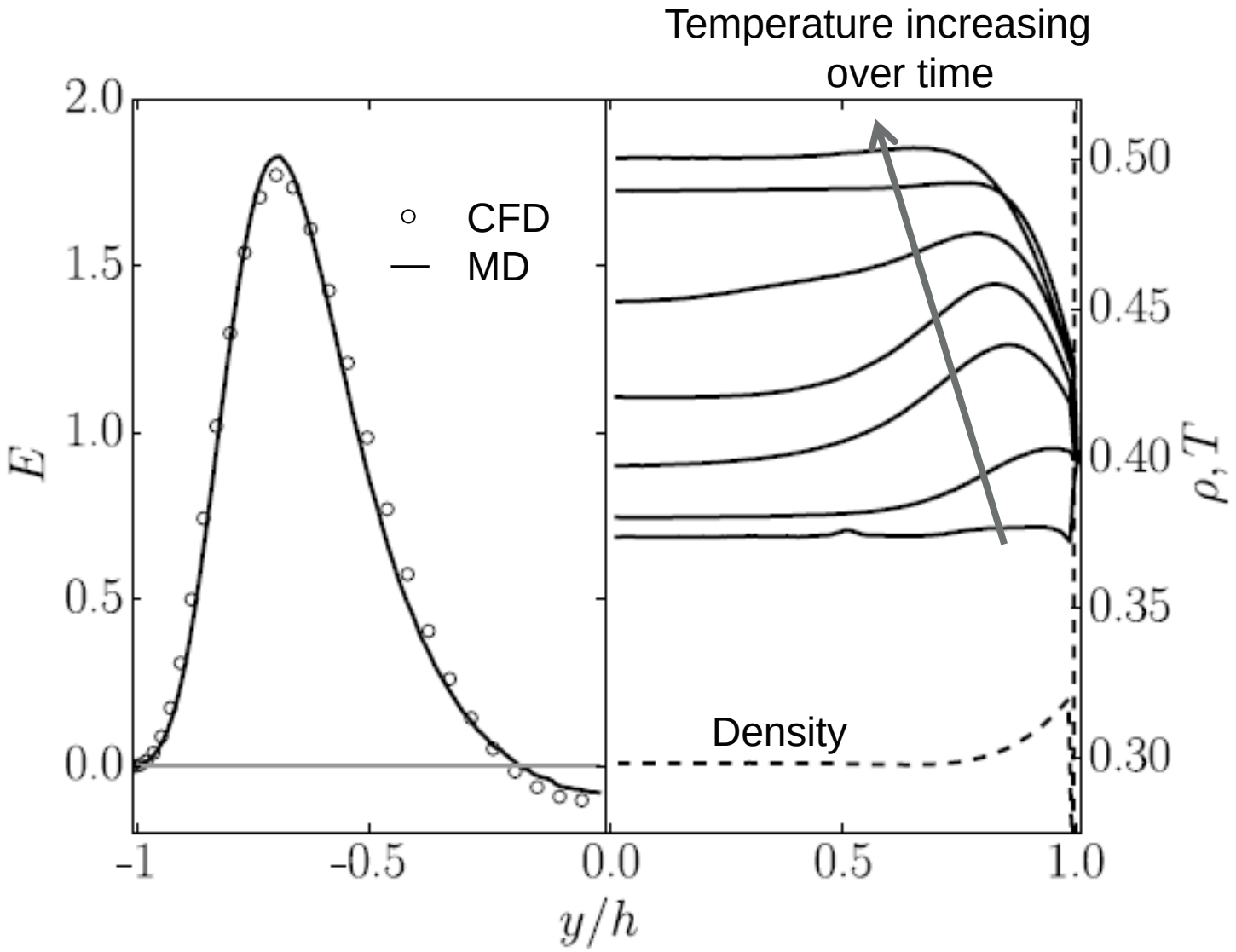
MD

Own code written in Fortran and parallelised using MPI

CFD (Channelflow)

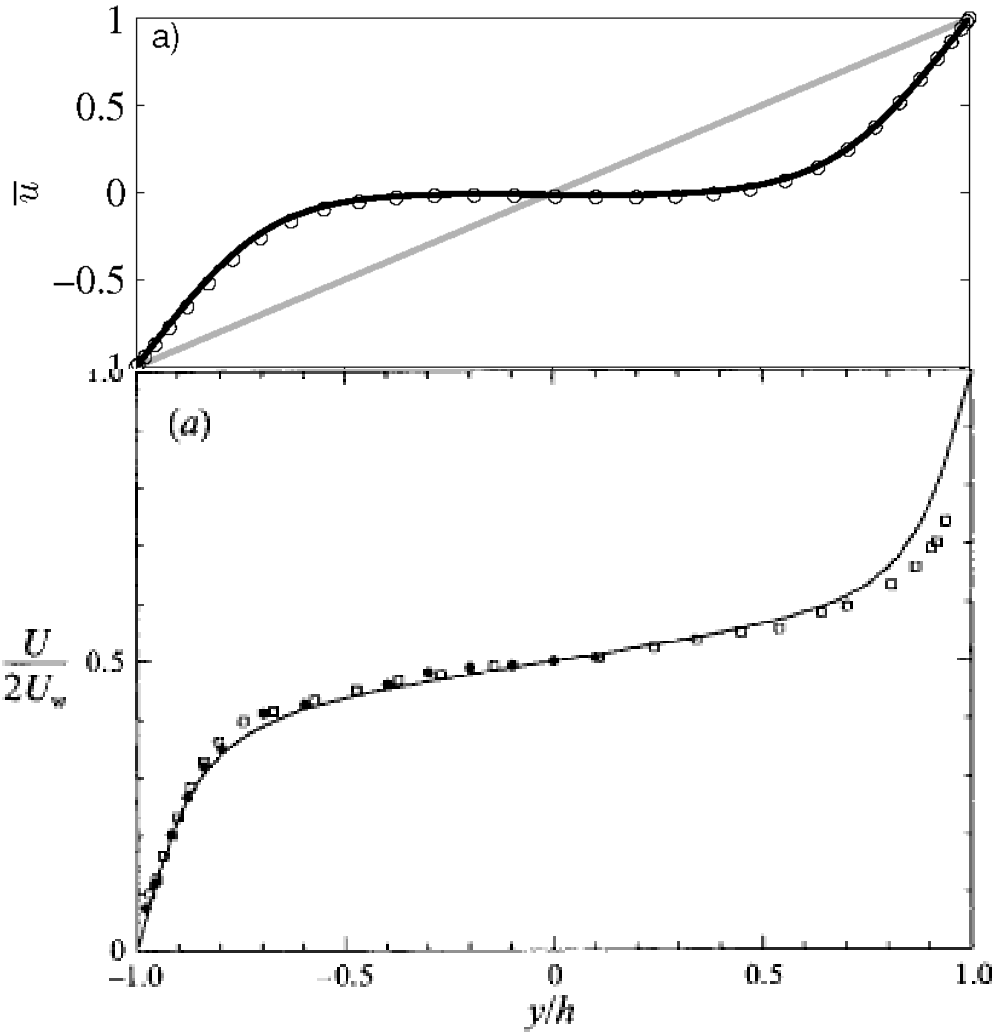
F. Gibson. Channelow: A spectral Navier-Stokes simulator in C++. Technical report, U. New Hampshire, 2012. Channelflow.org.

Turbulent Production and Temperature



Statistical Results

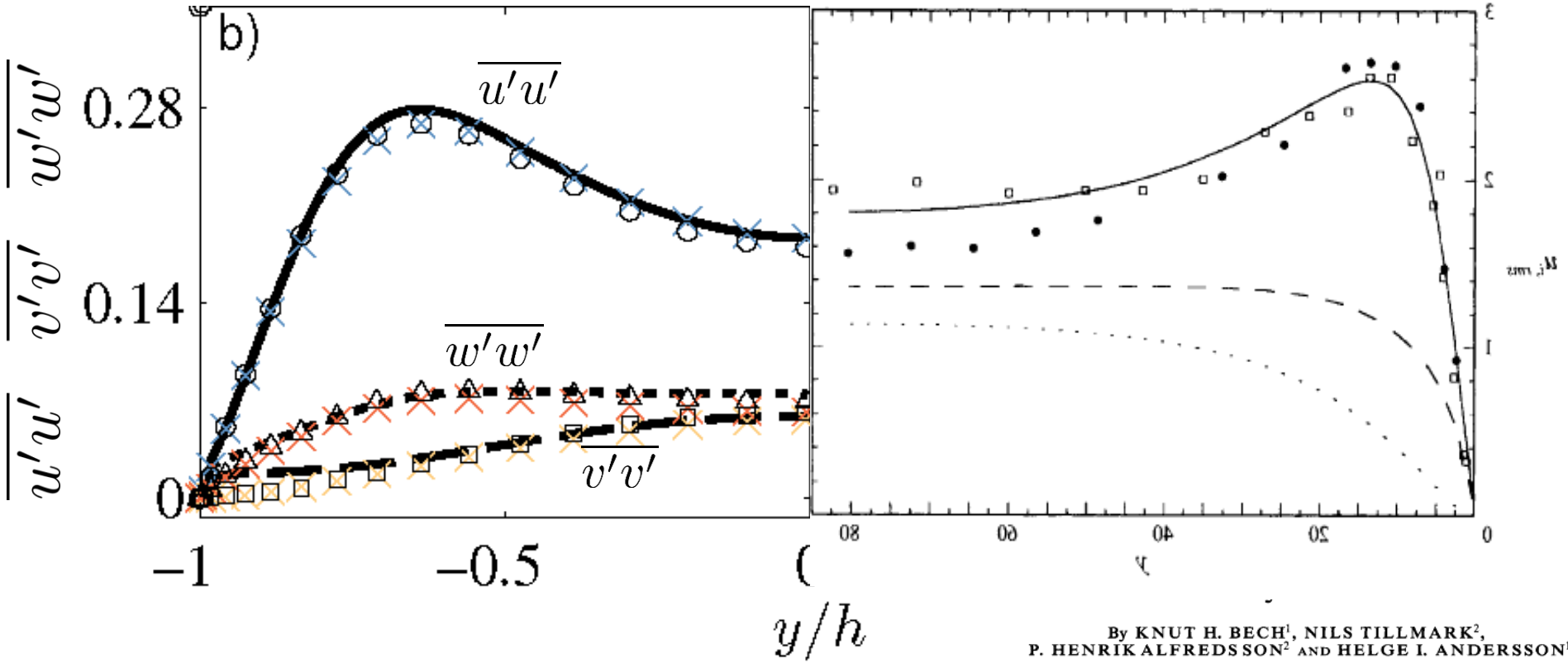
- Averaged velocity profile
- No longer Laminar profile across domain
- Good agreement with literature
  - Numerical continuum studies
  - Experimental results from turbulent simulations



By KNUT H. BECH[1], NILS TILLMARK[2], P. HENRIK ALFREDSSON[2] AND HELGE I. ANDERSSON[1]

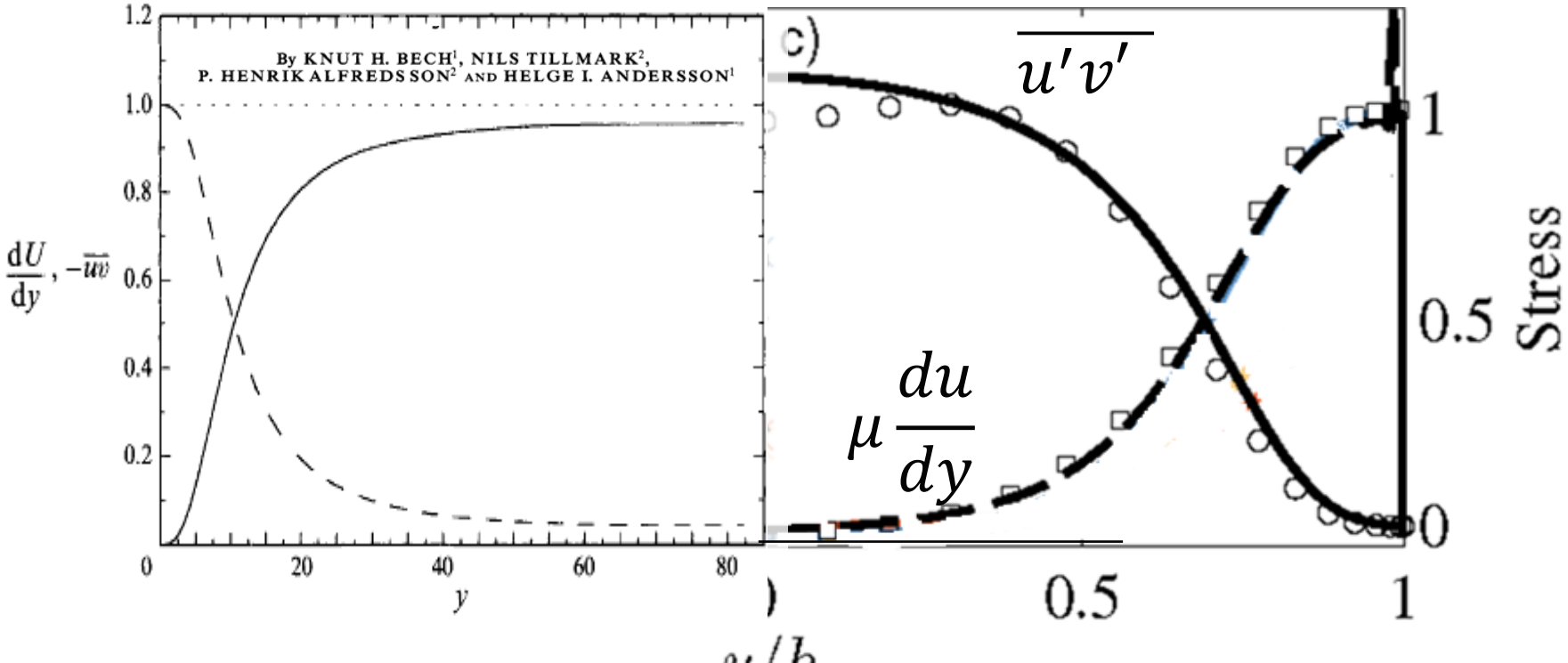
Statistical Results

- Observed RMS velocity profiles match literature
  - Numerical results match very well (Channelflow and CFD literature)
  - General profile is consistent with experimental data



Turbulent Stresses or Molecular Stresses

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

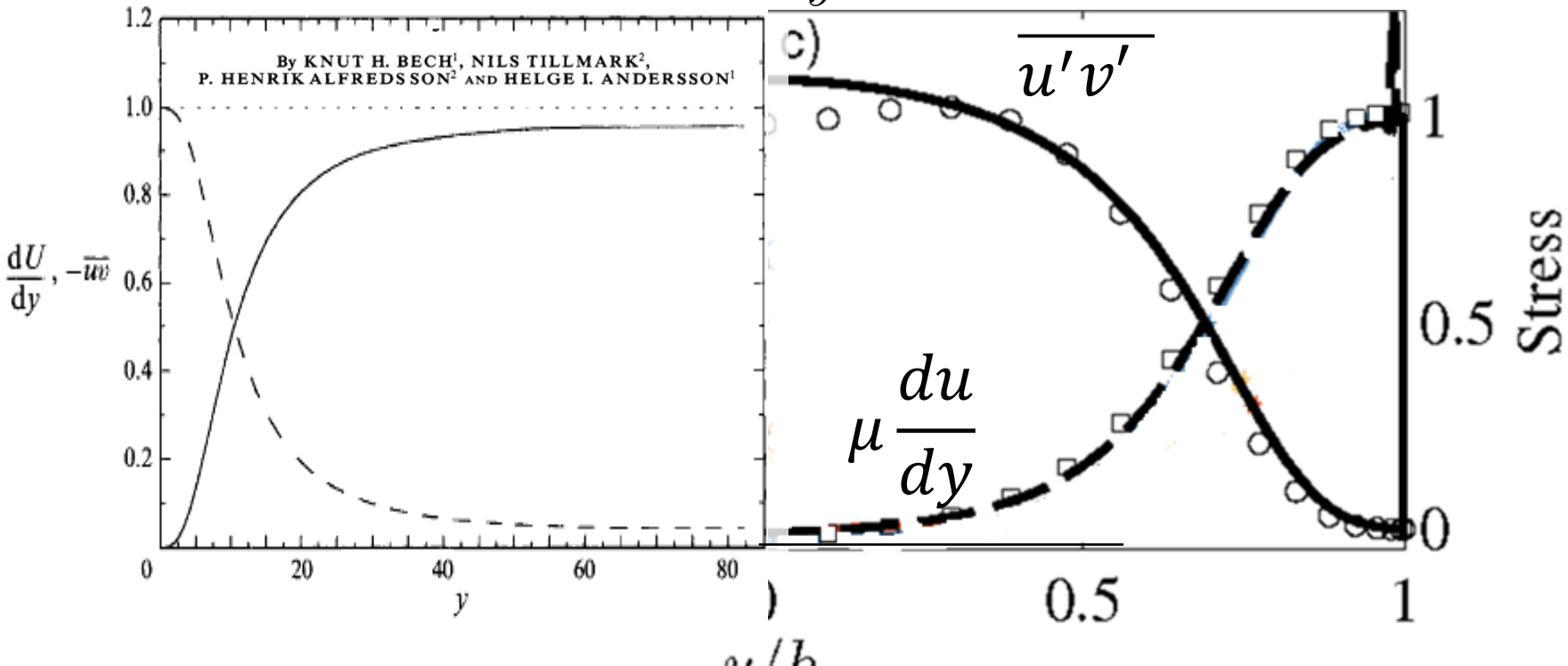


Turbulent Stresses or Molecular Stresses

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

$$\Pi_{xy} = \mu \frac{du}{dy}$$

Reynolds shear stress $\overline{u'v'} - \mu \frac{du}{dy} = 1$ Viscous shear stress



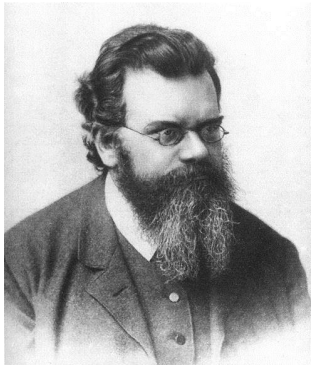
Pressure Tensor in an MD Simulation

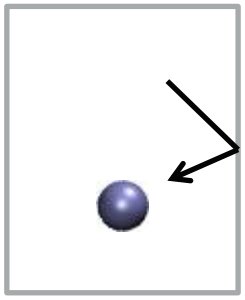
- Pressure definition in a dense molecular system
  - Kinetic part due to fluctuations
  - Configurational part due to liquid structure

$$\oint_S \Pi_{xy} \cdot dS_y = \underbrace{\sum_{i=1}^{N} \left\langle m_i v_{xi} v_{yi} dS_{yi} \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} \left\langle f_{xij} dS_{yij} \right\rangle}_{\text{Configurational}}$$

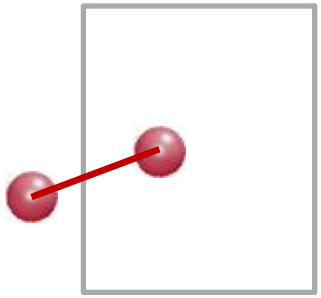
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





$$\dot{\boldsymbol{r}}_i = \boldsymbol{v}_i + \boldsymbol{u}$$

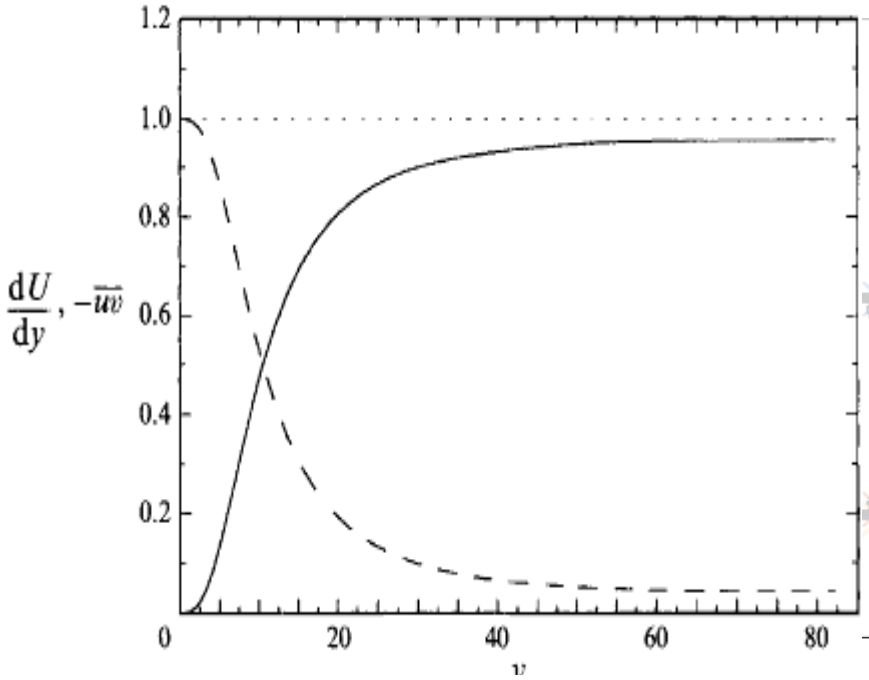


Configurational part

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

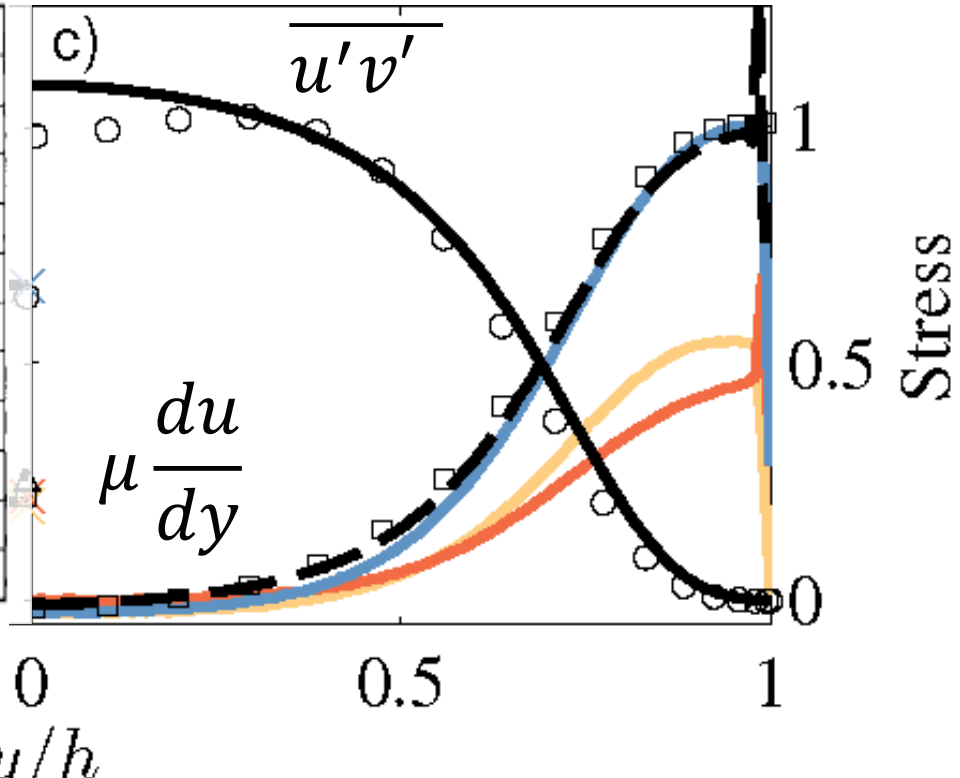
Turbulent Stresses or Molecular Stresses

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



An investigation of turbulent plane Couette flow at low Reynolds numbers

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



Same Concept, Different Scales

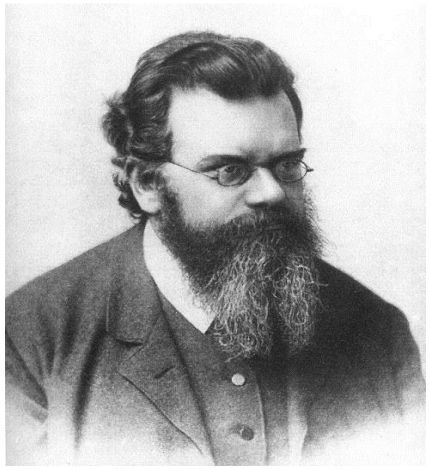
- Reynolds Decomposition

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

- Peculiar velocity

$$\dot{r}_i = u + v_i$$

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



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

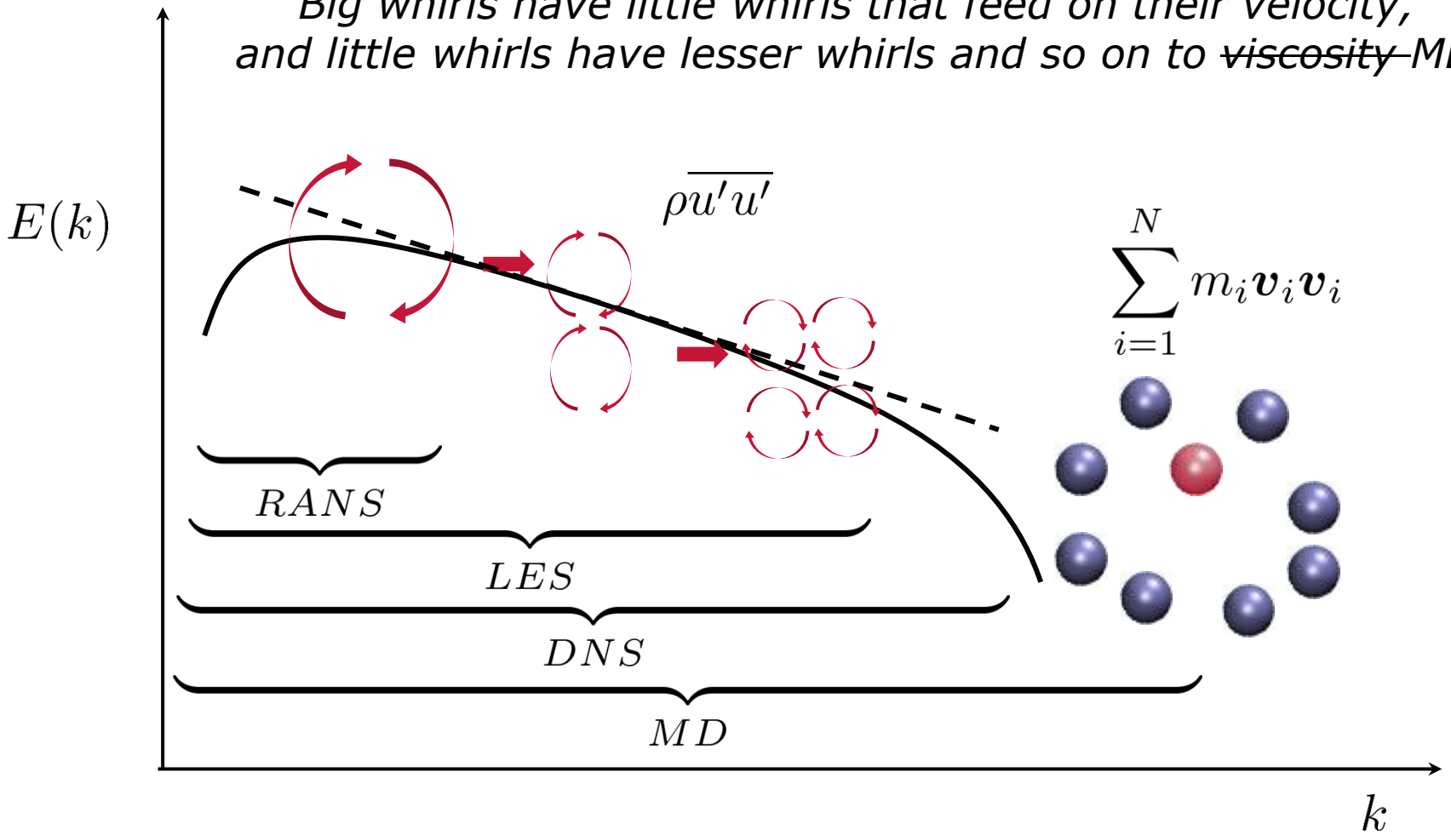
$$\overline{\sum \langle \dot{\boldsymbol{r}}_i \dot{\boldsymbol{r}}_i \rangle} = \overline{\sum \langle \boldsymbol{v}_i \boldsymbol{v}_i \rangle} + \overline{\boldsymbol{u}'\boldsymbol{u}'} + \overline{\boldsymbol{u}\boldsymbol{u}}$$

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

Is Reynolds Stress just Kinetic Pressure?

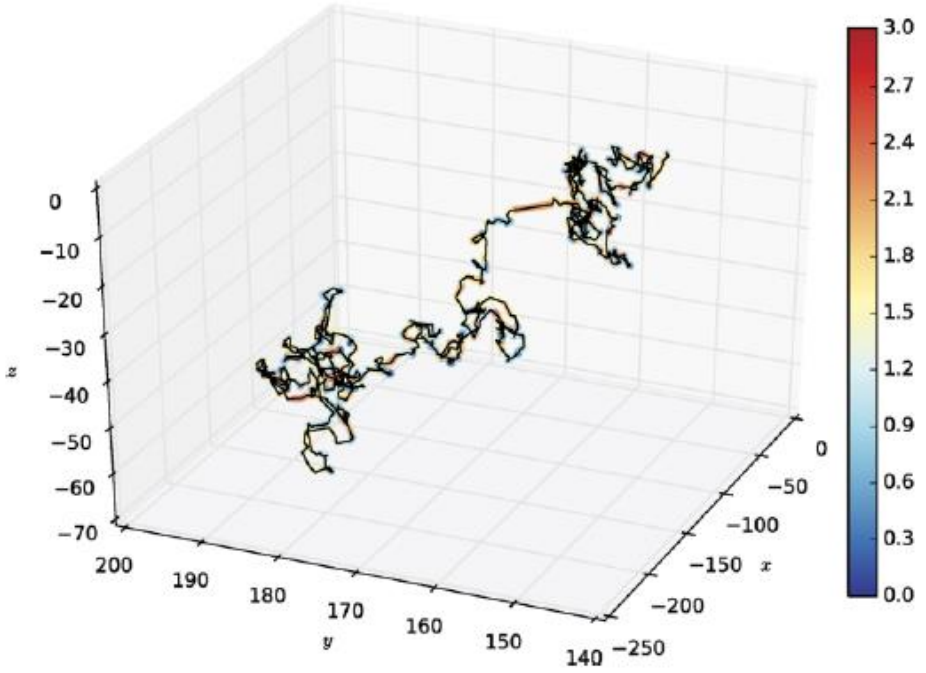
Brunel University London

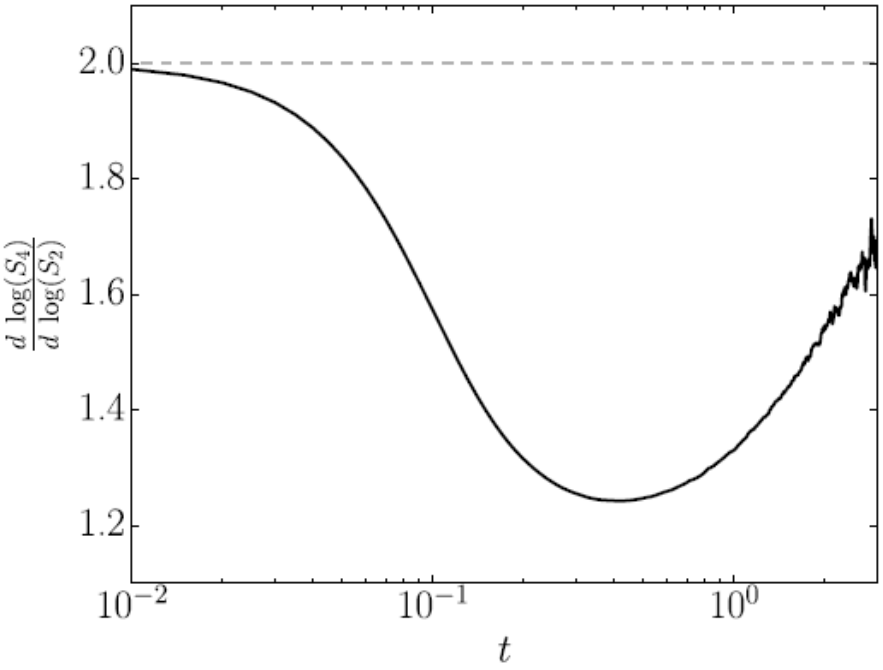
Big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to ~~viscosity~~ MD



The Molecular Cage and Small Scale Eddies

- Following individual molecular trajectories shows eddying motion
- Structure functions shows a similar trend to tracer particles in a turbulent flow

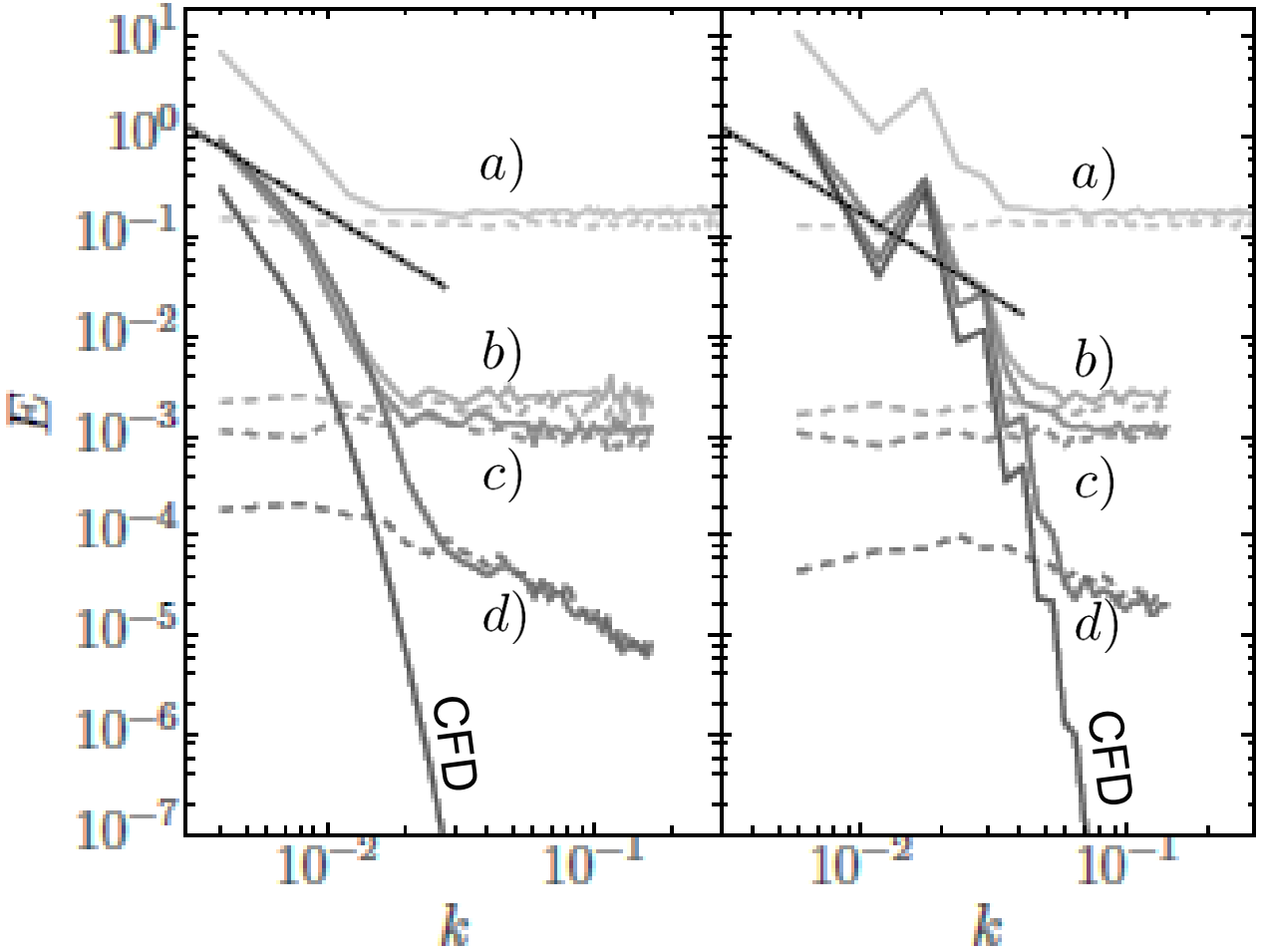


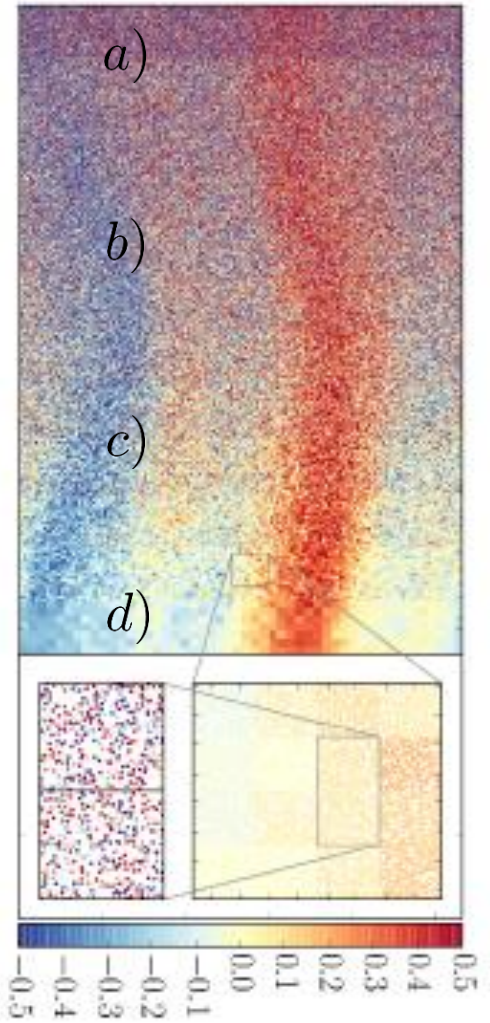


Energy Spectra

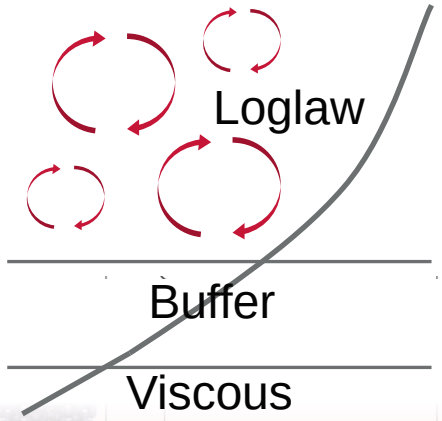
$$\boldsymbol{u} = \frac{1}{N_{cell}} \sum_{i=1}^{N_{cell}} \langle \boldsymbol{v}_i \rangle$$

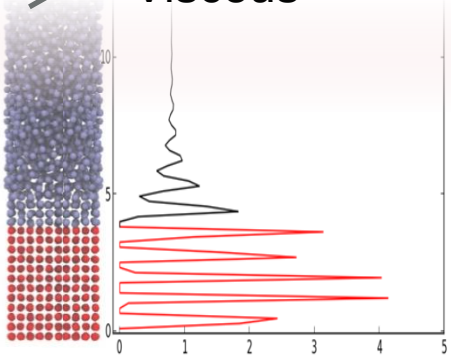
Case	τ_{MD}	Grid resolution
a)	0.005	$672 \times 198 \times 400$
b)	0.005	$84 \times 198 \times 50$
c)	8	$84 \times 198 \times 50$
d)	32	$84 \times 66 \times 50$



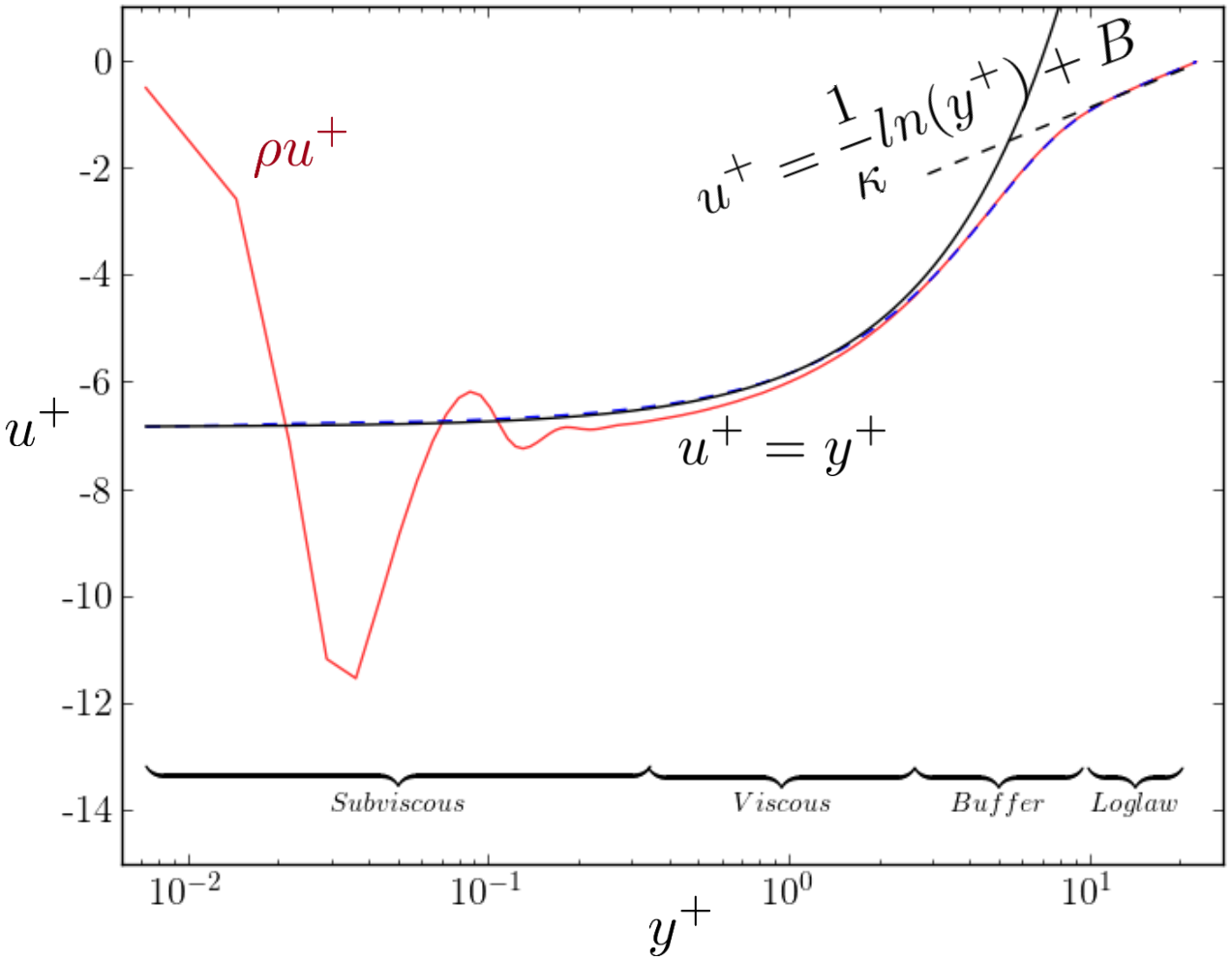


Law of the wall

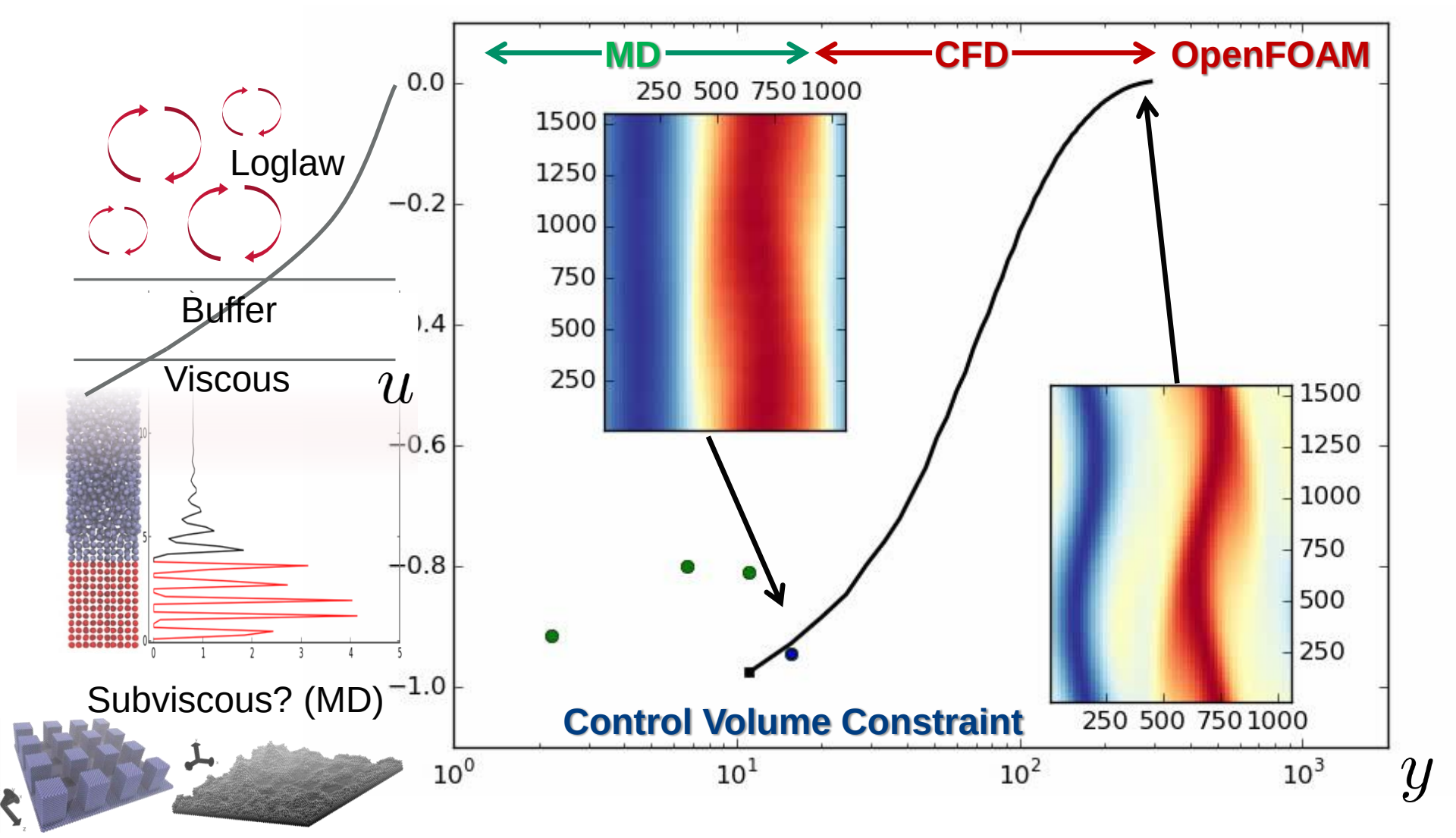




Subviscous? (MD)



Coupling Results – Turbulent Couette



Summary

- Introduction
- Molecular Dynamics
- The Minimal Channel

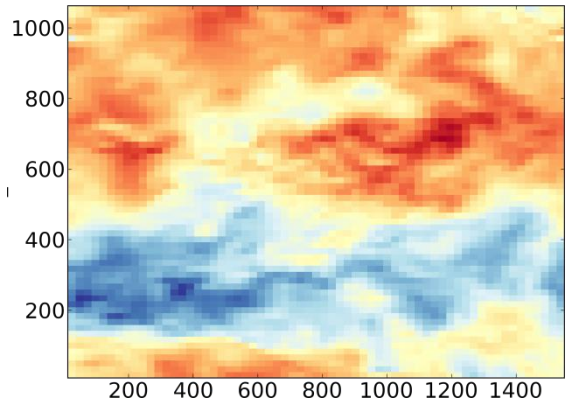
Brunel University London

Any Questions?

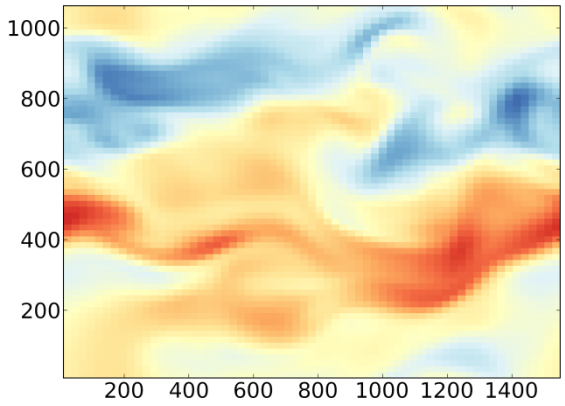
Three plots of decreasing Reynolds Number

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

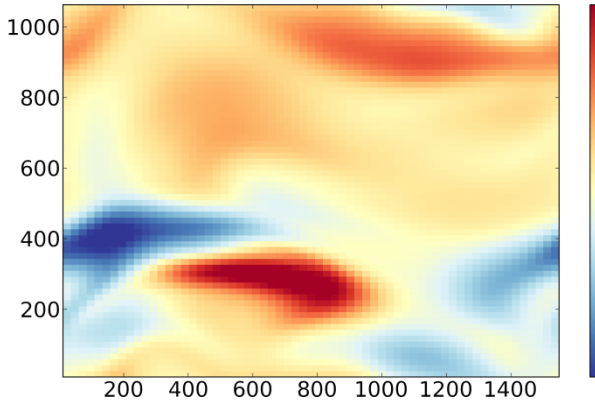
Re ≈ 4000

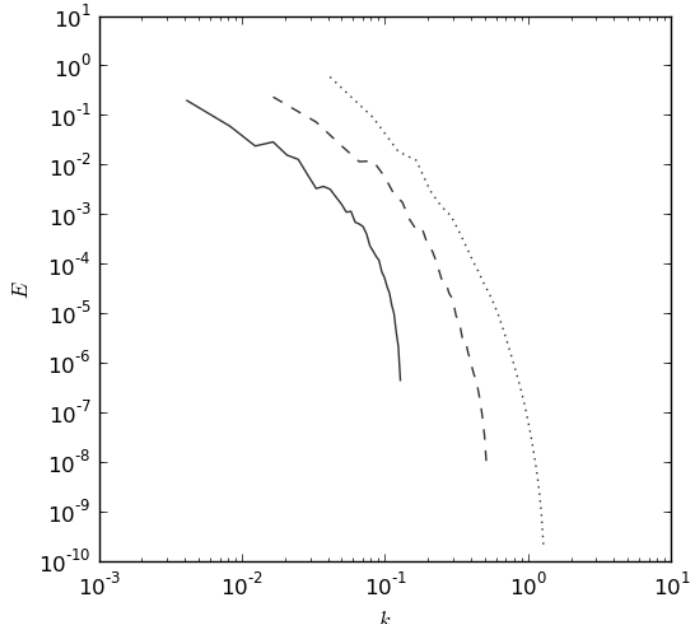


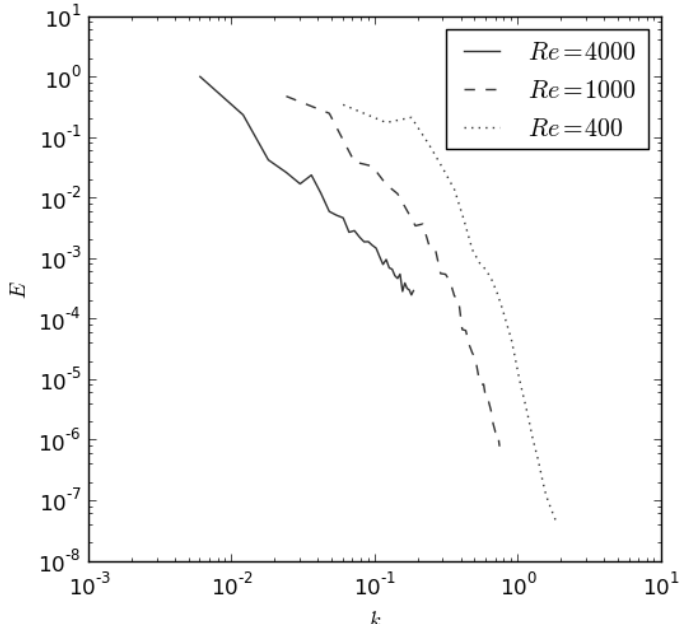
Re ≈ 1000



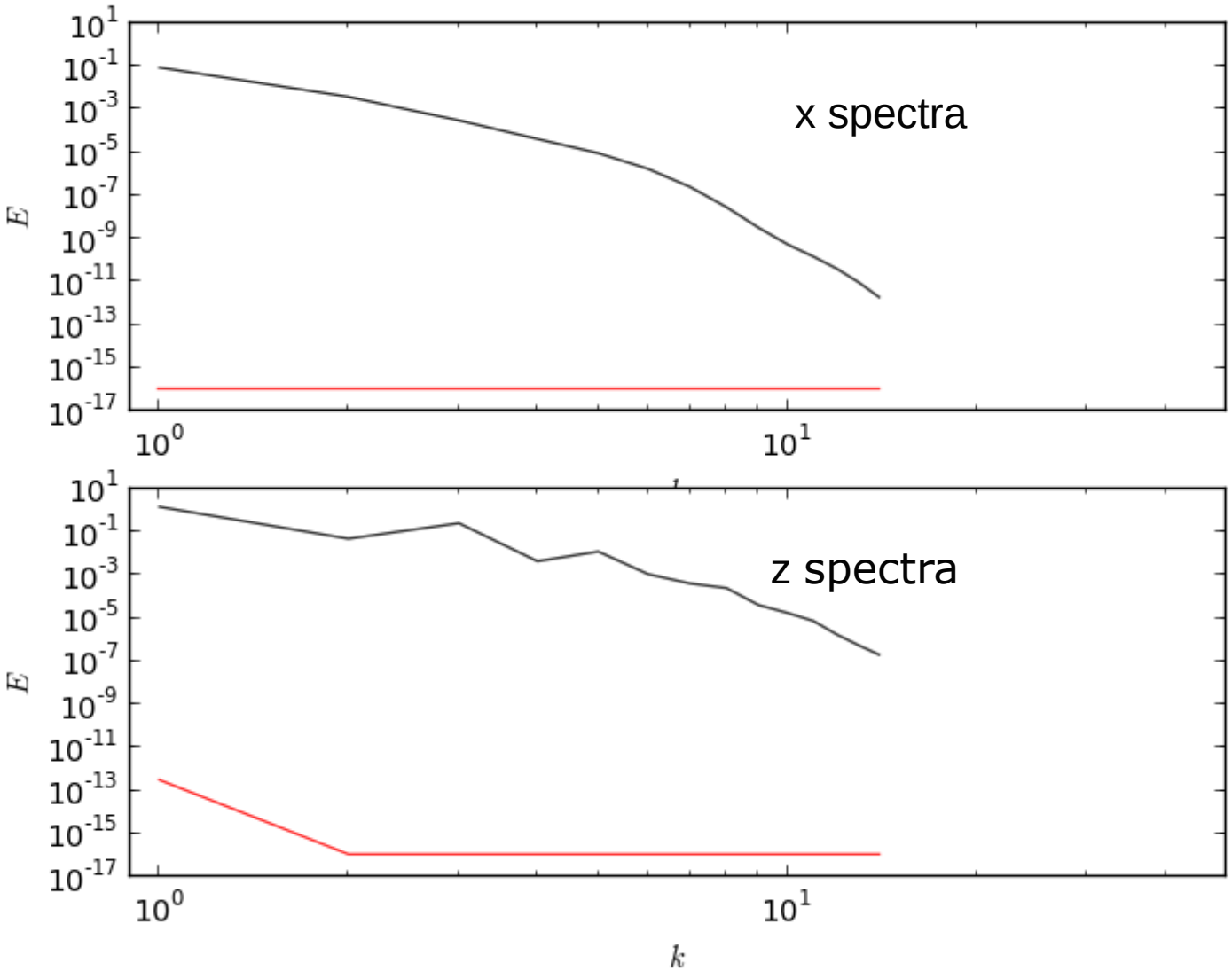
Re ≈ 400







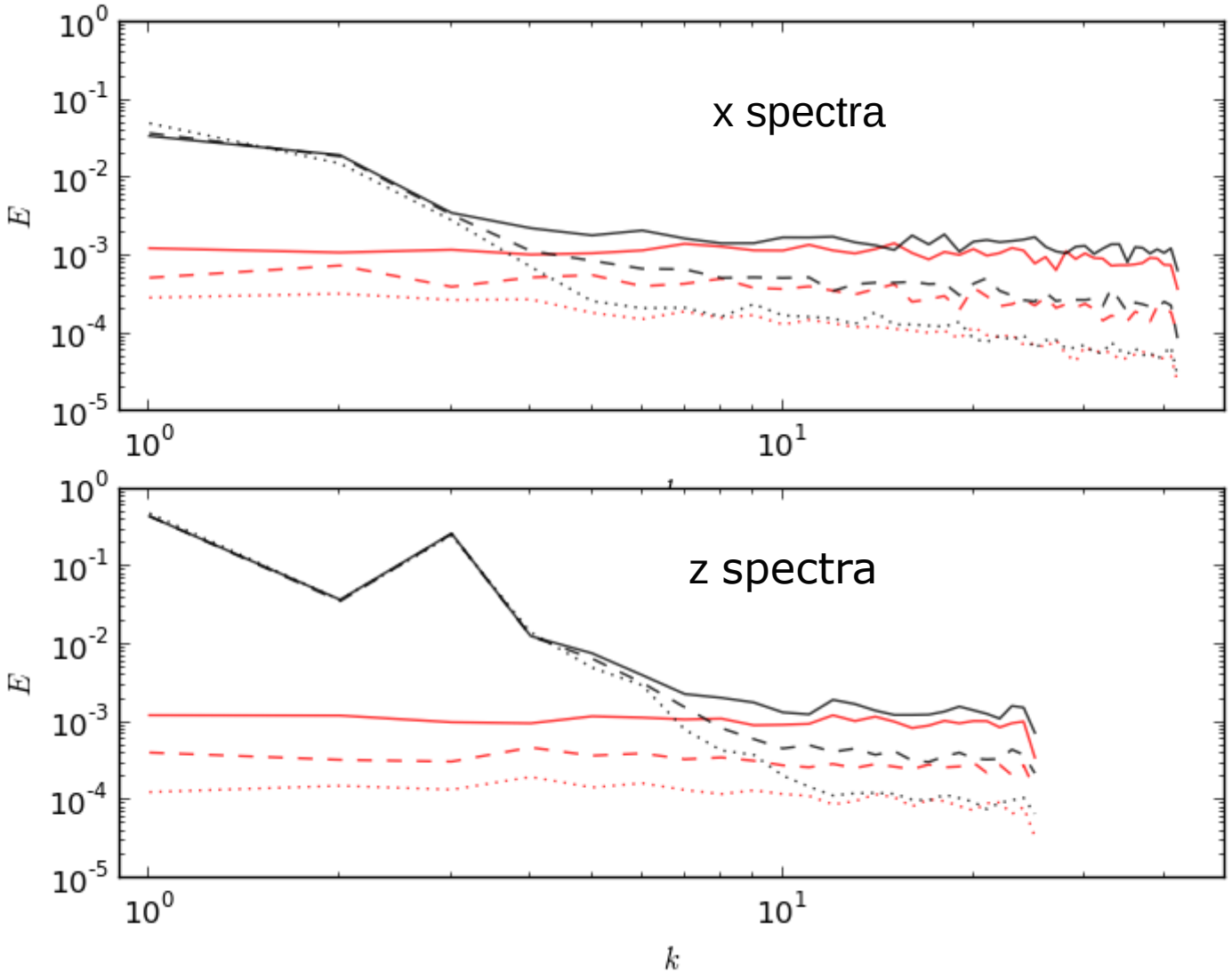
Velocity Spectra



Black Lines
Turbulent CFD Flow

Red Lines
Laminar CFD Flow

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