Interface Between Molecular and Continuum Simulation of Fluid Dynamics

Edward Smith

Fluid Mechanics Seminar

29/05/19

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Summary

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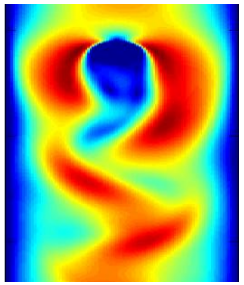
Master's → PhD Mechanical Engineering → EPSRC Fellowship

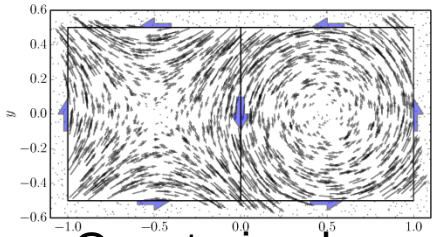


Lattice Boltzmann

Coupled MD simulation

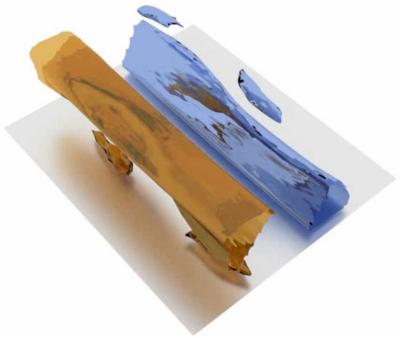
$$\vartheta_i \equiv \int_{x^-}^{x^+}\int_{y^-}^{y^+}\int_{z^-}^{z^+} \delta(x_i - x)\delta(y_i - y)\delta(z_i - z)dxdydz$$

Control Volume formulation



Constrained dynamics

Molecular Turbulence

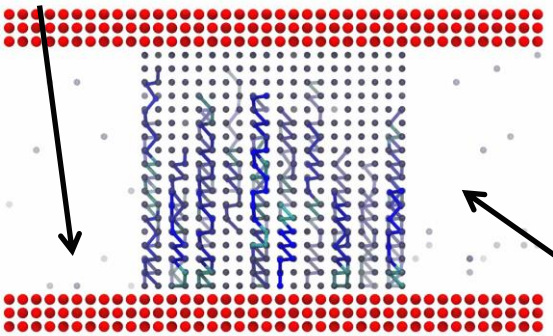


Swinburne → Chemical Eng. → Civil Eng. → Mechanical Eng.

Heat Flux

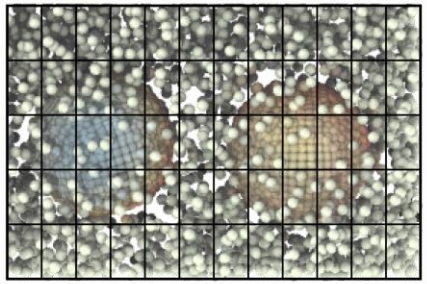
$$q = -\lambda\frac{\partial T}{\partial y} + \ldots$$

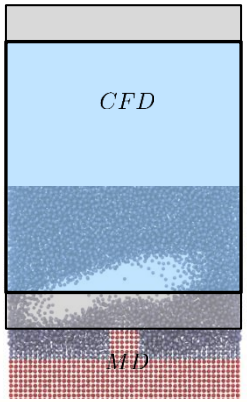
Moving Contact Line



Interface

Granular Mechanics





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Computational Fluid Dynamics

- Continuous field at every point in space
  - Mass Conservation

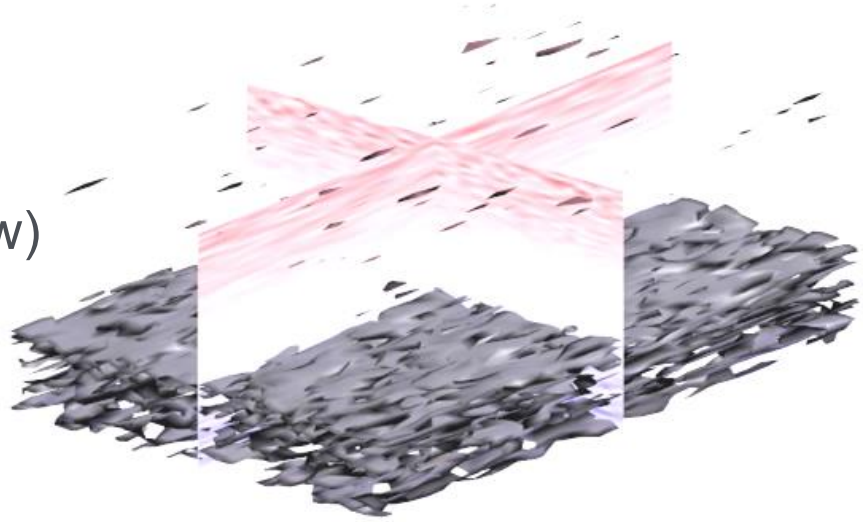
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - Momentum Balance (Newton's Law)

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

  - 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

Molecular Dynamics

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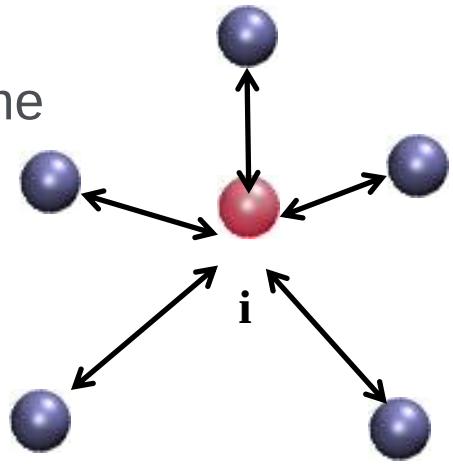
Discrete molecules in continuous space

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

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



Acceleration obtained from forces

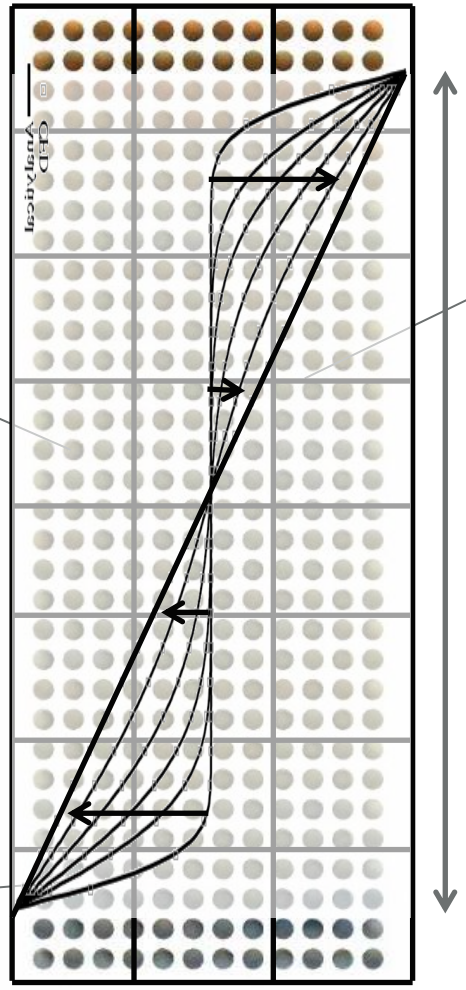
- Governed by Newton's law for an N-body system
- Point particles with pairwise interactions only

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

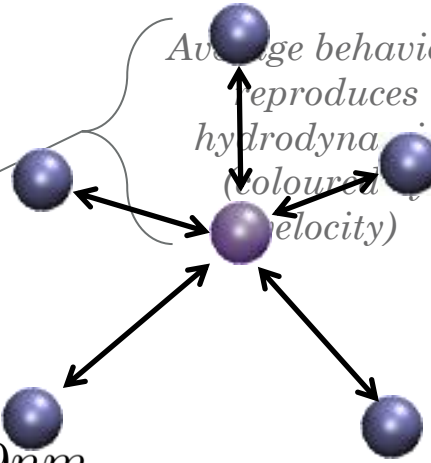
$$\Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

Molecular Dynamics

Liquid structure causes viscosity



Average behaviour reproduces hydrodynamics (coloured by velocity)



$H \approx 9nm$

Stick-slip near walls

Reynolds Number

$Re \approx 15$

with

4096 molecules

Molecular Dynamics
Complex Walls and Fluids

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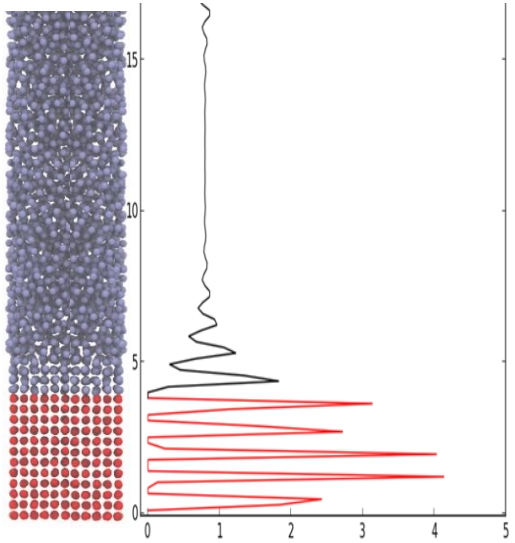
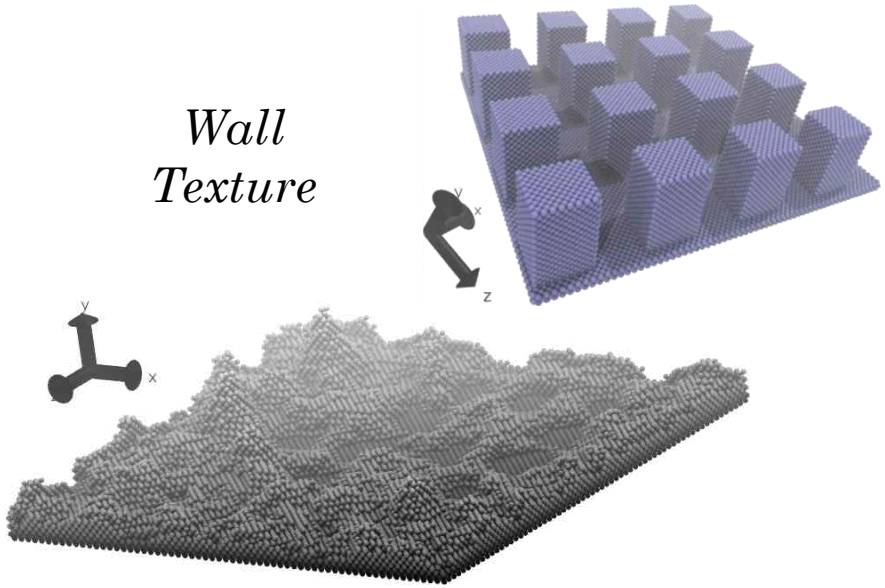
Liquid structure causes viscosity



Wall Texture



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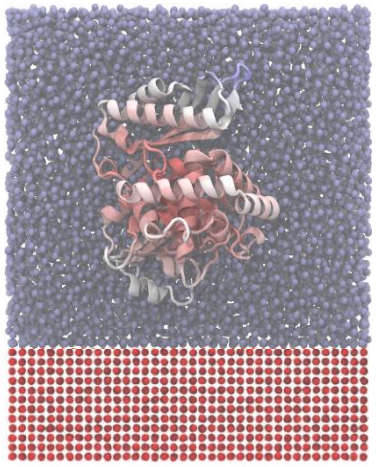
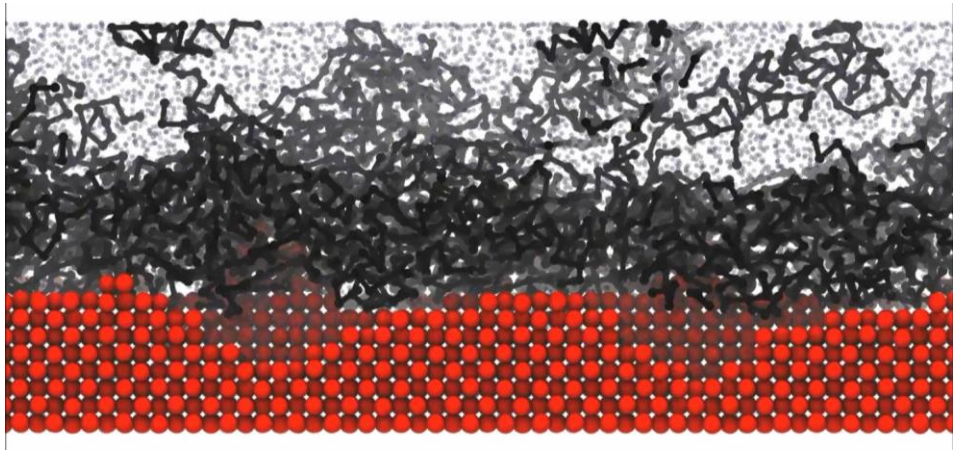


Molecules of arbitrary complexity



Oil, water and textured surface

Molecular Dynamics
Shocks and Multi-Phase

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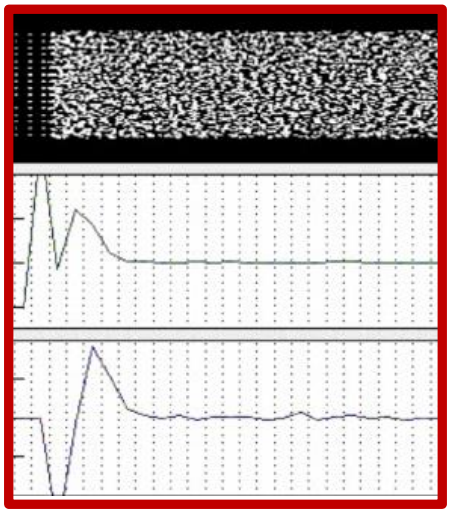
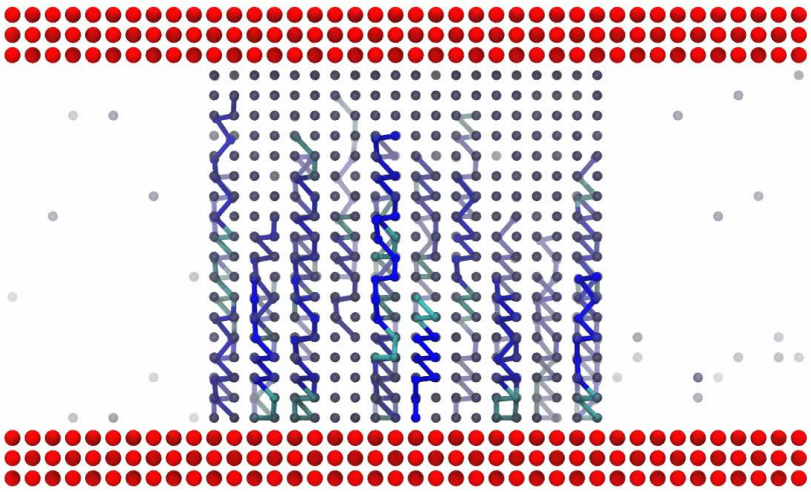
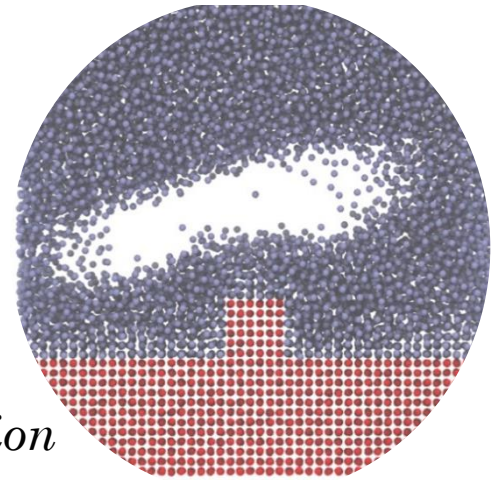
Shockwave



Droplet Formation



Contact line



Nucleation

Molecular Dynamics
Beyond The Continuum

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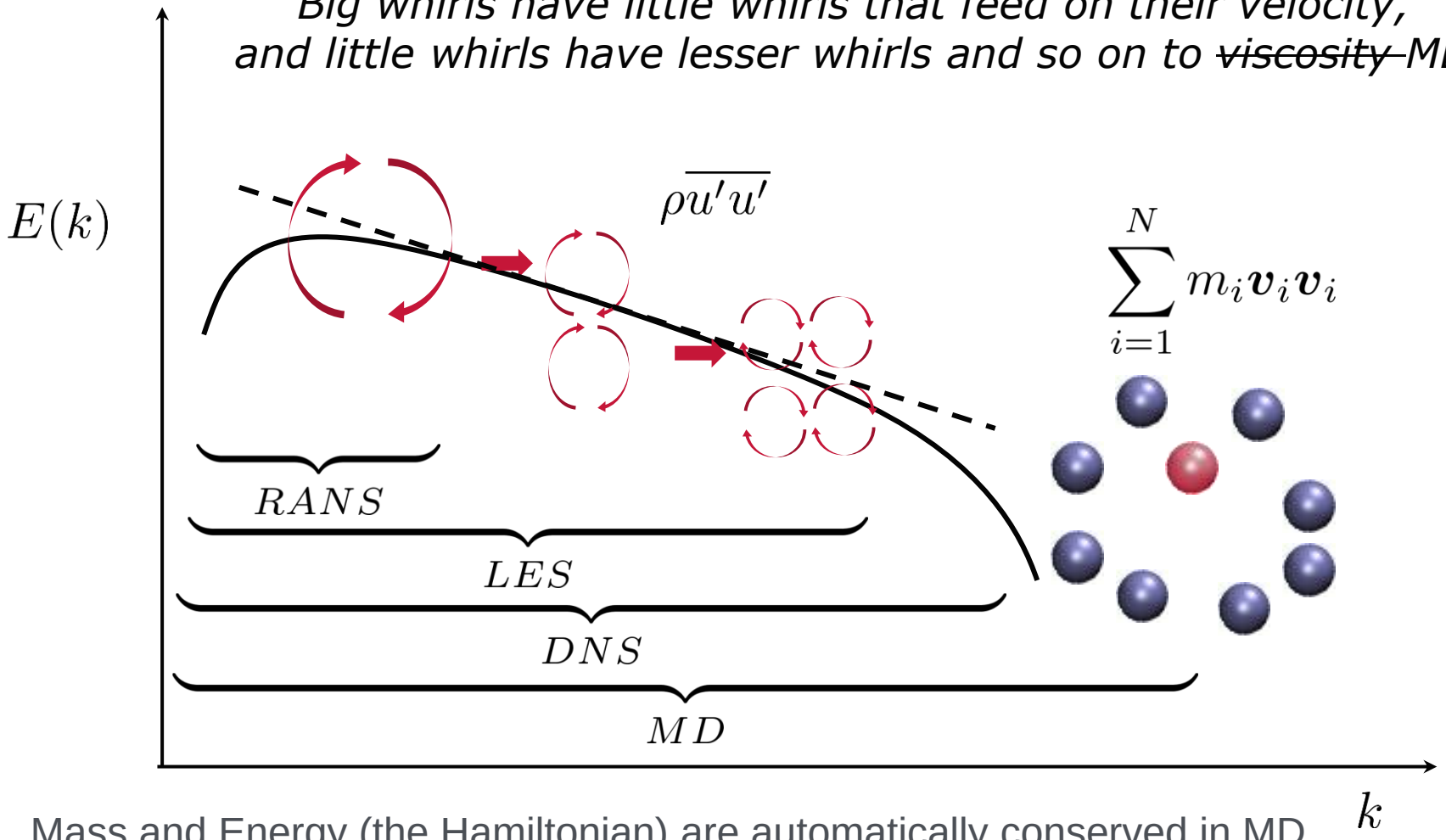
Big whirls have little whirls that feed on their velocity,
and little whirls have lesser whirls and so on to ~~viscosity~~ MD



Mass and Energy (the Hamiltonian) are automatically conserved in MD

Coupling Overview

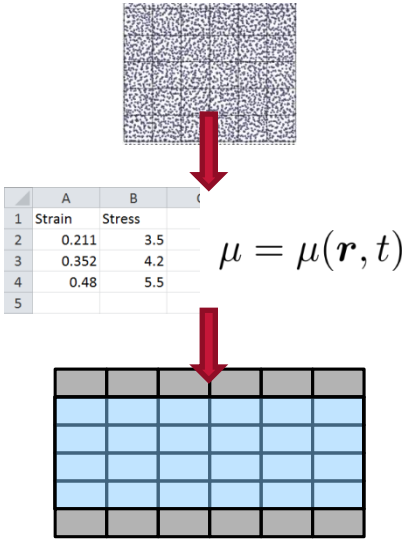
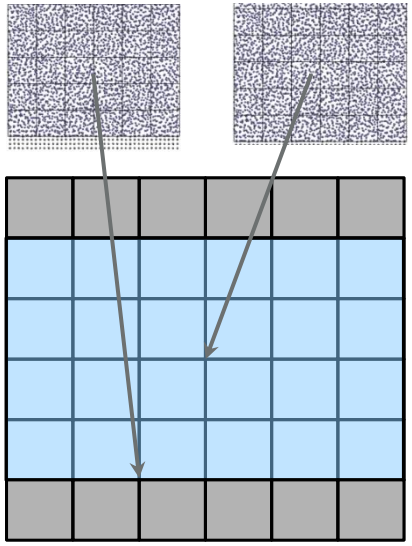


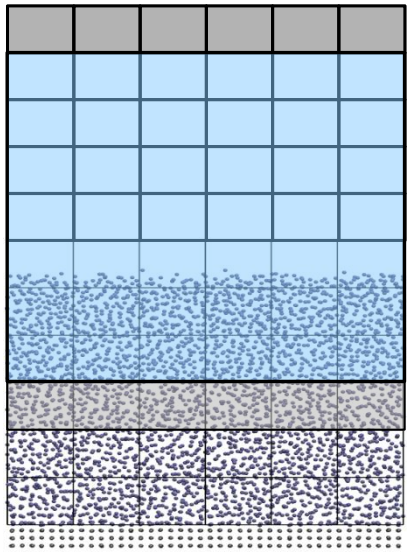
Table Lookup or Coefficients

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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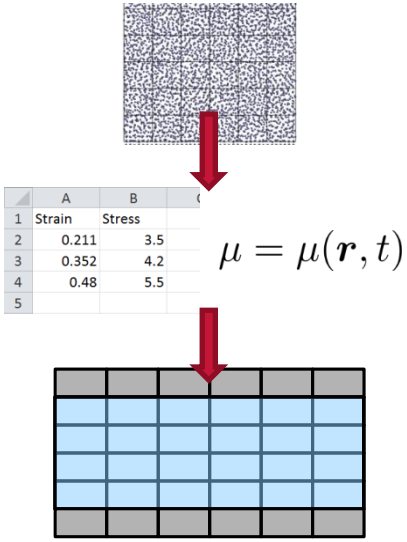

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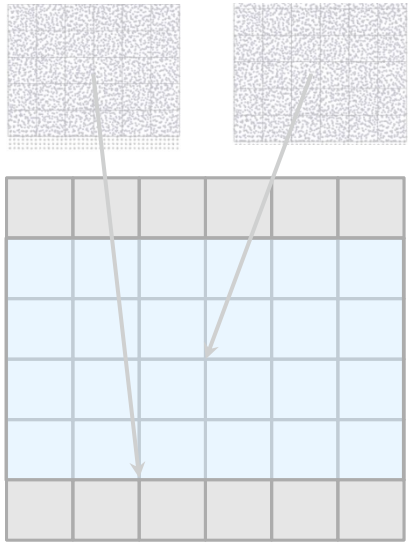

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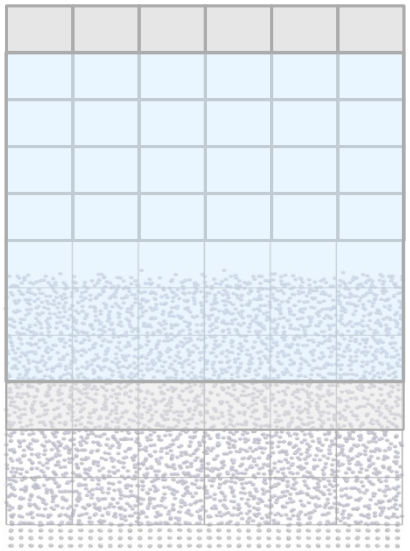

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Molecular Dynamics
Extracting Coefficients

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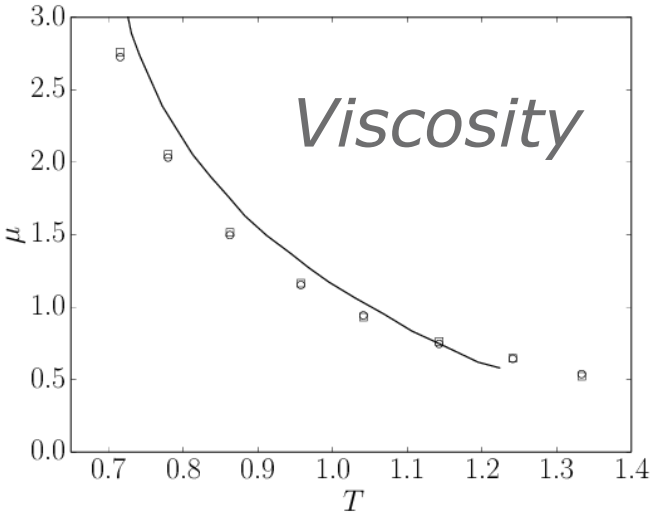
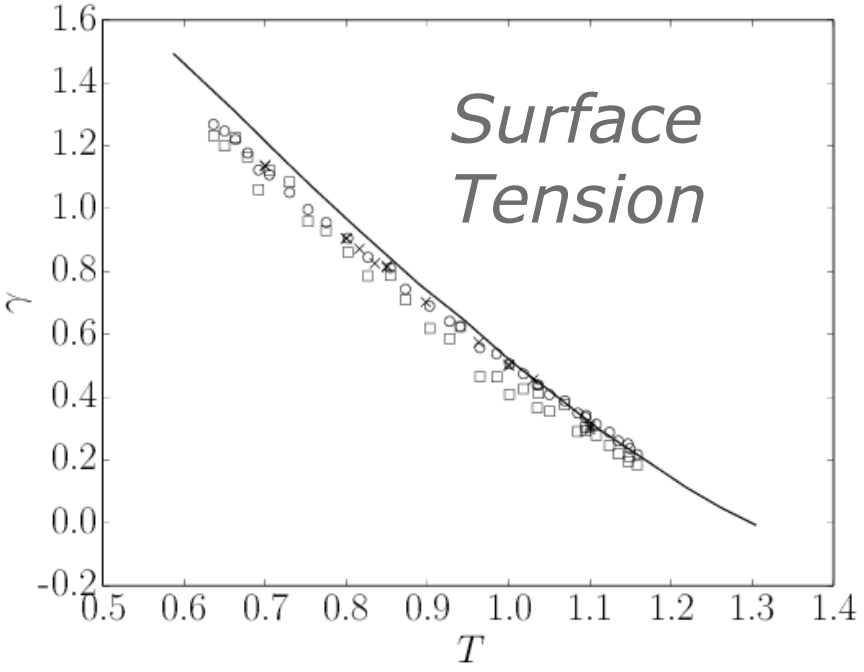
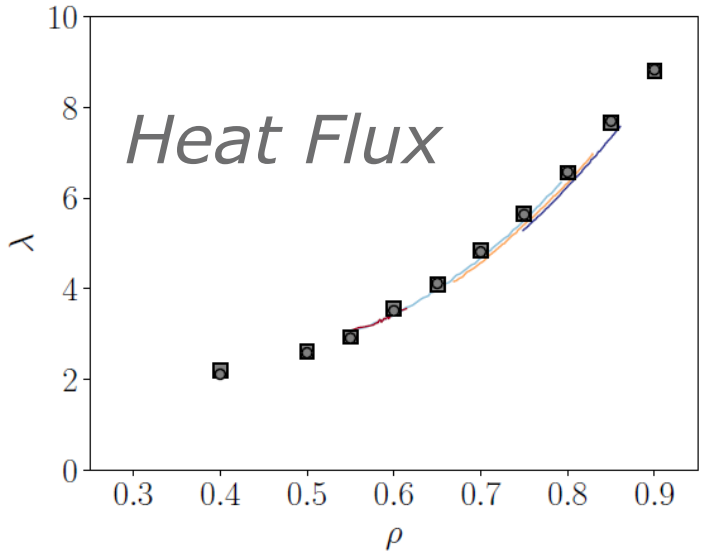
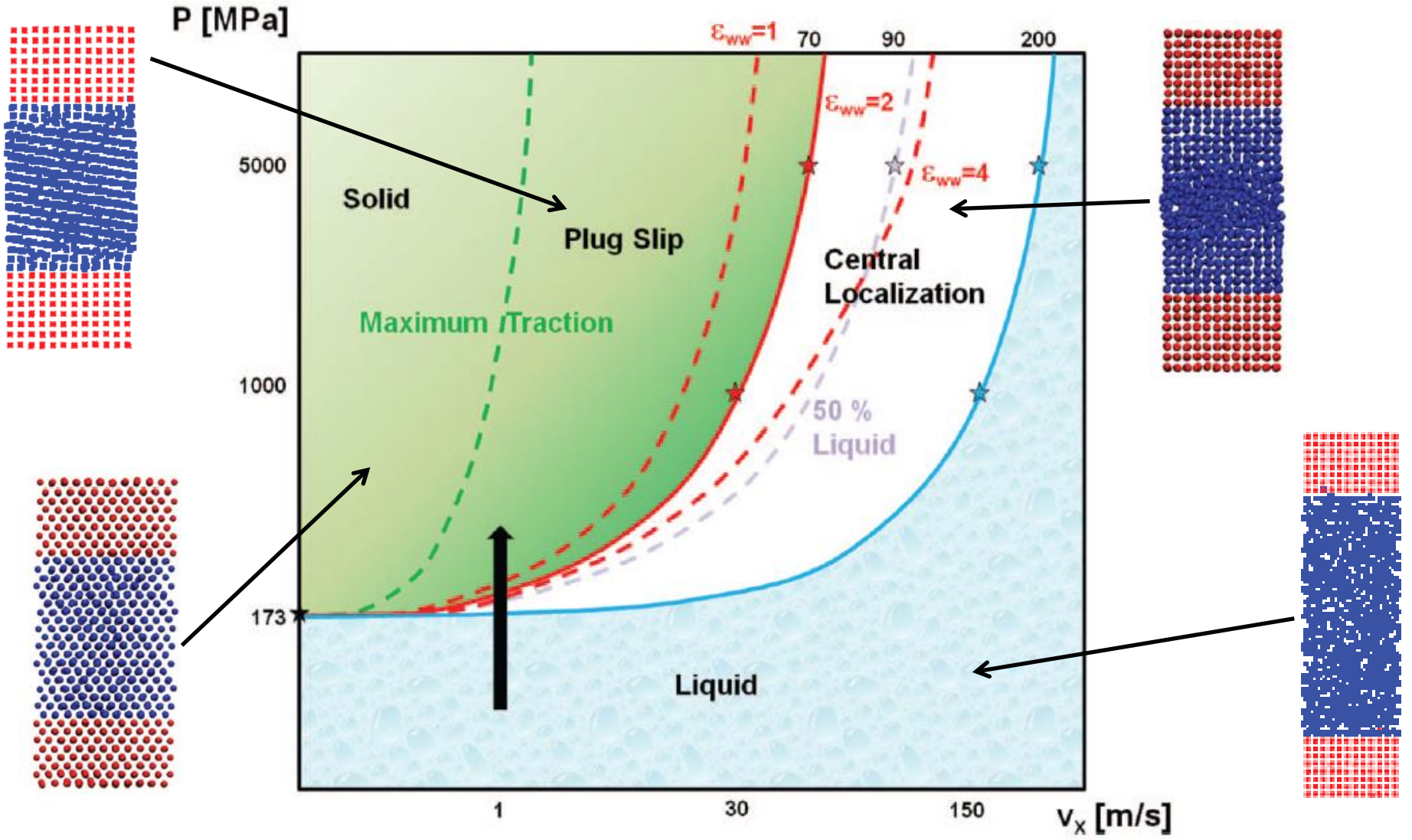






Non Continuum Shear Phase Map



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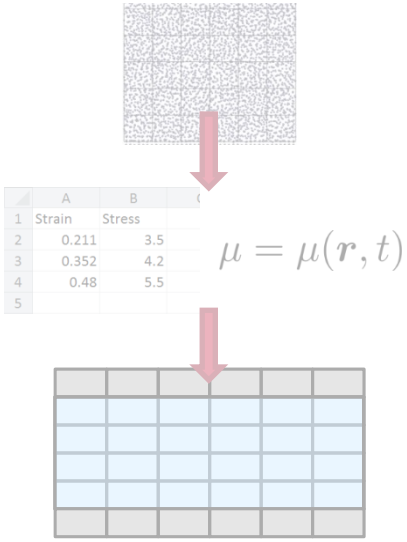

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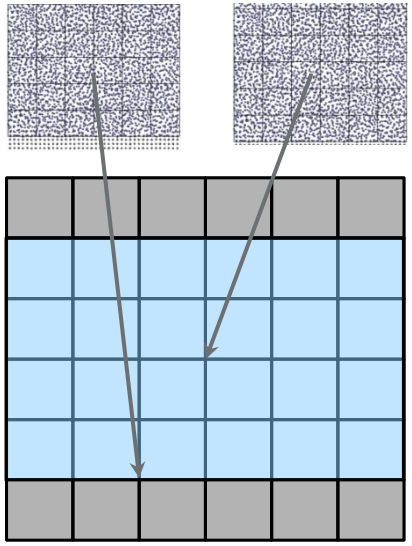

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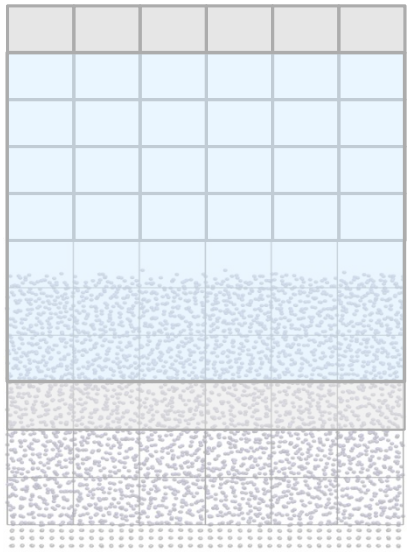

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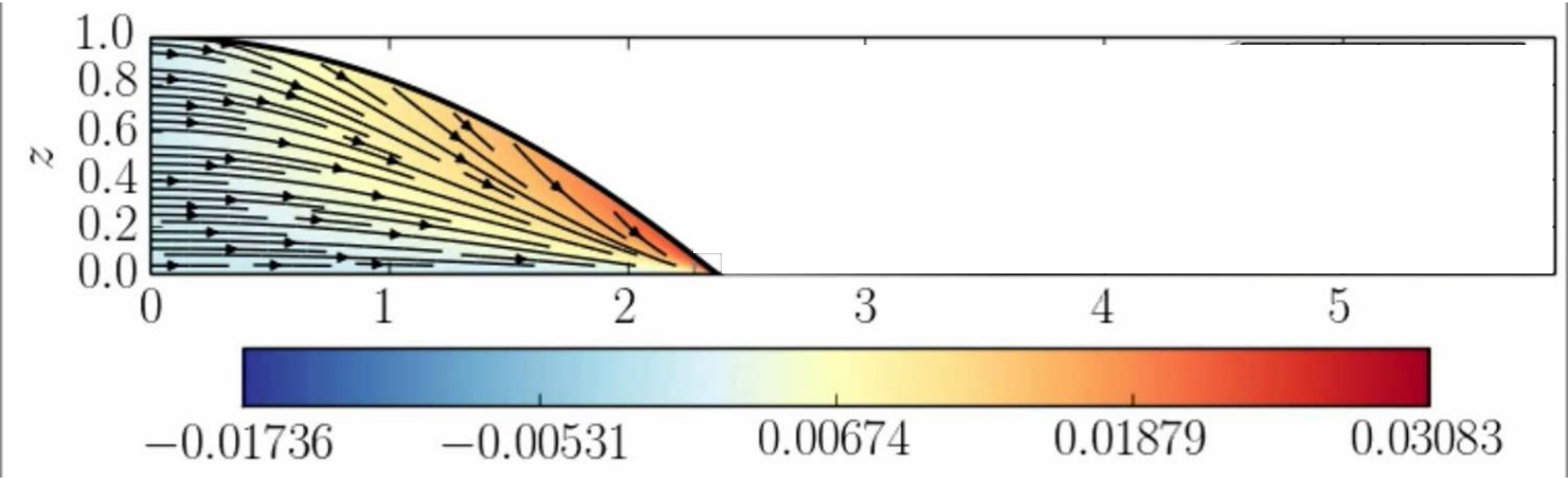
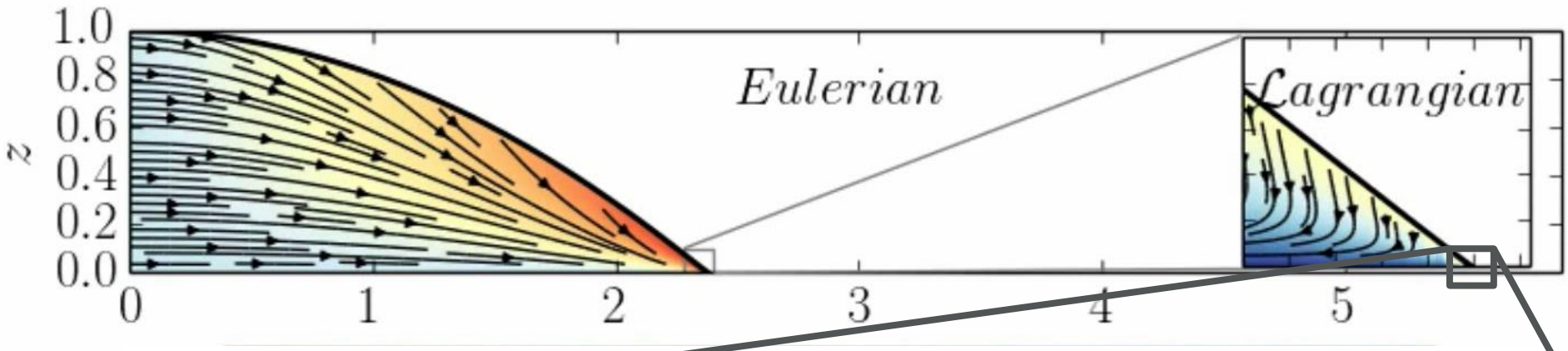
Coupled Droplet Spreading and MD



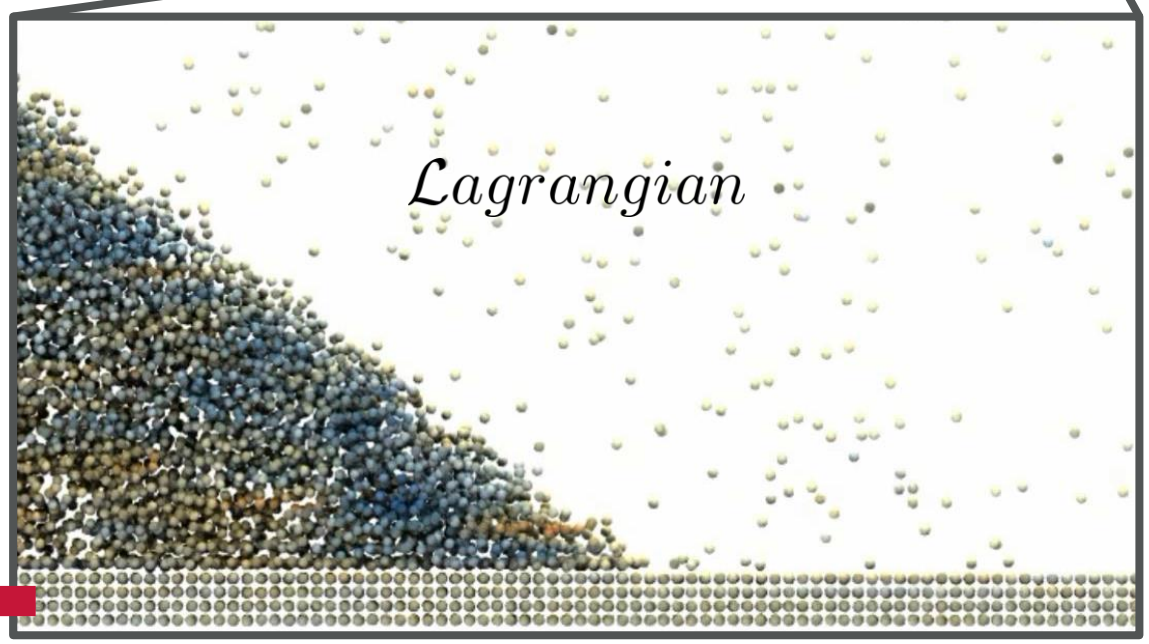
Coupled Droplet Spreading and MD

1) Thompson and Robbins (1989)



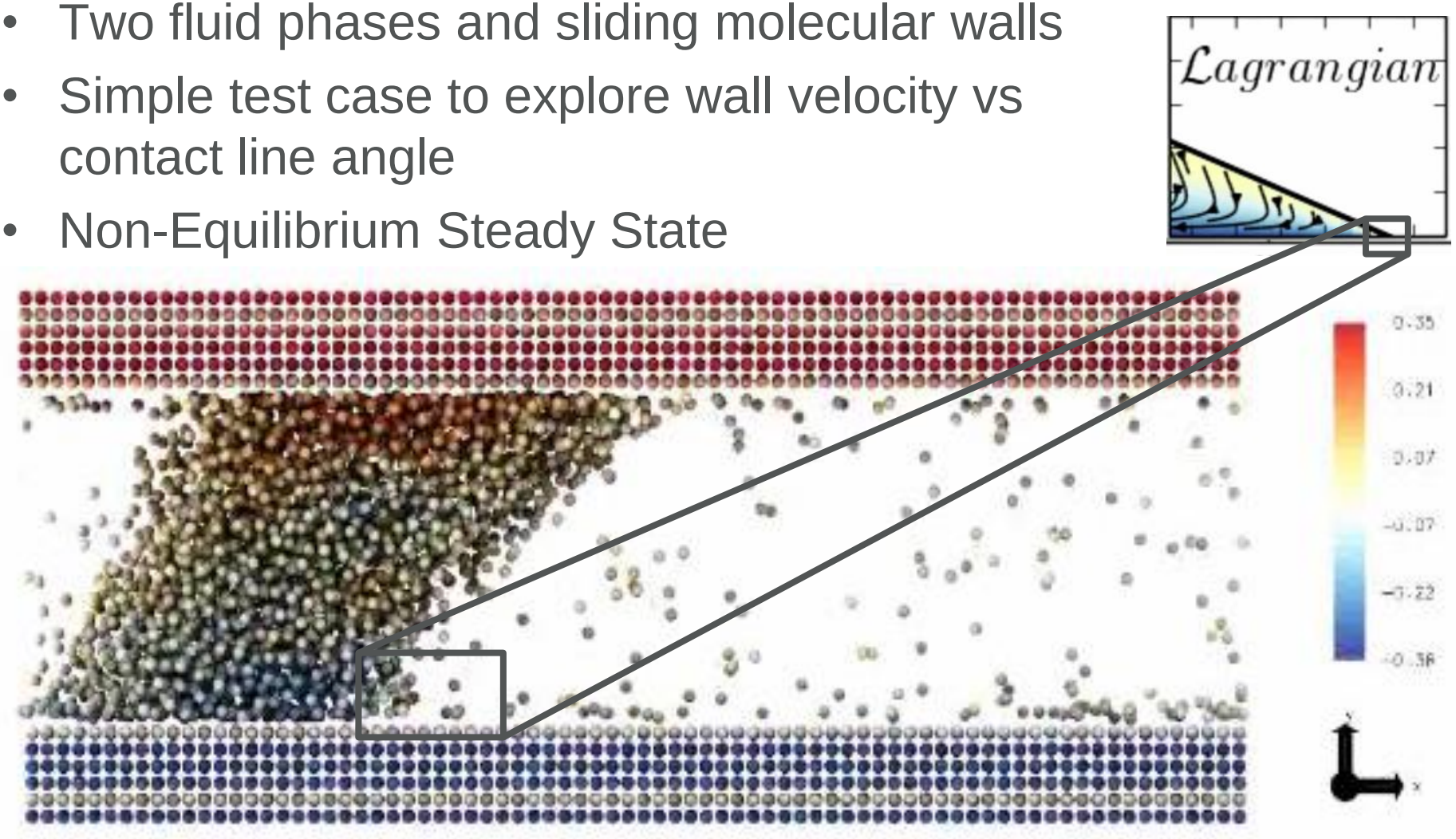
- Model the moving contact line with MD
- We want contact line speed as a function of continuum contact angle

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



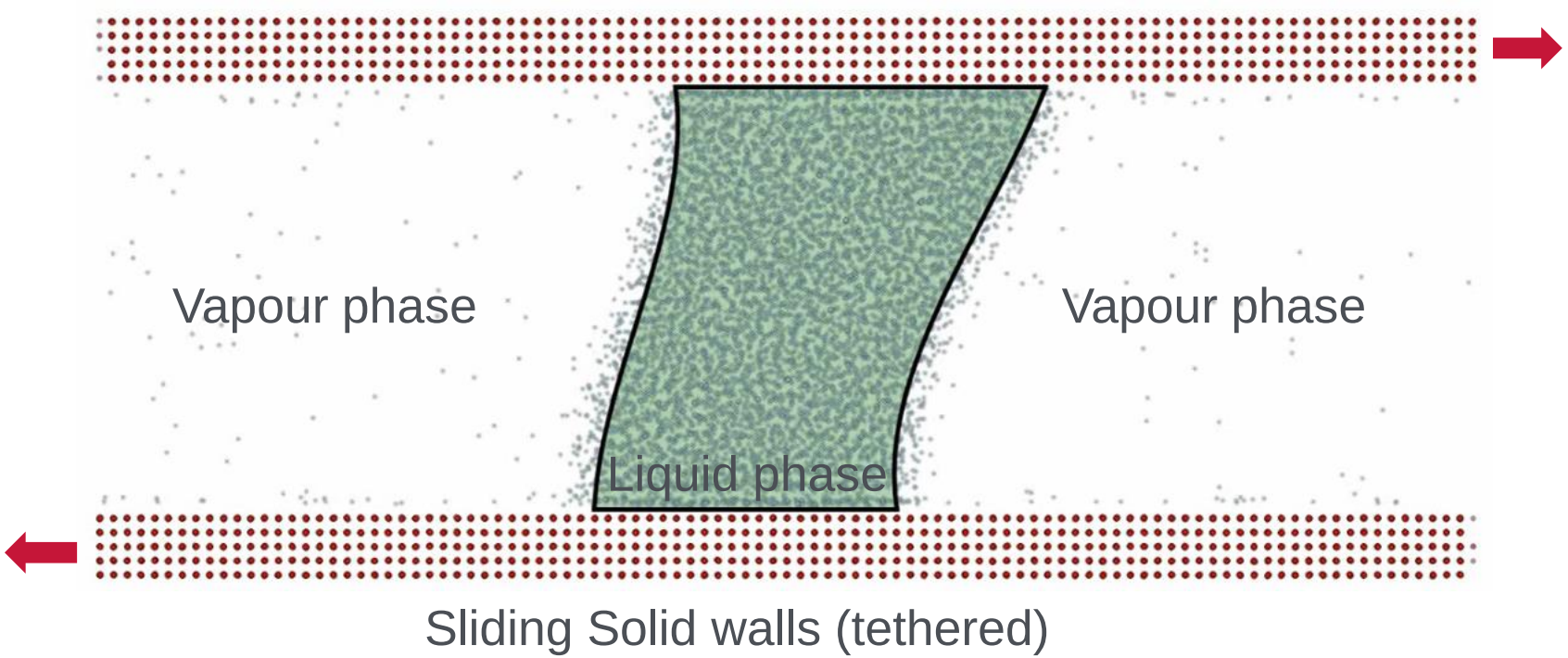
A Sheared Liquid Bridge

- Two fluid phases and sliding molecular walls
- Simple test case to explore wall velocity vs contact line angle
- Non-Equilibrium Steady State



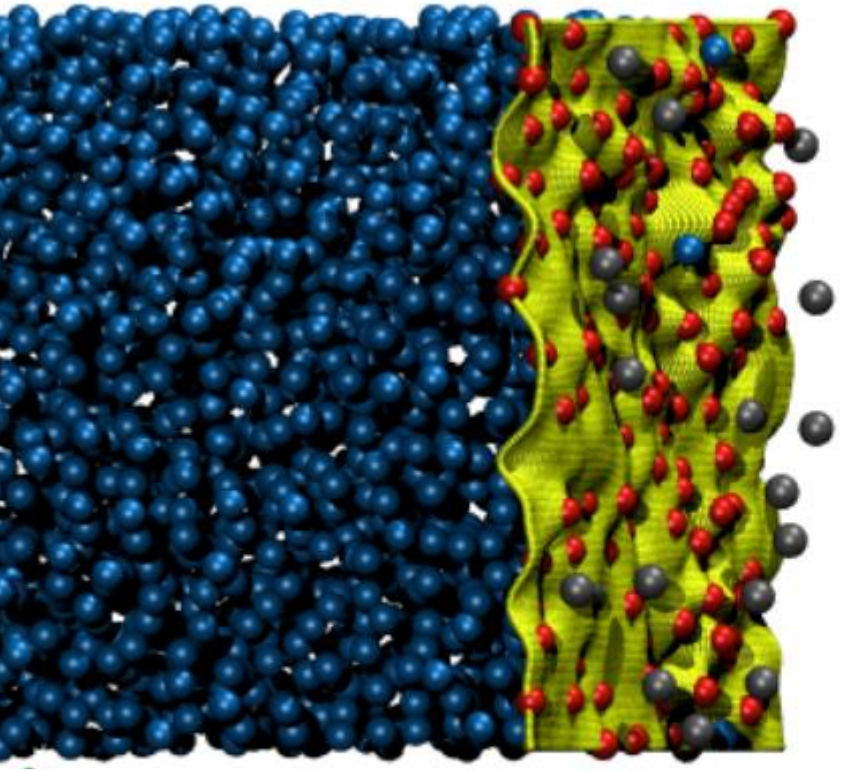
Moving liquid-vapour interfaces

- Molecular dynamics naturally forms an interface
- Mathematical framework to track moving surface
  - Dynamics, surface tension and curvature
  - Flow along surface of molecules (e.g. surfactants)



Intrinsic surface

- Intrinsic Surface by minimising a penalty function



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

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

Function of sines and cosines

Chacon & Tarazona (2003) PRL 91, 166103

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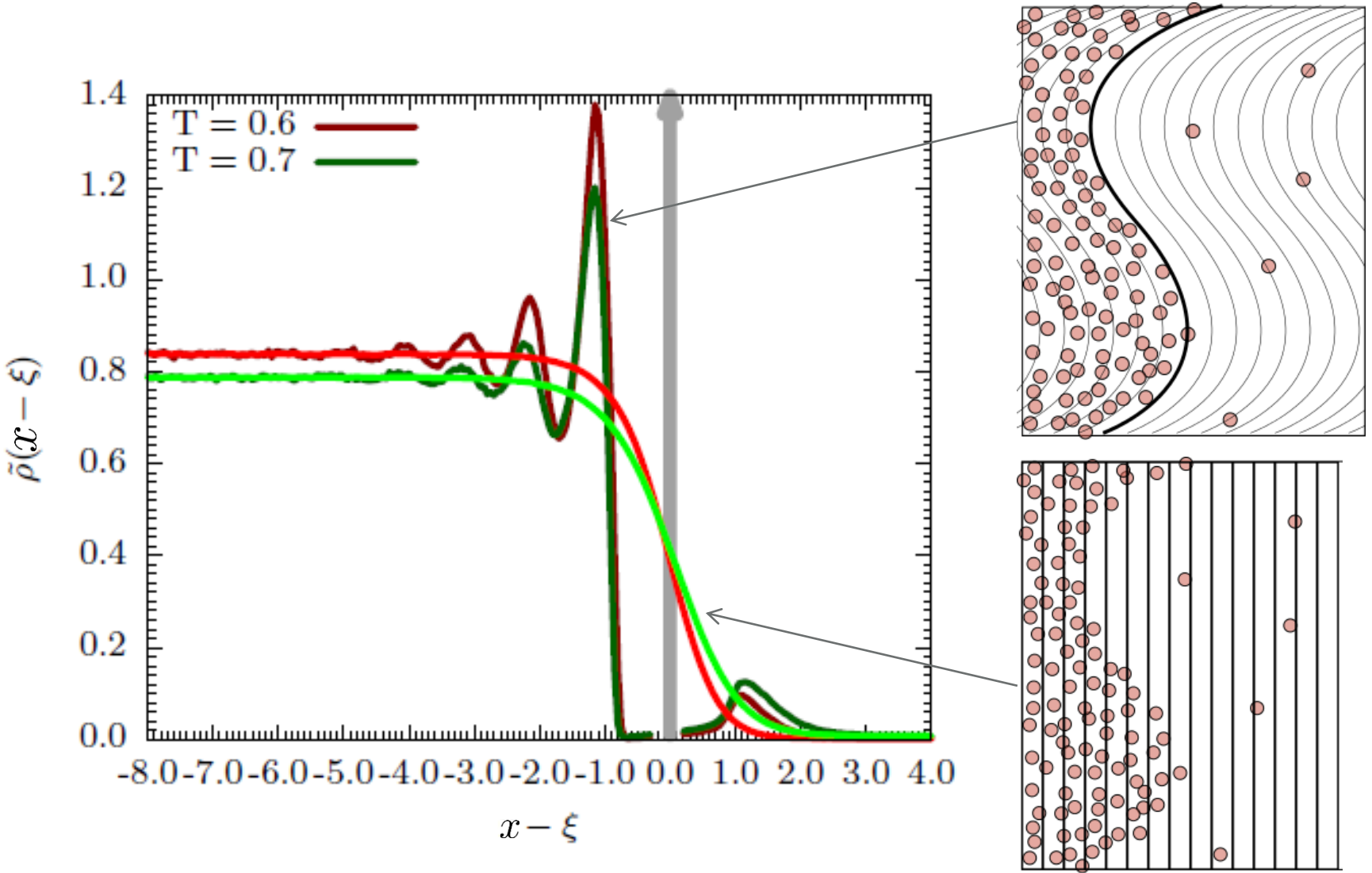
Interfaces Control Volume



Molecular Dynamics simulation of Nucleation

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Wall w
mo
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Isosurface of Density

EPSRC
Pioneering research and skills

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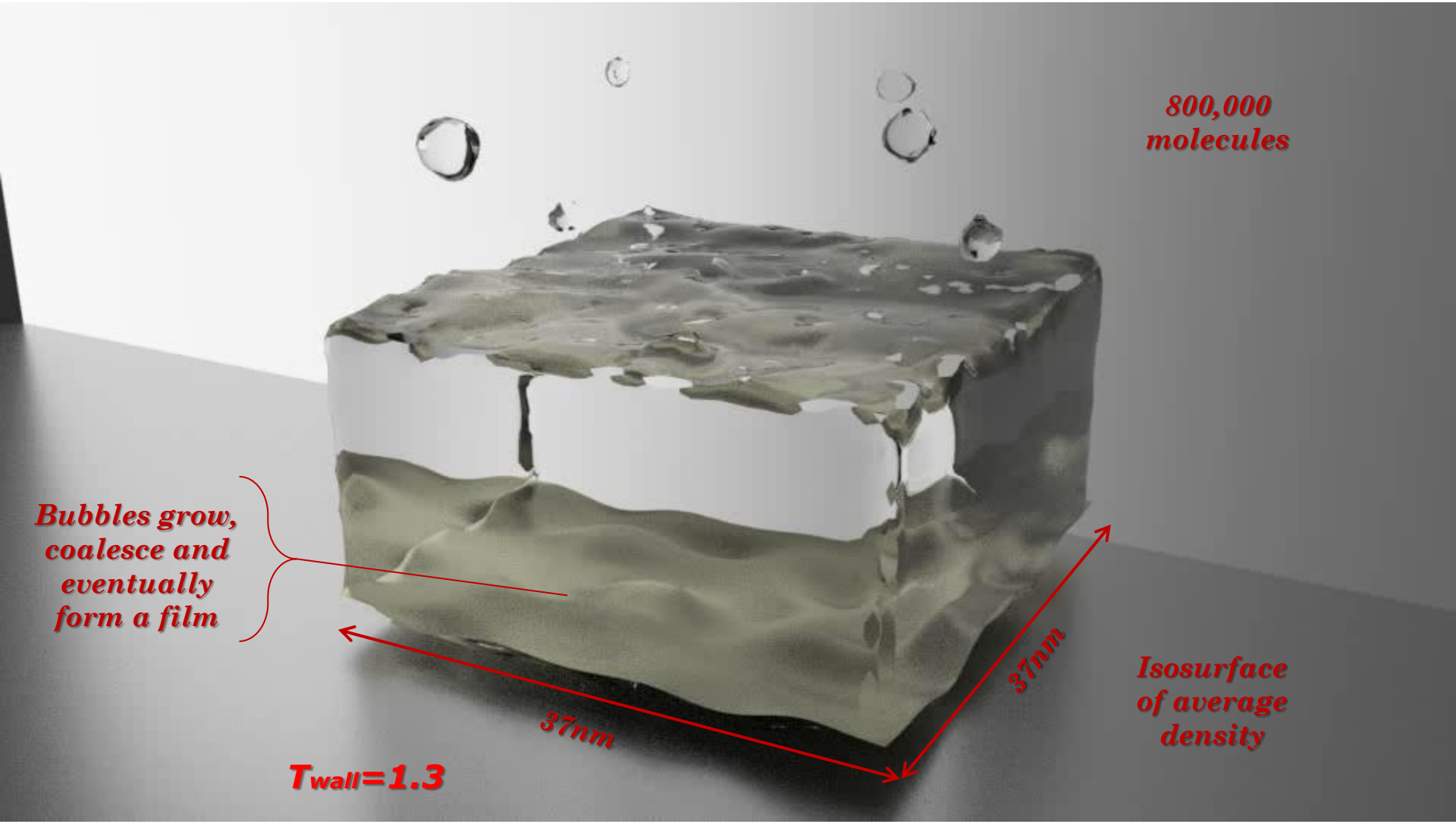
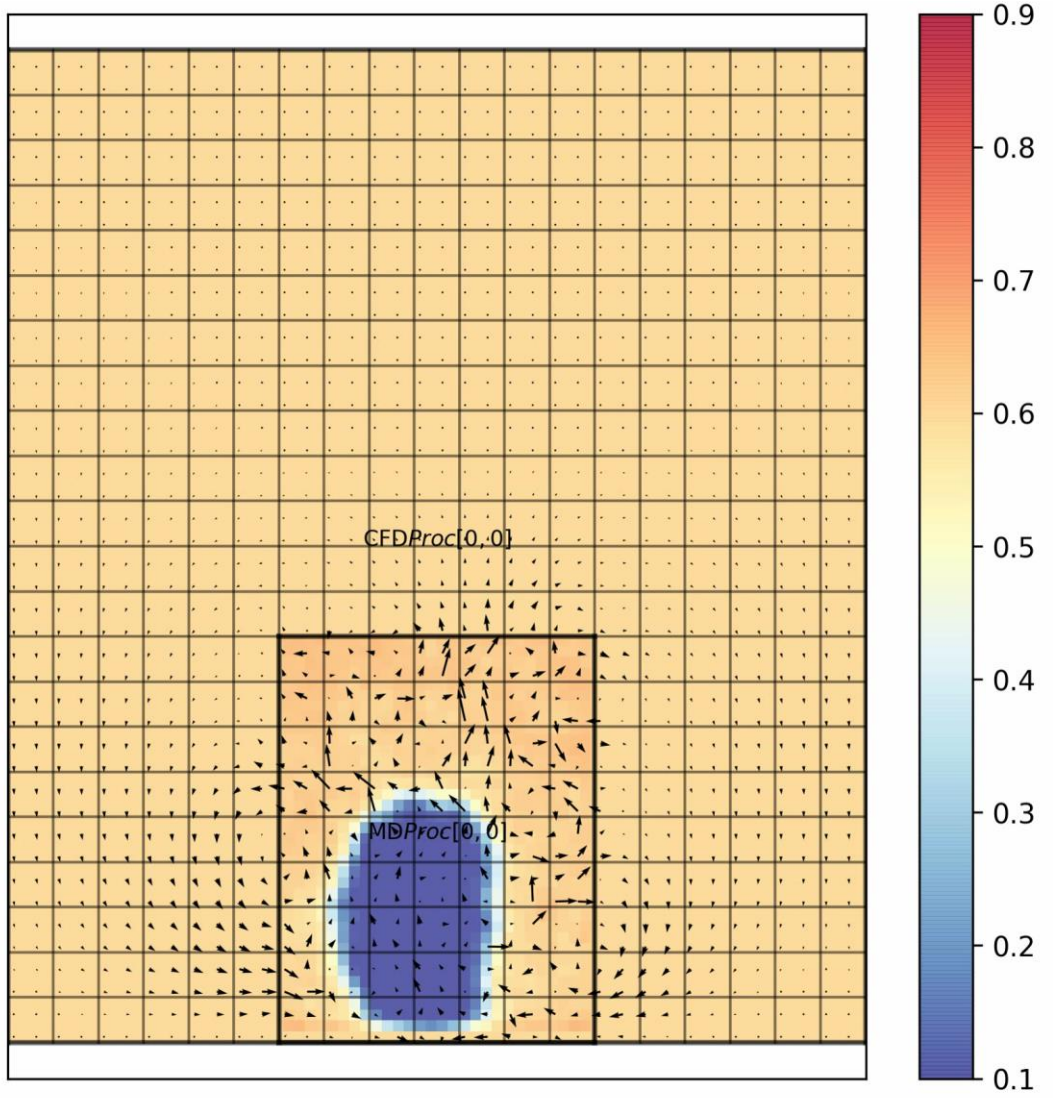


Coupled Simulation of Boiling

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



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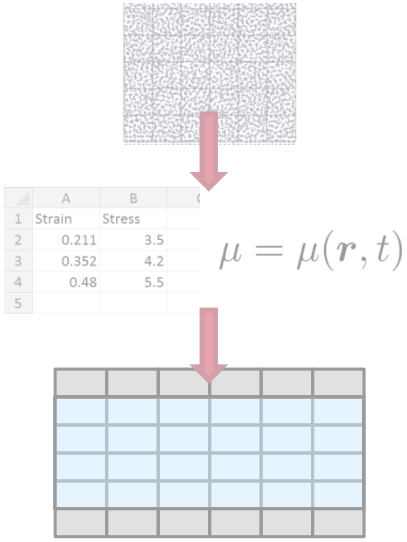

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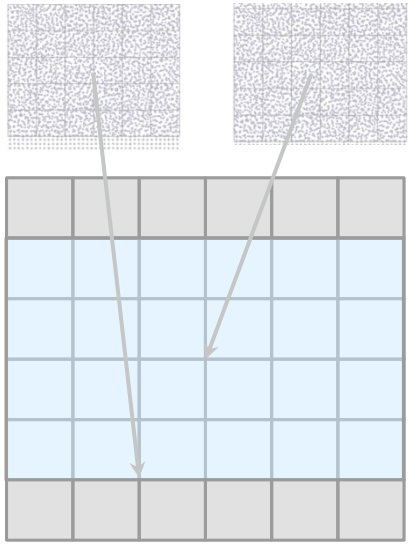

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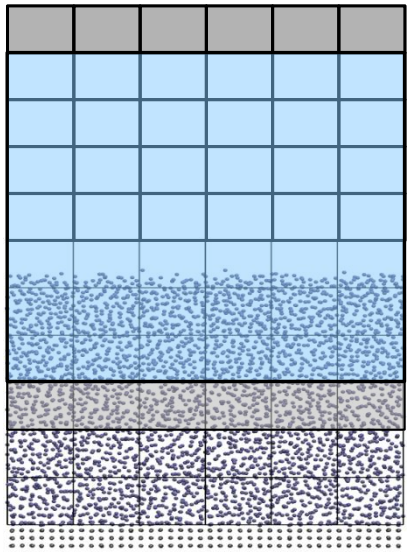

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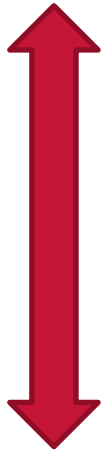
Coupled Simulation

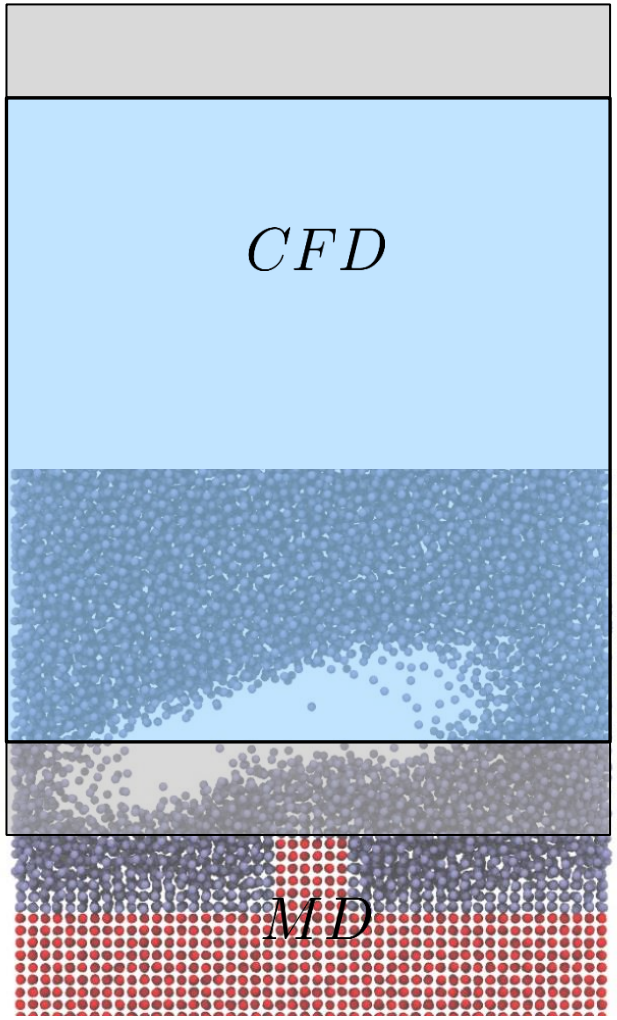
- Assumes a continuous field

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



- Discrete molecules

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



Coupled Simulation

- Control (Finite) Volume form

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

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

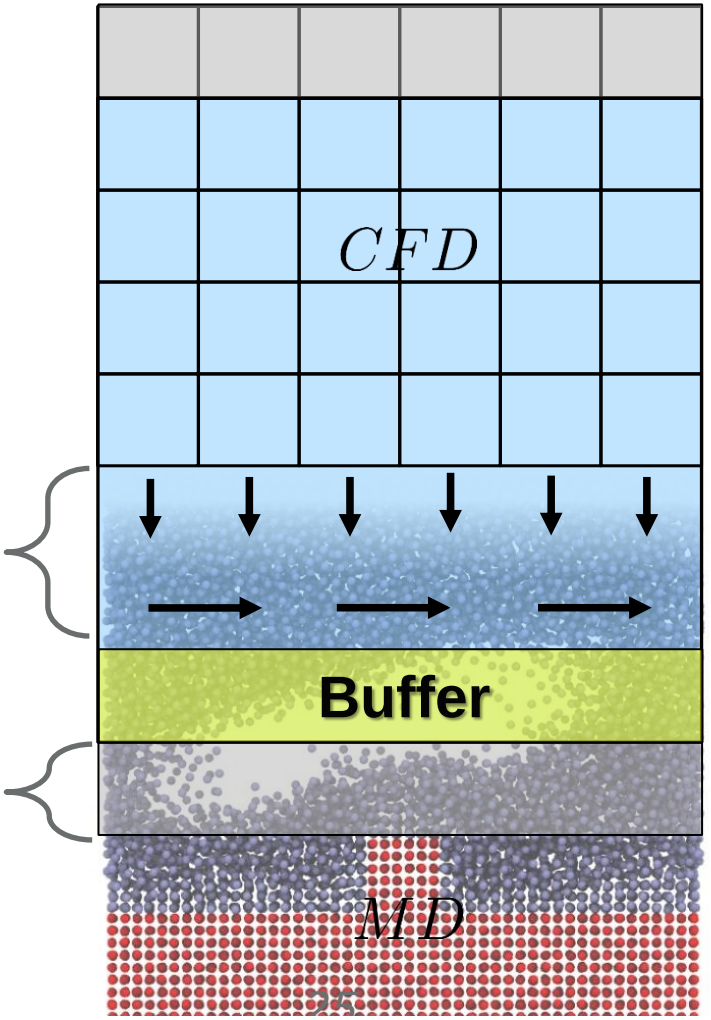
CFD→MD Boundary condition

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

MD→CFD Boundary condition

- Discrete molecules

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



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

Granular Mechanics

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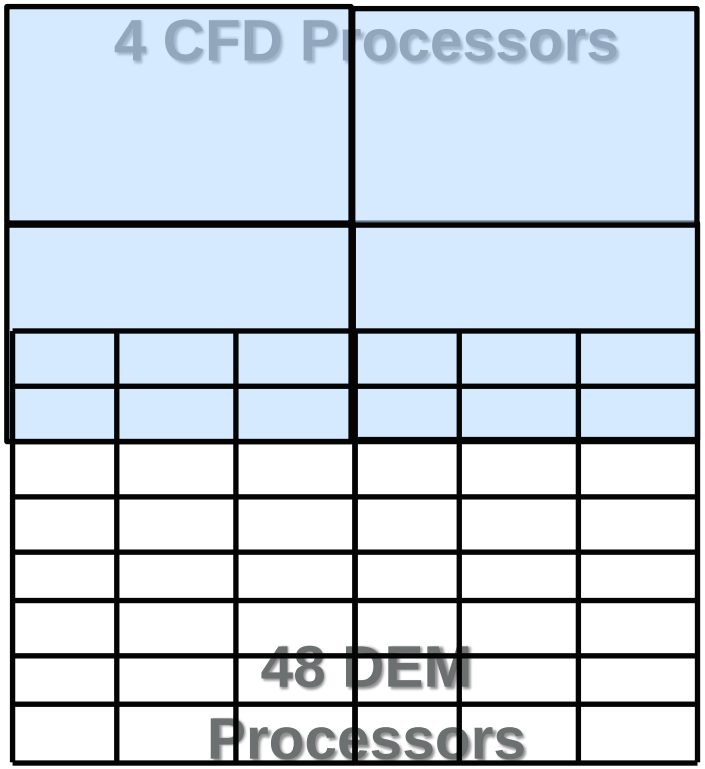
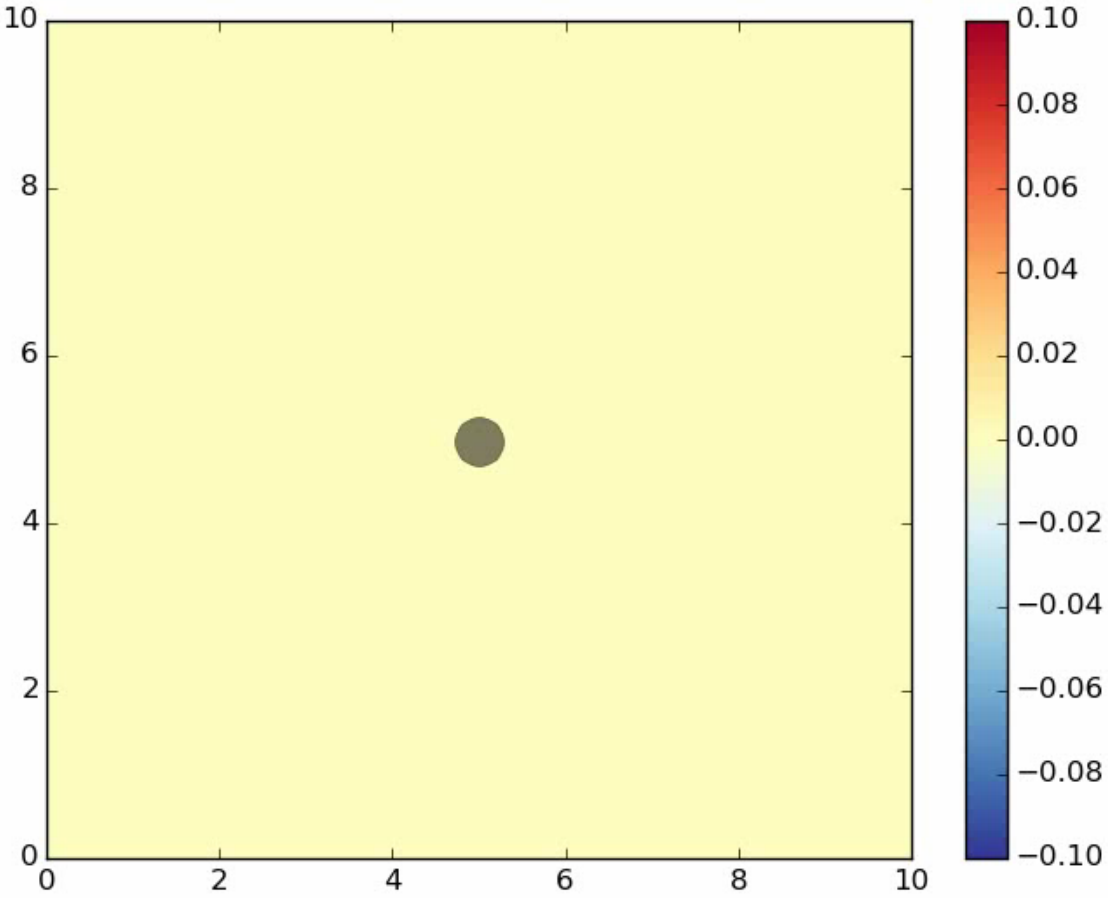


Particle in Flow (with Drag)

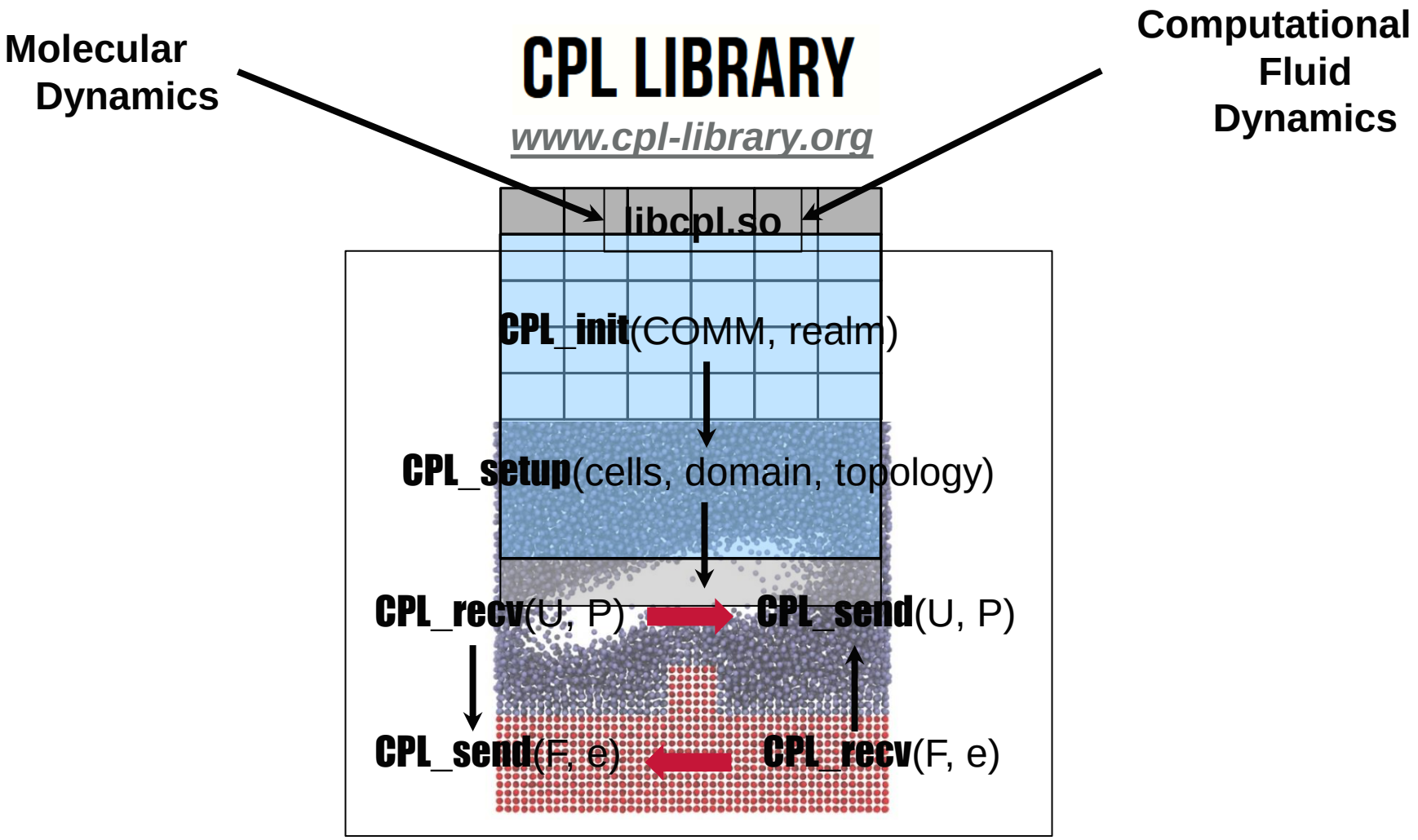


- Drag force applied to molecule with porosity calculated

$$f_i = A|u_i - u|(u_i - u)$$

- Equal and opposite force applied back to CFD

CPL Library

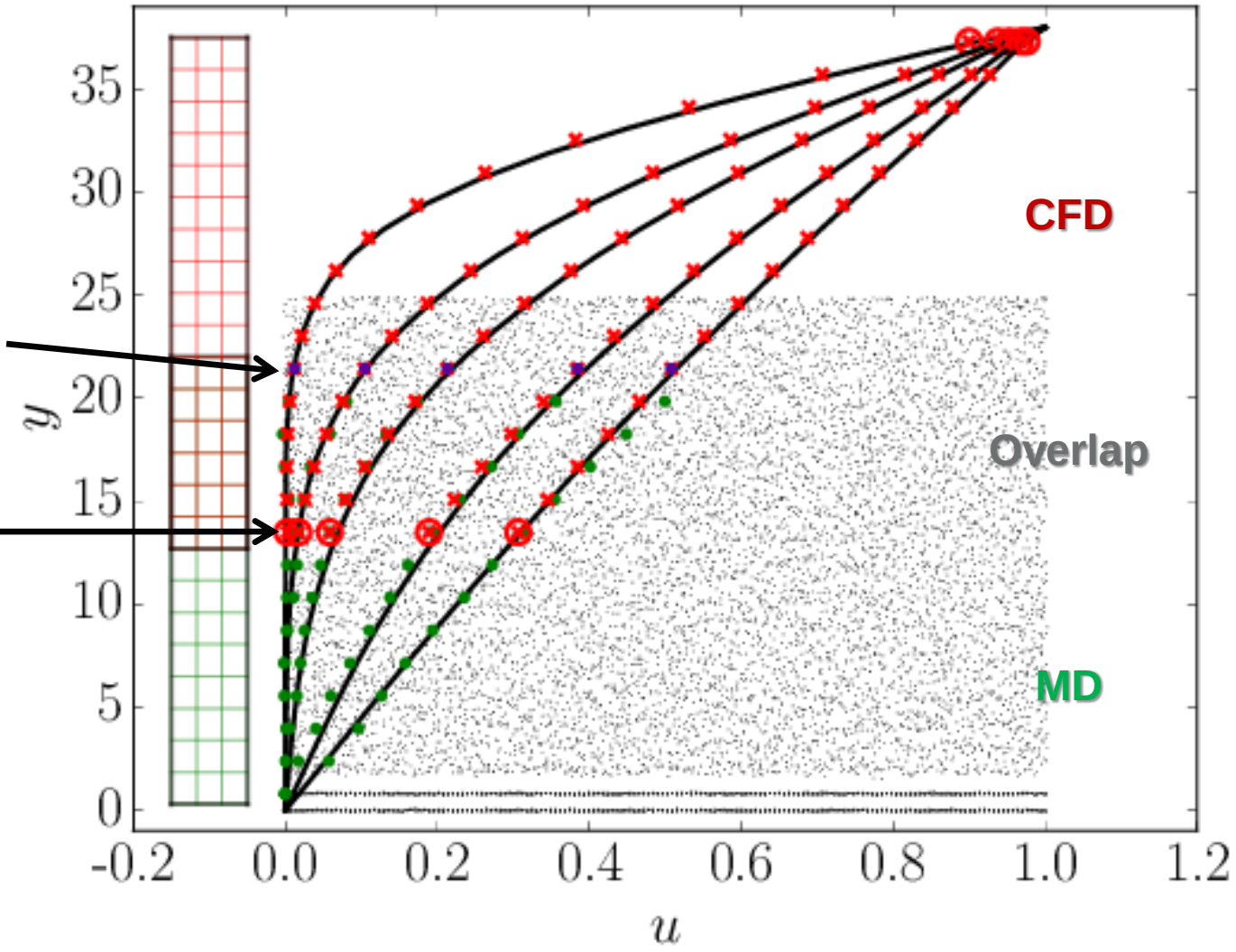

Molecular Dynamics
CPL LIBRARY
www.cpl-library.org
Computational Fluid Dynamics
libcpl.so
CPL_init(COMM, realm)
CPL_setup(cells, domain, topology)
CPL_recv(U, P)
CPL_send(U, P)
CPL_send(F, e)
CPL_recv(F, e)

Coupling Results – Couette Flow

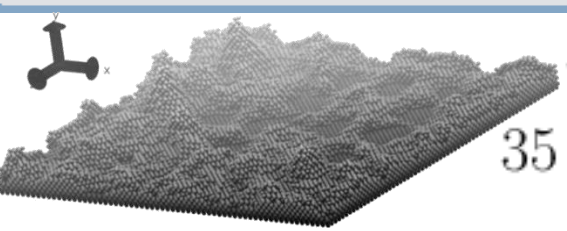
Brunel University London

Constraint

CFD Boundary



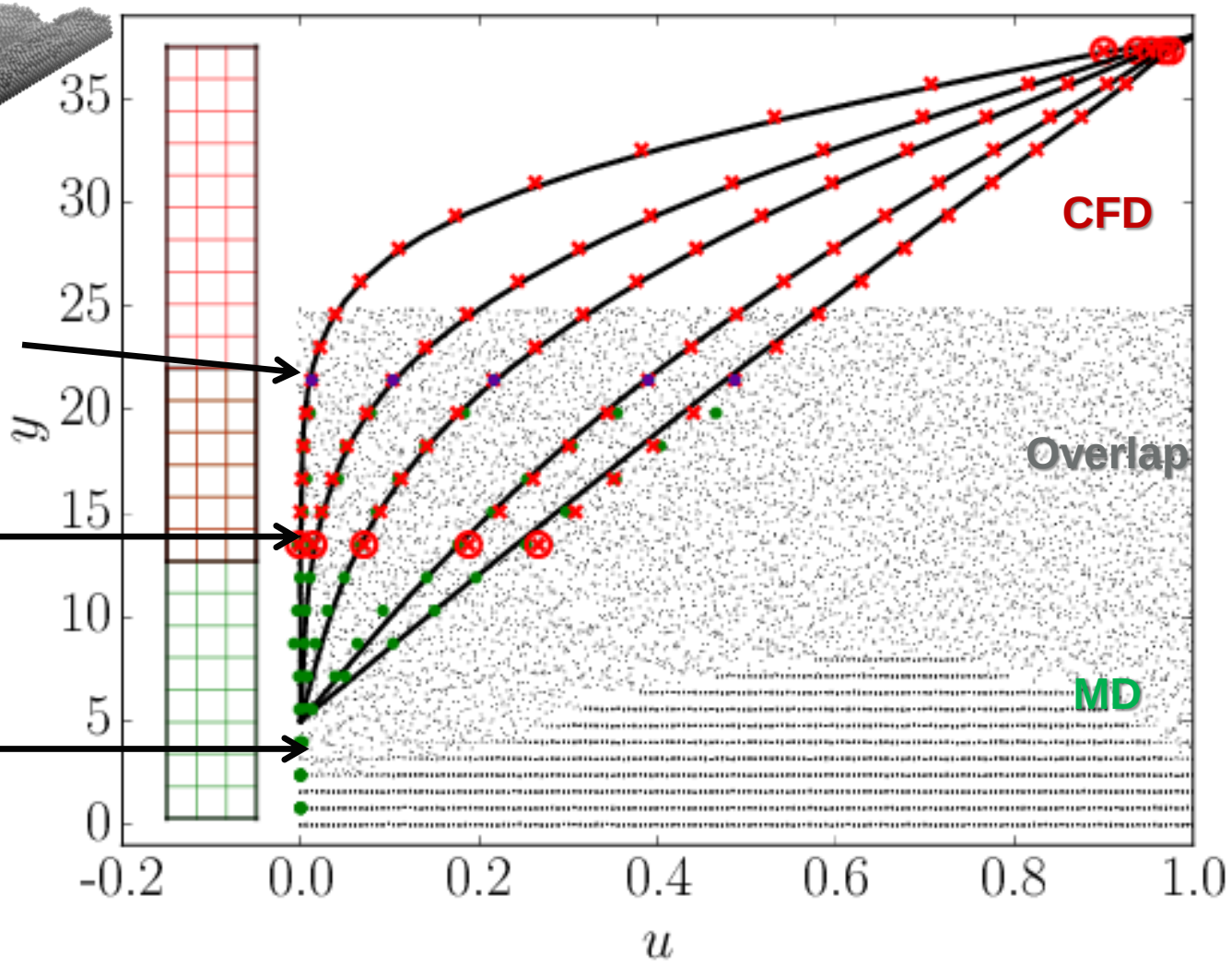
Coupling Results – Couette Flow



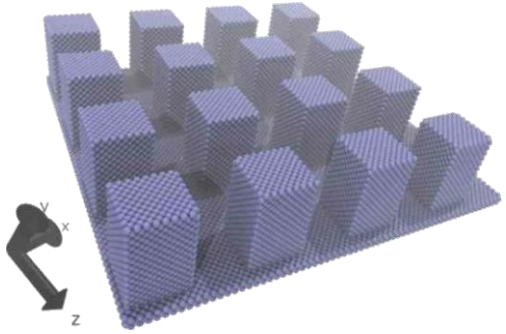
Constraint

CFD Boundary

Rough wall shifts zero velocity location



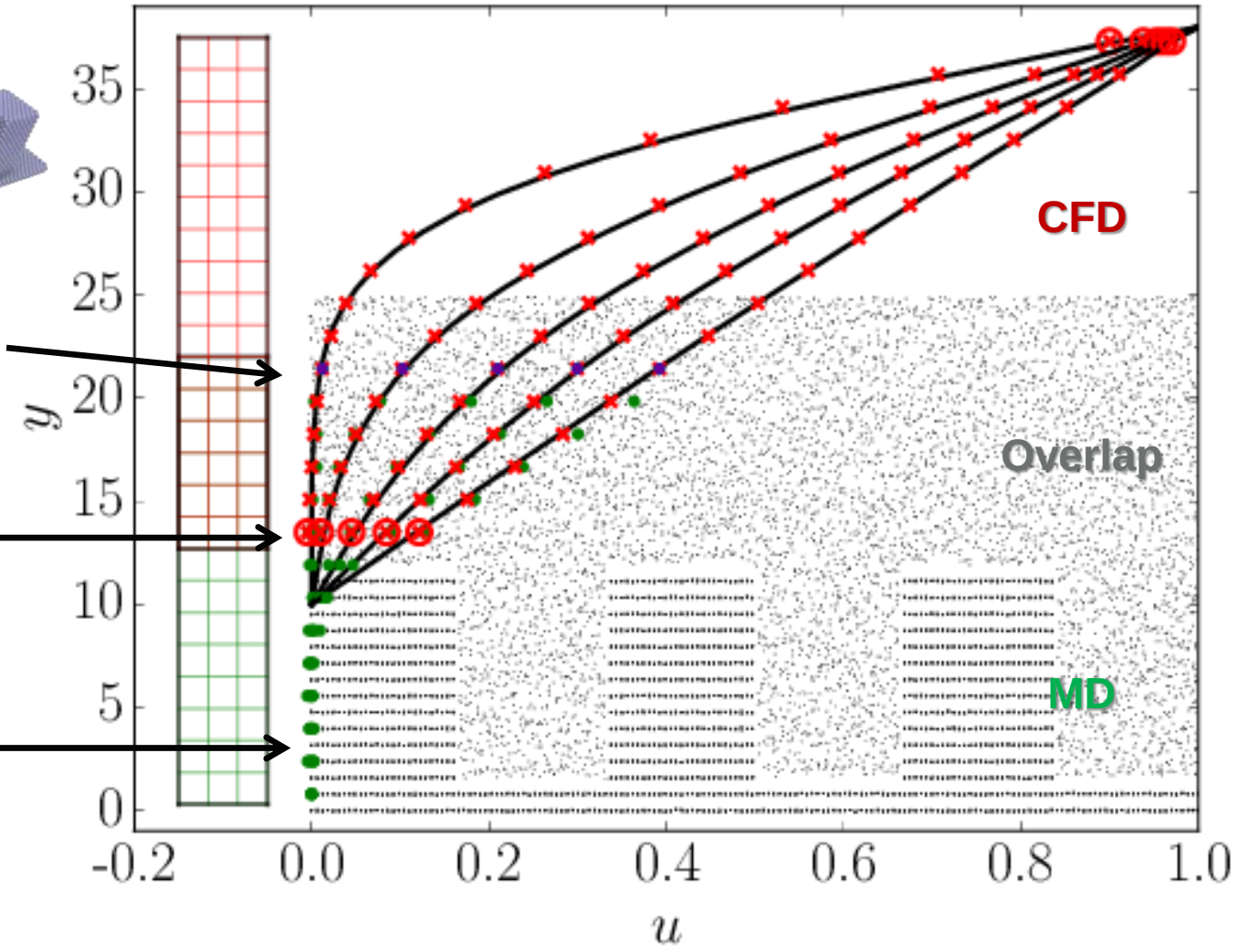
Coupling Results – Couette Flow



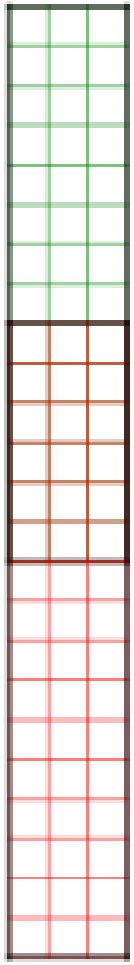
Constraint

CFD Boundary

Posts shifts zero velocity location



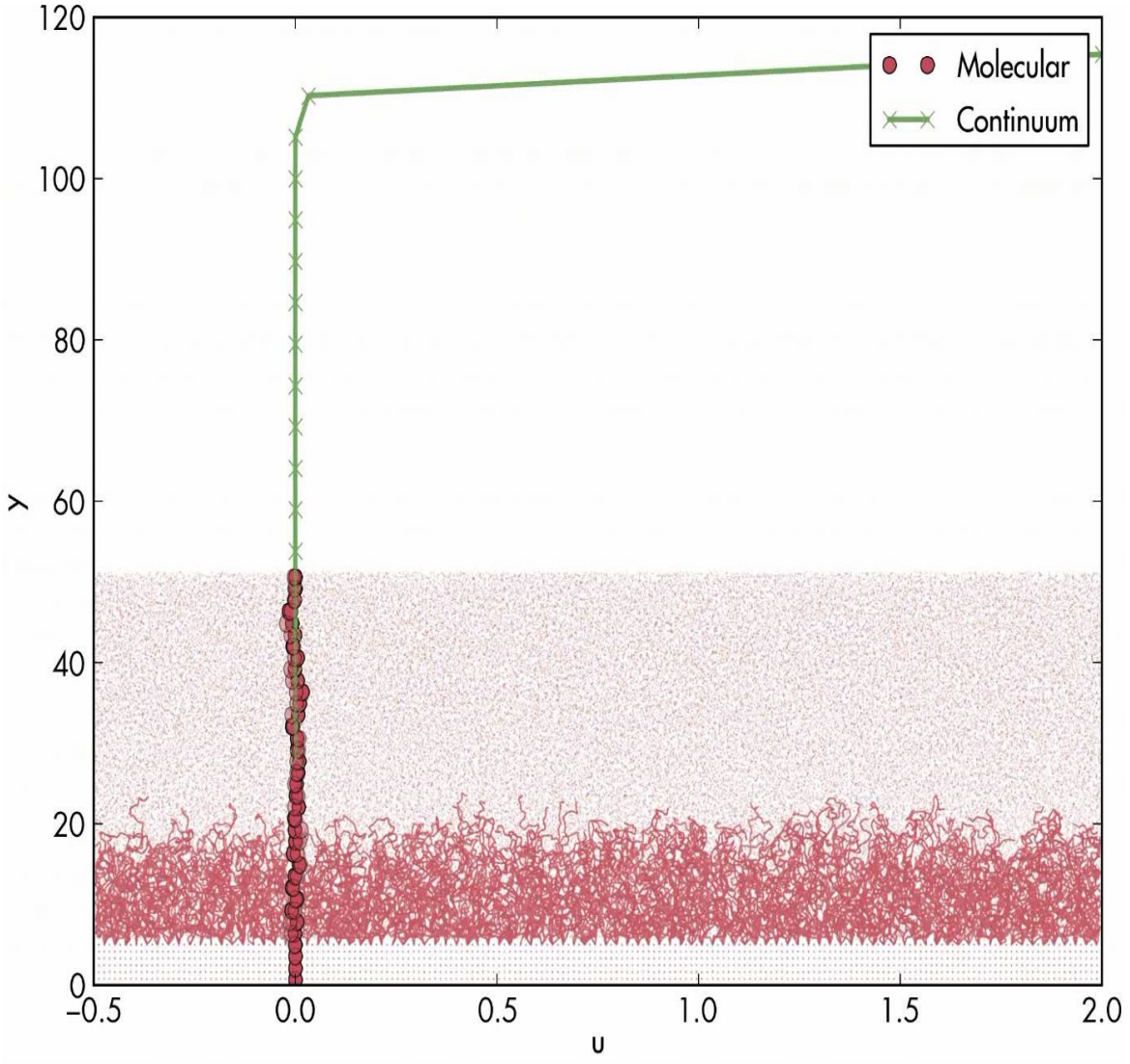
Coupling Results – Polymer Brushes



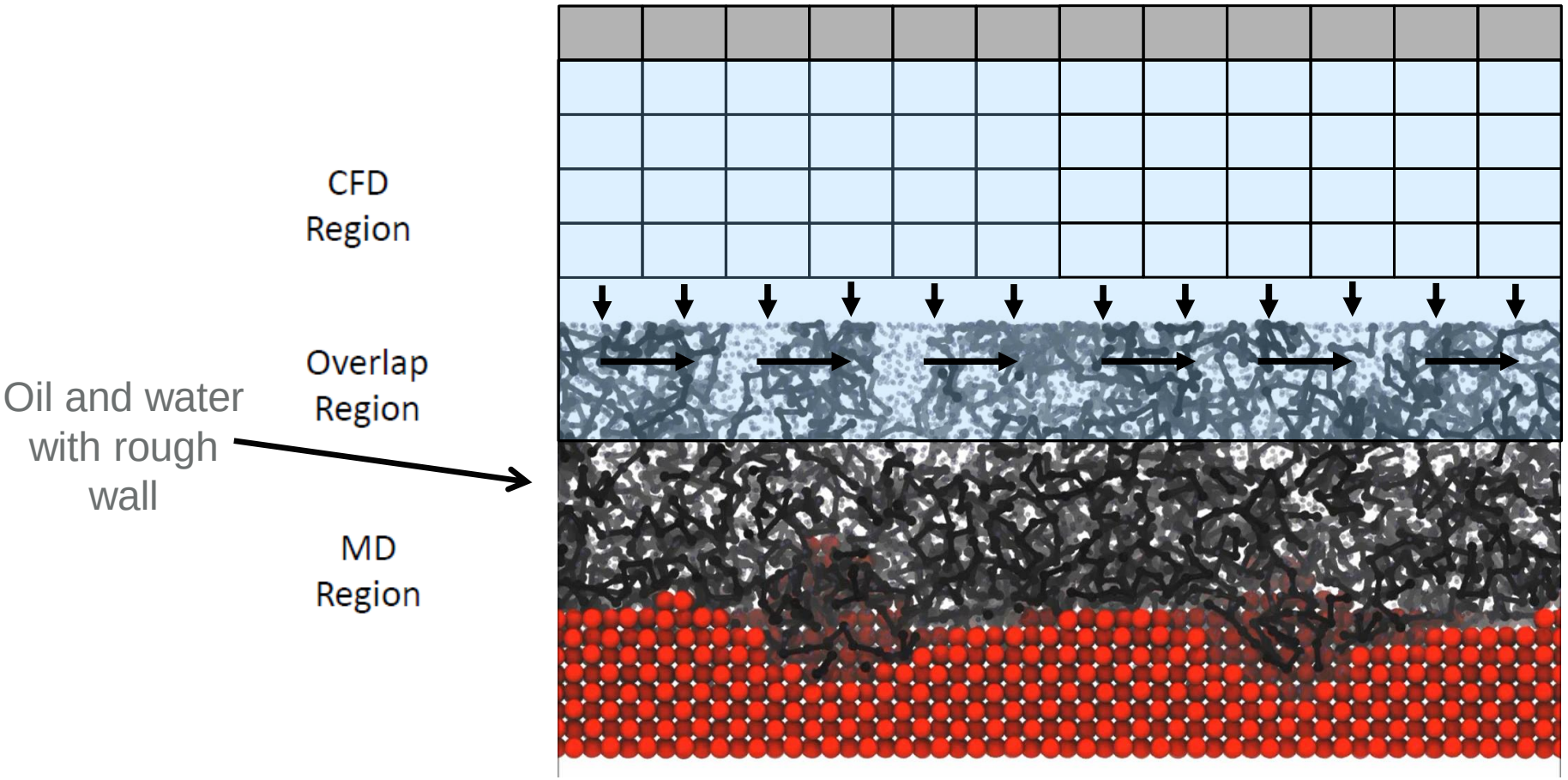
CFD Region

Overlap Region

MD Region



Coupling Results – Couette Flow



Molecular Simulation of Turbulence

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Molecular Simulation of Turbulence

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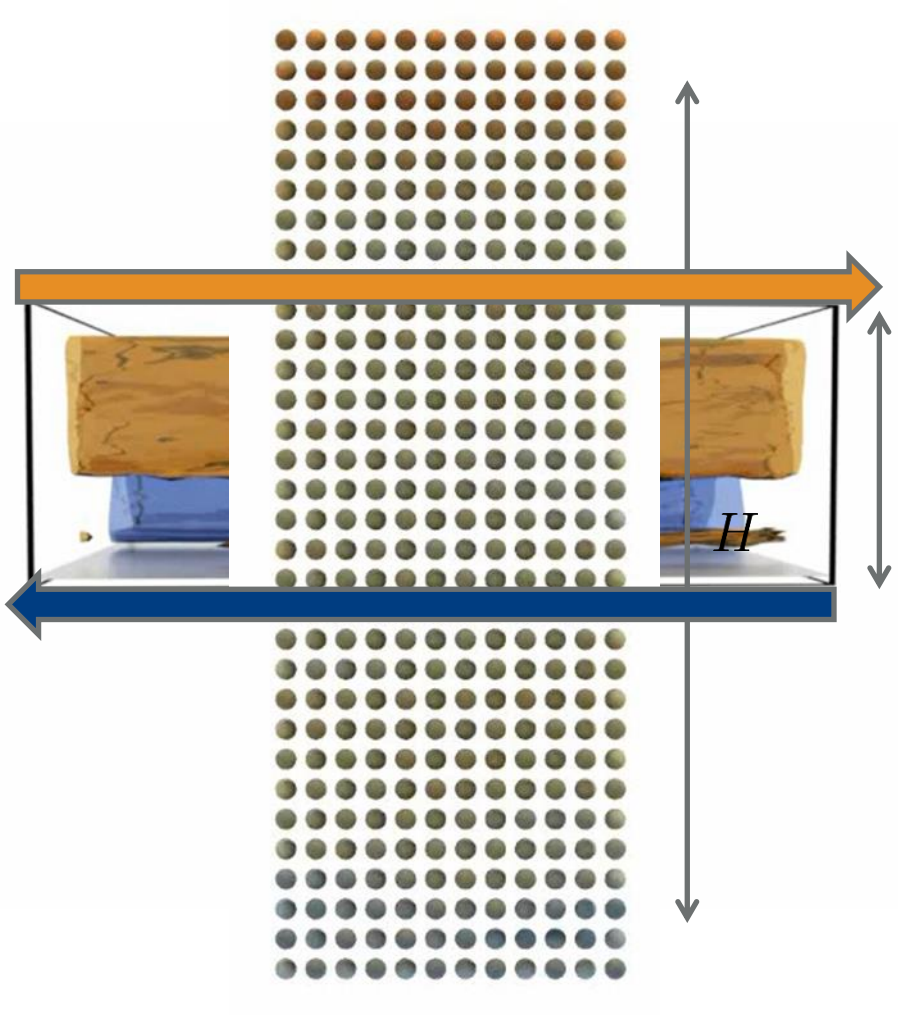

Reynolds Number

$Re \approx 400$

with

300 million molecules

Molecular Simulation of Turbulence

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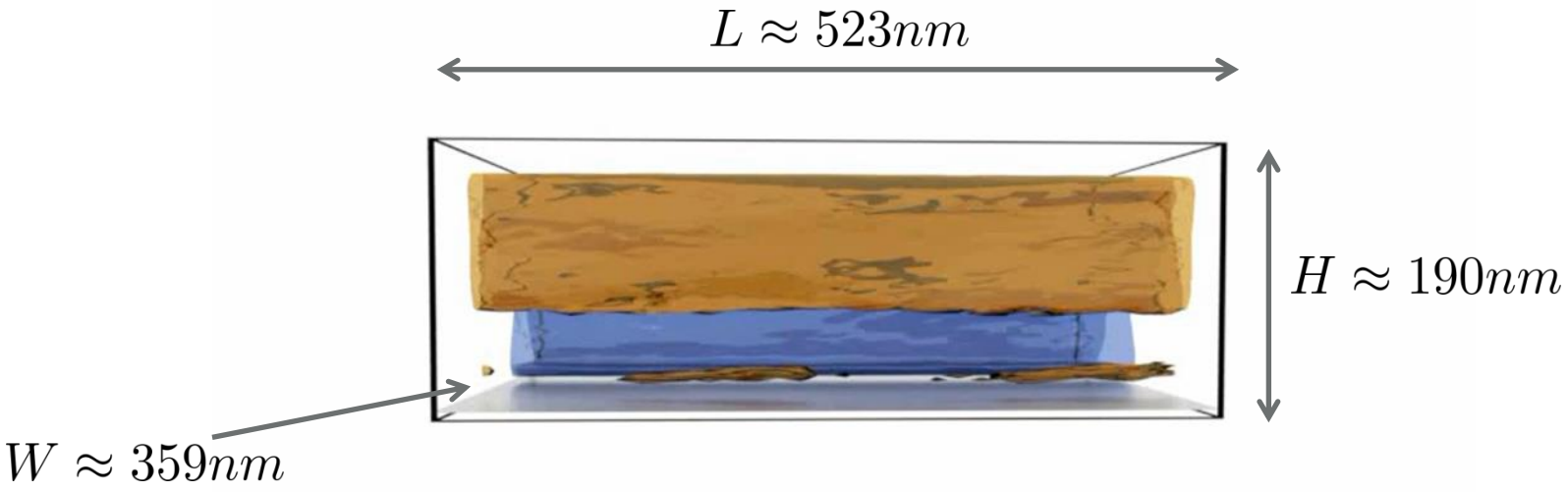
Minimal channel Couette flow



Reynolds Number

$Re \approx 400$

with
300 million molecules

Molecular Simulation of Turbulence

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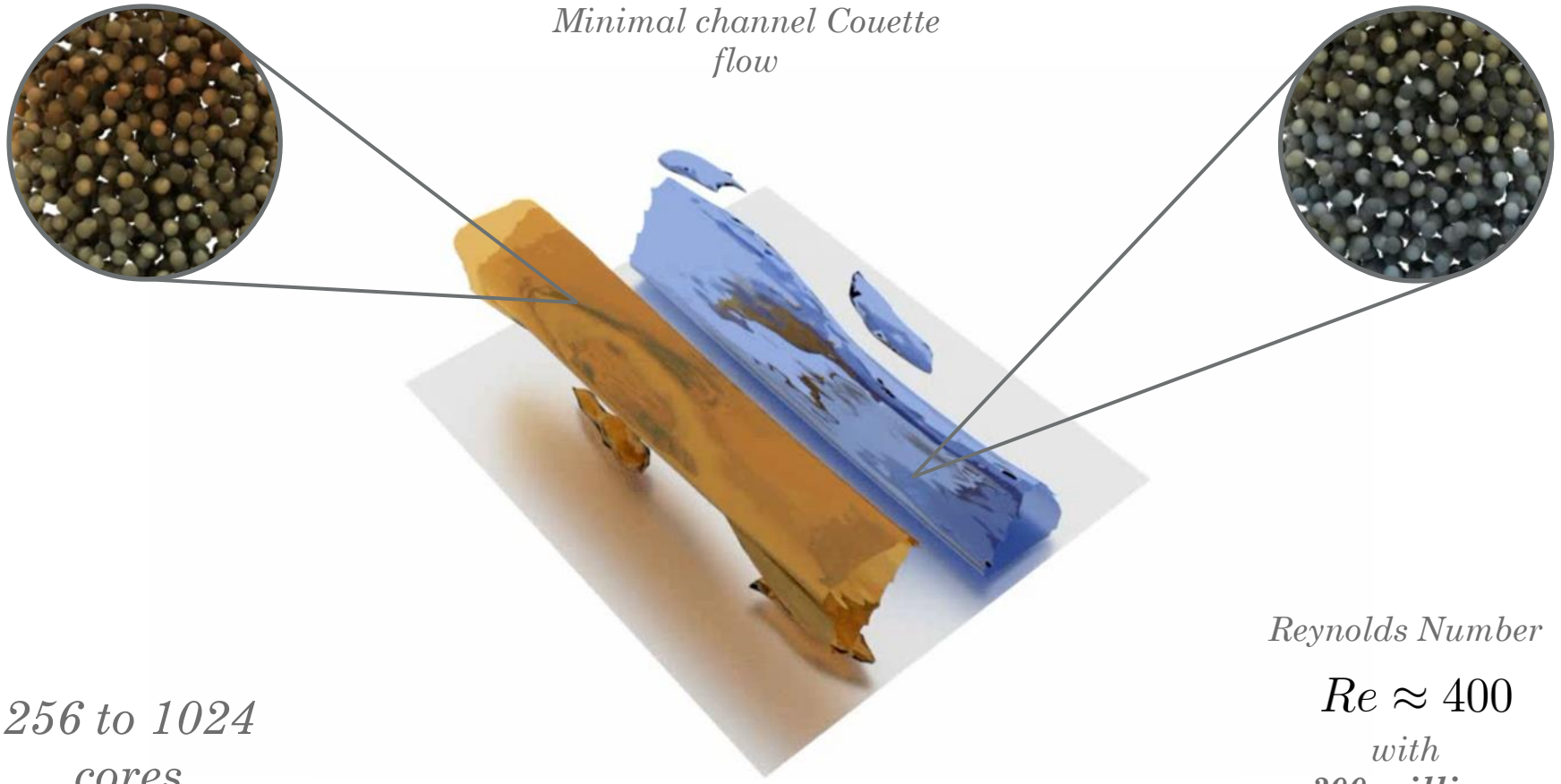
Minimal channel Couette flow



Isosurfaces of turbulent kinetic energy coloured by velocity

256 to 1024 cores Running for over a year

Reynolds Number

$Re \approx 400$

with ***300 million molecules***

Molecular Simulation of Turbulence

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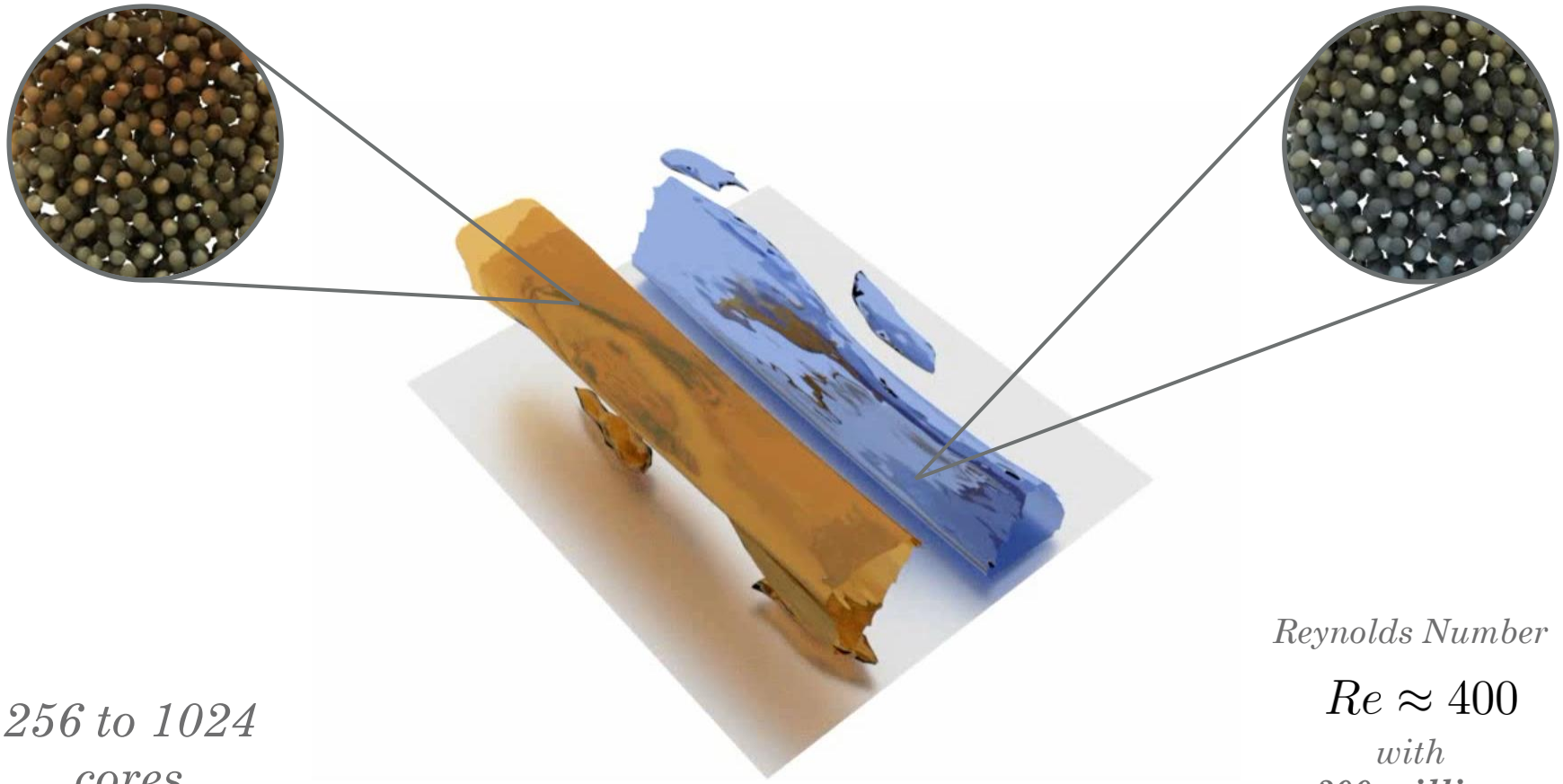

Isosurfaces of turbulent kinetic energy coloured by velocity

256 to 1024 cores Running for over a year

Reynolds Number

$Re \approx 400$

with ***300 million molecules***

Molecular Simulation of Turbulence

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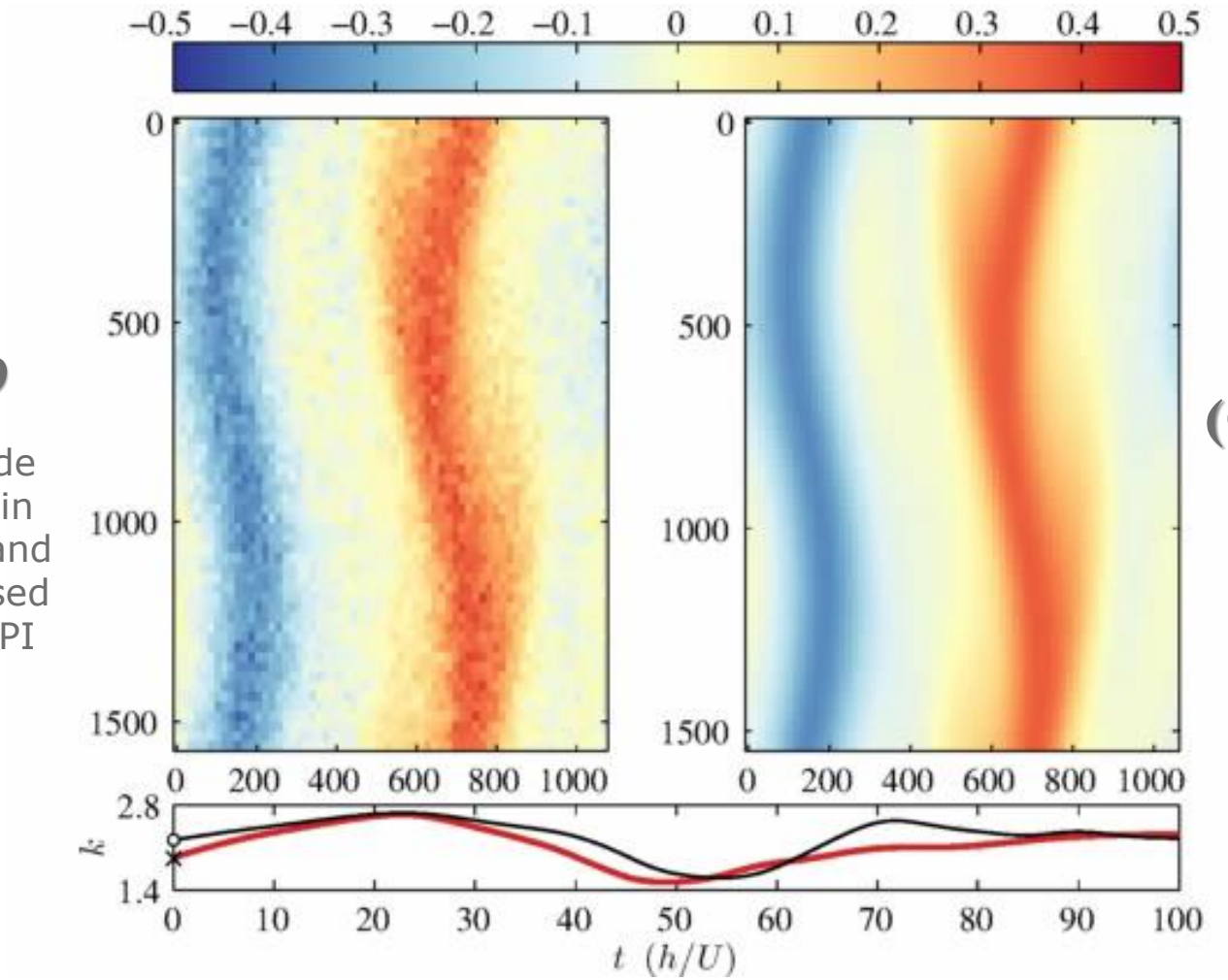
Centre slice velocity



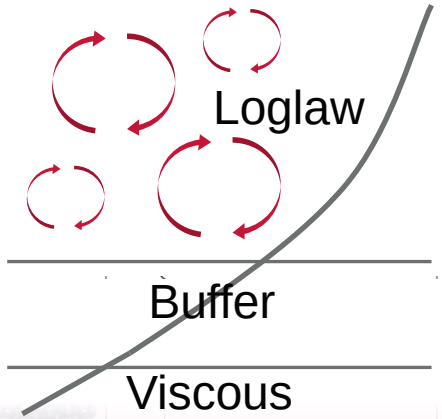
MD

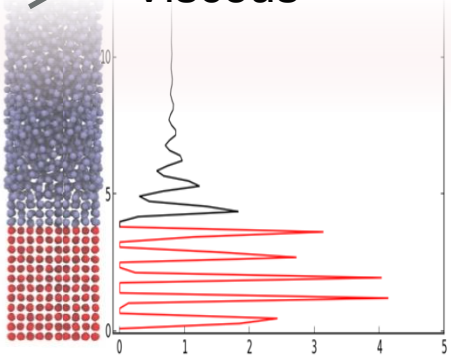
Own code written in Fortran and parallelised using MPI

CFD (Channelflow)

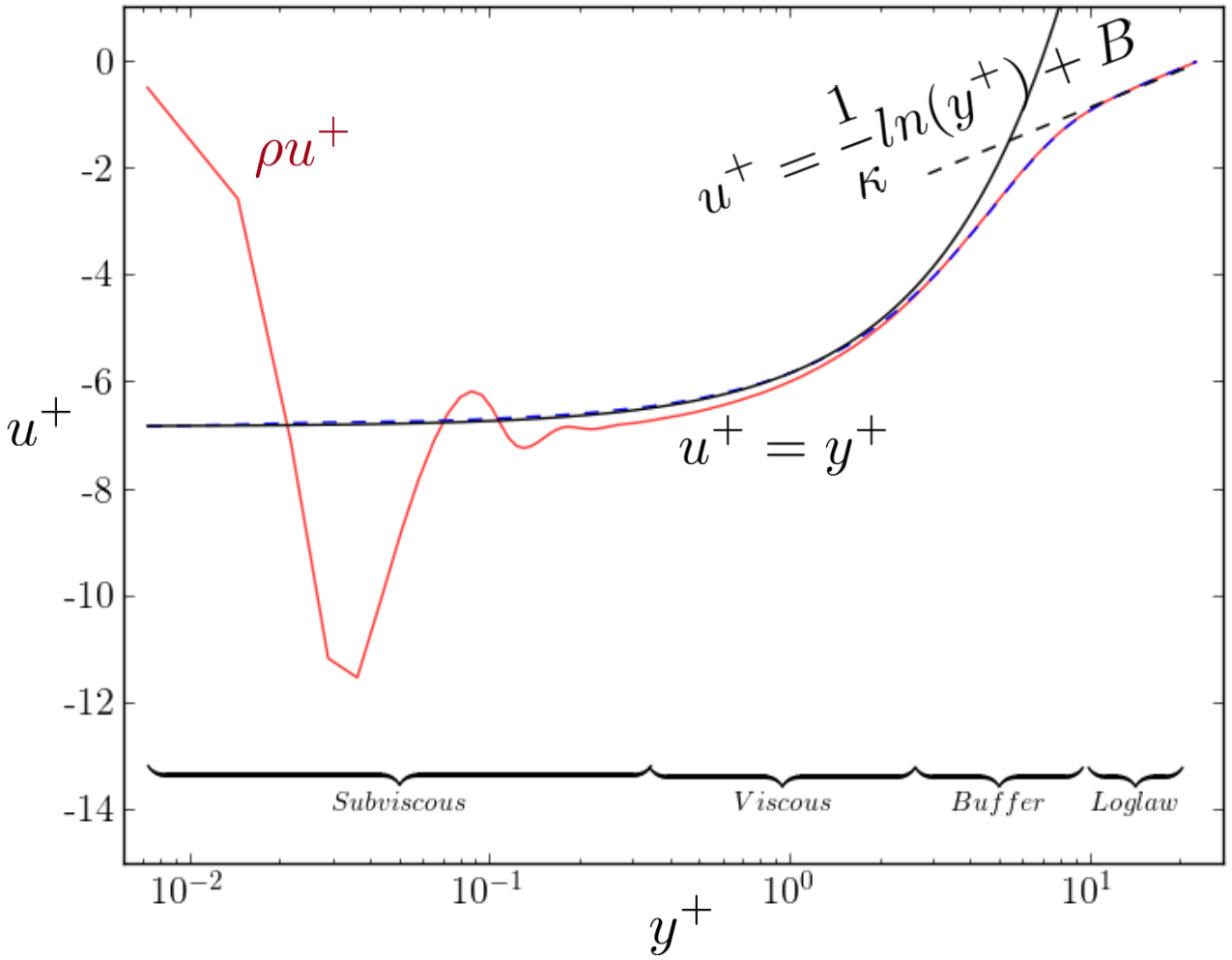
F. Gibson. Channelow: A spectral Navier-Stokes simulator in C++. Technical report, U. New Hampshire, 2012. Channelflow.org.

Law of the wall

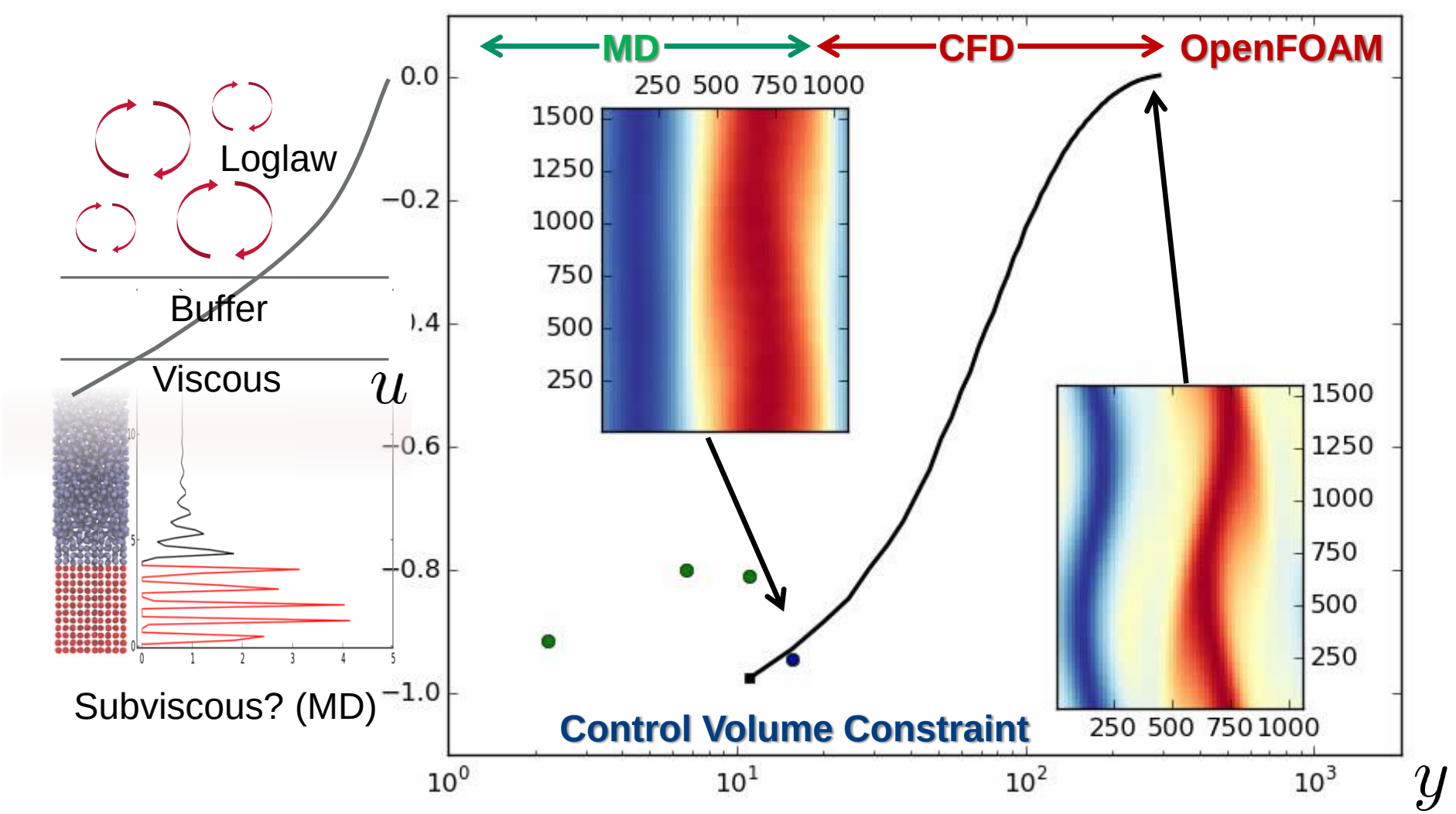




Subviscous? (MD)



Coupling Results – Turbulent Couette



Summary

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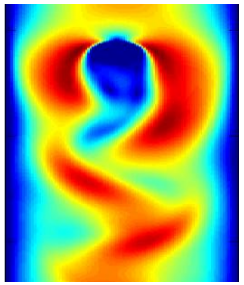
Master's → PhD Mechanical Engineering → EPSRC Fellowship

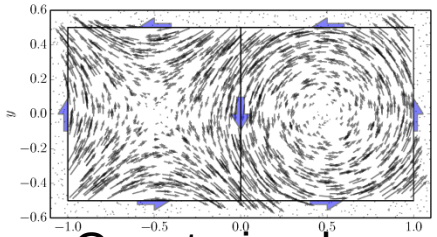


Lattice Boltzmann

Coupled MD simulation

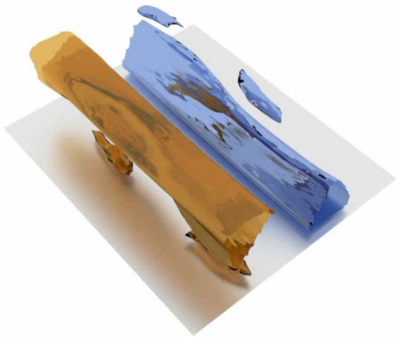
$$\vartheta_i \equiv \int_{x^-}^{x^+}\int_{y^-}^{y^+}\int_{z^-}^{z^+} \delta(x_i - x)\delta(y_i - y)\delta(z_i - z)dxdydz$$

Control Volume formulation



Constrained dynamics

Molecular Turbulence

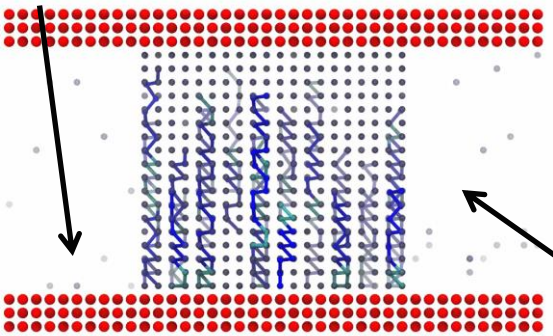


Swinburne → Chemical Eng. → Civil Eng. → Mechanical Eng.

Heat Flux

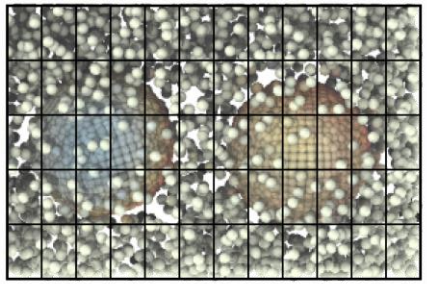
$$q = -\lambda\frac{\partial T}{\partial y} + \ldots$$

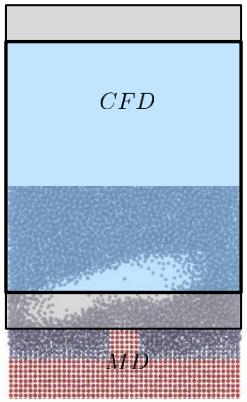
Moving Contact Line



Interface

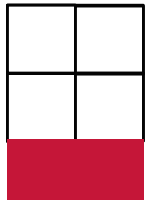
Granular Mechanics



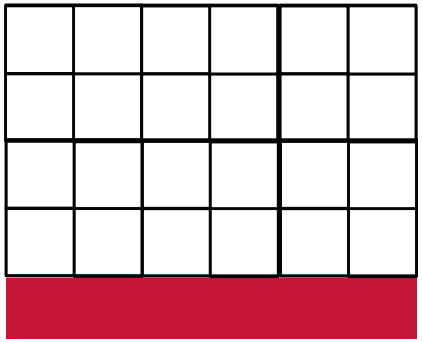


CPL LIBRARY

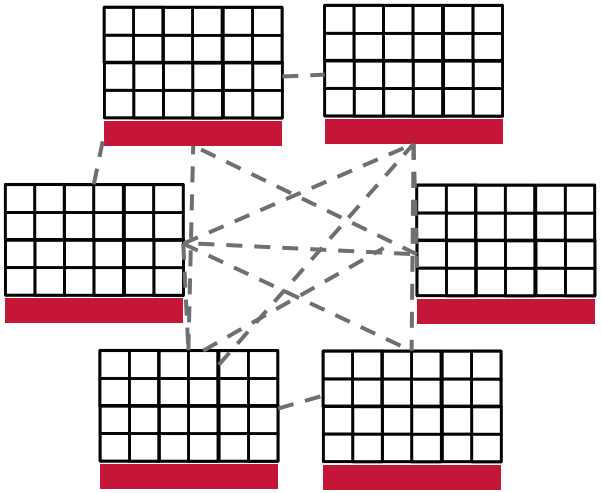
Computers



Laptop
~4 cores
Shared memory



Workstation
~24 cores
Shared memory



Supercomputer
1000+ cores
Individual memory
interconnected

Core
Memory
Interconnect

Parallel Computing

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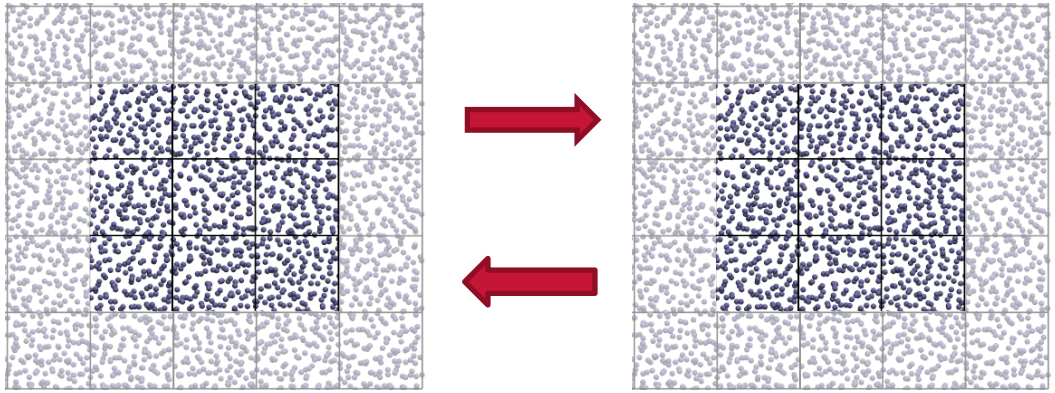
Localisations lends itself to parallel computing using MPI

- Spatial decomposition employed
- Halo cells (ghost molecules) used to link regions



Halo exchange of variable amounts of data

- MPI_Send
- MPI_Recv

Innovate UK

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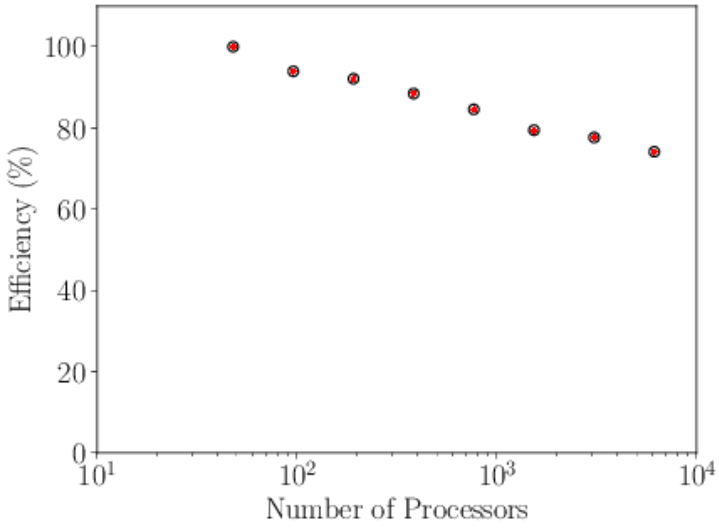
Computational

- All my results come from my own parallelised MD code
  - Validated against experiments
  - Optimised for good scaling



- Python GUI for Masters' students and collaborators (inc. BP)

- **CPL LIBRARY** is open-source (www.cpl-library.org),
  - Fortran, C++, Python with OpenFOAM interface
  - Best Practice (SSI), Git, Unit test & Docker
  - Minimal Python code to test and understand

Software Sustainability Institute