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# Coupling Molecular Dynamics to Continuum Models for Fluid Mechanics

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20/07/17

Collaborations with David Heyes, Daniele Dini, Tamer Zaki,
David Trevelyan, Eduardo Fernando-Ramos,
Omar Matar, Erich Muller and Richard Craster

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# Overview

- Introduction
  - Continuum Fluid Dynamics (CFD)
  - Molecular Dynamics (MD)
  - Coupling
- Some Work on the Derivation of a Conservative Coupling Schemes
  - Mathematical Framework
  - Constrained Dynamics
- Simulation Results
  - Laminar Couette Flow and Nucleation
  - Minimal Channel Turbulent Couette Flow

# Computational Fluid Dynamics

- Assumed continuous at every point in space
  - Mass Conservation

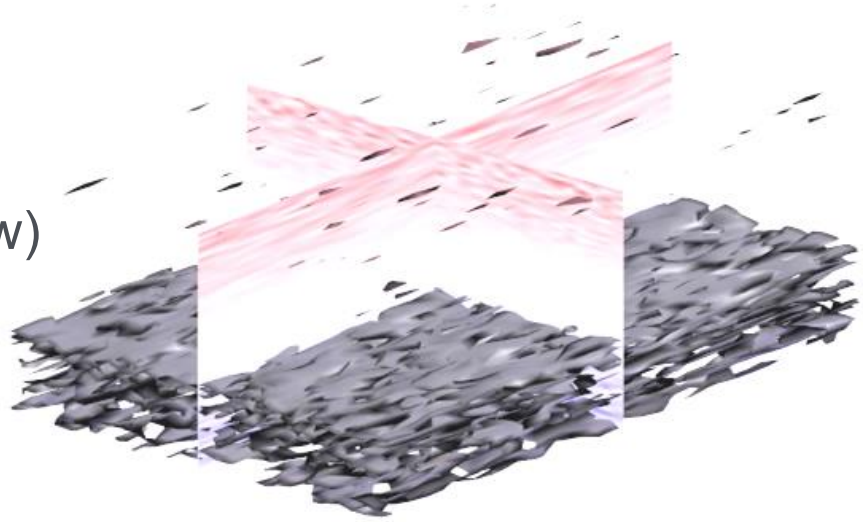
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - 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

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# Computational Fluid Dynamics

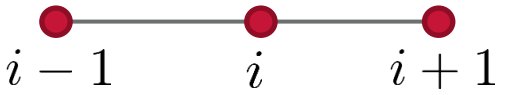
- The Navier-Stokes Equation

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

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

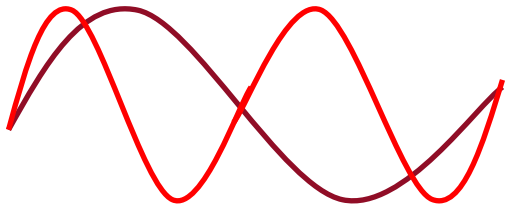
- Finite Difference Method

$$\frac{\partial u_i}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$



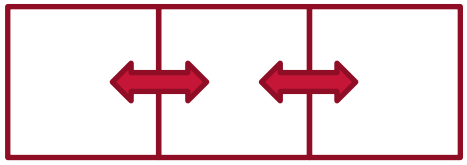

- Spectral Methods

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



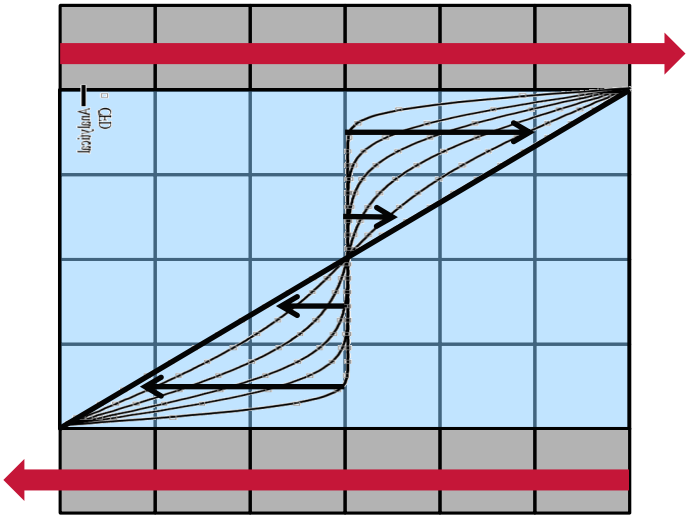
- Finite Volume ($0^{th}$ order element) Method

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



# Computational Fluid Dynamics

- Domain split into a number of cells (points)
  - 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
  - Local thermodynamic equilibrium vs. hydrodynamic scales
  - Knudsen Number fairly useless for dense fluids

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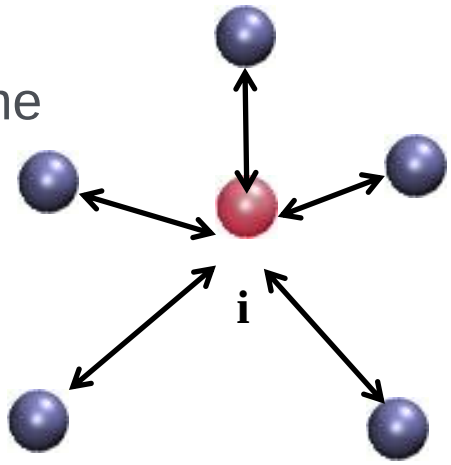
# Molecular Dynamics

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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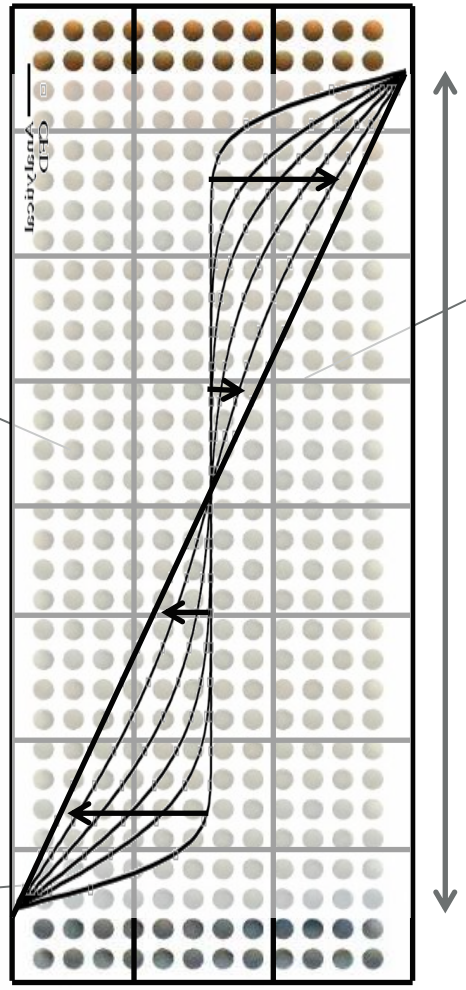
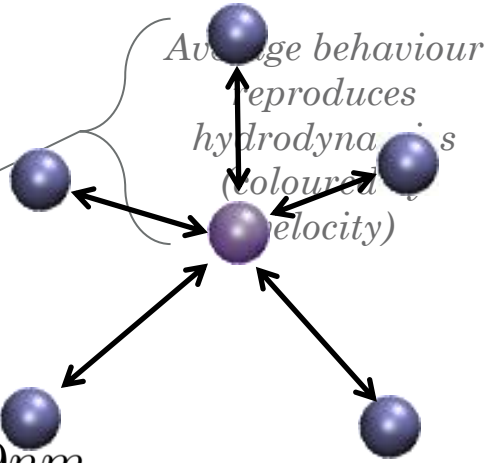
# Molecular Dynamics

*Liquid structure causes viscosity*



*Stick-slip near walls*



$H \approx 9nm$

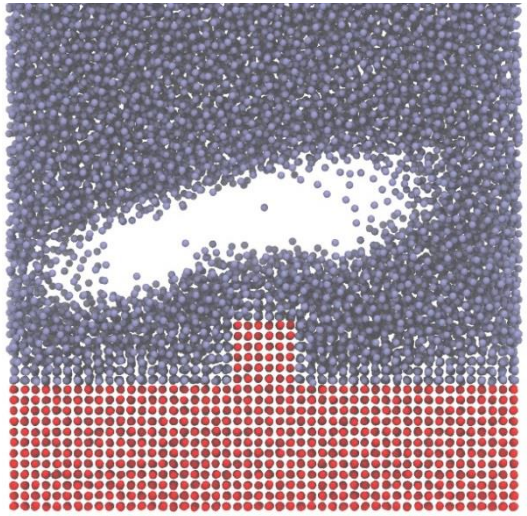
*Reynolds Number*

$Re \approx 15$

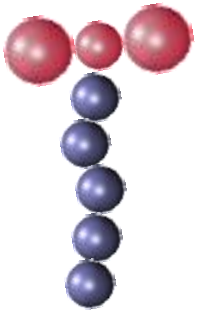
*with*

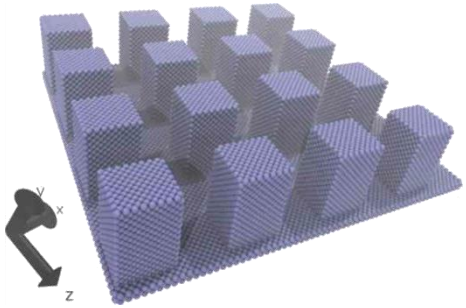
***4096 molecules***

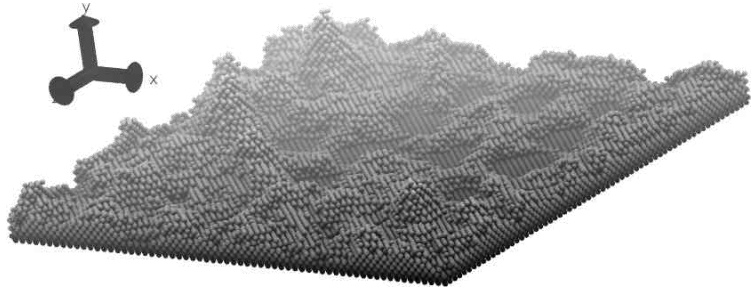
# Molecular Dynamics

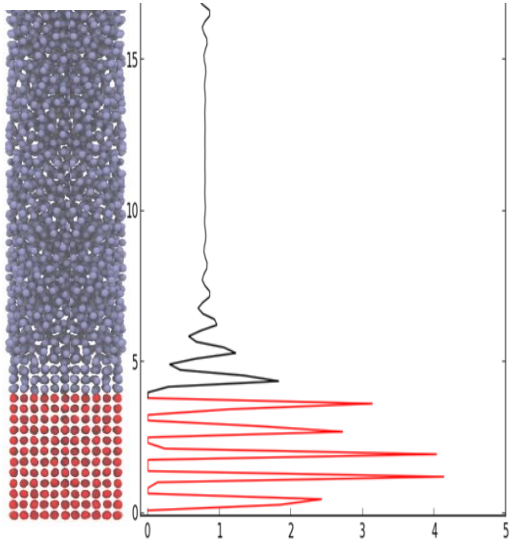


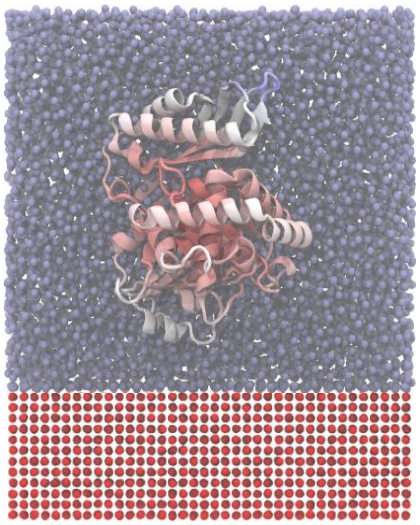
*Superspreading Surfactant, e.g. Silwet-L77*









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# Coupling Overview

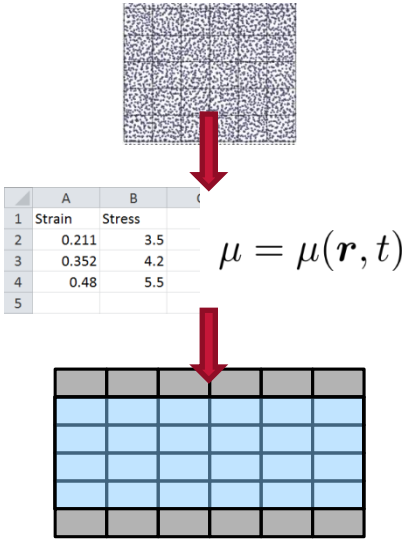
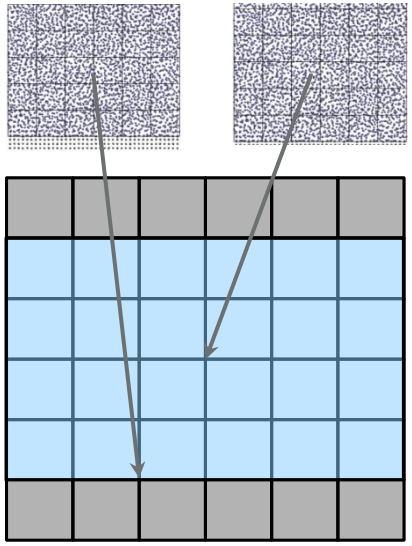


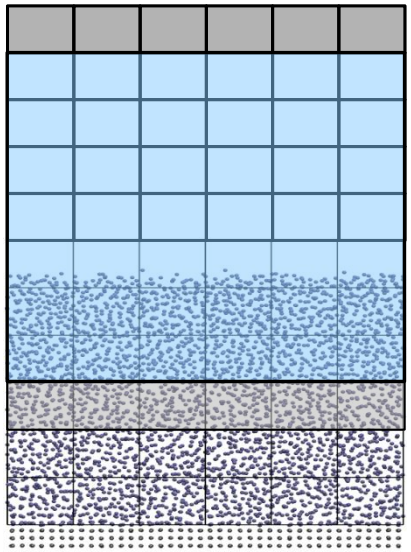

**Table Lookup or Coefficients**

MD parameter study stored in table and CFD uses data



**Embedded Models (HMM)**

MD – embedded in a CFD simulation [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)

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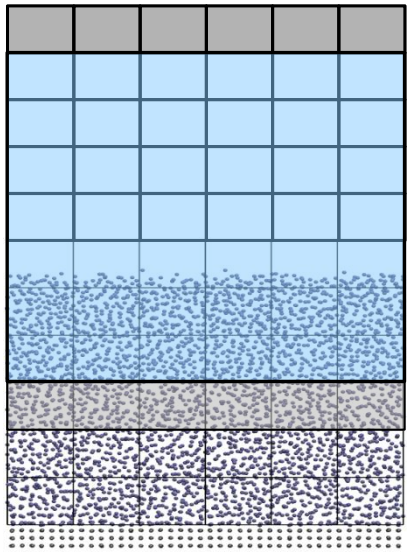
# Coupling Assumptions

- **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

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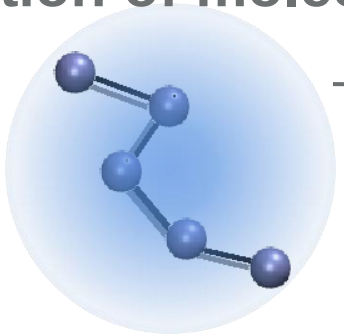
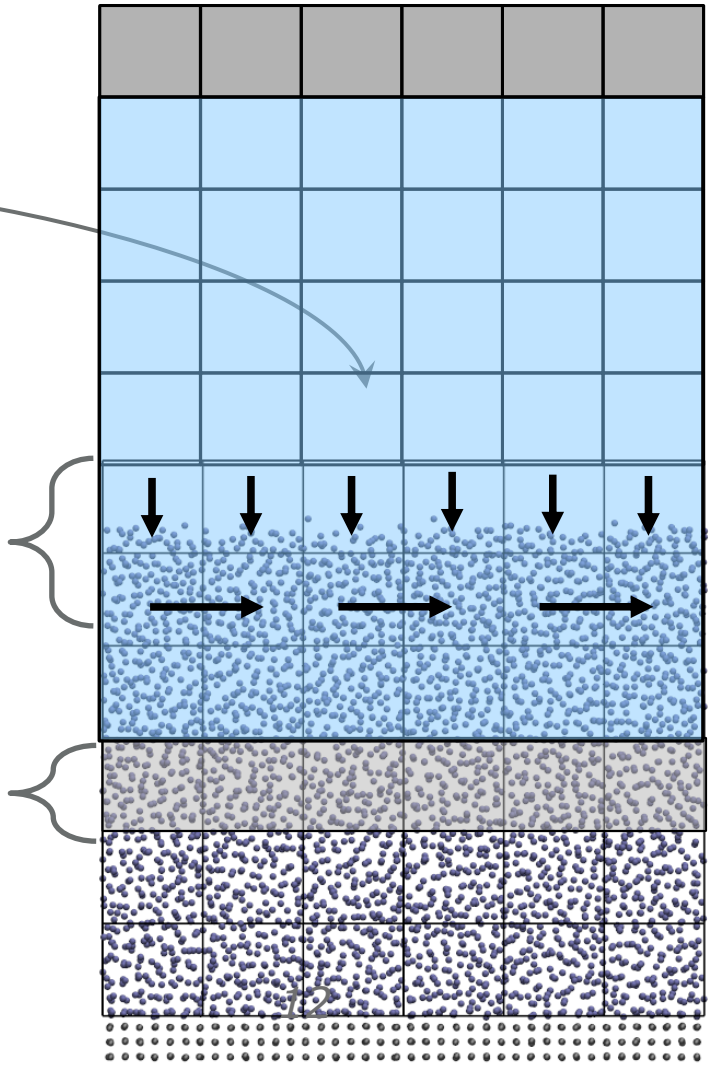
# Domain Decomposition

## Boundary force and insertion of molecules



*USHER, AdRES and Fade RDF based force*



**CFD→MD Boundary condition**

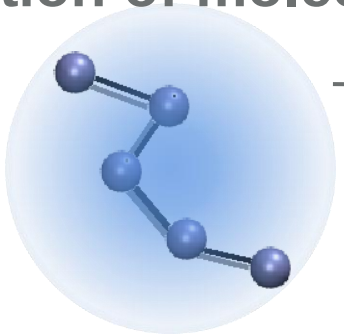
**MD→CFD Boundary condition**

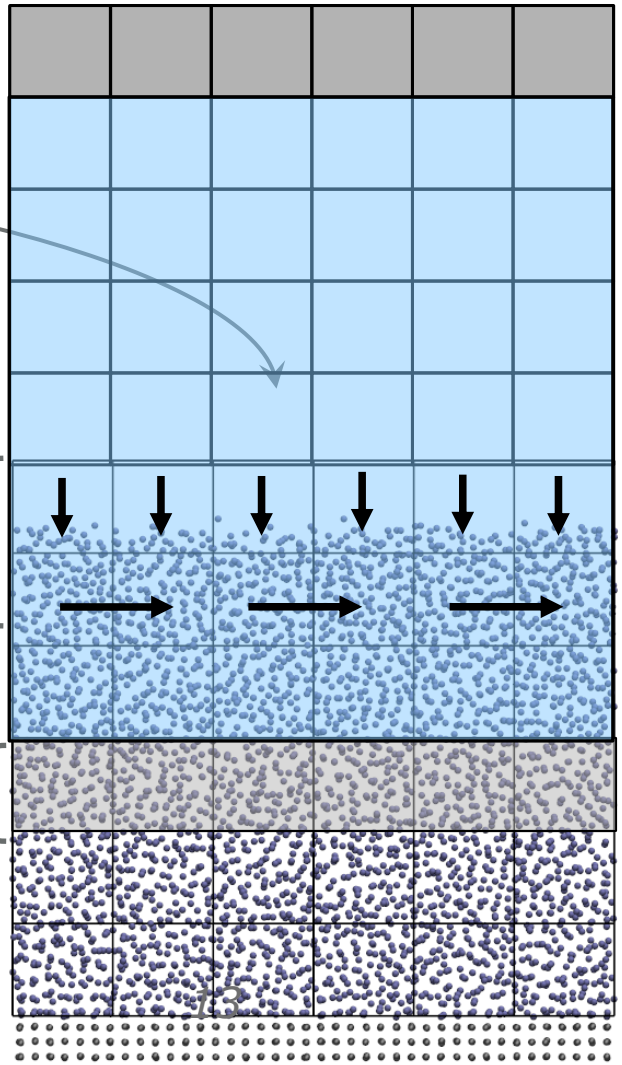
*O'Connell Thompson (1995), Hadjiconstantinou (1998), Flekkoy (2000), Nie et al (2004). All since 1995, and we have over 100 years of statistical mechanics*

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

# 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 $2\times396$, 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*

J. H. Irving and John G. Kirkwood
Gates and Crellin Laboratories of Chemistry† No. 1463, Pasadena, California

(Received November 21, 1949)

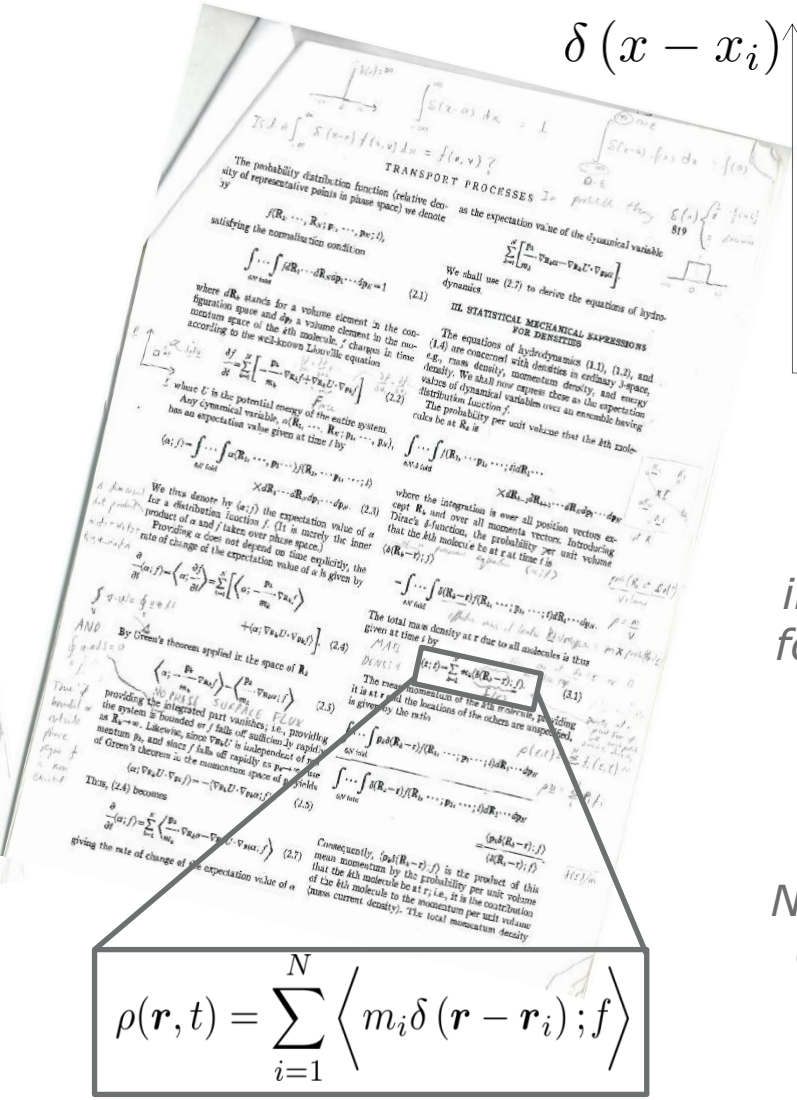
The equations of hydrodynamics—continuity equation, equation of motion, and equation of energy transport—are derived by means of the classical statistical mechanics. Thereby, expressions are obtained for the stress tensor and heat current density in terms of molecular variables. In addition to the familiar 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

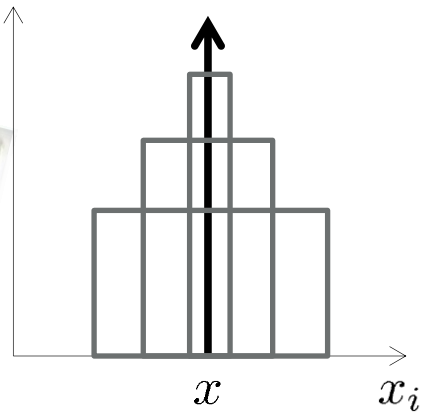
* This work was supported by the U. S. ONR under Contract Nonr-244 w/h the California Institute of Technology.
† Contribution No. [illegible].
[1] J. G. Kirkwood, J. Chem. Phys. 14, 180 (1946).
[2] M. Born and H. S. Green, Proc. Roy. Soc. A188, 10 (1946).
[3] Kirkwood, Buff, and Green, J. Chem. Phys. 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*

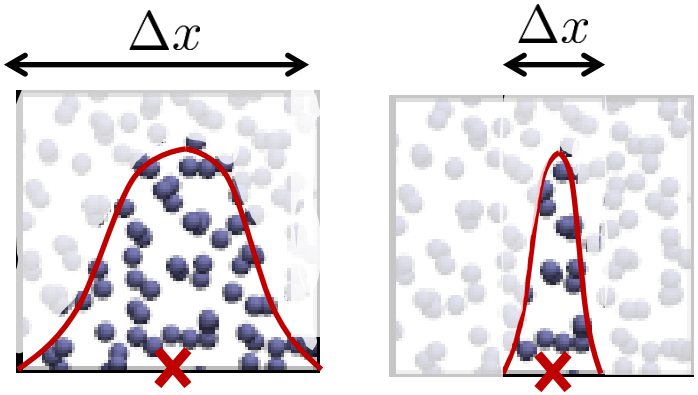
***BUT***

*No molecule is ever exactly at a point*

# Linking the two formulations

- Irving and Kirkwood (1950) express field based quantities using the Dirac delta functional and ensemble averages

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




- Same **temporal** scale

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

$$\delta(x)=\lim_{\Delta x\to 0}\frac{1}{\Delta x}e^{x^2/\Delta x^2}$$

- Same **spatial** scale
  - Dirac delta formally correct but no molecule ever at point r
  - Any approximation to the Dirac delta is no longer formally correct
  - A discrete system can only be approximately represented using a continuous field

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# The Control Volume Formulation

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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

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



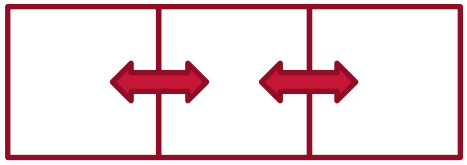

- Spectral Methods

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



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

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



# The Control Volume (Weak) Form

- The “weak formulation” expressed the equations in integrated form

$$\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right) dV$$

- Integrating the Dirac delta function exactly provides a combination of Heaviside functions

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*Integrating the Dirac delta functional gives a combination of Heaviside functionals, which can:*

- *Be mathematically manipulated to give fluxes and forces*
- *Be implemented directly in MD codes*
- *Be linked to the continuum control volume.*

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# The Control Volume Functional

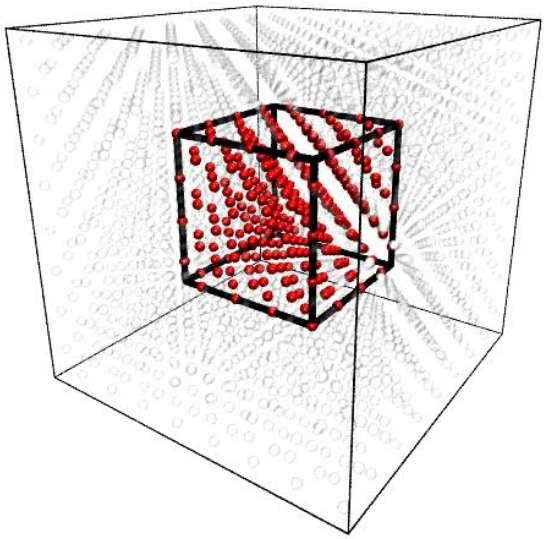
- The Control volume functional is the formal integral of the Dirac delta functional in 3 dimensions (3D top hat or box car function)

$$\vartheta_i \equiv \int_{x^-}^{x^+}\int_{y^-}^{y^+}\int_{z^-}^{z^+} \delta(x_i - x)\delta(y_i - y)\delta(z_i - z)dxdydz$$

$$= \left[H(x^+ - x_i) - H(x^- - x_i)\right]$$

$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$

$$\times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$



- In words

$$\vartheta \equiv \begin{cases} 1 & \text{if molecule is inside volume} \\ 0 & \text{if molecule is outside volume} \end{cases}$$

# Derivative yields surface fluxes and stresses

- Taking the Derivative of the CV function

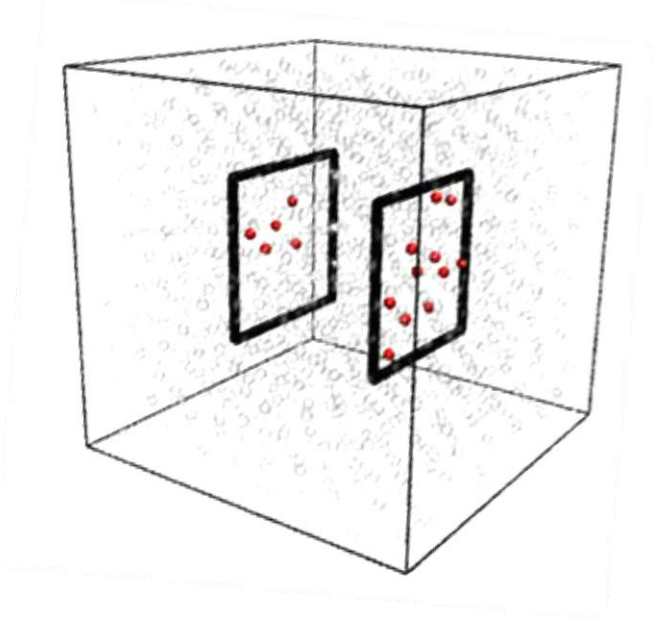
$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right] \times \left[H(y^+ - y_i) - H(y^- - y_i)\right] \times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

- Vector form defines six surfaces

$$d\mathbf{S}_i = \boldsymbol{i} dS_{xi} + \boldsymbol{j} dS_{yi} + \boldsymbol{k} dS_{zi}$$

- Or in words

$$d\mathbf{S}_i \equiv \begin{cases} \infty & \text{if molecule on surface} \\ 0 & \text{otherwise} \end{cases}$$



# The Control Volume (Weak) Form

- The “weak formulation” expressed the equations in integrated form

$$\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)dV = \sum_{i=1}^{N} m_i\vartheta_i \equiv \sum_{i\in\mathrm{Cell}}^{N_{\mathrm{Cell}}} m_i$$

$$\frac{d}{dt}\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i\frac{d\vartheta_i}{dt} = \sum_{i=1}^{N} m_i\frac{d\boldsymbol{r}_i}{dt}\cdot\frac{d\vartheta_i}{dr_i} = \sum_{i=1}^{N} m_i\boldsymbol{v}_i\cdot d\mathbf{S}_i$$

- Integrating the Dirac delta function exactly provides a combination of Heaviside functions, which can:
  - Be mathematically manipulated to give fluxes and forces
  - Be implemented directly in MD codes (assembly version)
  - Be linked to the continuum control volume (or finite volume) equations as they are no expressed in the same form

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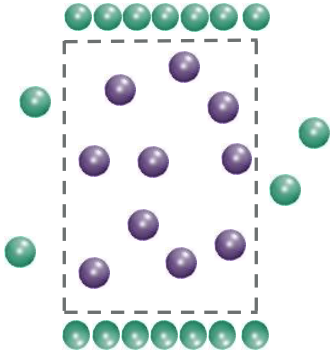
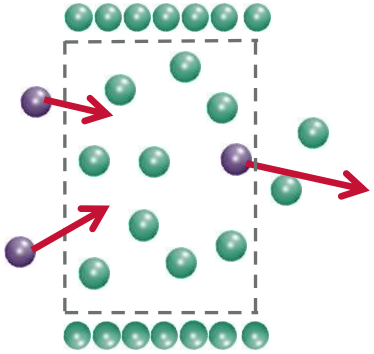
# Control Volume Functional

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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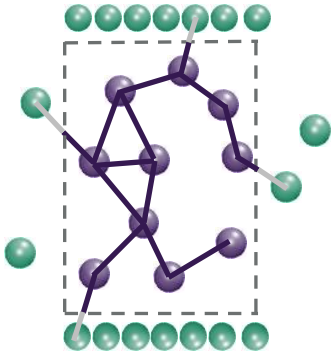
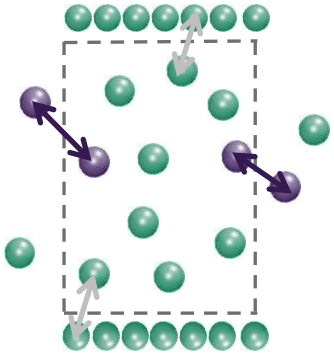
# Control Volume Functional - Forces

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

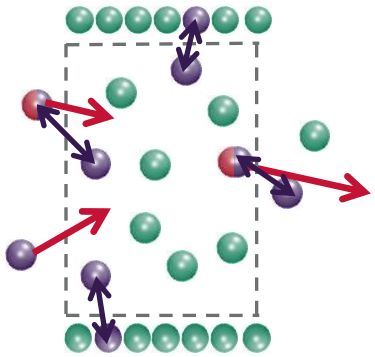
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\boldsymbol{S}_i$$

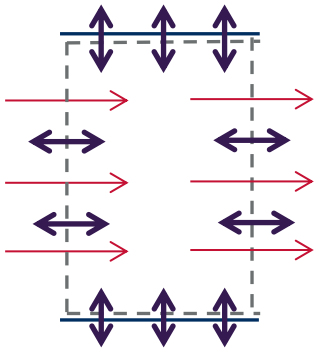
$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u} \cdot d\mathbf{S}$$

- 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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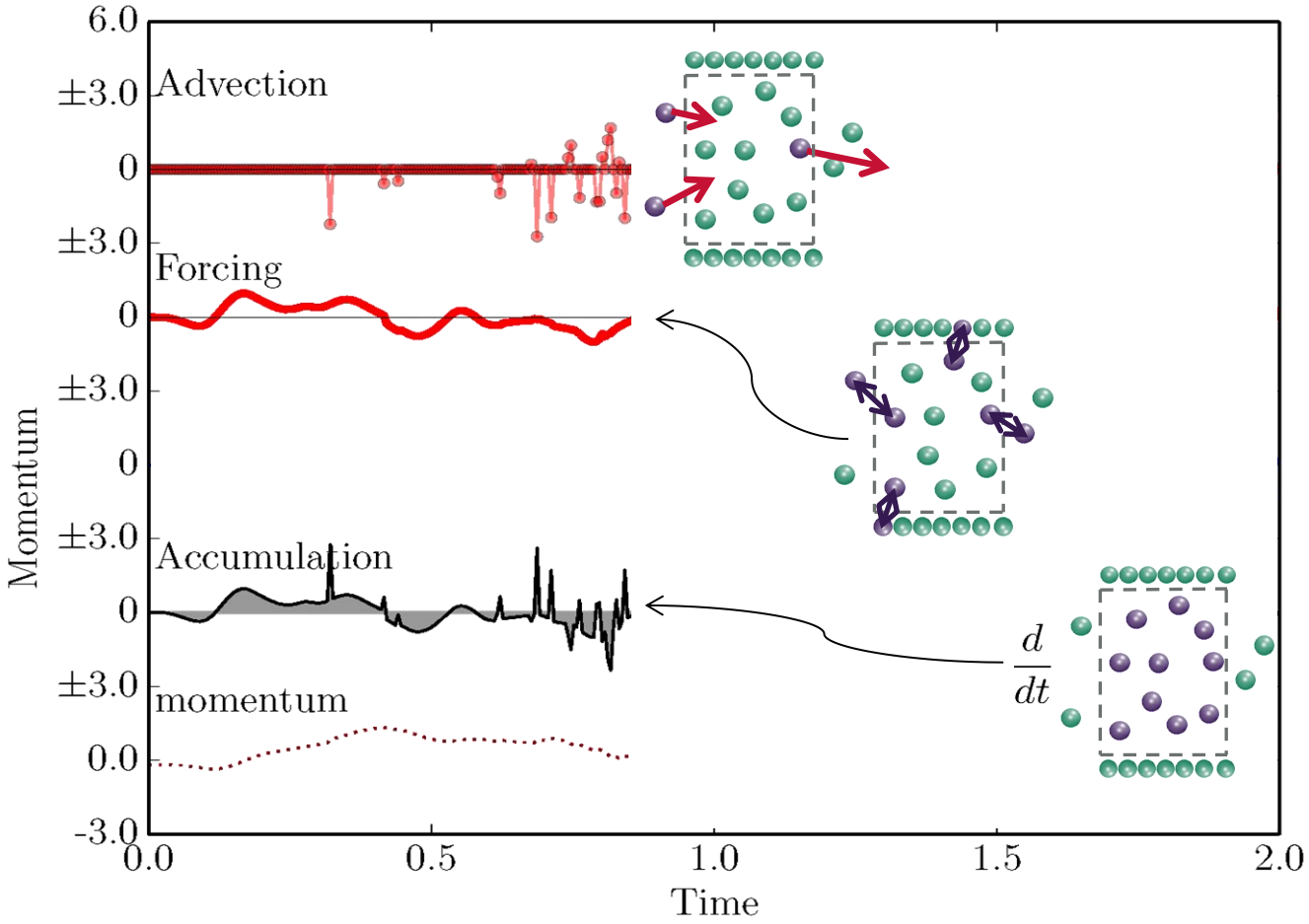
# Exact Conservation

## 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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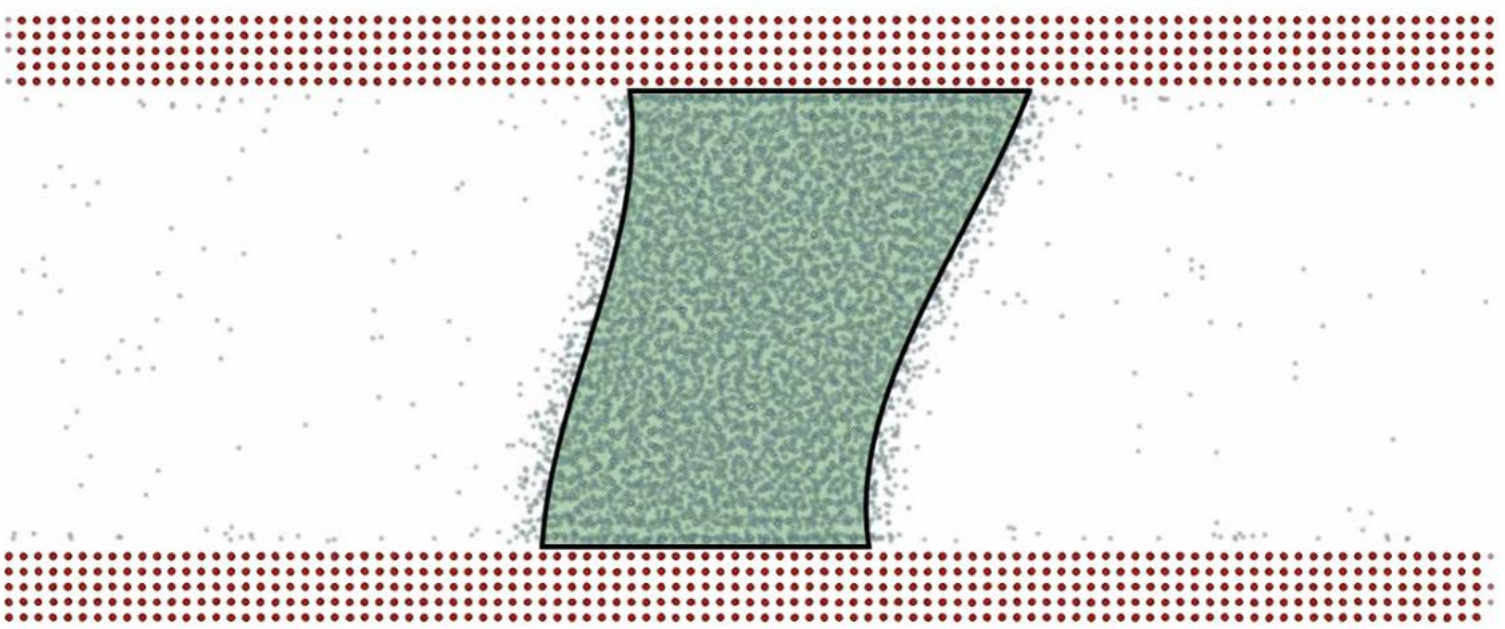
# Exact Conservation – Arbitrary Volume

**Results from any arbitrary volume**

- Accumulation = Forcing + Advection



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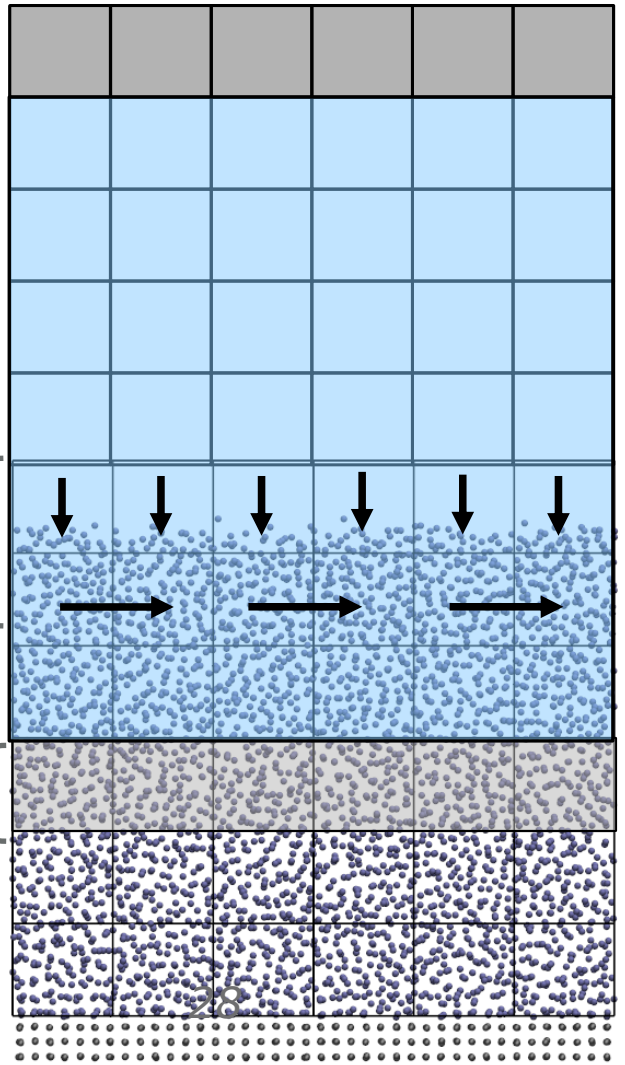
# Domain Decomposition

Consistent Framework ✓

CFD→MD Boundary condition

MD→CFD Boundary condition



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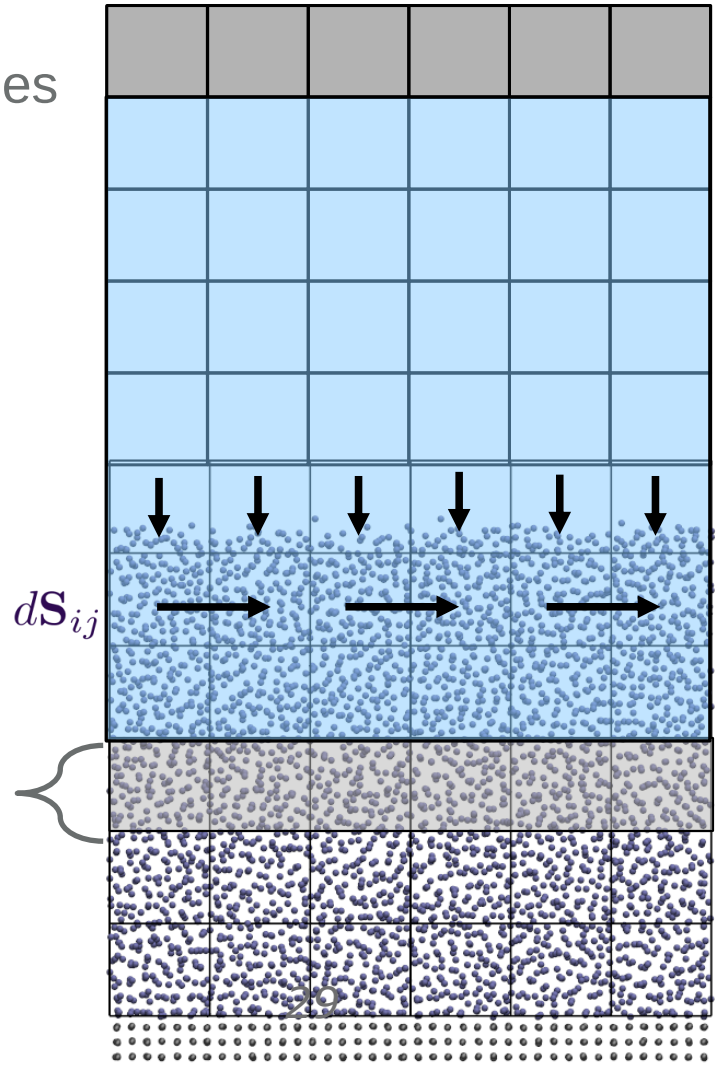
# Domain Decomposition

Only volume averages, fluxes and stresses

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

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

**MD→CFD Boundary condition**



# 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 (mathematical framework)
- Control Volumes are the only meaningful way to relate the two systems

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# Constrained Dynamics

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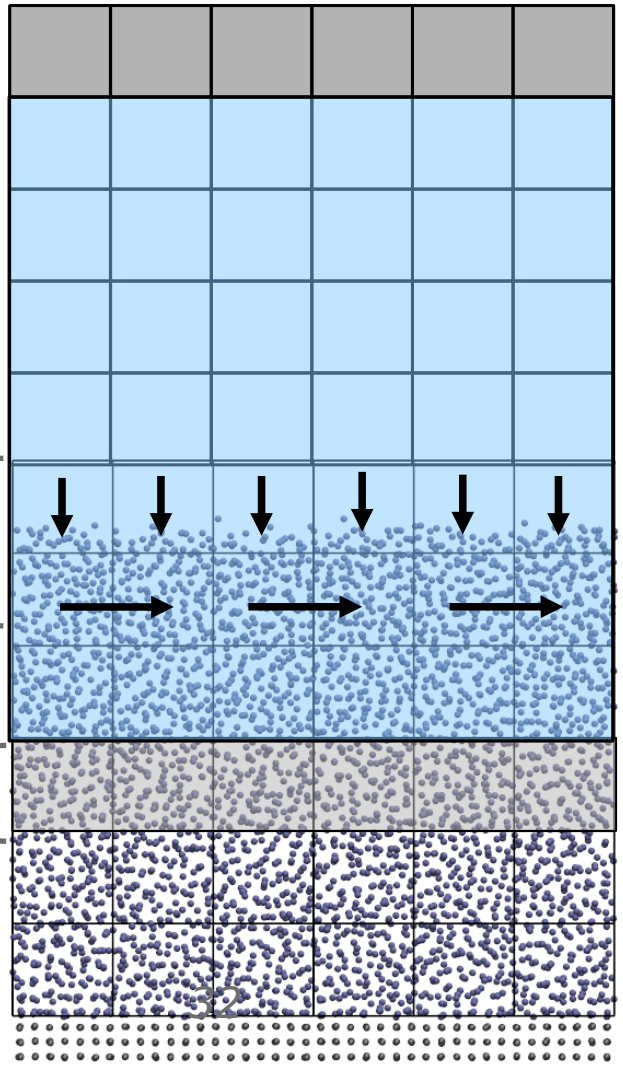
# Domain Decomposition

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 (Based on years of NEMD theory)

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

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# Constrained Control Volume

## Gauss Principle of Least Constraint Applied

- Valid for any form of constraint (Based on years of NEMD theory)

$$\frac{\partial}{\partial \boldsymbol{r}_{ij}} \sum_{i=1}^{N} \left[\boldsymbol{F}_i - \boldsymbol{r}_{ij}\right]^2 - \boldsymbol{\lambda} \cdot \boldsymbol{g} = 0 \qquad g(\boldsymbol{r}_i, \dot{\boldsymbol{r}}_i) = \sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i - \int_V \rho \boldsymbol{u} dV = 0$$

## Resulting equation is Newton's Law plus a correction

- Exact control of momentum to machine precision
- Iteration needed to convergence

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i \vartheta_i}{M_I} \left[ \frac{d}{dt} \int_V \rho \boldsymbol{u} dV - \frac{d}{dt} \sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i \right]$$

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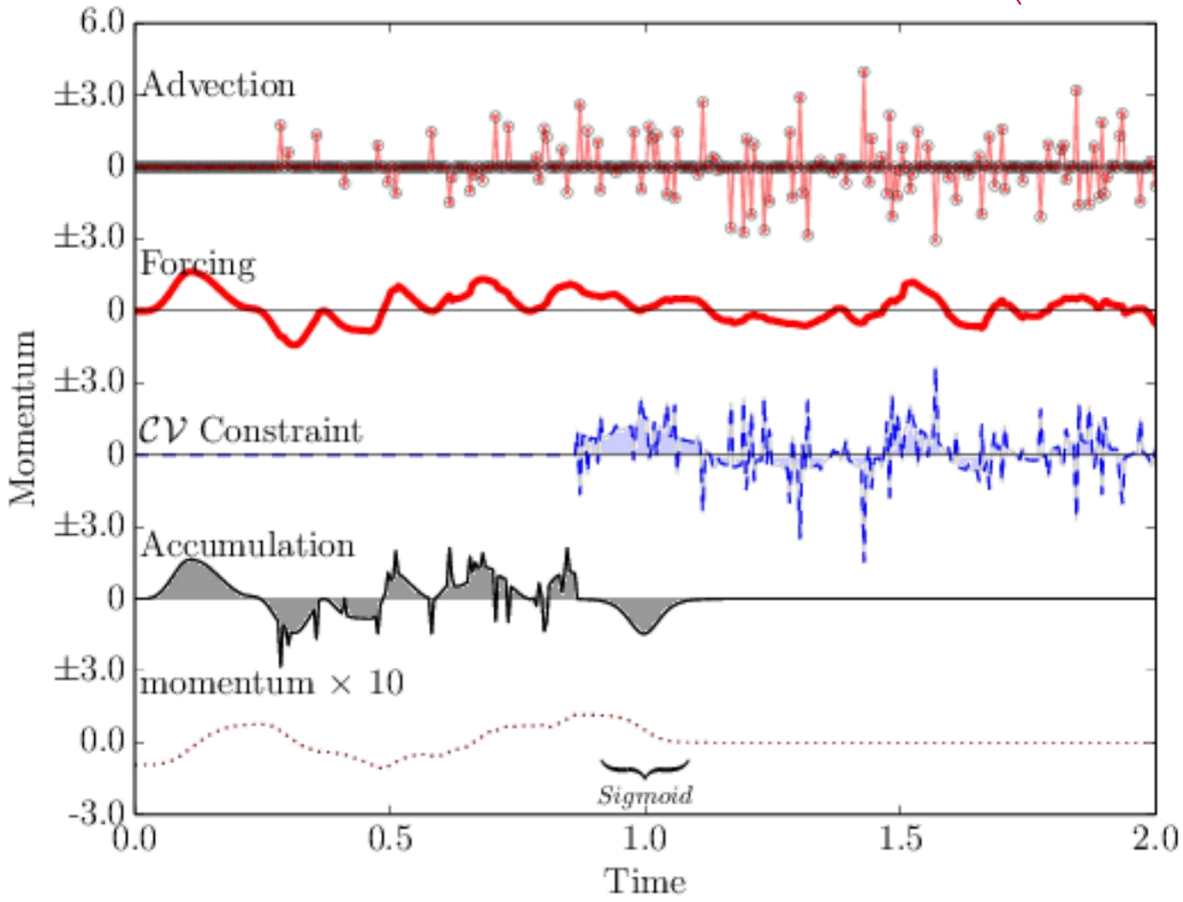
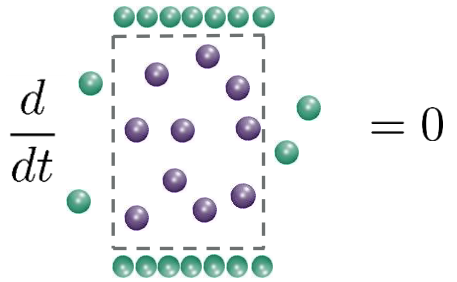
# Constrained Control Volume

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i \vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho \boldsymbol{u} dV - \frac{d}{dt}\sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i\right]$$

$0$




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



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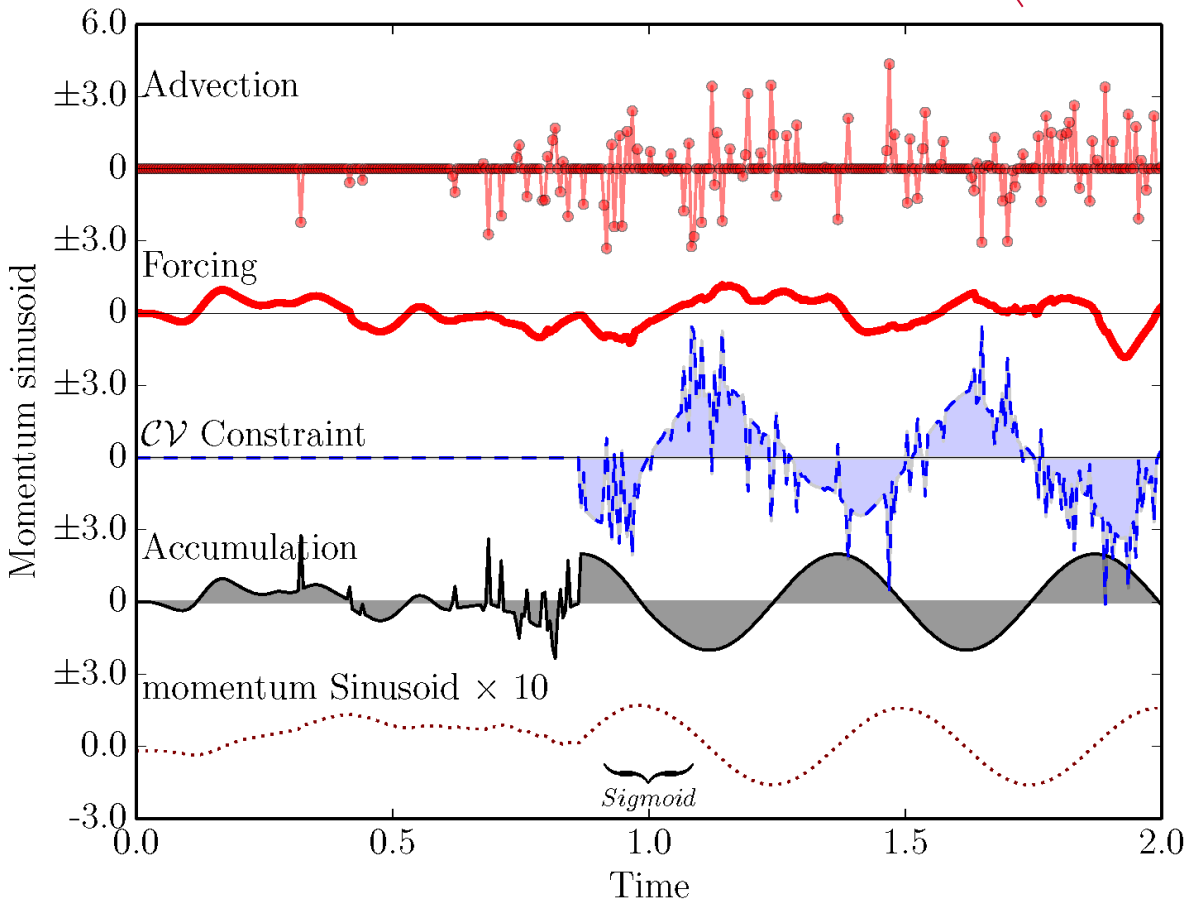
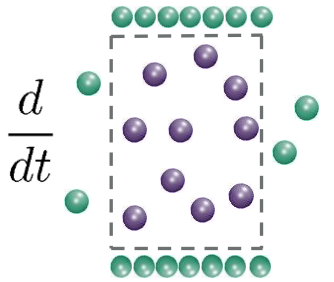
# Constrained Control Volume

$$\sim cos(t)$$

$$m_i\ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV - \frac{d}{dt}\sum_{i=1}^{N} m_i\dot{\boldsymbol{r}}_i\vartheta_i\right]$$




- 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

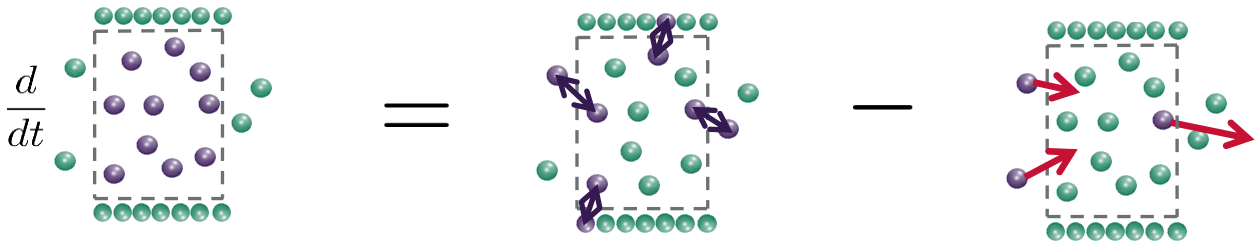
## Only the average for the whole control volume is constrained

- Force is the same for all molecules in volume form

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + \frac{m_i \vartheta_i}{M_I} \left[ \frac{d}{dt} \int_V \rho \boldsymbol{u} dV - \frac{d}{dt} \sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i \right]$$

## By distributing over molecules, we can prevent jumps and add extra constraints

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



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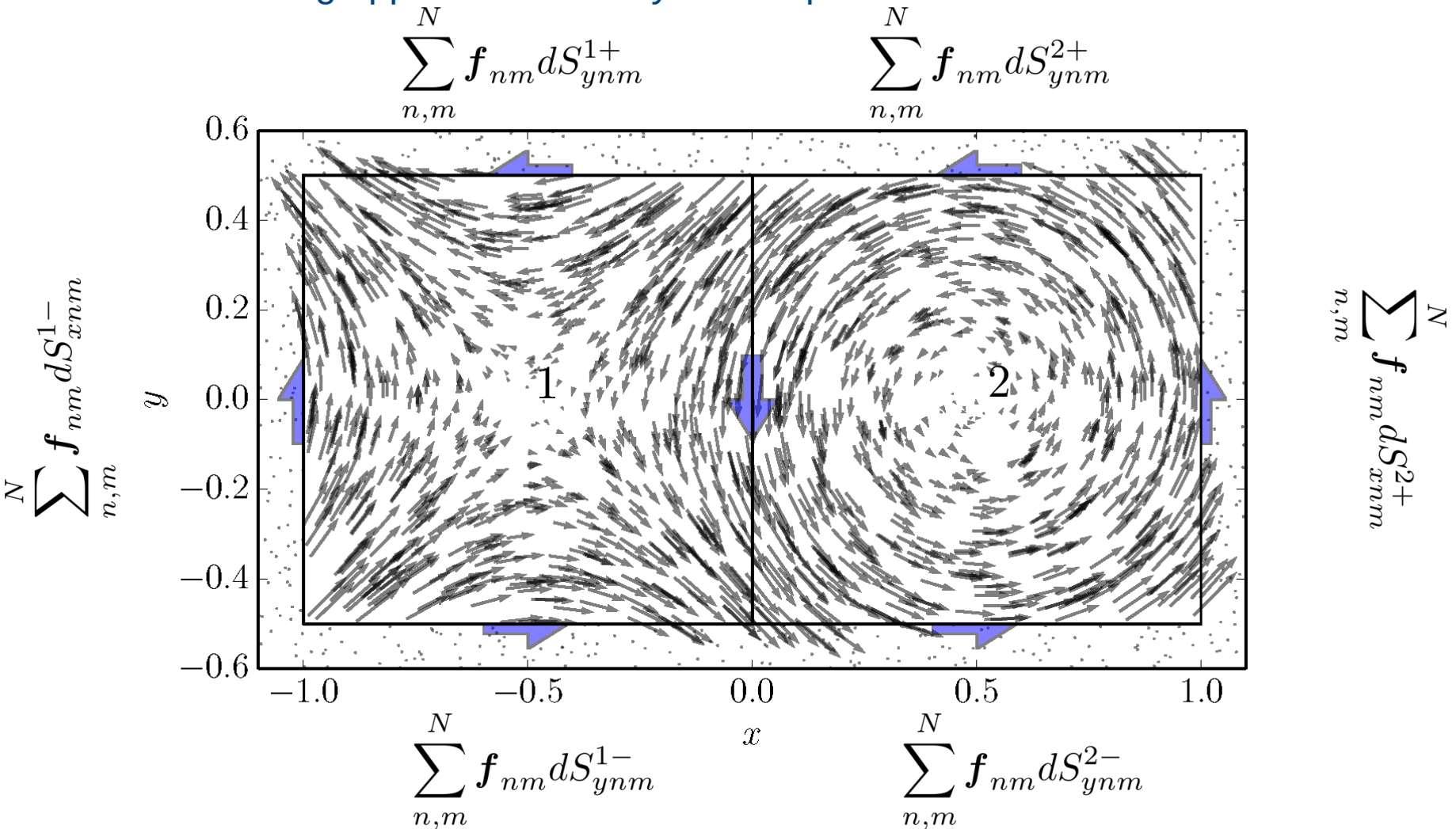
# Constrained Control Volume

- Forcing applies an arbitrary 18 component 3D stress field



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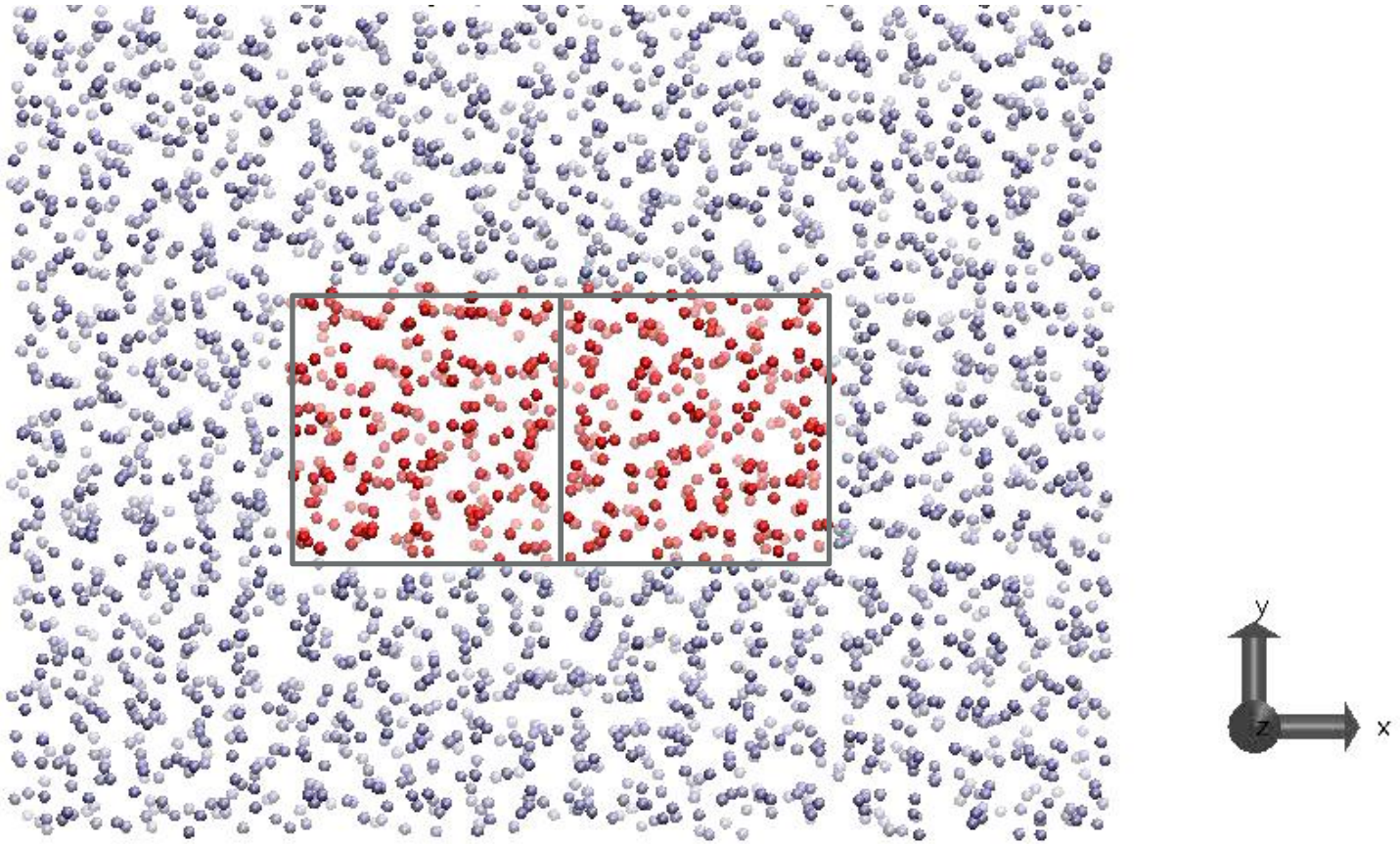
# Constrained Control Volume



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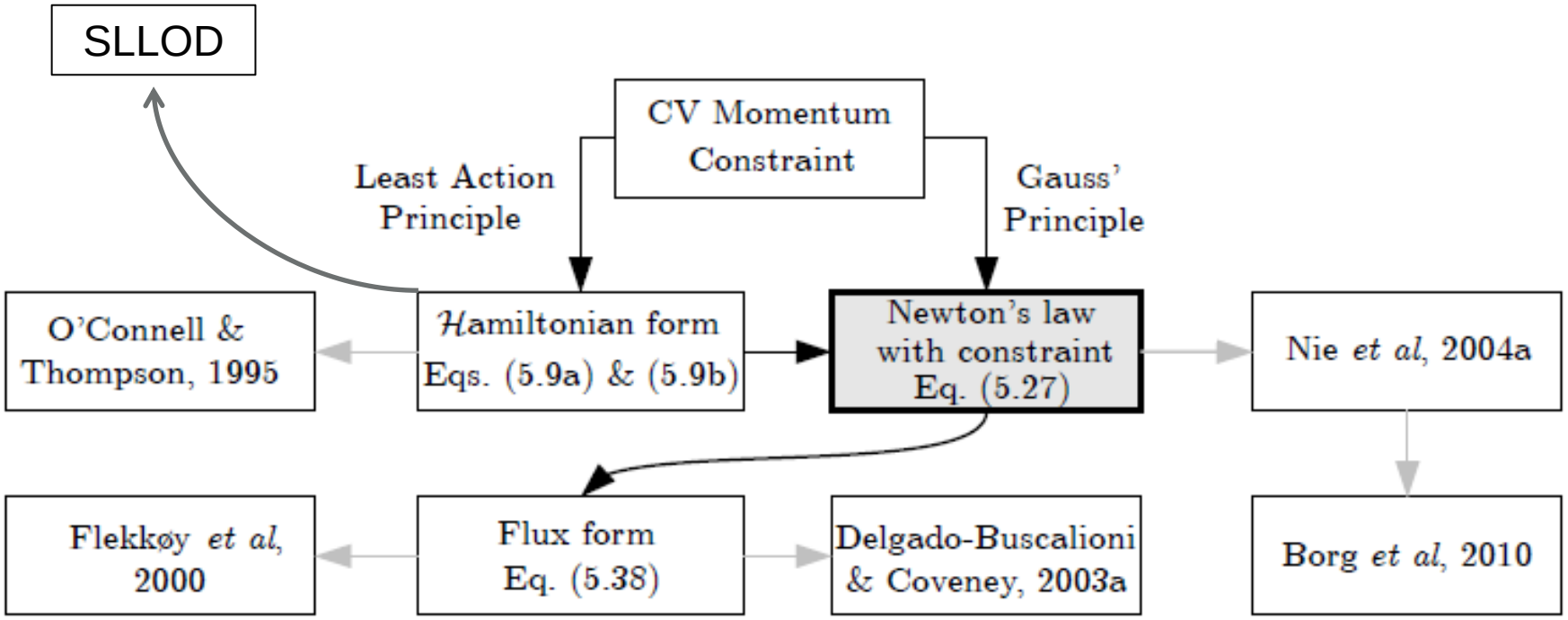
# Constrained Control Volume



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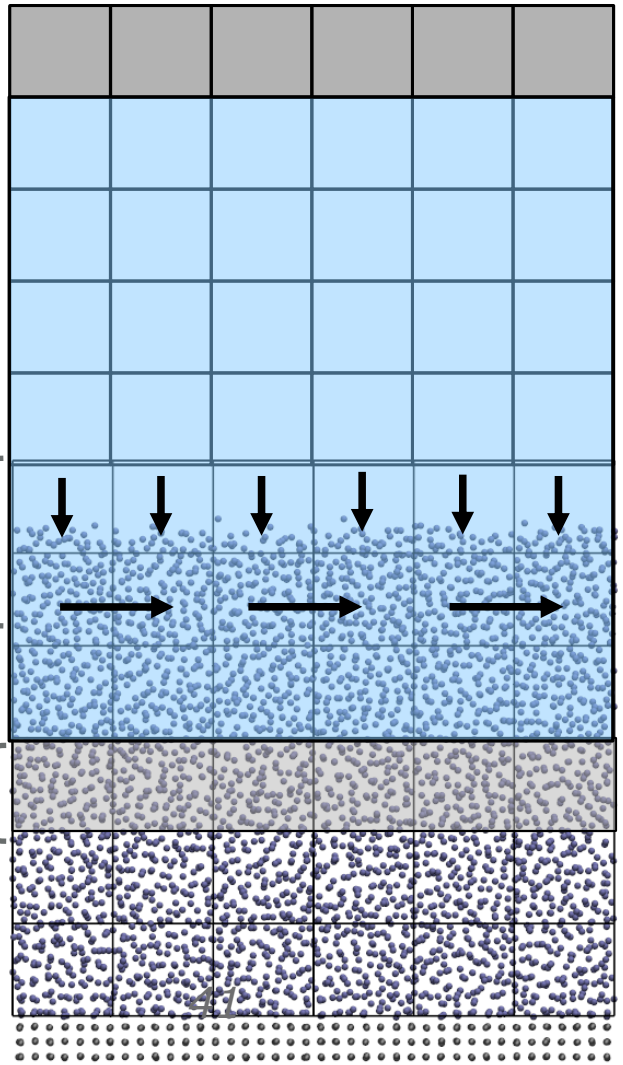
# Domain Decomposition

Consistent Framework ✓

- CFD→MD Boundary condition ✓
- MD→CFD Boundary condition ✓



# Key Points

- How do we ensure conservation between domains?
- Attempted to do this with a consistent CV formulation and exact constraints derived from energy minimisation formulations
- Ideally we would have no overlap and a sharp interface with flux between MD-CFD solvers
- Lots of things not considered: fluctuations, complex molecules, multi-phases, timesteps, overlap, buffer, insertion, etc

# Coupled Simulation Results

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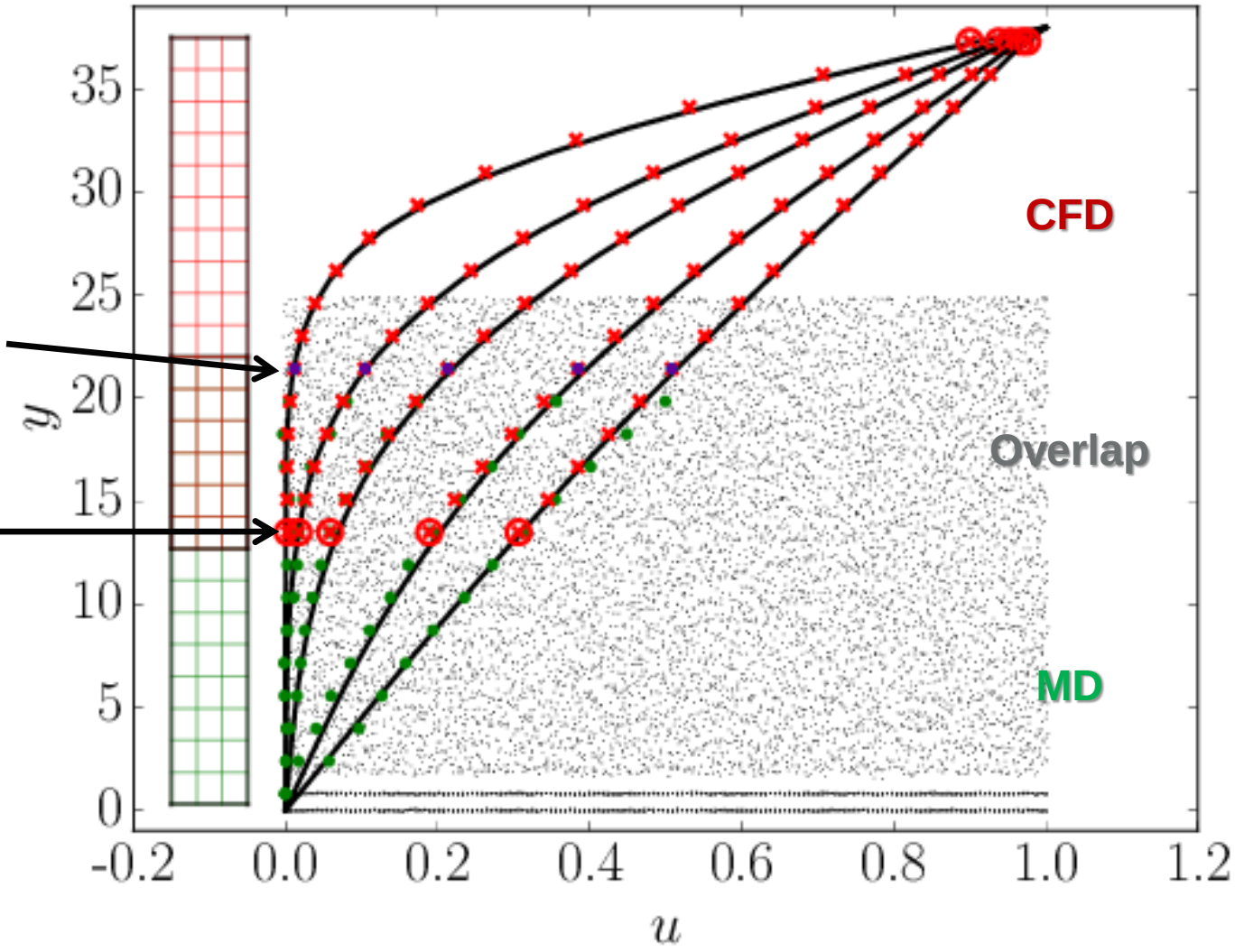
# Coupling Results – Couette Flow



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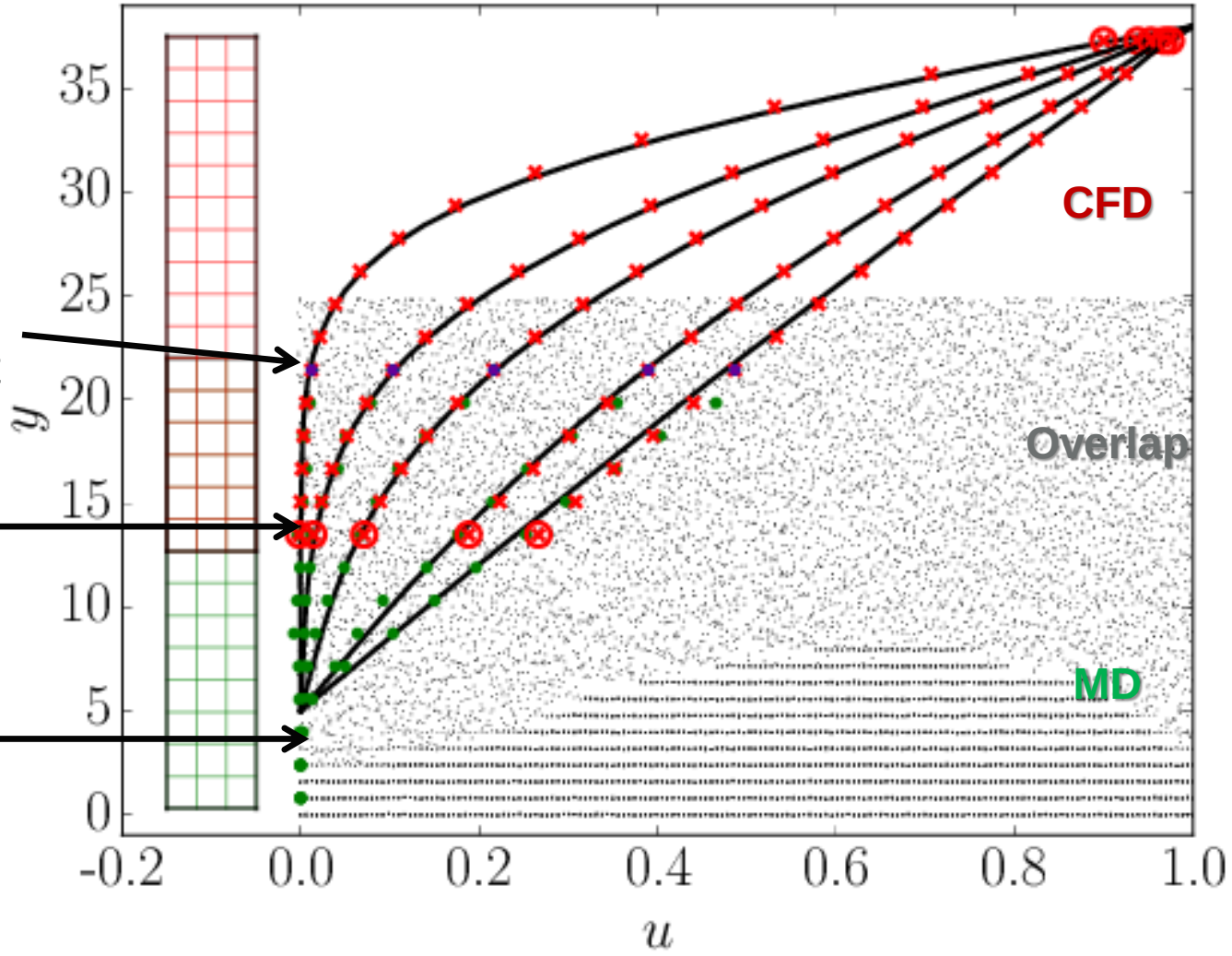
# Coupling Results – Couette Flow

Exact Control Volume Constraint

CFD Boundary

Rough wall shifts zero velocity location



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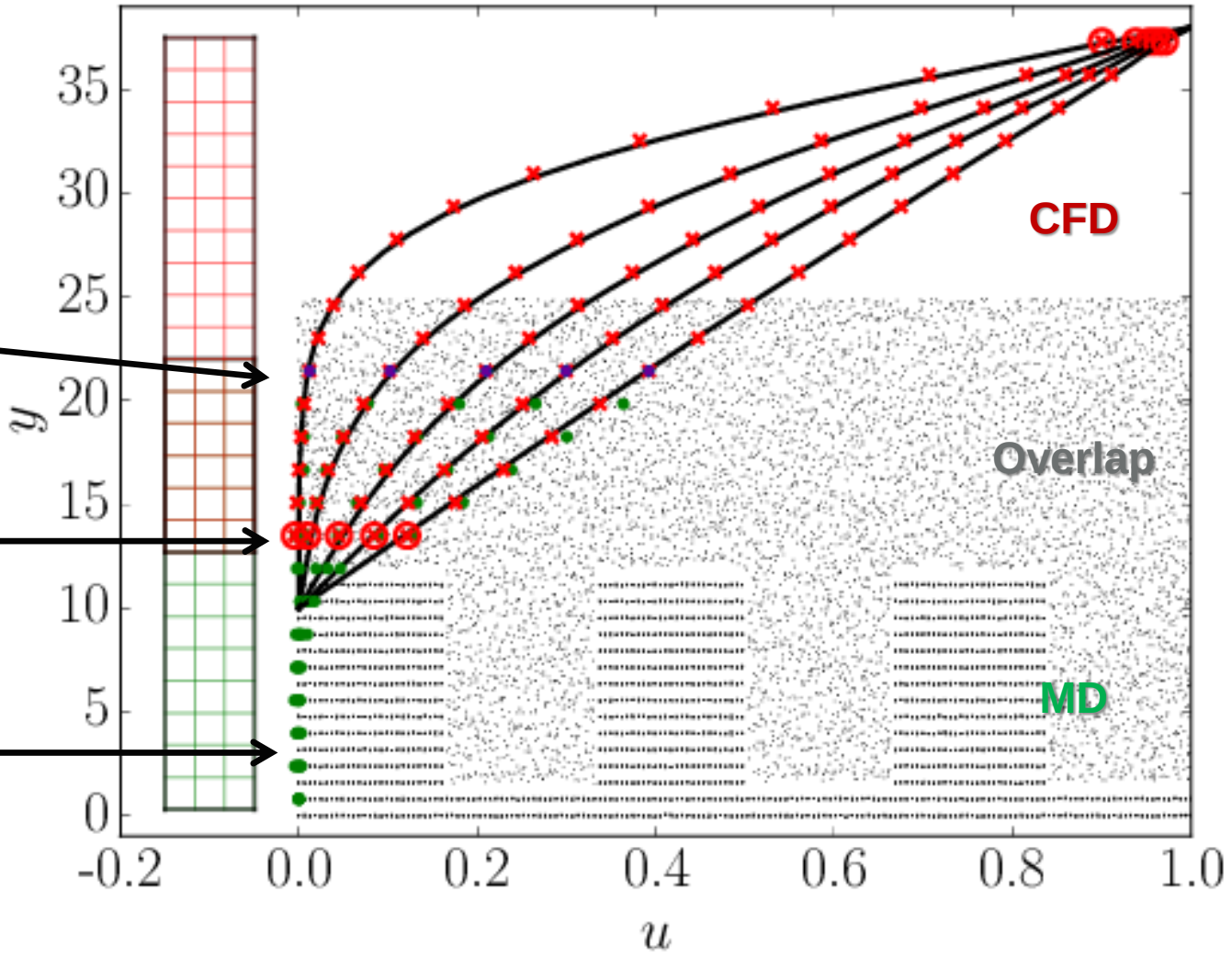
# Coupling Results – Couette Flow

Exact Control Volume Constraint

CFD Boundary

Posts shifts zero velocity location



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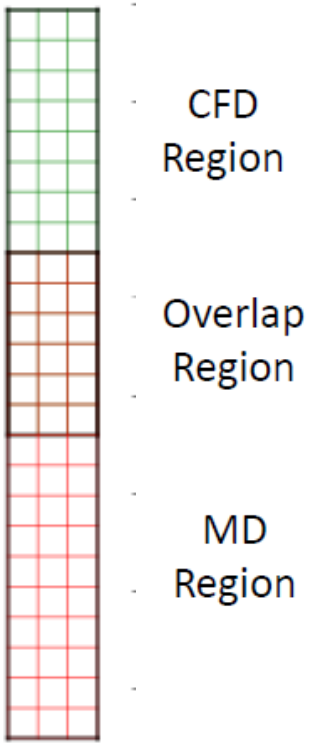
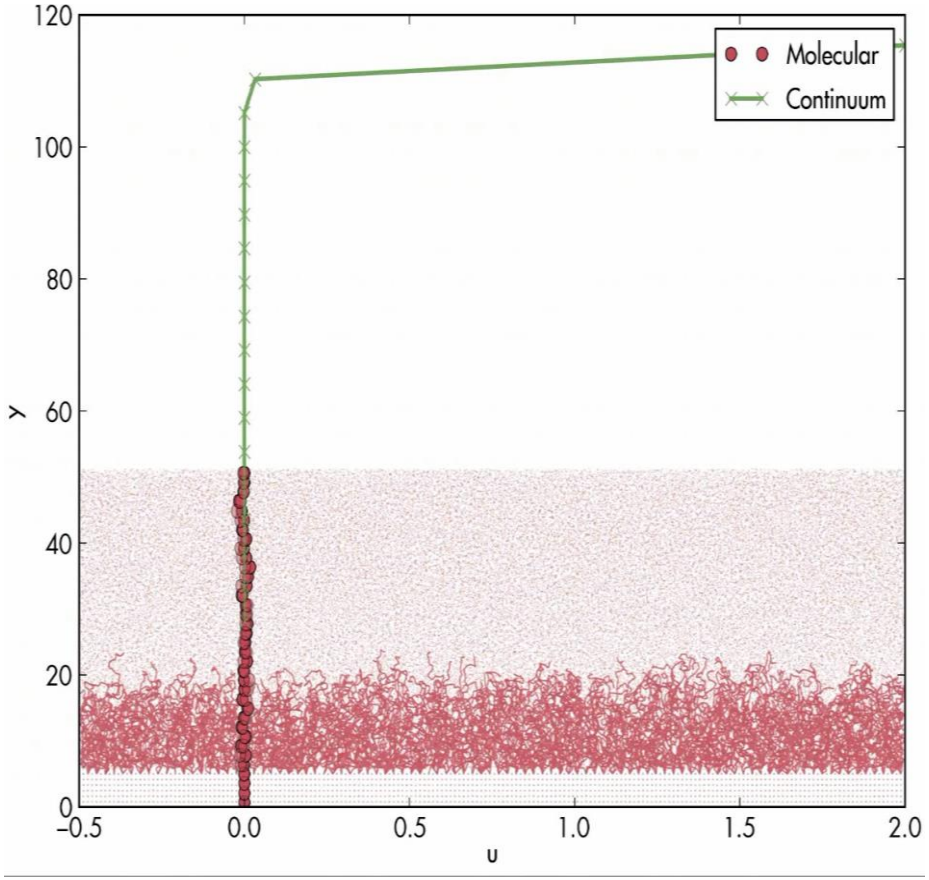
# Coupling Results – Couette Flow




By David Trevelyan

Imperial College London

# Beyond Single Phase Laminar Flow

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# Molecular Dynamics simulation of Nucleation


*Wall w*
*mo*
*rou*

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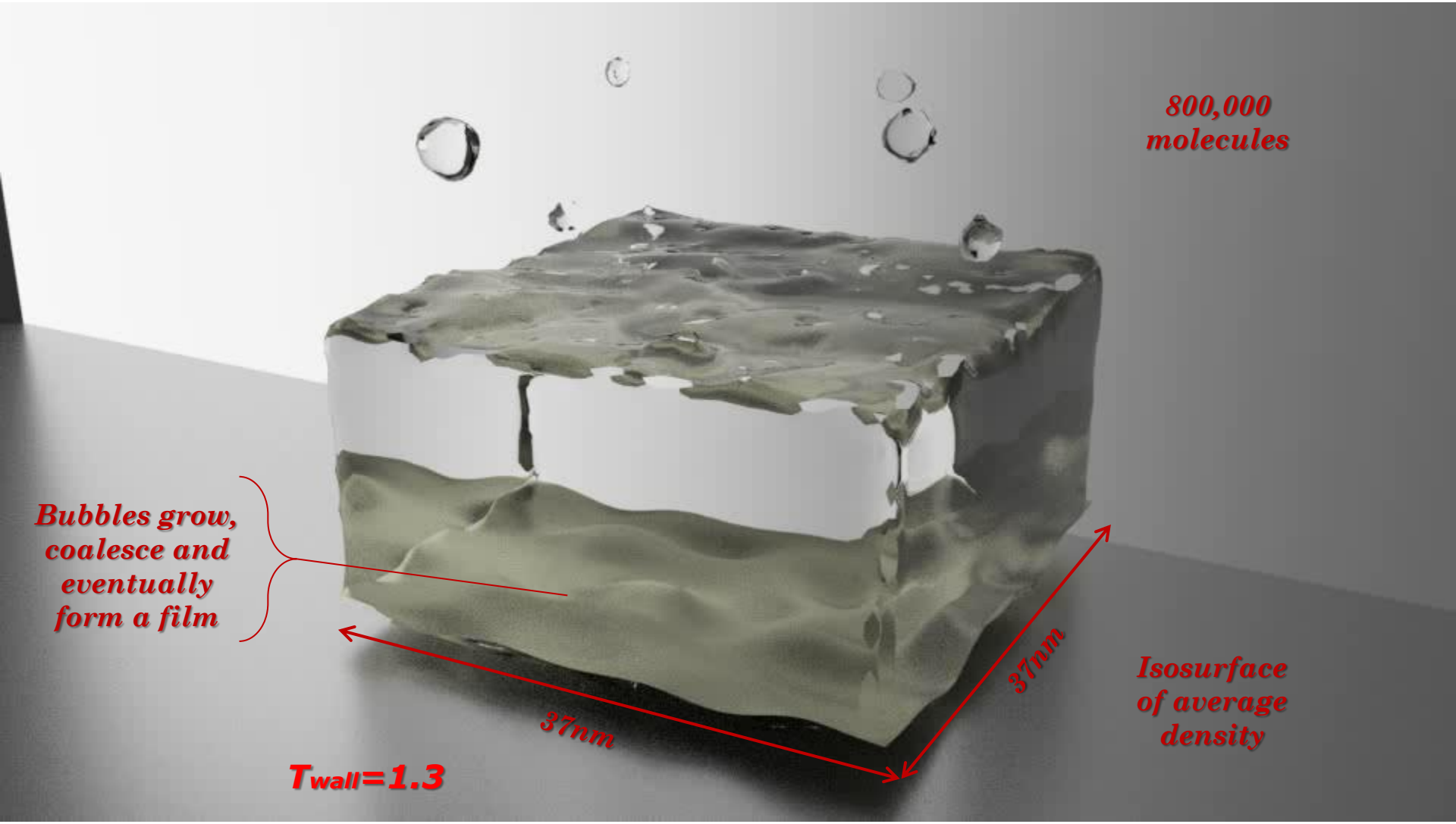
# Isosurface of Density



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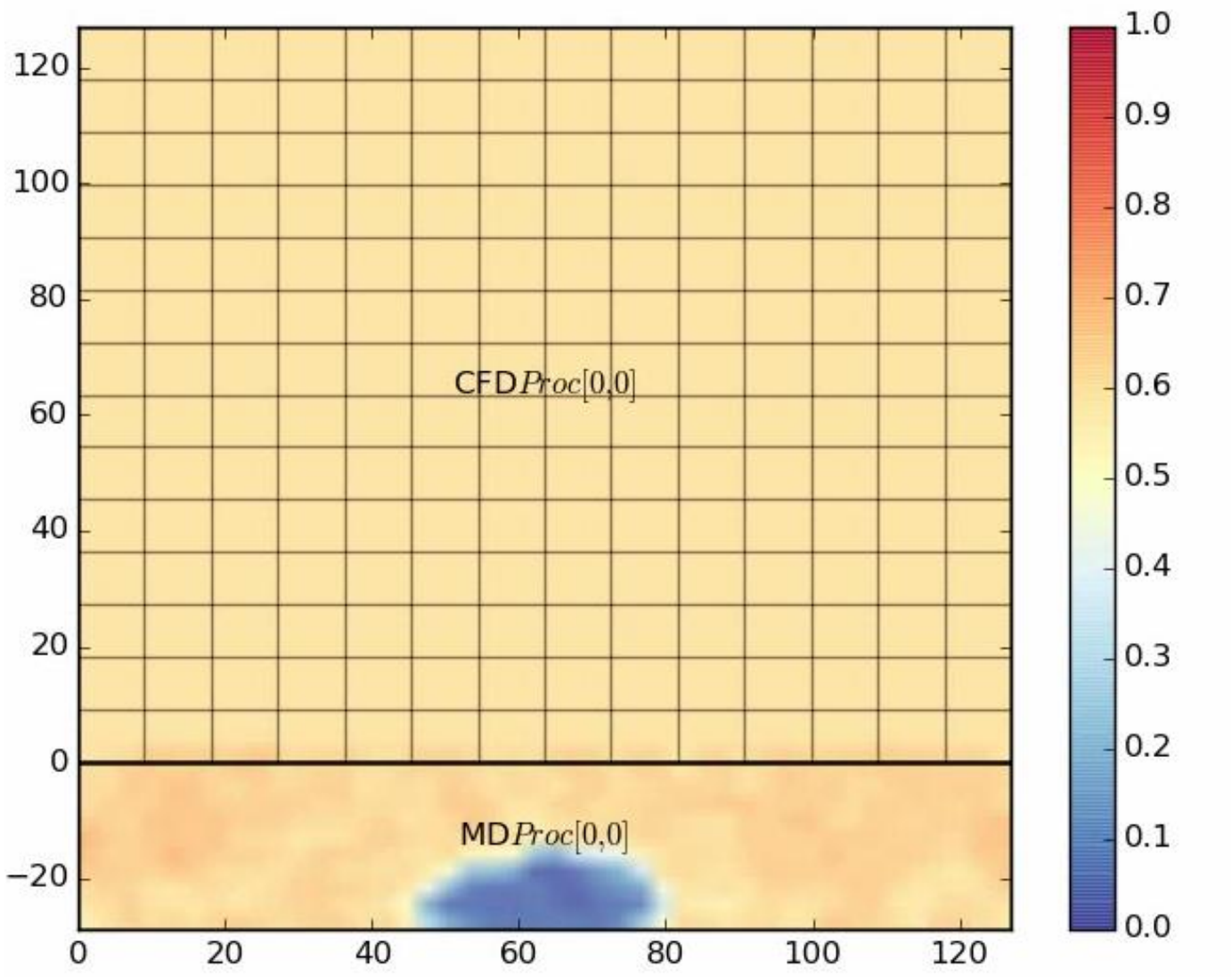
# Coupled Simulation of Boiling



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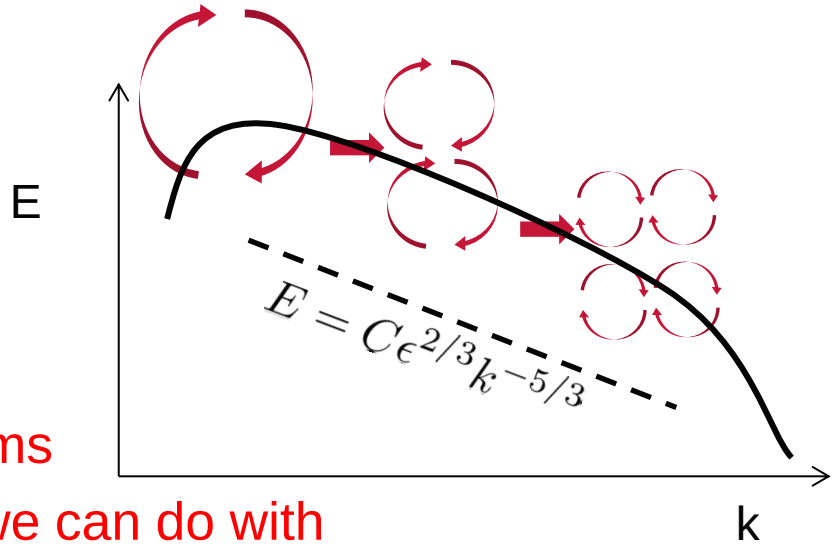
# Molecular Simulation of Turbulence

- 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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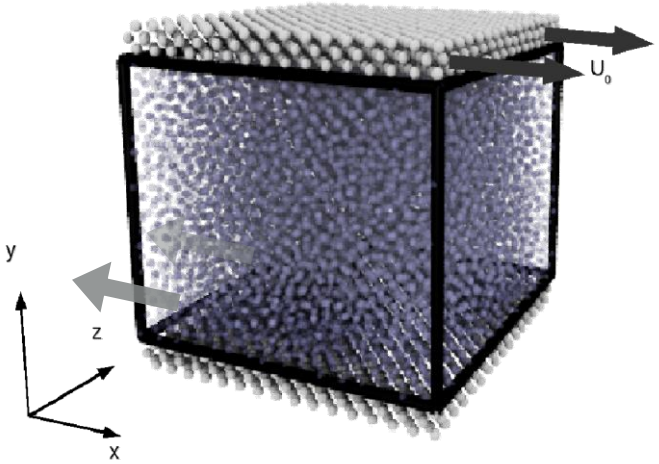
# Domain Overview

- 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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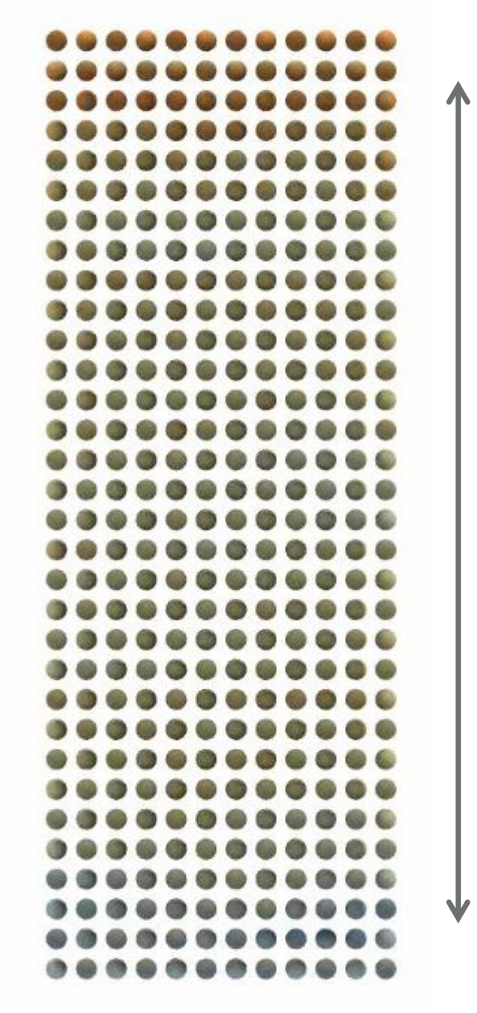
# Molecular Simulation of Turbulence



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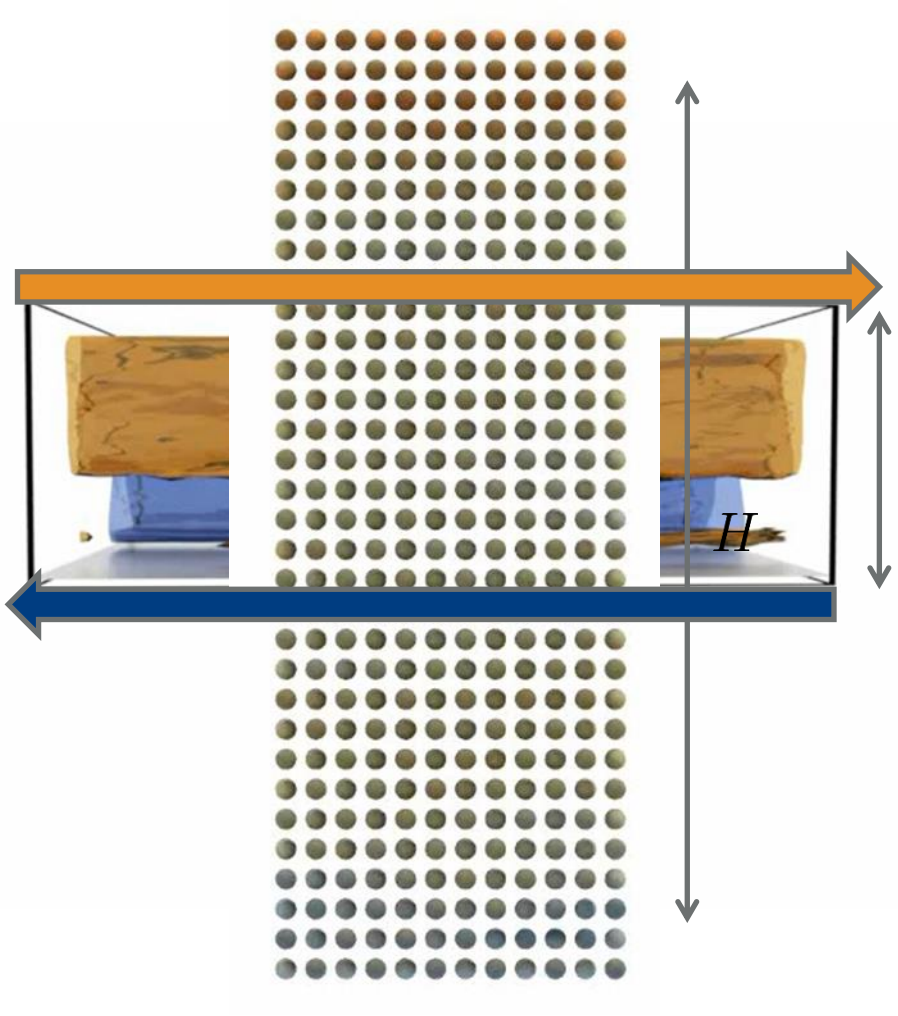
# Molecular Simulation of Turbulence




*Reynolds Number*

$Re \approx 400$

*with*

***300 million molecules***

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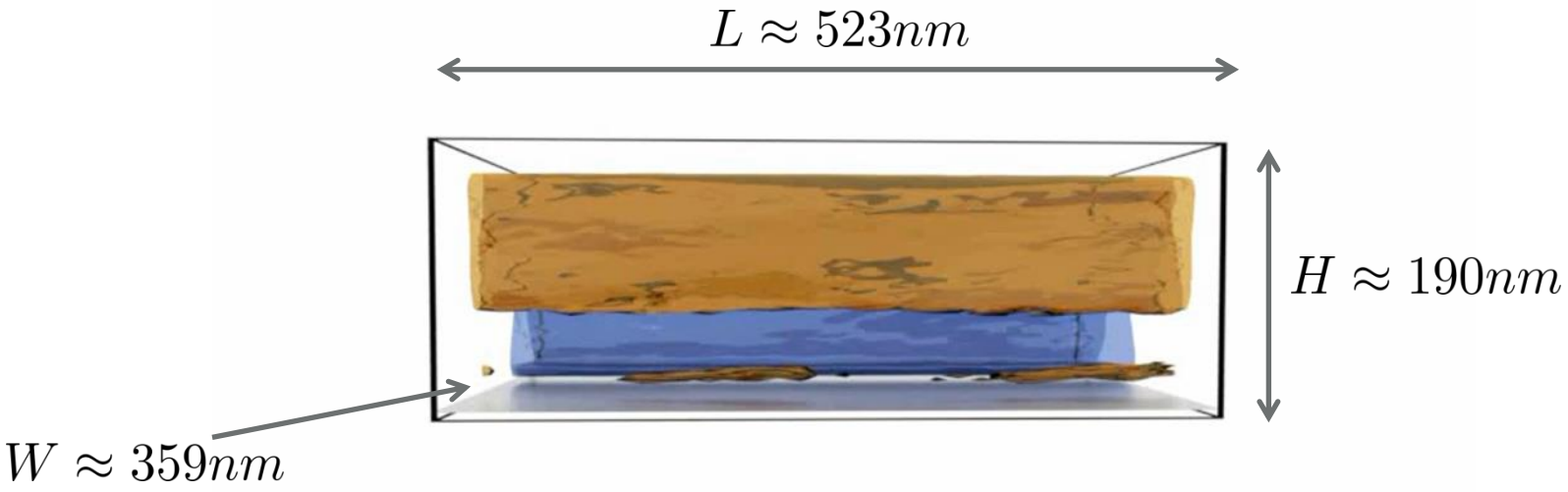
# Molecular Simulation of Turbulence

*Minimal channel Couette flow*




*Reynolds Number*

$Re \approx 400$

*with*
***300 million molecules***

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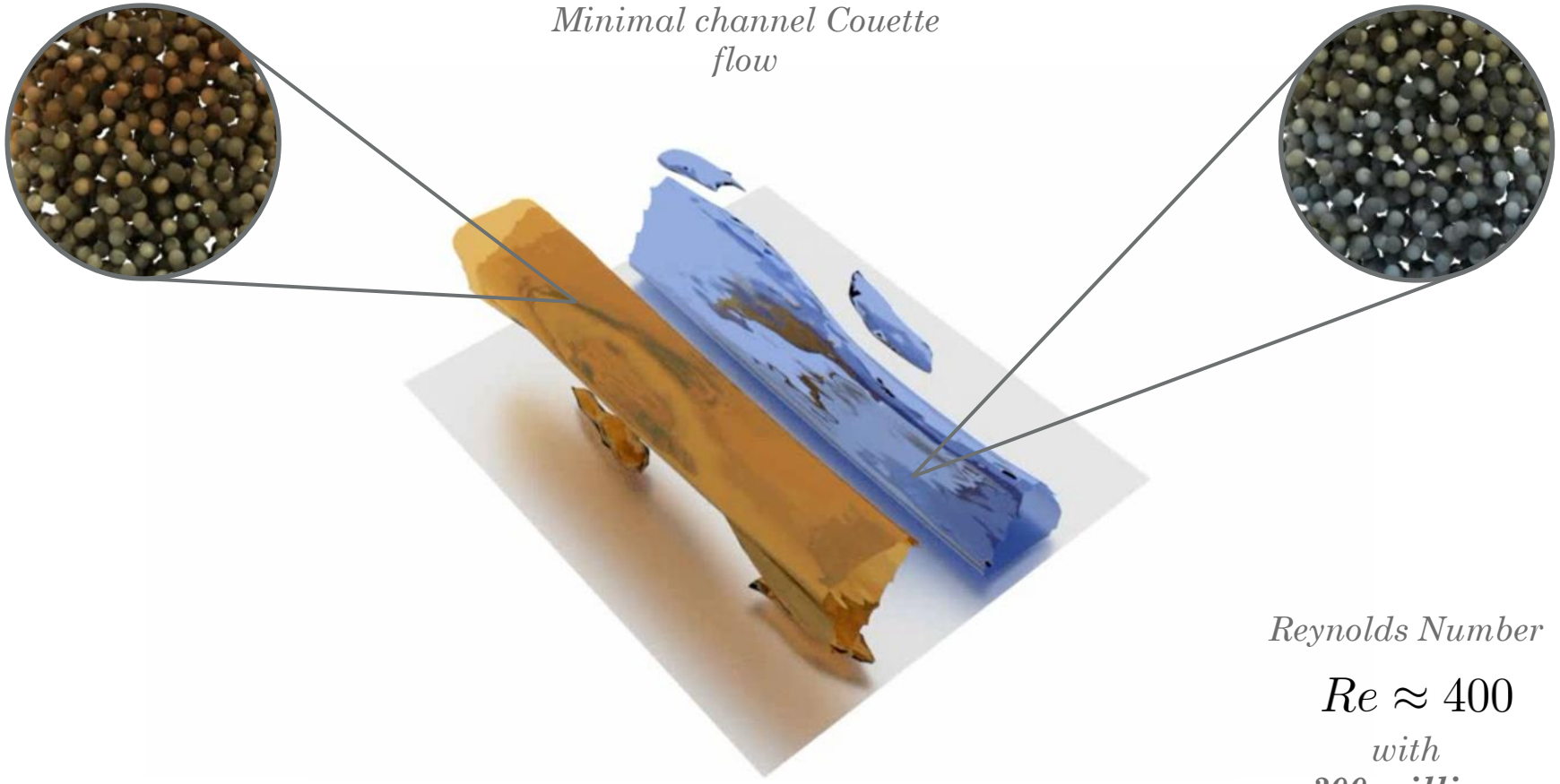
# Molecular Simulation of Turbulence

*Minimal channel Couette flow*



*Isosurfaces of turbulent kinetic energy coloured by velocity*

*Reynolds Number*

$Re \approx 400$

*with*

***300 million molecules***

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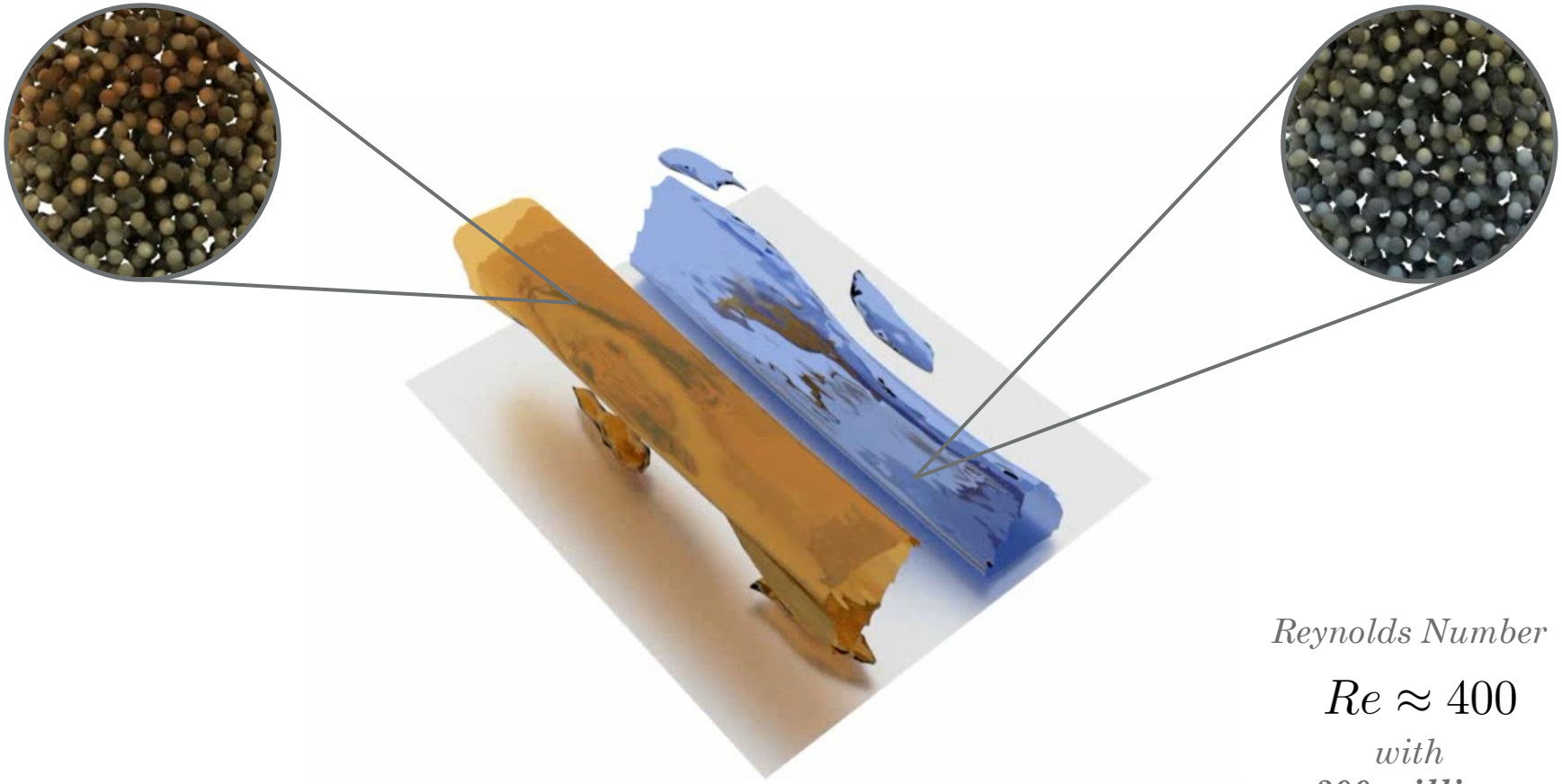
# Molecular Simulation of Turbulence



*Isosurfaces of turbulent kinetic energy coloured by velocity*

*Reynolds Number*

$Re \approx 400$

*with*

***300 million molecules***

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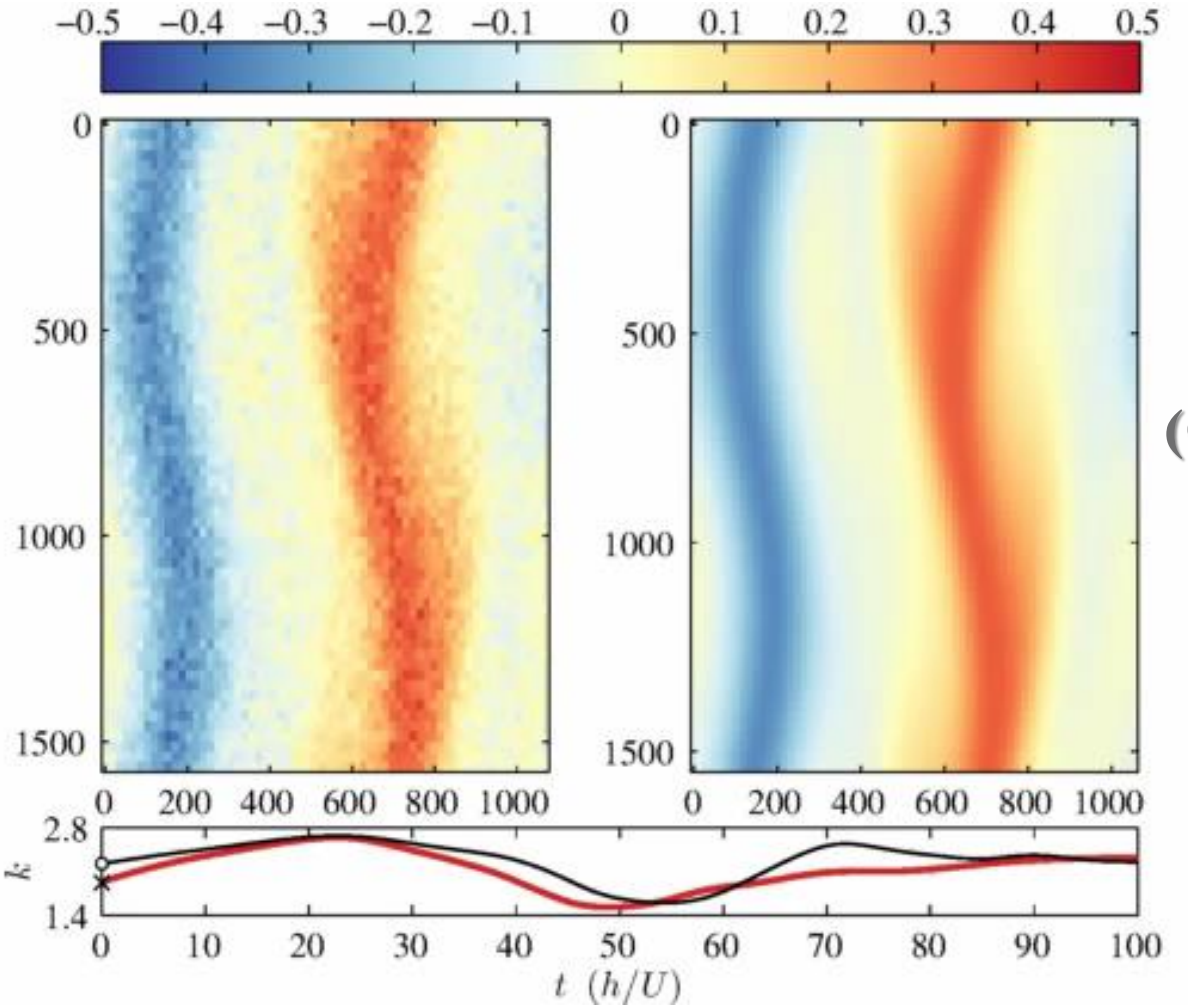
# Molecular Simulation of Turbulence

## *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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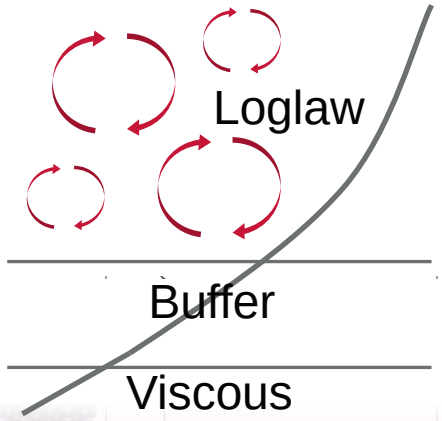
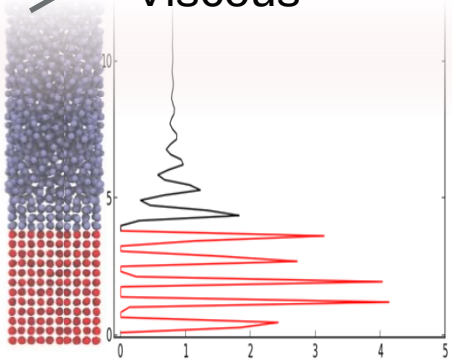
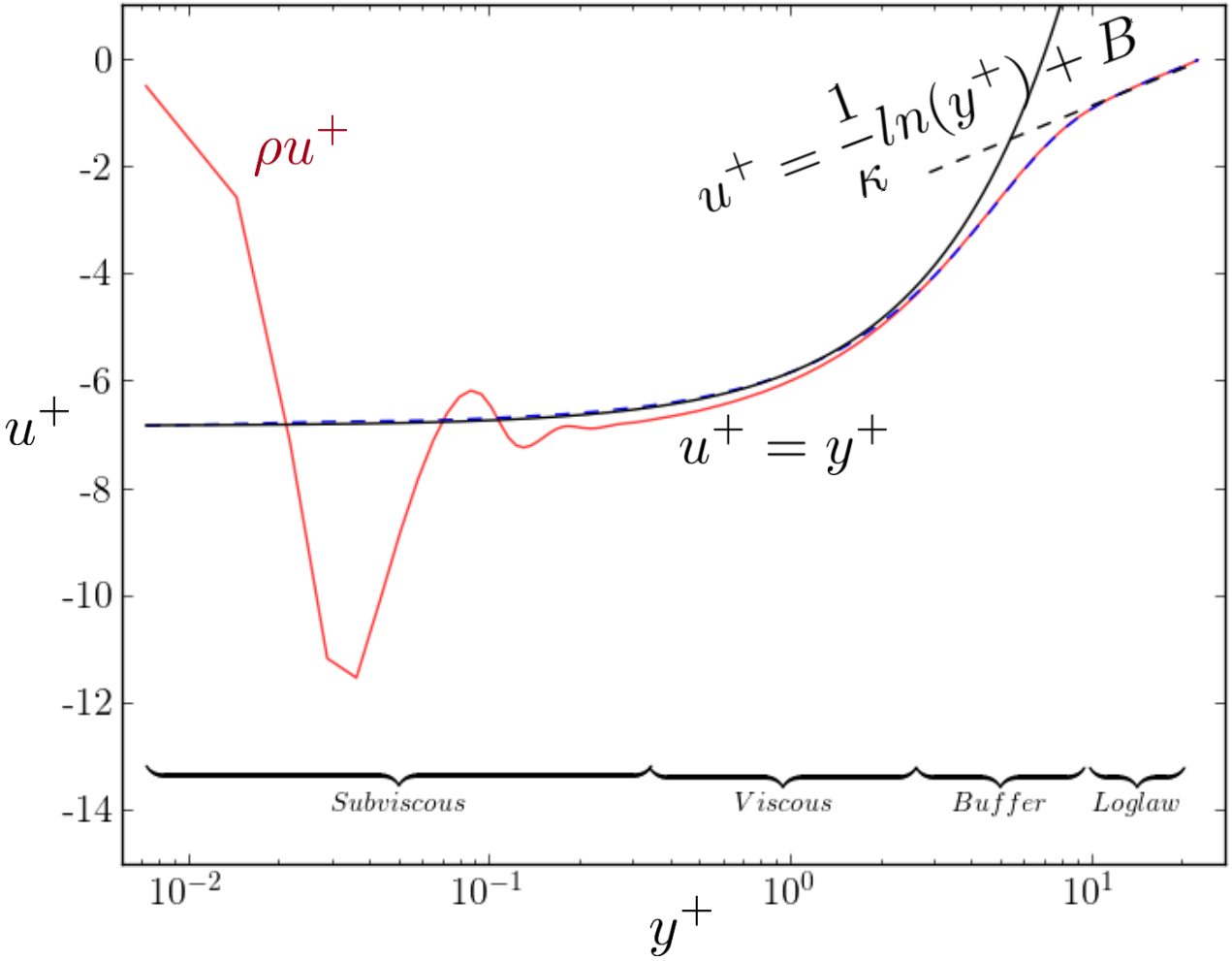
# Law of the wall



Subviscous? (MD)



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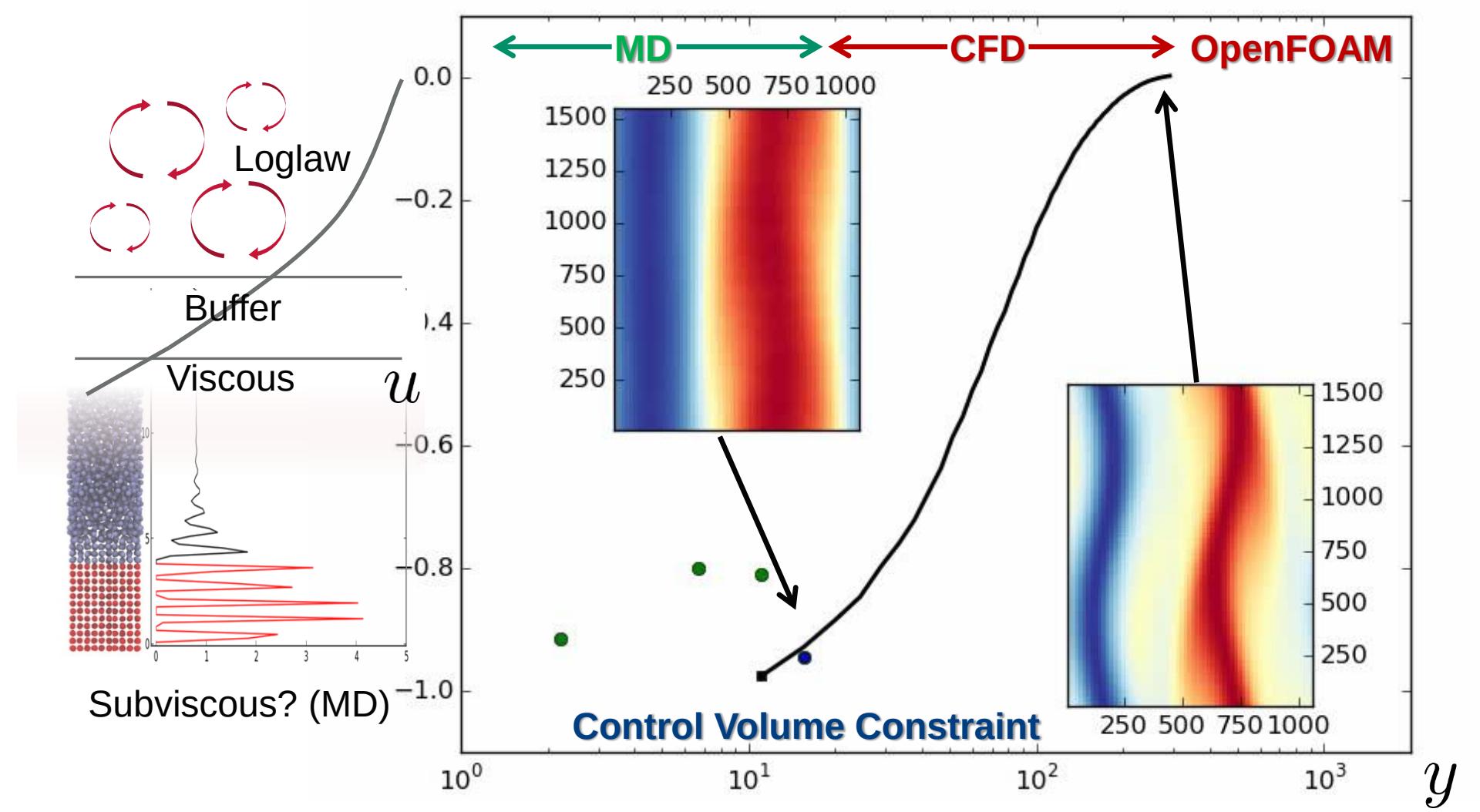
# Coupled Turbulent Couette



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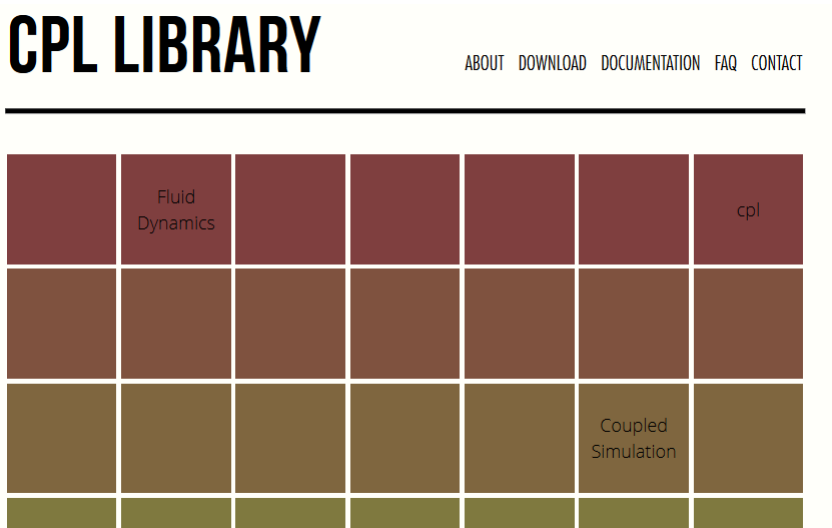
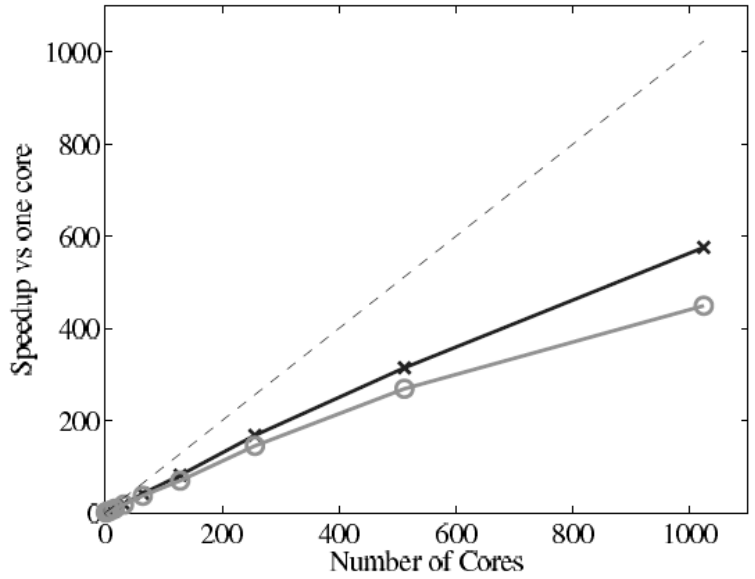
# Large Scale Simulation : CPL library

- Open Source Fortran, C, C++ and Python bindings
- Designed to facilitate the linking of massively parallel codes
- No external dependencies beyond standard packages
- Suite of Python and google tests with continuous integration testing
- Minimal set of functions and examples to lower barrier to entry for coupled simulation **CPL_init CPL_setup CPL_send CPL_recv**




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

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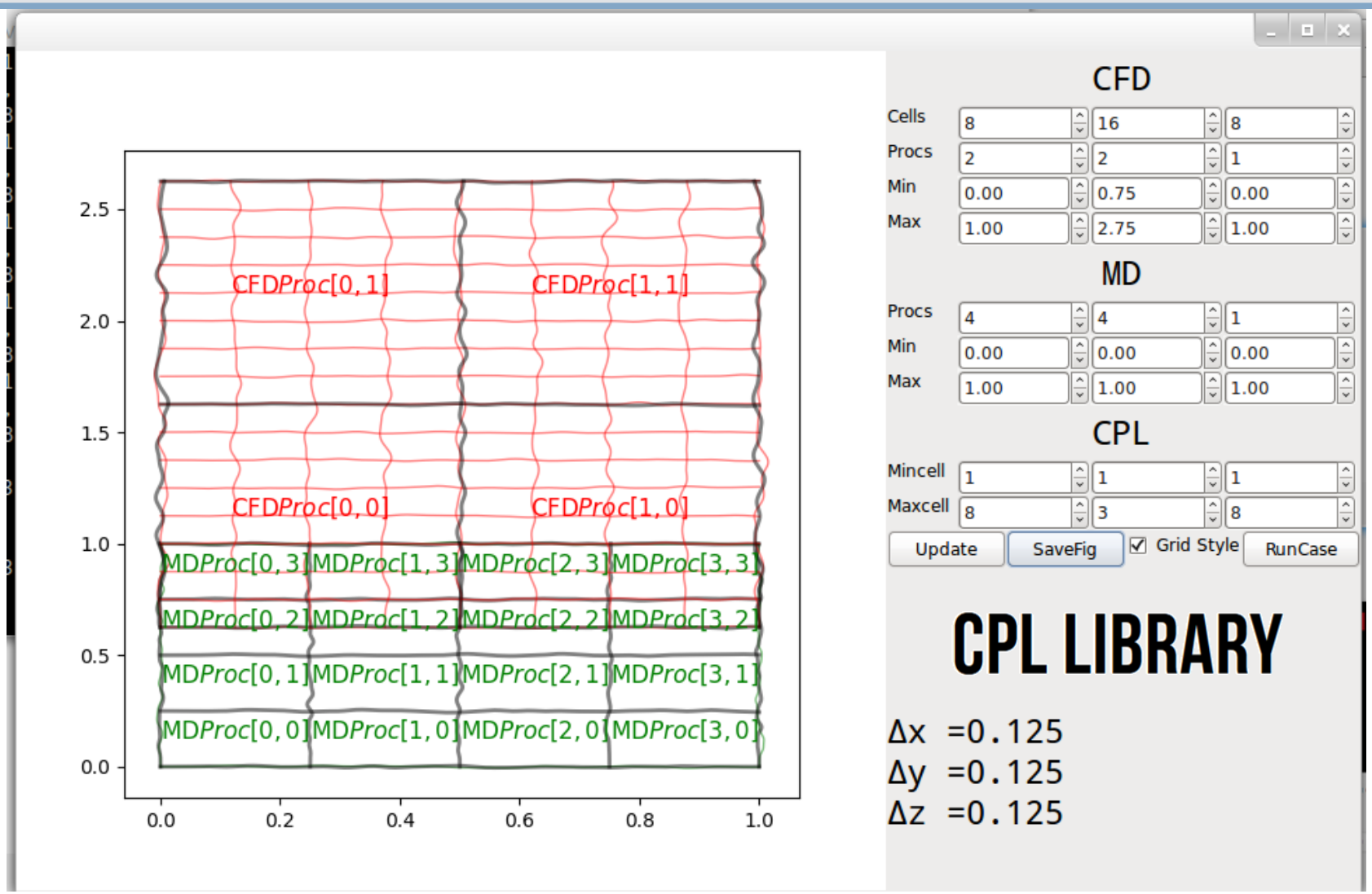
# Topology Design Tool



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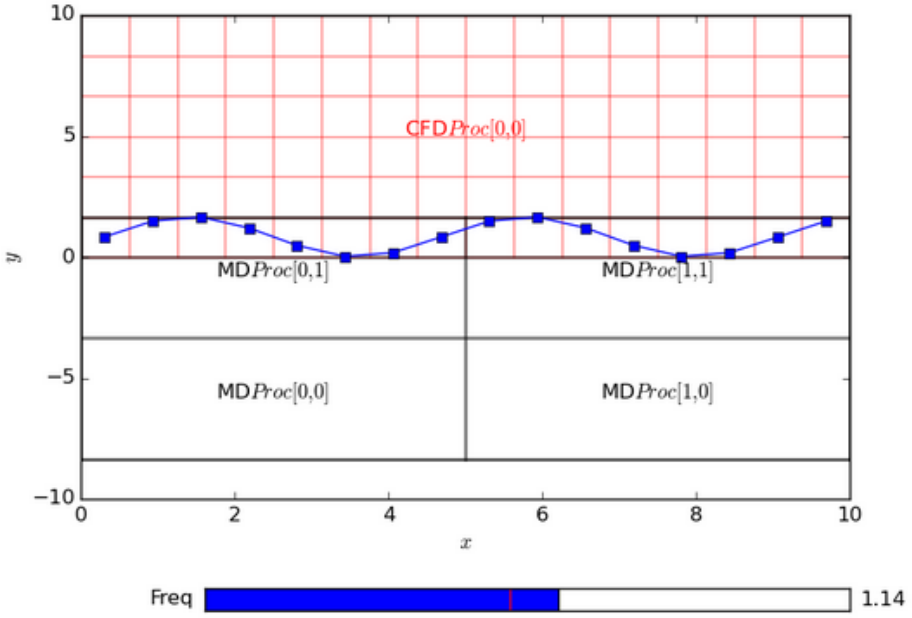
# Minimal Examples to Lower Barrier to Entry




(www.cpl-library.org)

## 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,

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

# Conclusions

- Molecular dynamics (MD) allows unique insight into wall textures, chemical coatings, bio-molecules, etc
- Coupled simulation links continuum CFD to extend to system sizes which would be too expensive with MD
- The control volume relates continuum and discrete system with both expressed in conservative form
- Mathematical operator framework (CV functional) helps to get CV values and fluxes in a molecular system
- CV functional applied to derive a local constraint using constrained dynamics which unifies literature
- Applied to laminar Couette flow, turbulent flow with examples of texture, chemical and nucleation

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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