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Coupled Simulation of Continuum and Molecular Dynamics using Domain Decomposition

Edward Smith

Edinburgh 03/05/16

Collaborations with David Heyes, Daniele Dini,Tamer Zaki
Omar Matar, Erich Muller and Richard Craster

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Overview

- Coupled Simulation
- Toward a consistent framework
- Constrained Dynamics
- Large scale computations and cpl-library
- Turbulent Molecular Dynamics

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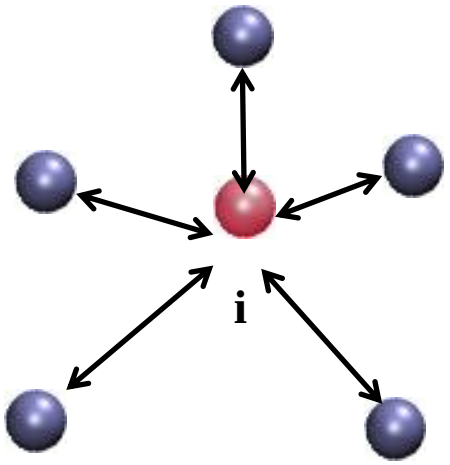
Molecular Dynamics

Discrete molecules in continuous space

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

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



Acceleration obtained from forces

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

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

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

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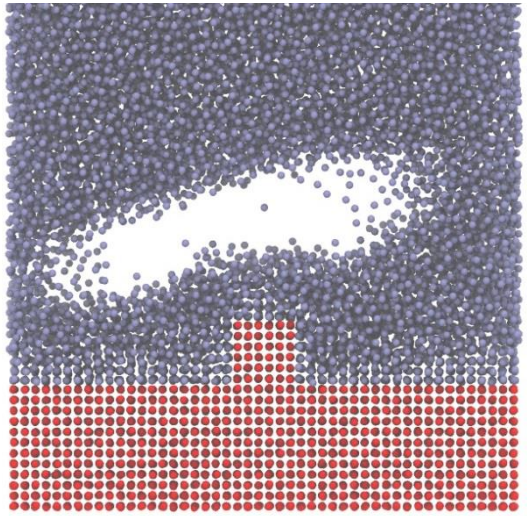
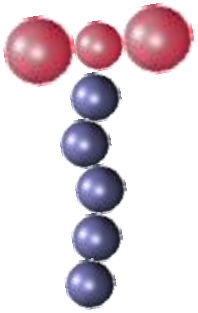
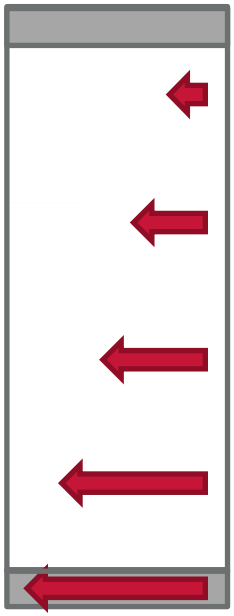
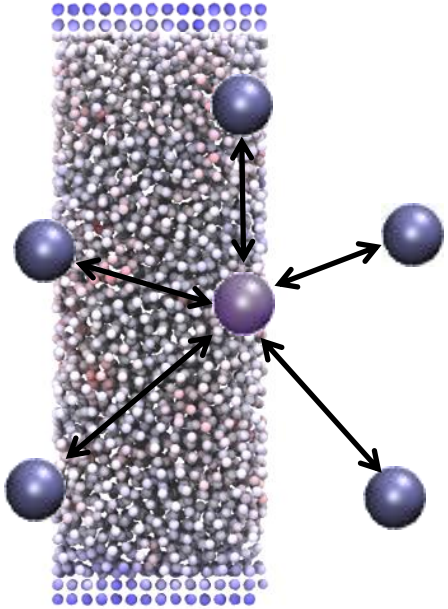
Molecular Dynamics

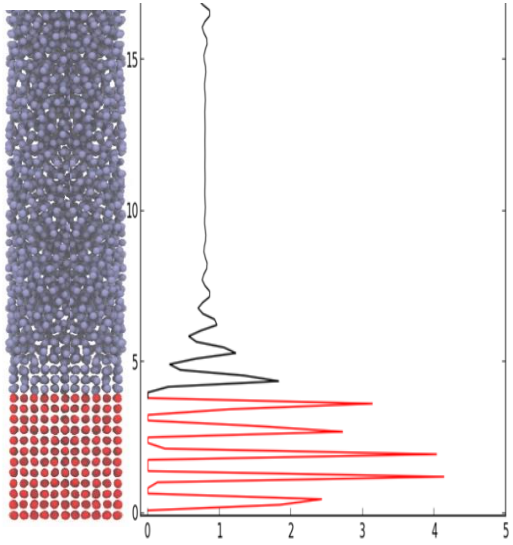


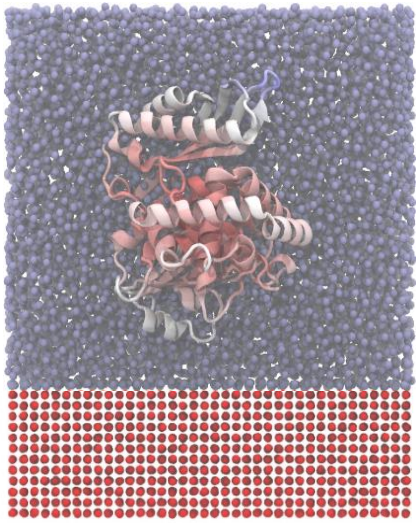
Superspreading Surfactant, e.g. Silwet-L77











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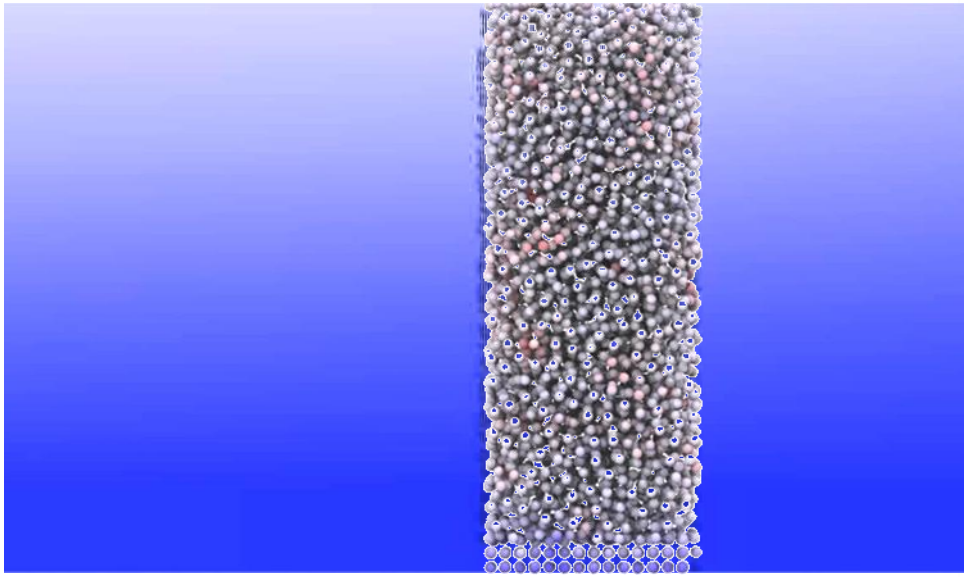
Continuum Solver

- **Mass conservation**

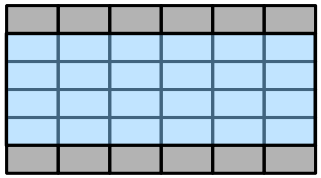
$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u}\cdot d\mathbf{S}$$

- **Momentum Balance**

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



Direct Numerical Simulation of Turbulent Couette Flow



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Coupling Overview

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 and Coveney, (2003)

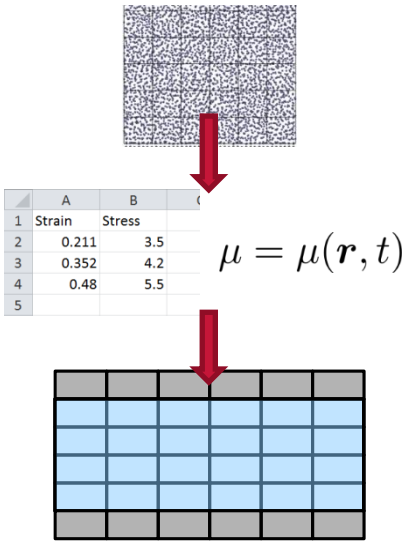
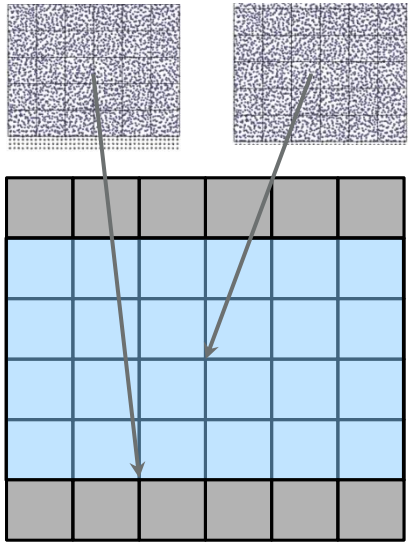


Table Lookup or Coefficients

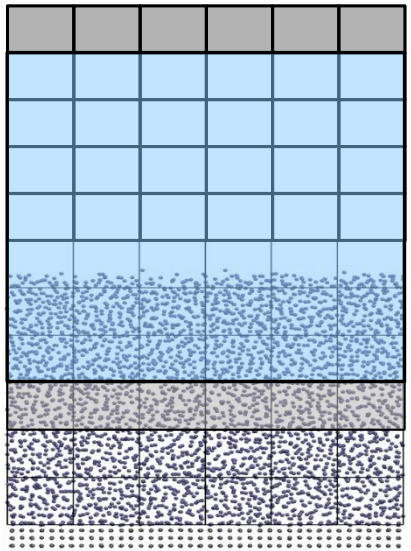
MD parameter study stored in table and CFD uses data



Embedded Models (HMM)

MD – embedded in a CFD simulation

Used for Non-Newtonian effects [1)]



Domain Decomposition

MD –CFD linked along an interface

Local features e.g. contact line [2)]

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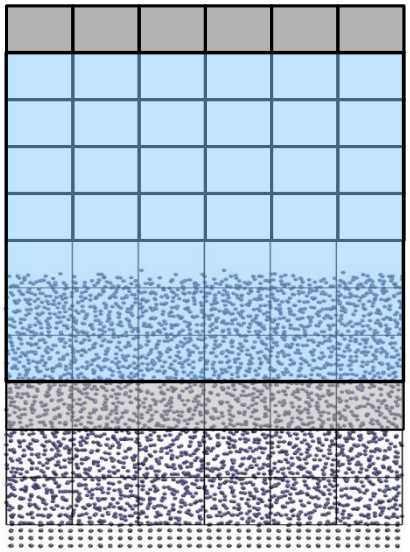

Domain Decomposition

MD –CFD linked along an interface

Local features e.g. contact line [2)]

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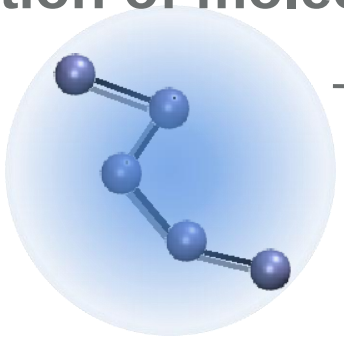
Coupling Challenges

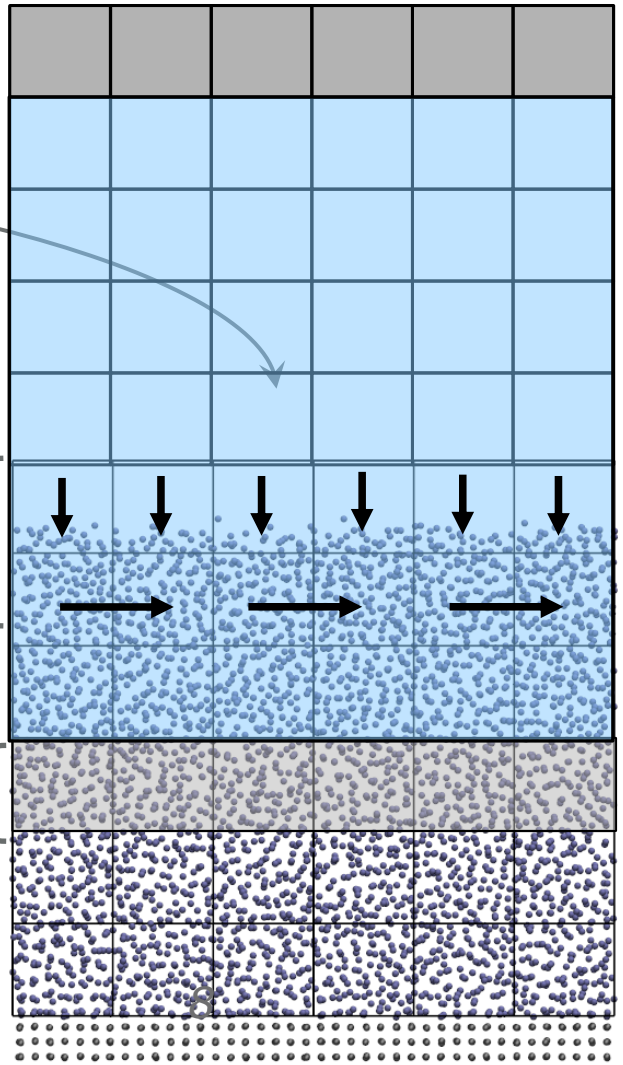
Boundary force and insertion of molecules



Consistent Framework

CFD→MD Boundary condition

MD→CFD Boundary condition



$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i \overset{?}{\Longleftrightarrow} \frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = \boldsymbol{\nabla}\cdot\boldsymbol{\Pi}$$

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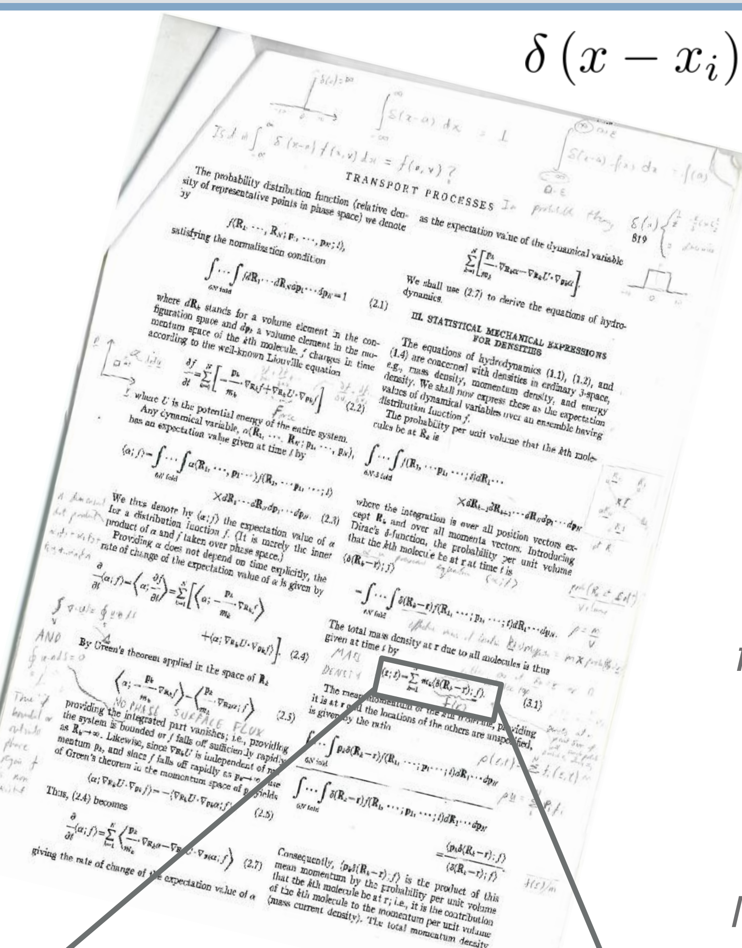
Irving and Kirkwood (1950)

The Journal of Chemical Physics — Volume 18, Number 6 — June, 1950

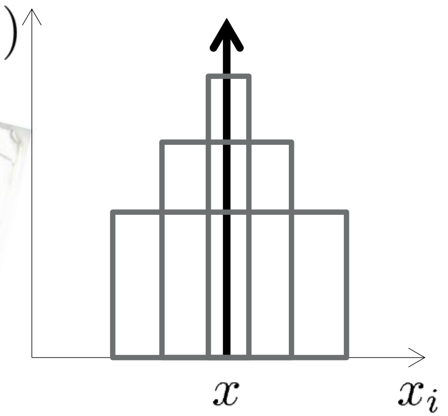
The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics

J. H. Irving and John G. Kirkwood



TRANSPORT PROCESSES

III. STATISTICAL MECHANICAL EXPRESSIONS FOR DENSITIES

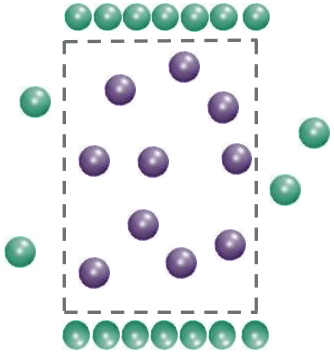


$$\rho(\boldsymbol{r}, t) = \sum_{i=1}^{N} \left\langle m_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right); f \right\rangle$$

The Dirac delta infinitely high, infinitely thin peak formally equivalent to the continuum differential formulation
BUT
No molecule is ever exactly at a point

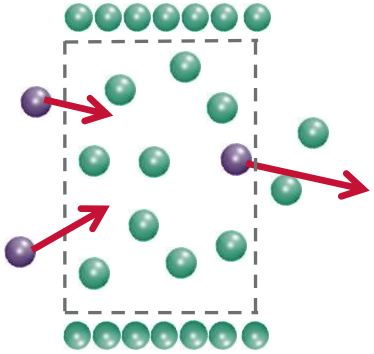
Control Volume Functional

- The Control volume function is the integral of the Dirac delta function in 3 dimensions



$$\vartheta_i \equiv \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

- Its derivative gives the fluxes over the surface



$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i}$$

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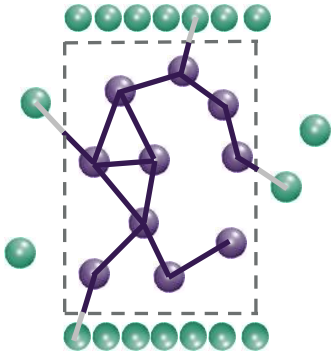
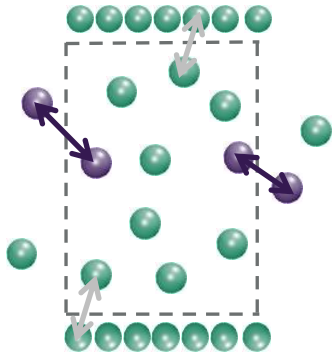
Control Volume Functional - Forces

- A CV based on the length of intermolecular interaction inside the volume (used in the volume average stress)



$$\vartheta_s \equiv \int_V \delta(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) dV$$

- Its derivative gives the forces over the surface (as in the method of planes stress)



$$dS_{xij} \equiv \int_0^1 \frac{\partial \vartheta_s}{\partial x} ds$$

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The Control Volume Equations

- Mass Conservation

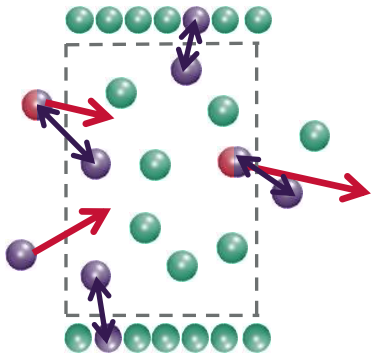
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\boldsymbol{S}_i$$

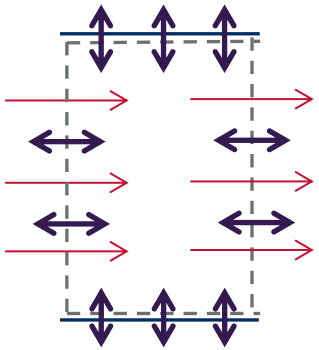
$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u} \cdot d\mathbf{S}$$

- Momentum Balance

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\mathbf{n} \cdot d\mathbf{S}_{ij}$$

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





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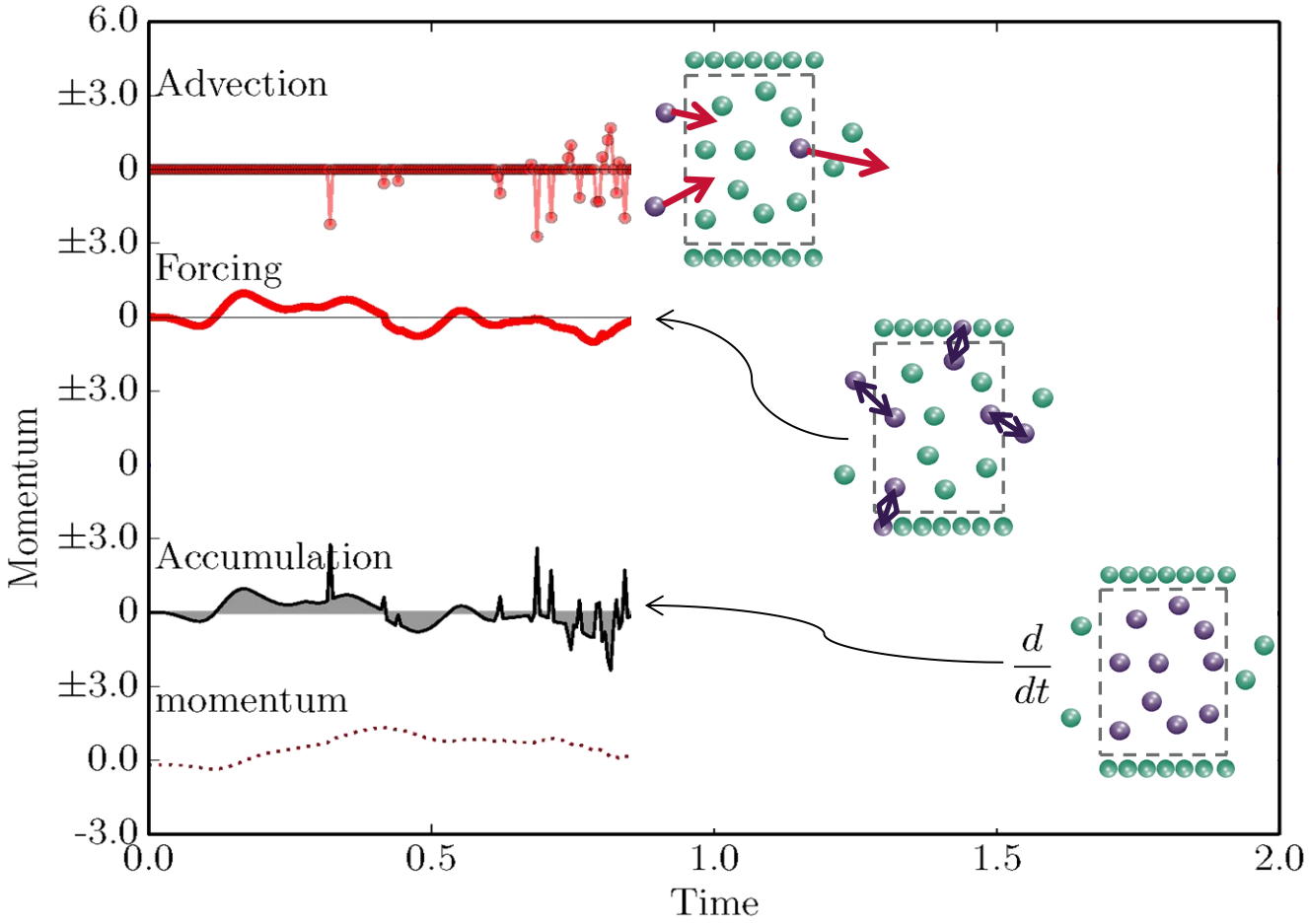
Exact Conservation

- **Results from any arbitrary volume**
  - Accumulation = Forcing + Advection
  - Momentum evolution is the integral of accumulation



$$\underbrace{\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\textit{Advection}} \underbrace{- \frac{1}{2} \sum_{i,j}^{N} \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij}}_{\textit{Forcing}} = \underbrace{\frac{d}{dt} \sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i}_{\textit{Accumulation}}$$

Key Points

- We can’t get molecular values at an infinitesimal point in space
- But, by integrating over a known control volume average changes inside a volume and flux over the surface can be related
- Exactly satisfaction of the conservation laws in both descriptions
- Only meaningful way to relate the two systems

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Coupling Challenges

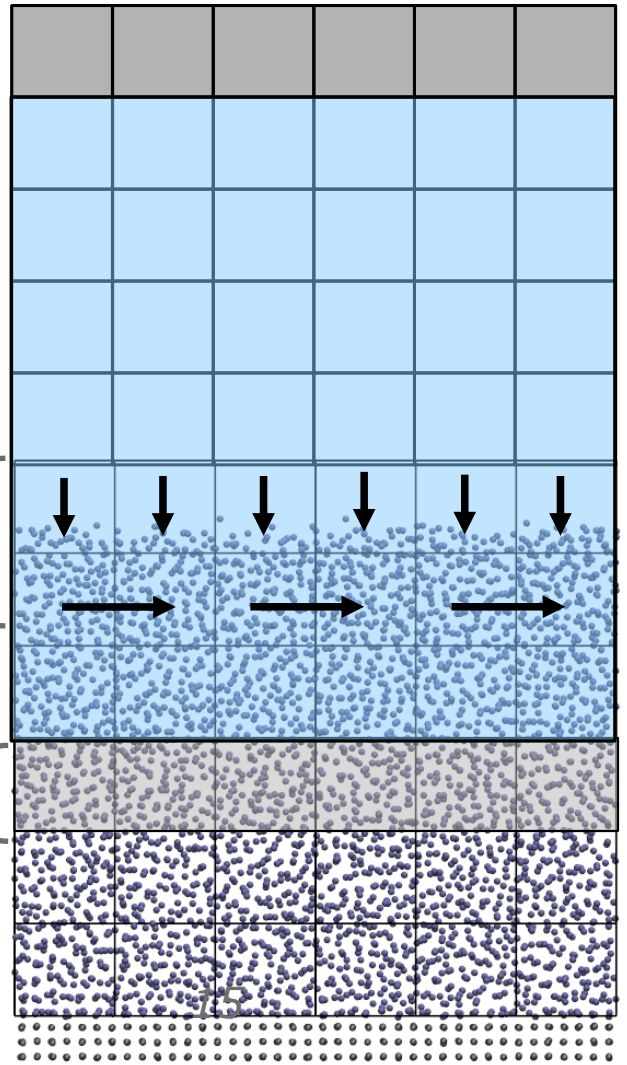
Both in Control Volume form

$$\sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i - \int_V \rho \boldsymbol{u} dV = 0$$

Consistent Framework ✓

CFD→MD Boundary condition

MD→CFD Boundary condition ✓



$$\oint_S \boldsymbol{\Pi} \cdot d\boldsymbol{S} = \sum_{i=1}^{N} m_i \boldsymbol{v_i} \boldsymbol{v_i} \cdot d\mathbf{S}_i + \frac{1}{4} \sum_{i,j}^{N} \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij}$$

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Constrained Control Volume

- **Non-unique solution**
  - Continuum field properties must specify N molecules
  - Hamilton's principle (subject to a constraint) used in the first fluids coupling scheme (O'Connell and Thompson 1995)
- **But now we want to apply a constraint localised using the control volume function**
  - CV function takes care of the localisation for us
  - Non-holonomic constraint

$$g(\boldsymbol{r}_i, \dot{\boldsymbol{r}}_i) = \sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i - \int_V \rho \boldsymbol{u} dV = 0$$

- **Gauss Principle of Least Constraint Applied**
  - Valid for any form of constraint

$$\frac{\partial}{\partial \boldsymbol{r}_{ij}} \sum_{i=1}^{N} \left[\boldsymbol{F}_i - \boldsymbol{r}_{ij}\right]^2 - \boldsymbol{\lambda} \cdot \boldsymbol{g} = 0$$

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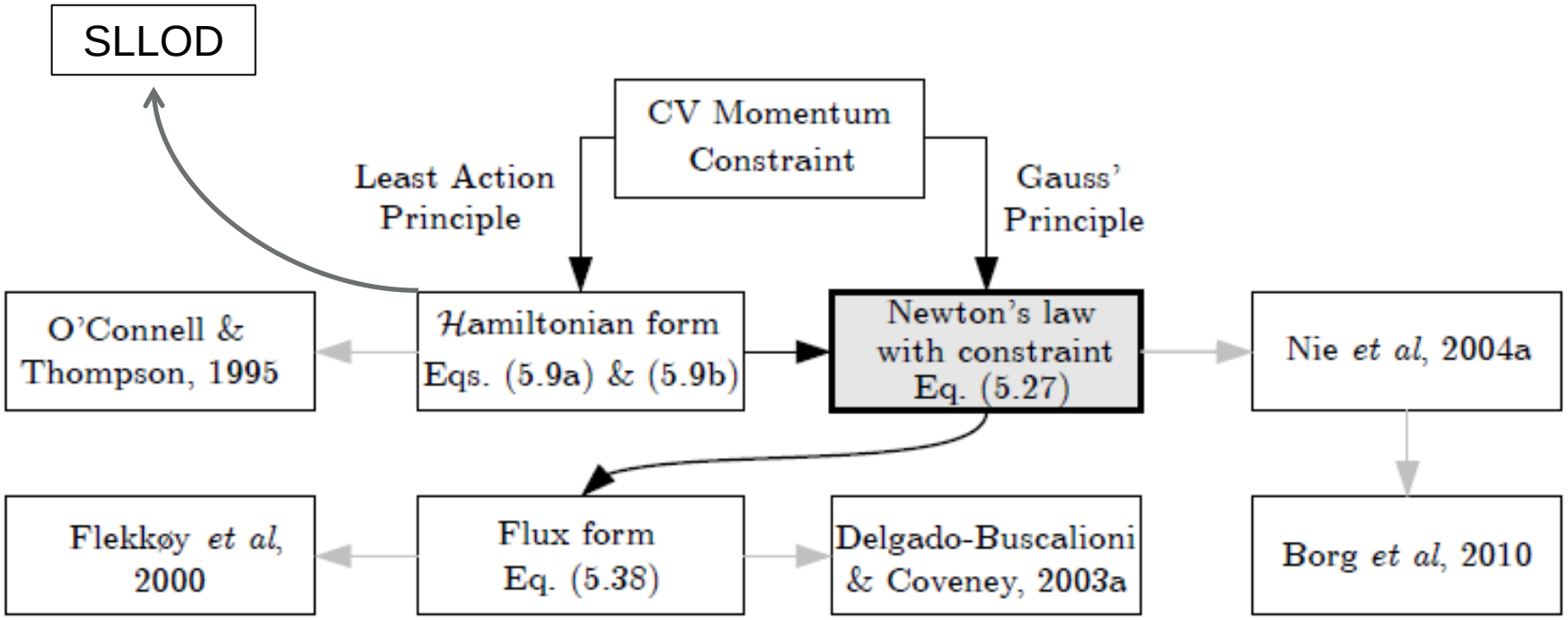
Constrained Control Volume



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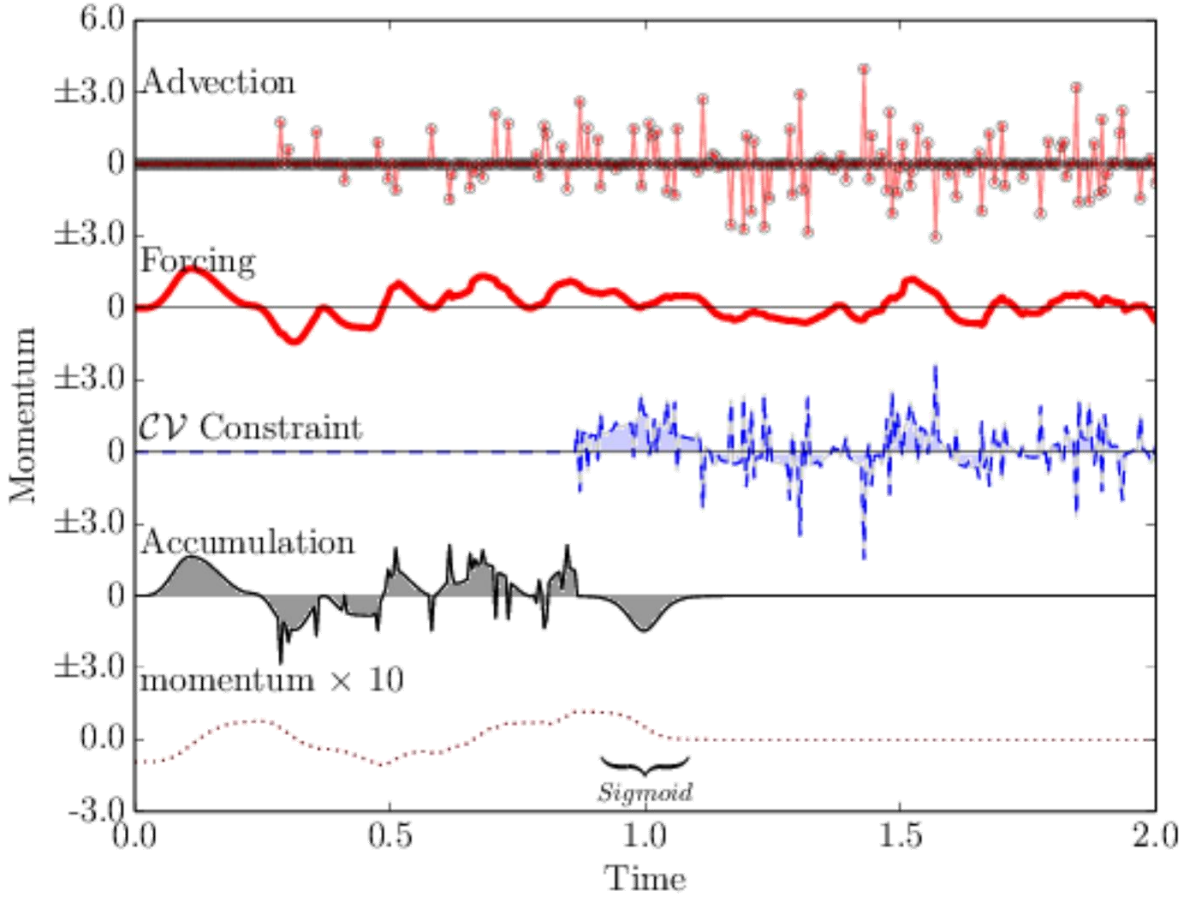
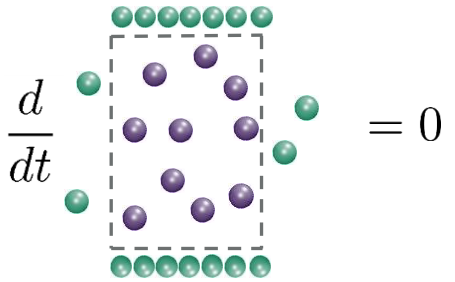
Constrained Control Volume

$$m_i\ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV + \overbrace{\sum_{n=1}^{N} m_i\dot{\boldsymbol{r}}_{\boldsymbol{n}}\dot{\boldsymbol{r}}_n\cdot d\mathbf{S}_n}^{\text{Advection}} - \overbrace{\sum_{n,m}^{N}\boldsymbol{f}_{nm}\mathbf{n}\cdot dS_{nm}}^{Forcing}\right]$$



- Zero time evolution applied
- No velocity evolution results
- Exact control of momentum using iteration to cancel both Forcing and Advection



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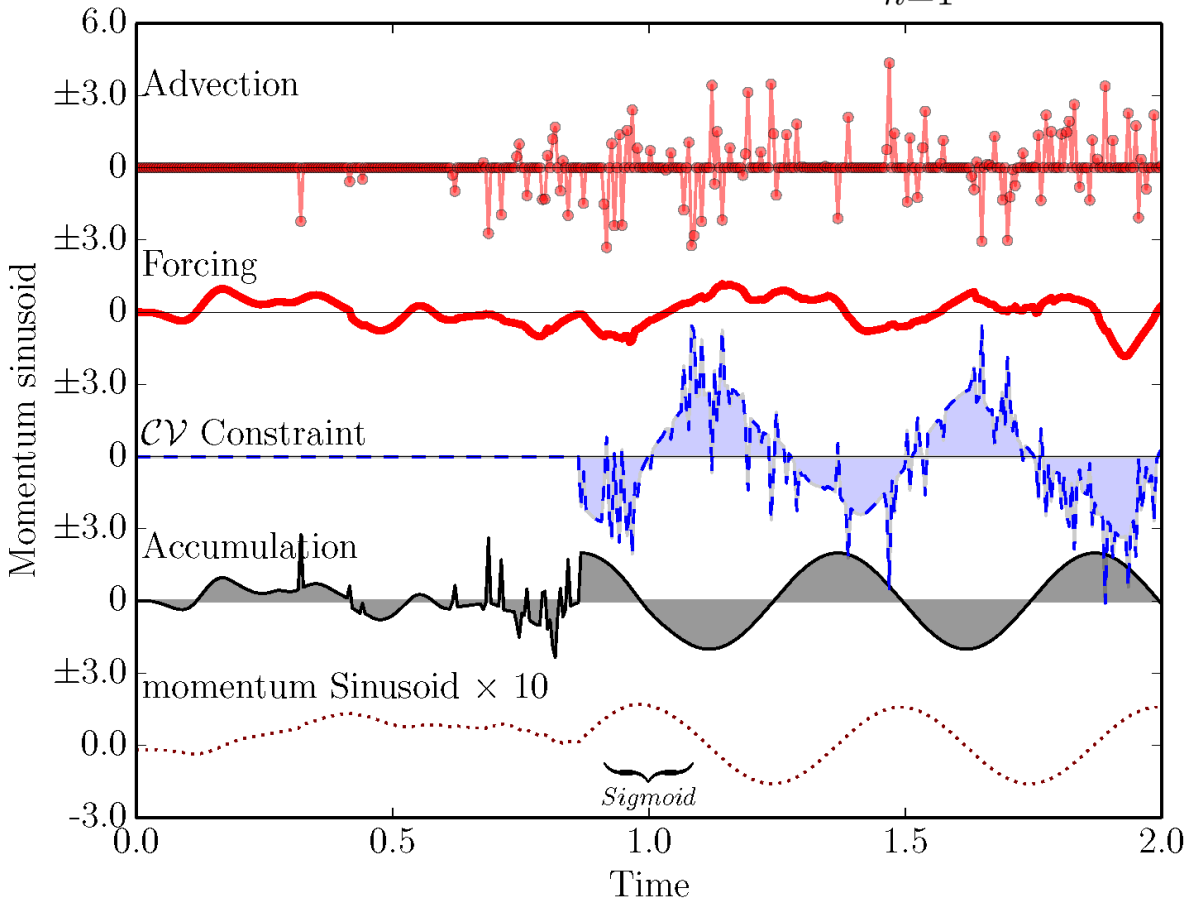
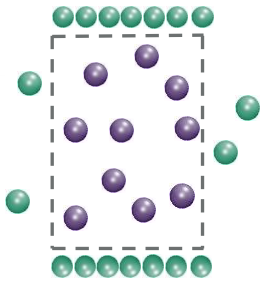
Constrained Control Volume

$$m_i\ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV + \overbrace{\sum_{n=1}^{N} m_i\dot{\boldsymbol{r}}_n\dot{\boldsymbol{r}}_n\cdot d\mathbf{S}_n}^{\text{Advection}} - \overbrace{\sum_{n,m}^{N}\boldsymbol{f}_{nm}\mathbf{n}\cdot dS_{nm}}^{Forcing}\right]$$



- Cosinusoidal time evolution applied
- Sinusoidal velocity evolution results
- Exact control of momentum using iteration to cancel both Forcing and Advection



$$\frac{d}{dt} = \frac{d}{dt}\int_V \rho\boldsymbol{u}dV$$

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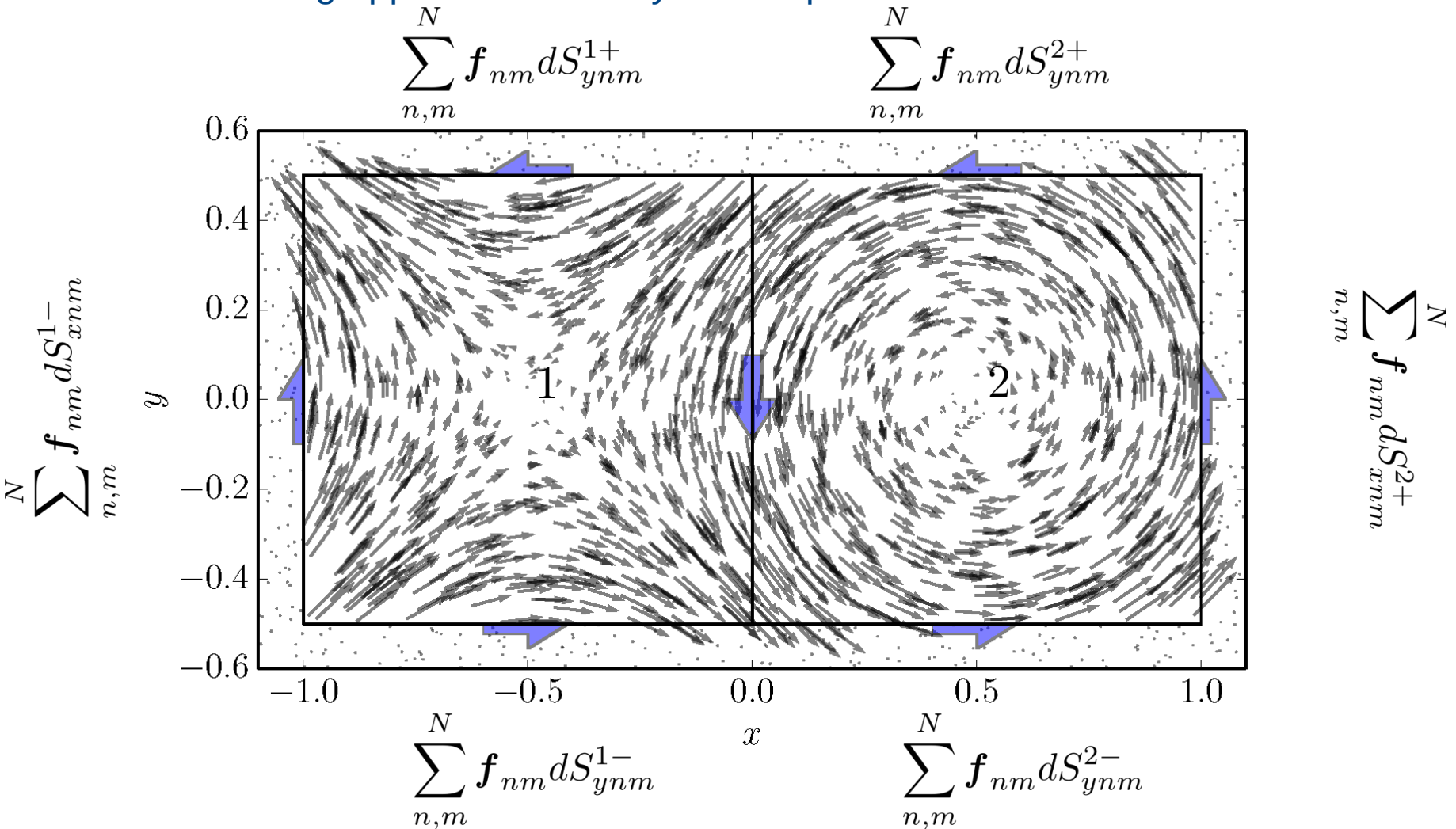
Constrained Control Volume

- Forcing applies an arbitrary 18 component 3D stress field



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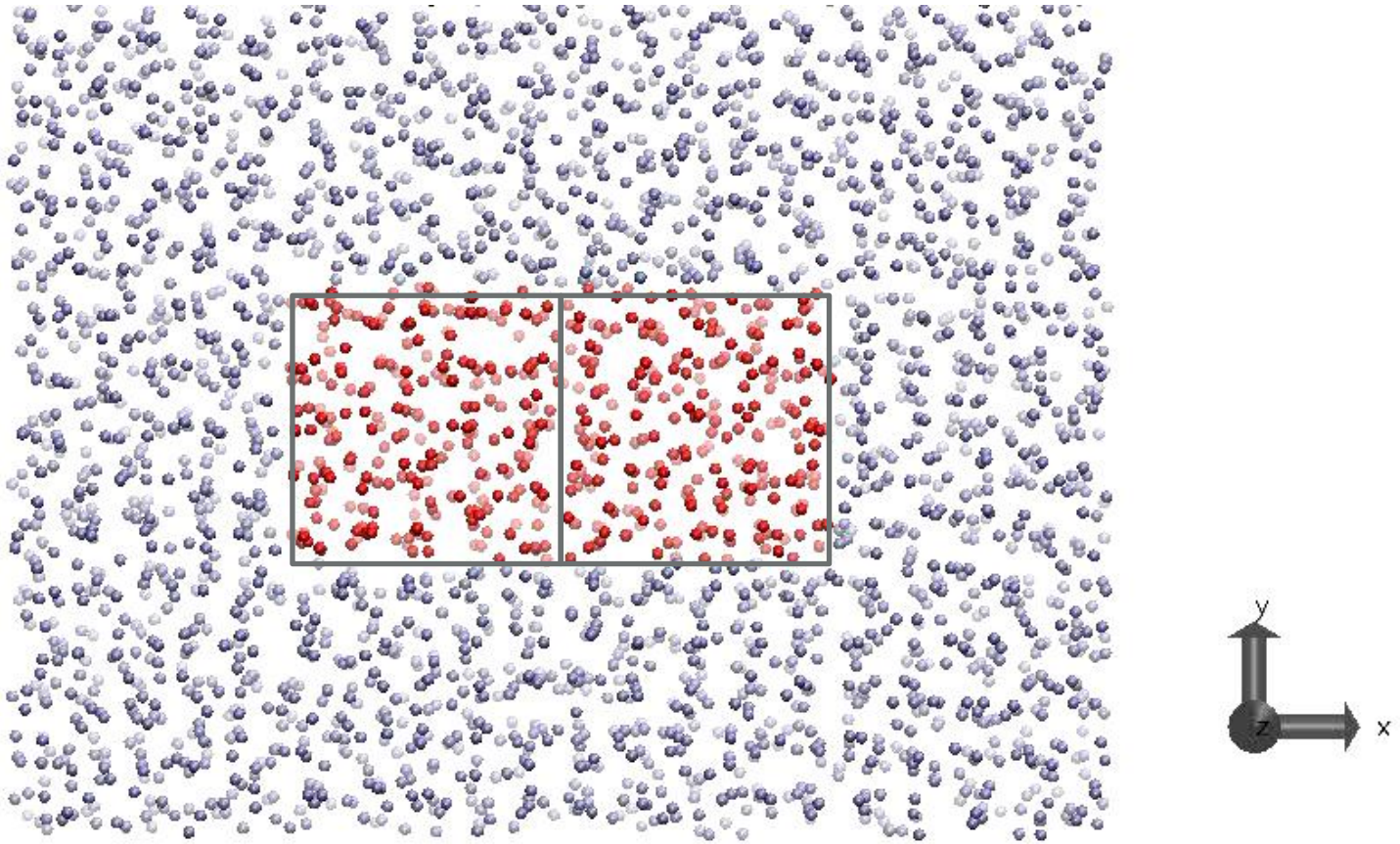
Constrained Control Volume



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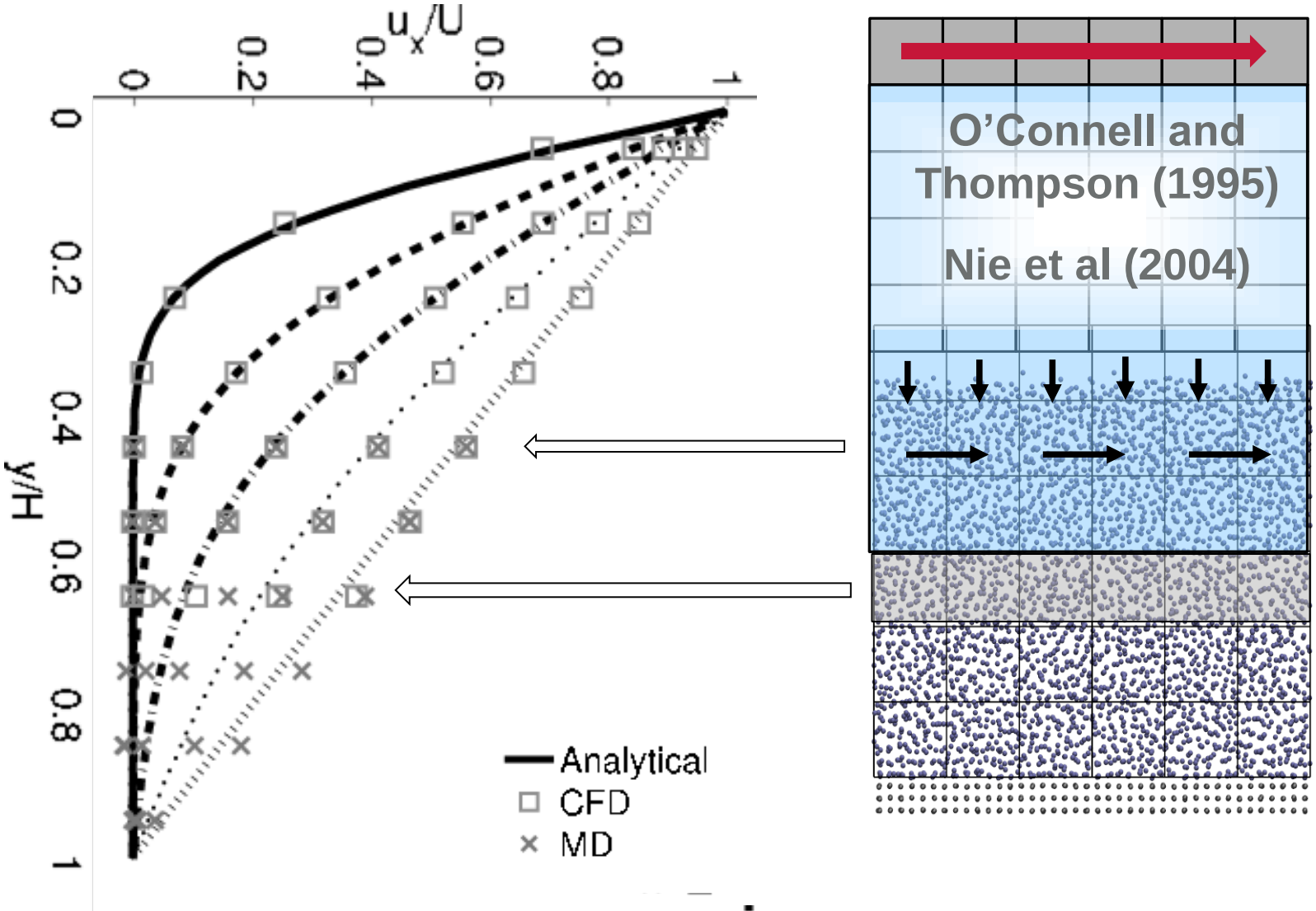
Coupling Results – Couette Flow



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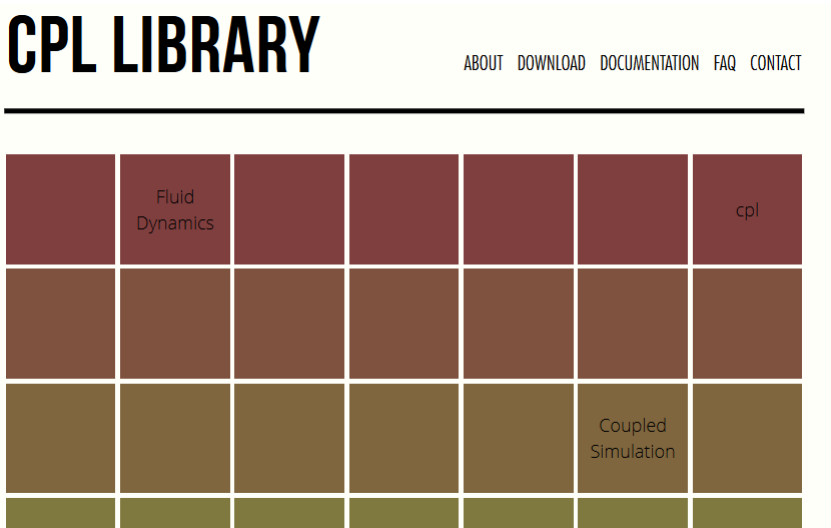
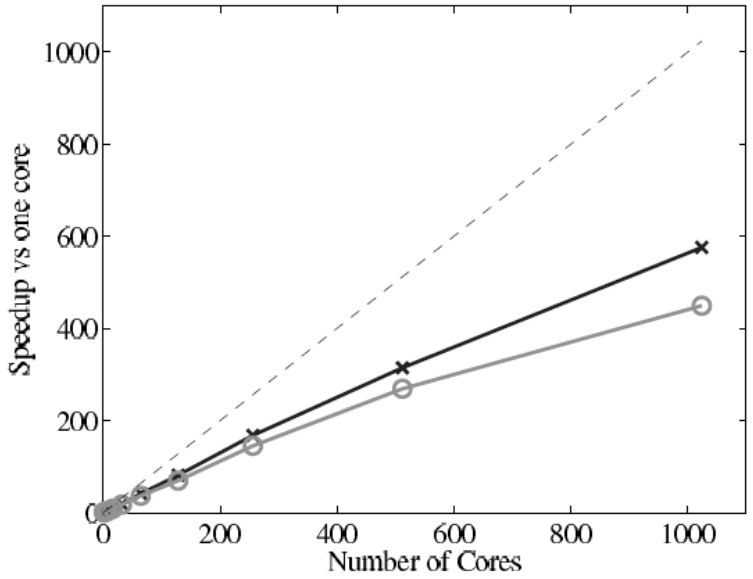
Large Scale Simulation : cpl-library

- Open Source (www.cpl-library.org) Fortran, c, c++ and python bindings
- Designed to facilitate the linking of massively parallel codes with minimal impact on performance of each code
- Continuous integrated build testing, no external dependencies beyond standard packages and suite of python unit tests
- Minimal set of function based on MPI to remove learning curve and lower barrier to entry for coupled simulation





(a) Parallel speedup of the MD solver only (×), coupled code (○) against the ideal speedup (——)

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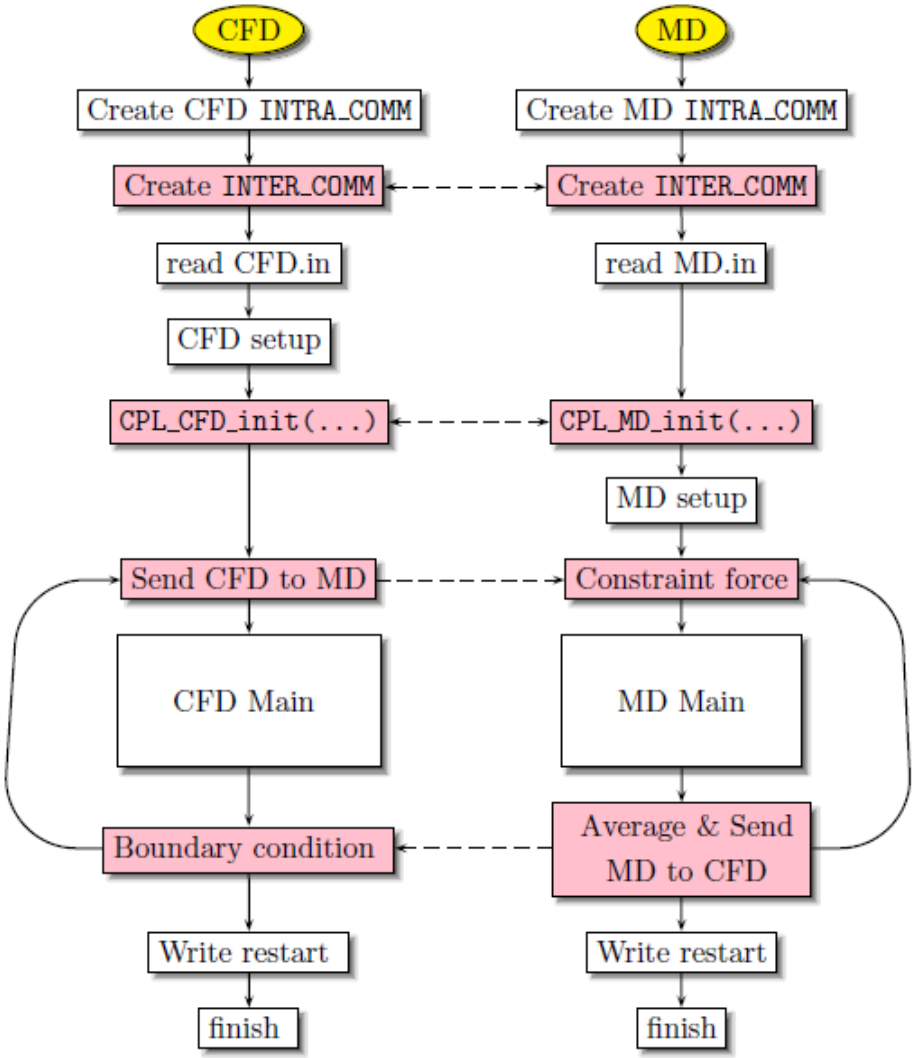
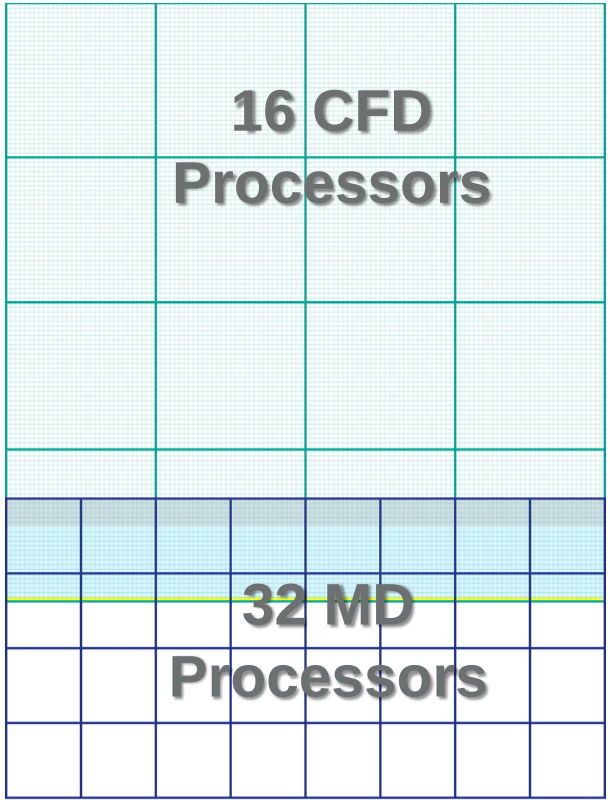
Large Scale Simulation : cpl-library



mpiexec –n 32./md.exe : -n 16 ./cfd.exe



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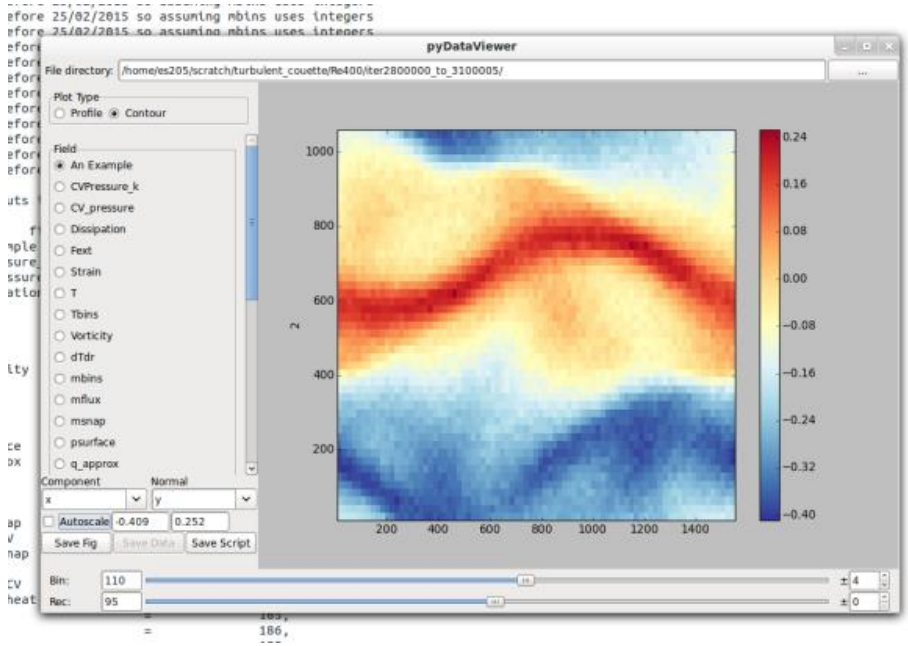
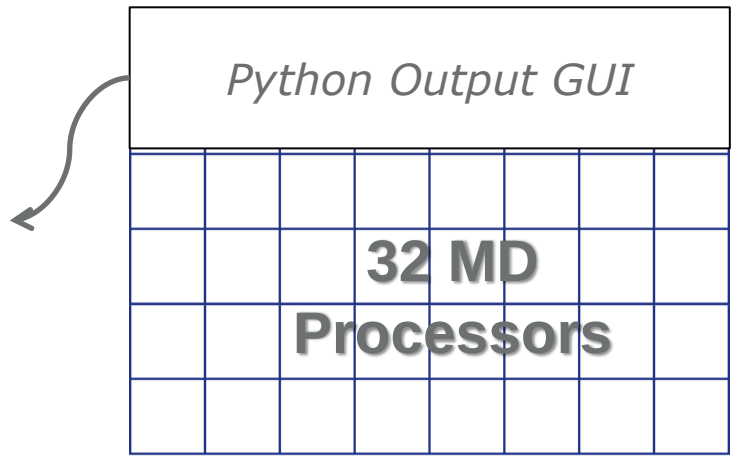
Large Scale Simulation : cpl-library

- Dummy python test routines to plot grid or display coupled exchange to encourage the tested modular development of codes
- Interfaces to LAMMPS and OpenFOAM provided with the library
- Works for domain decomposition overlap region and fully overlapping case to facilitate HMM as a possible extension??
- Aim is to allow large scale coupled MD and CFD simulation





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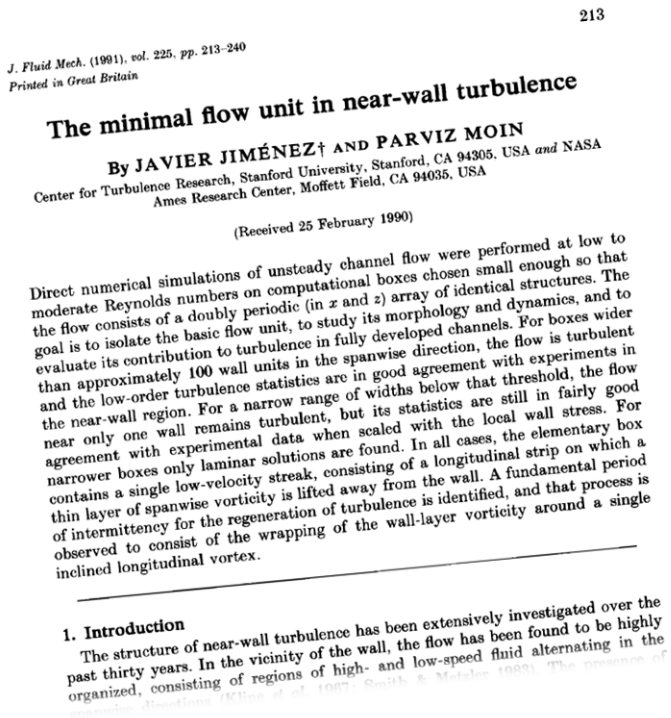
The Minimum Scale of Turbulence

- The minimum domain size required to sustain turbulent flow

Poiseuille flow, Re ≈ 2000



213

J. Fluid Mech. (1991), vol. 225, pp. 213–240
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The minimal flow unit in near-wall turbulence

By JAVIER JIMÉNEZ† AND PARVIZ MOIN
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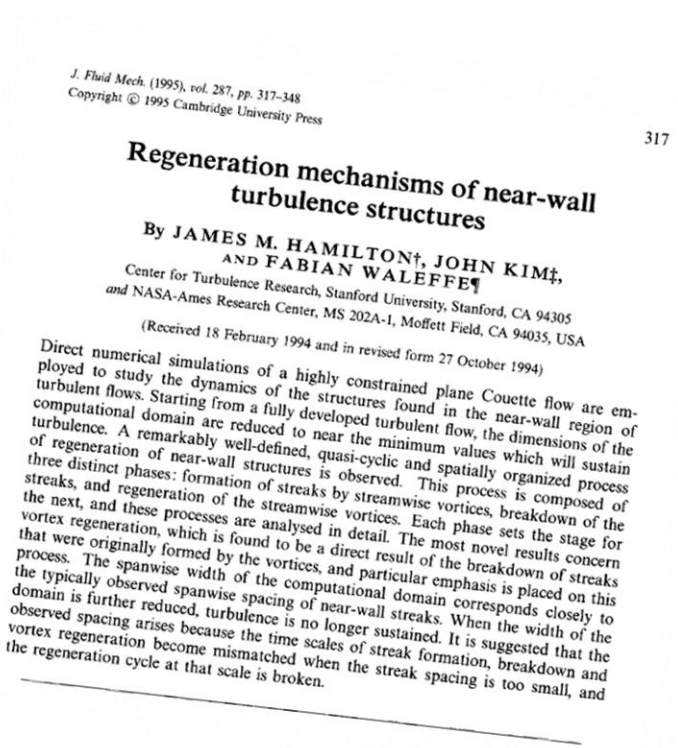
(Received 25 February 1990)

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¶
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(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.

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Literature On the Minimum Flow Unit

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

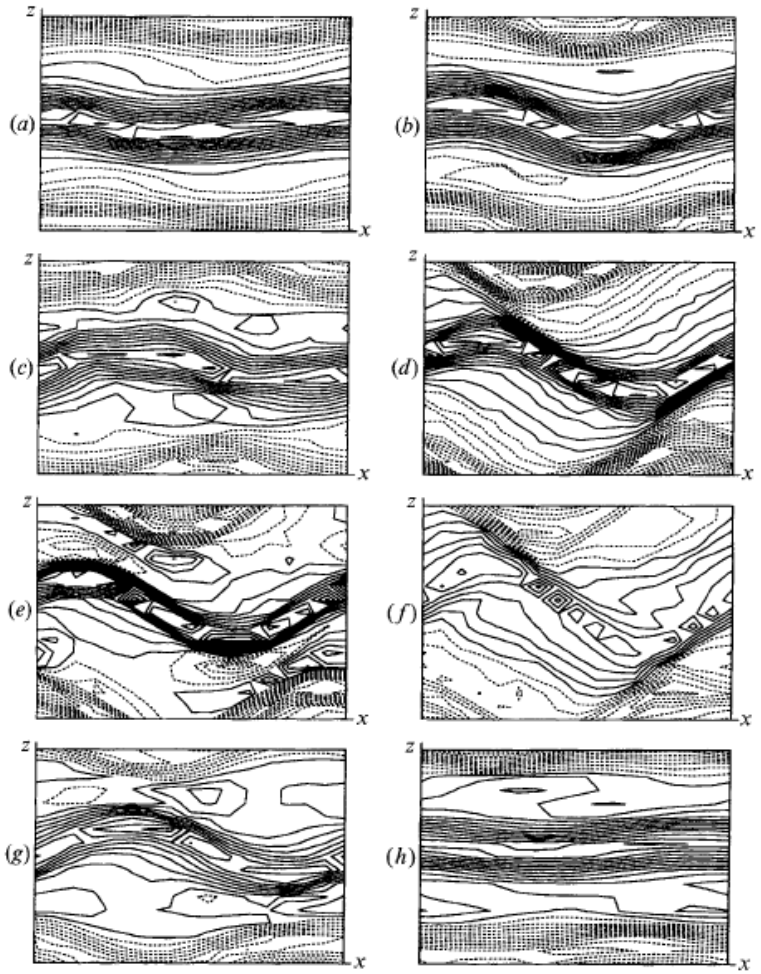

FIGURE 2. Iso-contours of u-velocity in the (x, z)-plane centred between the walls; solid contours positive, dashed contours negative. Contour interval 0.032. (*a*) $t = 757.5$, (*b*) $t = 764.8$, (*c*) $t = 772.0$, (*d*) $t = 777.8$, (*e*) $t = 783.0$, (*f*) $t = 794.1$, (*g*) $t = 808.2$, (*h*) $t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

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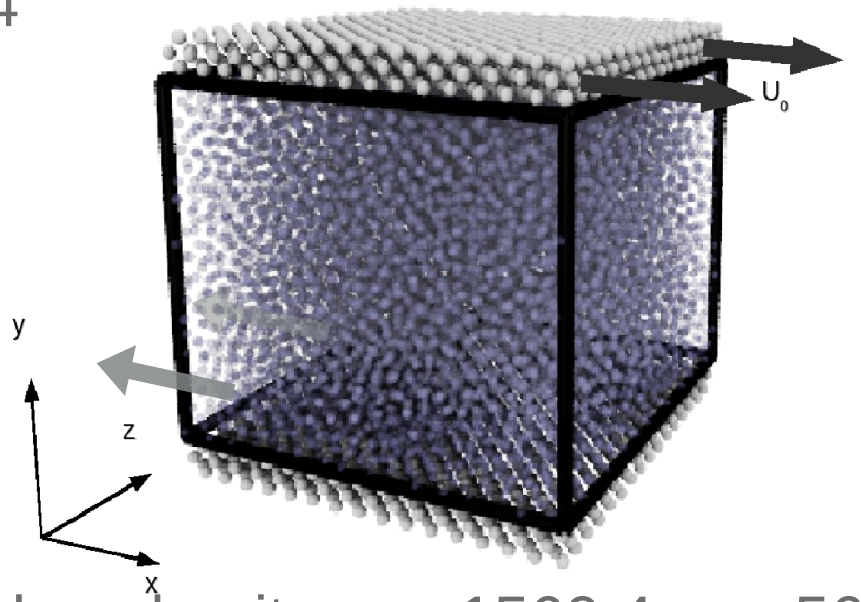
Domain Overview

- Simulation Setup
  - Sliding top and bottom walls in y with u = ± 1
  - Periodic in x and z directions
  - Walls are tethered, sliding molecules with NH thermostat with T=0.4



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

Molecular Turbulent Couette Flow

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

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

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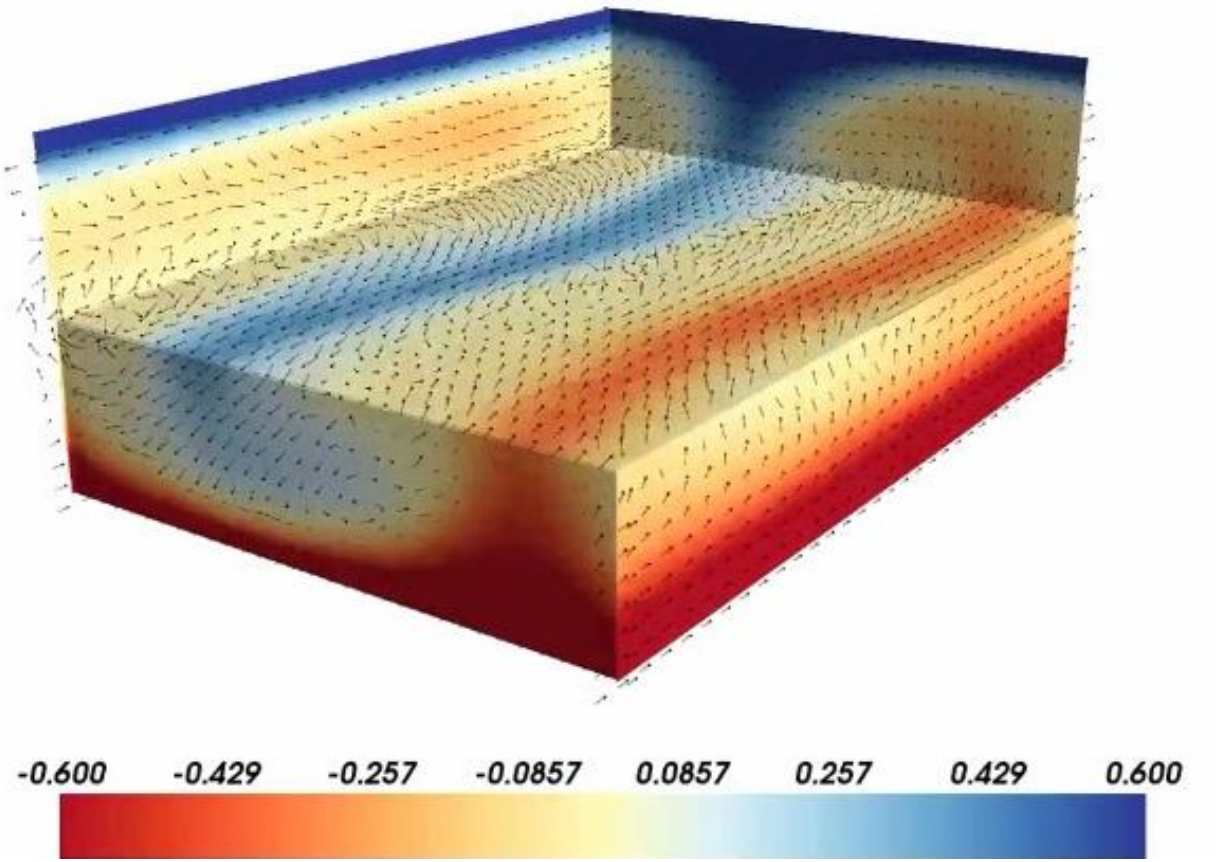
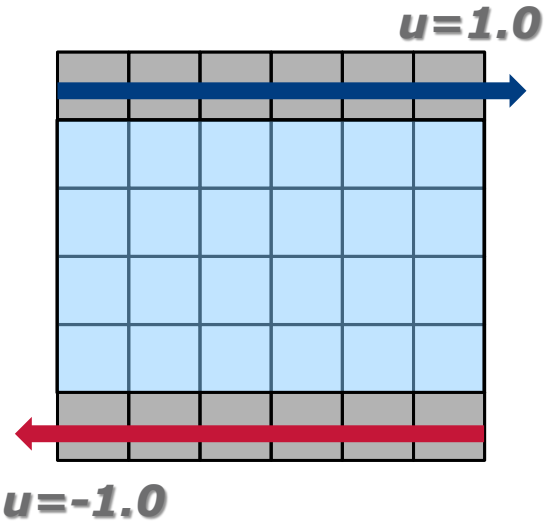
From Smith E, under review in Phys. Fluid (2015) http://arxiv.org/pdf/1508.01163v1.pdf

Molecular Simulation of Minimal Channel Flow

- Vortex breakdown and reformation





- Simulation time
  - MD 6 months on 360 cores supercomputer
  - CFD overnight on a laptop

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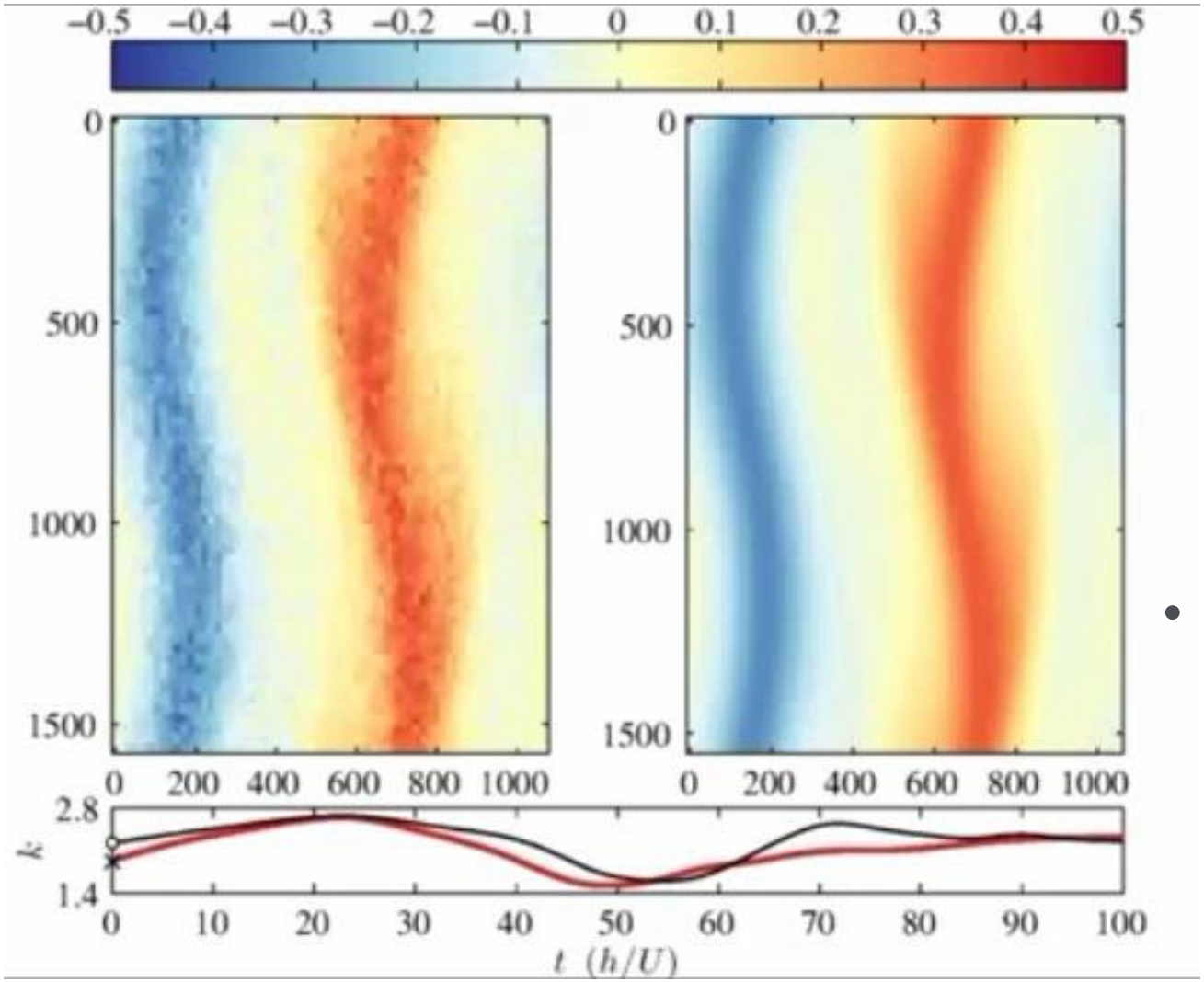
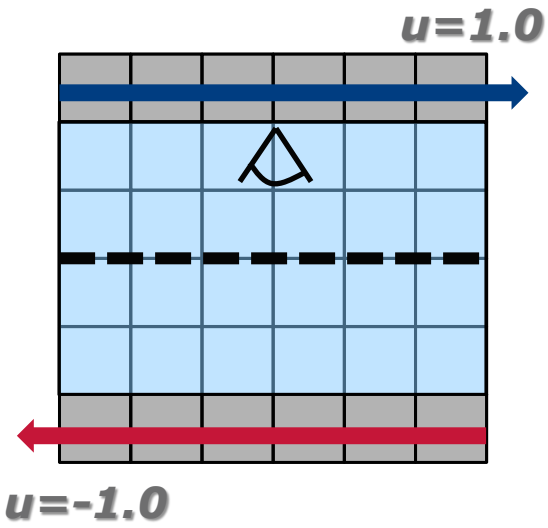
From Smith E, under review in Phys. Fluid (2015)
http://arxiv.org/pdf/1508.01163v1.pdf

Molecular Simulation of Minimal Channel Flow





- Simulation time
  - MD 6 months on 360 cores supercomputer
  - CFD overnight on a laptop

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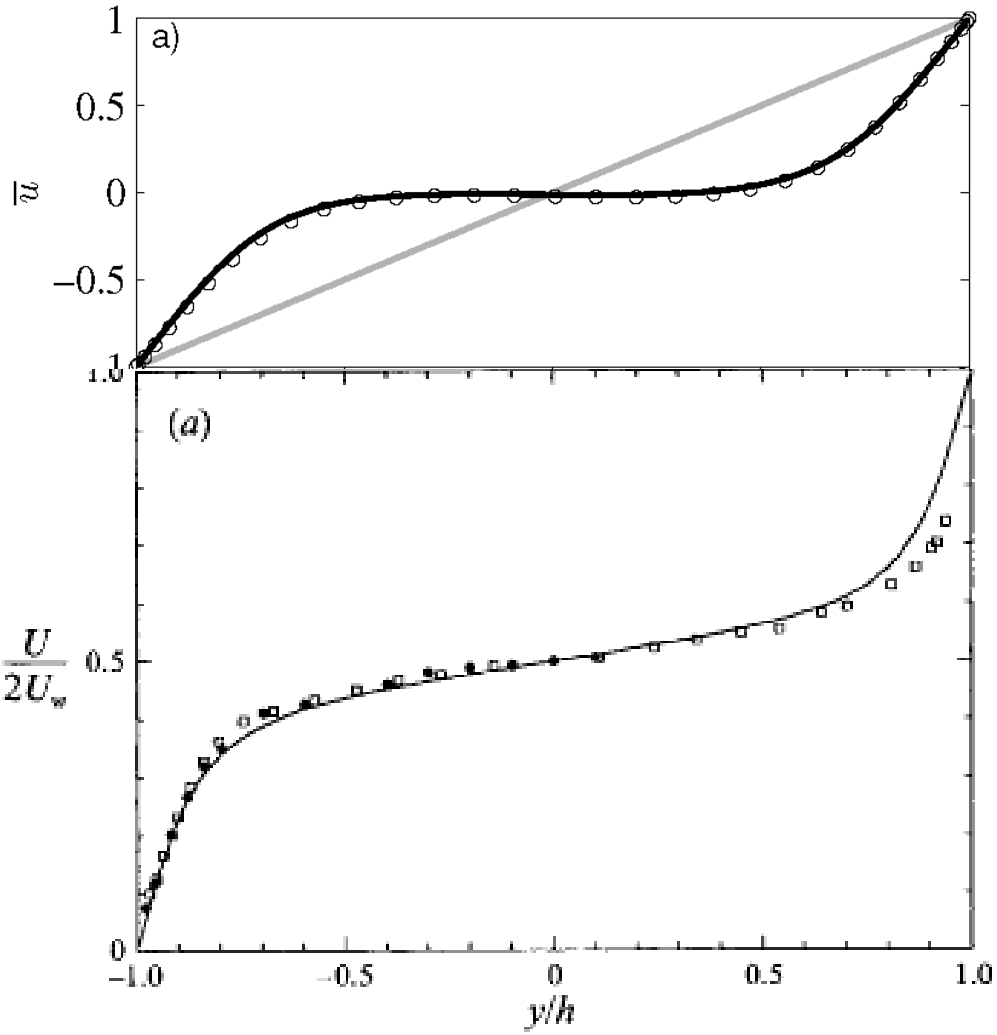
Statistical Results

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



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

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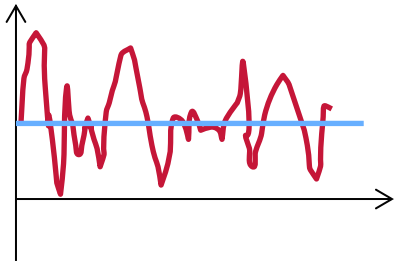
Reynolds Decomposition

- Split the motion into time average and fluctuating part



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

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

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

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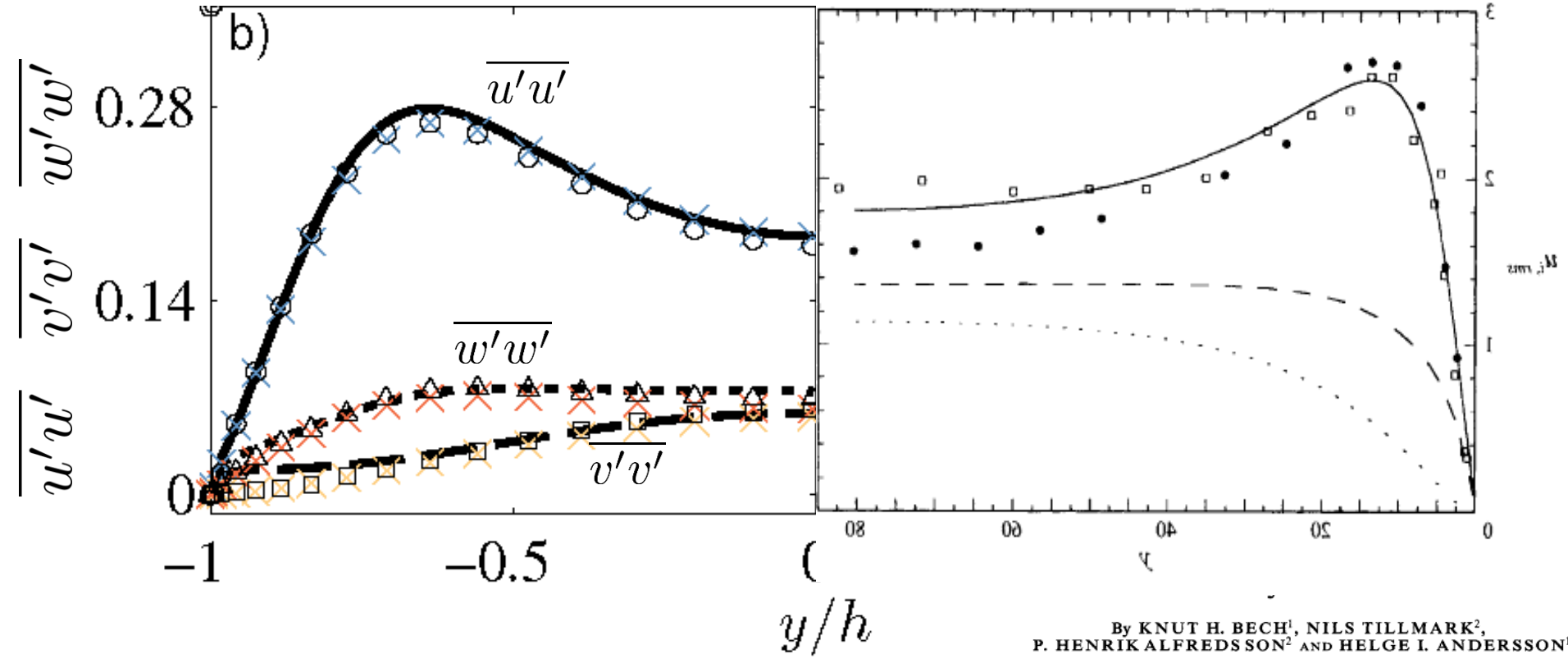
Statistical Results

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



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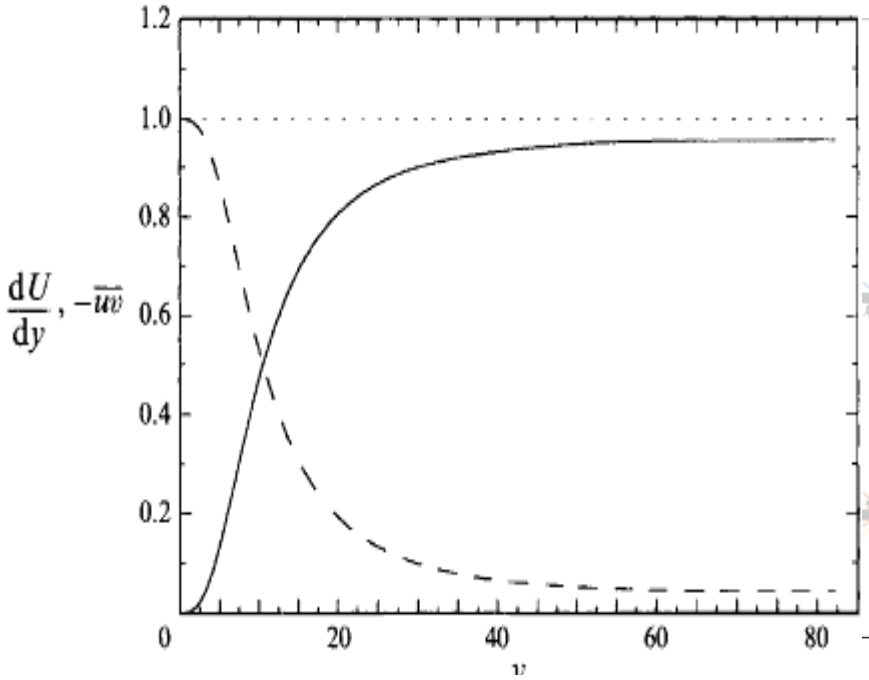
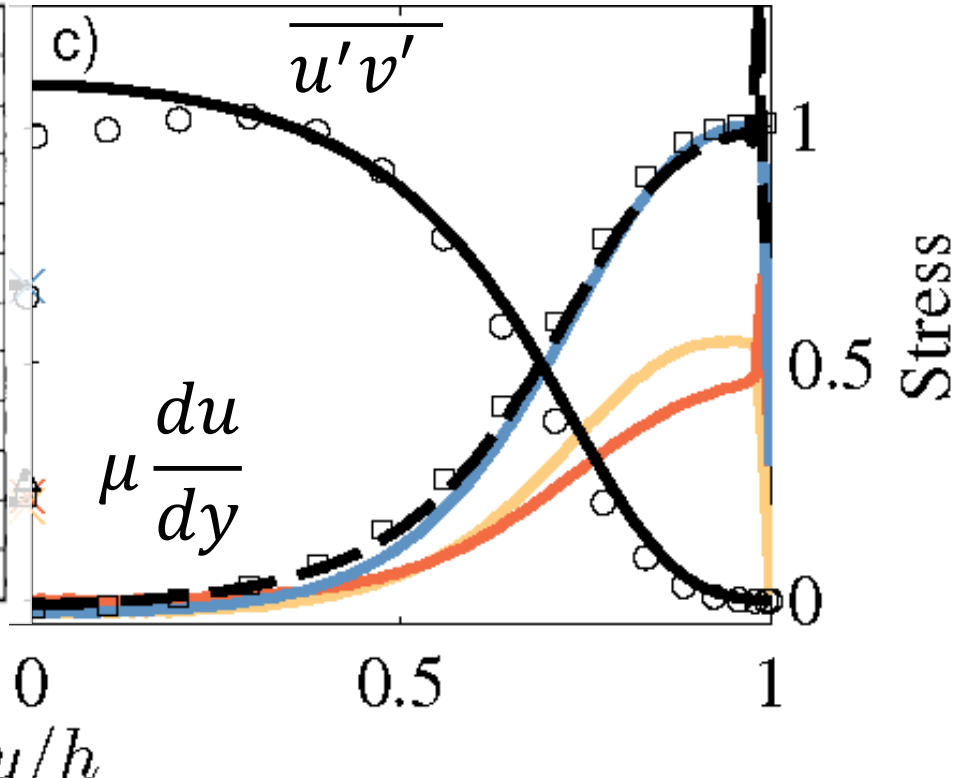
Turbulent Stresses or Molecular Stresses

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



An investigation of turbulent plane Couette flow at low Reynolds numbers

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



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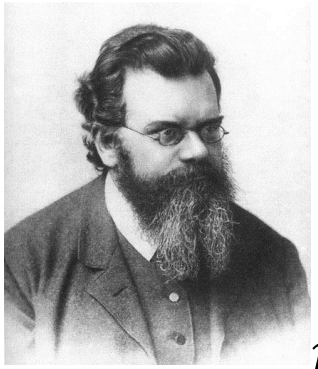
Pressure Tensor in an MD Simulation

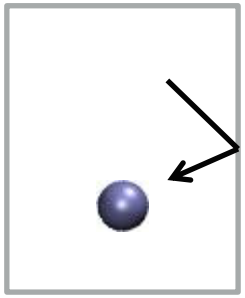
- Pressure definition in a dense molecular system has a long history
  - Virial form given by Rudolf Clausius in 1870
  - Irving and Kirkwood (1950) gave a full localised description,
  - Expressed as forces/fluxes over a plane (Todd, Evans and Daivis,1995)

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

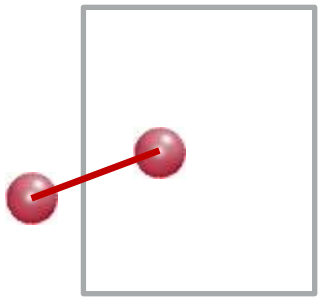
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





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



Configurational part

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

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Same Concept, Different Scales

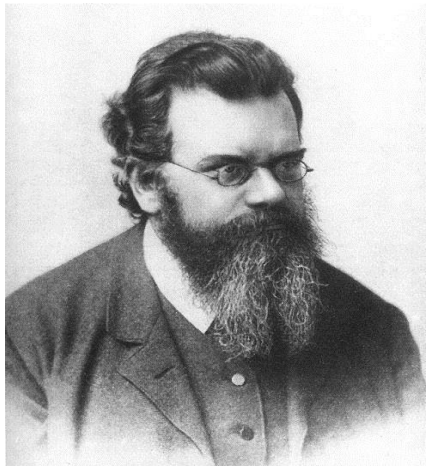
- Reynolds Decomposition

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

- Peculiar velocity

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

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



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

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

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

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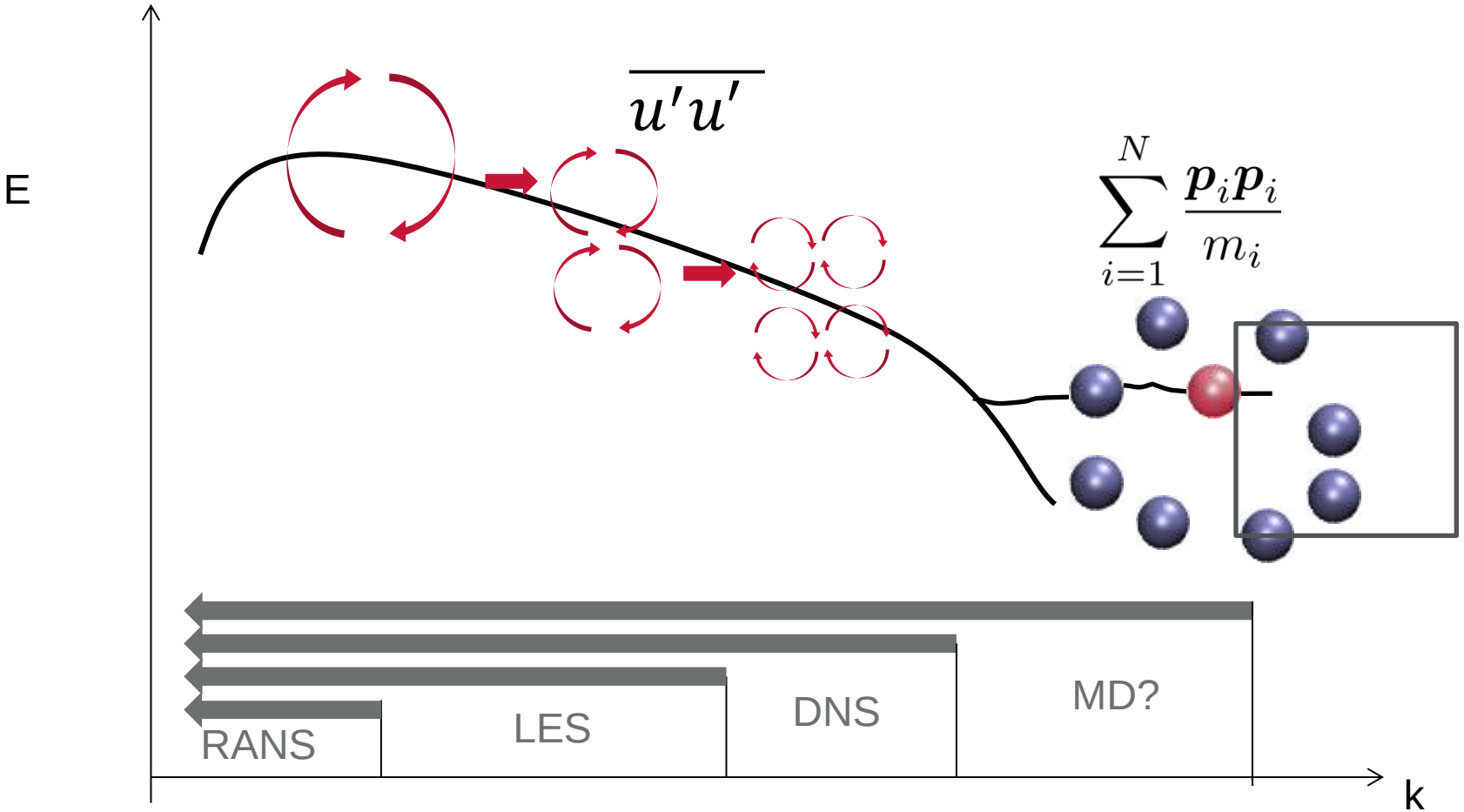
Is Reynolds Stress just Kinetic Pressure?

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



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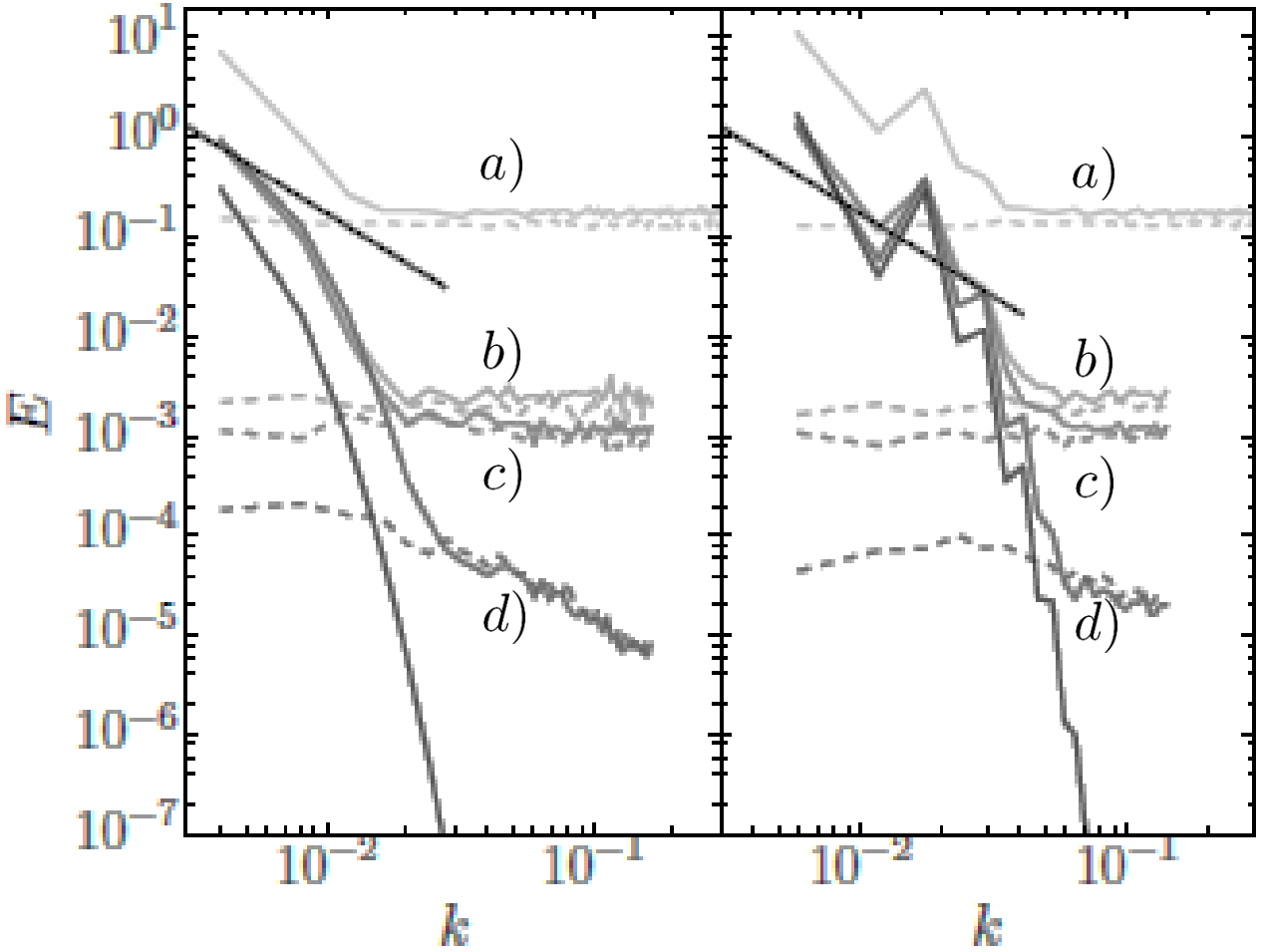
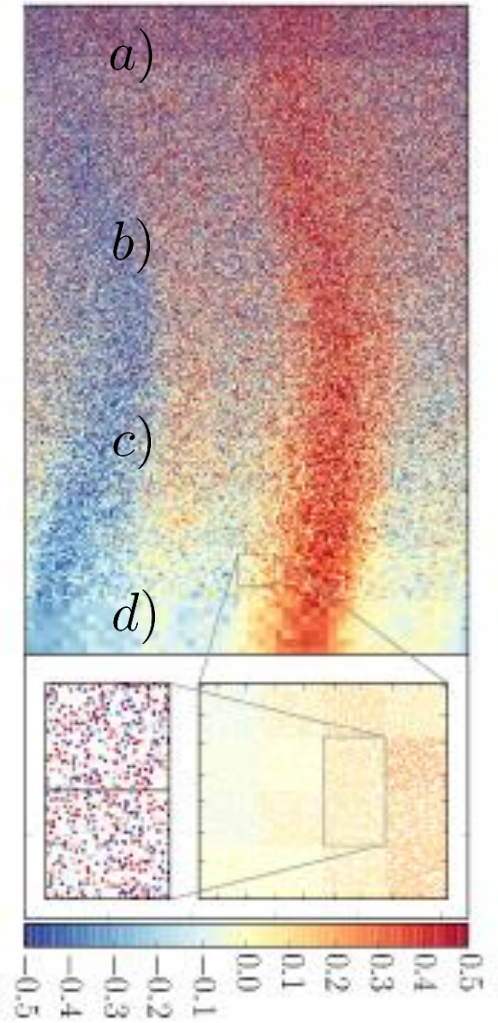
Energy Spectra

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	$84 \times 66 \times 50$





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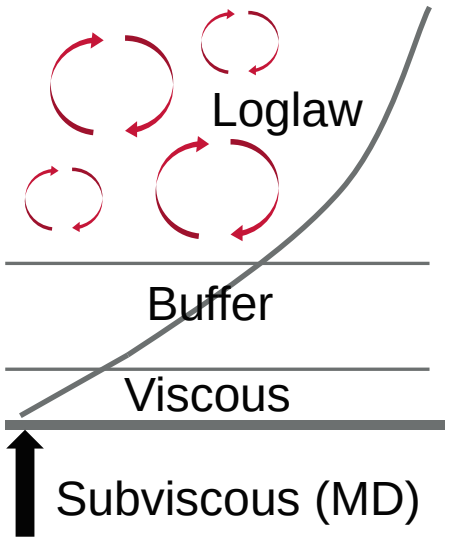
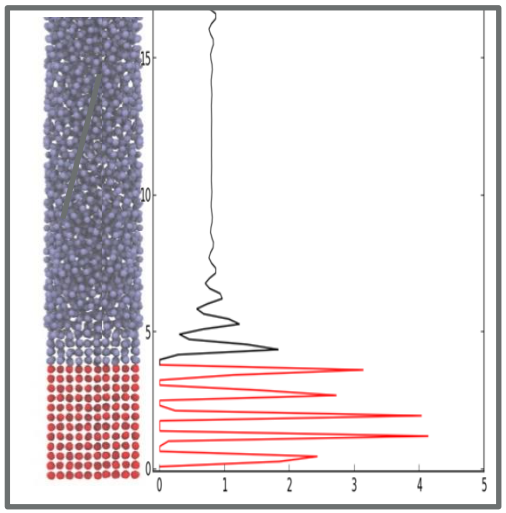
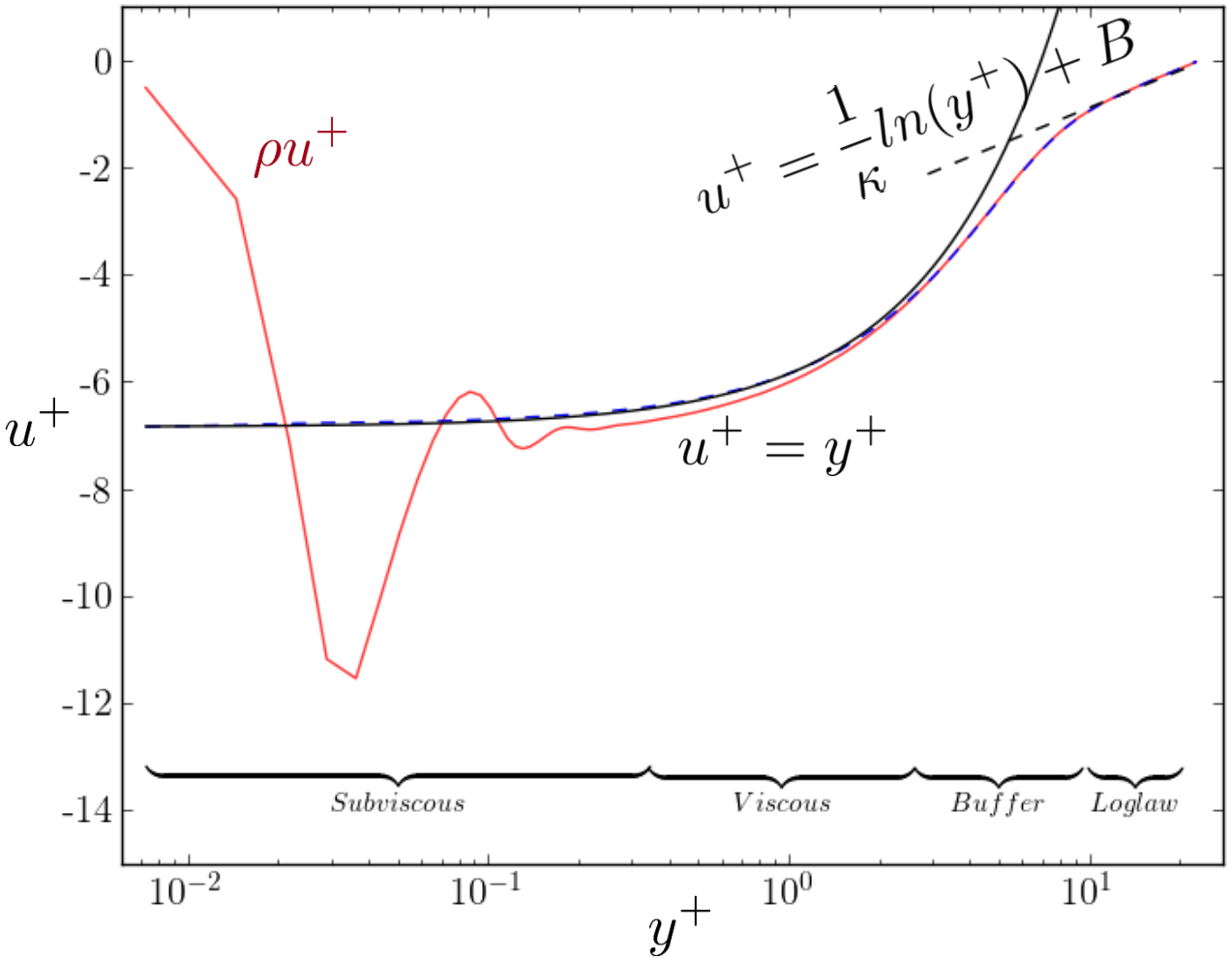
Law of the wall







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Summary

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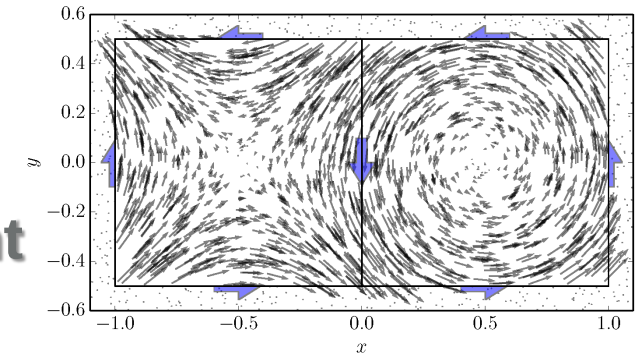
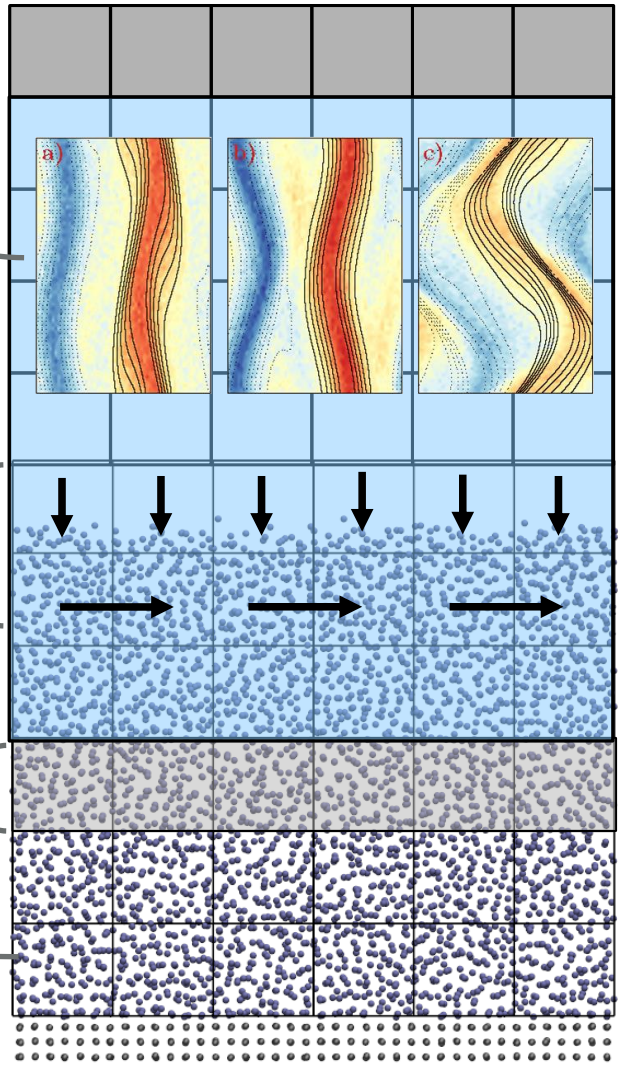
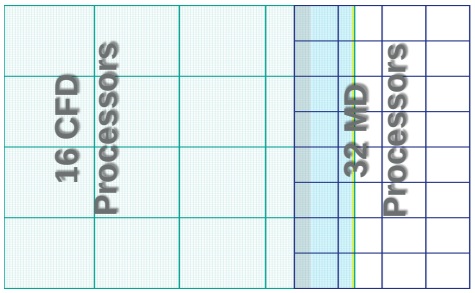
Control Volume Constraint







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Overview

- Coupled Simulation
- Toward a consistent framework
- Constrained Dynamics
- Large scale computations and cpl-library
- Turbulent Molecular Dynamics

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Acknowledgements and Questions

Thank you, Any Questions

- Coupling theory work with David Heyes, Daniele Dini and Tamer Zaki
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