A Molecular Simulation of the Turbulent Minimal Channel Flow

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Summary

- Introduction
- Molecular Dynamics (MD)
- The Minimal Channel

Section 0

INTRODUCTION

Computational Fluid Dynamics

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

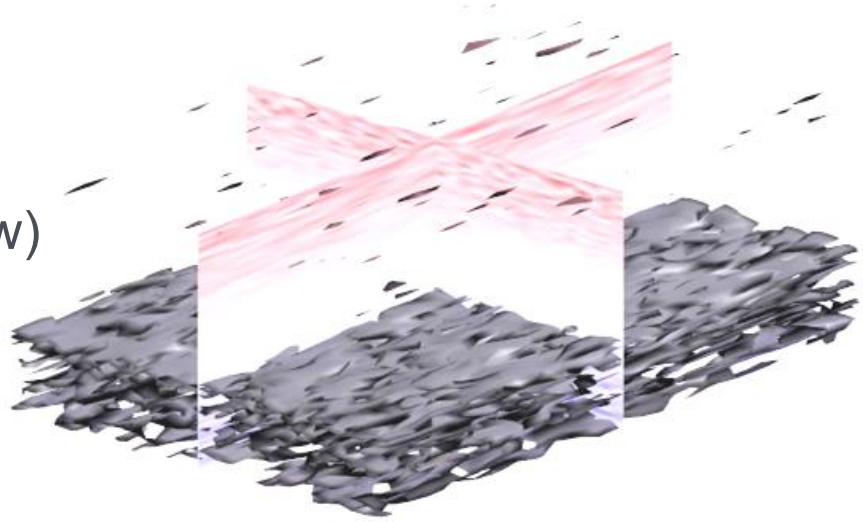
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - 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

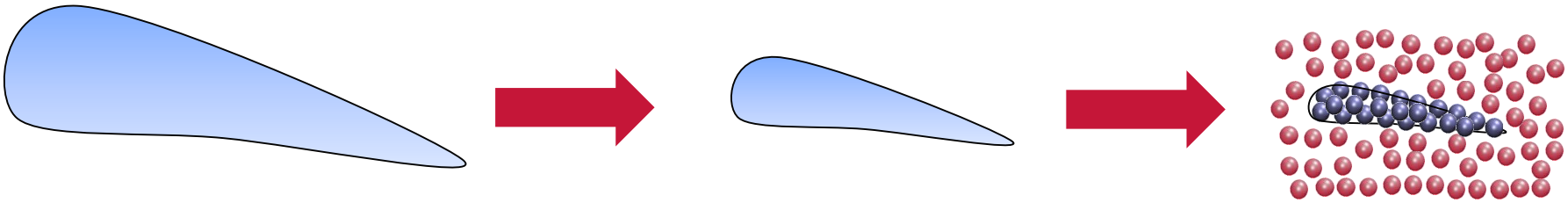
- The Incompressible Navier-Stokes Equation

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

- 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?



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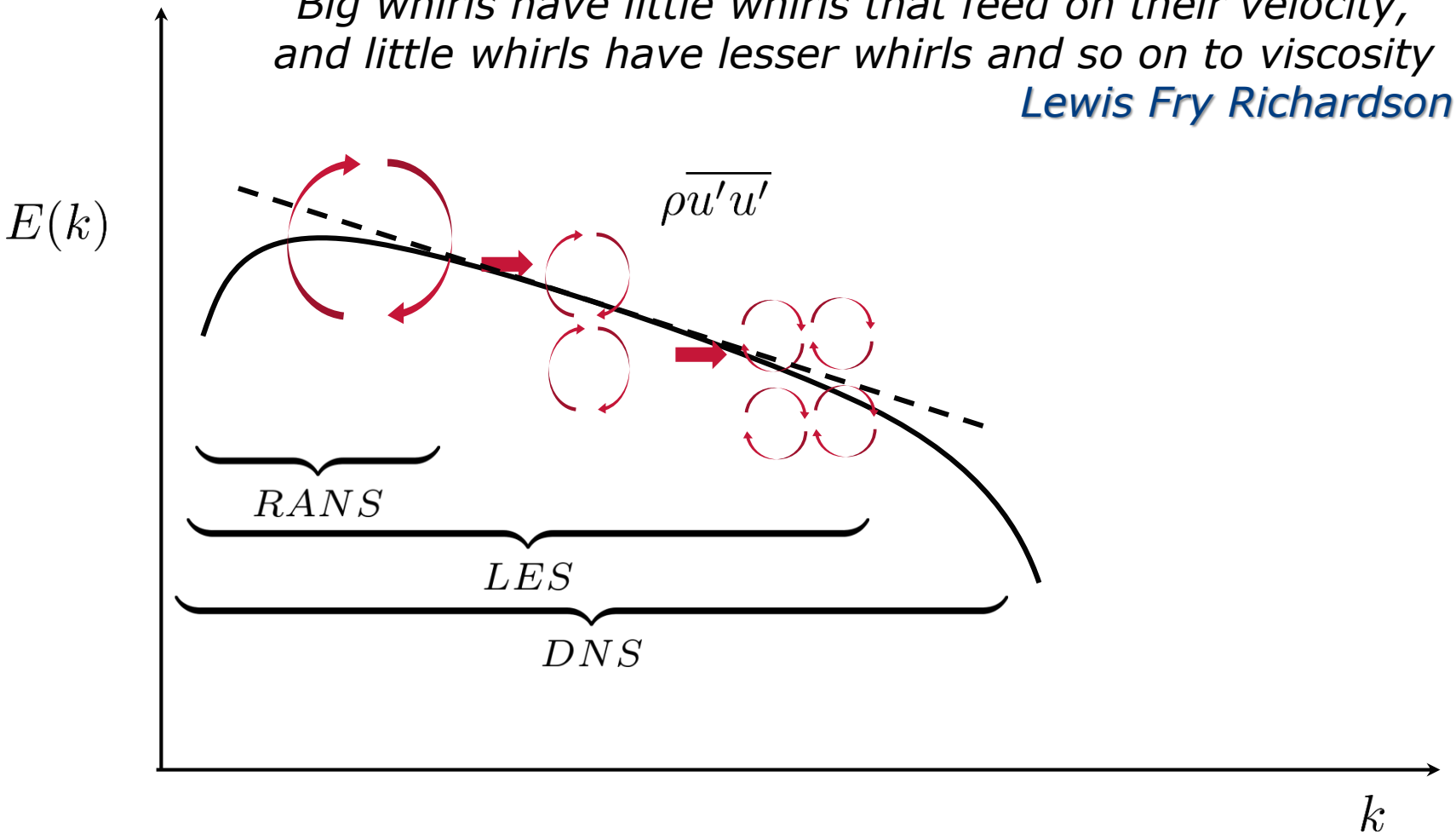
- Reynolds number
  - Scaling argument applied to any scale
- Is there a minimum?
  - Travis et al (1997) single phase valid down to nanometers
  - Local thermodynamic equilibrium vs. hydrodynamic scales
  - Knudsen Number fairly useless for dense fluids

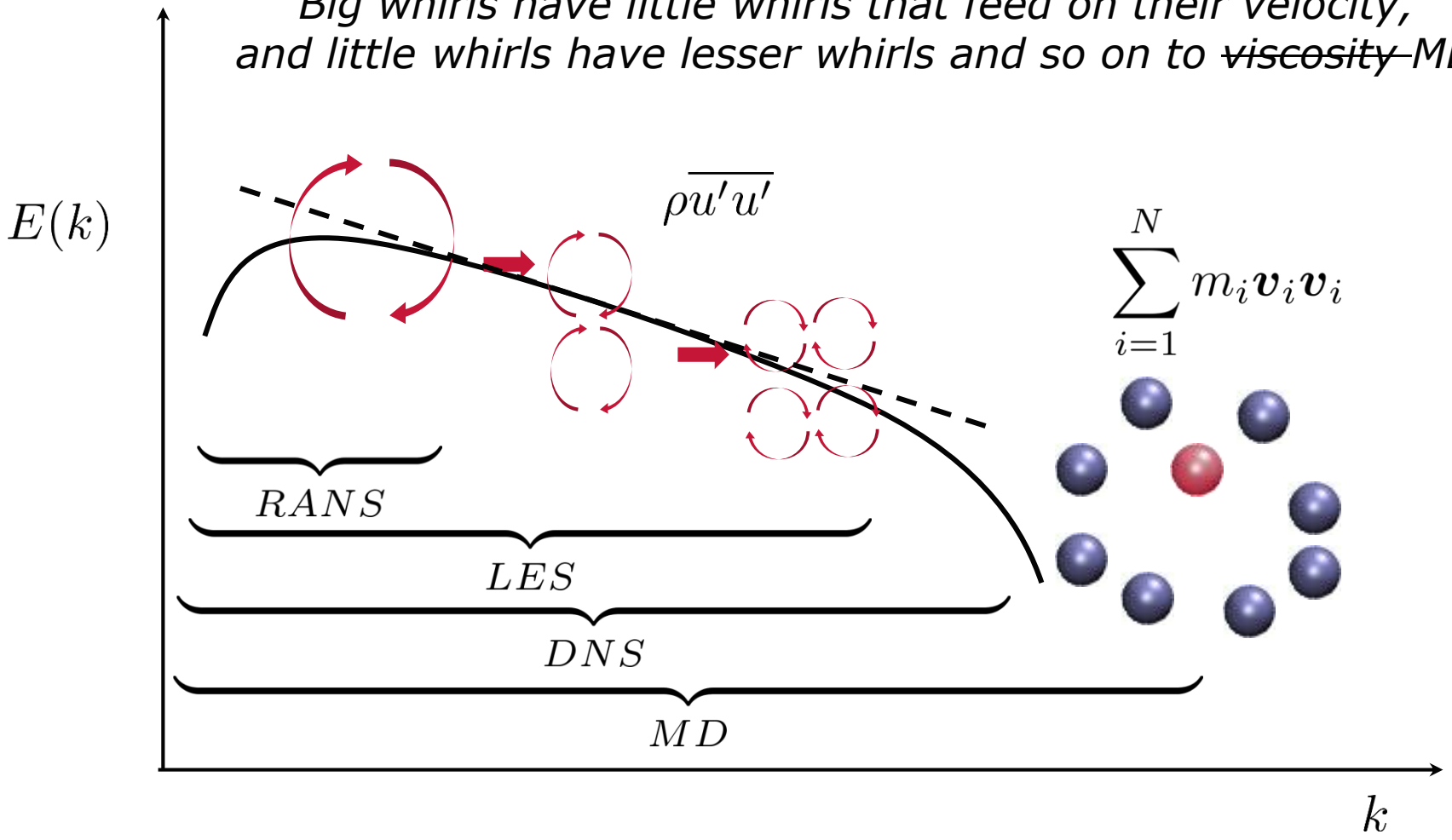
The Continuum

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



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



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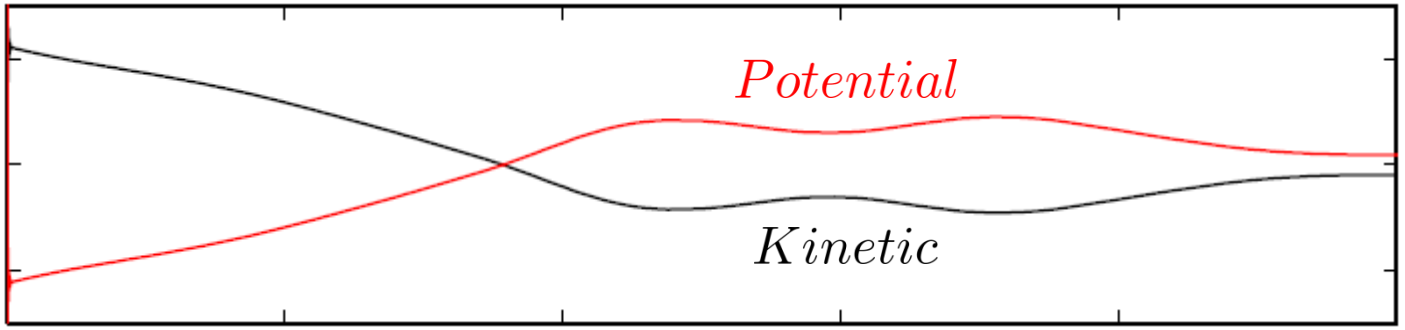
Section 1

MOLECULAR DYNAMICS

Molecular Dynamics

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

$\frac{dE}{dt}$



  - 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

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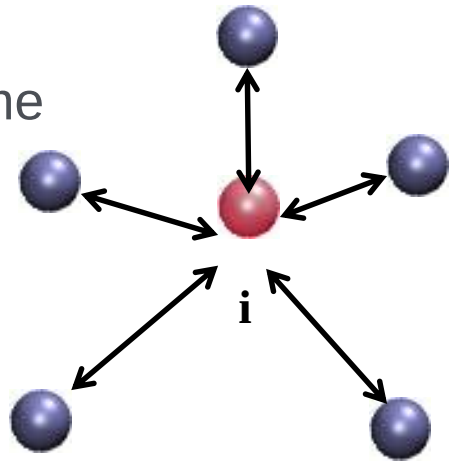
Discrete molecules in continuous space

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

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

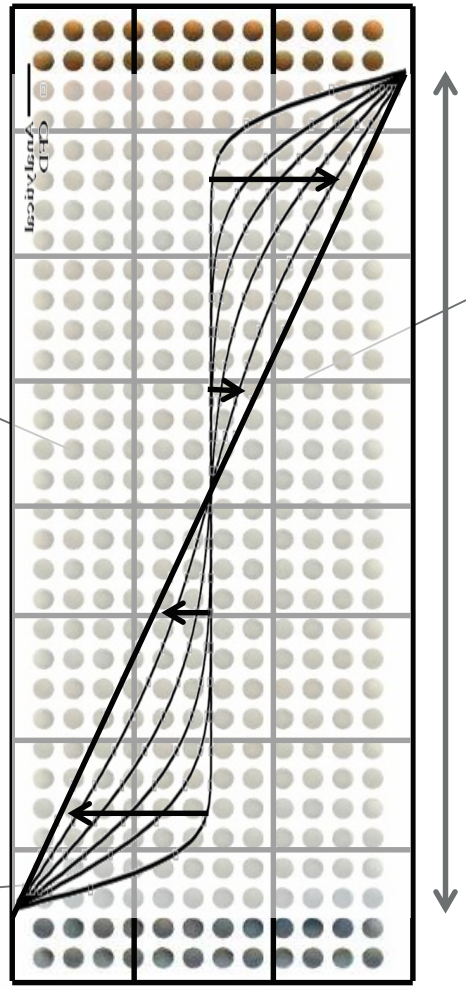


Acceleration obtained from forces

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

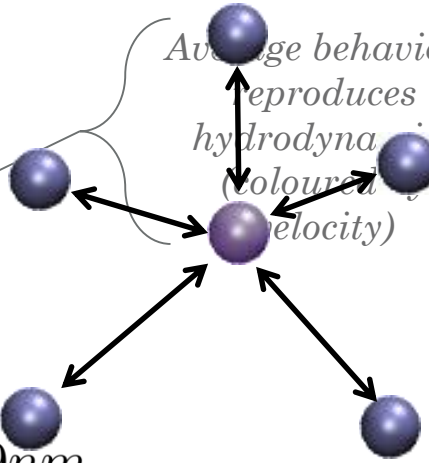
$$m_i\ddot{\mathbf{r}}_i = \mathbf{F}_i = \sum_{i\neq j}^{N} \boldsymbol{f}_{ij} = \sum_{i\neq j}^{N} \boldsymbol{\nabla}\Phi_{ij} \qquad \Phi(r_{ij}) = 4\epsilon\left[\left(\frac{\ell}{r_{ij}}\right)^{12} - \left(\frac{\ell}{r_{ij}}\right)^{6}\right]$$

Molecular Dynamics



Liquid structure causes viscosity

Stick-slip near walls



Average behaviour reproduces hydrodynamics (coloured by velocity)

$H \approx 9nm$

Reynolds Number

$Re \approx 15$

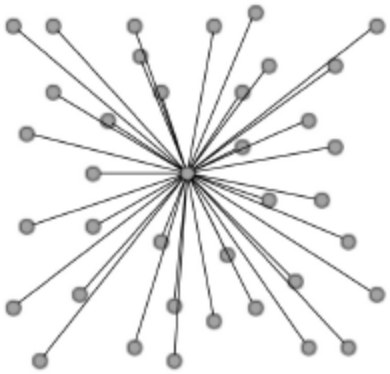
with

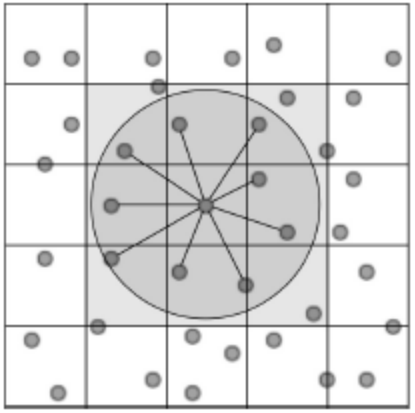
4096 molecules

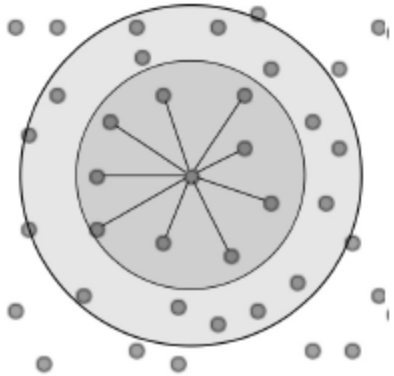
MD Computing

- 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

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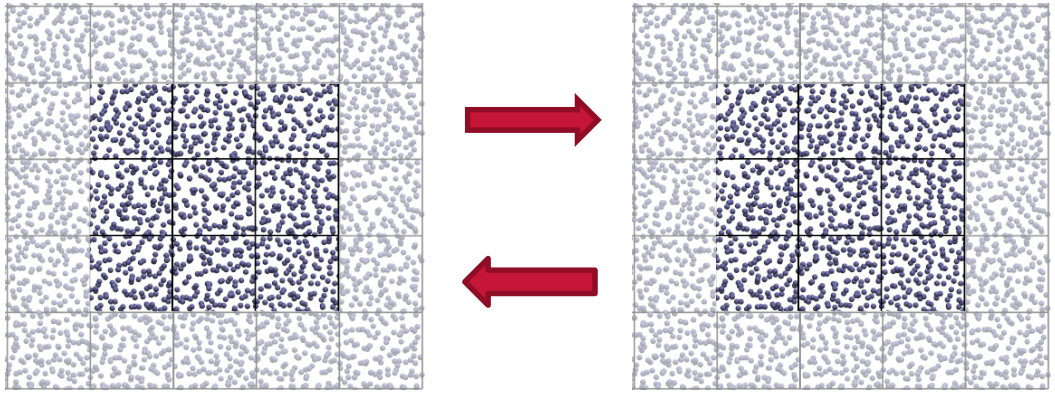
Localisations lends itself to parallel computing using MPI

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



Halo exchange of variable amounts of data

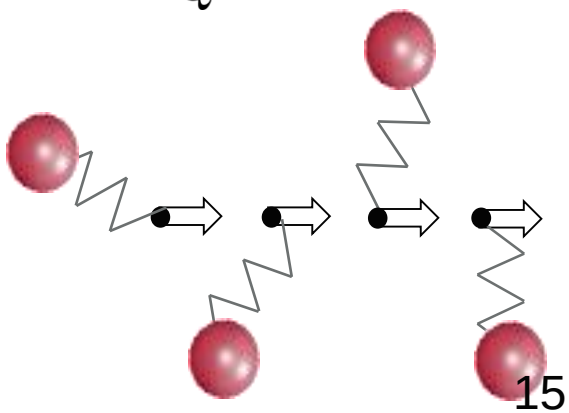
- MPI_Send
- MPI_Probe and MPI_Recv

NEMD - Tethering and Thermostatting

- Non Equilibrium Molecular Dynamics (NEMD) is the study of cases beyond thermodynamic equilibrium, with:
  - Temperature gradients
  - Flow of fluid (e.g. Couette or Poiseuille flow)
- We induce temperature gradients and flows
  - Thermostats (e.g. Nosé Hoover)
    - Remove heat from system
  - Tethered molecules
    - (An)harmonic spring to tether site
  - With sliding
    - Slide site and (optionally) molecules

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \boldsymbol{F}_i^{teth} - \psi m_i \boldsymbol{c}_i$$

$$\dot{\psi} = \frac{1}{Q}\left[T - 3T_{target}\right]$$



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

NEMD - Tethering and Thermostatting

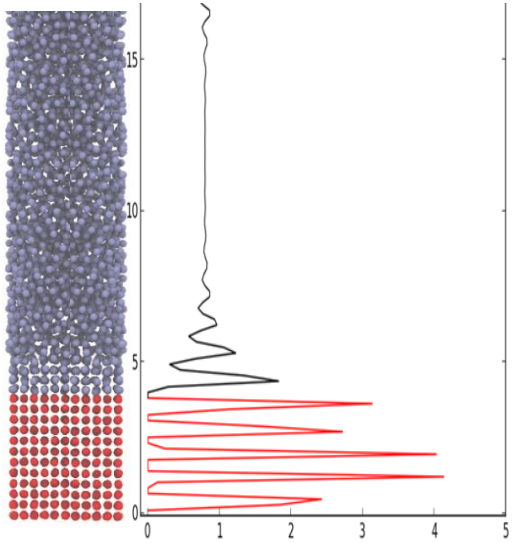
- Non Equilibrium Molecular Dynamics (NEMD) is the study of cases beyond thermodynamic equilibrium, with:
  - An MD system is completely described by position $\boldsymbol{r}_i$ and velocity $\boldsymbol{v}_i$ of all N molecules in the system
  - Theoretical underpinning in the form of the Liouville equation – a continuity equation in 6N degrees $f = f(\boldsymbol{r}_i, \boldsymbol{v}_i)$ which gives,

$$\frac{df}{dt} = \sum_{i=1}^{N} \left[\frac{\partial \boldsymbol{r}_i}{\partial t} \frac{\partial f}{\partial \boldsymbol{r}_i} + \frac{\partial \boldsymbol{v}_i}{\partial t} \frac{\partial f}{\partial \boldsymbol{v}_i} \right]$$

- Just awarded a special interest group (SIG) in NEMD
  - Please let me know if you're interested in joining
  - Potential applications in a wide range of problems in fluid dynamics so need help identifying interesting challenges
  - The microscopic underpinnings of fluid dynamics

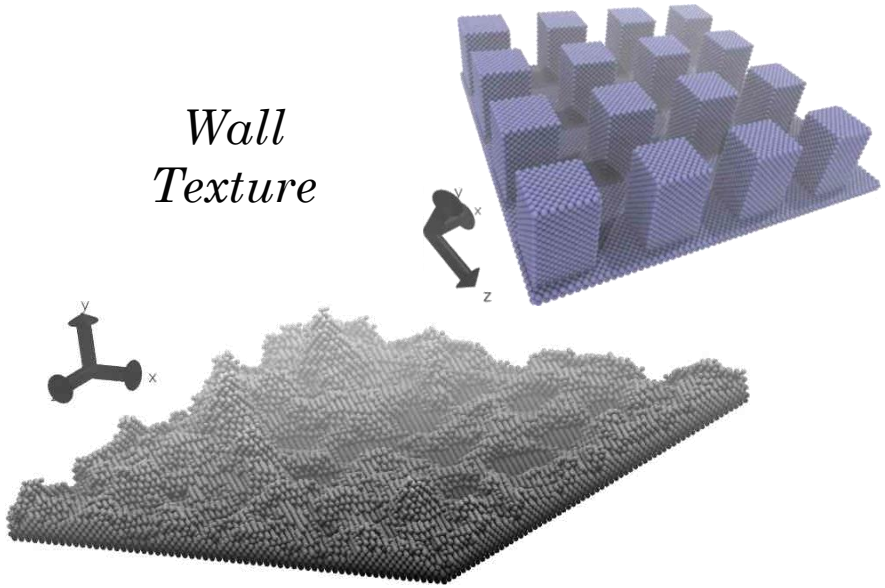
Molecular Dynamics – Complex Walls and Fluids

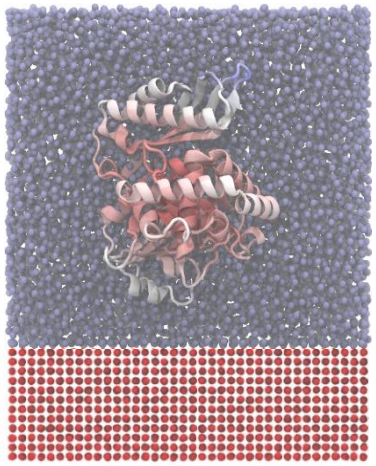
Liquid structure causes viscosity



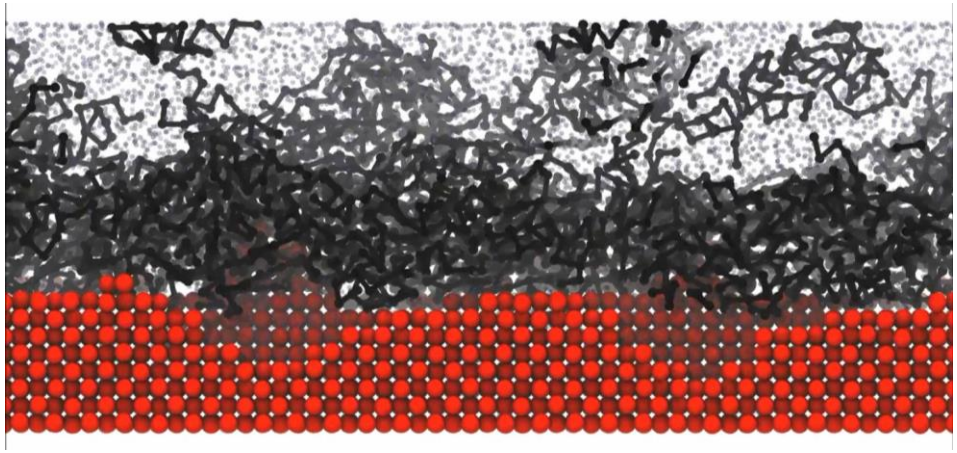
Stick-slip near walls

Wall Texture





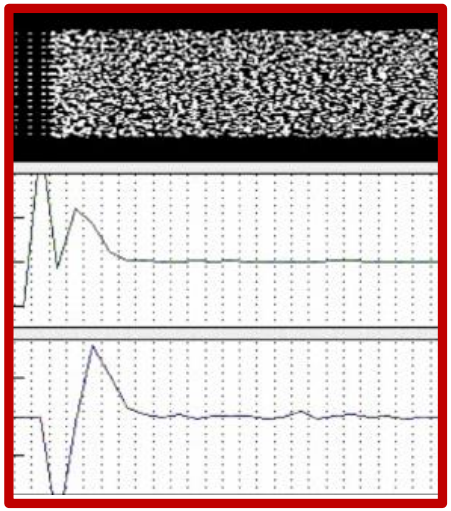
Molecules of arbitrary complexity



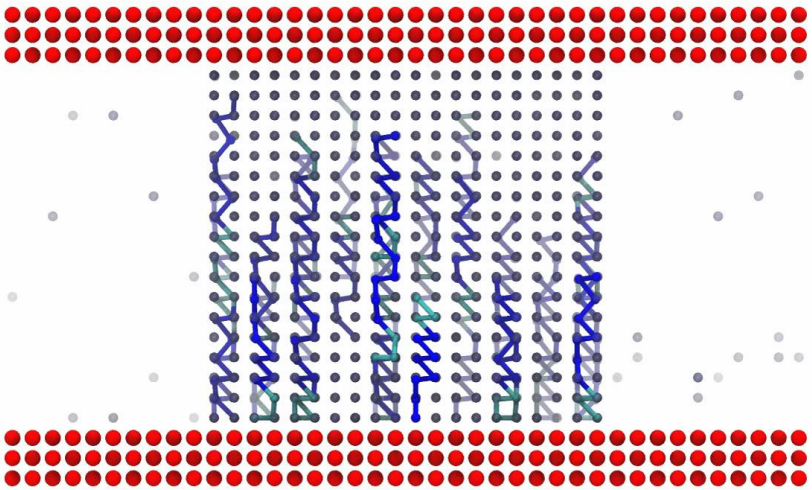
Oil, water and textured surface

Molecular Dynamics – Shocks and Multi-Phase

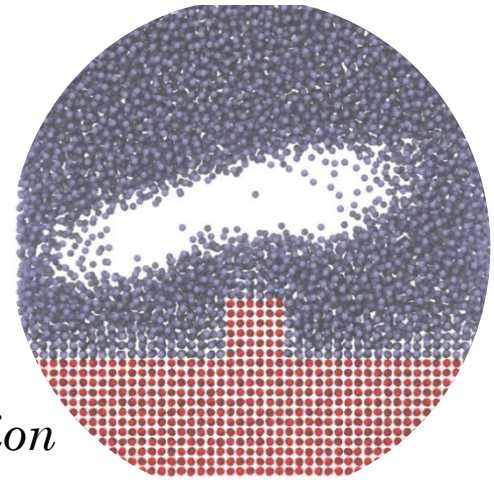
Shockwave



Droplet Formation

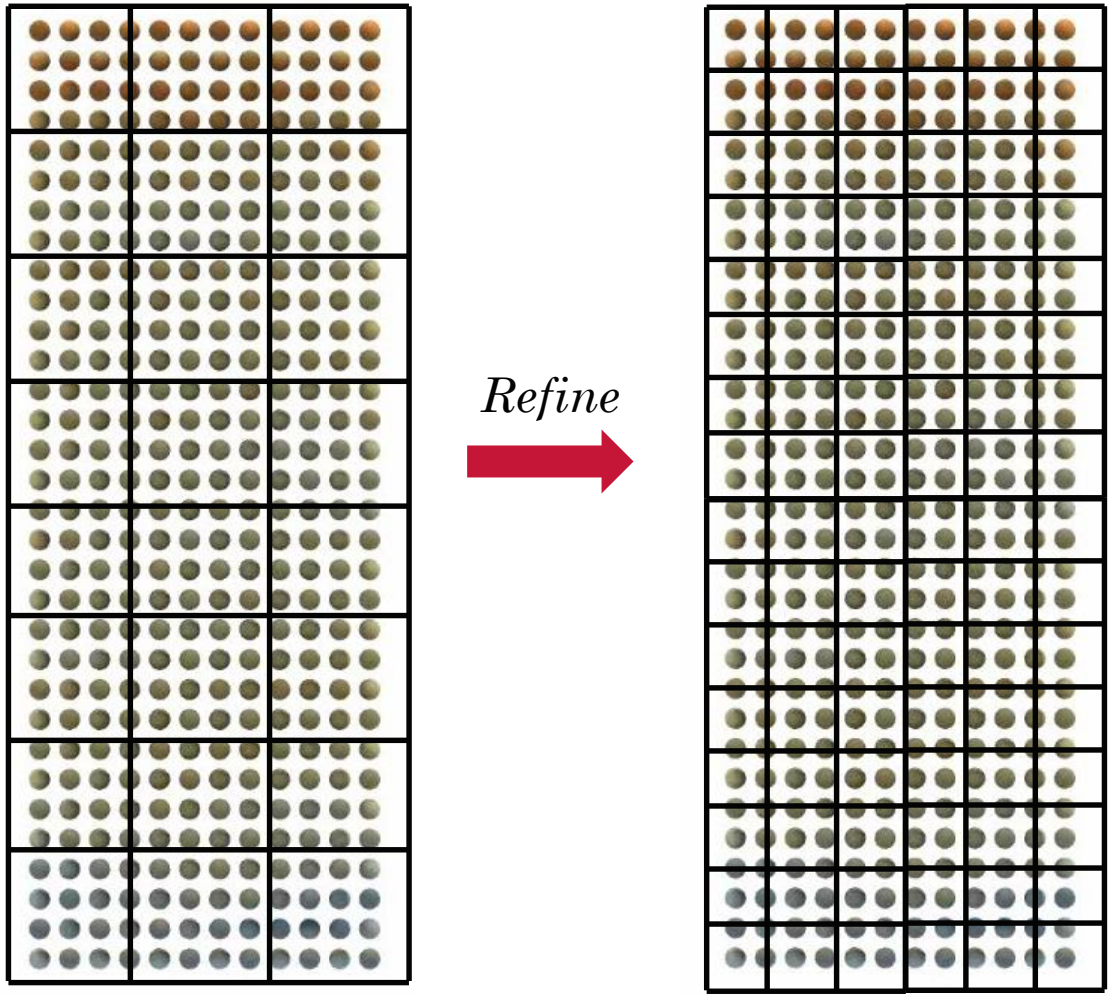


Nucleation



Contact line

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

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

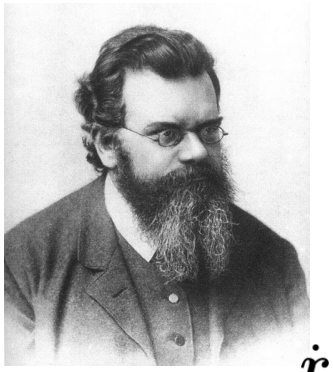
Pressure (stress) in an MD Simulation

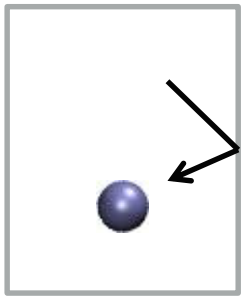
- Pressure definition in a dense molecular system
  - Kinetic part due to fluctuations
  - Configurational part due to liquid structure

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

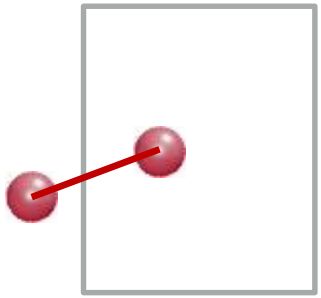
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





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

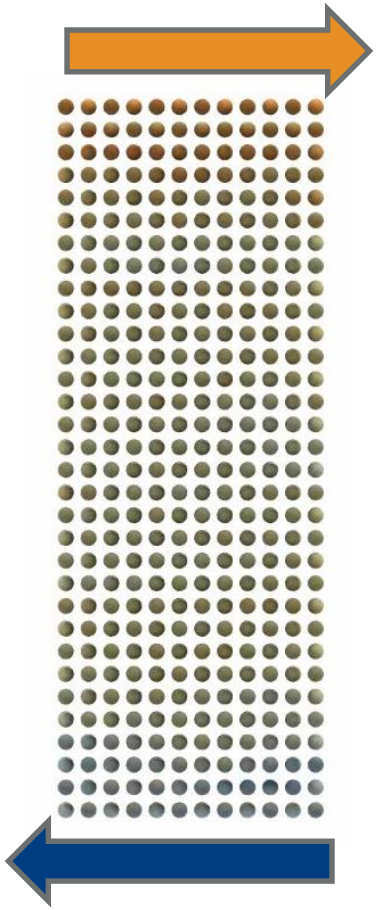


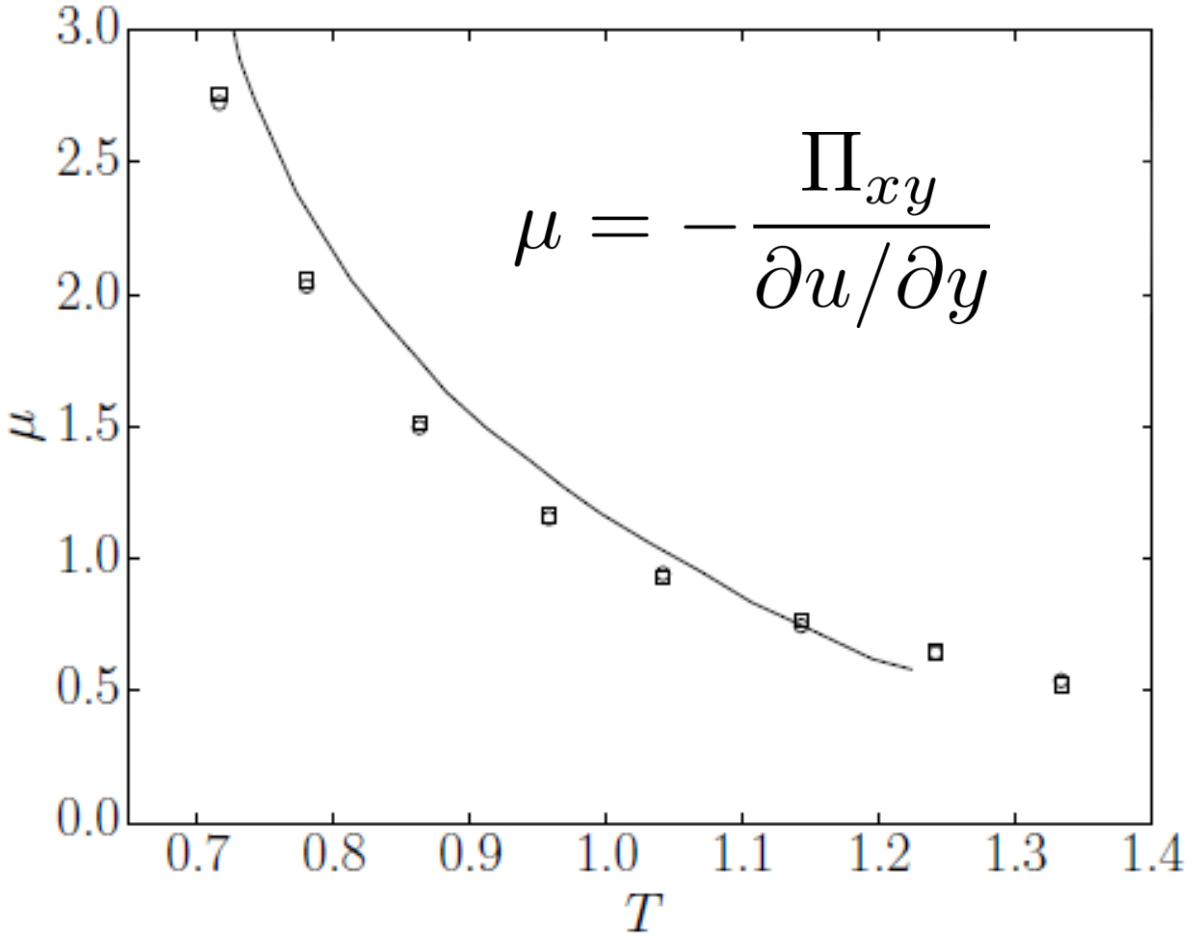
Configurational part

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

Viscosity

- Good agreement with experiments





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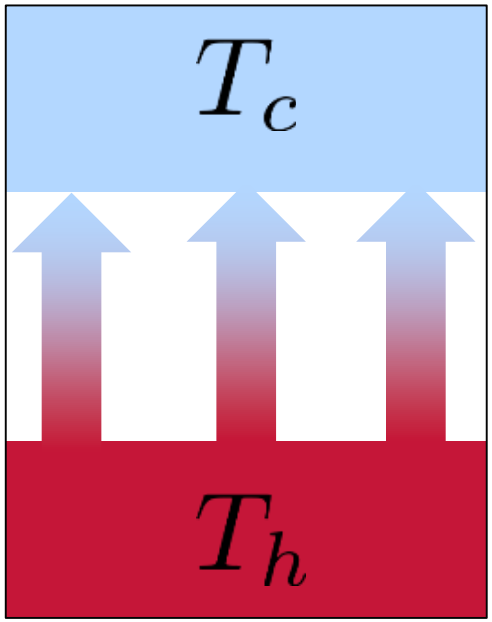
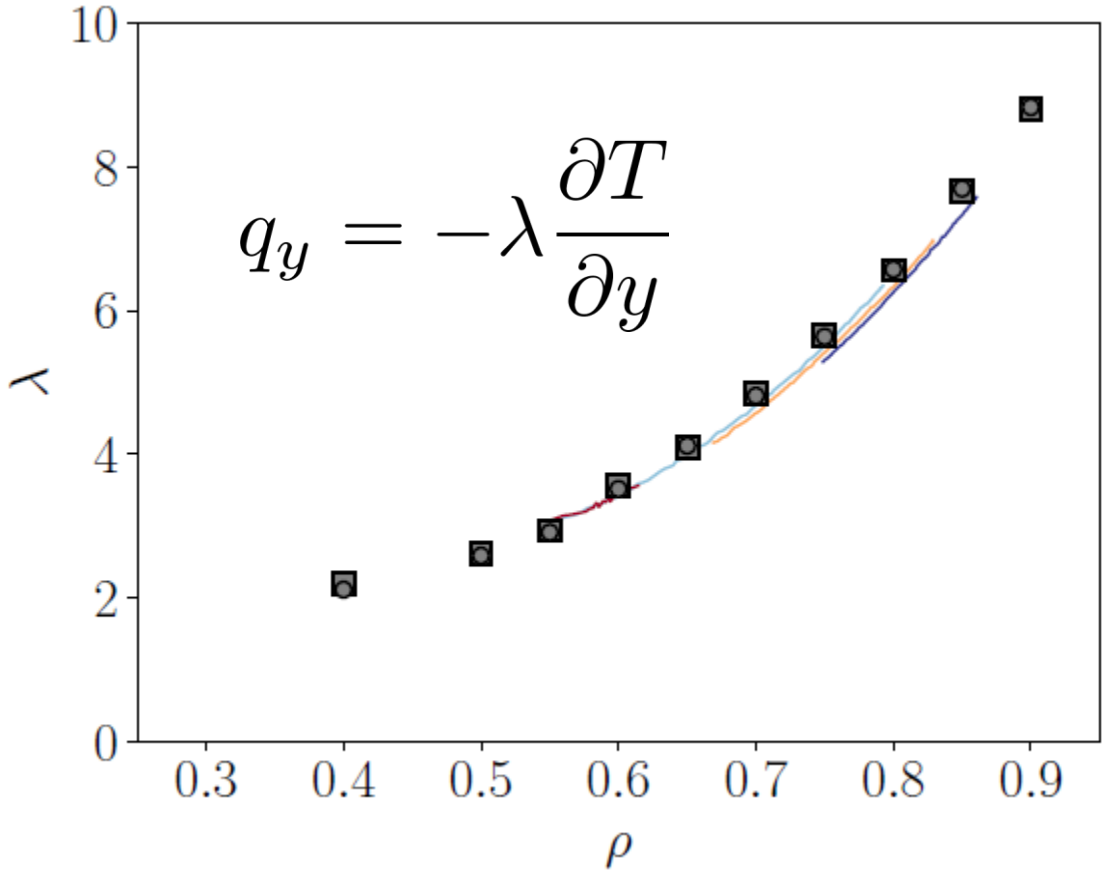
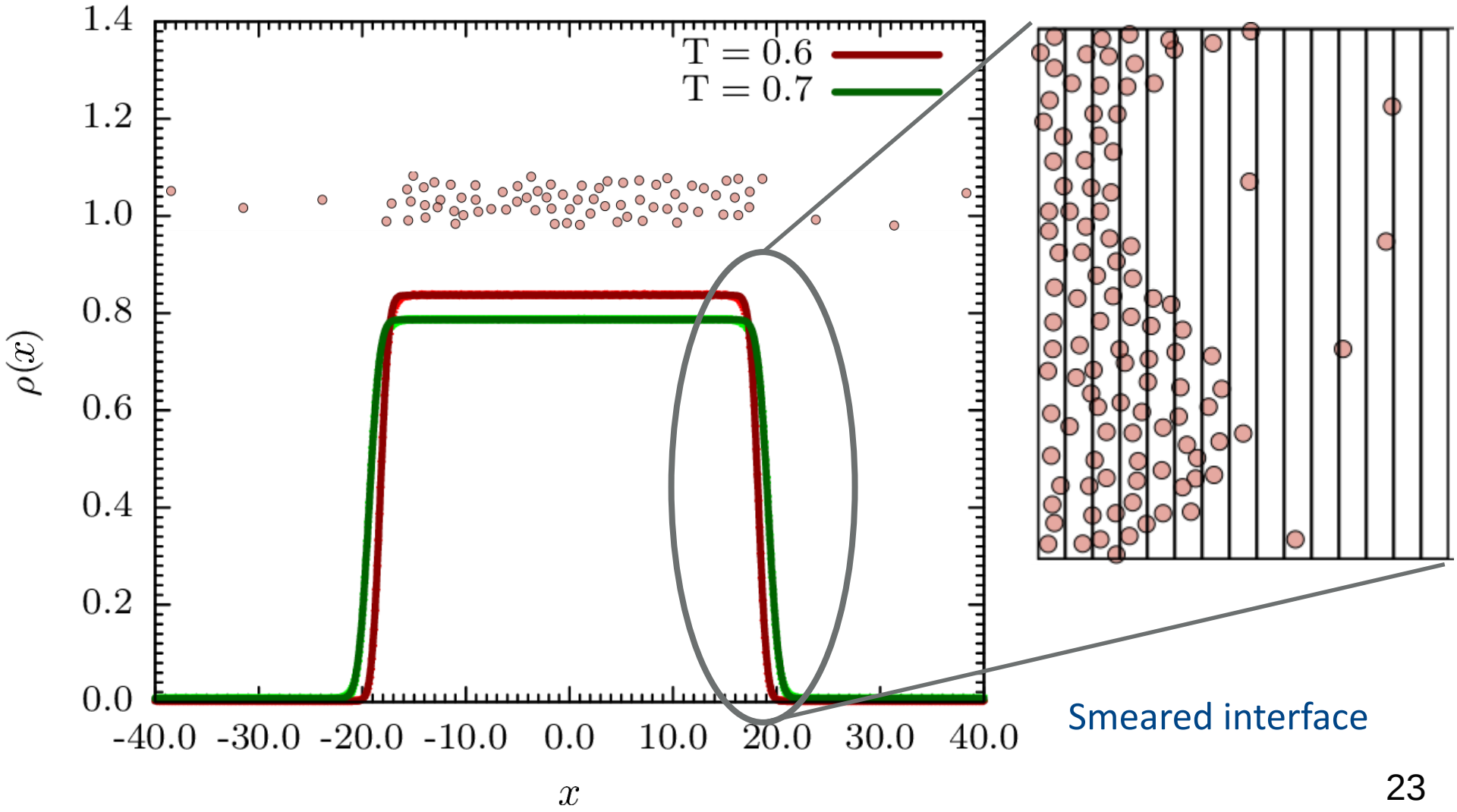
Fourier's law of heat conduction

- Good agreement with experiments





Multiphase Flows



Smeared interface

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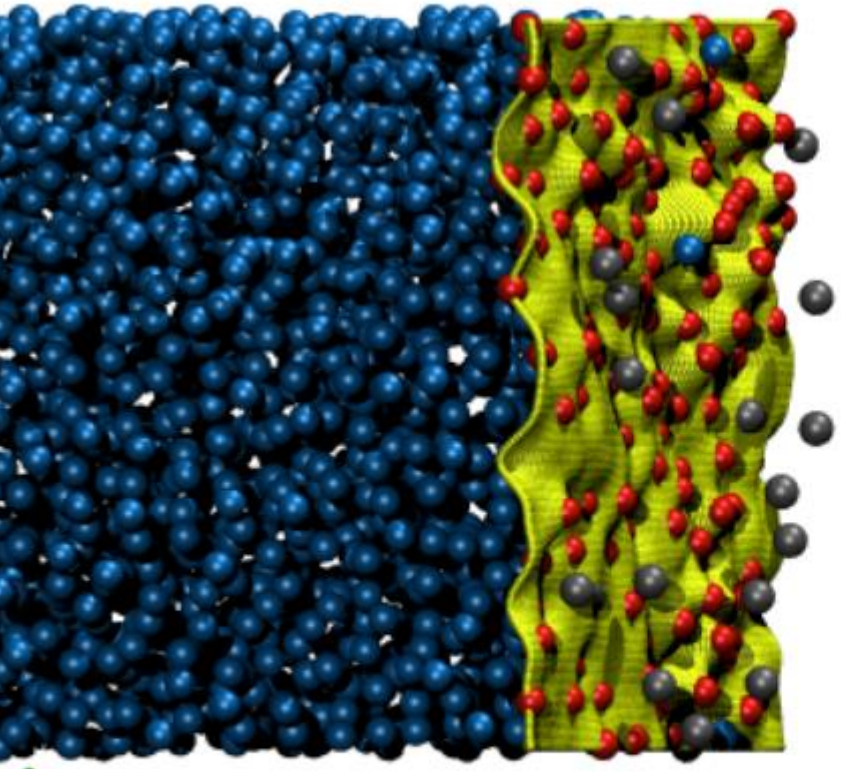
Intrinsic surface

- 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

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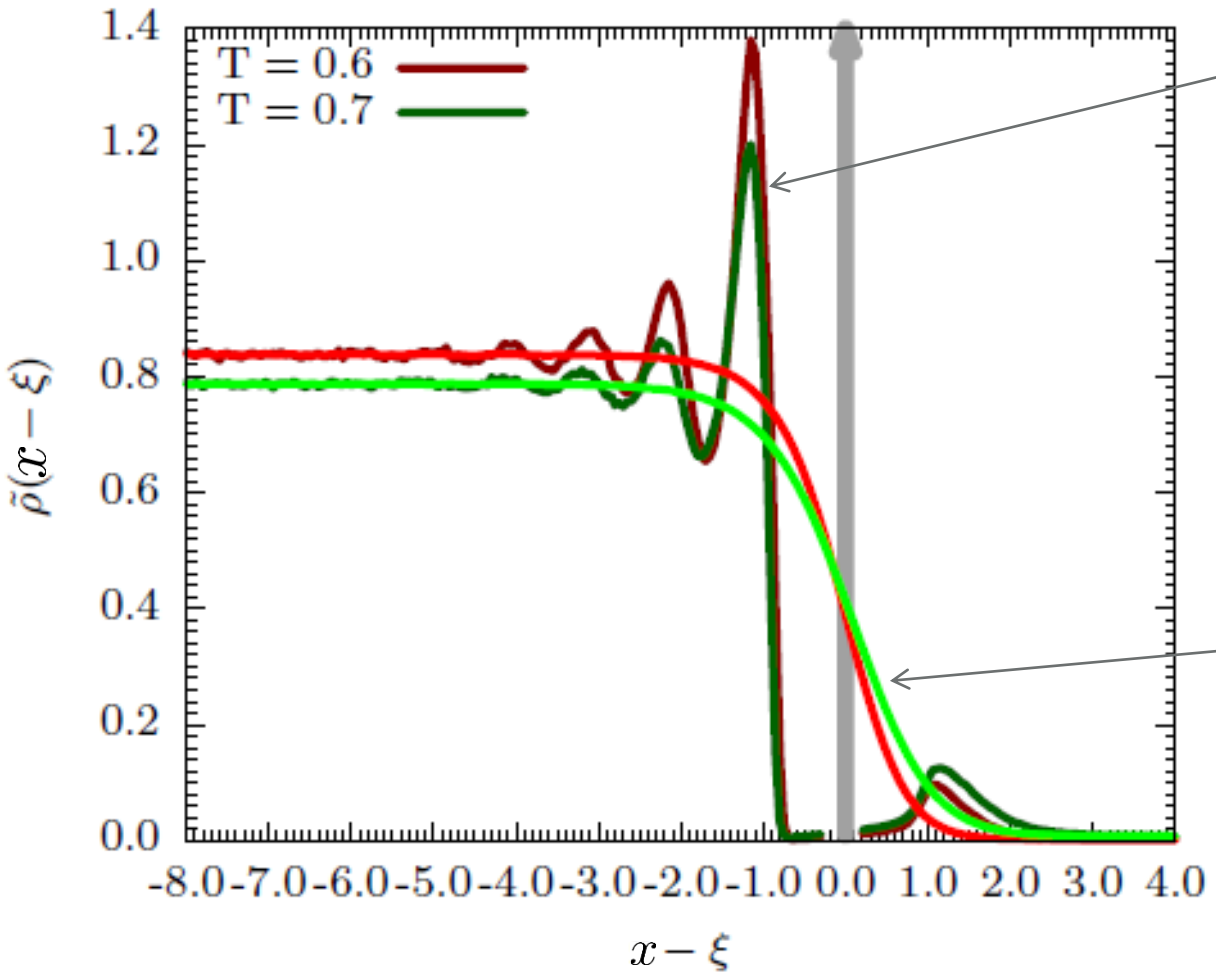
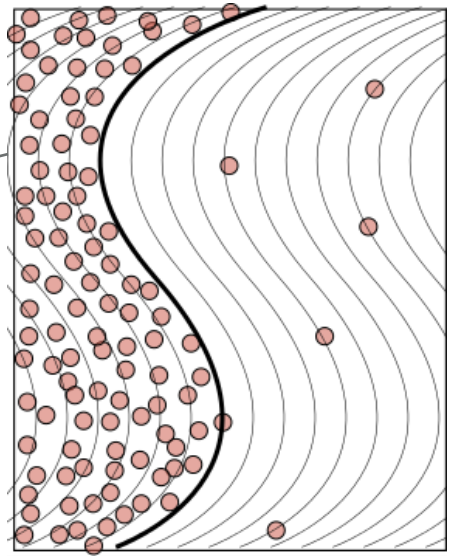
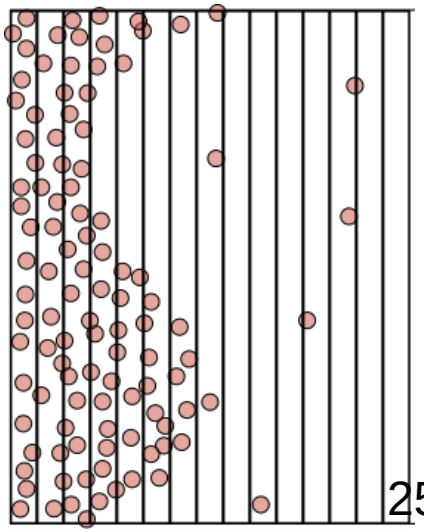
Results for Density







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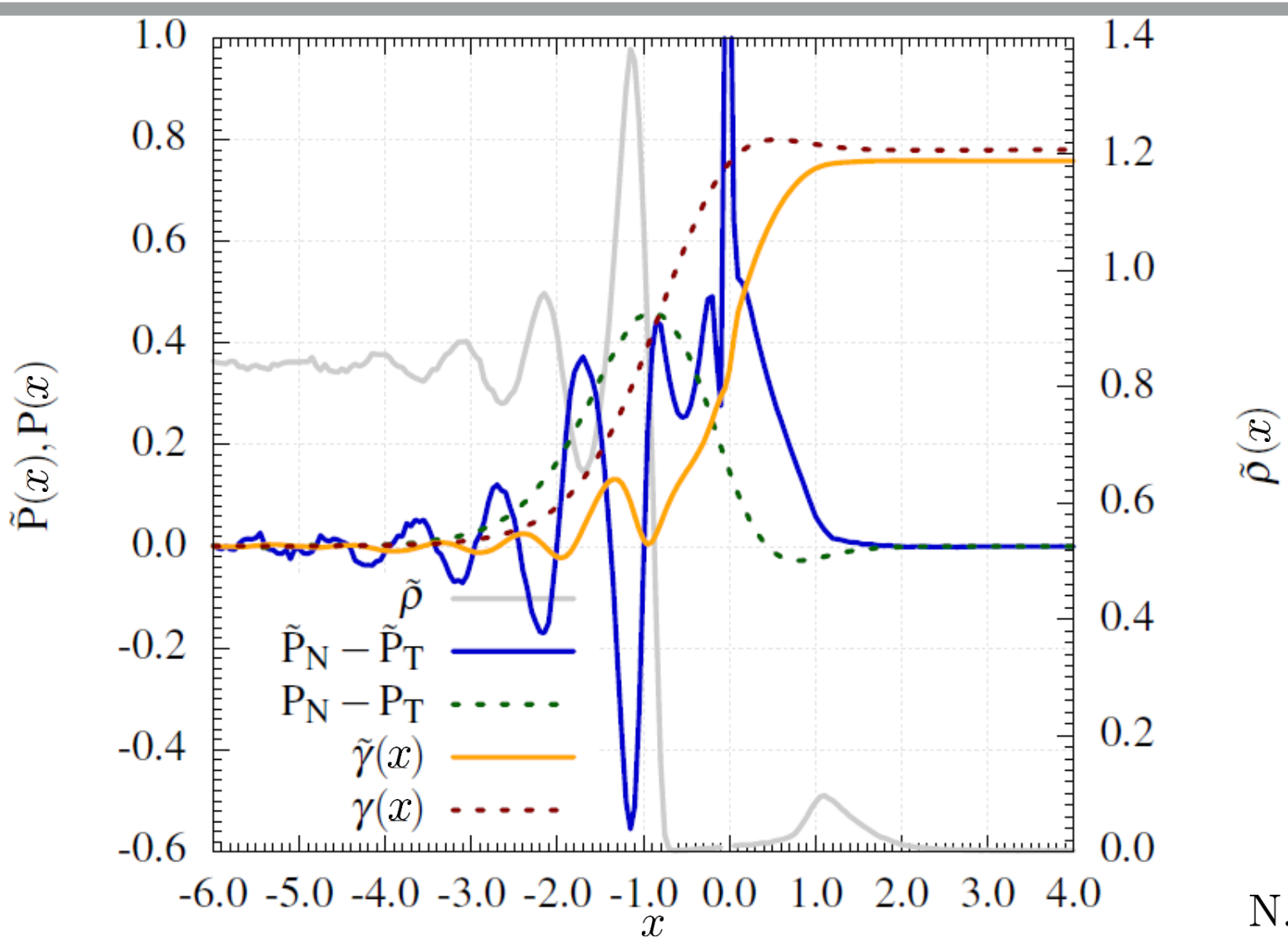
Results for Pressure

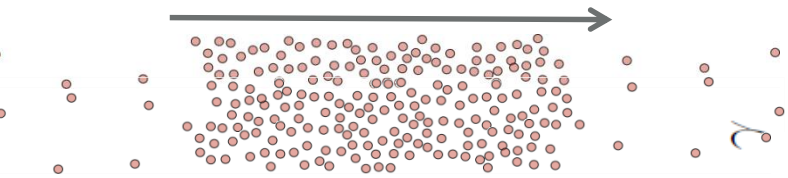


N.B. $\Pi \equiv P$

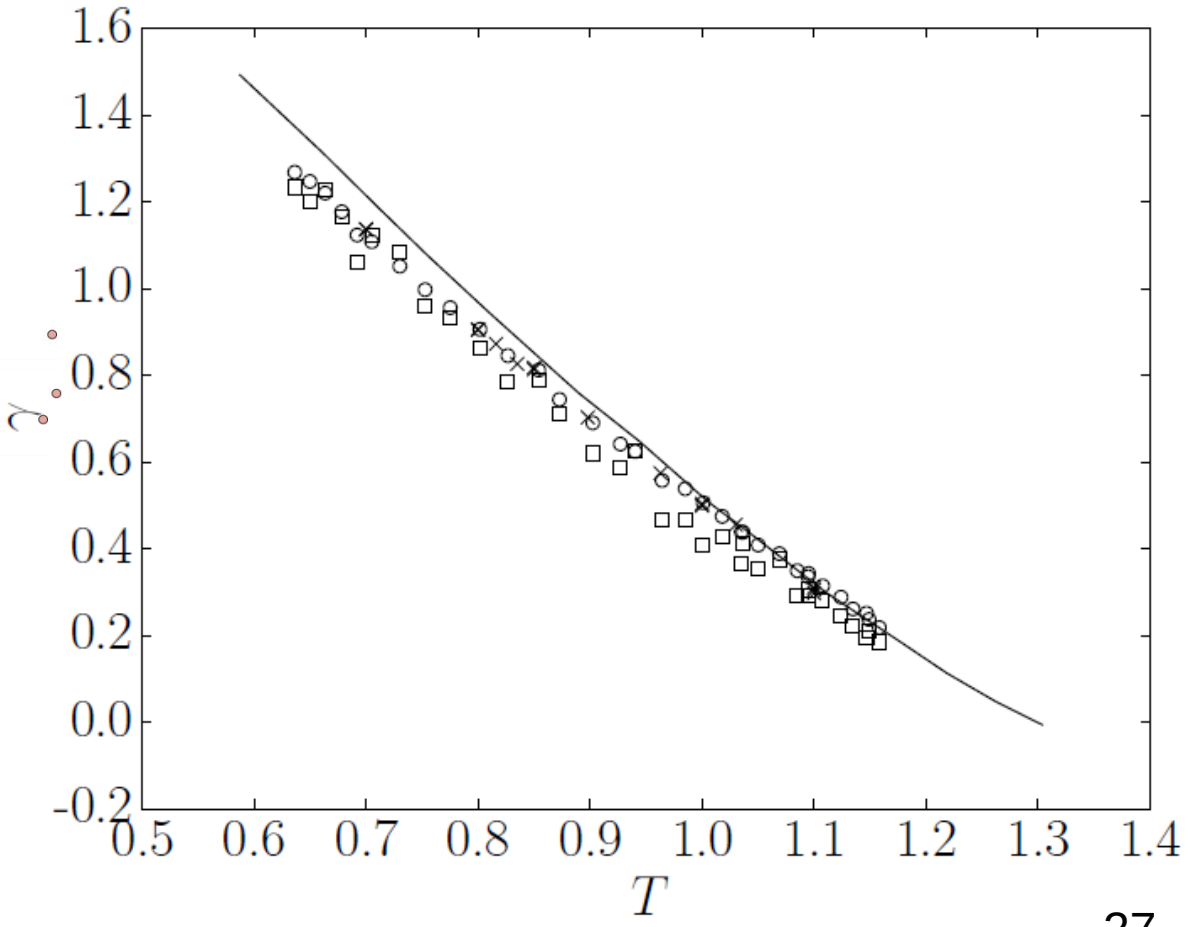
Results for Surface Tension

- Good agreement with experiments

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



Integrate over Liquid Vapour interface(s)



Work with Omar Matar - recently funded EMBOSS EPSRC grant

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Molecular Dynamics simulation of Nucleation

Wall w
mo
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Work with Omar Matar - recently funded EMBOSS EPSRC grant

Isosurface of Density

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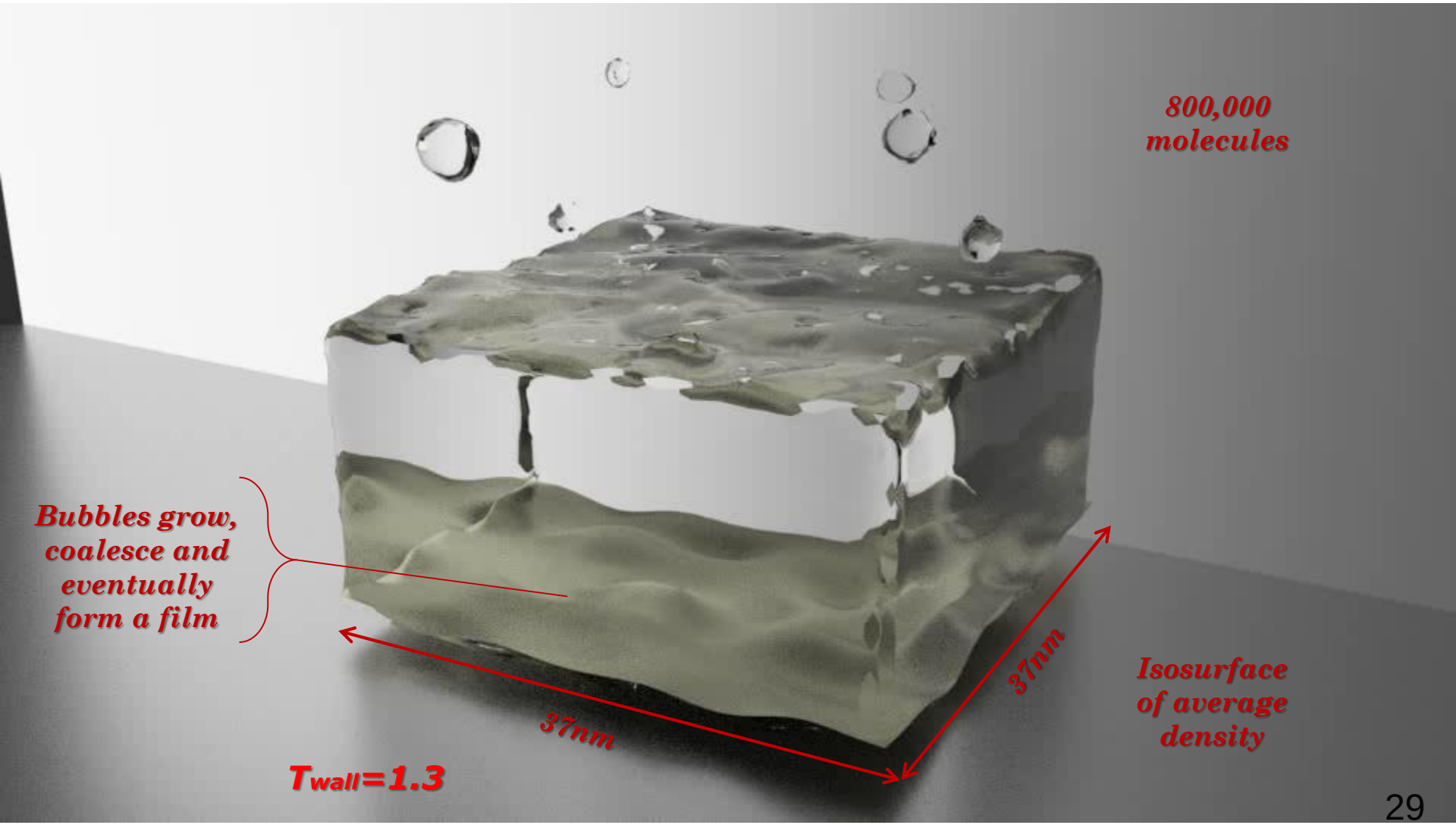


Coupling – Using MD with CFD

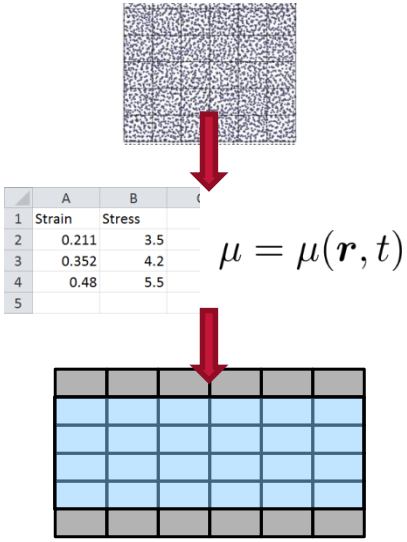
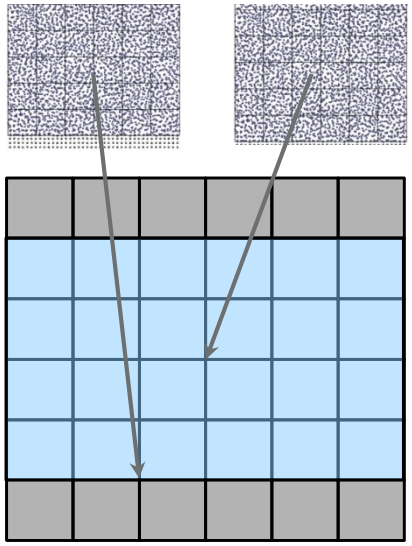


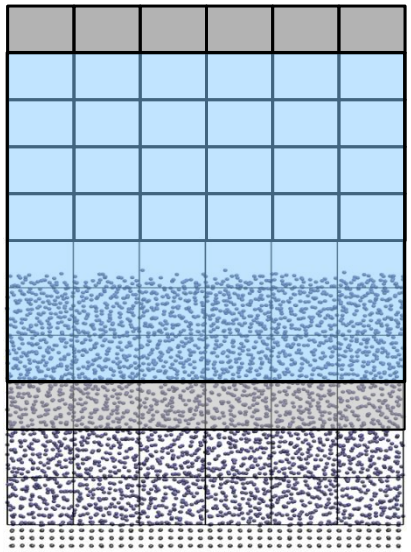
Table Lookup or Coefficients

MD parameter study stored in table and CFD uses data



Embedded Models (HMM)

MD – embedded in a CFD simulation [1)]

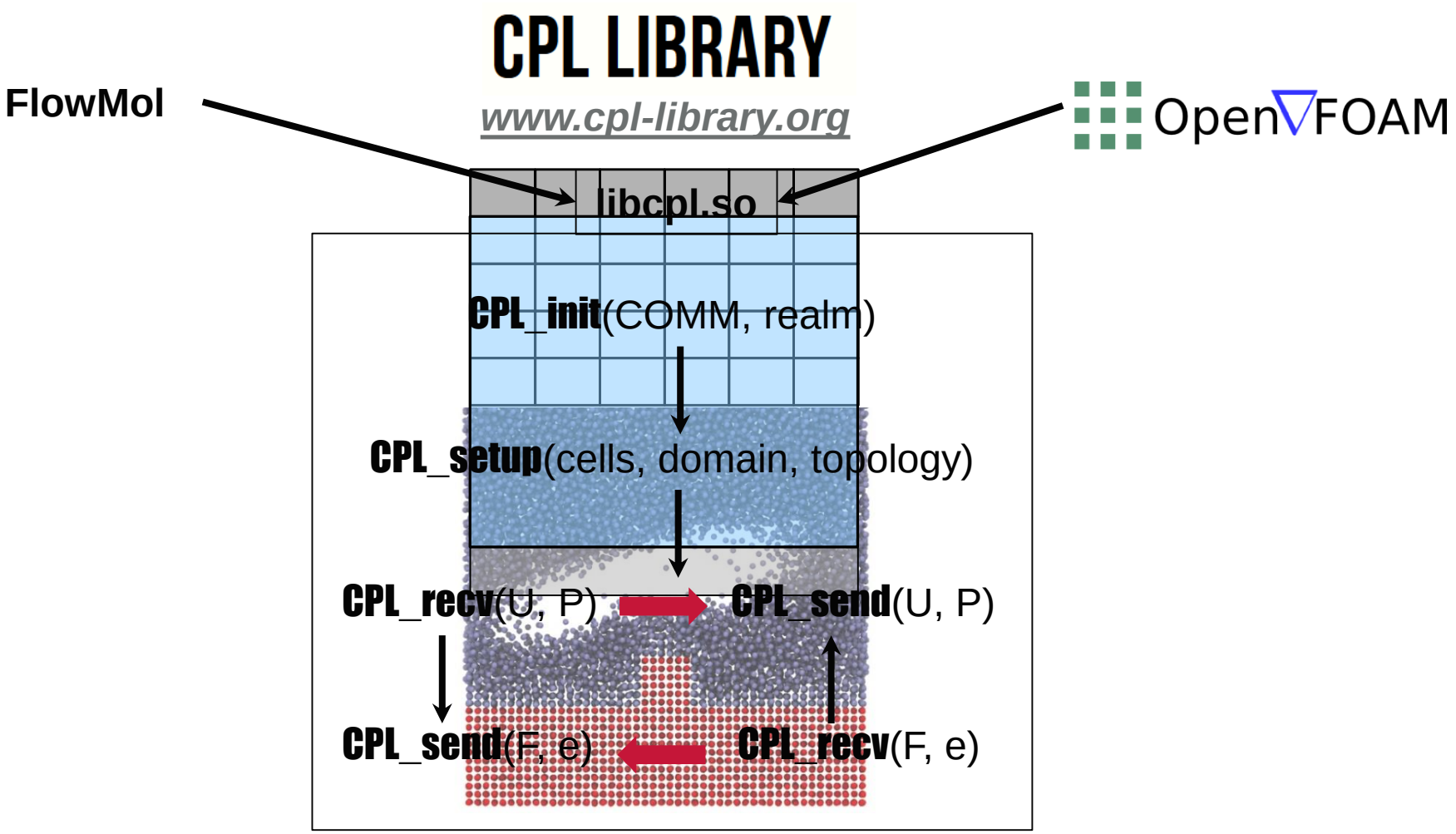


Domain Decomposition

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



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Coupled CFD-MD Simulation

- Finite Volume Solver

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

$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i + \mathbf{F}_i^C \quad i \in \text{cell}$$

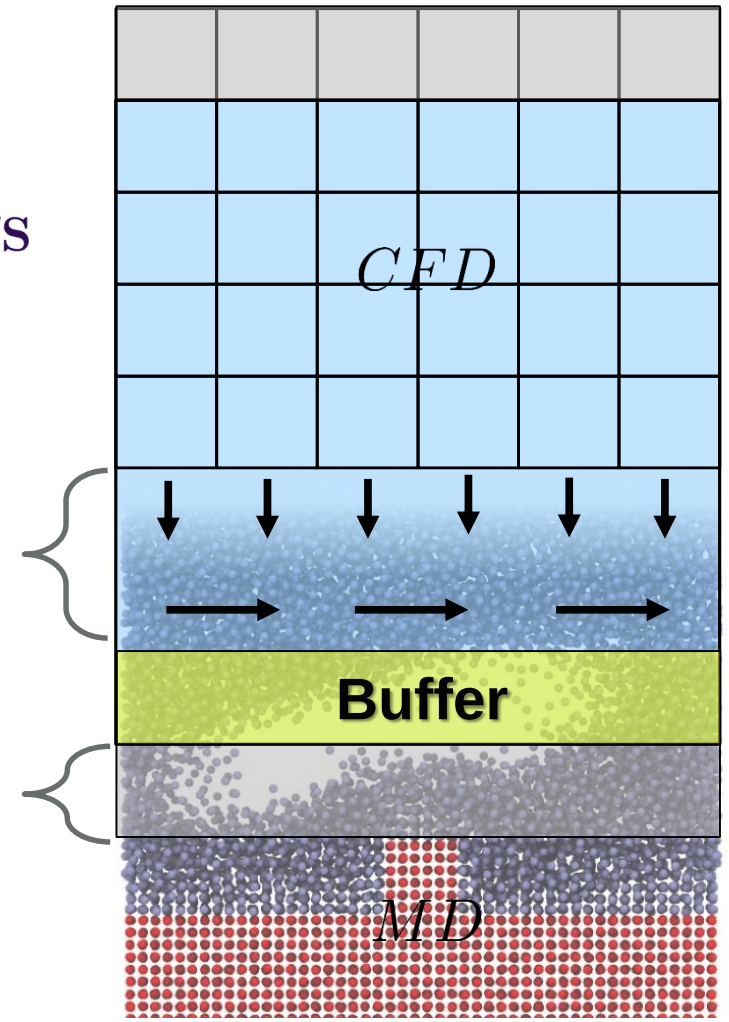
CFD→MD Boundary condition

$$\boldsymbol{u}^{BC} = \sum_{i\in\text{cell}} \boldsymbol{v}_i$$

MD→CFD Boundary condition

- Discrete molecules

$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i \text{ for all i in N}$$



O'Connell Thompson (1995), Hadjiconstantinou (1998), Flekkoy (2000), Nie et al (2004).

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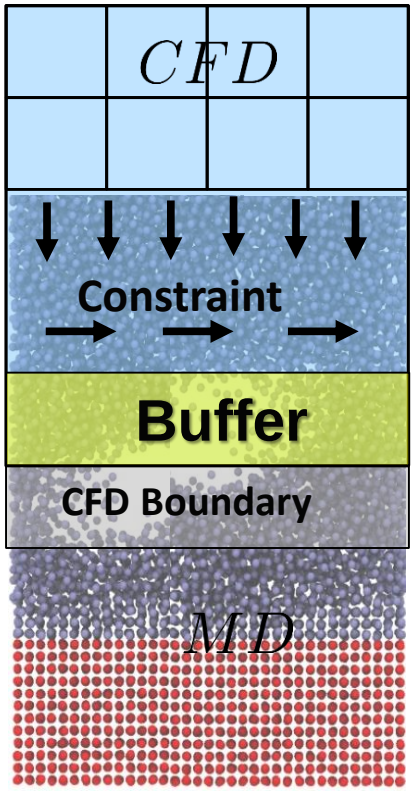
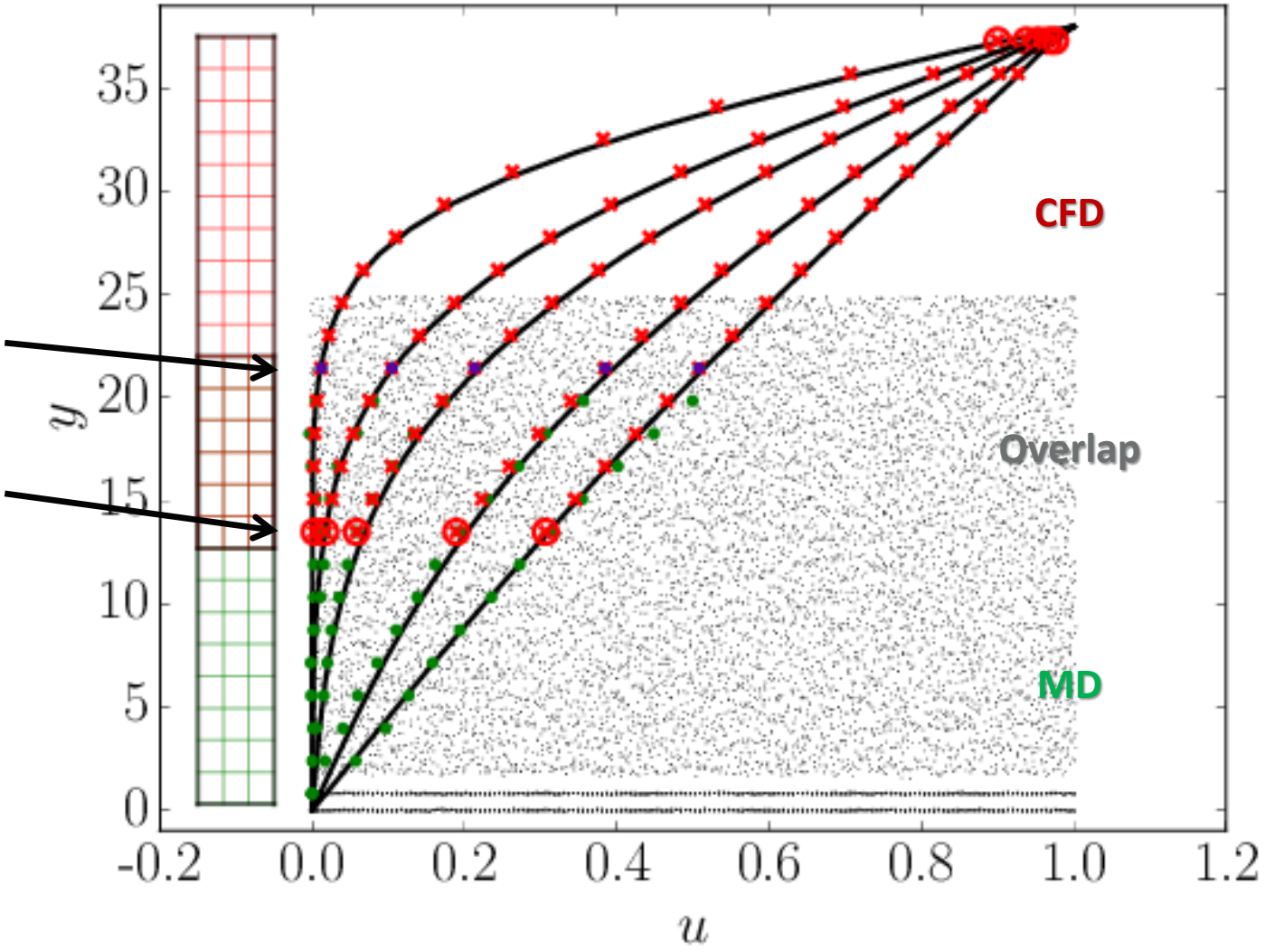
Coupling Results – Couette Flow





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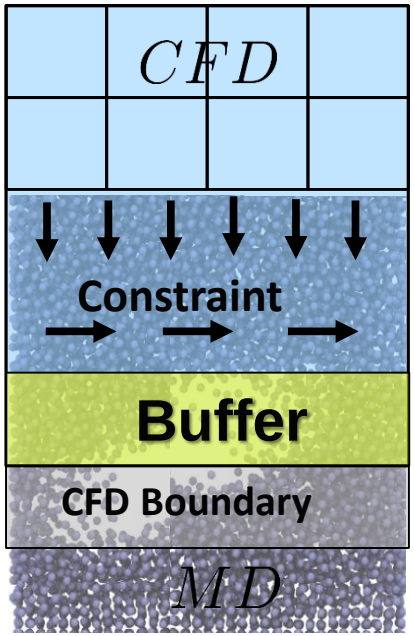
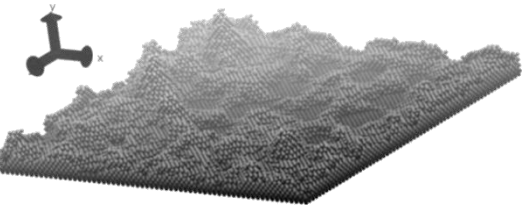
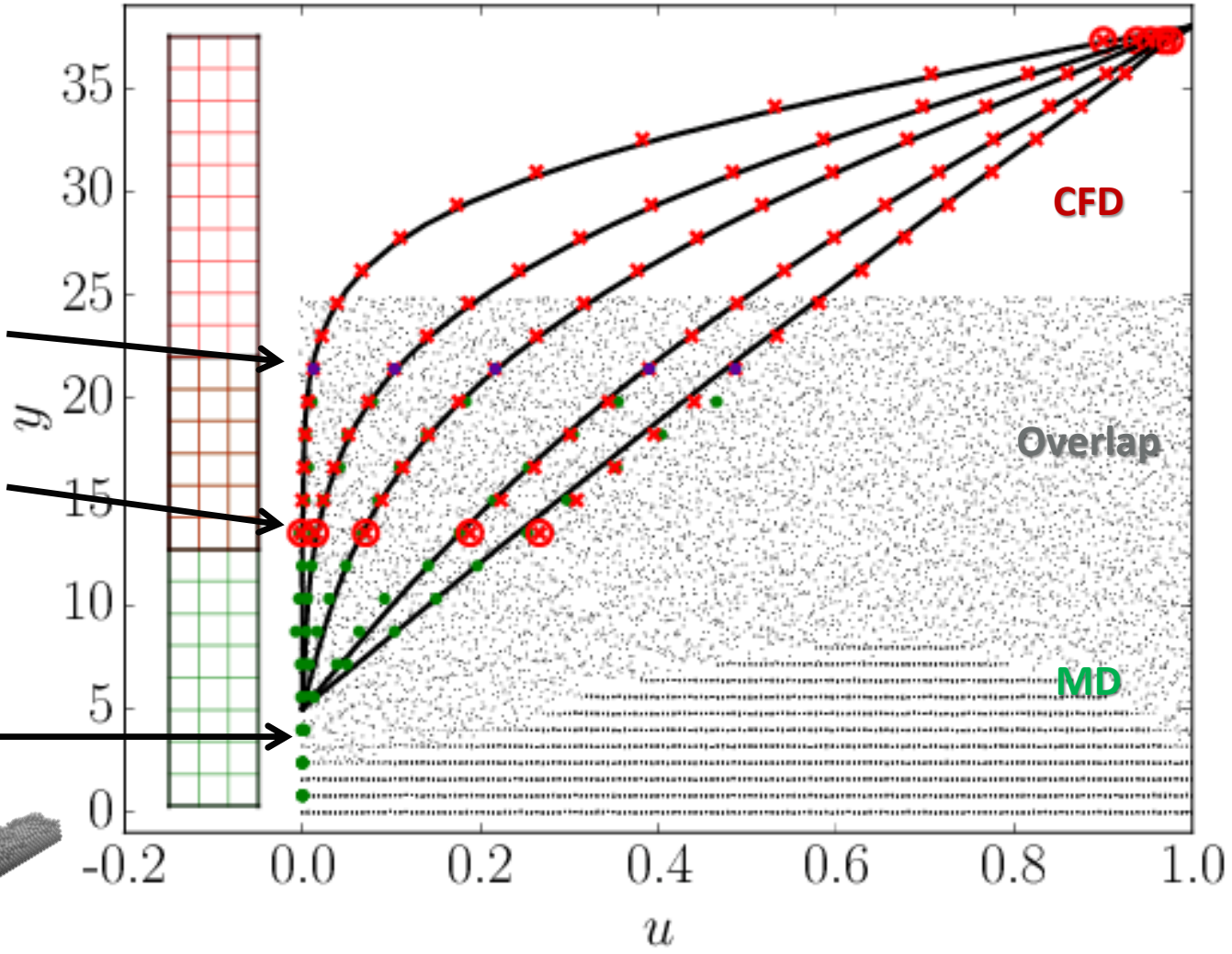
Coupling Results – Couette Flow



Rough wall shifts zero location





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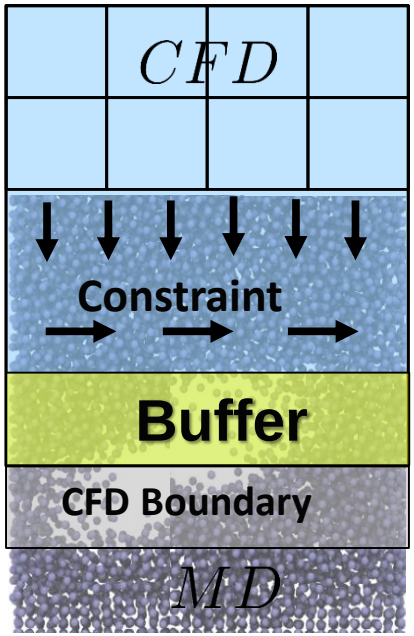
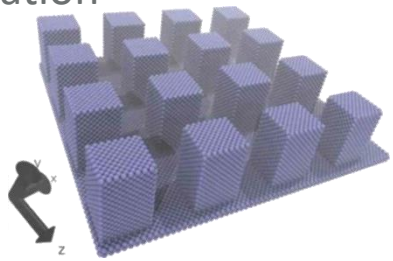
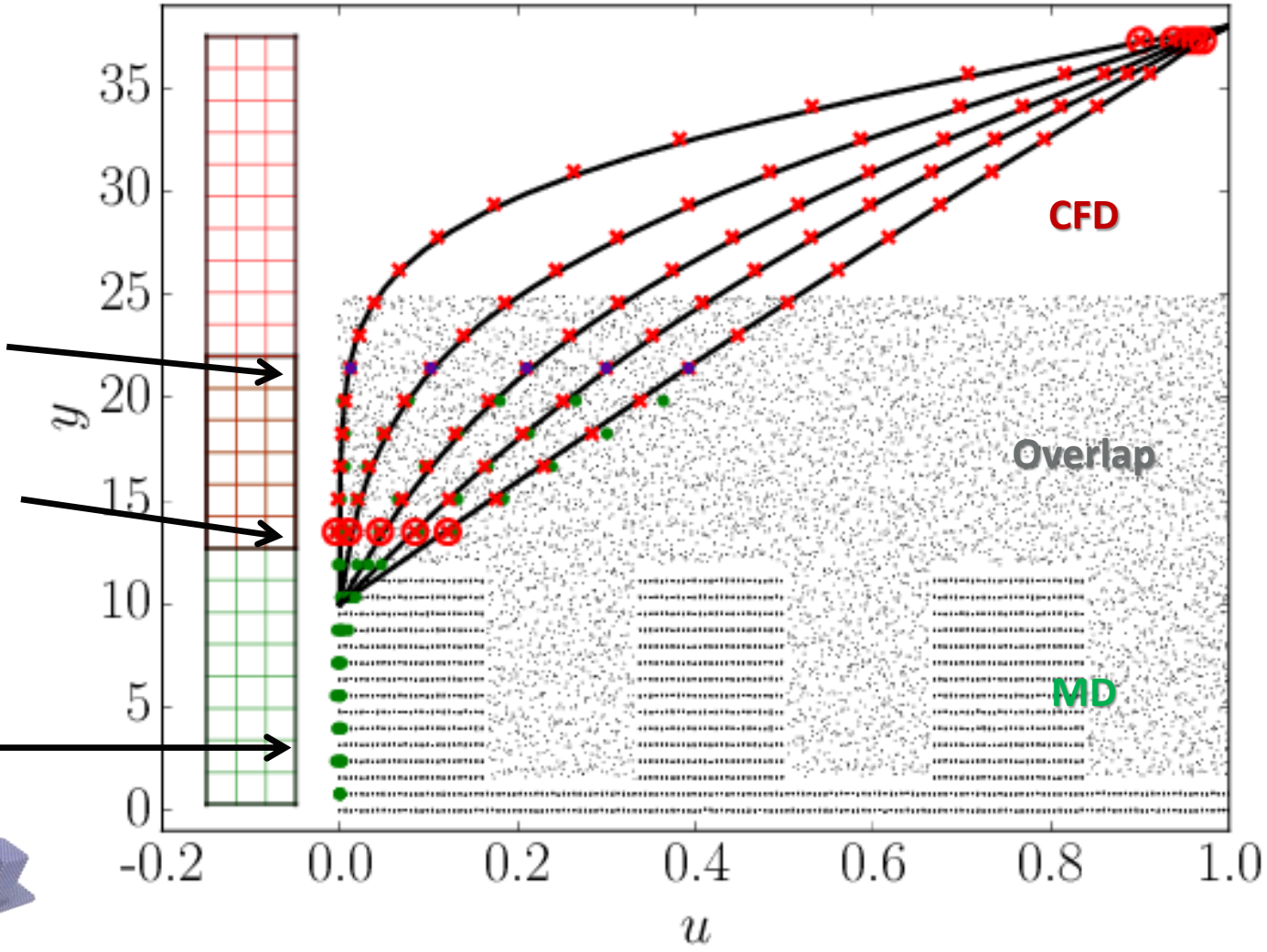
Coupling Results – Couette Flow



Posts shift zero location





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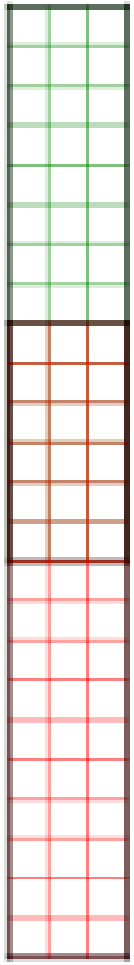
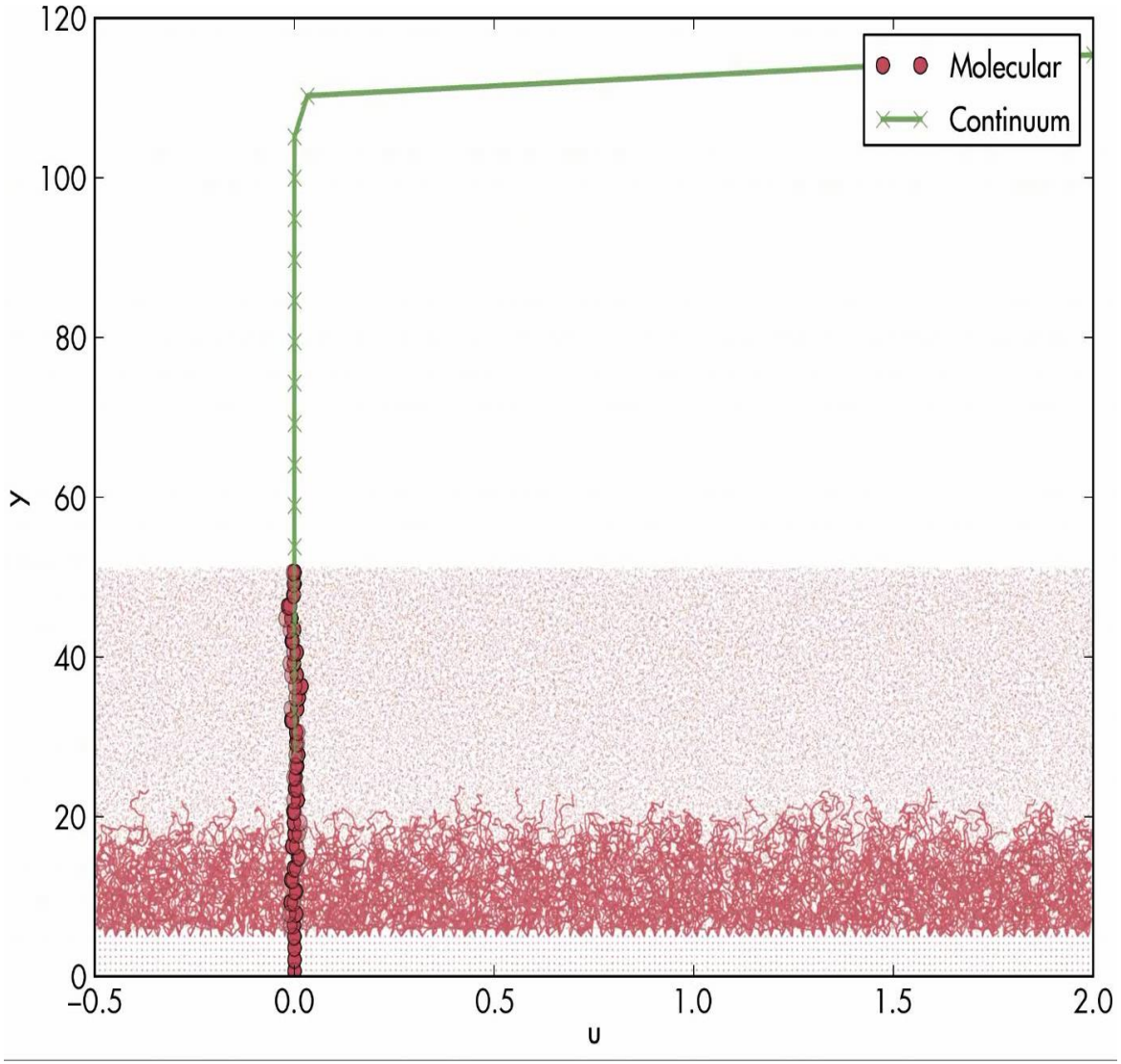
Coupling Results – Polymer Brushes



CFD Region

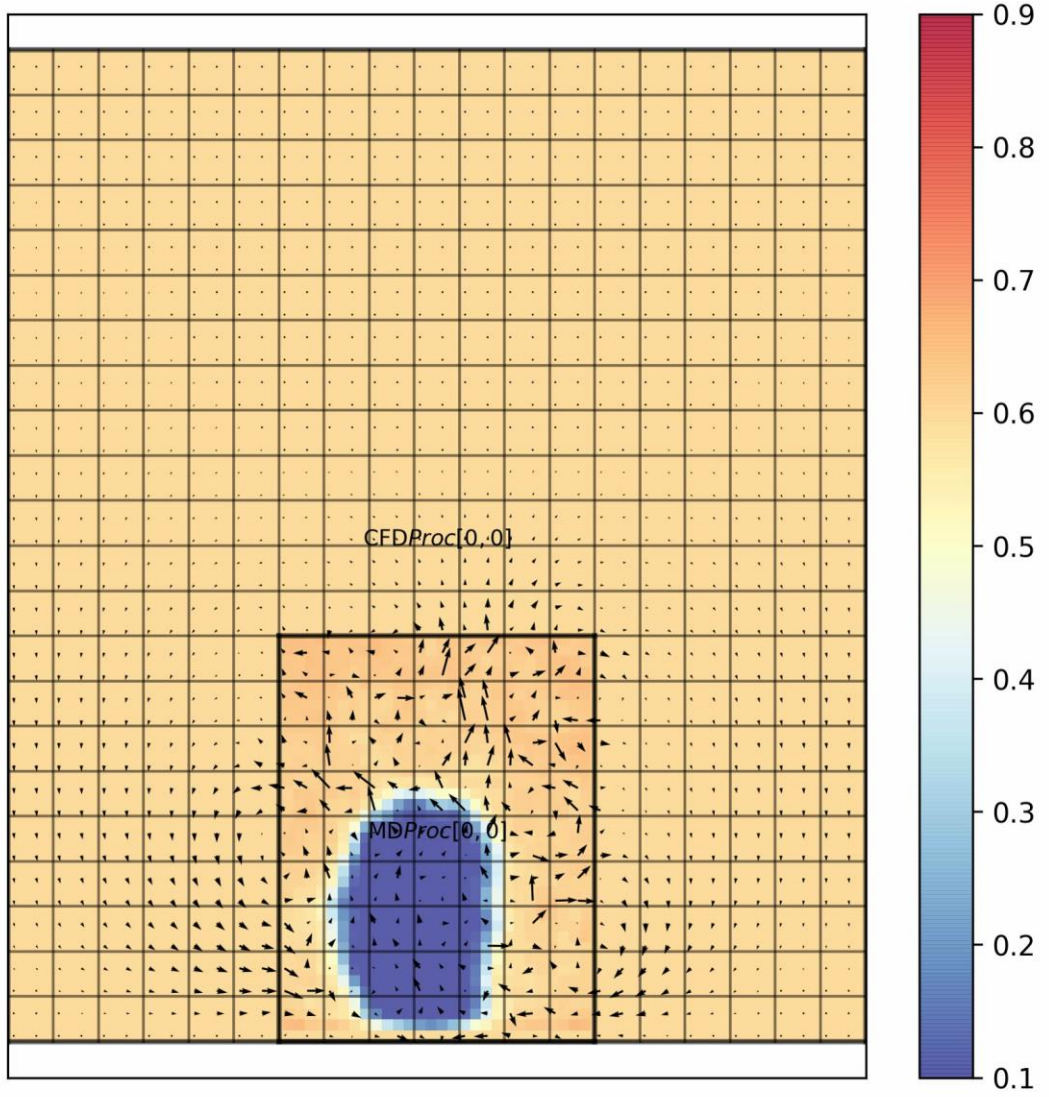
Overlap Region

MD Region



Coupled Simulation of Boiling

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

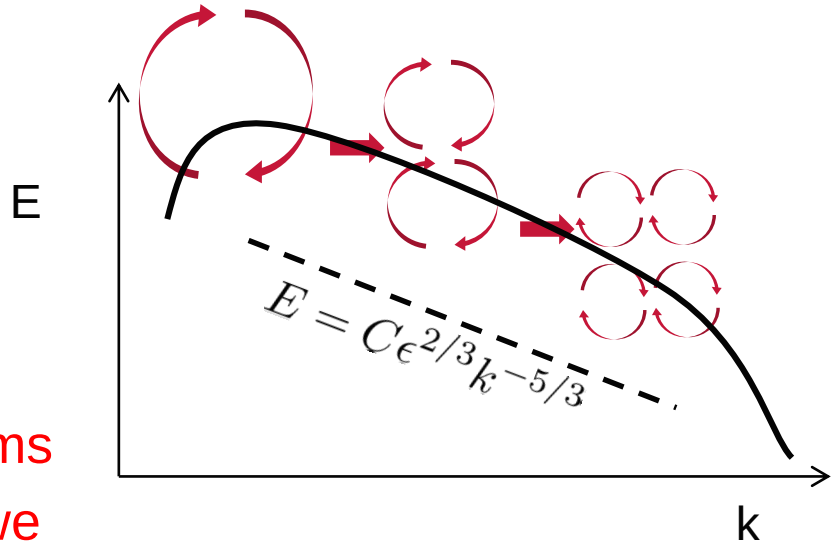


Section 2

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

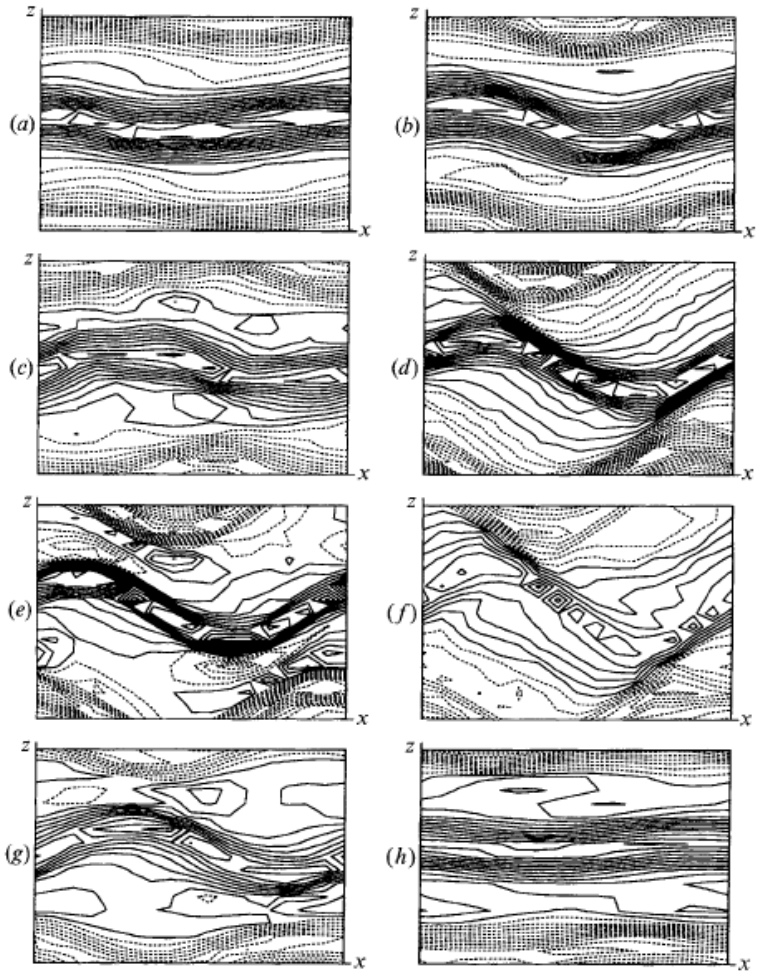
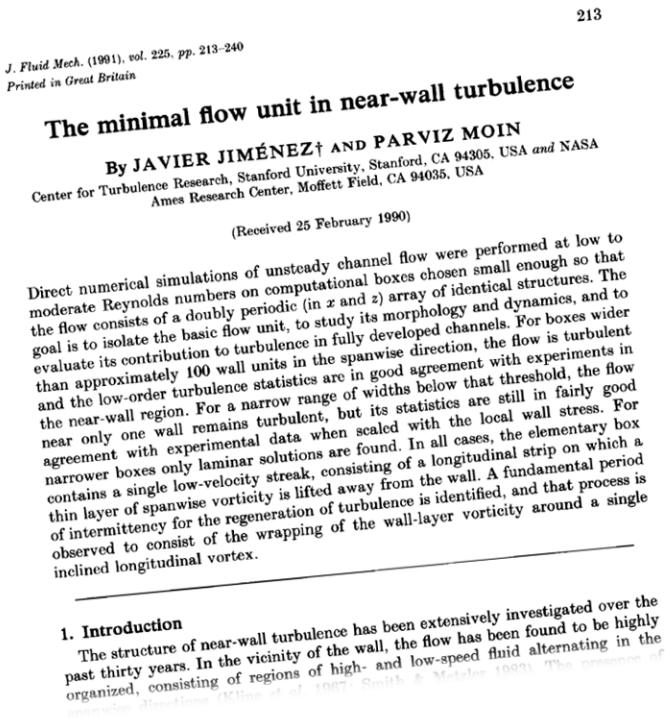


FIGURE 2. Iso-contours of u-velocity in the (x, z)-plane centred between the walls; solid contours positive, dashed contours negative. Contour interval 0.032. (*a*) $t = 757.5$, (*b*) $t = 764.8$, (*c*) $t = 772.0$, (*d*) $t = 777.8$, (*e*) $t = 783.0$, (*f*) $t = 794.1$, (*g*) $t = 808.2$, (*h*) $t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

Molecular Simulation of Turbulence

- The minimum domain size required to sustain turbulent flow

Poiseuille flow, Re ≈ 2000



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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

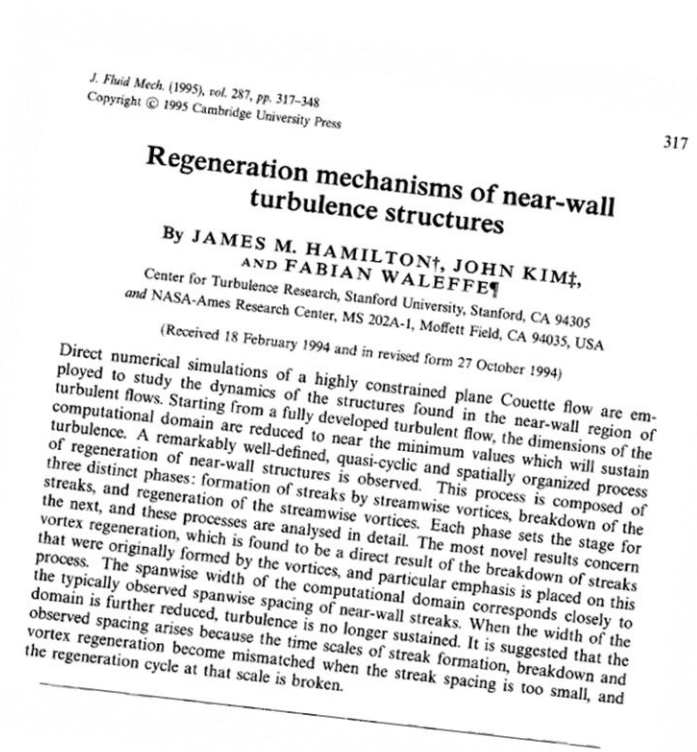
(Received 25 February 1990)

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

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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 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

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

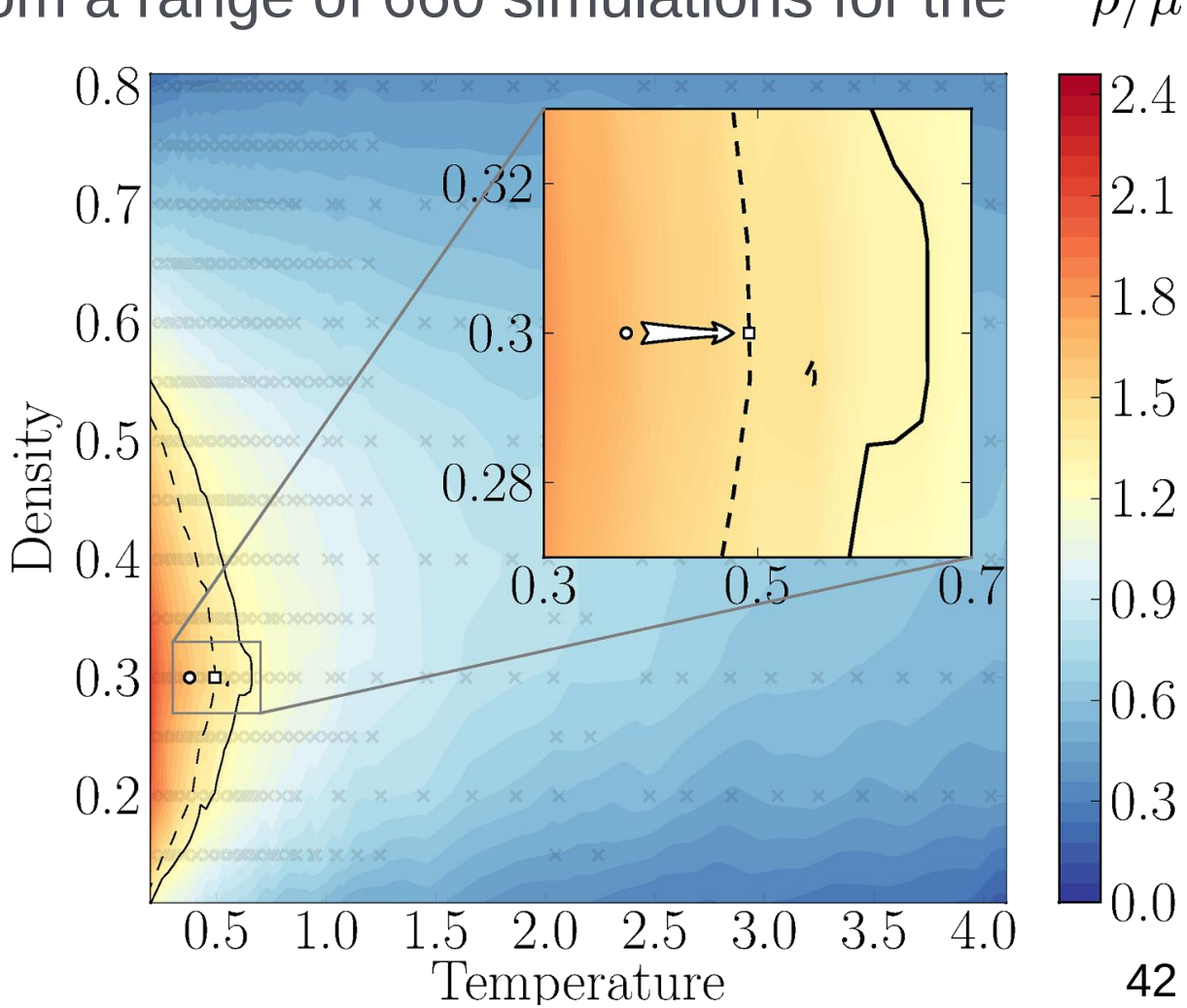
$$Re > 400$$

- The target value

$$u = \pm 1$$

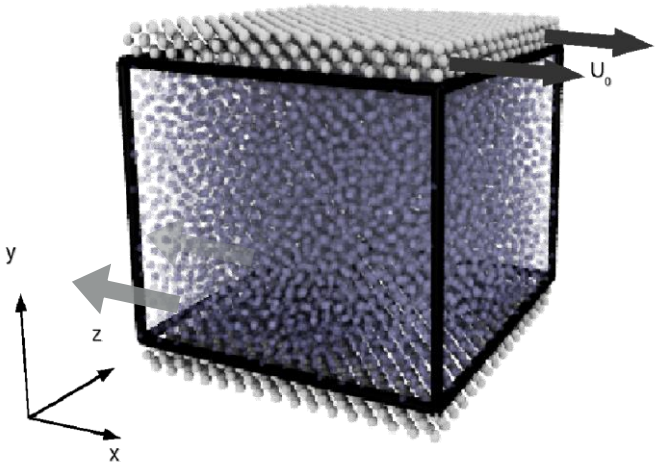
$$\rho/\mu > 1.4$$

$$L = 560$$



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

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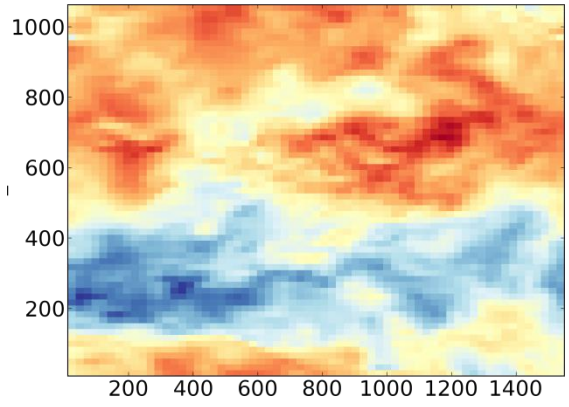
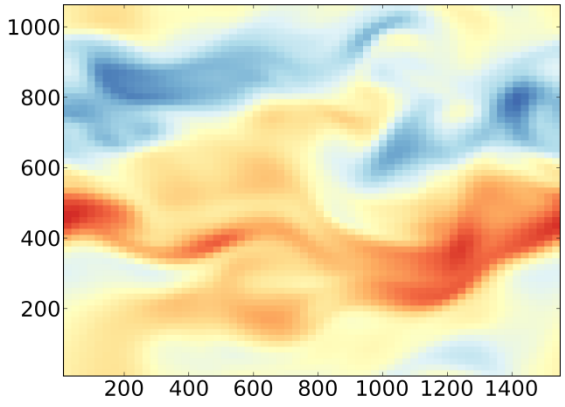
- From Jimenez and Moin (1991):

  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.

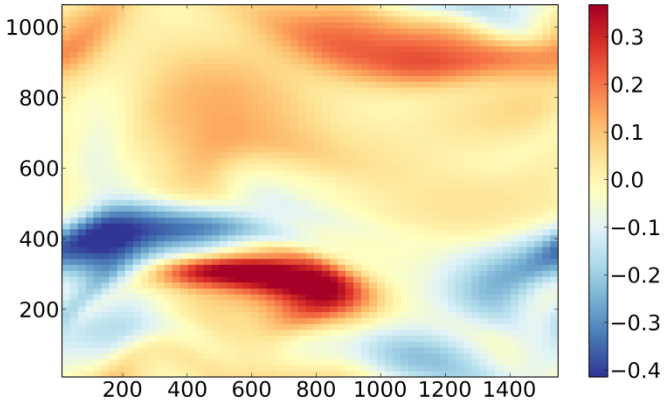
Re ≈ 4000



Re ≈ 1000



Re ≈ 400



Molecular Simulation of Turbulence

Molecular Simulation of Turbulence

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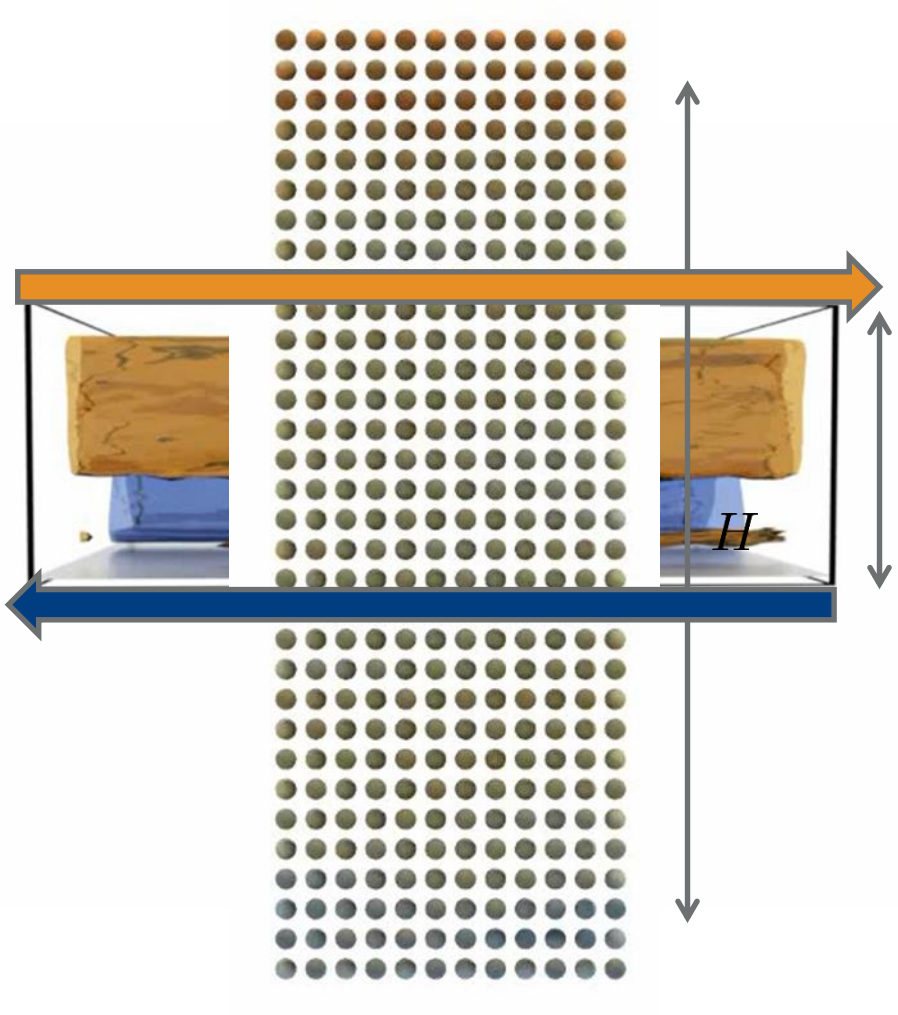

Reynolds Number

$Re \approx 400$

with

300 million molecules

Molecular Simulation of Turbulence

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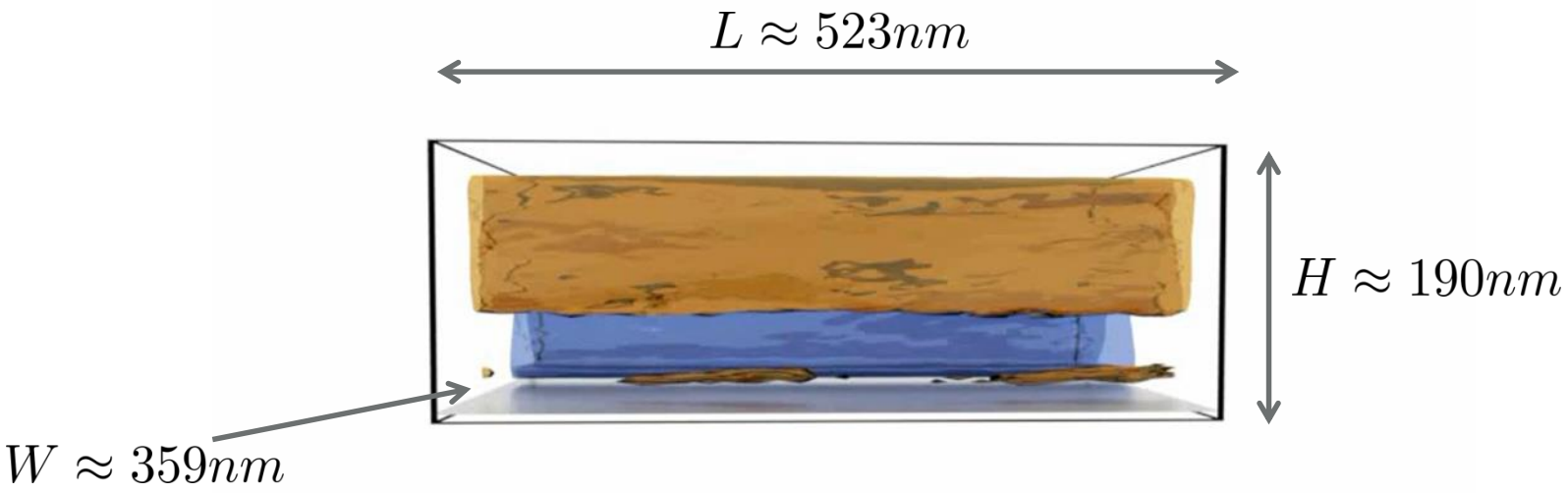
Minimal channel Couette flow



Reynolds Number

$Re \approx 400$

with
300 million molecules

Molecular Simulation of Turbulence

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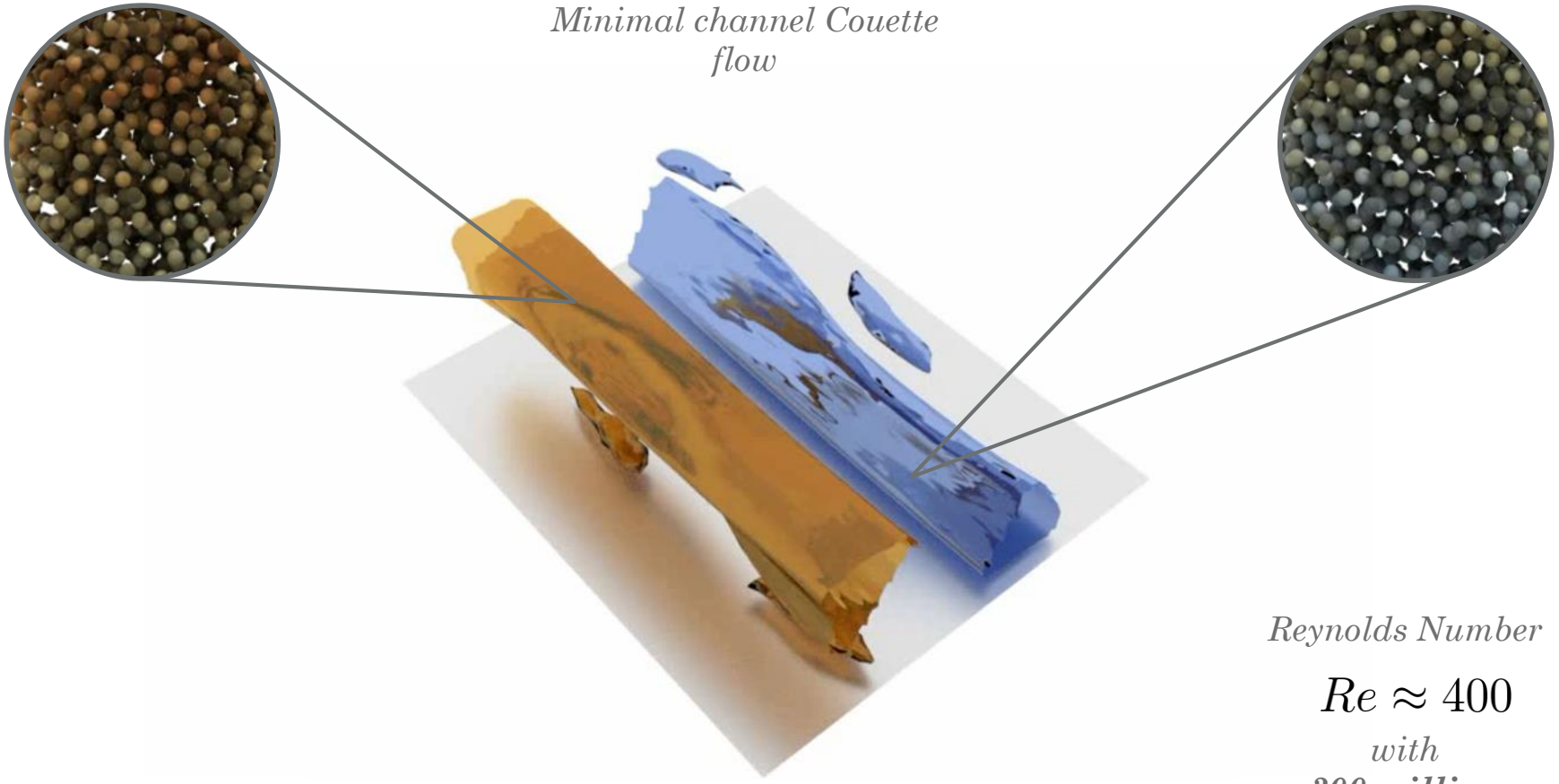
Minimal channel Couette flow



Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$Re \approx 400$

with

300 million molecules

Molecular Simulation of Turbulence

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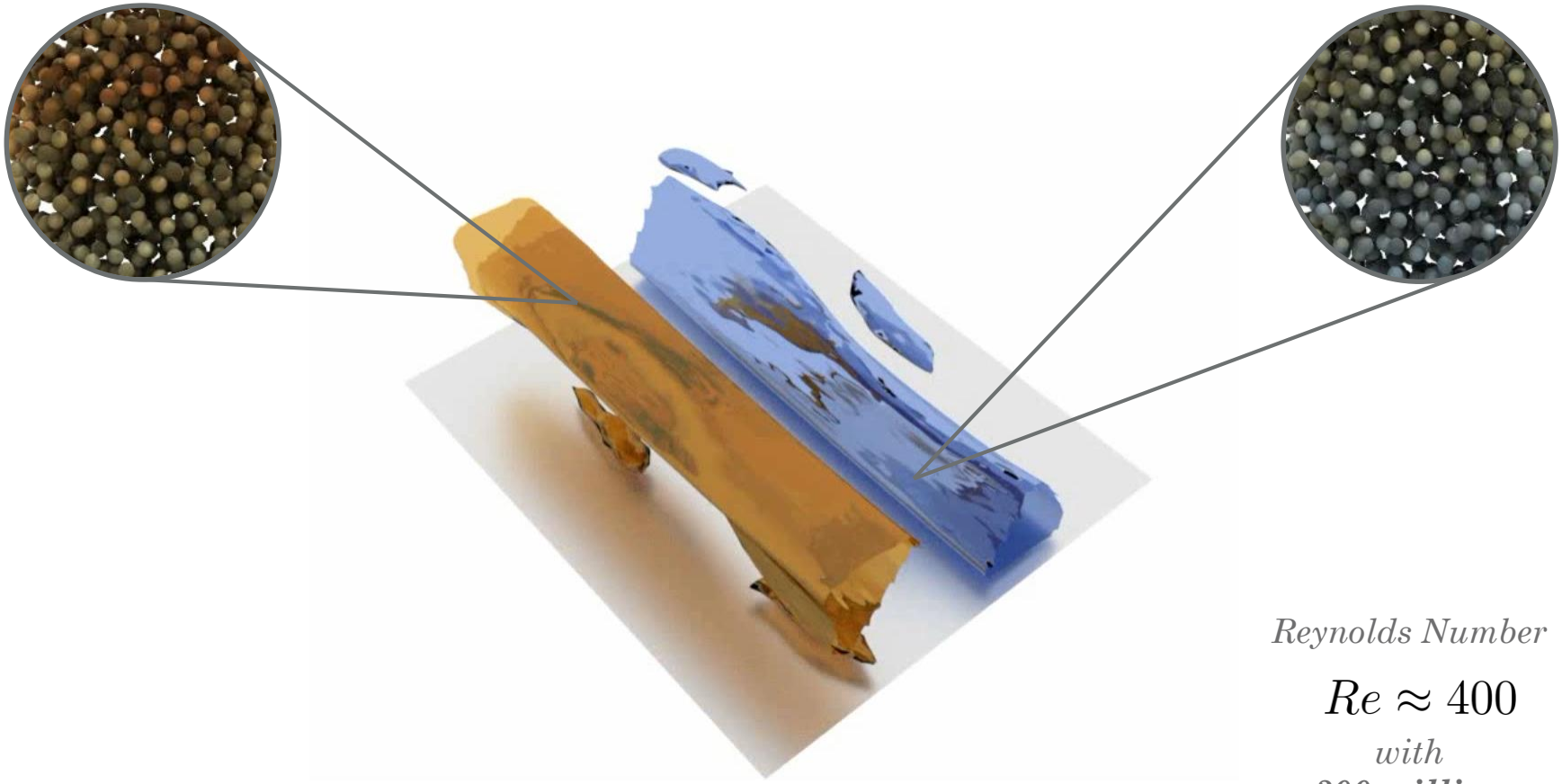


Isosurfaces of turbulent kinetic energy coloured by velocity

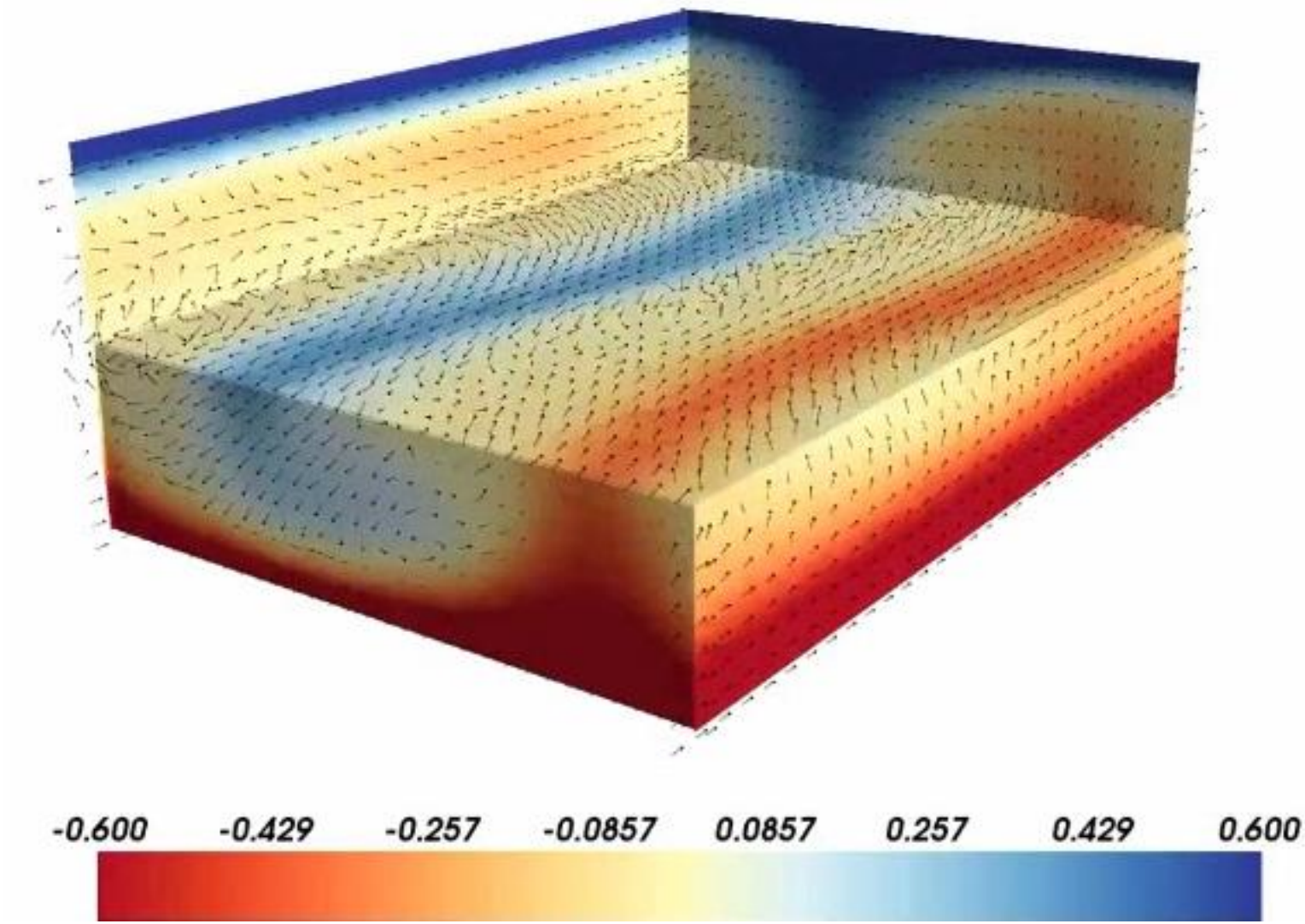
Reynolds Number

$Re \approx 400$

with

300 million molecules

Molecular Turbulent Couette Flow



MD vs CFD

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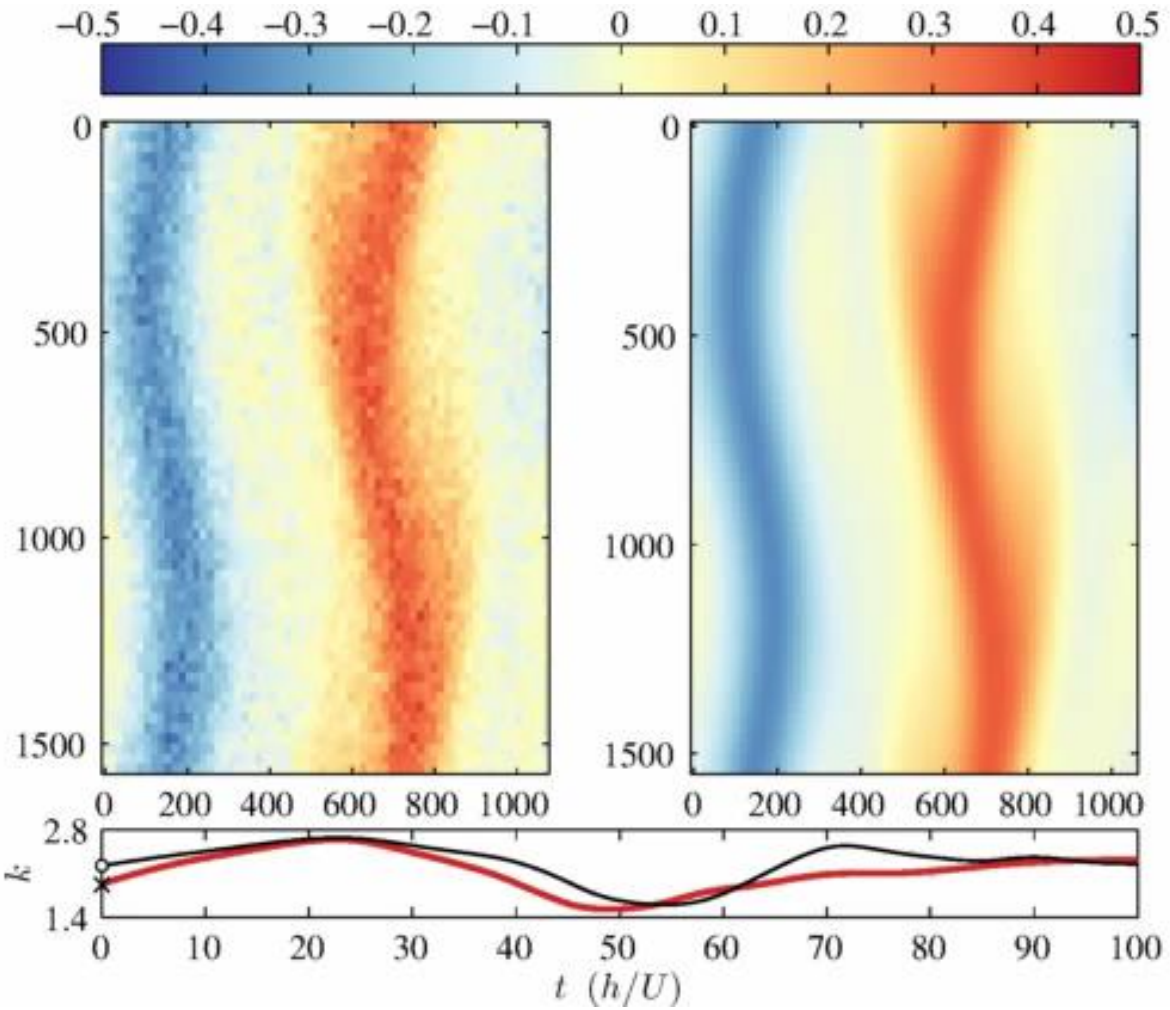
Centre slice velocity



MD

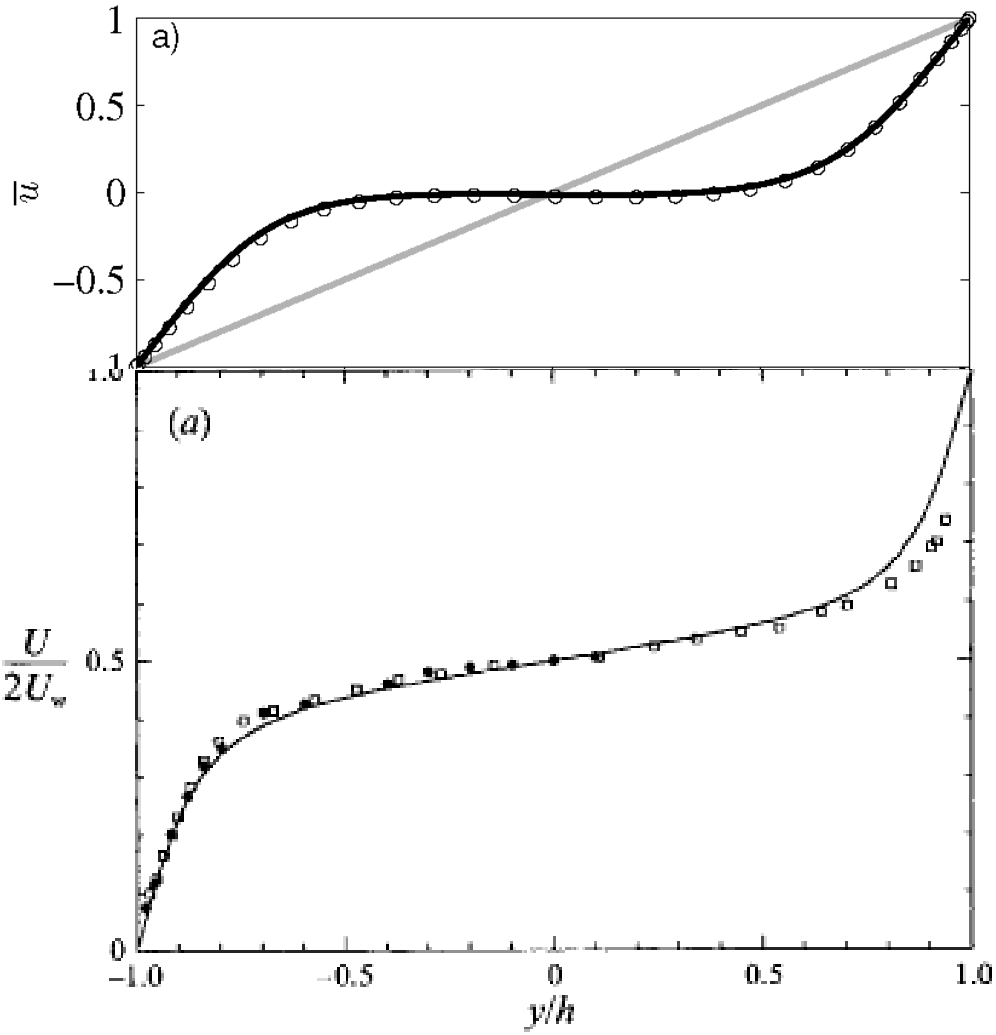
Own code written in Fortran and parallelised using MPI

CFD (Channelflow)

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

Statistical Results

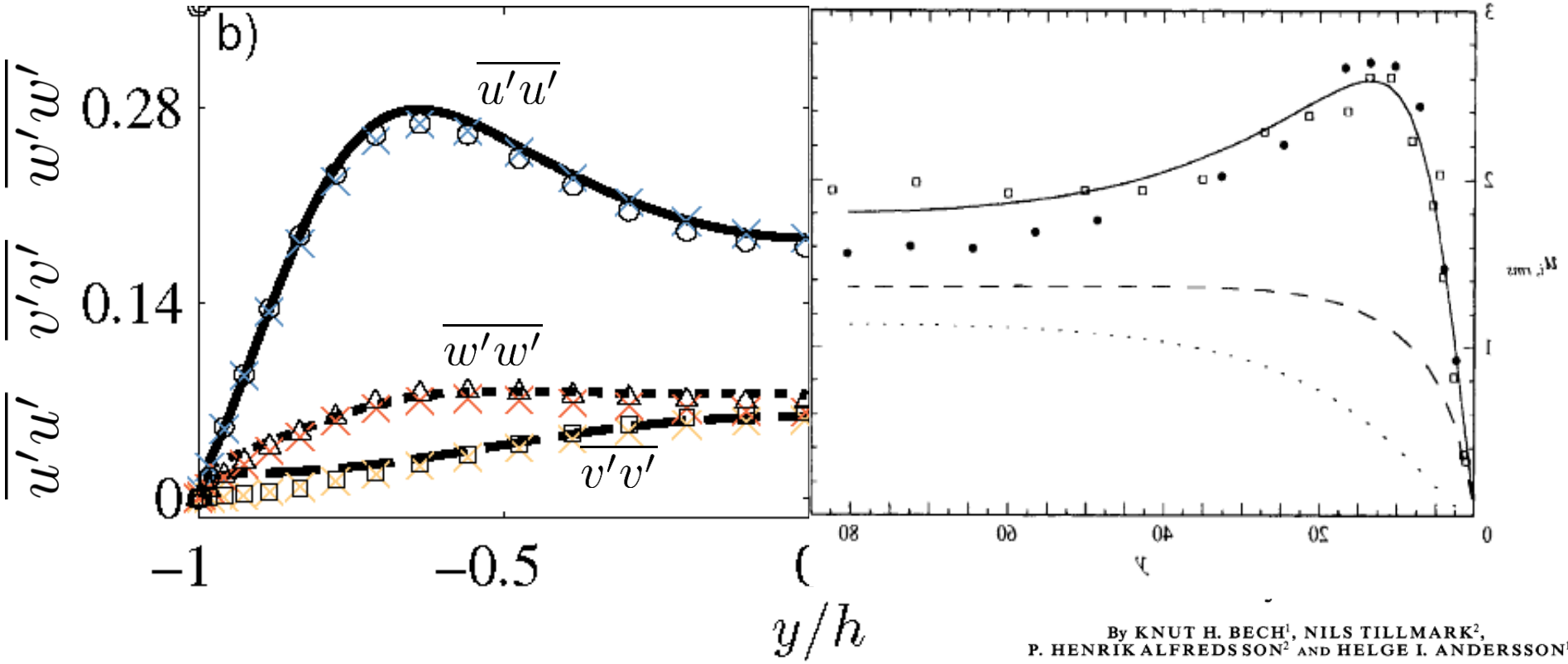
- Averaged velocity profile
- No longer Laminar profile across domain
- Good agreement with literature
  - Numerical continuum studies (points)
  - Experimental results from turbulent simulations (bottom graph)



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

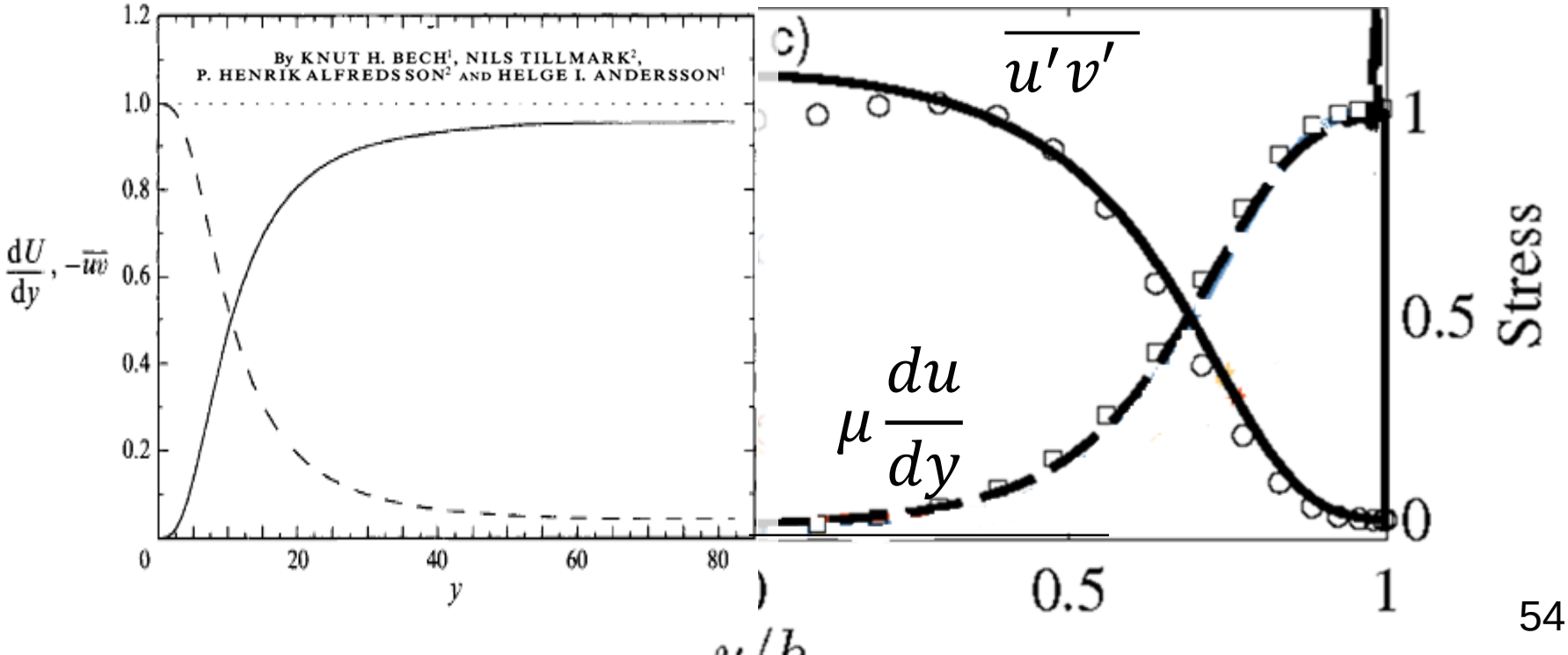
Statistical Results

- Observed RMS velocity profiles match literature
  - Numerical results match well (coloured crosses are Channelflow and symbols are CFD literature)
  - General profile is consistent with experimental data (right)



Turbulent Stresses or Molecular Stresses

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

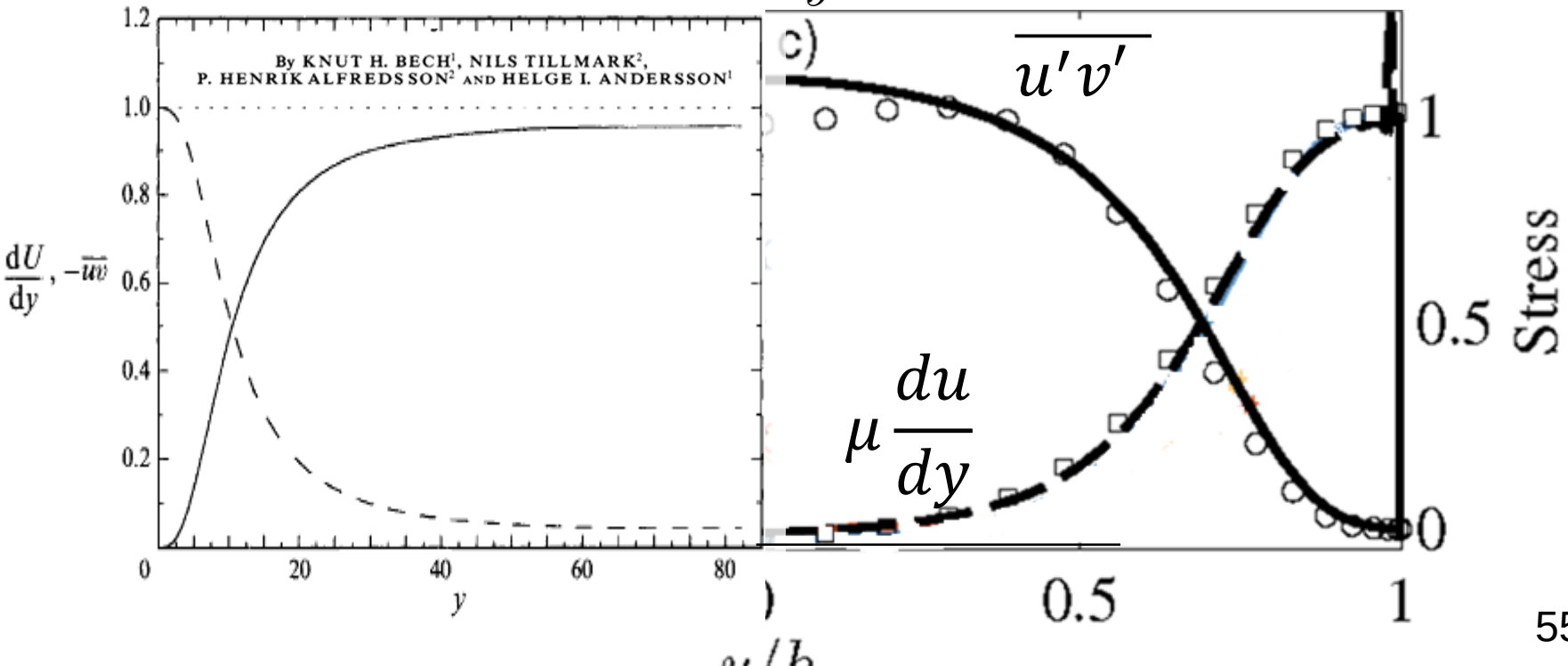


Turbulent Stresses or Molecular Stresses

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

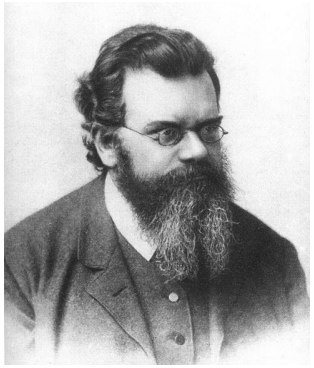


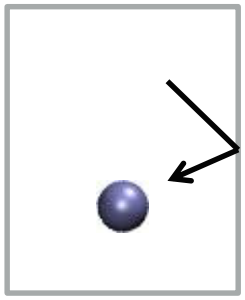
Pressure Tensor in an MD Simulation

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

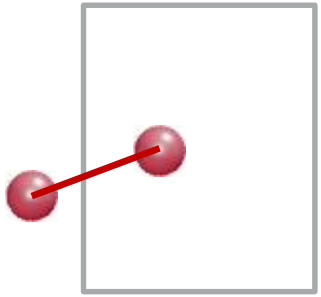
$$\oint_S \Pi_{xy} \cdot dS_y = \underbrace{\sum_{i=1}^{N} \left\langle m_i v_{xi} v_{yi} dS_{yi} \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} \left\langle f_{xij} dS_{yij} \right\rangle}_{\text{Configurational}}$$

Kinetic theory part
Momentum due to average of molecules crossing a plane and returning





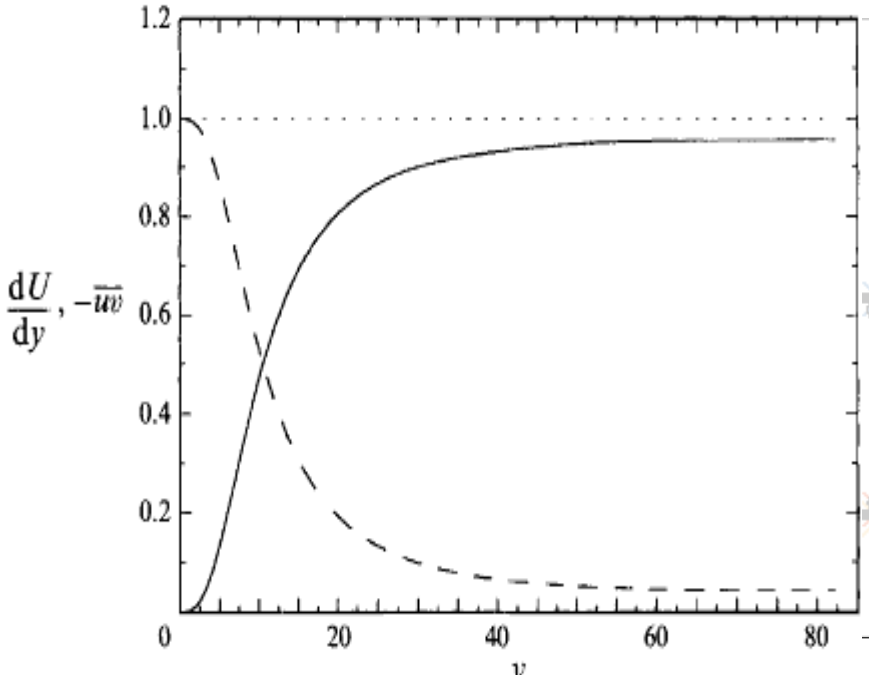
$$\dot{\boldsymbol{r}}_i = \boldsymbol{v}_i + \boldsymbol{u}$$



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

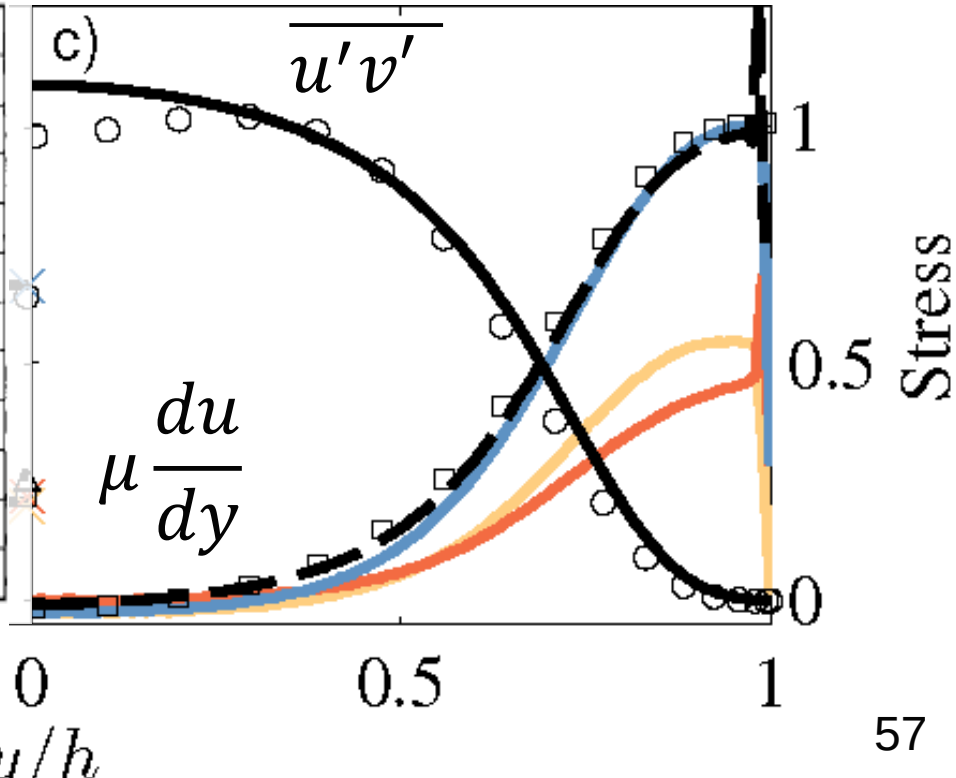
Turbulent Stresses or Molecular Stresses

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



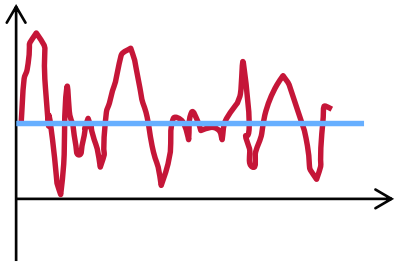
An investigation of turbulent plane Couette flow at low Reynolds numbers

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



Reynolds Decomposition

- Inspired by kinetic theory, Osborne Reynolds split fluid motion into average and fluctuating part

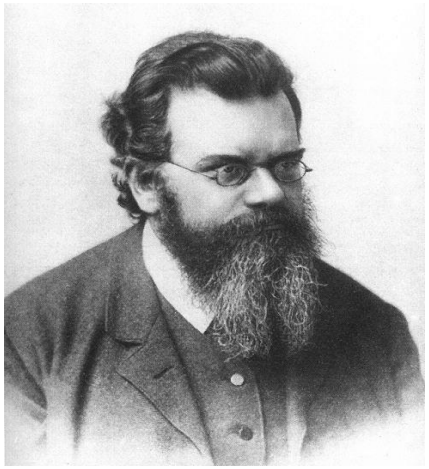


$$u = \overline{u} - u'$$

- Time average to get the Reynold Averaged Navier-Stokes equations
  - Reynolds stress tensor doesn't disappear
  - Approximated by eddy viscosity

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

Same Concept, Different Scales



Peculiar velocity

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

Reynolds' Decomposition

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

- Kinetic part of the pressure tensor and Reynolds stress same mathematical quantity averaged over different length/time scales

$$\sum_{i=1}^{N} \overline{\langle \dot{\boldsymbol{r}}_i \dot{\boldsymbol{r}}_i \rangle} = \sum_{i=1}^{N} \overline{\langle \boldsymbol{v}_i \boldsymbol{v}_i \rangle} + \overline{\boldsymbol{u}'\boldsymbol{u}'} + \overline{\boldsymbol{u}\boldsymbol{u}}$$

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

Is Reynolds Stress just Kinetic Pressure?

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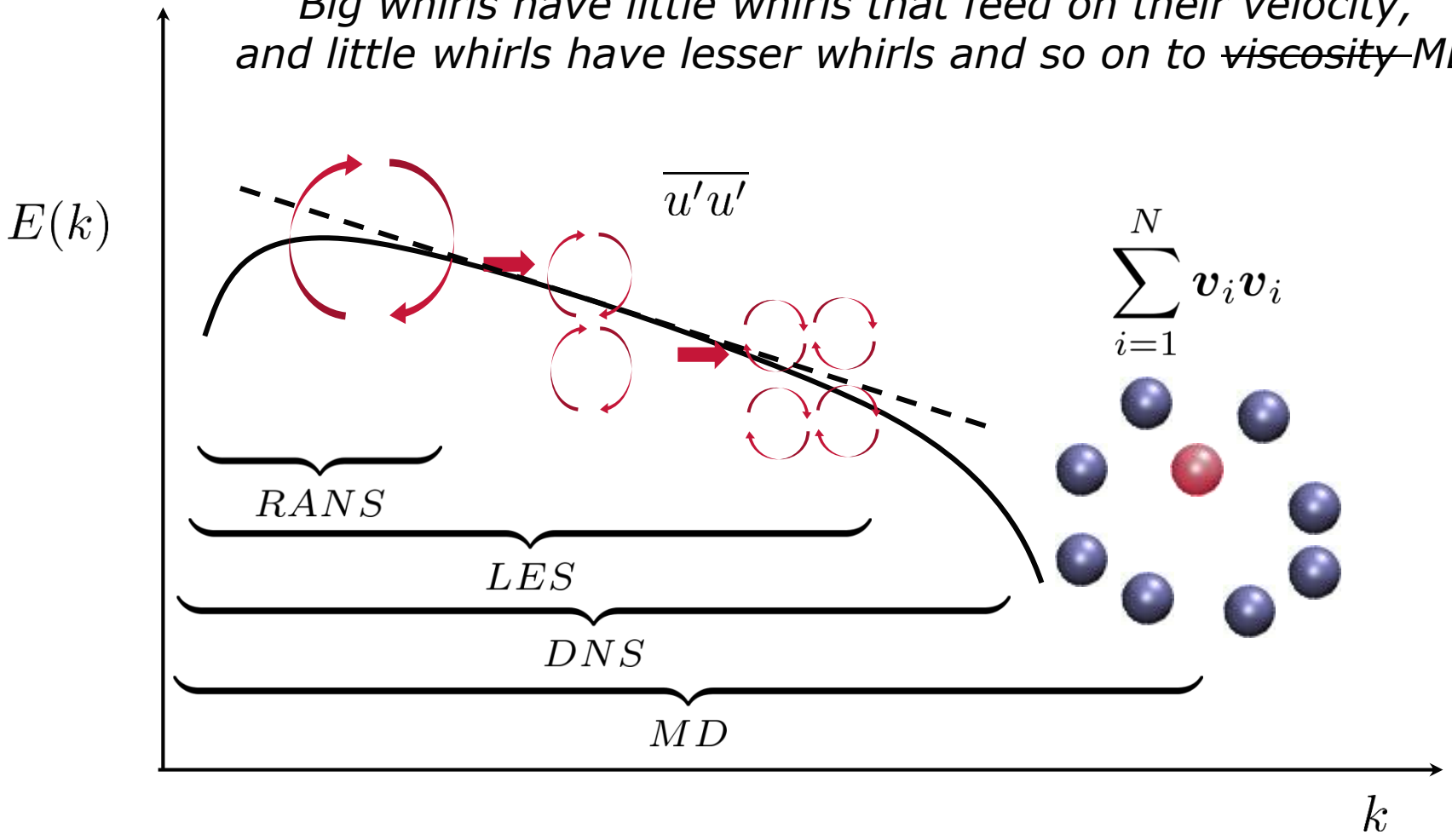
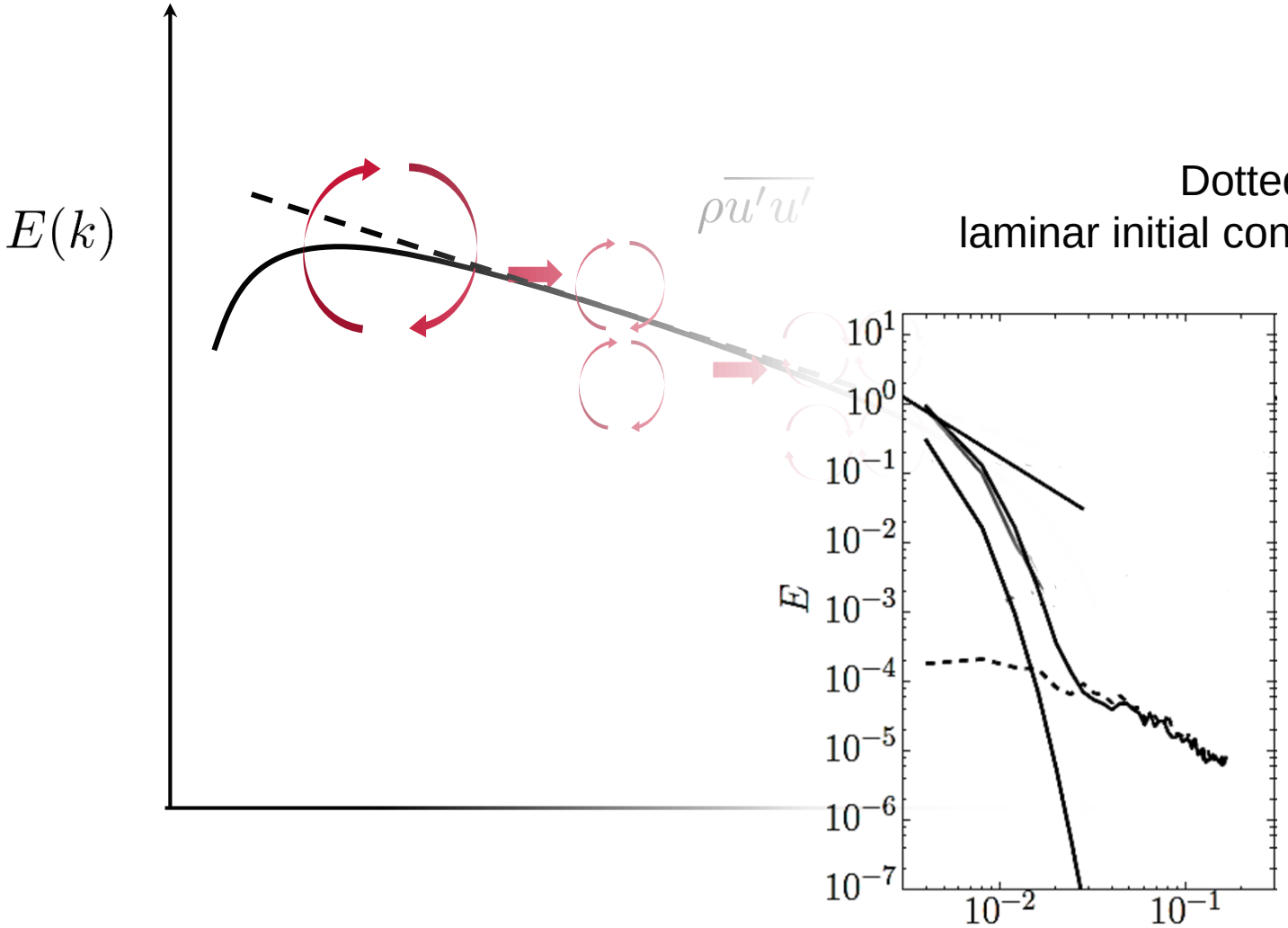
Big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to ~~viscosity~~ MD

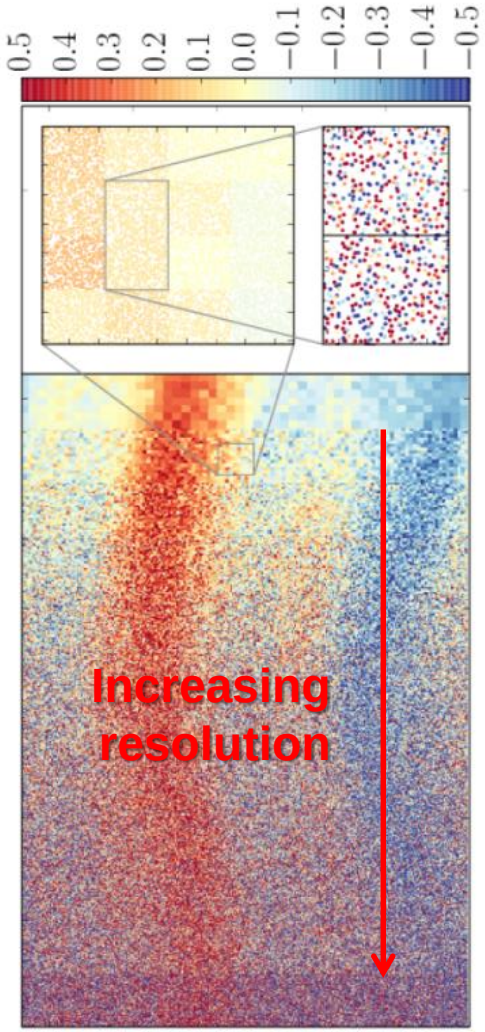


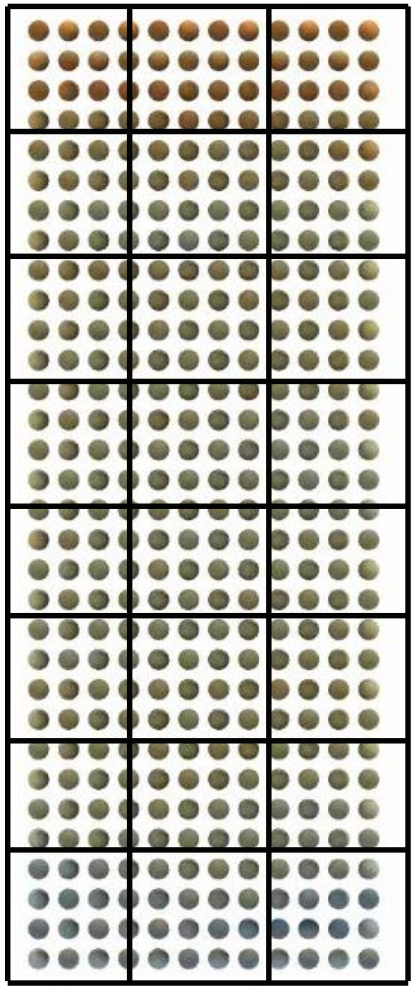
Is Reynolds Stress just Kinetic Pressure?



Dotted lines
laminar initial condition at same Re

Molecular Dynamics

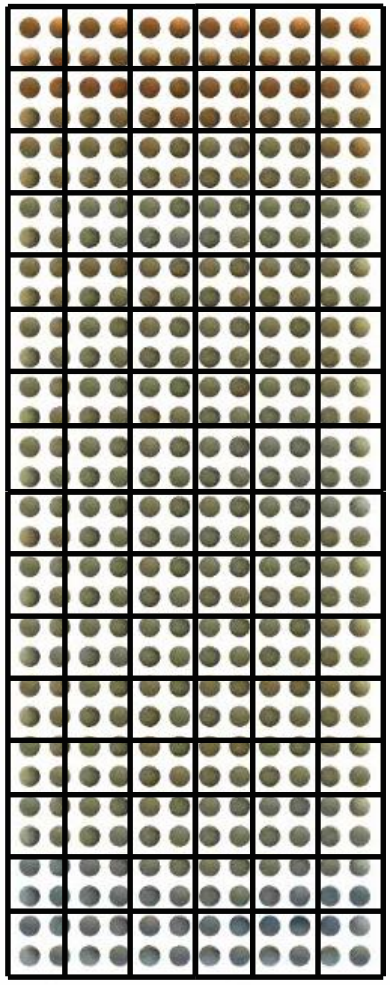




$$\boldsymbol{u} = \frac{1}{N}\sum_{i=1}^{N}\langle \dot{\boldsymbol{r}}_i \rangle$$

Increasing resolution

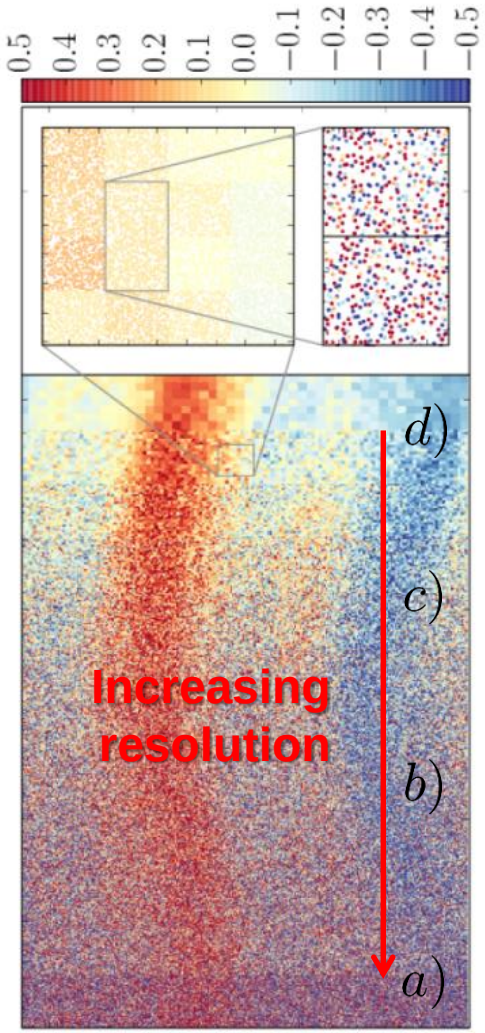
$$T = \frac{1}{3N}\sum_{i=1}^{N}\left\langle \frac{\boldsymbol{p}_i^2}{m_i} \right\rangle$$

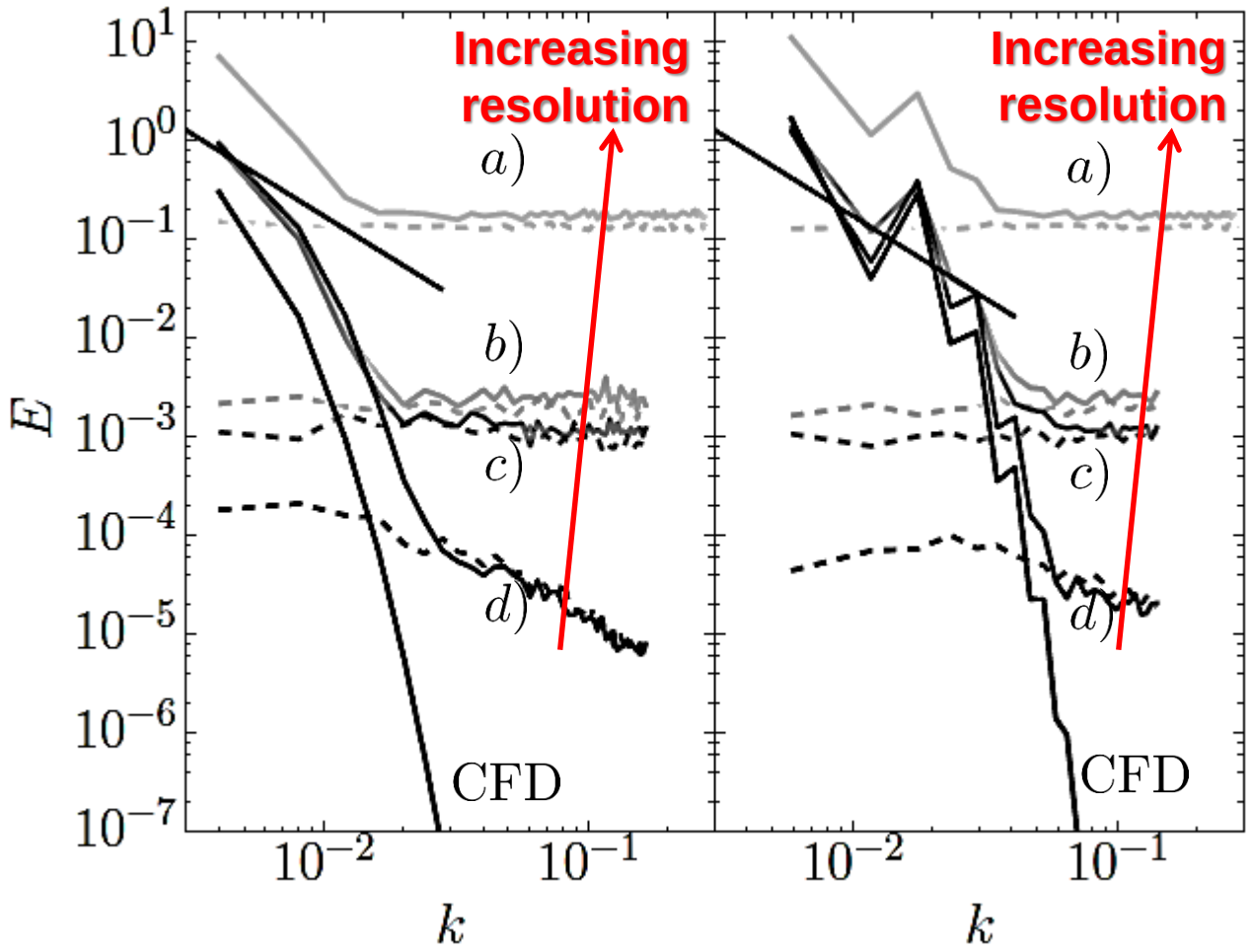


Spectra

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

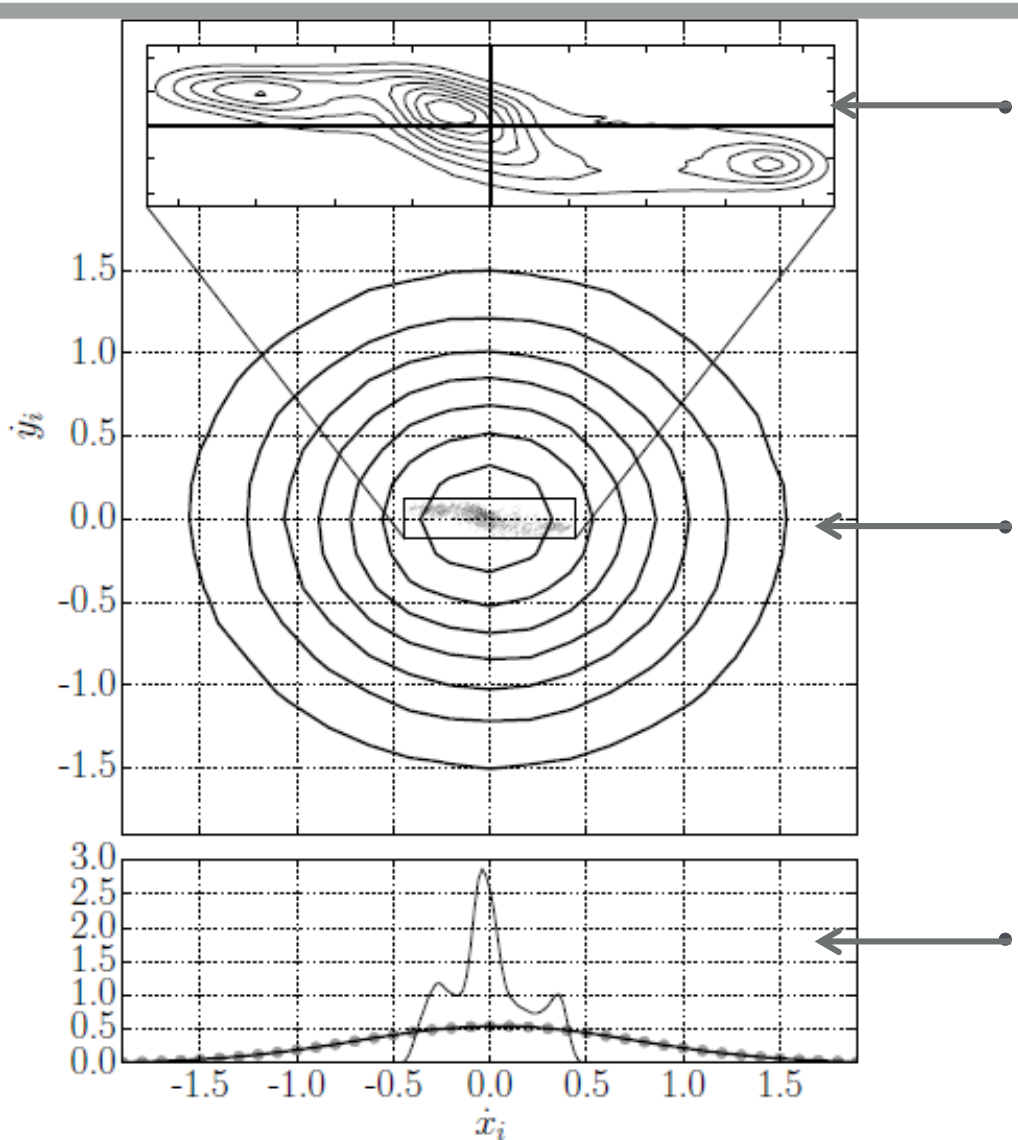
Case	τ_{MD}	Grid resolution
a)	0.005	$672 \times 198 \times 400$
b)	0.005	$84 \times 198 \times 50$
c)	8	$84 \times 198 \times 50$
d)	32	$84 \times 66 \times 50$





Dotted lines - laminar initial condition at same Re

Probability density functions (PDF)



PDF of average velocity shows sweeps and ejections

- Seen in near wall turbulence
- Isolates signal from the noise

PDF of molecular velocities show Gaussian behaviour

- Much wider range of velocities
- Symmetrical in x and y
- No observable flow

Side view of PDFs

- Projection of x

Molecular Structure

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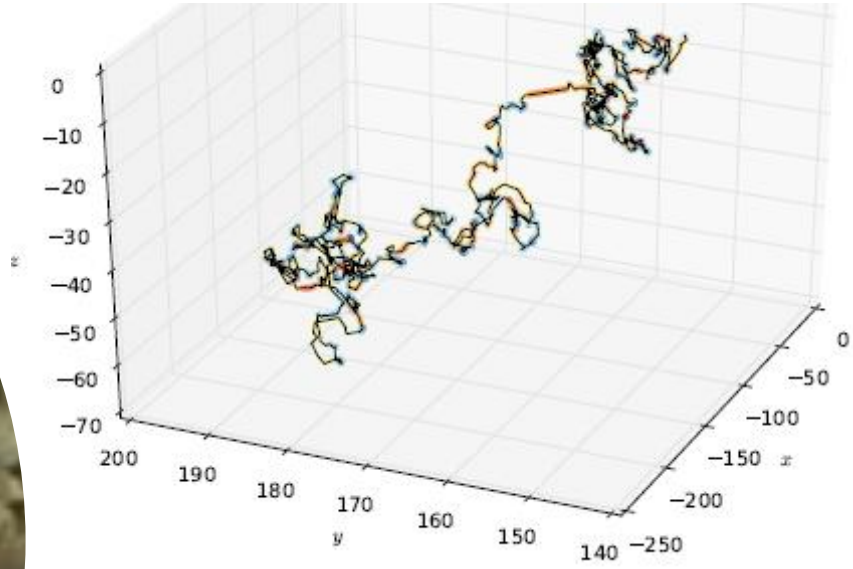
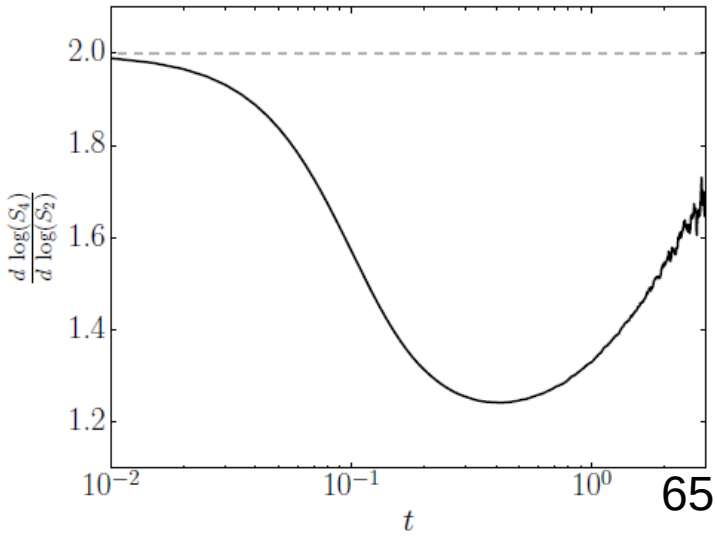




Energy Input and Dissipation

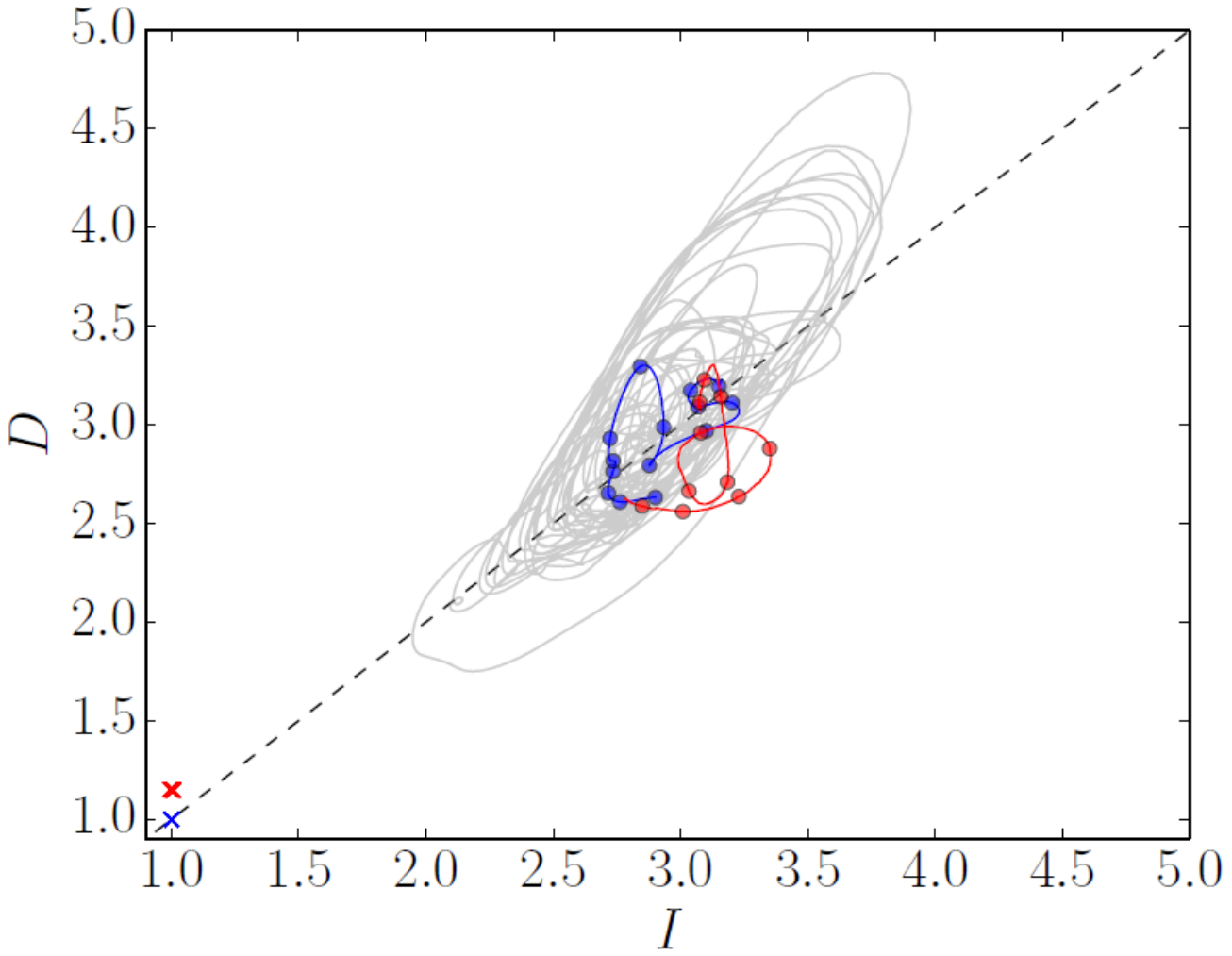
- Dissipation (D)

$$D = \frac{1}{V}\int_V \left(|\nabla u|^2 + |\nabla v|^2 + |\nabla w|^2\right) dV$$

- Energy Input (I)

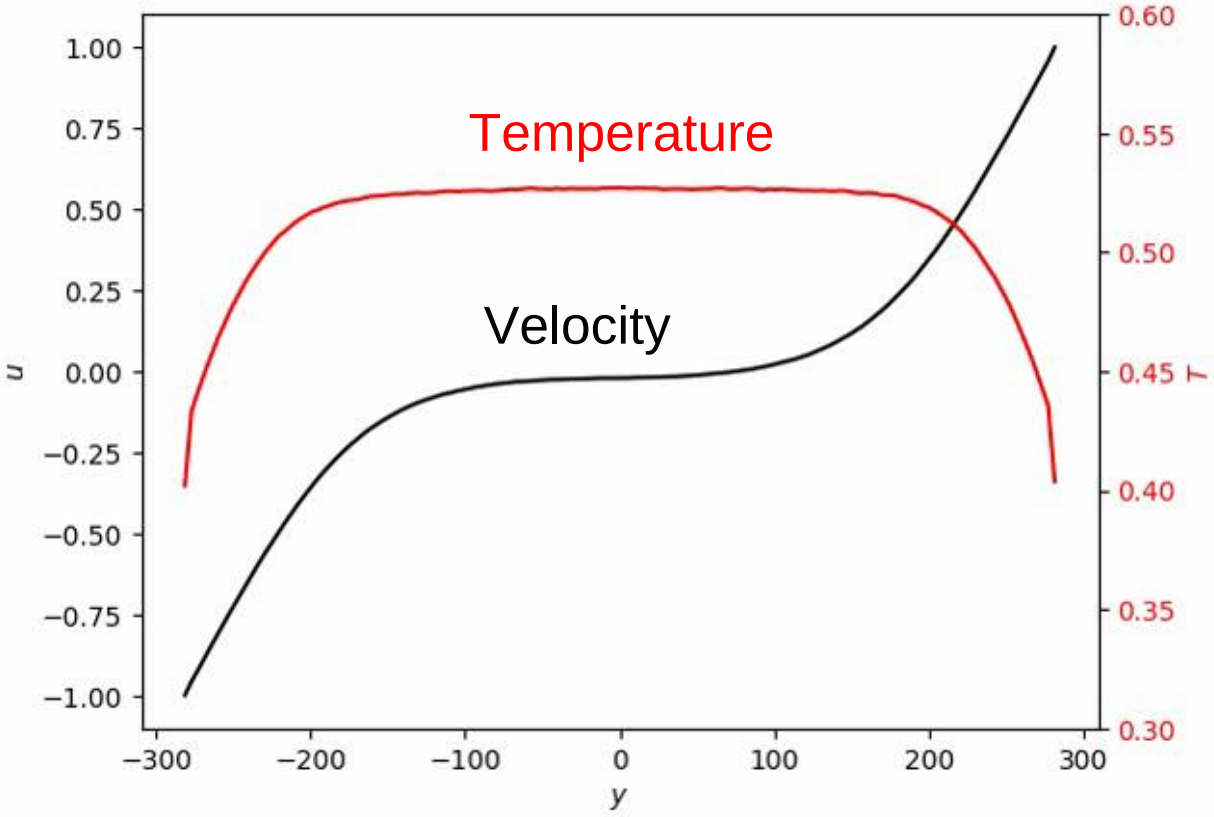
$$I = \frac{1}{A}\int_A \left(\left.\frac{\partial u}{\partial y}\right|_{y=-h} + \left.\frac{\partial u}{\partial y}\right|_{y=h} \right) dA.$$

- Dotted line for I=D
- MD is red
- CFD is blue
- Crosses show laminar solutions



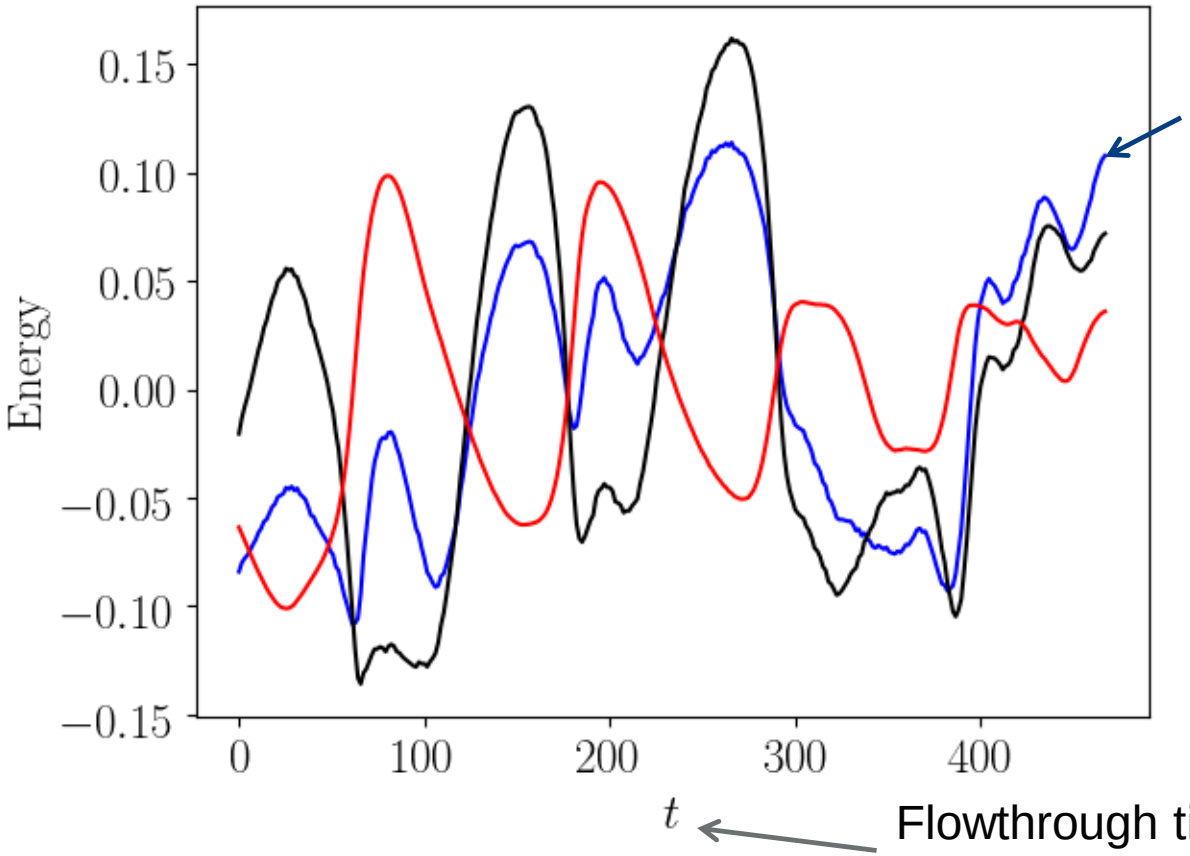
MD Conserves Energy

- Run over ~5 cycles or 500 flow through times
  - Temperature and Velocity are interconnected over a regeneration cycle



MD Conserves Energy

$$\mathcal{H} = Kinetic + Potential = \frac{1}{2}\sum_{i=1}^{N} m_i v_i^2 + \sum_{i=1}^{N}\sum_{j\neq i} \phi_{ij}$$



Total energy added by shearing walls and removed by thermostat

Flowthrough time (h/U)
A cycle is ~100

Normalised by Total Energy

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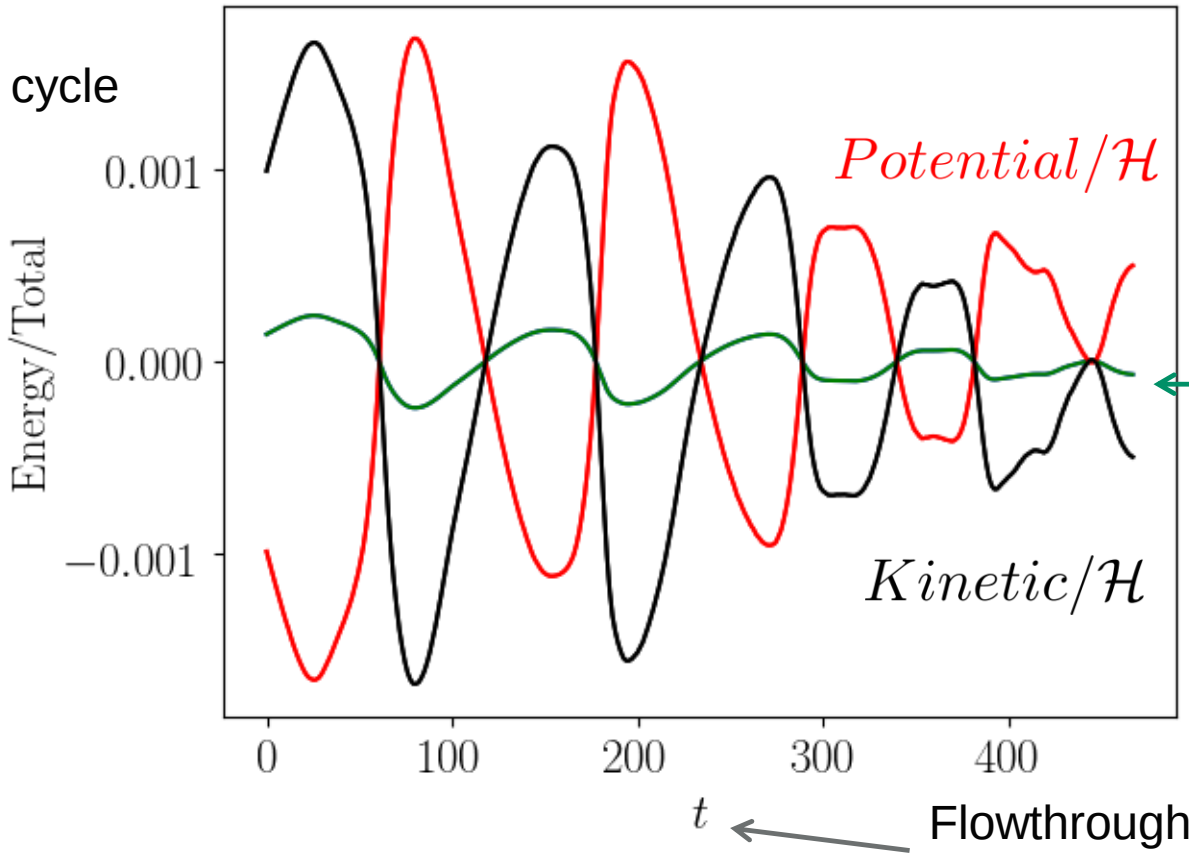
Interchange of kinetic, potential &TKE energy following the regeneration cycle

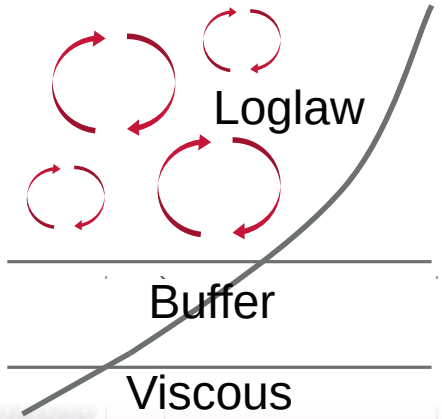
$$\frac{Kinetic}{\mathcal{H}} + \frac{Potential}{\mathcal{H}} = 1$$

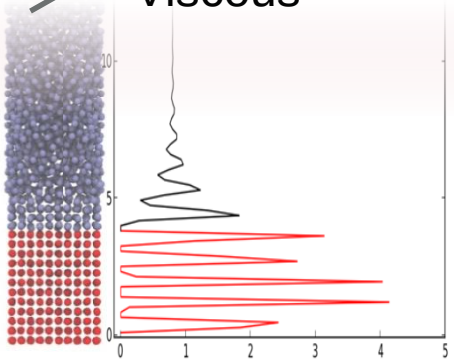


Turbulent Kinetic Energy (TKE) a small part of kinetic, shown scaled up

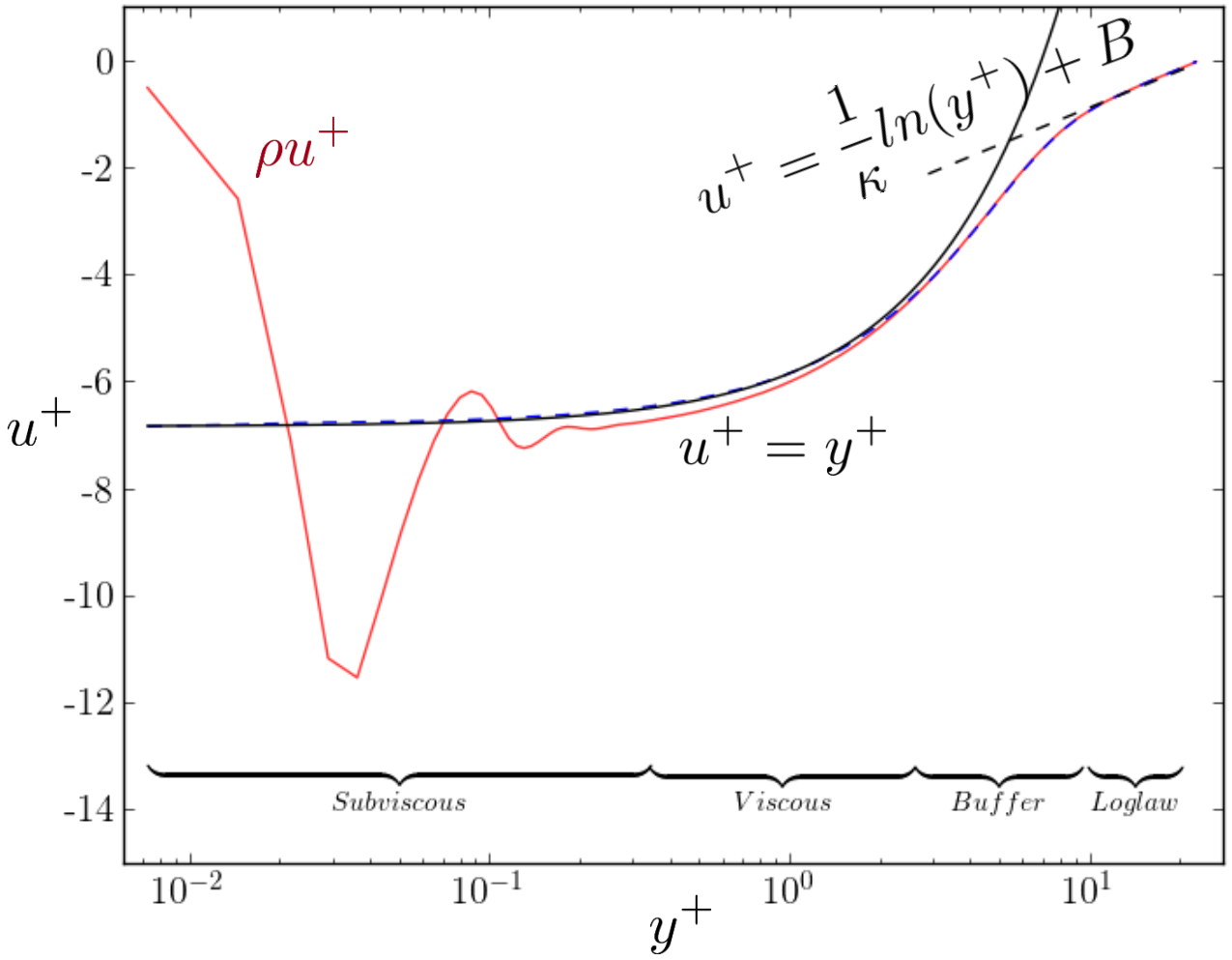
Flowthrough time (h/U)
A cycle is ~100

Law of the wall

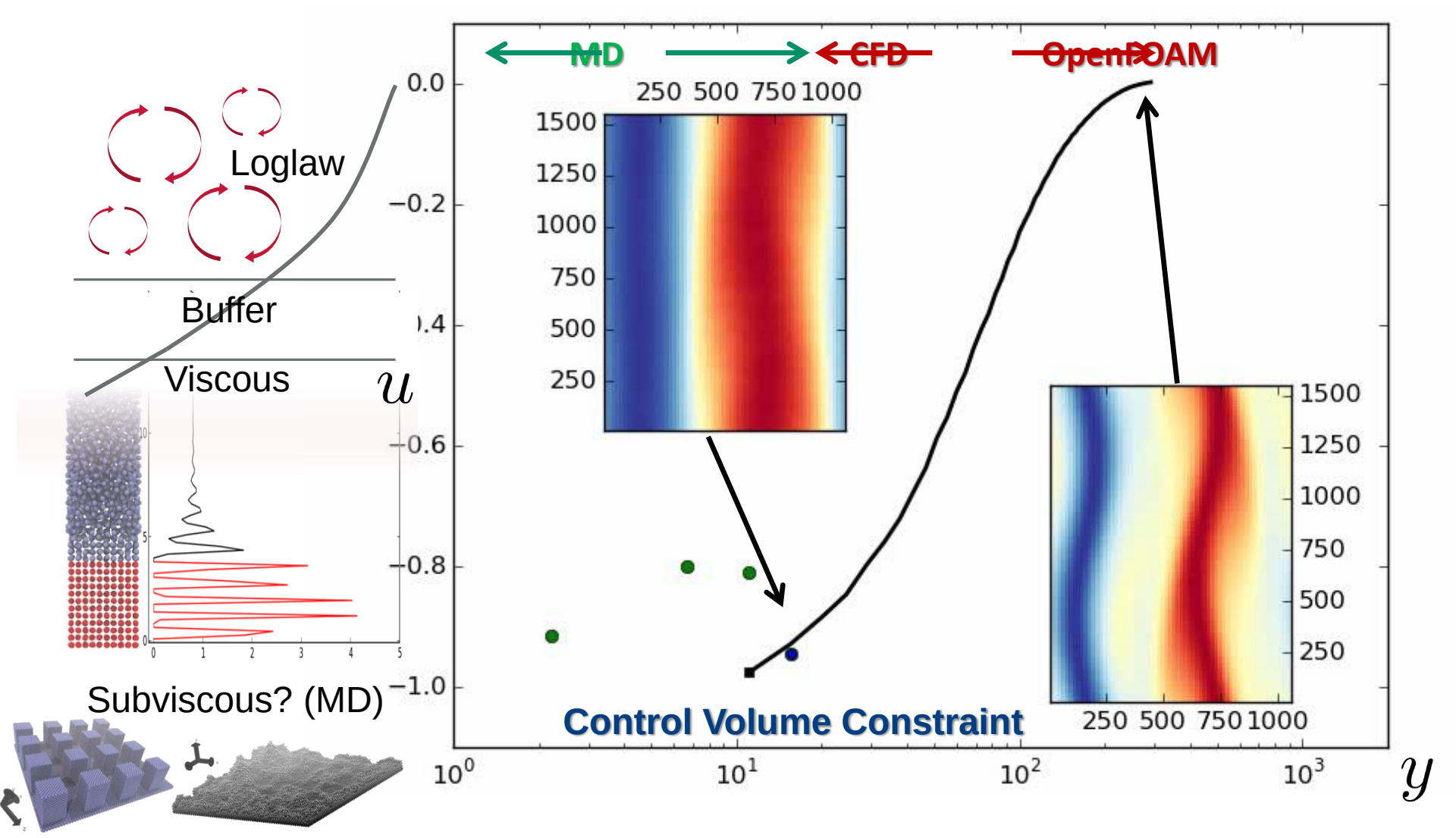




Subviscous? (MD)



Coupling Results – Turbulent Couette



Summary

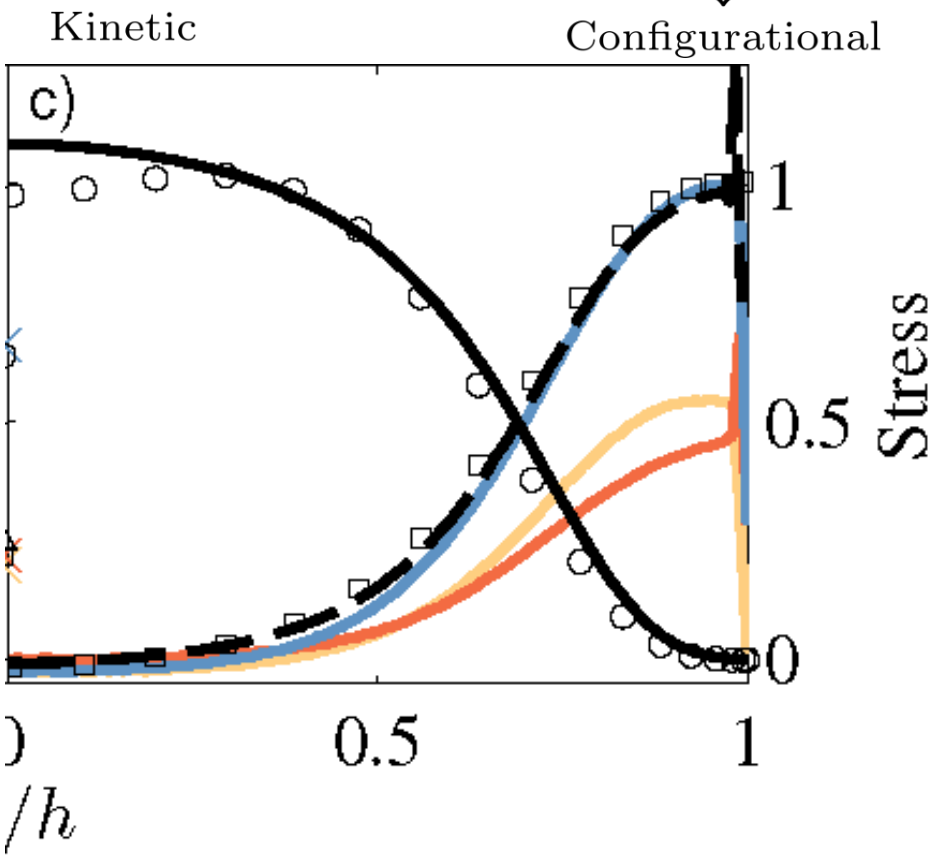
- Minimal Channel Molecular Dynamics look promising
  - Reproduces the key features of turbulence
  - Fewer modelling assumptions in MD, more fundamental than DNS
- Matches CFD and provides a range of additional insights
  - Regeneration cycle, statistics, law of the wall
  - Insights from PDFs, spectra and sub-grid Lagrangian statistics
- MD Reproduces More Physics and Full Range of Scales
  - Energy conserved, changing between thermal, fluid and structural
  - Reynolds stress tensor ***is*** the kinetic pressure tensor suggesting that the minimal eddy size could be molecular rotations

Thank you and Questions

Wall Units

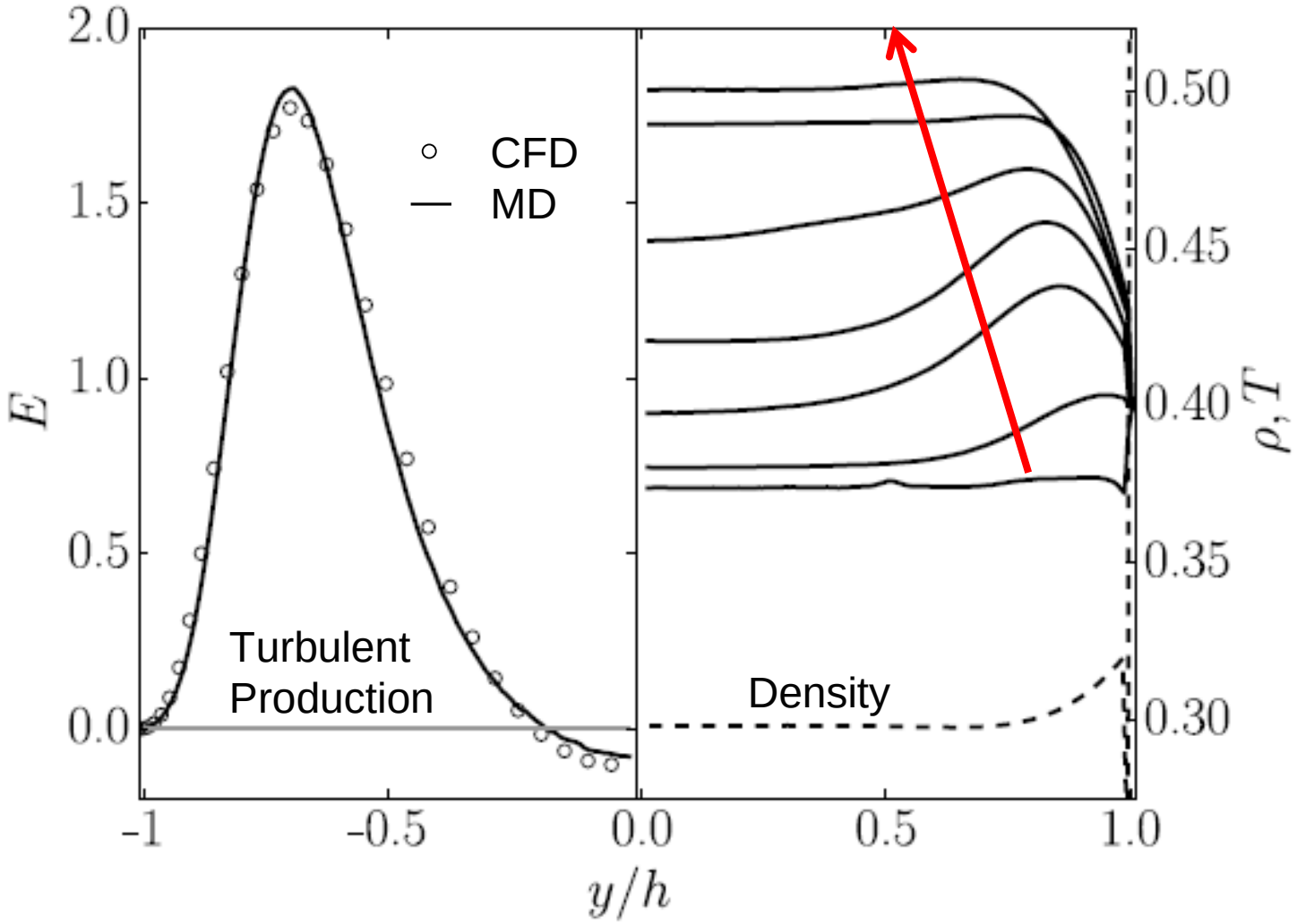
$$u^+ = \frac{u}{u_w} \quad u_w = \frac{\tau_w}{\rho} \quad \tau_w = \underbrace{\sum_{i=1}^{N} \left\langle m_i v_{xi} v_{yi} dS_{yi} \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle f_{xij} dS_{yij} \right\rangle}_{\text{Configurational}}$$

- The definition of wall stress τ_w is ambiguous in a molecular system due to
  - Stick slip
  - Deformation of the wall
  - Molecular stacking
- Evaluated 7ℓ away from the wall. The location at which shear stress equals the continuum analytical value in laminar MD channel of same dimensions.



Turbulent Production and Temperature

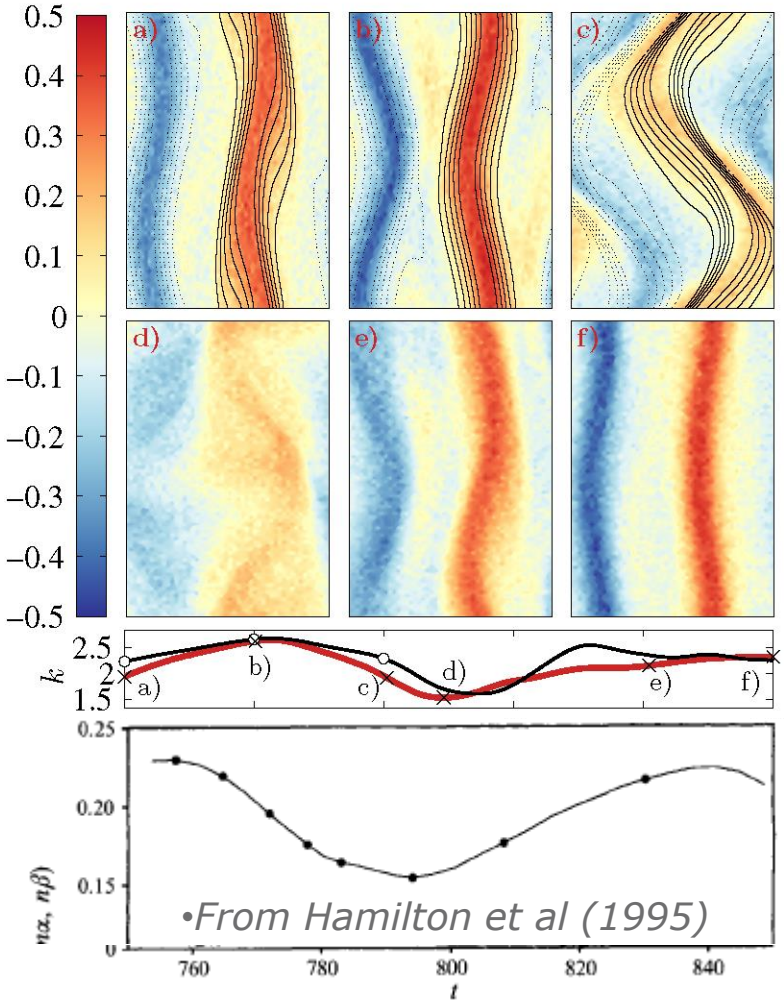
- Initial run over ~200 flowthrough times - Temperature increased over time



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



MD vs CFD

- Dissipation (D)

$$D = \frac{1}{V}\int_V \left(|\nabla u|^2 + |\nabla v|^2 + |\nabla w|^2\right) dV$$

- Energy Input (I)

$$I = \frac{1}{A}\int_A \left(\left.\frac{\partial u}{\partial y}\right|_{y=-h} + \left.\frac{\partial u}{\partial y}\right|_{y=h} \right) dA.$$

- Dotted line for I=D
- MD is red
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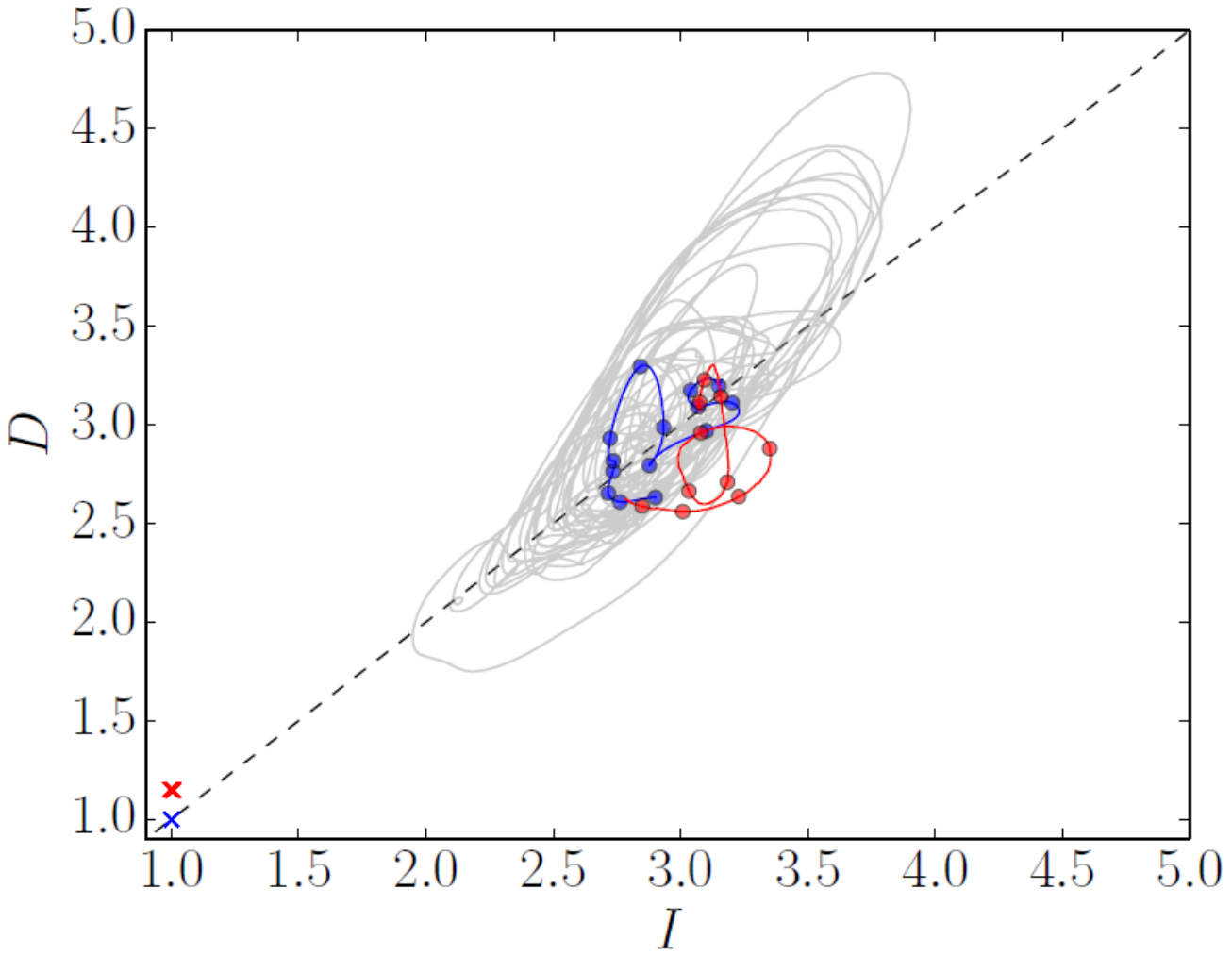
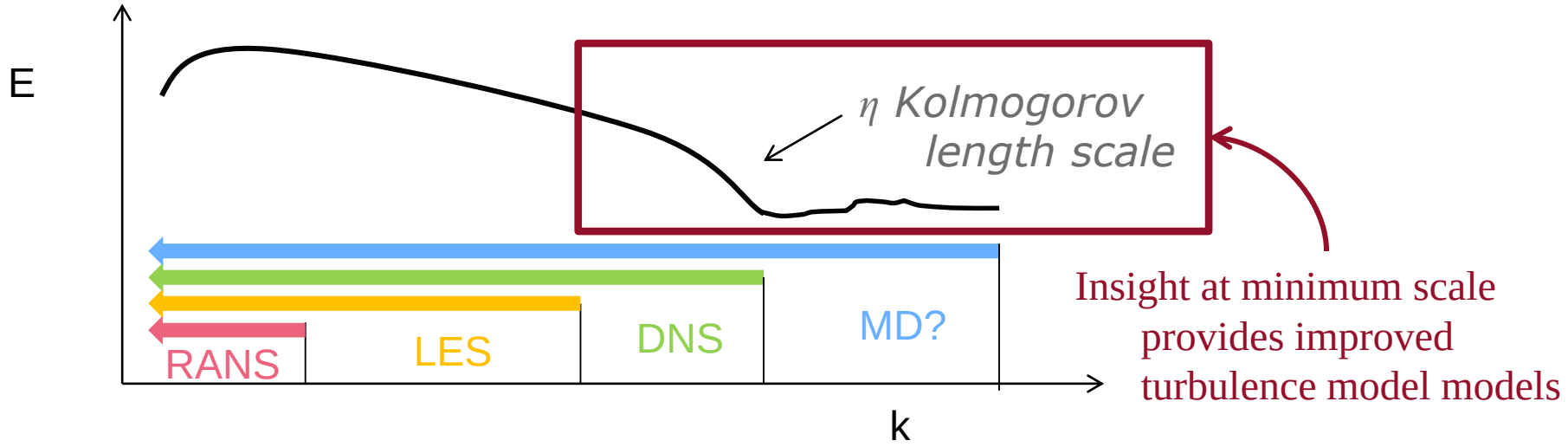
- Crosses show laminar solutions



The Minimum Scale of Turbulence

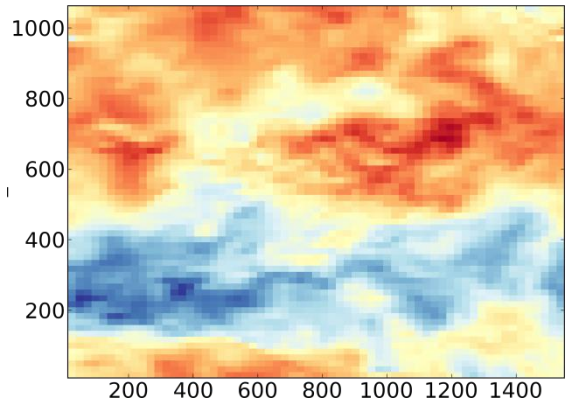
- Kolmogorov scaling arguments suggest a minimum scale
  - Based on dimensional analysis $\eta \sim Re^{-3/4}$
- Used to determine the minimum scale required in a CFD simulation and the number of grid cells
  - Direct Numerical Simulation (DNS) solves the full range
  - Large Eddy Simulation (LES) models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



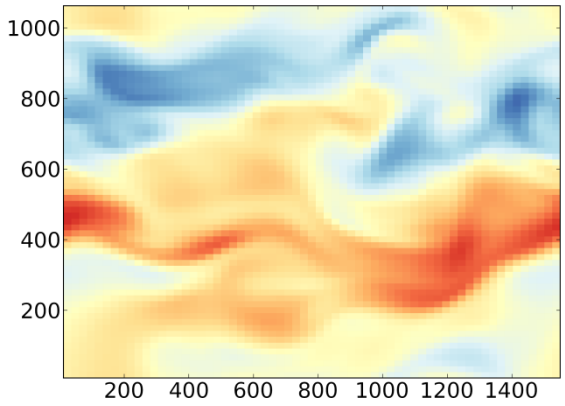
Three plots of decreasing Reynolds Number

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

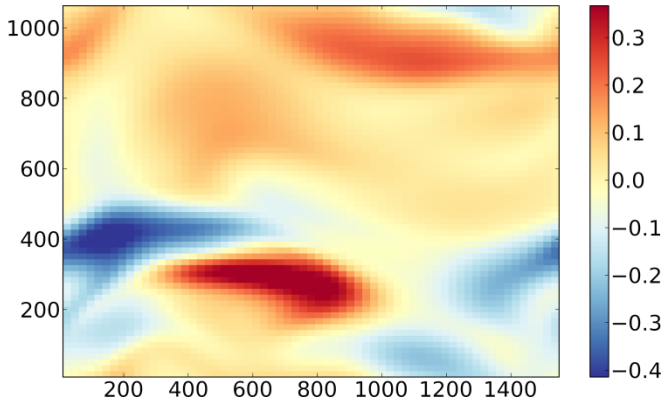
Re ≈ 4000

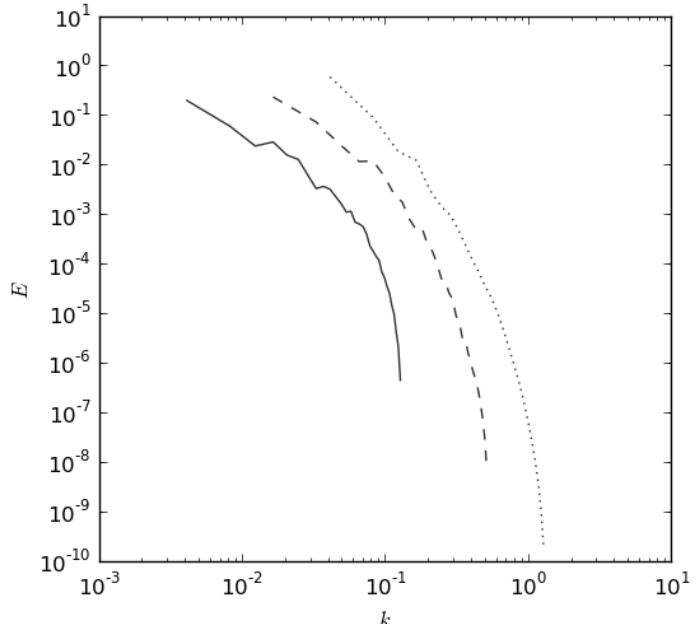


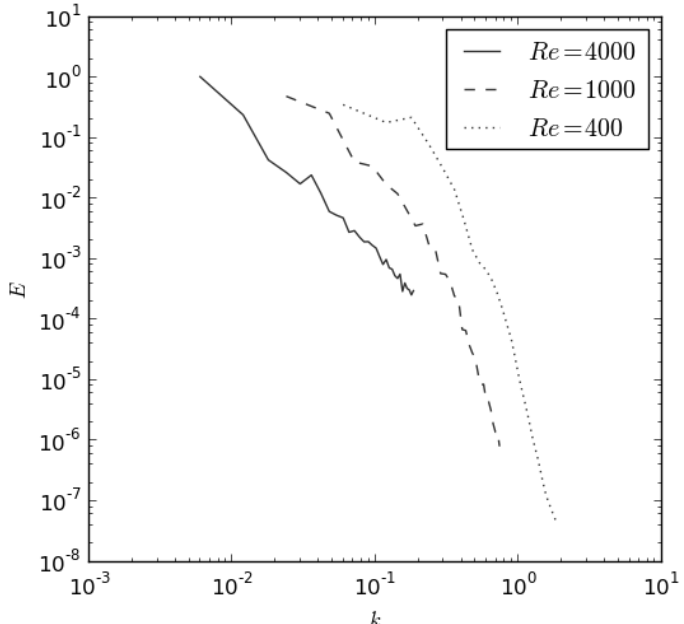
Re ≈ 1000



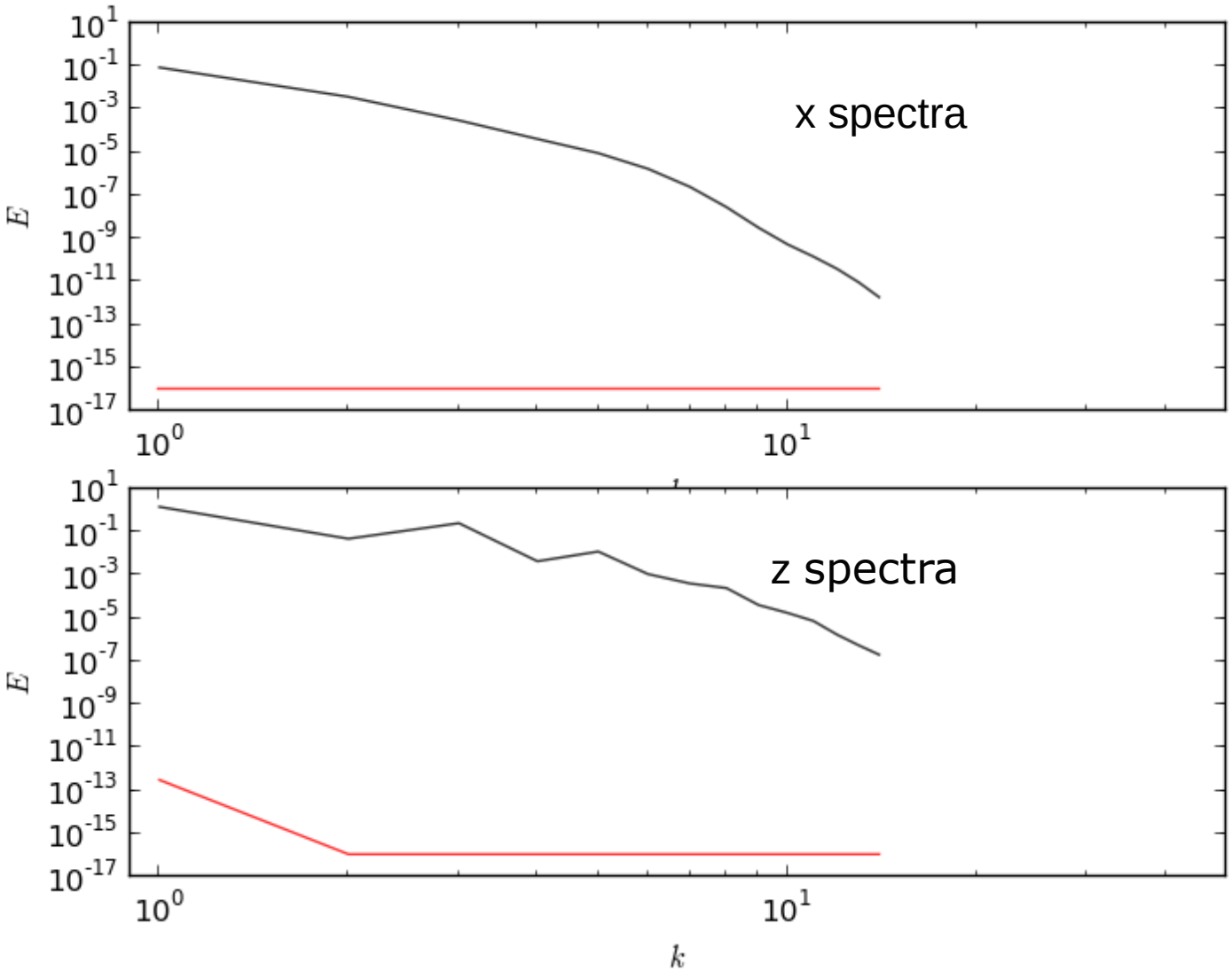
Re ≈ 400







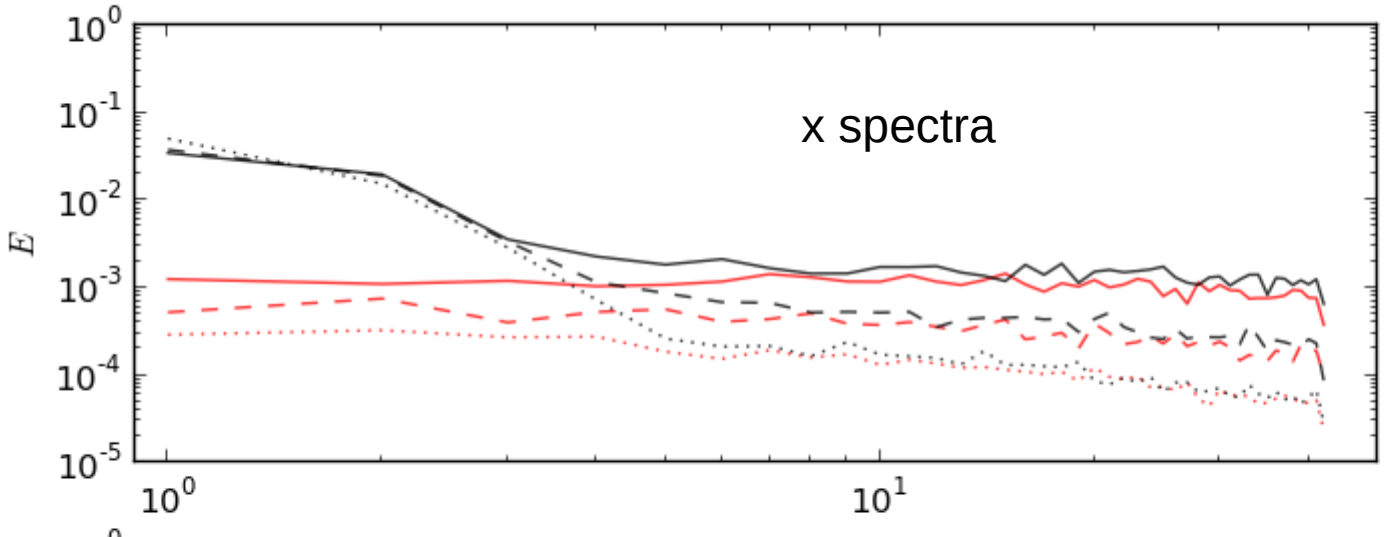
Velocity Spectra

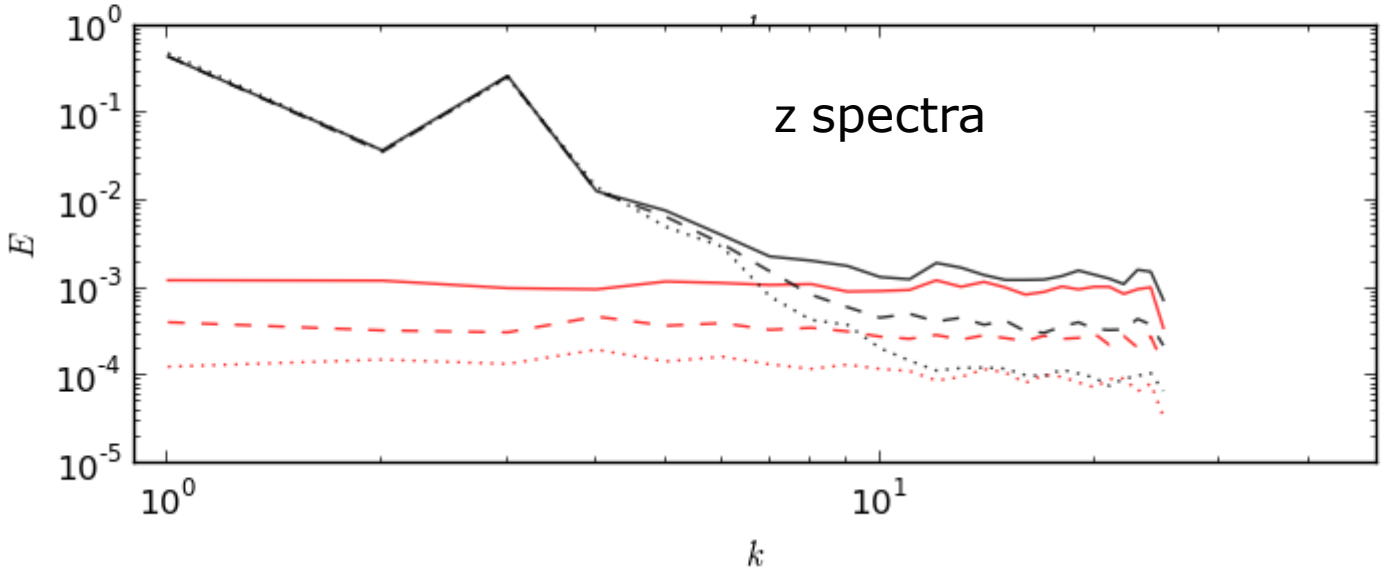


Black Lines
Turbulent CFD Flow

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