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Direct Coupling of Computational Fluid Dynamics and Molecular Dynamics: Conservation, Computation and Timesteps

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Overview

- Introduction to Molecular Dynamics, Continuum Fluid Dynamics and Coupling
- Some Work on the Derivation of a Conservative Coupling Schemes
- Coupling Software Development

Computational Fluid Dynamics

- Assumed continuous at every point in space
  - Mass Conservation

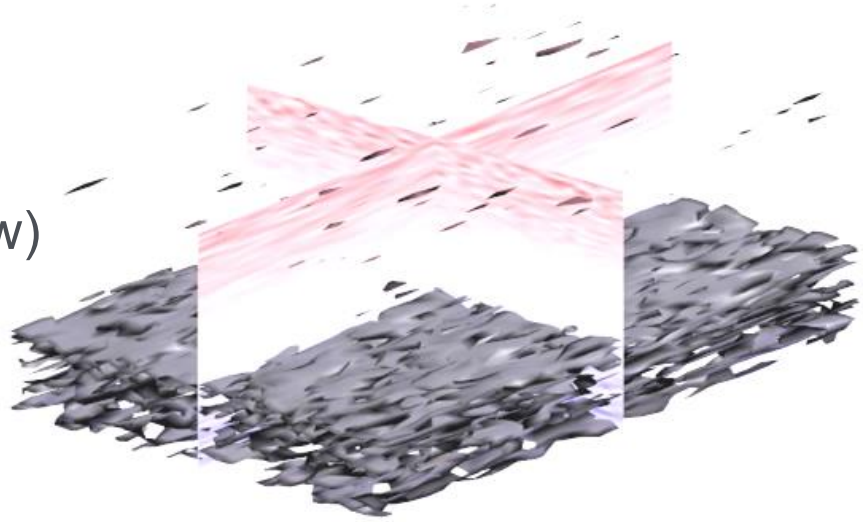
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - Momentum Balance (Newton's Law)

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

  - Energy Conservation

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



Direct Numerical Simulation of
Turbulent Couette Flow

Computational Fluid Dynamics

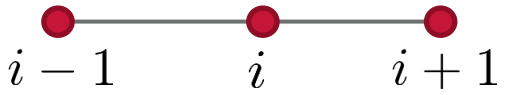
- The Navier-Stokes Equation

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

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

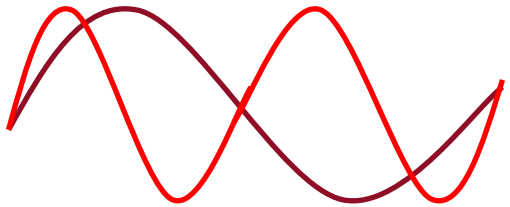
- Finite Difference Method

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



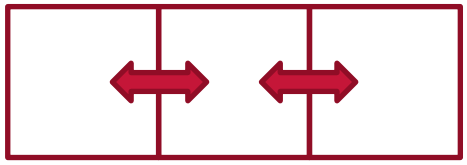
- Spectral Methods

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



- Finite Volume (0th order element) Method

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



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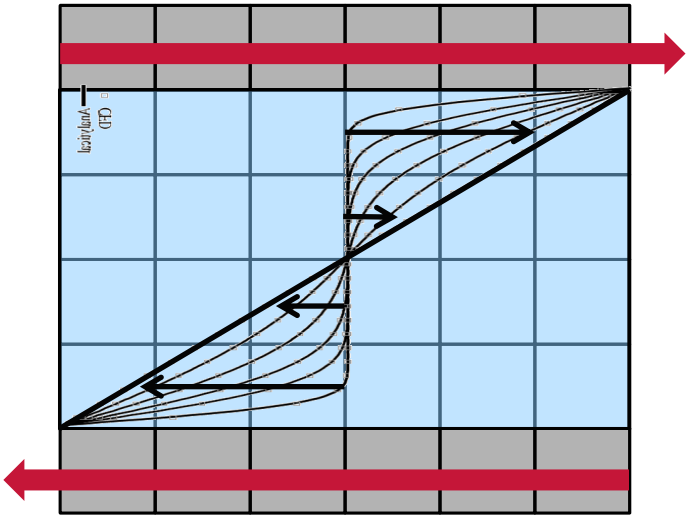
Computational Fluid Dynamics

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



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

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
  - Scaling argument applied to any scale
- Is there a minimum?
  - Travis et al (1997) single phase valid down to nanometers
  - Theodorakis, Muller, Craster & Matar (2015) not in droplets
  - Local thermodynamic equilibrium vs. hydrodynamic scales
  - Knudsen Number

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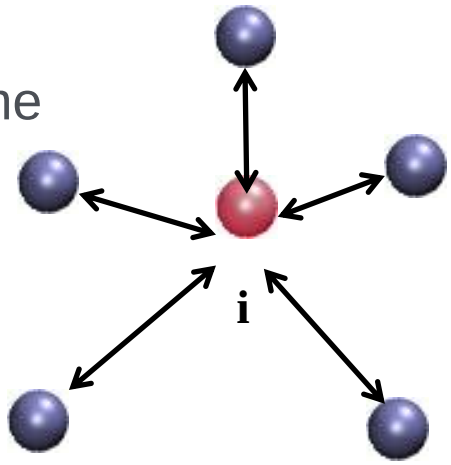
Molecular Dynamics

Discrete molecules in continuous space

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

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



Acceleration obtained from forces

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

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

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

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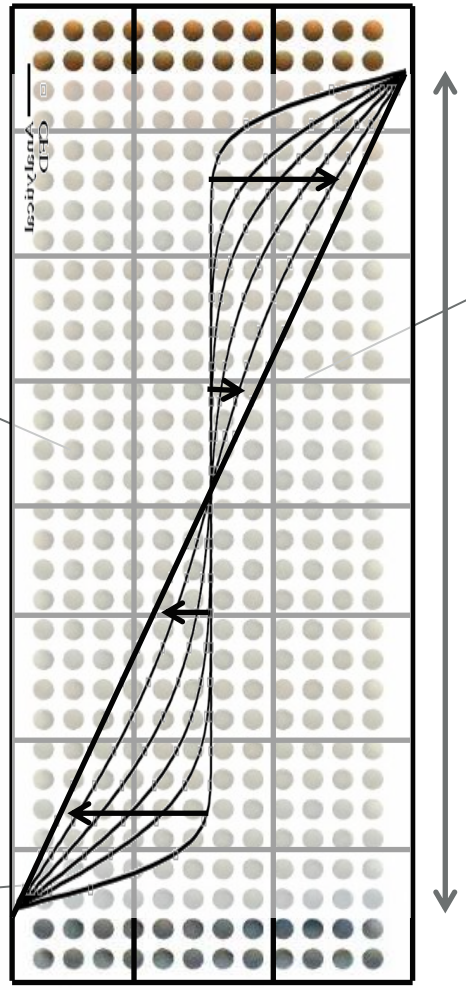
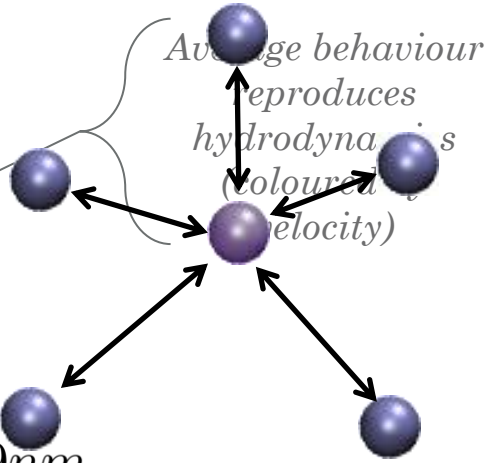
Molecular Dynamics

Liquid structure causes viscosity



Stick-slip near walls



$H \approx 9nm$

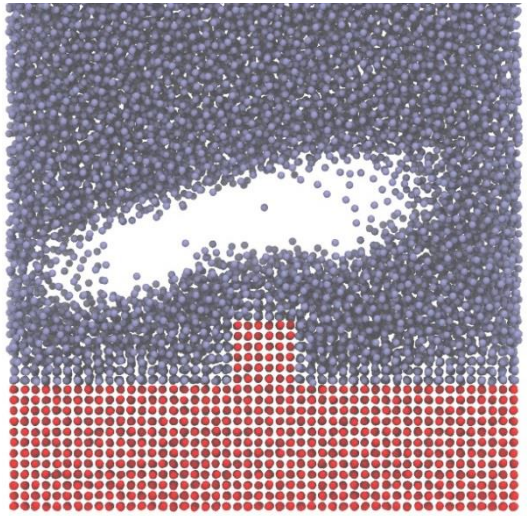
Reynolds Number

$Re \approx 15$

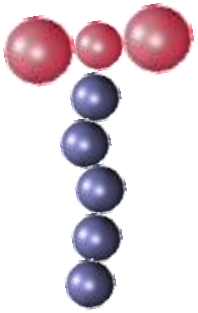
with

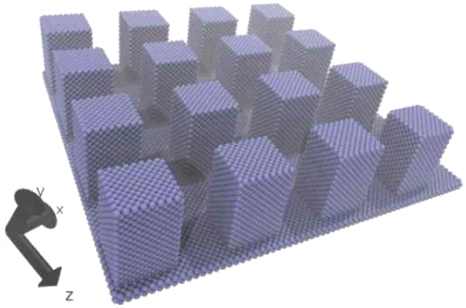
4096 molecules

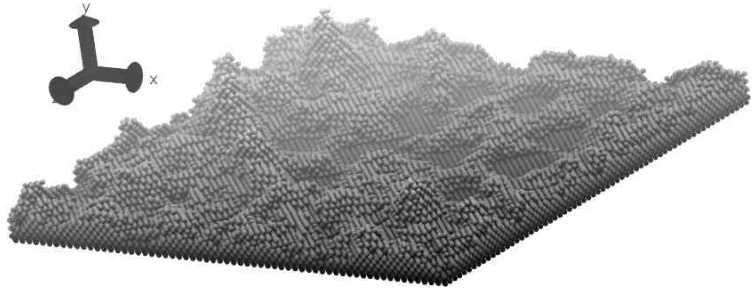
Molecular Dynamics

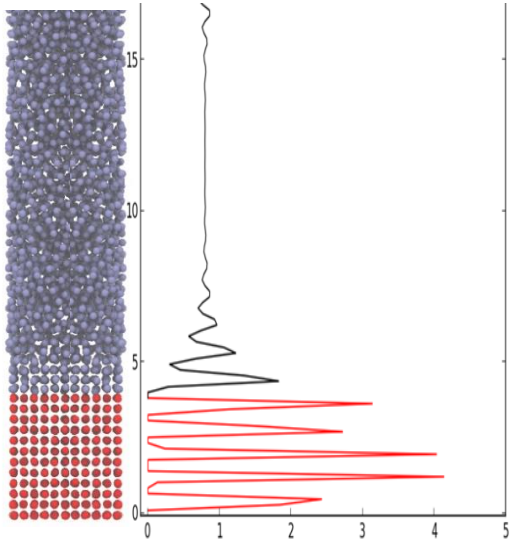


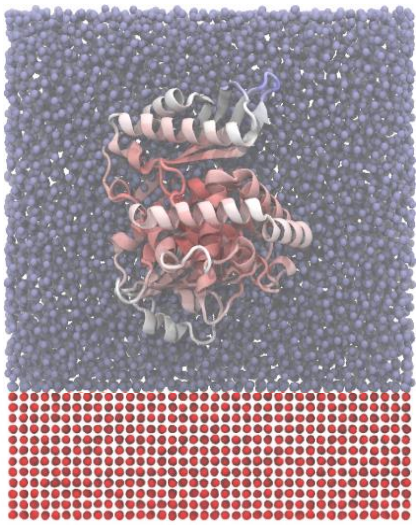
Superspreading Surfactant, e.g. Silwet-L77











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Coupling Overview

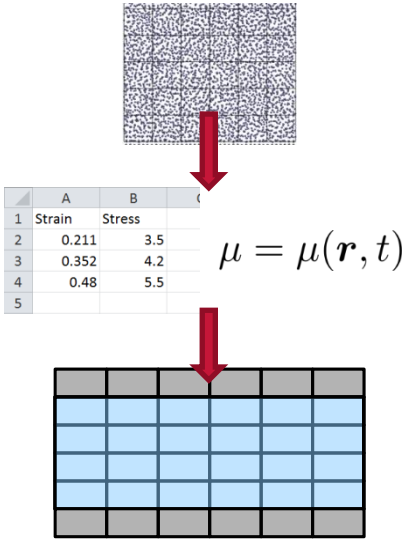
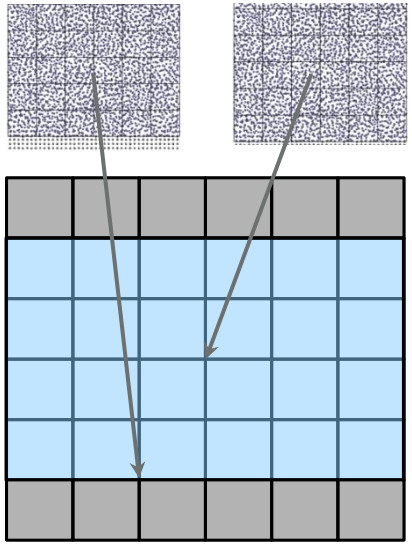


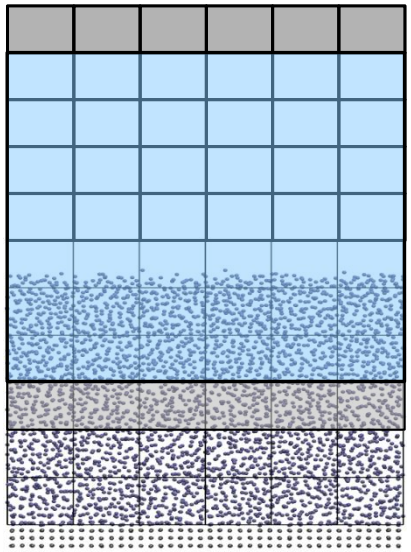
Table Lookup or Coefficients

MD parameter study stored in table and CFD uses data



Embedded Models (HMM)

MD – embedded in a CFD simulation



Domain Decomposition

MD –CFD linked along an interface

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Coupling Assumptions

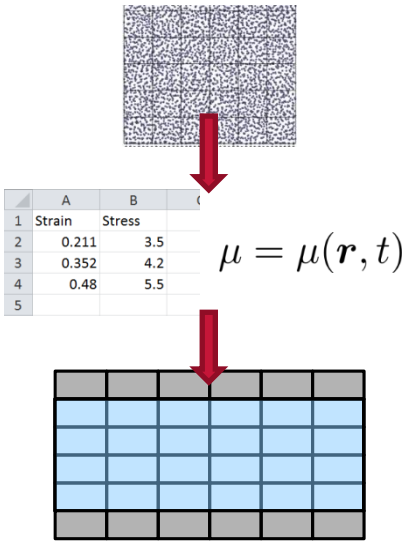


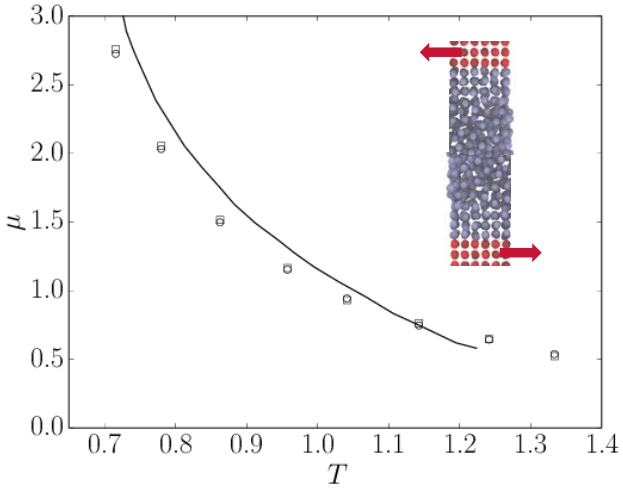
Table Lookup or Coefficients

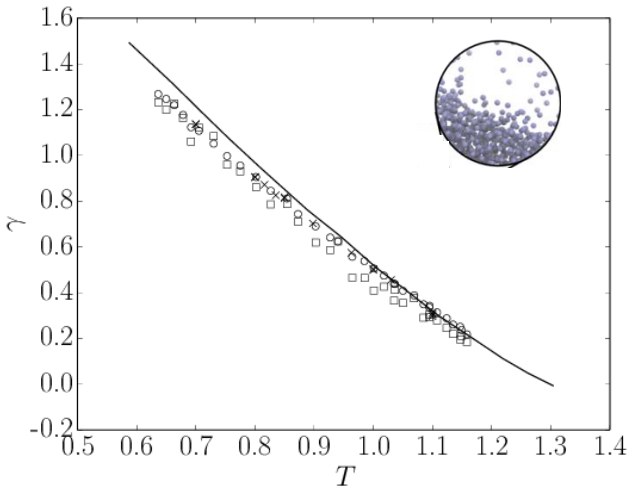
MD parameter study stored in table and CFD uses data

Essence of science get a relationship between e.g. stress and strain with MD simply a cheap experiment

Assumes validity of MD as representative for larger scale models (Similitude)

Arguably not actually coupling, simply "molecular fluid dynamics"





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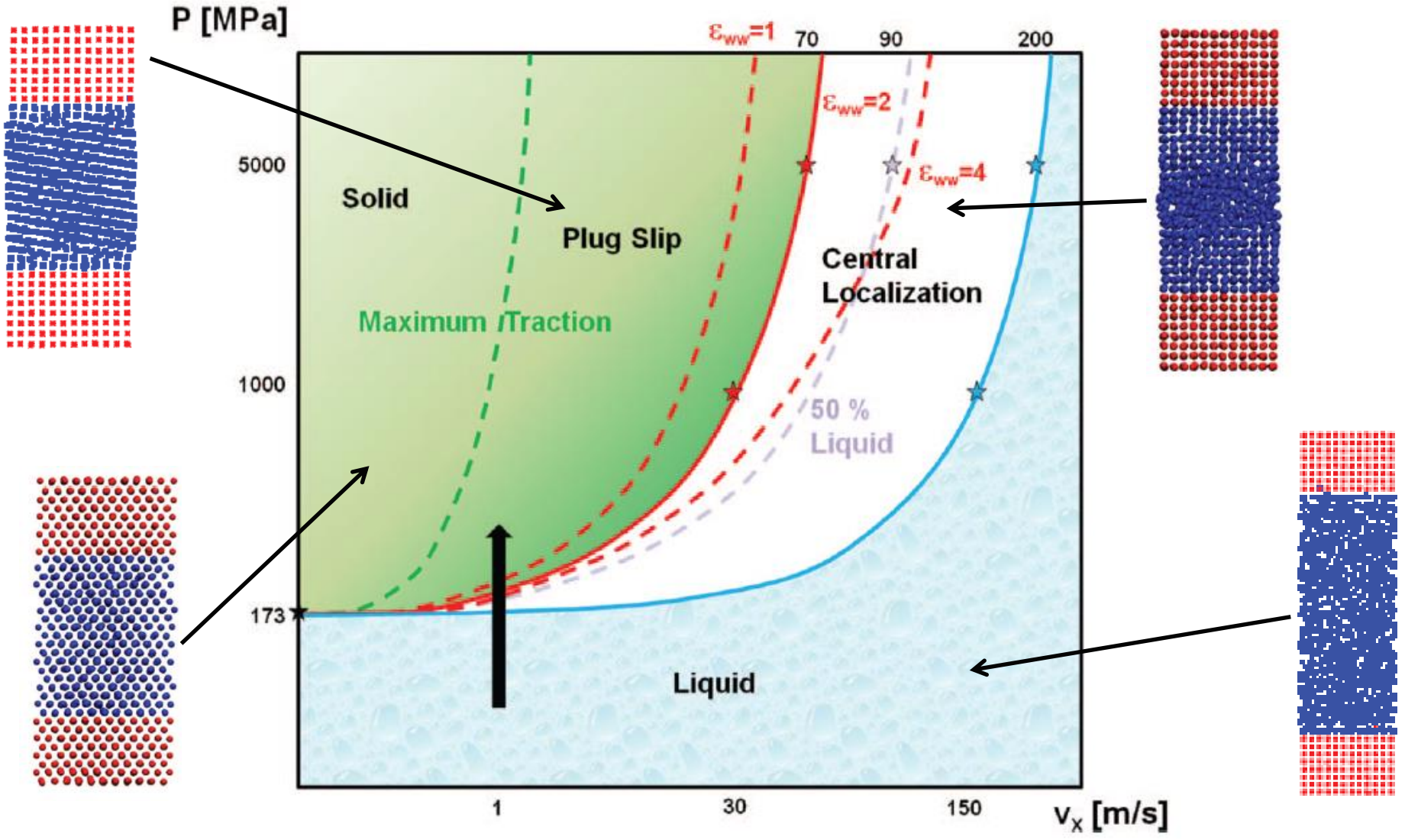
Non-Equilibrium (Non Continuum?) Phase Map



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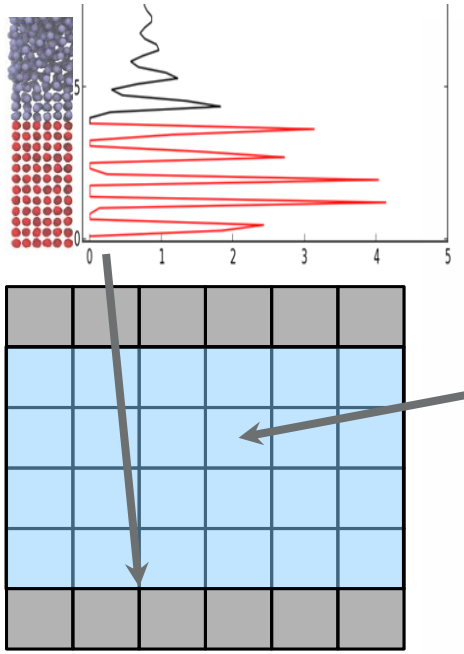
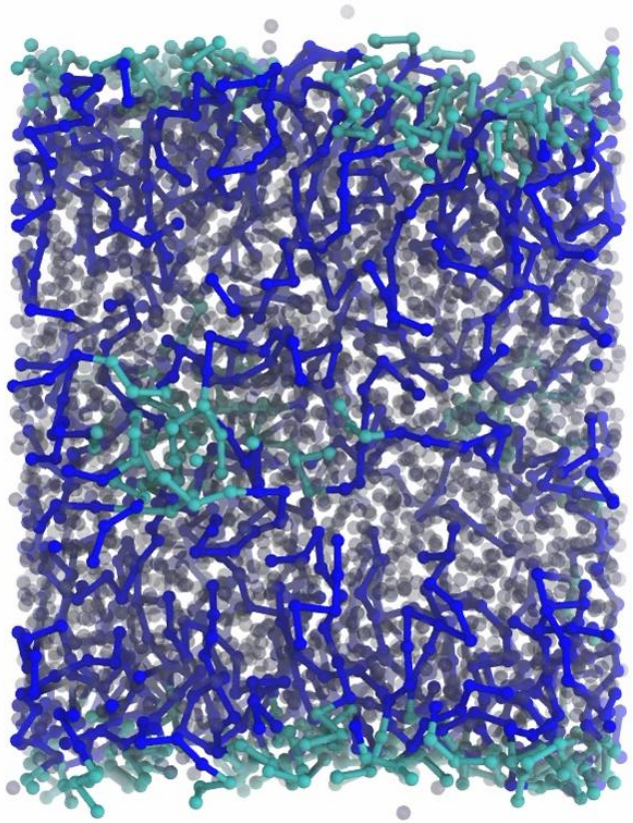
Coupling Assumptions

When we can't build a table due to large space or complexity

Assume the time and space scales are decoupled

Possible to observe a relationships later (machine learning opportunity)





Embedded Models (HMM)

MD – embedded in a CFD simulation

Used for Non-Newtonian effects [1)]

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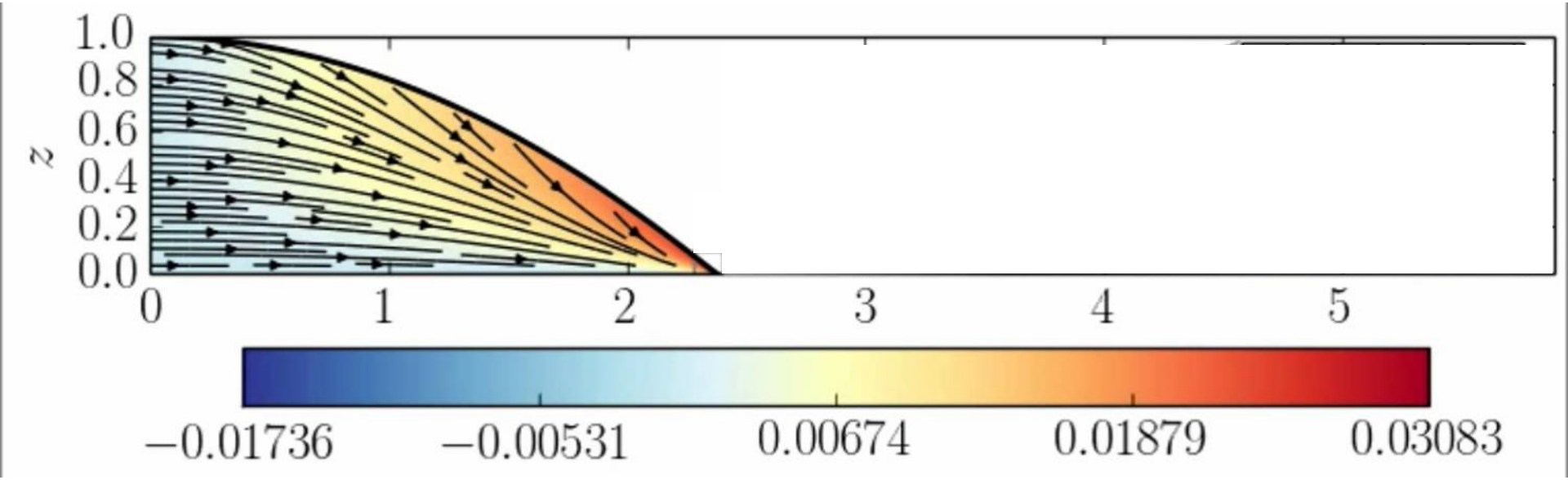
Coupled Droplet Spreading



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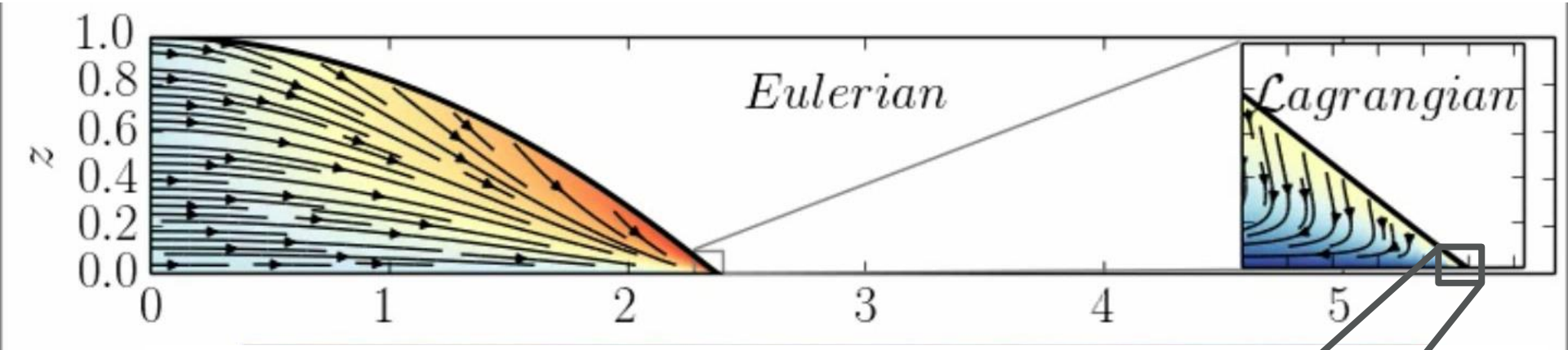
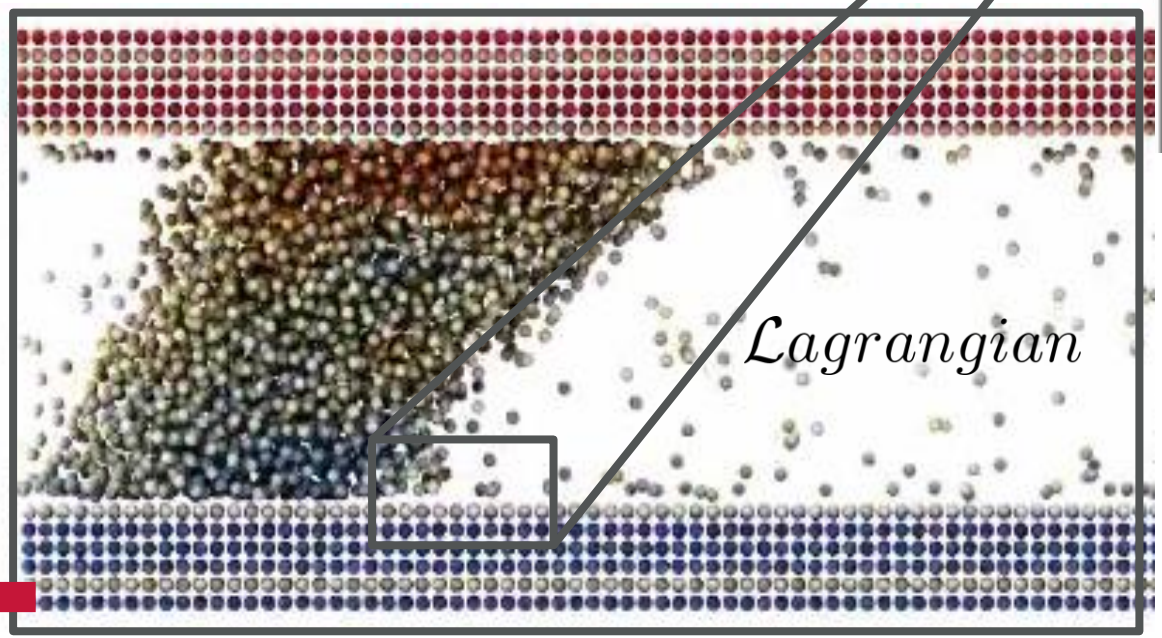
Coupled Droplet Spreading



- Model the moving contact line with MD
- We want contact line speed as a function of continuum contact angle



$$\frac{dx_c}{dt}$$

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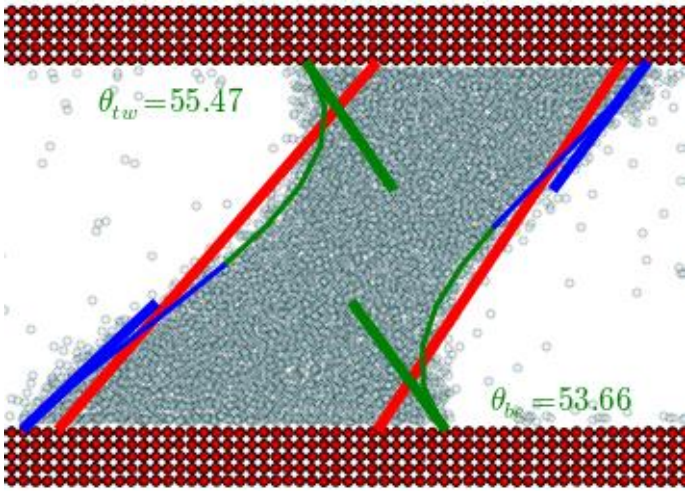
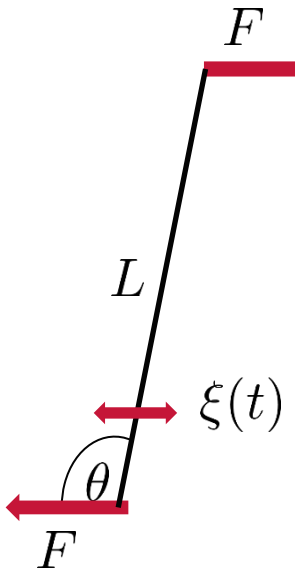
Building this into the Continuum Model

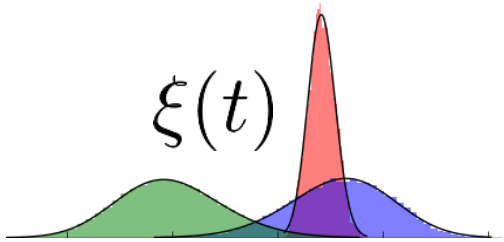
- Model the movement of the contact line as a torsional system





Spring mass + a random noise term

$$I\ddot{\theta} + \Gamma\dot{\theta} + k\theta - \xi = \mathcal{T}$$



- Torque $\mathcal{T} = F \times L$ approximately equal to wall sliding

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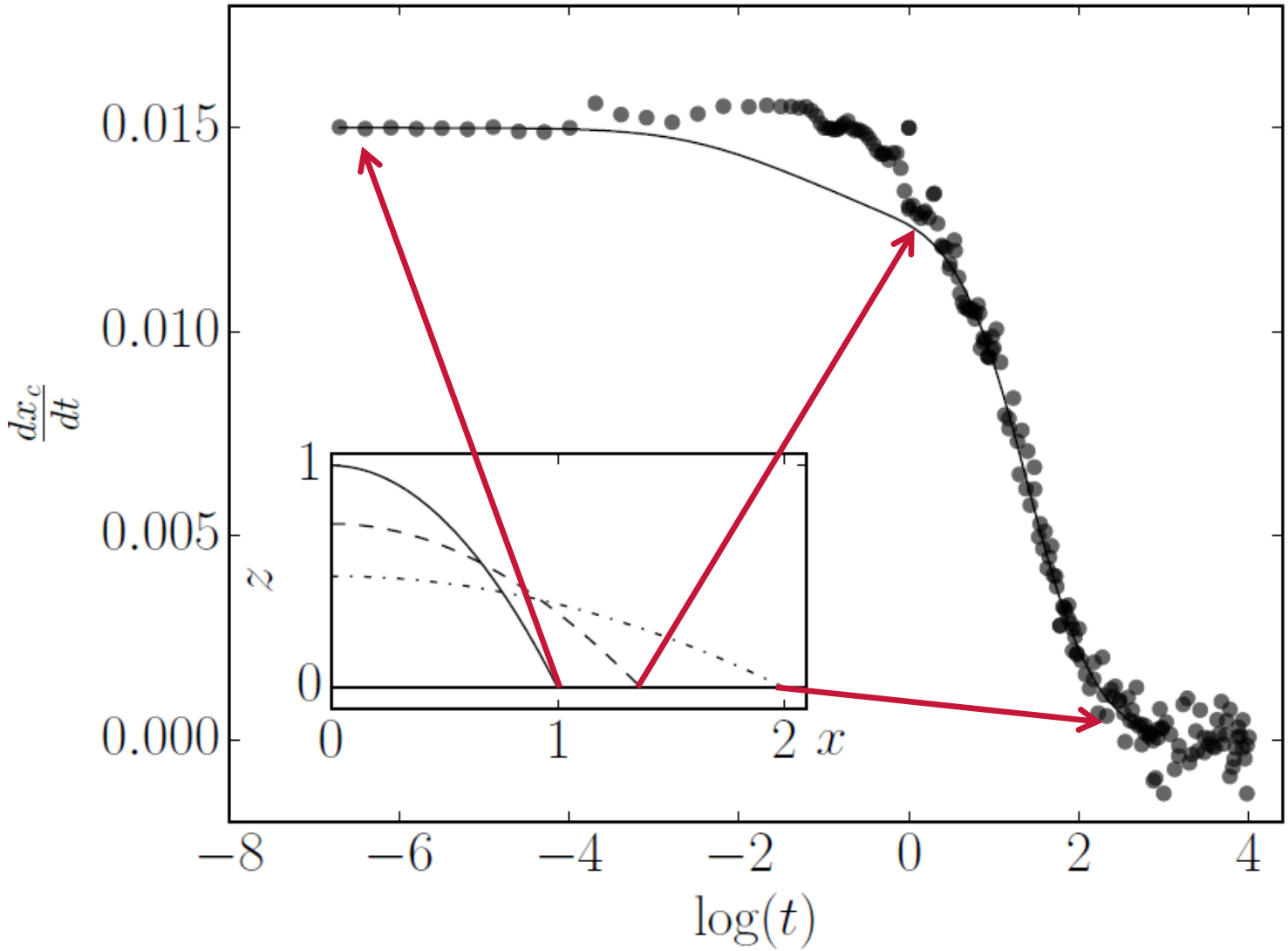
Building this into the Continuum Model



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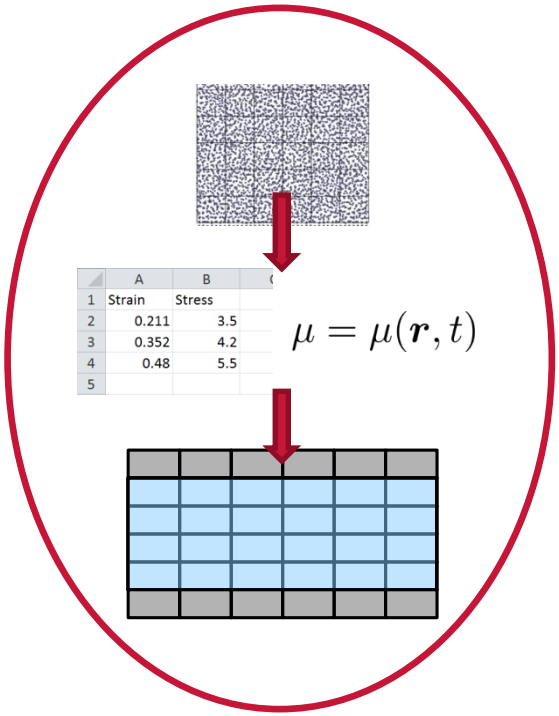
Coupling Assumptions



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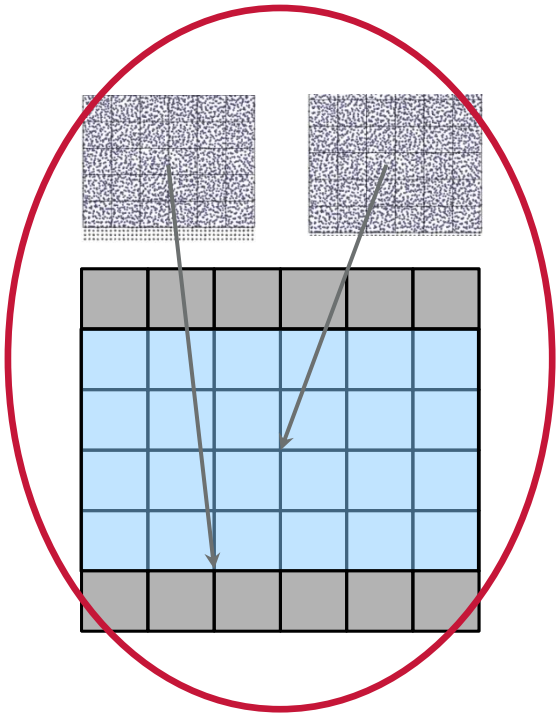

Embedded Models (HMM)

MD – embedded in a CFD simulation

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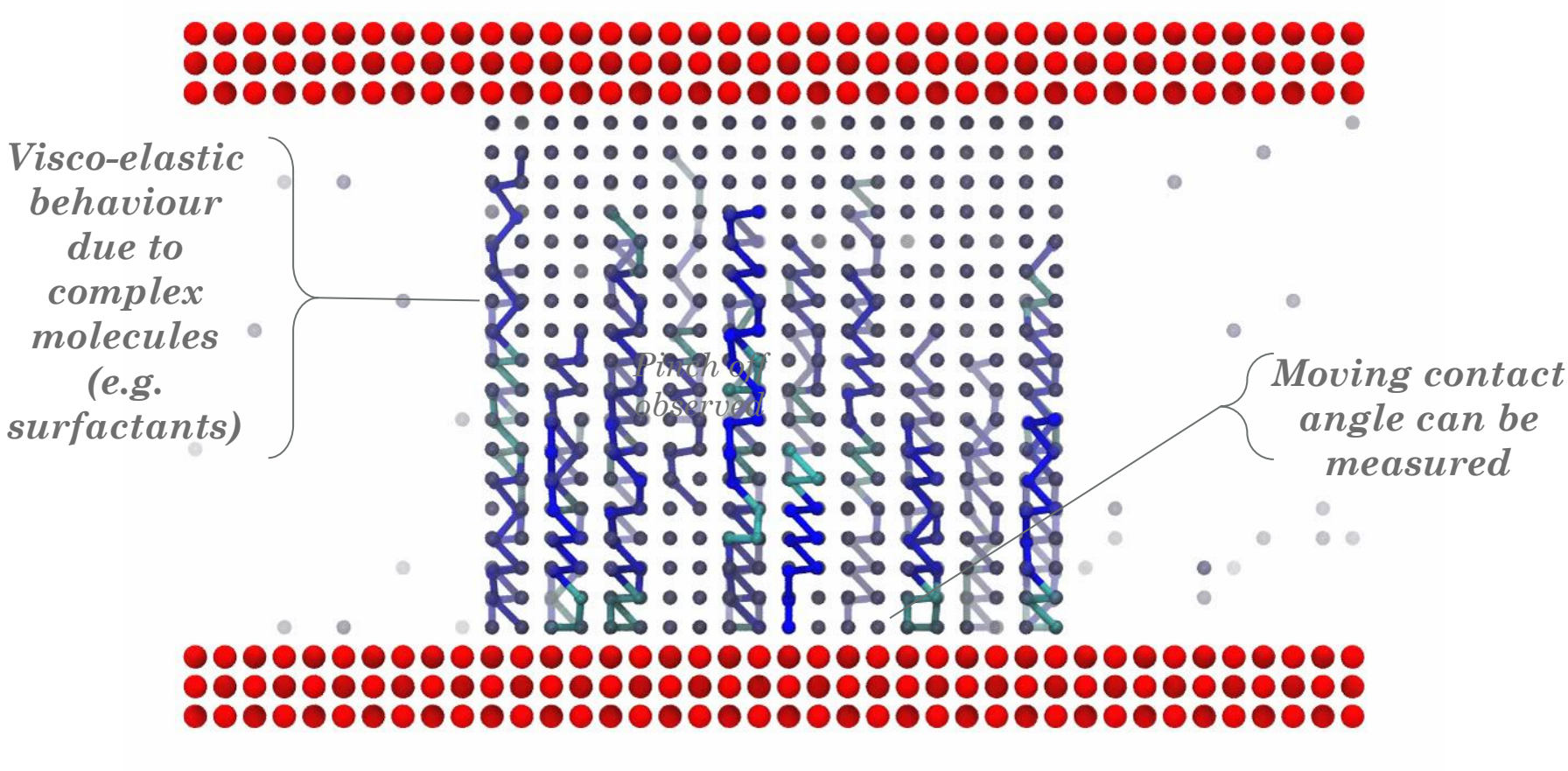
Extension to more complex flows



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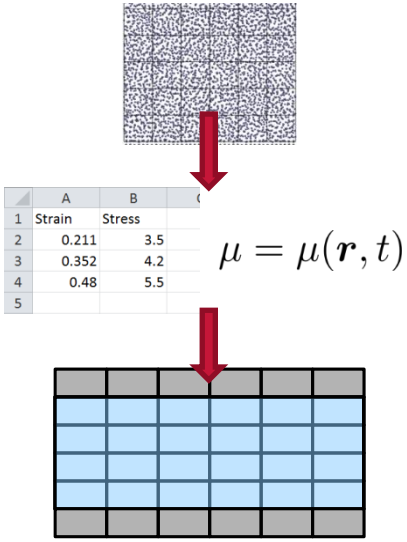
Coupling Assumptions



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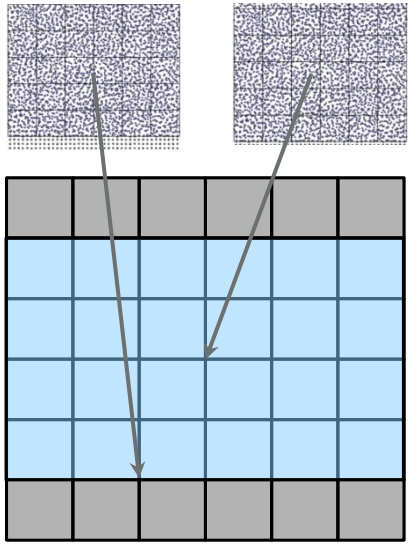

Embedded Models (HMM)

MD – embedded in a CFD simulation

Can we really reduce all the molecular complexity down to a close form relationship, table or embedded exchange?

We don't get the true evolution of the droplet with molecular detail

System size effects may mean similitude is not valid

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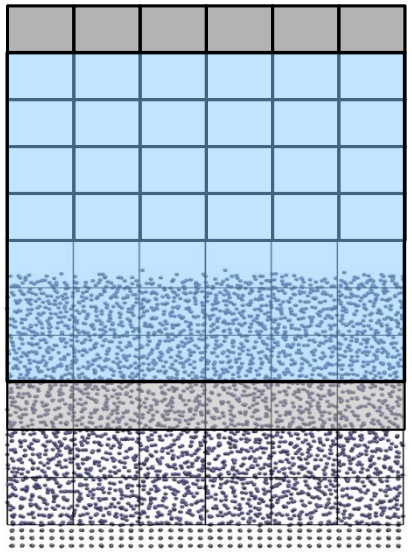
Coupling Assumptions

- **Domain decompositions makes no assumptions – full MD linked to CFD**
- **BUT, the length scales are the same and the timescales evolve together**
- **For accelerating molecular simulation NOT a boundary for CFD**
- **The most complex coupling**
  - How to link the two descriptions of reality?
  - “Noise” in MD can cause problems (fluctuating hydrodynamic or smarter/better averaging)
  - If we solve this, we can provide insight and techniques for the other coupling



Domain Decomposition

MD –CFD linked along an interface

Local features[2)]

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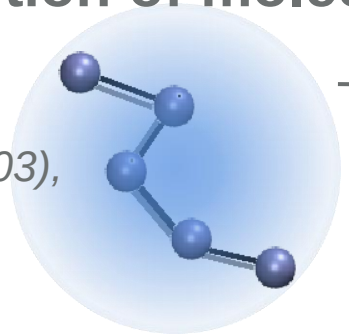
Domain Decomposition

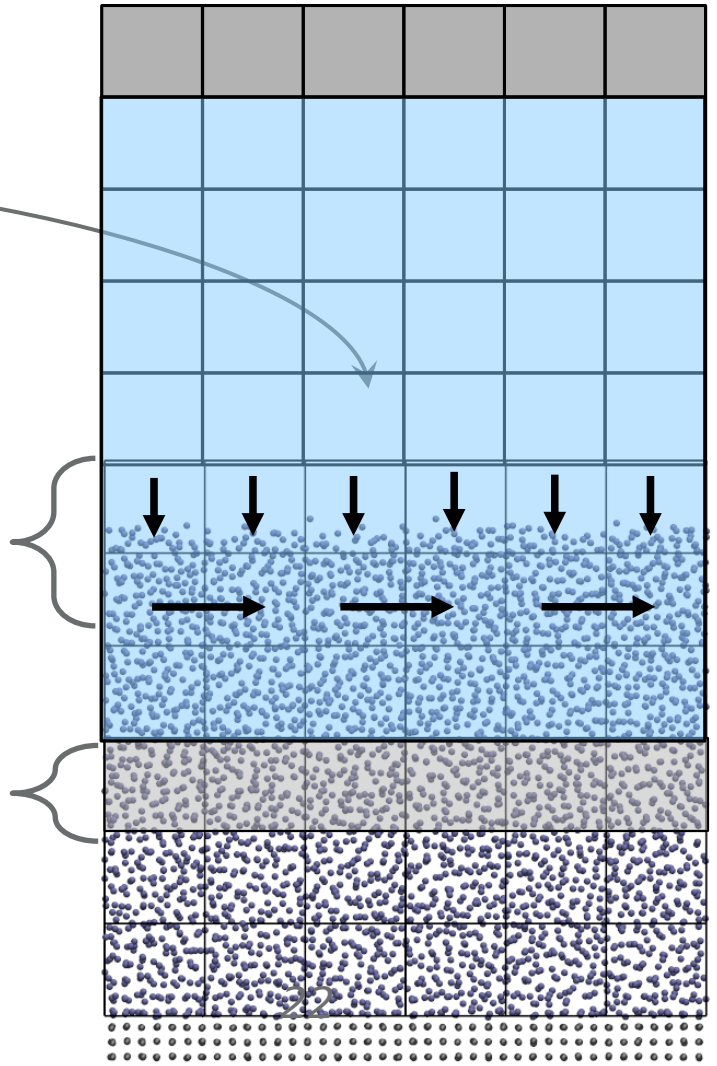
Boundary force and insertion of molecules



USHER (Delgado-Buscalioni 2003), Fade (Borg, Lockerby & Reese (2014)

CFD→MD Boundary condition

MD→CFD Boundary condition



O'Connell Thompson (1995), Hadjiconstantinou (1998), Flekkoy (2000), Nie et al (2004). All since 1995, and we have over 100 years of statistical mechanics

Many tuneable parameters – an art? Overlap size, timestep ratio, boundary force, etc

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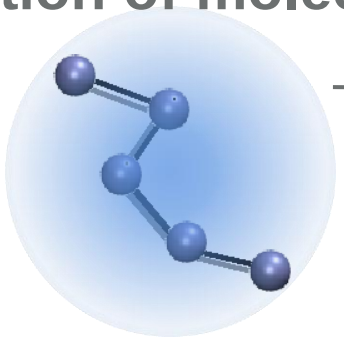
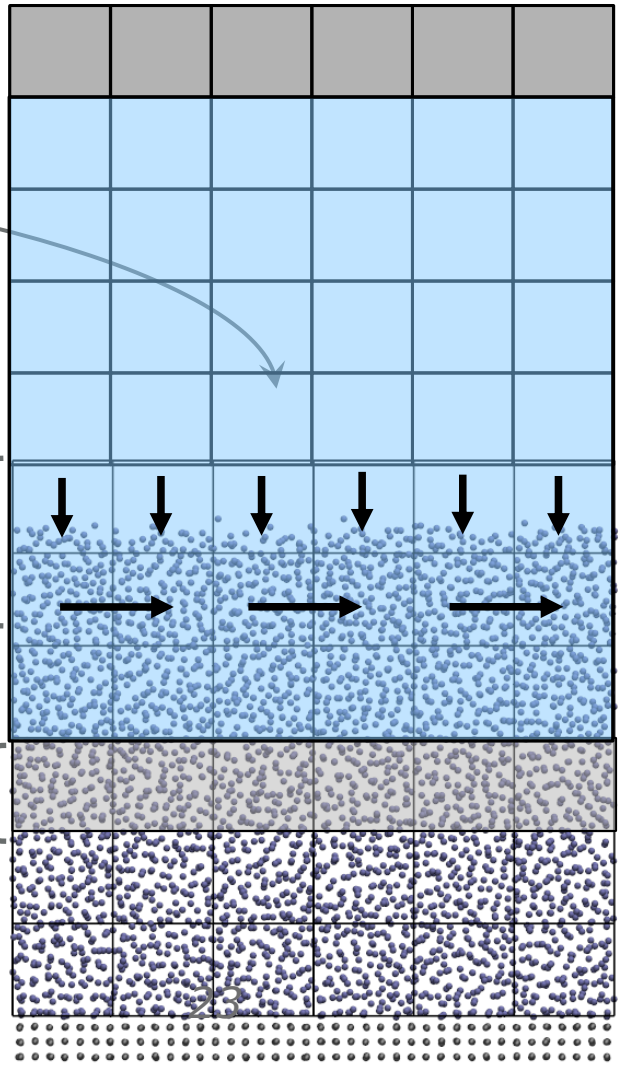
Domain Decomposition

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)

TRANSPORT PROCESSES

817

777.9 cm^{-1}. The band at 809.7 cm^{-1} has been interpreted as 2×396, the rather large difference between calculated and observed frequency being ascribed to the proximity to the A_g fundamental. However, this band could be an upper-stage band corresponding to 819 cm^{-1}.

The interpretation of the faint sharp band at 760.4 cm^{-1} as an upper-stage band, $778+\nu_6-\nu_3$, seems more plausible than its interpretation as the B_{1g} combination, $210+558$ cm^{-1}. The faint sharp Raman band at 838.7 cm^{-1} has been interpreted as an upper-stage band, $2\times407+\nu_6-\nu_3$, rather than as the B_{2u} difference band, $1340-510$ cm^{-1}, because the corresponding sum band has not been observed. If the preferred interpretations are correct, the group of Raman bands, 760, 778, 819, and 839 cm^{-1}, are related to each other in much the same manner as similar groups in the spectra of CO_2 and CS_2.

ACKNOWLEDGMENTS

The writers wish to express their indebtedness to Dr. C. F. Hammer and E. I. du Pont de Nemours and Company for the samples; to Doctors Isabelle and Jerome Karle for electron diffraction data; and to Dr. E. K. Plyler and the National Bureau of Standards for data in the long wave-length region.

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 18, NUMBER 6 JUNE, 1950

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

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(Received November 21, 1949)

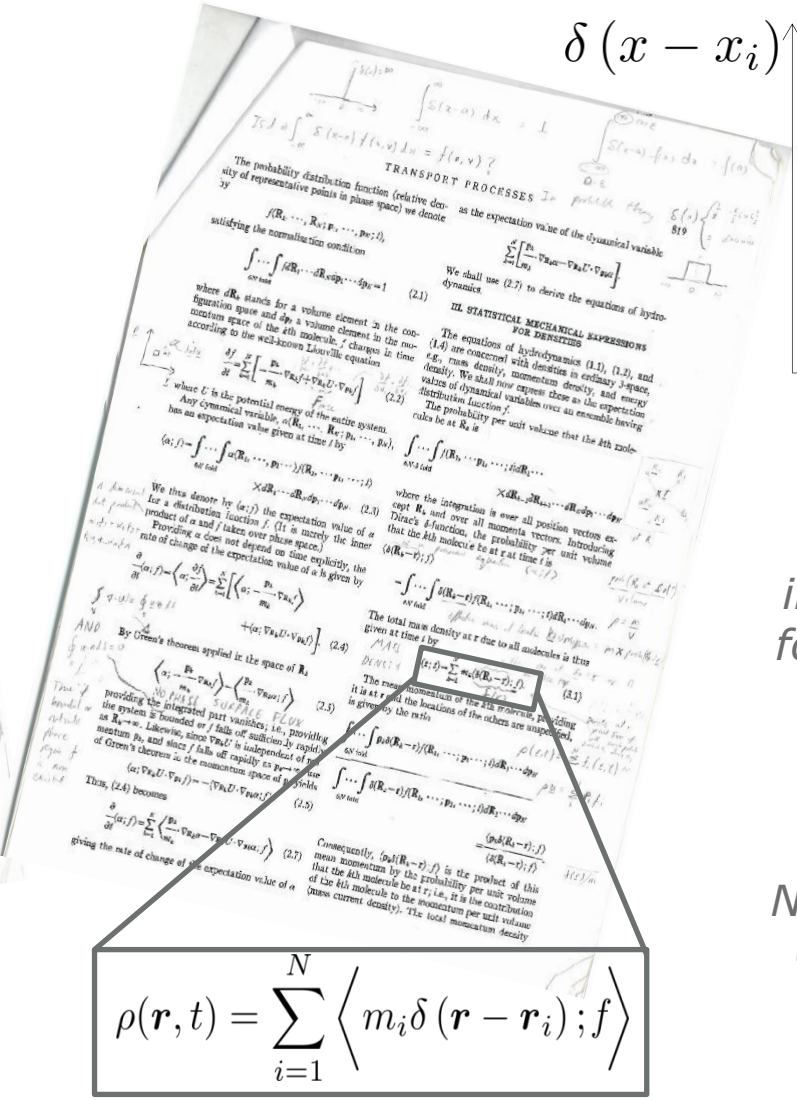
The equations of hydrodynamics—continuity equation, equation of motion, and equation of energy transport—are derived by means of the classical statistical mechanics. Thereby, expressions are obtained for the stress tensor and heat current density in terms of molecular variables. In addition to the familiar terms occurring in the kinetic theory of gases, there are terms depending upon intermolecular force. The contributions of intermolecular force to the stress tensor and heat current generally are expressed, respectively, as quadratures of the density and current density in the configuration space of a pair of molecules.

INTRODUCTION

THIS paper will be concerned with a derivation of the equations of hydrodynamics from the principles of the classical statistical mechanics. In particular, the equations of continuity, the equation of motion, and the equation of energy transport will be derived. By so doing, the stress tensor and heat current density can be expressed in terms of molecular variables. The stress tensor consists of a kinetic part (which occurs in the kinetic theory of gases) and another term (dominant for a liquid) which will be expressed as a quadrature involving the potential of intermolecular force and the density of pairs of molecules. The heat current density is the sum of the potential of intermolecular force and the density and current density in the configuration space of a pair of molecules. The results were previously stated in the first article of this series,[1] which this derivation was prompted.

To obtain explicit expressions for the pair probability density and probability current density one would in principle need to solve the Liouville equation (Eq. (2.2)) for the probability distribution in Gibbs phase space and then perform repeated integrations. Since this program is untenable for a liquid, various attempts have been made to obtain a closed equation satisfied approximately by the probability distribution function in the phase space of a pair of molecules. One such equation has been derived by Born and Green[2] using a generalized "superposition" assumption. Another, a generalization of the well-known Fokker-Planck equation of stochastic theory, has been derived by Kirkwood by introducing the concepts of time smoothing and a friction constant. This latter equation has been applied to obtain an expression for the stress tensor linear in gradients of fluid velocity and, thereby, expressions in terms of molecular variables) for coefficients of shear and volume viscosity.[3] The same equation generalized to non-uniform temperature, after linearizing in the temperature gradient and thereby an explicit expression for the heat current and thereby an expression for the coefficient of thermal conductivity.[4] We shall assume, for purposes of mathematical simplicity, a single component, simple phase fluid system consisting of molecules which interact under central forces only. It is not difficult to generalize the treatment to a multiple component or multiple

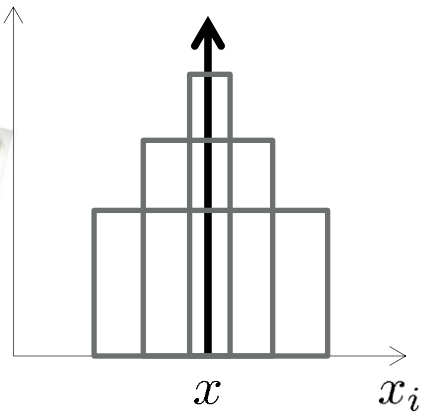
* This work was supported by the U. S. ONR under Contract Nonr-244 w/h the California Institute of Technology.
† Contribution No. [illegible].
[1] J. G. Kirkwood, J. Chem. Phys. 14, 180 (1946).
[2] M. Born and H. S. Green, Proc. Roy. Soc. A188, 10 (1946).
[3] Kirkwood, Buff, and Green, J. Chem. Phys. 17, 988 (1949).
[4] Kirkwood, Brinkley, and Irving (to be published). The [illegible] exhibits terms a more precise construction of the [illegible] distribution function.



TRANSPORT PROCESSES

819

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



The Dirac delta infinitely high, infinitely thin peak formally equivalent to the continuum differential formulation

BUT

No molecule is ever exactly at a point

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Computational Fluid Dynamics

- The Navier-Stokes Equation

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

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

- Finite Difference Method

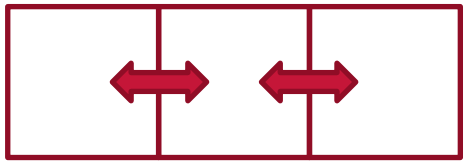
$$\frac{\partial u_i}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{\Delta x}$$

- Spectral Methods

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

- Finite Volume (0^{th} order element) Method

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



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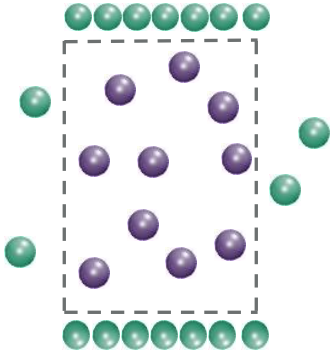
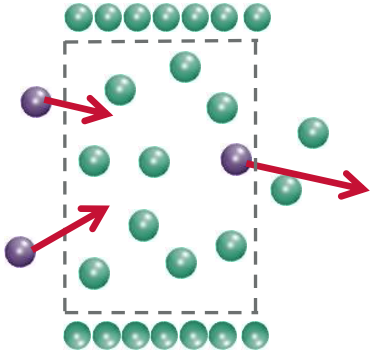
Control Volume Functional

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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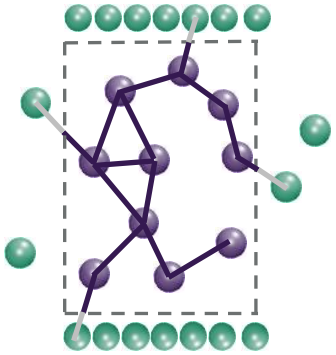
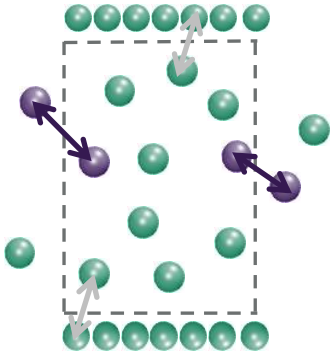
Control Volume Functional - Forces

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

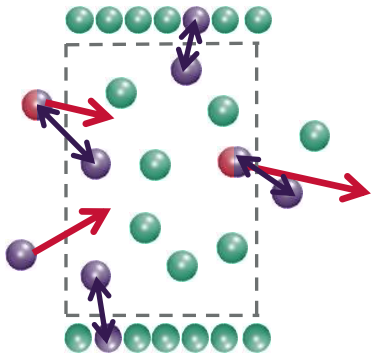
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\boldsymbol{S}_i$$

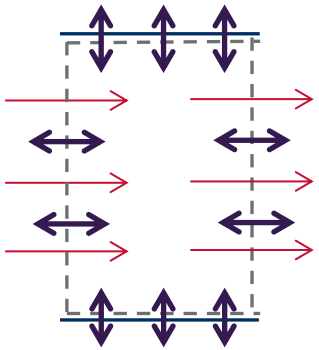
$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u} \cdot d\mathbf{S}$$

- 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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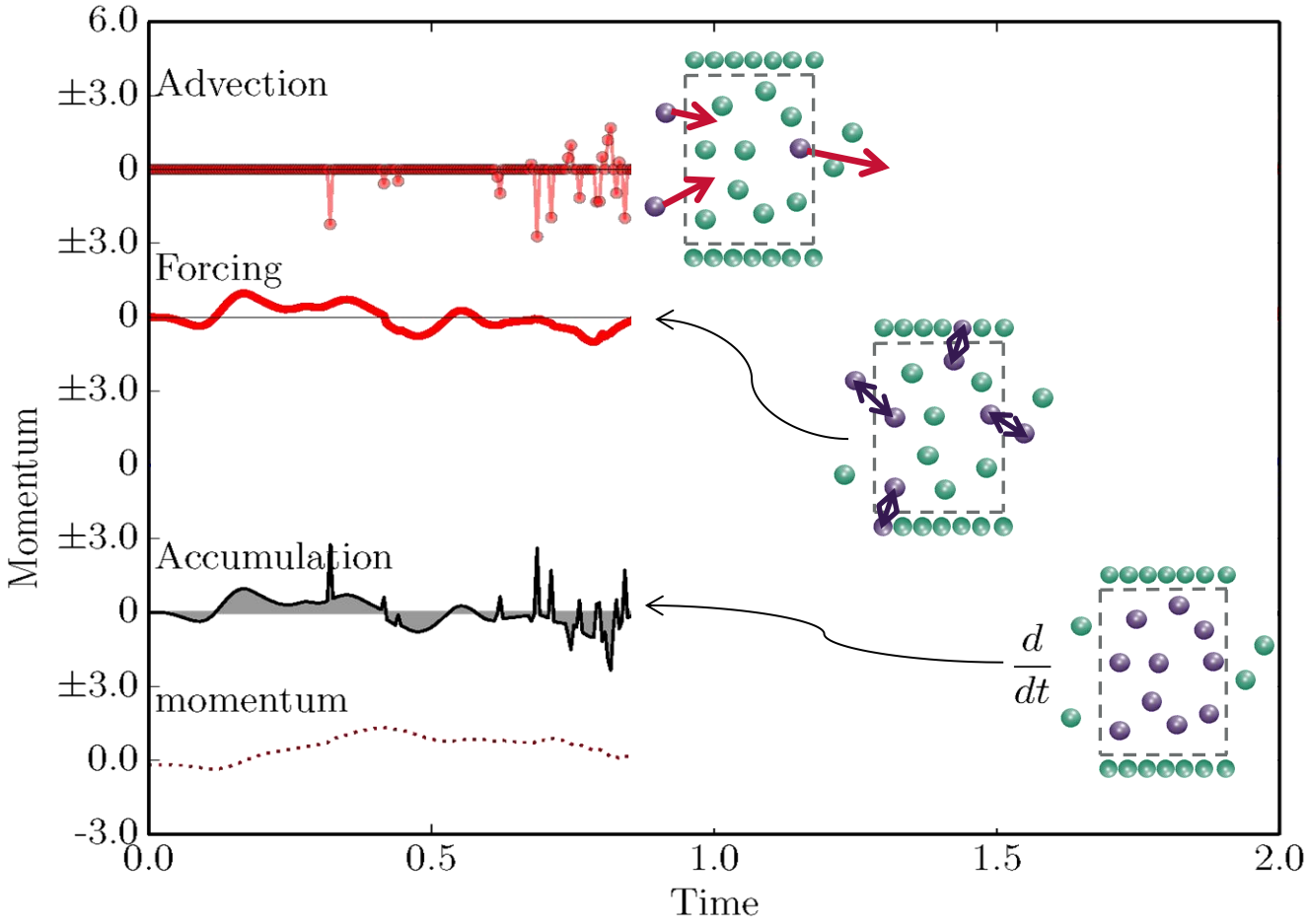
Exact Conservation

Results from any arbitrary volume

- Accumulation = Forcing + Advection



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

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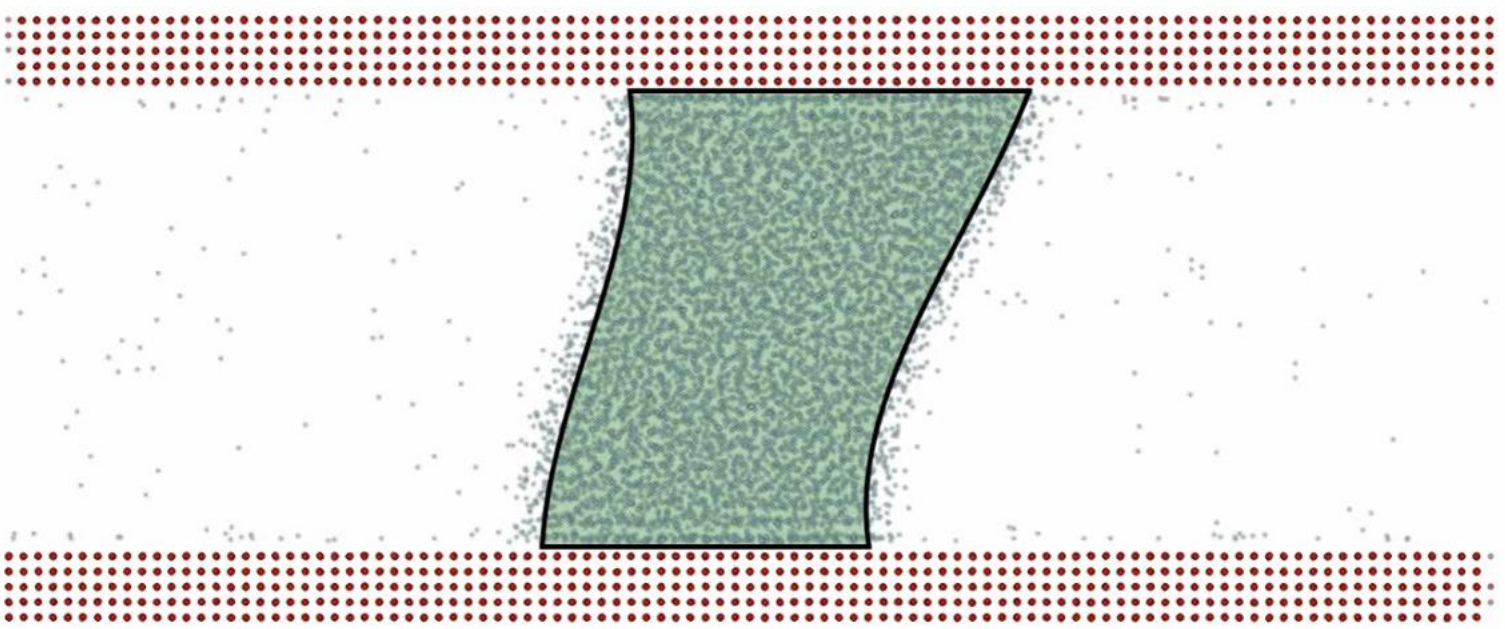
Exact Conservation – Arbitrary Volume

Results from any arbitrary volume

- Accumulation = Forcing + Advection



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
- Control Volumes are the only meaningful way to relate the two systems

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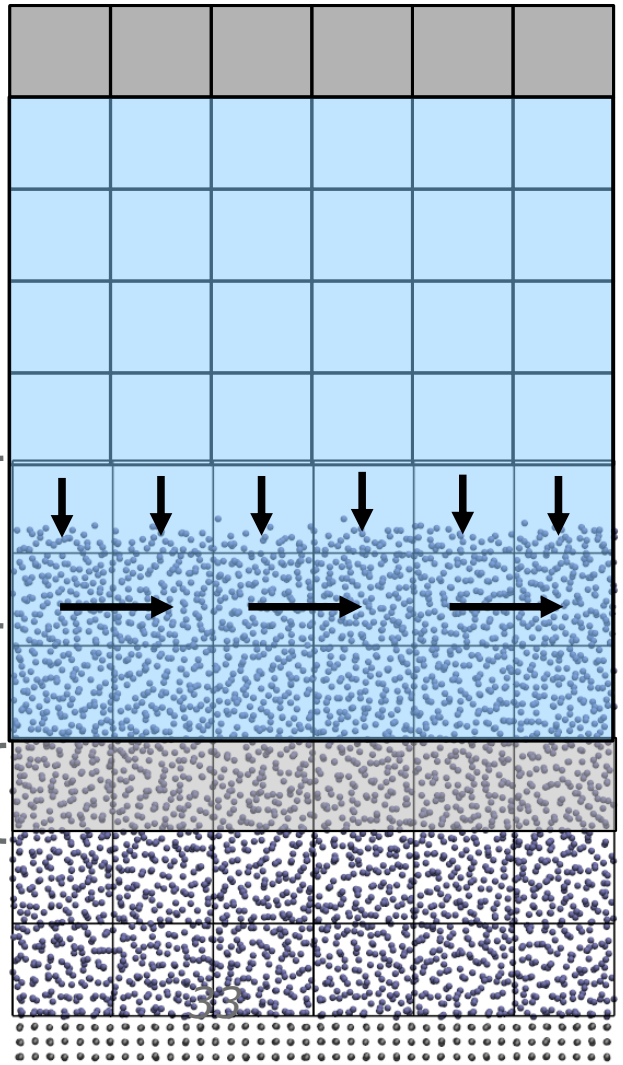
Domain Decomposition

Consistent Framework ✓

CFD→MD Boundary condition

MD→CFD Boundary condition ✓



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Constrained Control Volume

Non-unique solution

- Continuum field properties must specify dynamics of N molecules
- Hamilton's principle (subject to a constraint) used in the first fluids coupling scheme (O'Connell and Thompson 1995)

We 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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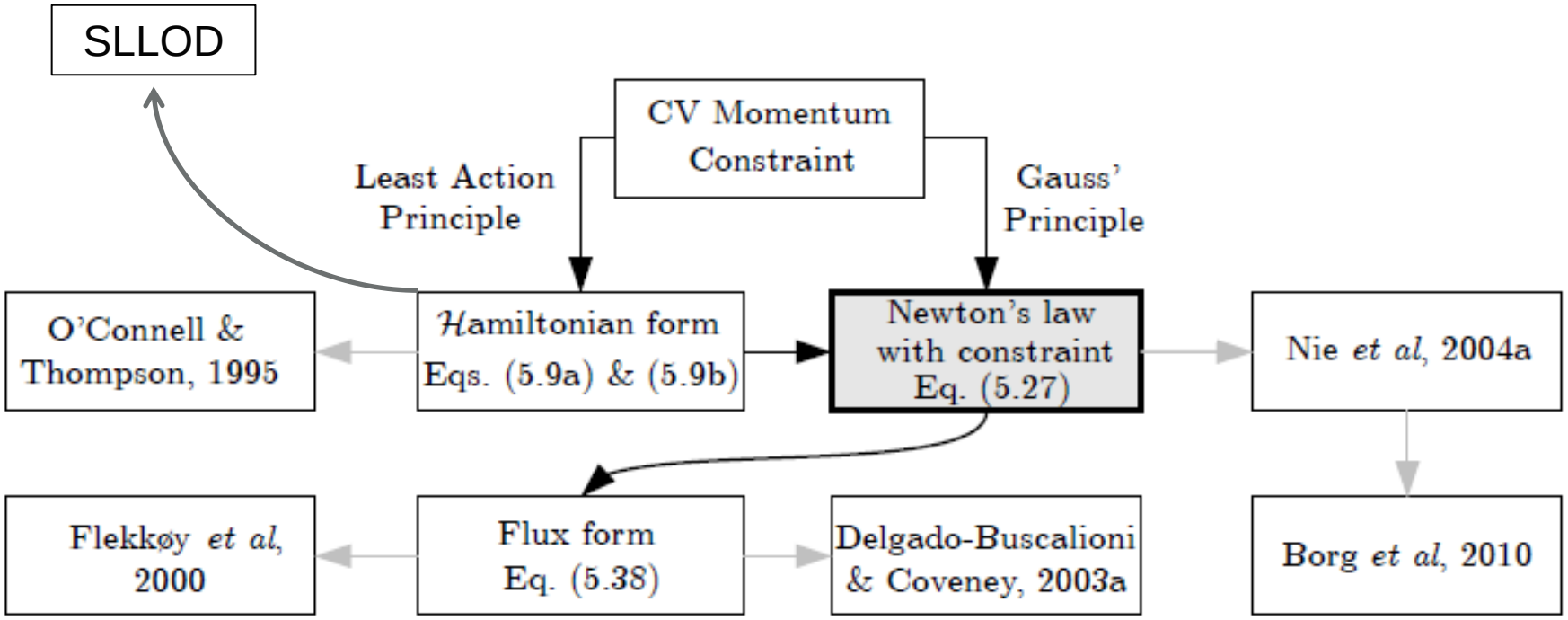
Constrained Control Volume



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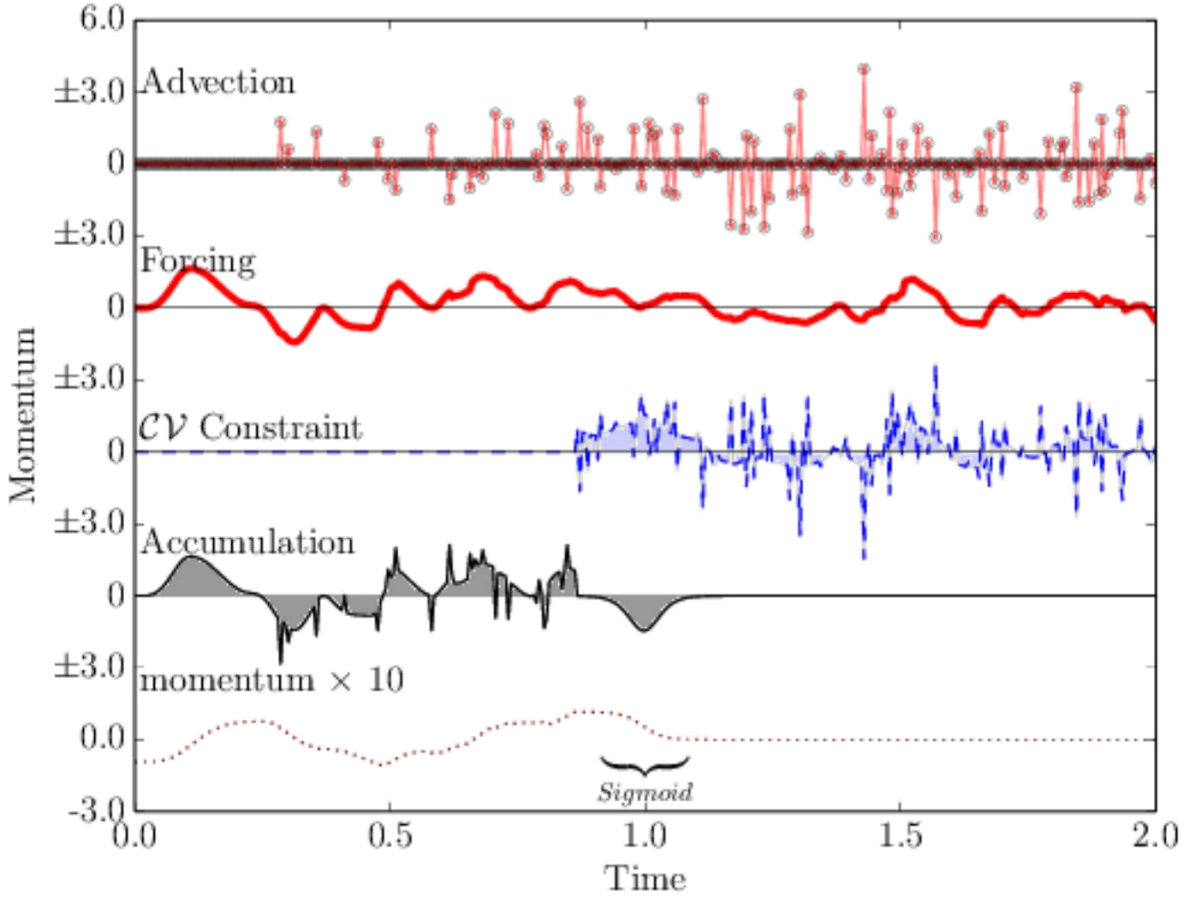
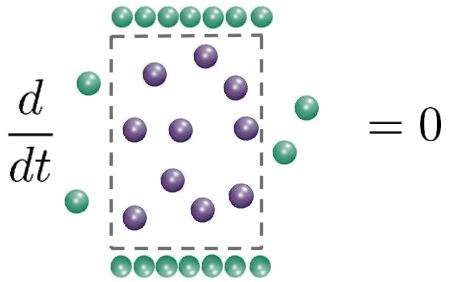
Constrained Control Volume

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



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



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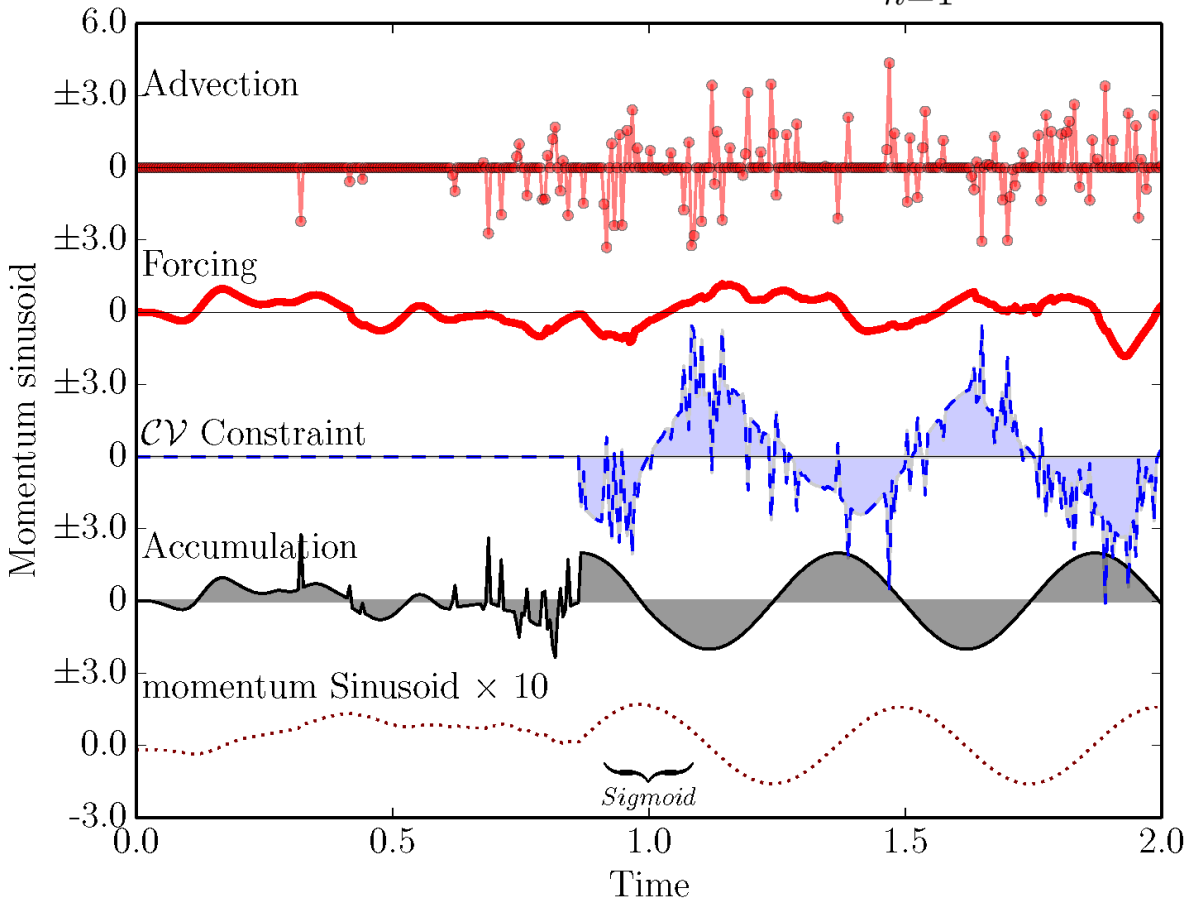
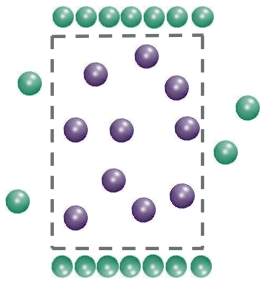
Constrained Control Volume

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



- 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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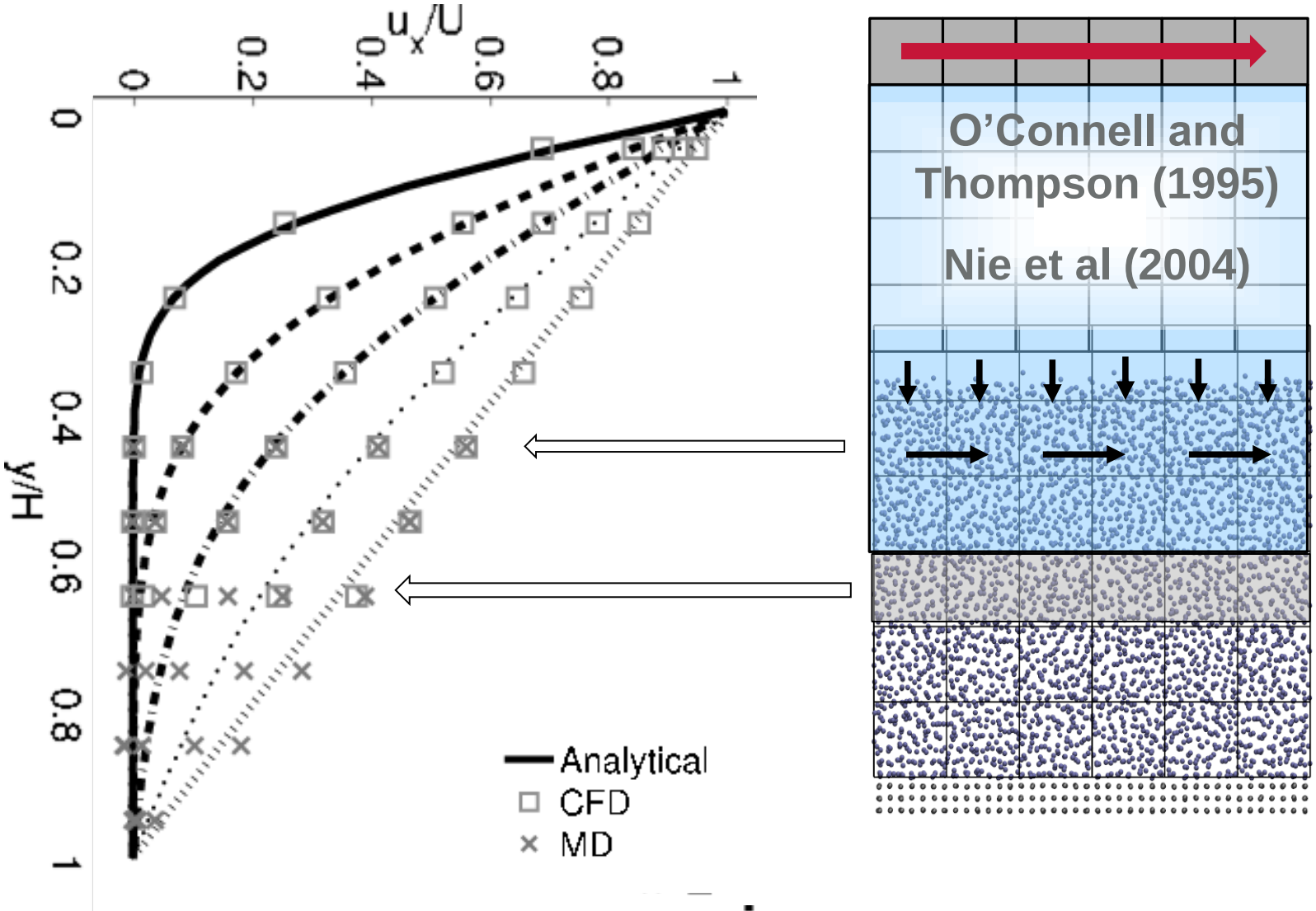
Coupling Results – Couette Flow



Key Points

- How do we ensure conservation equations are satisfied between domains
- A consistent framework and exact constraints derived from sound physical theories help
- Still lots of work needed to elevate from an art to a science (pressure solver, order of accuracy, complex molecules, interfaces, etc)

Some Examples

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Molecular Dynamics simulation of Nucleation

Wall w
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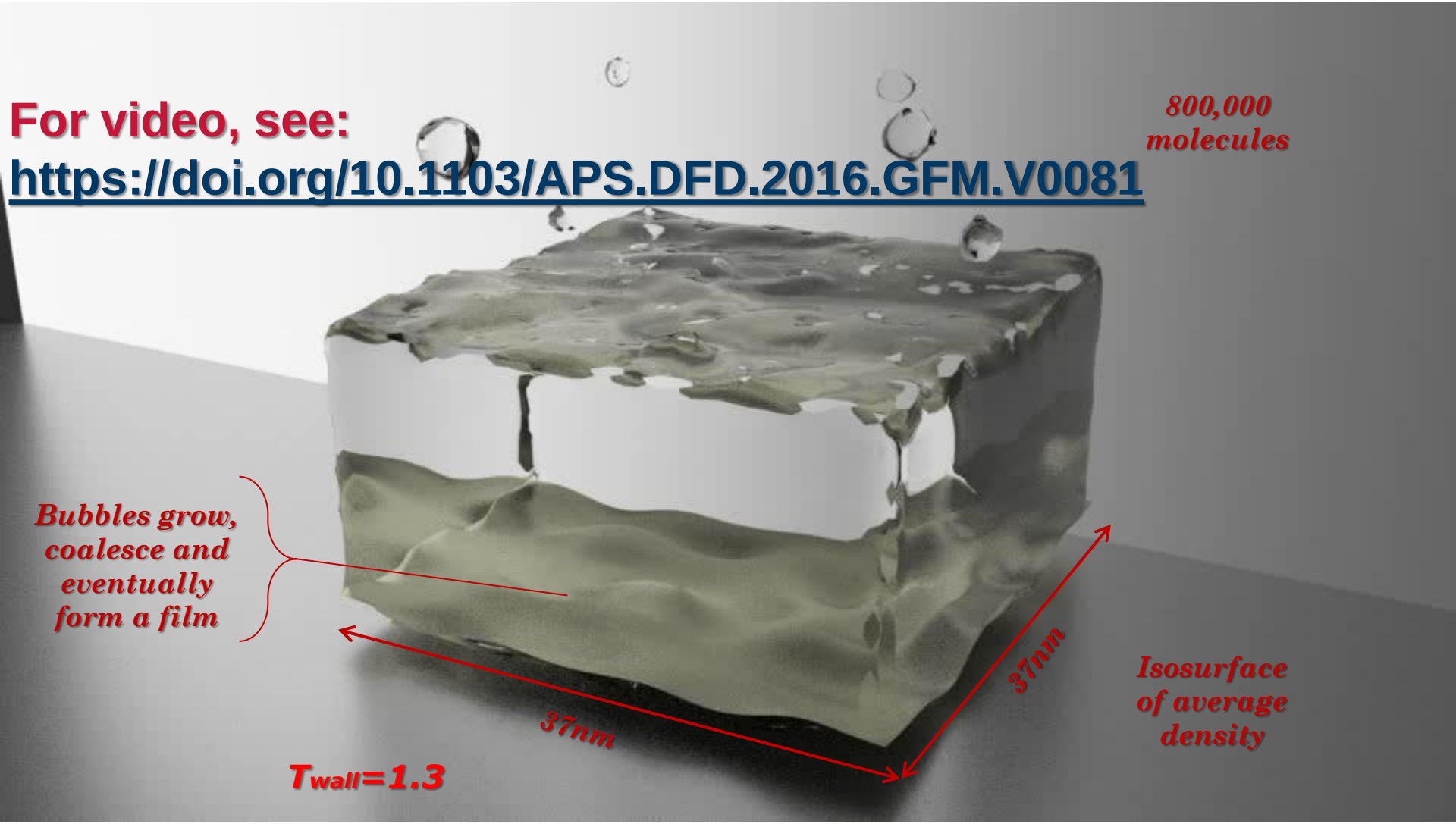
Isosurface of Density



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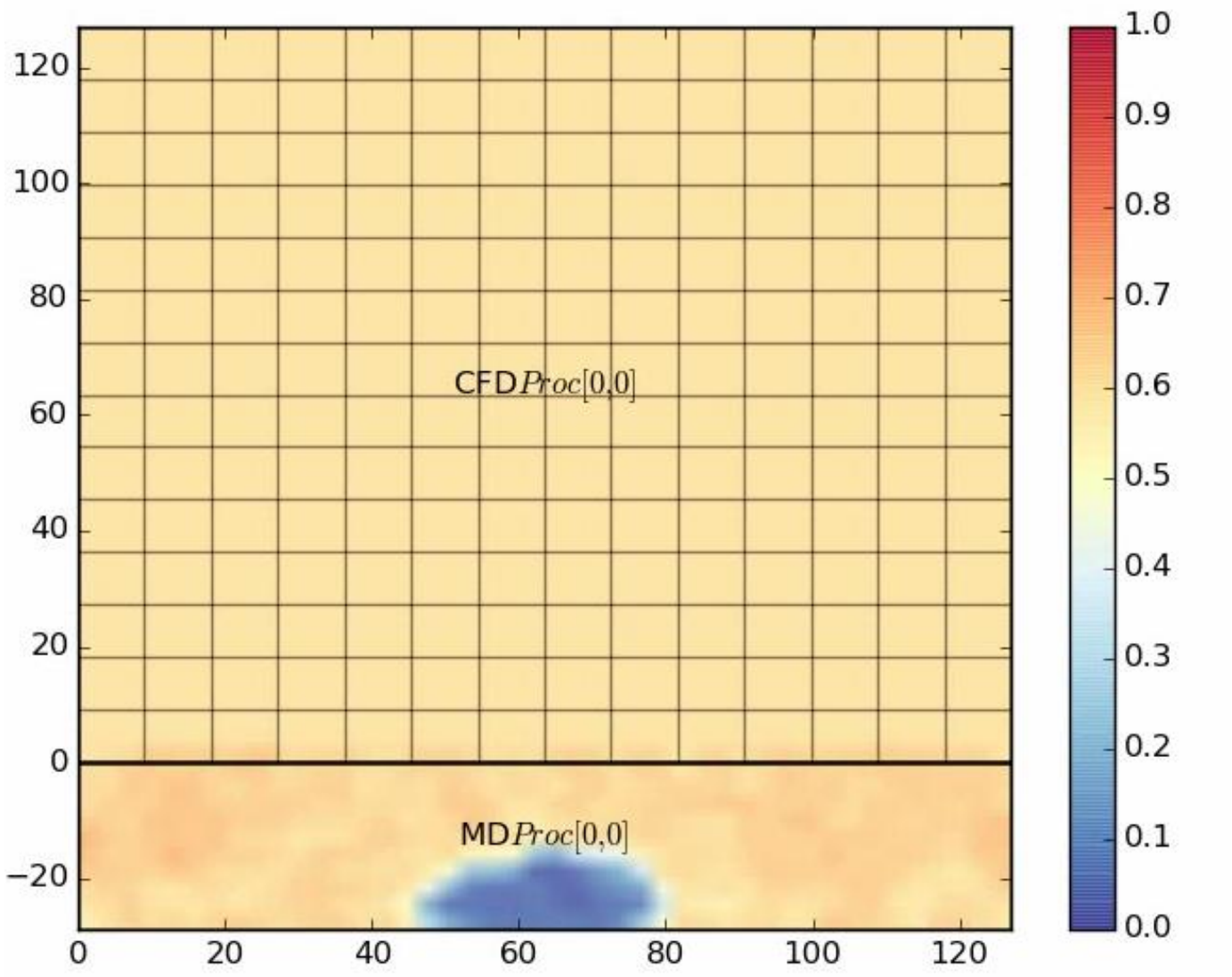
Coupled Simulation of Boiling



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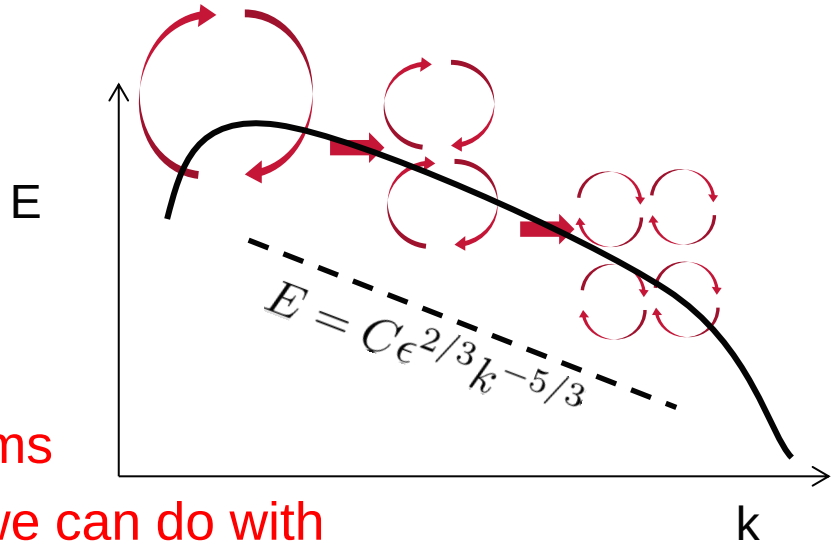
Molecular Simulation of Turbulence

- 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



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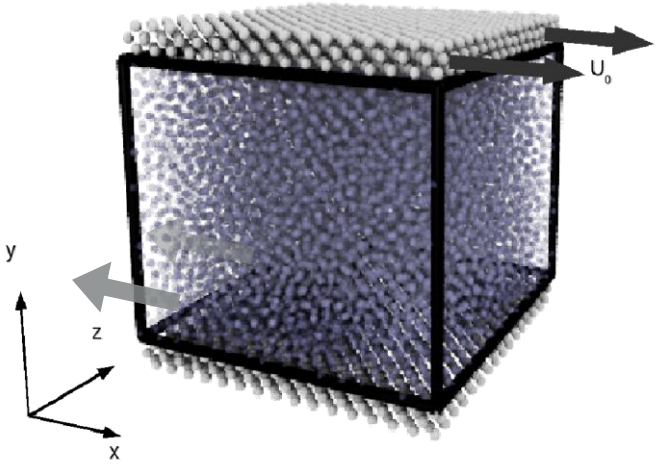
Domain Overview

- Simulation Setup
  - All Molecular Dynamics (not coupled)
  - 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 density=0.3, ~300 million molecules on 256+ processors

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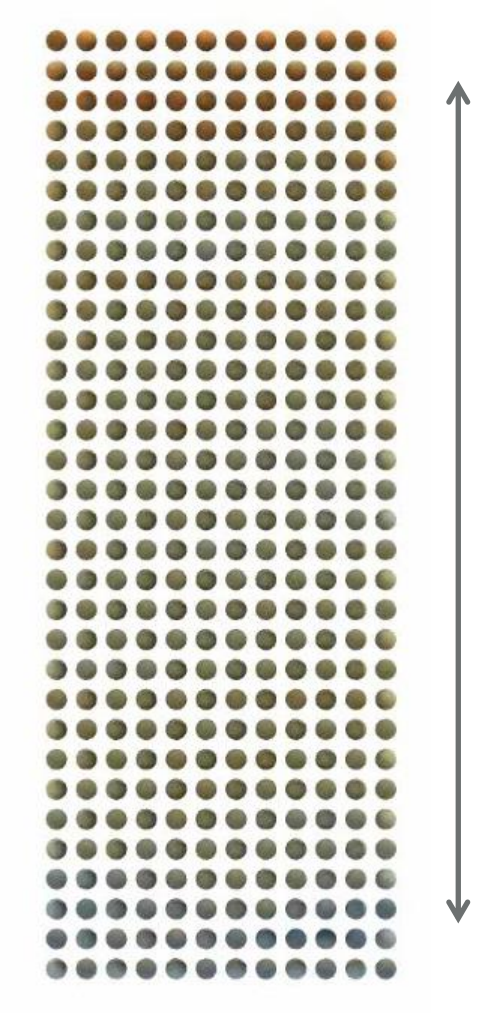
Molecular Simulation of Turbulence



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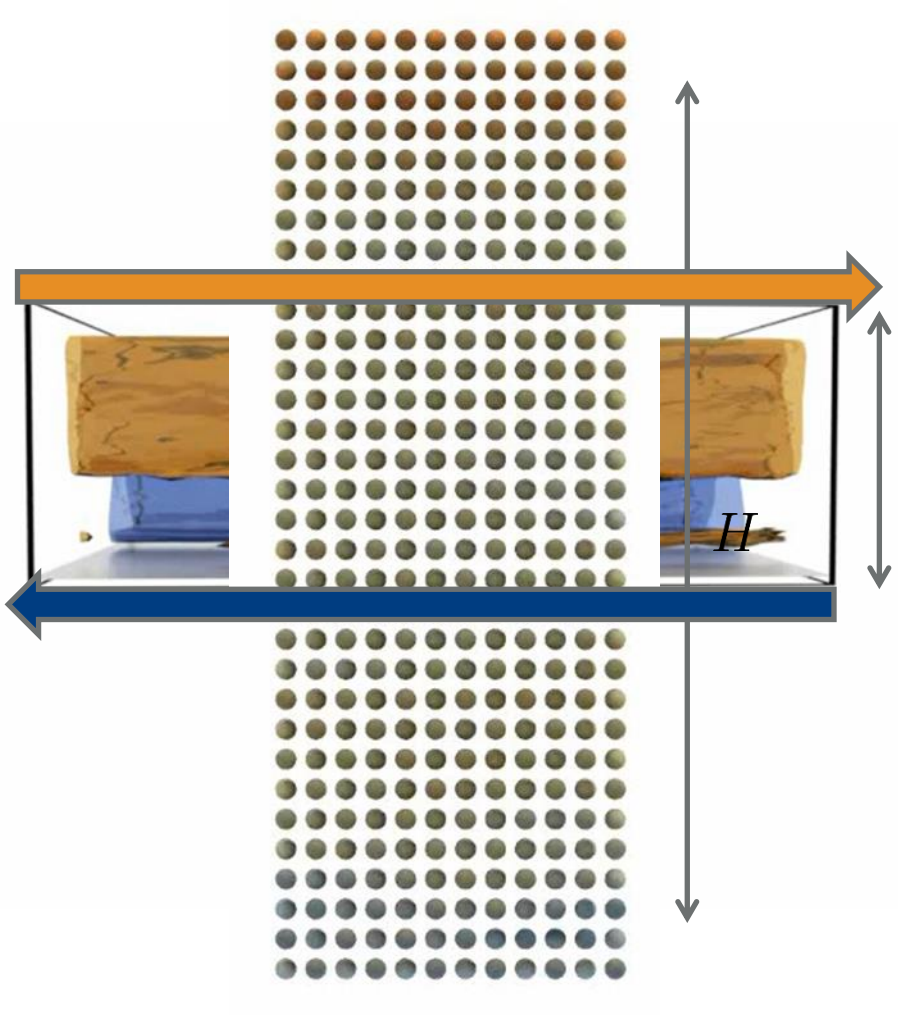
Molecular Simulation of Turbulence



Reynolds Number

$Re \approx 400$

with

300 million molecules

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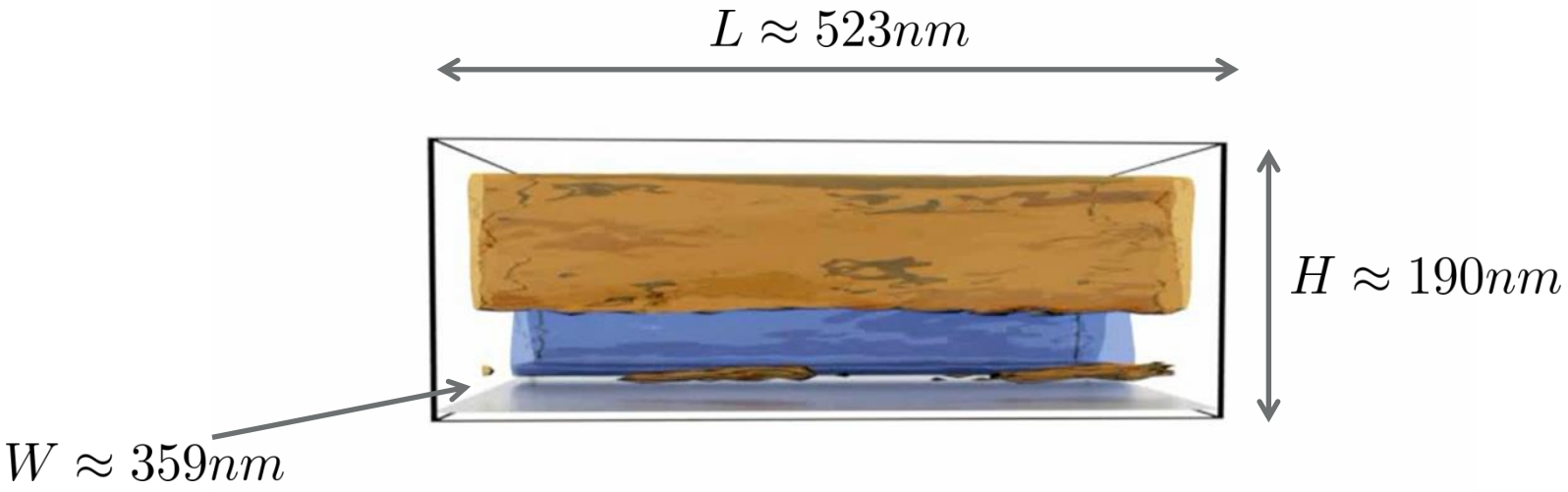
Molecular Simulation of Turbulence

Minimal channel Couette flow



Reynolds Number

$Re \approx 400$

with
300 million molecules

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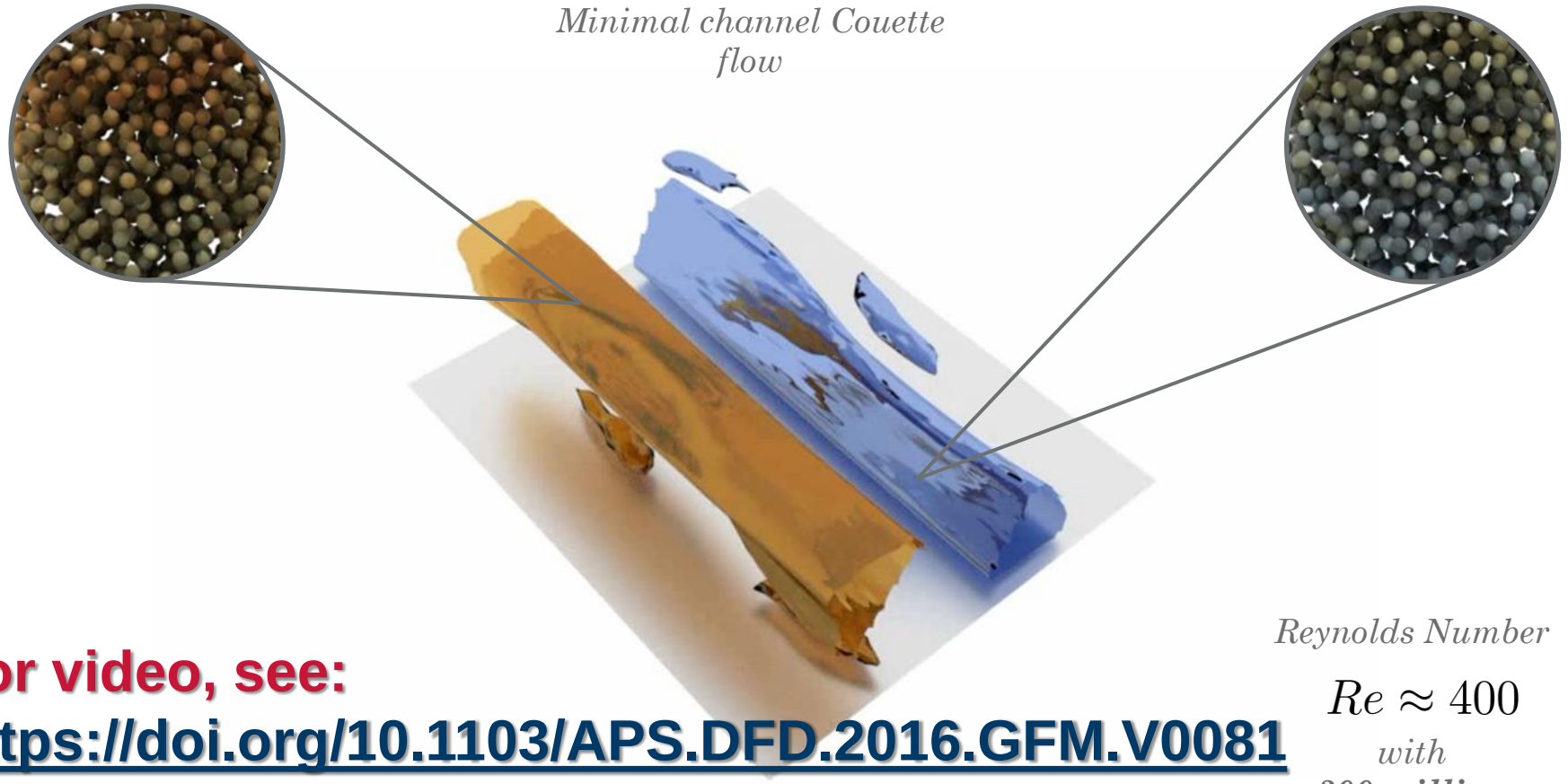
Molecular Simulation of Turbulence

Minimal channel Couette flow



For video, see:
https://doi.org/10.1103/APS.DFD.2016.GFM.V0081

Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$Re \approx 400$

with
300 million molecules

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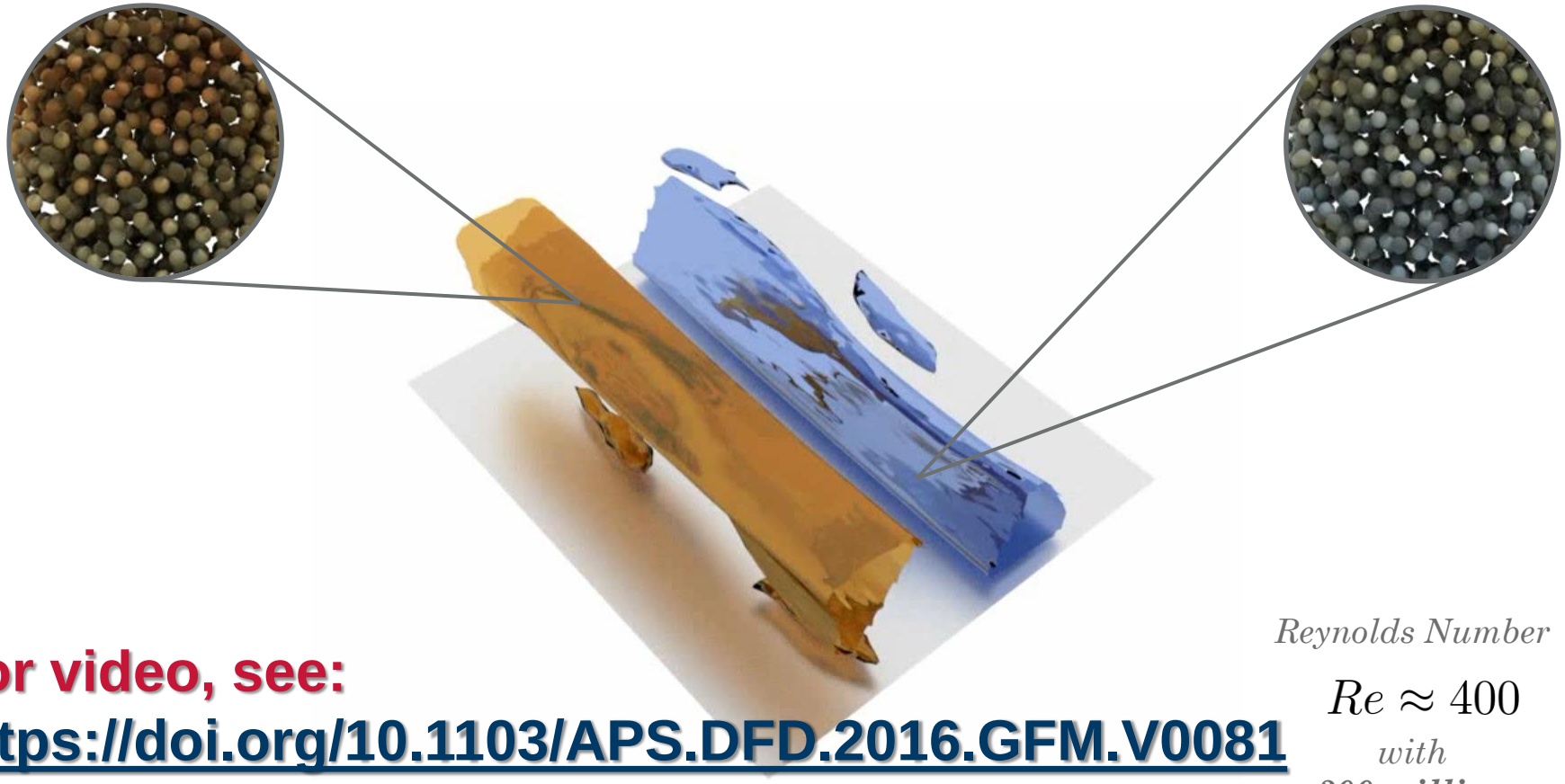
Molecular Simulation of Turbulence



For video, see:
https://doi.org/10.1103/APS.DFD.2016.GFM.V0081

Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$Re \approx 400$

with
300 million molecules

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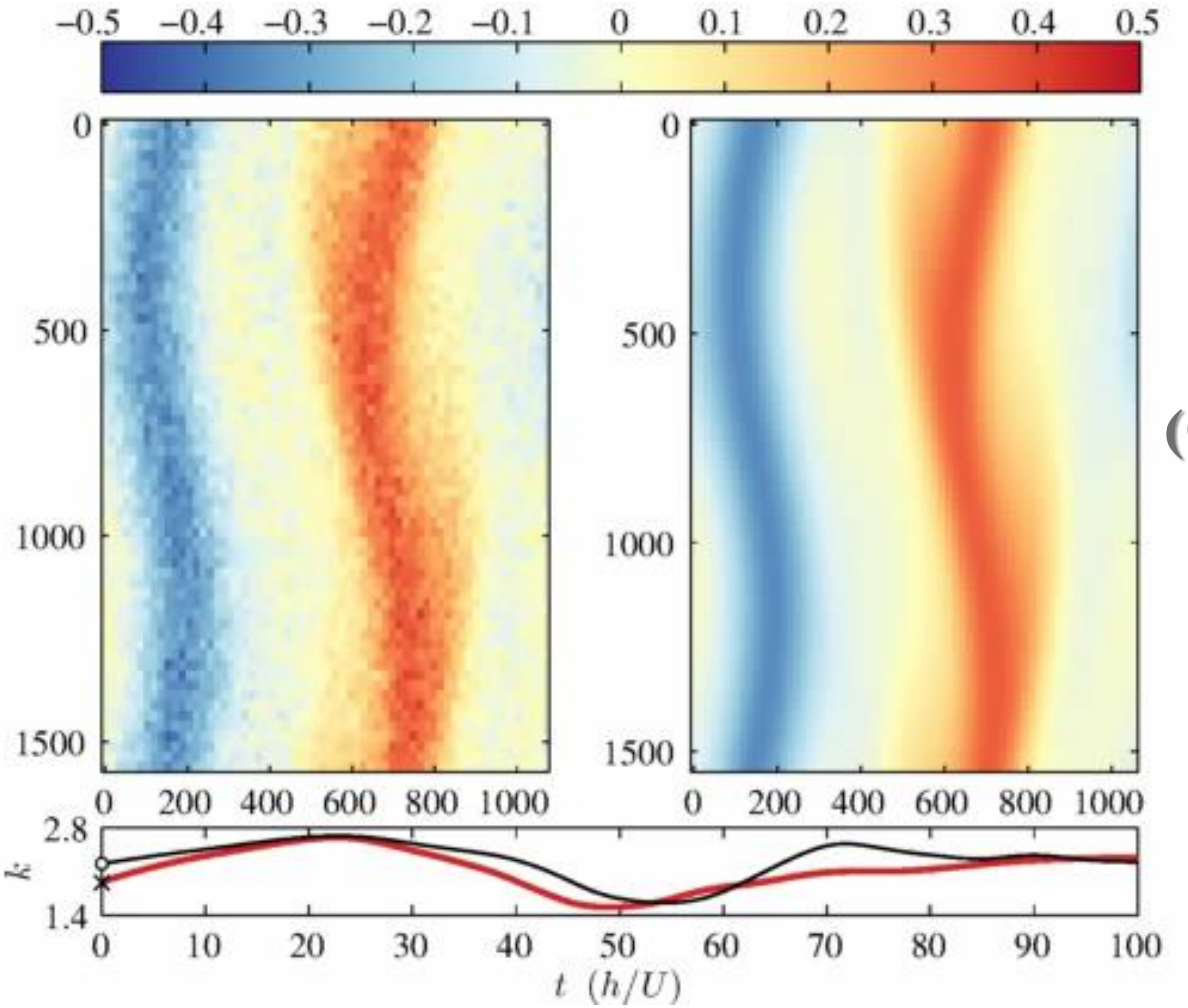
Molecular Simulation of Turbulence

Centre slice velocity



MD

Own code written in Fortran and parallelised using MPI

CFD (Channelflow)

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

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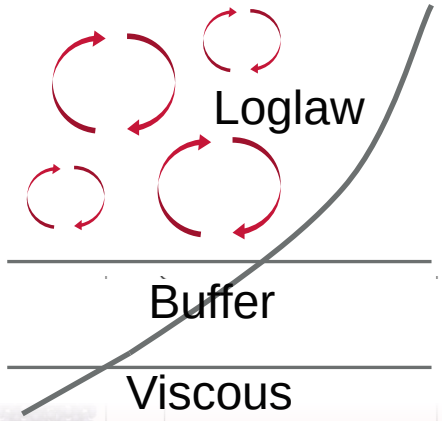
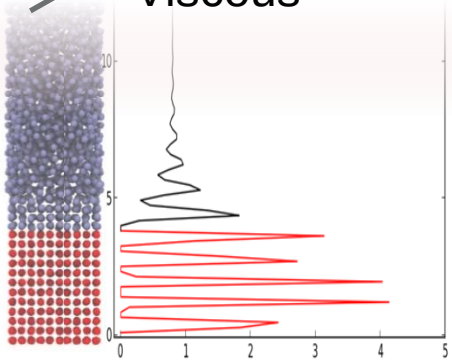
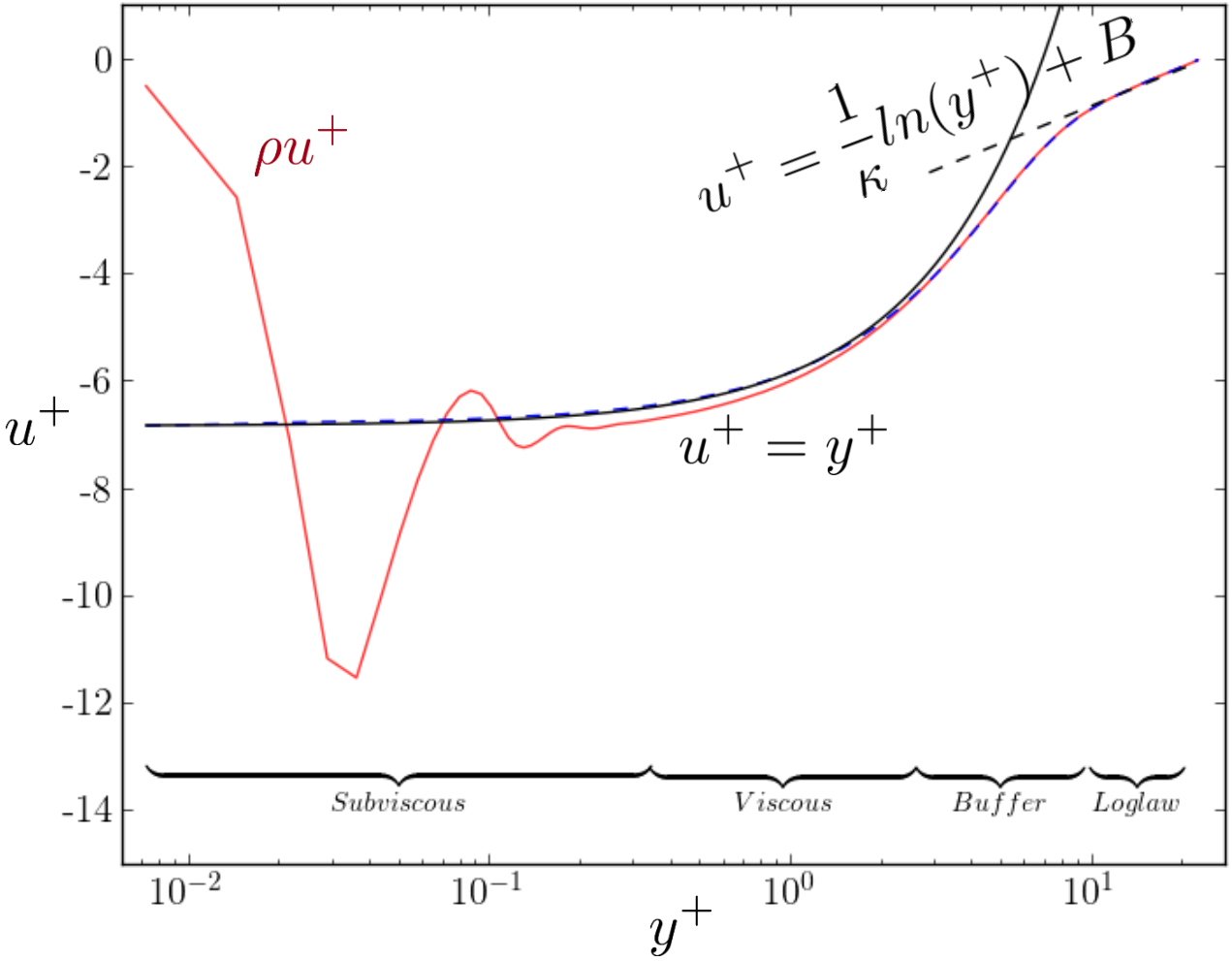
Law of the wall





Subviscous? (MD)



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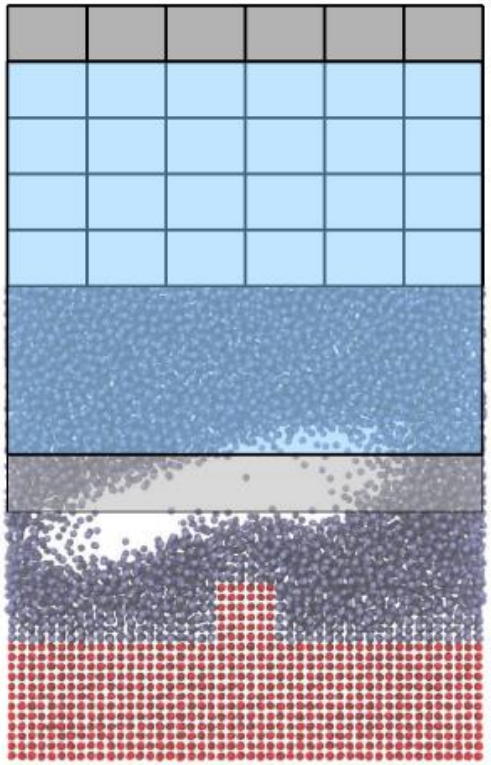
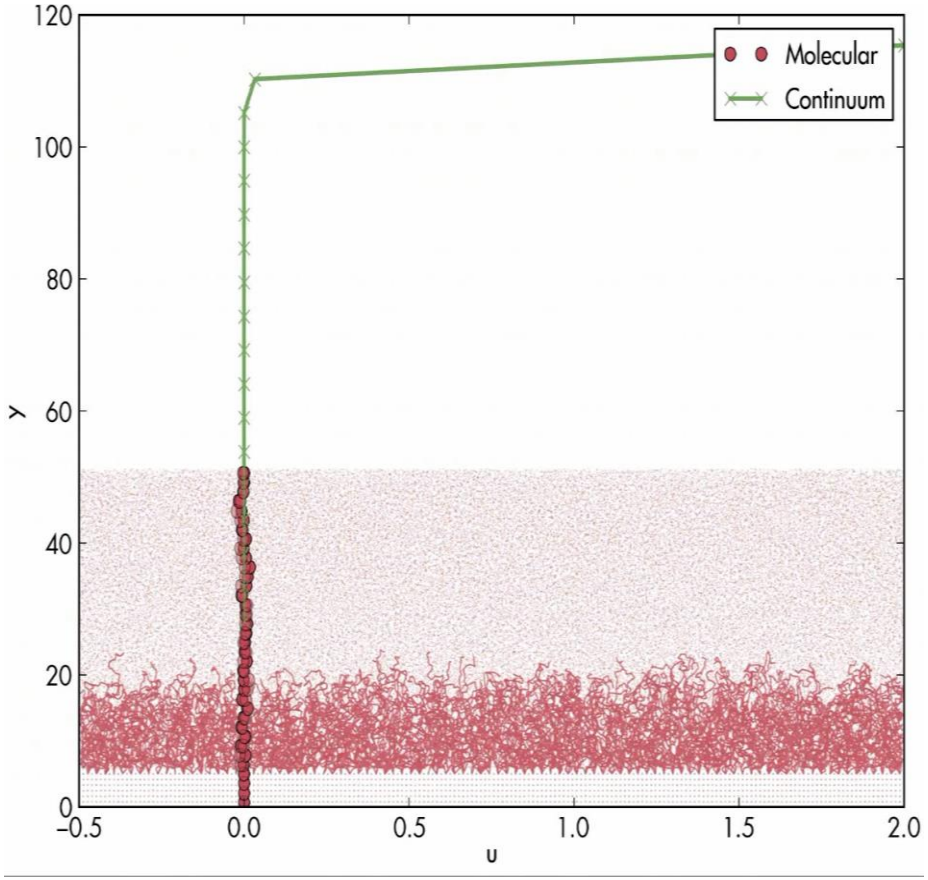
Coupled Simulation (The Extension to Coupling)



CFD Region

Overlap Region

MD Region



With David Trevelyan, Lucian Anton, Eduardo Fernado-Ramez, David Heyes and Daniele Dini

Coupled Simulation

- For turbulent flow, the timescales must evolve together; We cannot separate into pseudo-steady cases
- For nucleation the molecular provides an instance of an evolving bubble to the continuum
- Gain unique insight into the effect of wall textures, chemical coatings, effects of fouling, etc
- The timescales are very far from industrial, but validity of dimensionless analysis means we gain insight
- This assumption is the same in all types of coupled simulation – MD is representative of larger scale
- We still need large scale simulations and coupling allows system sizes which would be too expensive with MD

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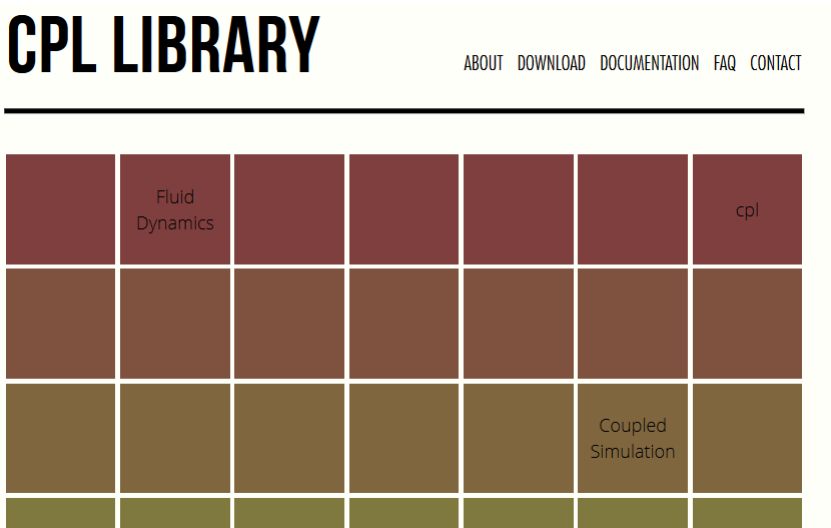
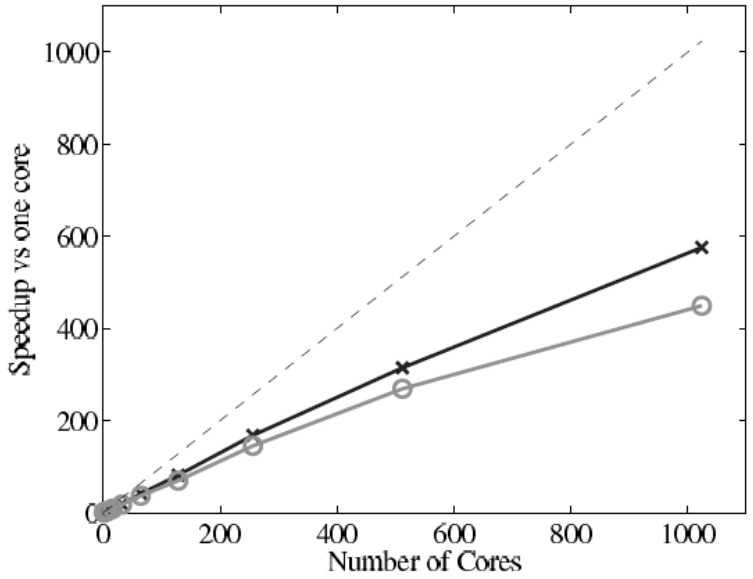
Large Scale Simulation : CPL library

- 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 integration testing, no external dependencies beyond standard packages and suite of Python and google tests
- Minimal set of functions and examples to 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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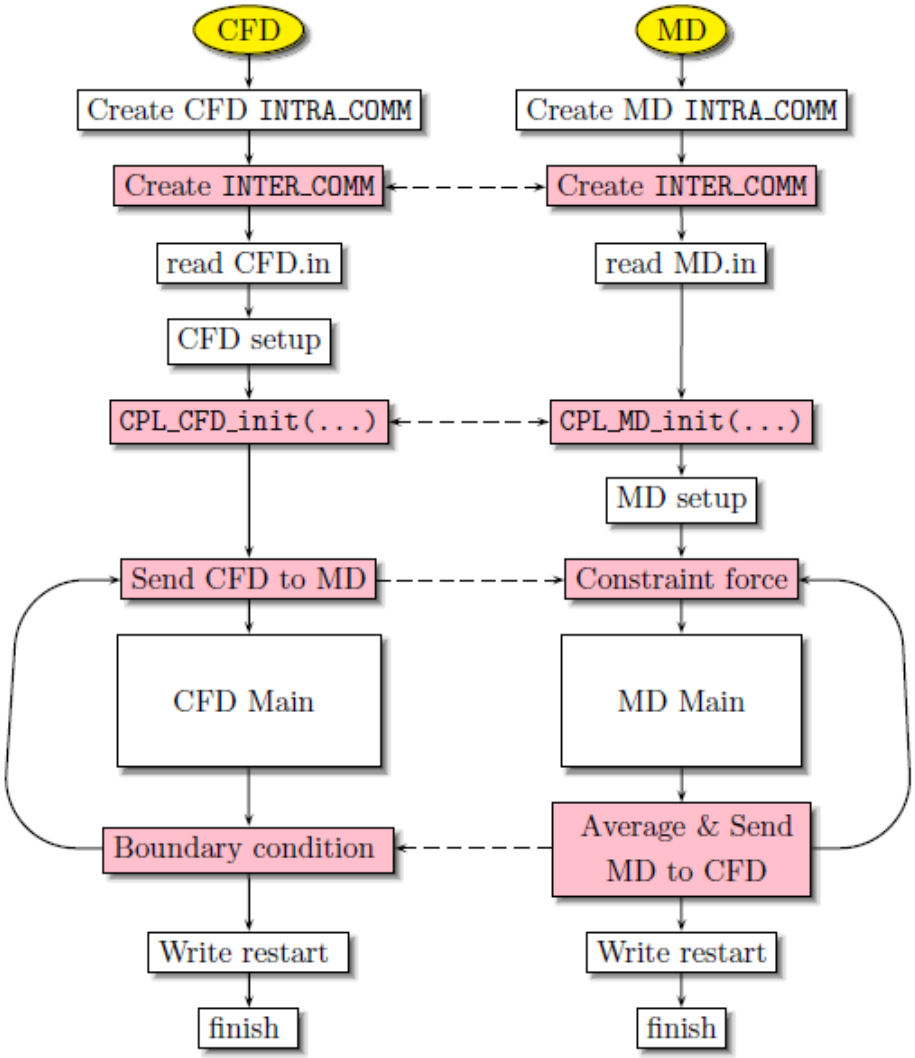
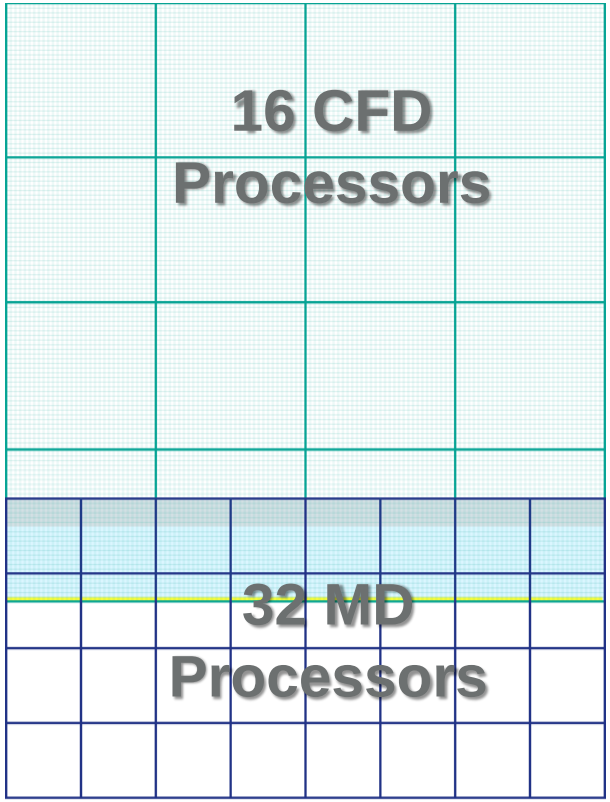
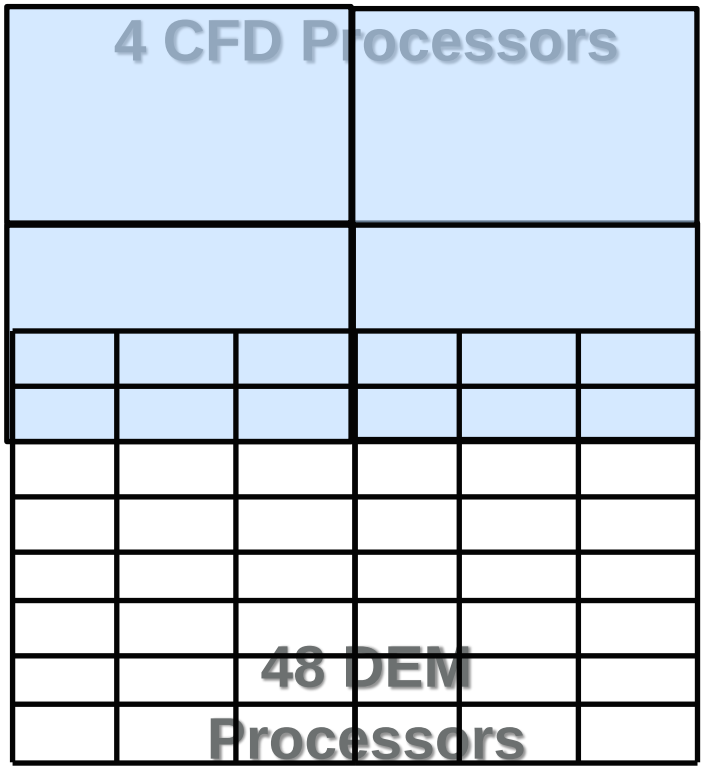
Large Scale Simulation : CPL-library



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



Granular Mechanics



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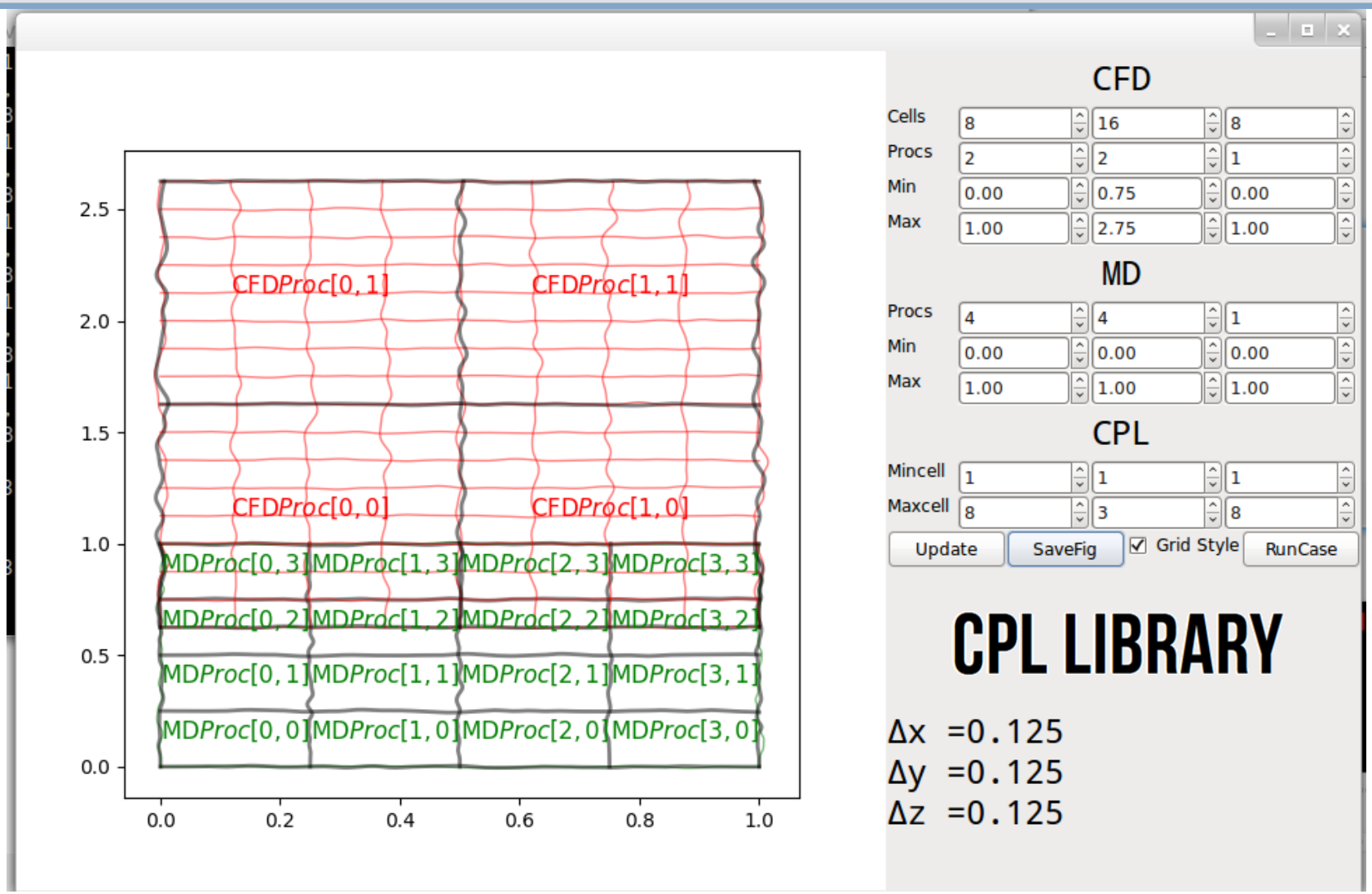
Topology Design Tool



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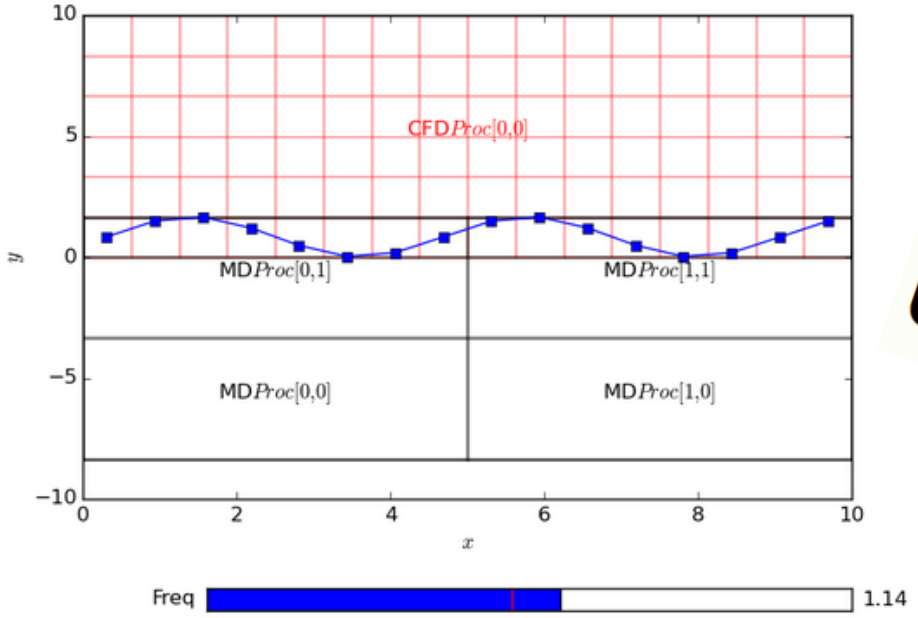
Minimal Examples to Lower Barrier to Entry



CPL LIBRARY

MINIMAL CFD AND MD CODE WITH COUPLING

Bringing the previous examples of topological setup and data exchange, along with a minimal CFD solver for the 2D unsteady diffusive equation,

$$\frac{\partial u}{\partial t} = \nu \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right]$$

Key Points

- We need easy to use, well tested and highly scalable computing to lower barrier to entry
- Molecular Fluid Dynamics has the potential to be a rich area of research at the molecular **timescale**!
- Domain decomposition is NOT a boundary for CFD, it is for accelerating molecular simulation
- Molecular details are not simply an inconvenience to be ignored, many important insights
- Direct benefits to industry both from the new cases which are only possible with coupled simulation and from development of new closure relationships

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Coupling Overview

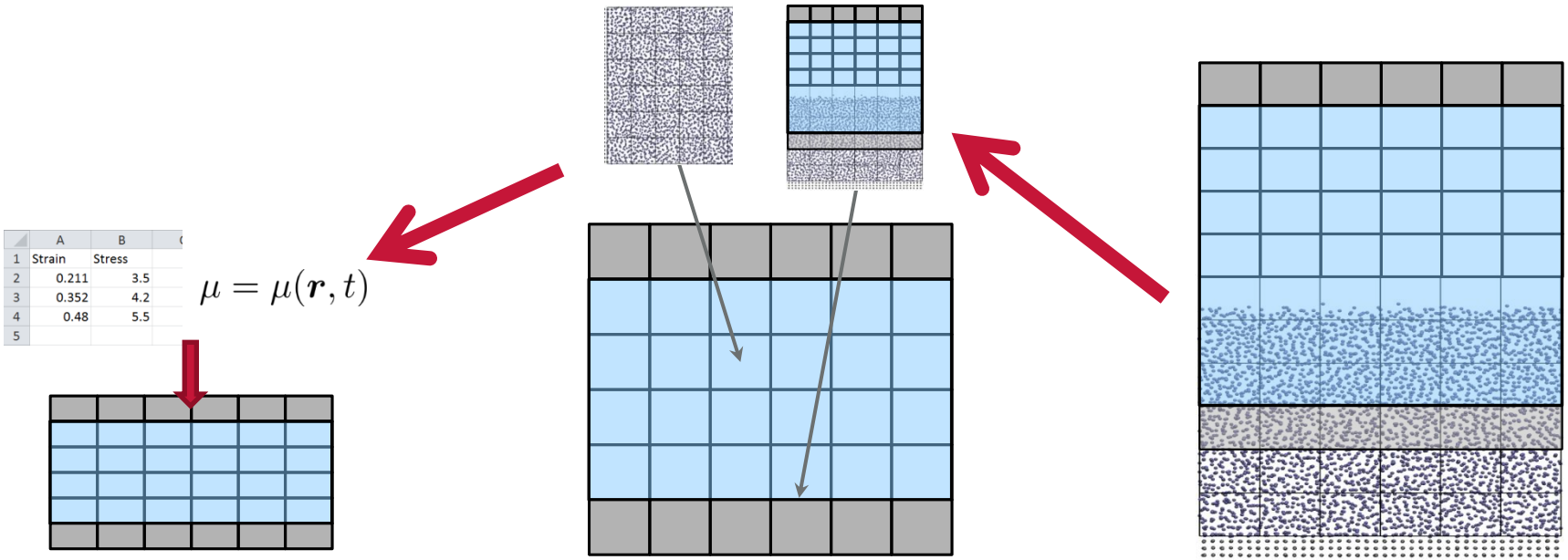

Table Lookup or Coefficients

- Assumes phenomenon can be parameterised
- By using coupling we gain new data and new ways of doing this

Embedded Models (HMM)

- Separate **timescales** and lengthscales
- Assumes phenomenon can be modelled using steady state cases

Domain Decomposition

- Same **timescale**
- Systems evolve together
- Limited to molecular scale studies but similarity is valid

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Thank you – Any Questions?

Collaborations with David Heyes, Daniele Dini, Tamer Zaki, David Trevelyan, Eduardo Fernando-Ramos,

Omar Matar, Erich Muller and Richard Craster