Brunel University London

MULTISCALE INVESTIGATION OF NUCLEATE-BOILING AND INTERFACES

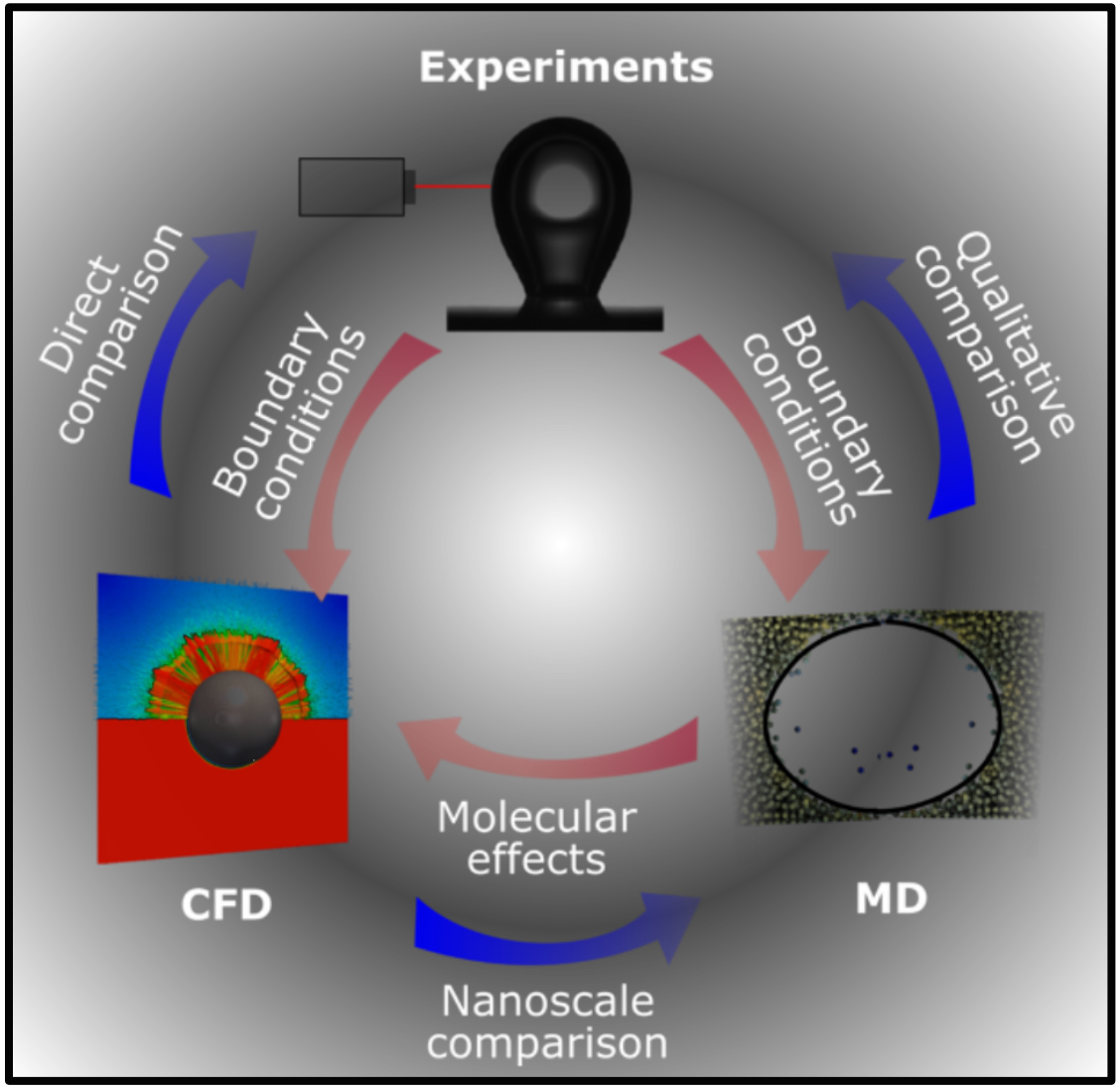
Edward Smith,
Mirco Magnini and Victor Voulgaropoulos

Talk 187 - UKHTC 2019

11:20-12:40 on 09/09/19

MINI - Project Scope

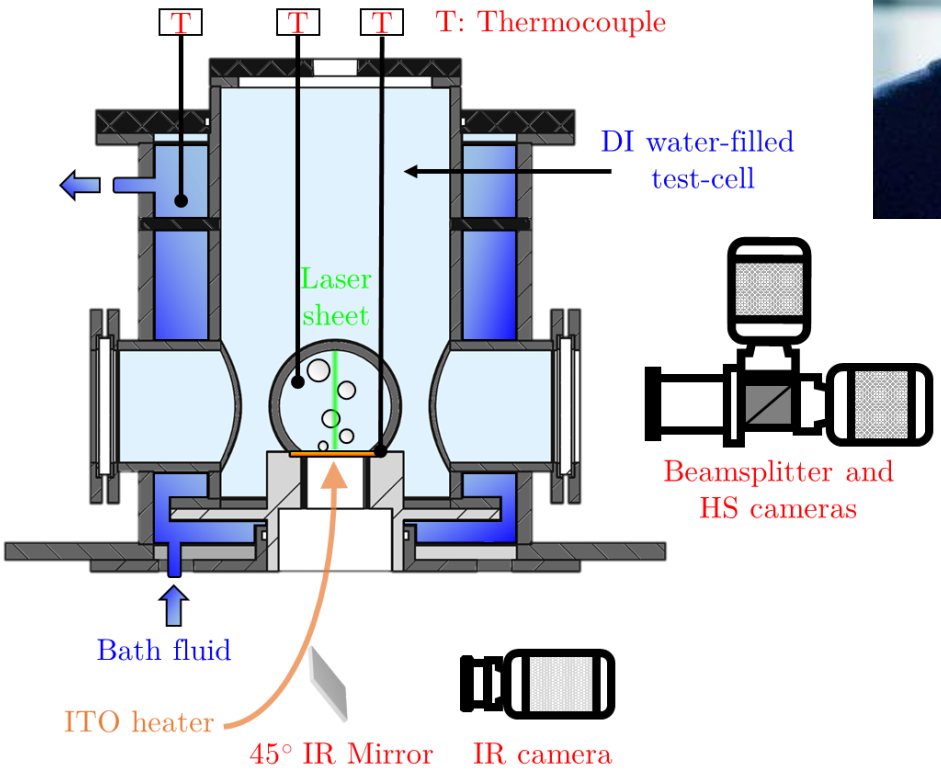
- A collaboration funded by the Julia Higgins fund at Imperial
- Combining
  - Computational fluid dynamics (CFD)
  - Molecular dynamics (MD)
  - Experiments
- Follow on in the form of EMBOSS EPSRC grant

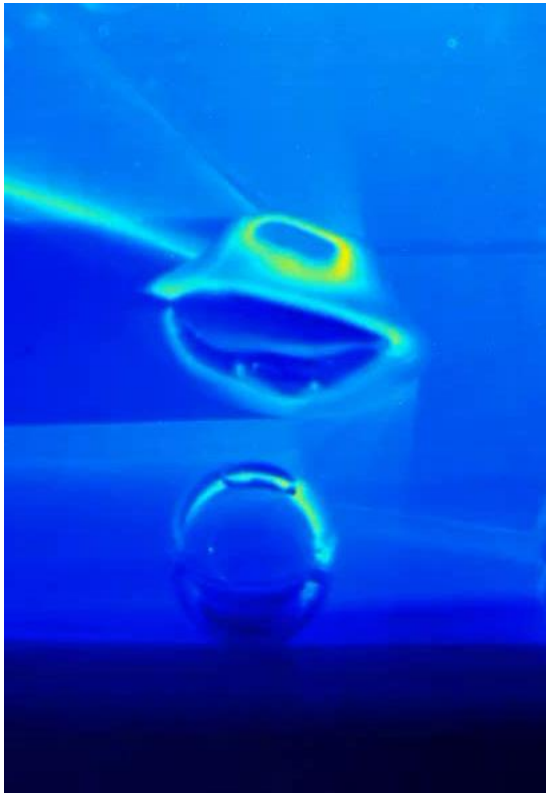


Experimental Results

- Victor Voulgaropoulos

Conference
theatre 16:15
Monday
Talk 175





Continuum CFD

- Mirco Magnini

Later this session

Talk 168

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \left[\mu\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)\right] + \boldsymbol{F_\sigma}$$

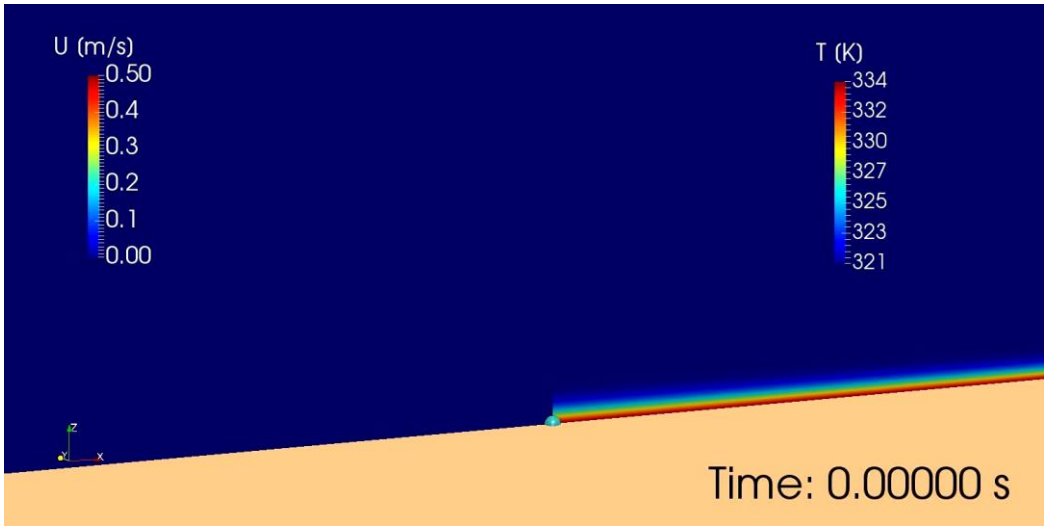
$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \boldsymbol{u}) = \frac{1}{\rho_v} m_i'' |\nabla \alpha|$$

$$\frac{\partial\left(\rho c_p T\right)}{\partial t} + \nabla \cdot \left(\rho c_p \boldsymbol{u} T\right) = \nabla \cdot (\lambda \nabla T) - m_i''\left[h_{lv} - \left(c_{p,v} - c_{p,l}\right)T\right]|\nabla \alpha|$$

$$\nabla \cdot \boldsymbol{u} = \left(\frac{1}{\rho_v} - \frac{1}{\rho_l}\right) m_i'' |\nabla \alpha|$$

$$m_i'' = \frac{h_i}{h_{lv}}\left(T_i - T_{sat}(p_v)\right),$$

$$h_i = \frac{2\gamma}{2-\gamma}\left(\frac{\bar{M}}{2\pi \bar{R}}\right)^{1/2} \frac{\rho_v h_{lv}^2}{{T_{sat}}^{3/2}(p_v)}$$



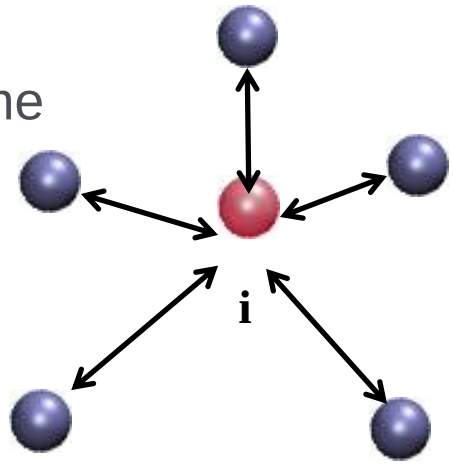
Molecular Dynamics

Brunel University London

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

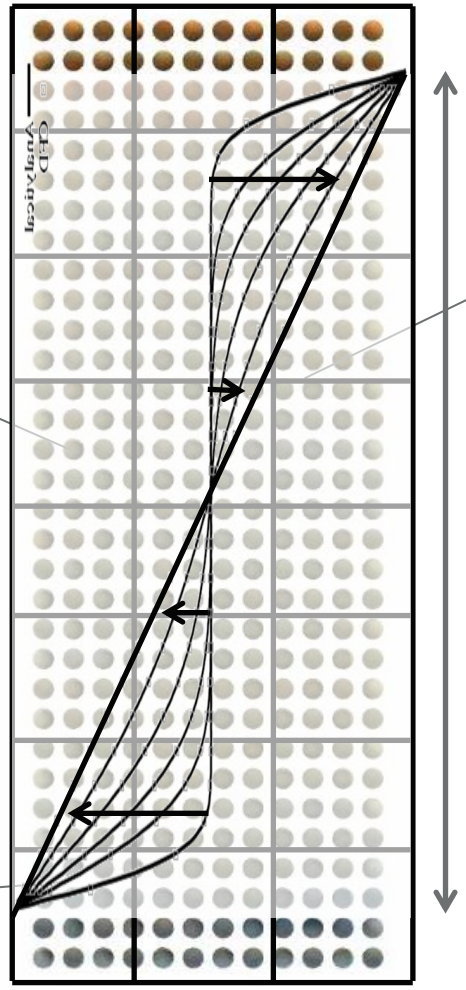
- Governed by Newton's law for an N-body system
- Point particles with electrostatic interactions

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

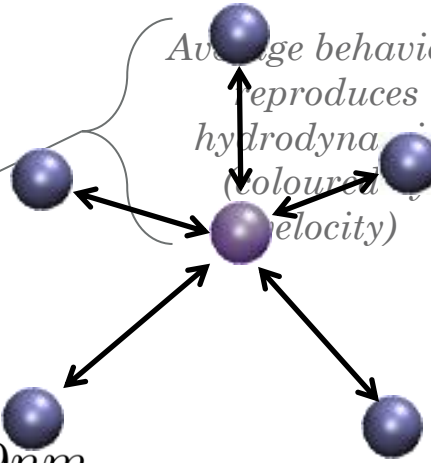
$$\Phi_{ij} = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

Molecular Dynamics

Liquid structure causes viscosity



Average behaviour reproduces hydrodynamics (coloured by velocity)



$H \approx 9nm$

Stick-slip near walls

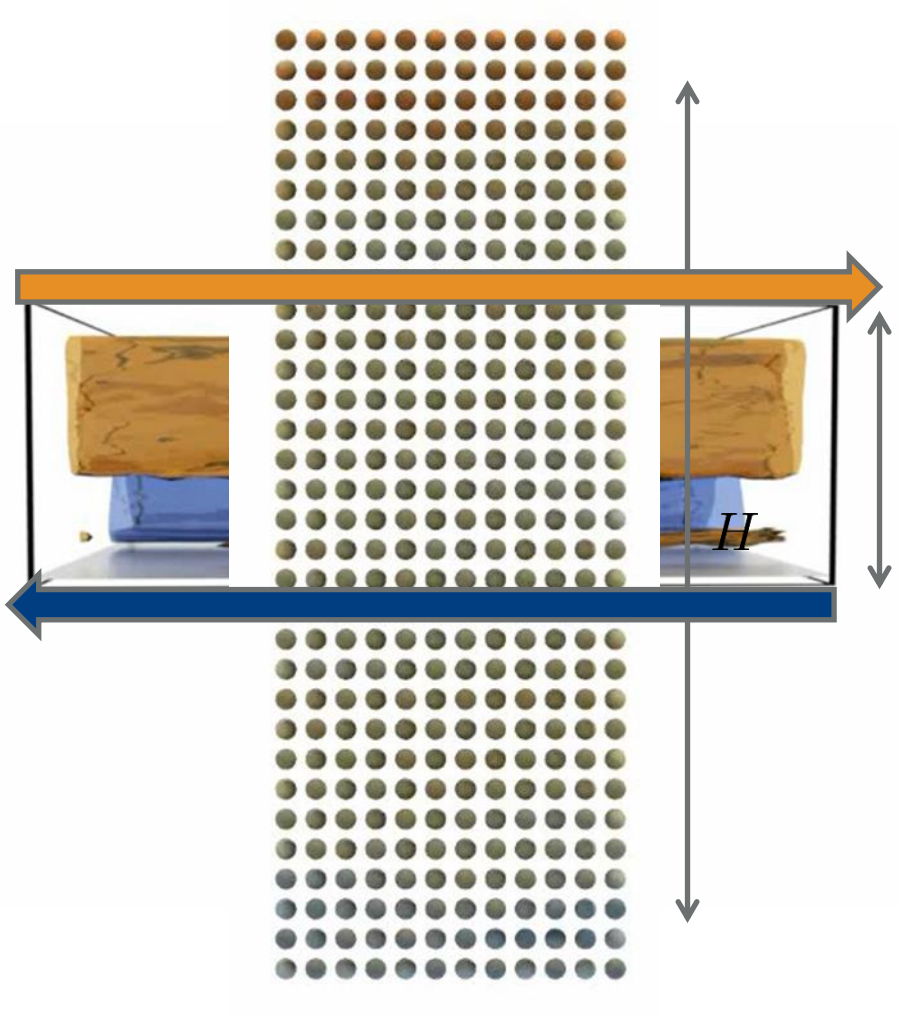
Reynolds Number

$Re \approx 15$

with

4096 molecules

Non-Dimensional Scaling



Reynolds Number

$Re \approx 400$

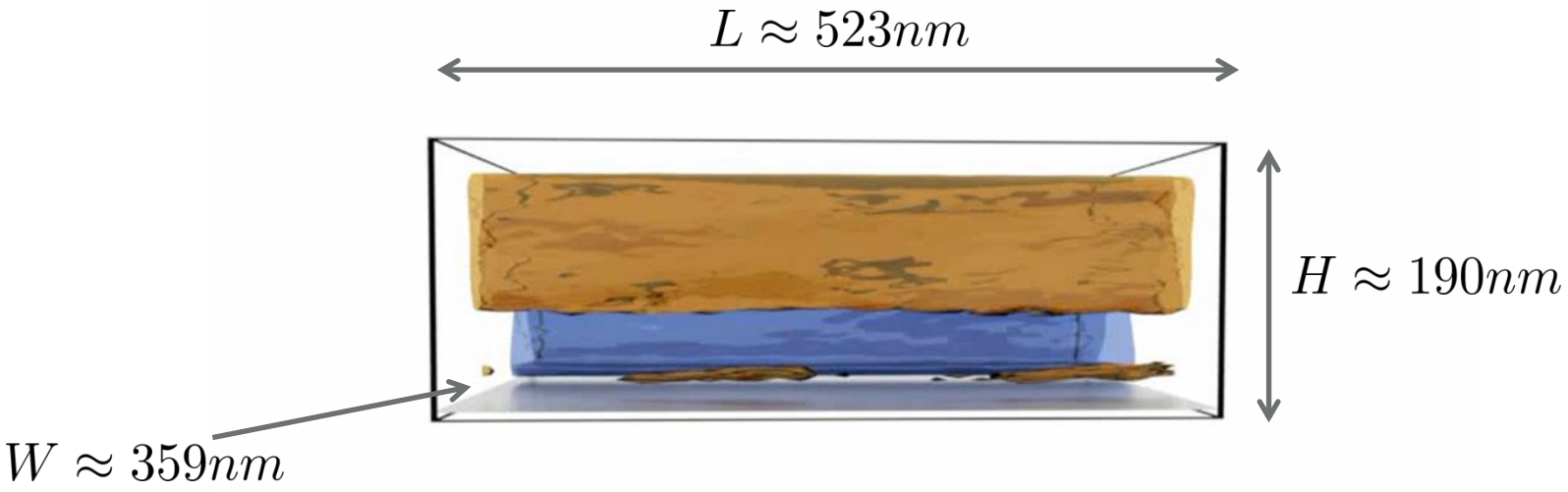
with

300 million molecules

Non-Dimensional Scaling

Brunel University London

Minimal channel Couette flow



Reynolds Number

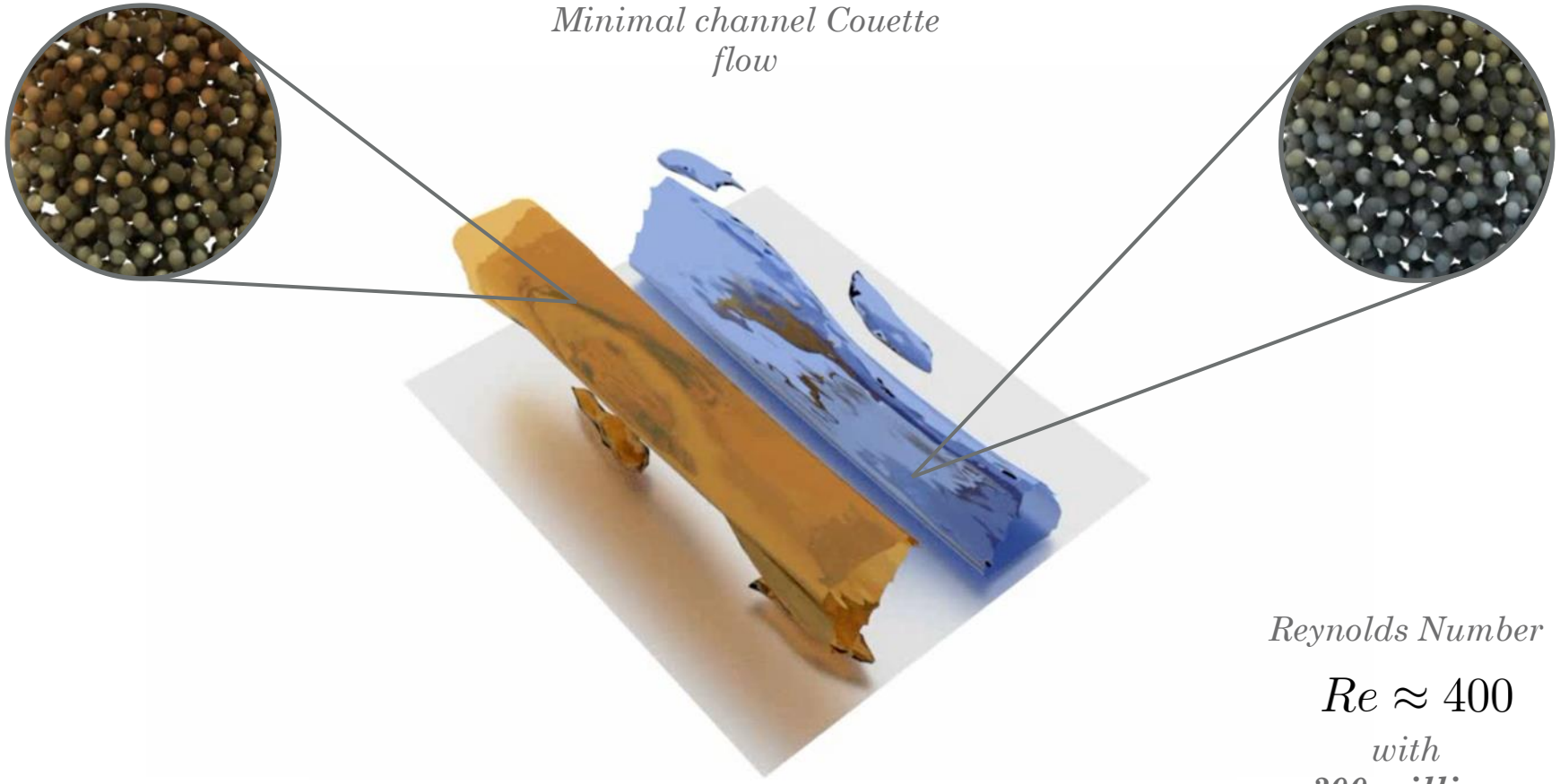
$Re \approx 400$

with
300 million molecules

Non-Dimensional Scaling

Brunel University London

Minimal channel Couette flow



Isosurfaces of turbulent kinetic energy coloured by velocity

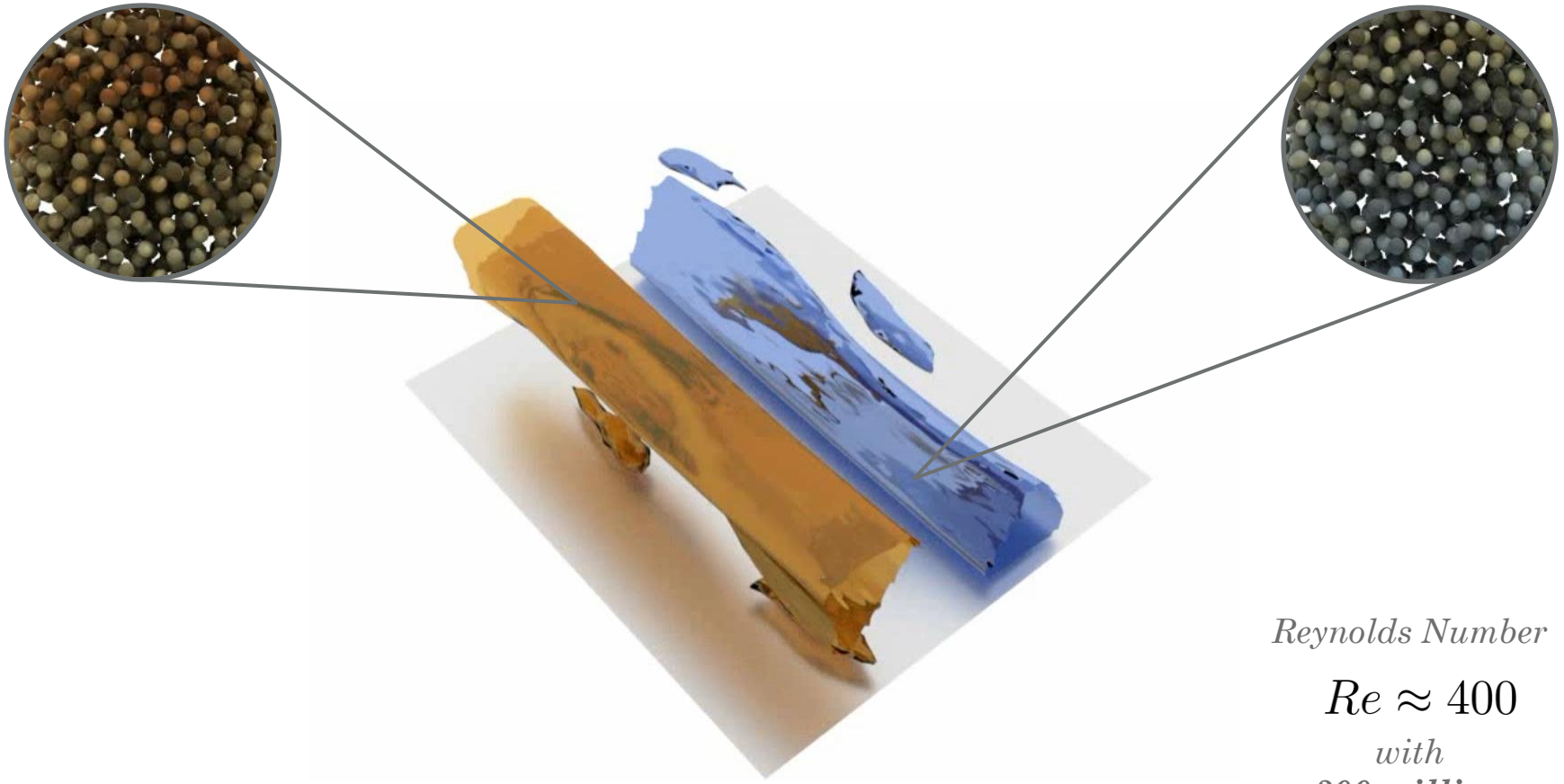
Reynolds Number

$Re \approx 400$

with

300 million molecules

Non-Dimensional Scaling



Isosurfaces of turbulent kinetic energy coloured by velocity

Reynolds Number

$Re \approx 400$

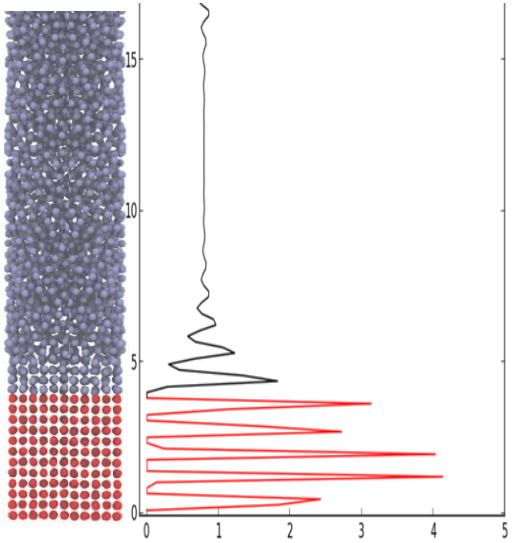
with

300 million molecules

Molecular Dynamics
Complex Walls and Fluids

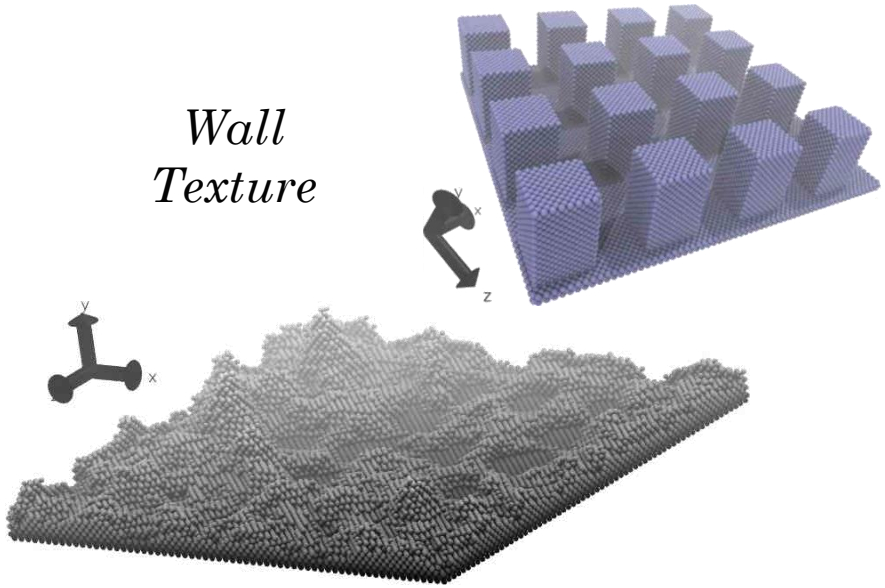
Brunel University London

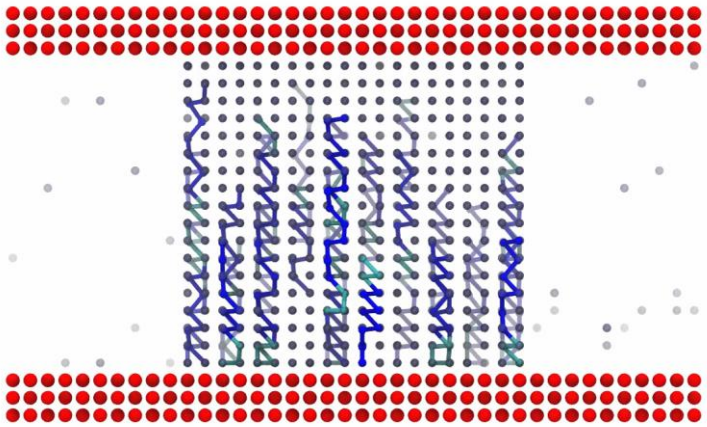
Liquid structure causes viscosity



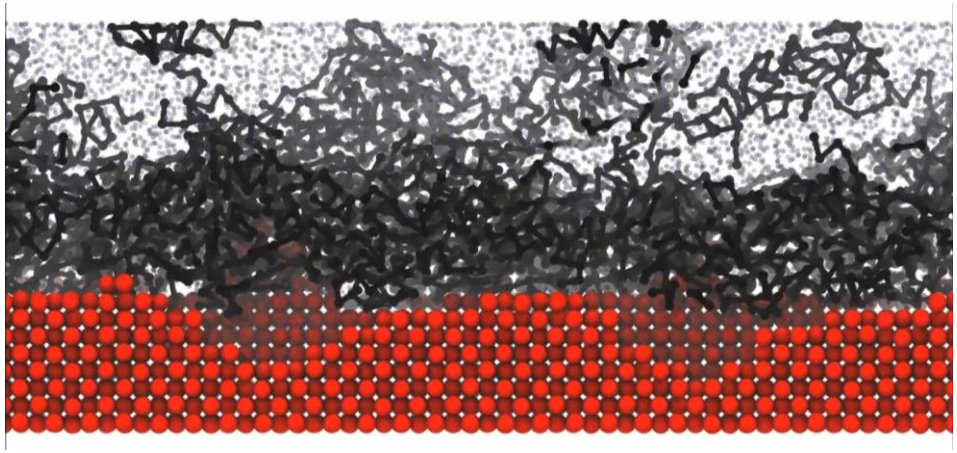
Stick-slip near walls

Wall Texture





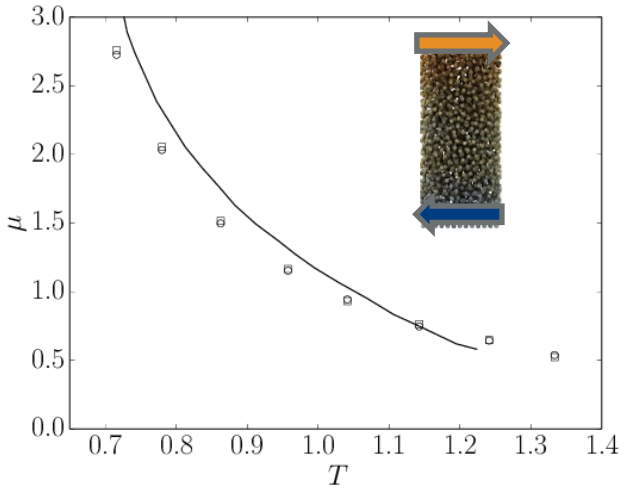
Contact line

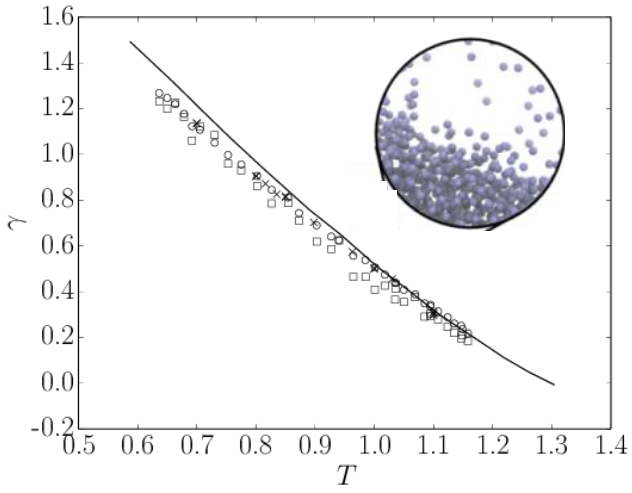


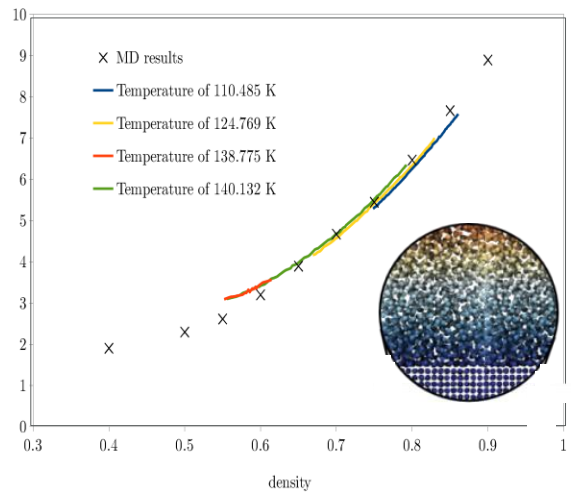
Oil, water and textured surface

Empirical Coefficients

- Outputs of the simulation match experiments, shown here for liquid Argon







- Viscosity

$$\mu = \frac{V}{k_B T} \langle \Pi_{xy}(t) \Pi_{xy}(0) \rangle$$

- Green-Kubo

- Surface tension

$$\gamma = \int (\Pi_N - \Pi_T)\, dx$$

Kirkwood Buff

- Heat Flux

$$\kappa = \frac{V}{k_B T} \langle q_y(t) q_y(0) \rangle$$

Green-Kubo

Non-Dimensional Scaling

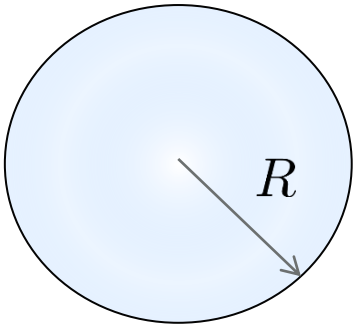
- Reynolds

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

- Eotvos (Bond)

$$Eo = \frac{\Delta \rho g R^2}{\gamma}$$

Bubble



- Capillary

$$Ca = \frac{\mu u}{\gamma}$$

- Marangoni

$$Ma = -\frac{\partial \gamma}{\partial T}\frac{R \Delta T}{\mu \kappa}$$

- Viscosity

$$\mu = \frac{V}{k_B T}\langle \Pi_{xy}(t)\Pi_{xy}(0)\rangle$$

- Green-Kubo

- Surface tension

$$\gamma = \int (\Pi_N - \Pi_T)\, dx$$

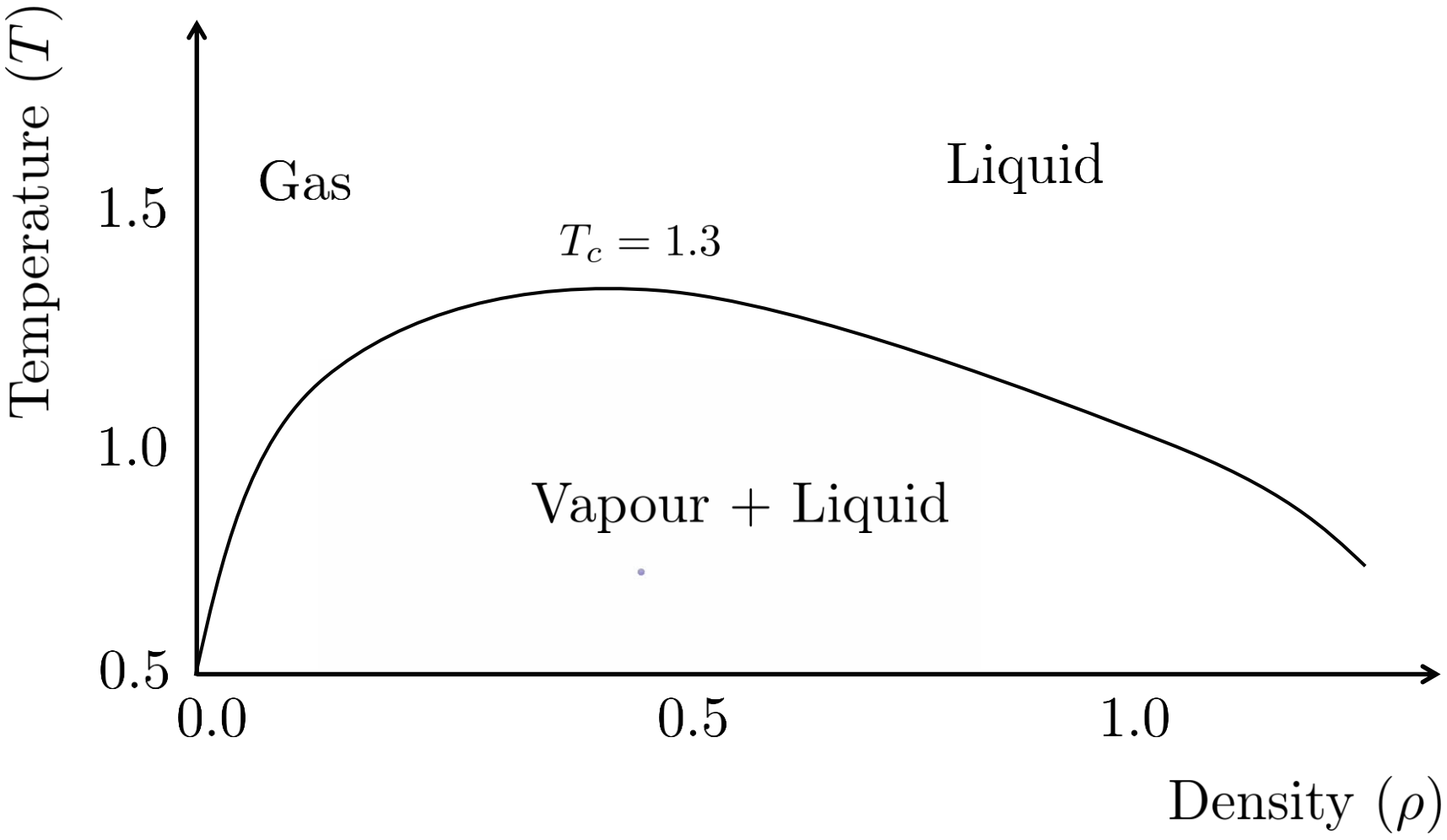
Kirkwood Buff

- Heat Flux

$$\kappa = \frac{V}{k_B T}\langle q_y(t) q_y(0)\rangle$$

Green-Kubo

Phase Diagram

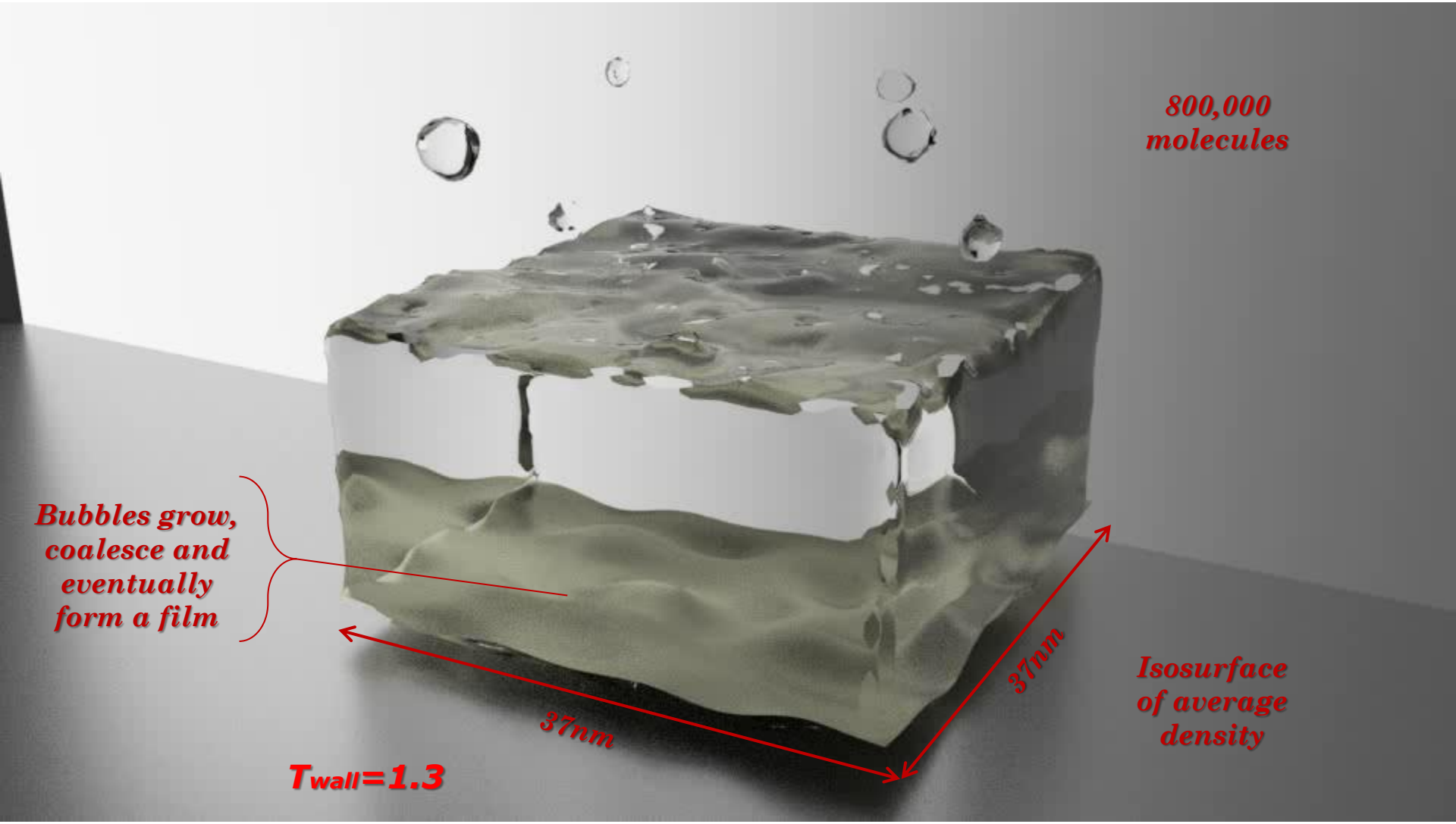


Molecular Dynamics simulation of Nucleation

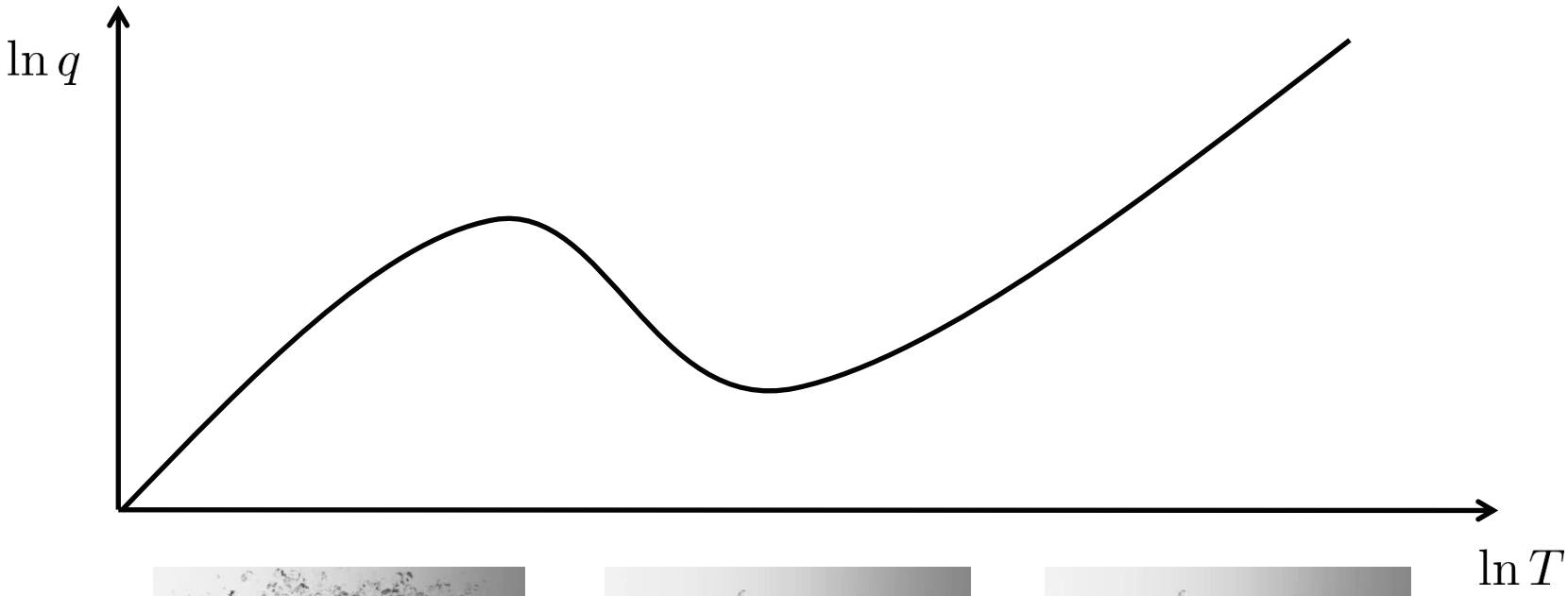
Brunel University London

Wall w
mo
rou

Isosurface of Density



Pool Boiling Curve



No nucleation and convection

Nucleate Boiling

Film Boiling

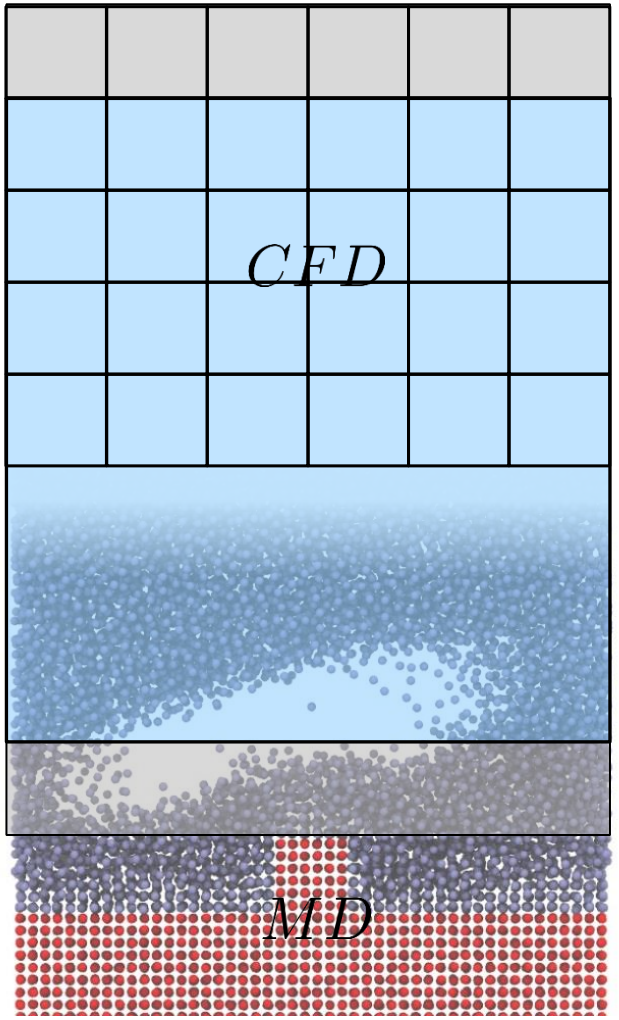
Coupled CFD-MD Simulation

- Assumes a continuous field

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

- Discrete molecules

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



Coupled CFD-MD Simulation

- Assumes a continuous field

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

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

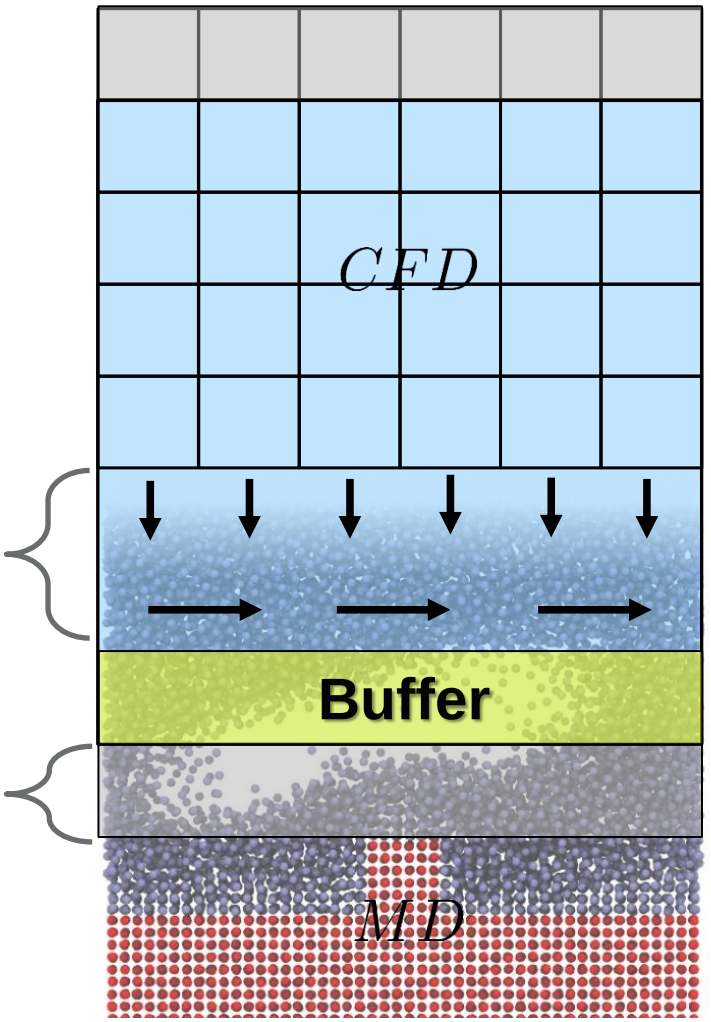
CFD→MD Boundary condition

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

MD→CFD Boundary condition

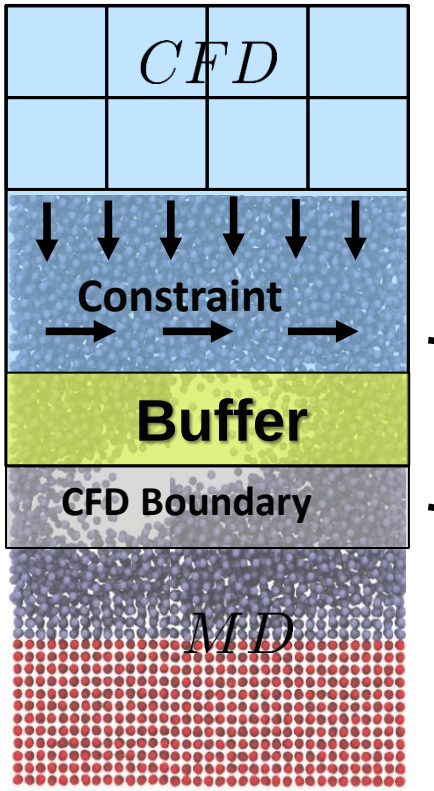
- Discrete molecules

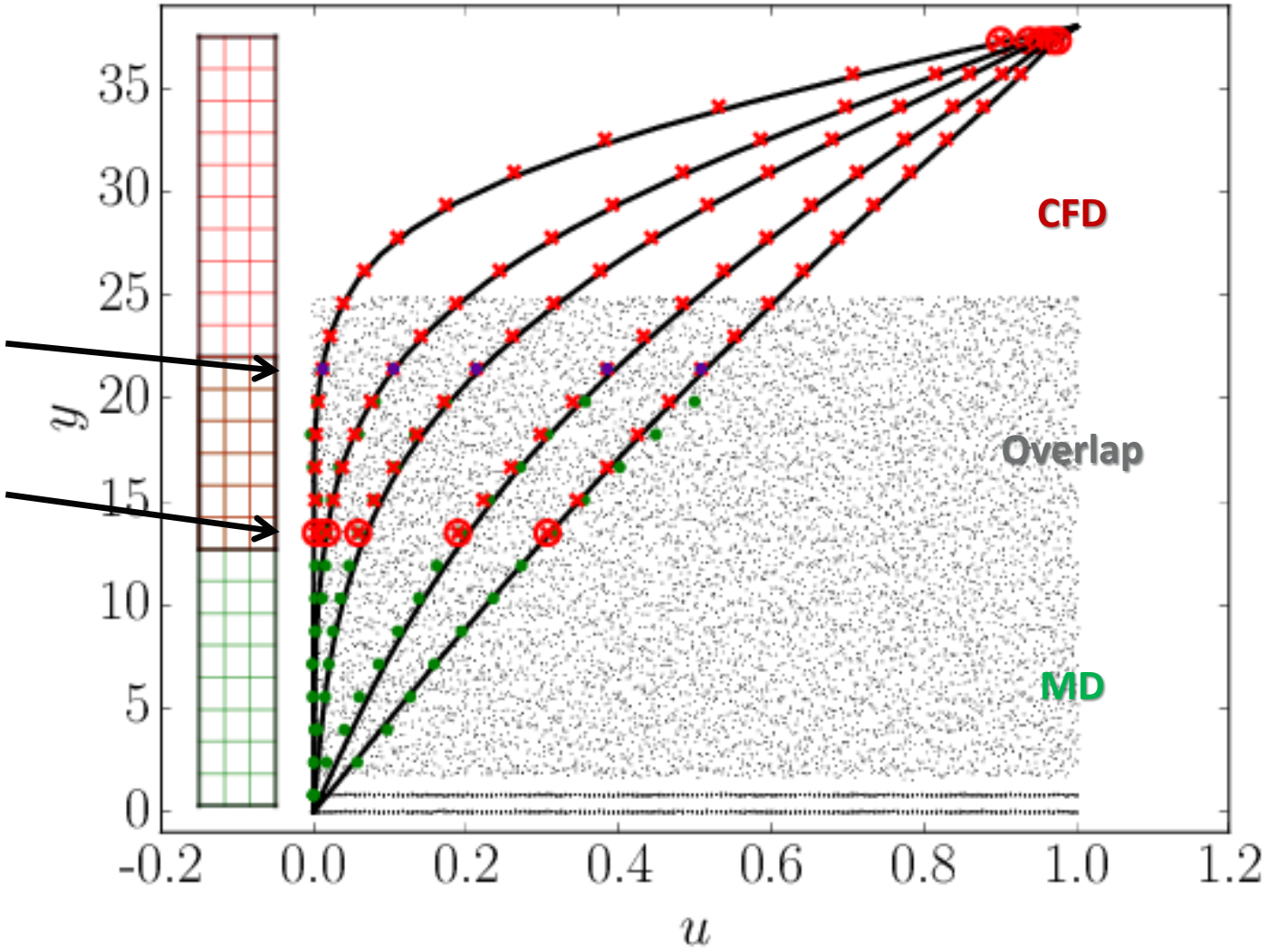
$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i \text{ for all i in N}$$



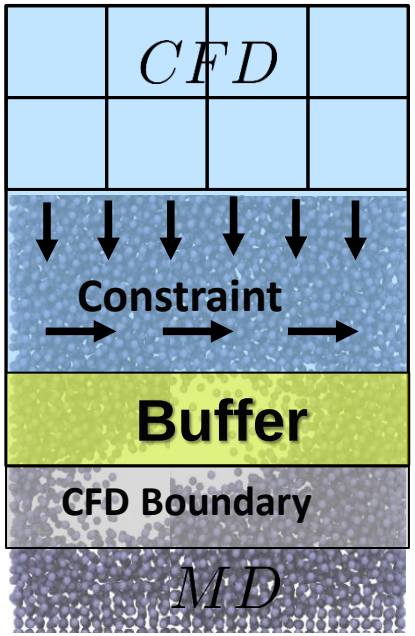
O'Connell Thompson (1995), Hadjiconstantinou (1998), Flekkoy (2000), Nie et al (2004).

Coupling Results – Couette Flow

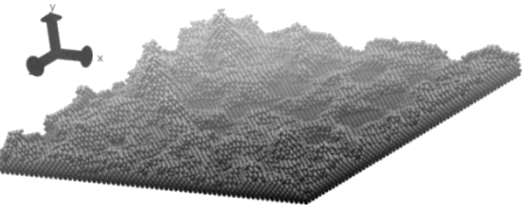


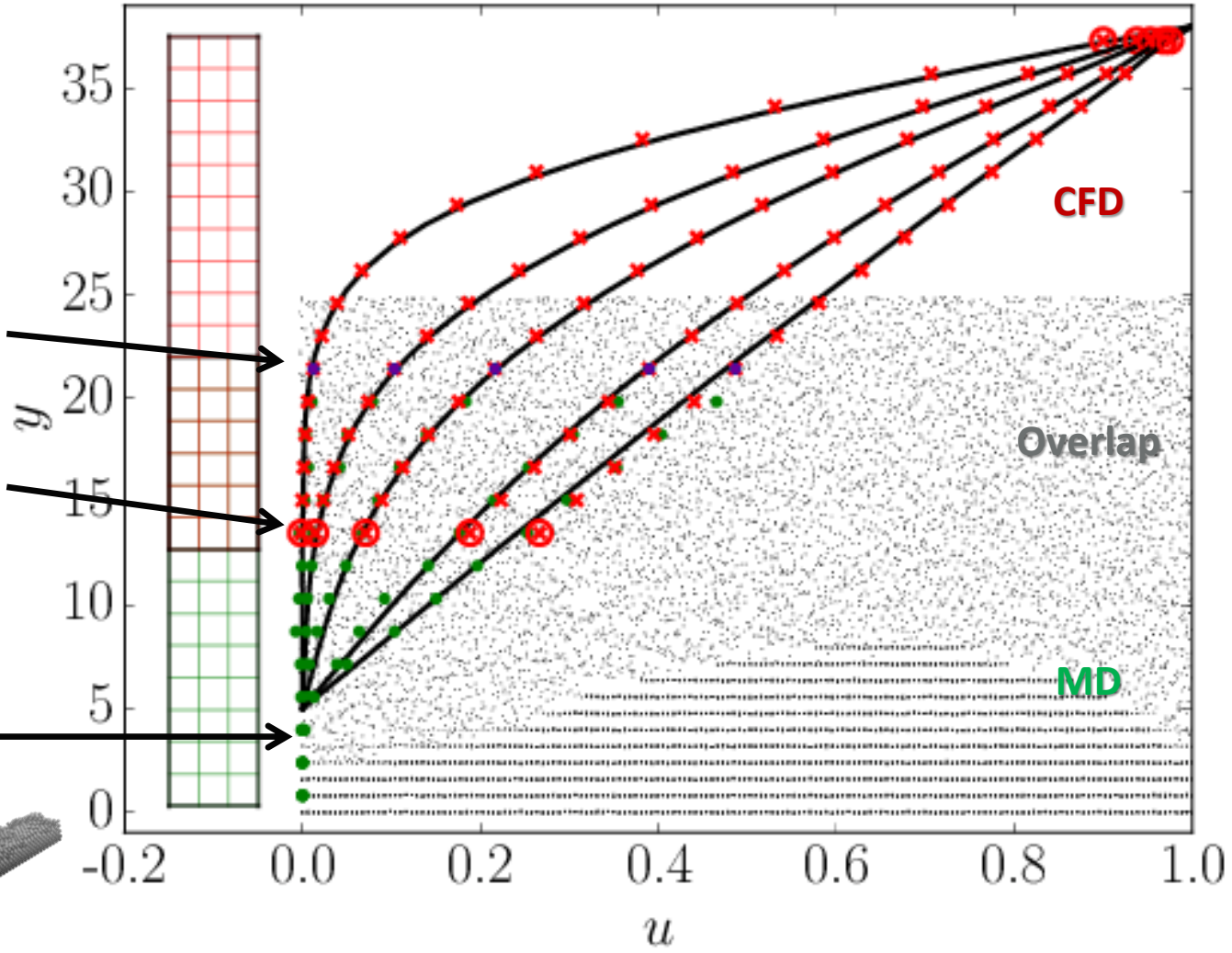


Coupling Results – Couette Flow

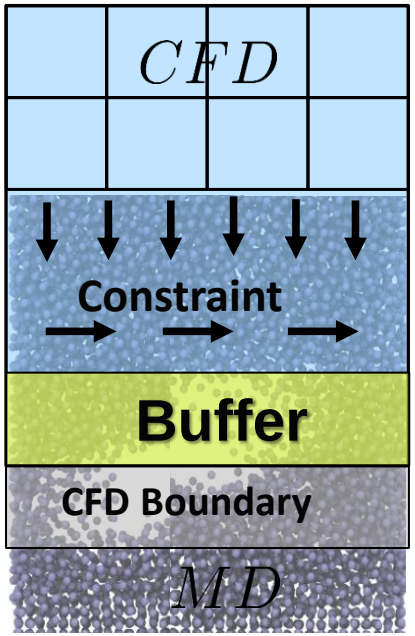


Rough wall shifts zero location

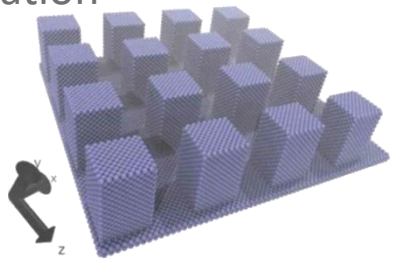


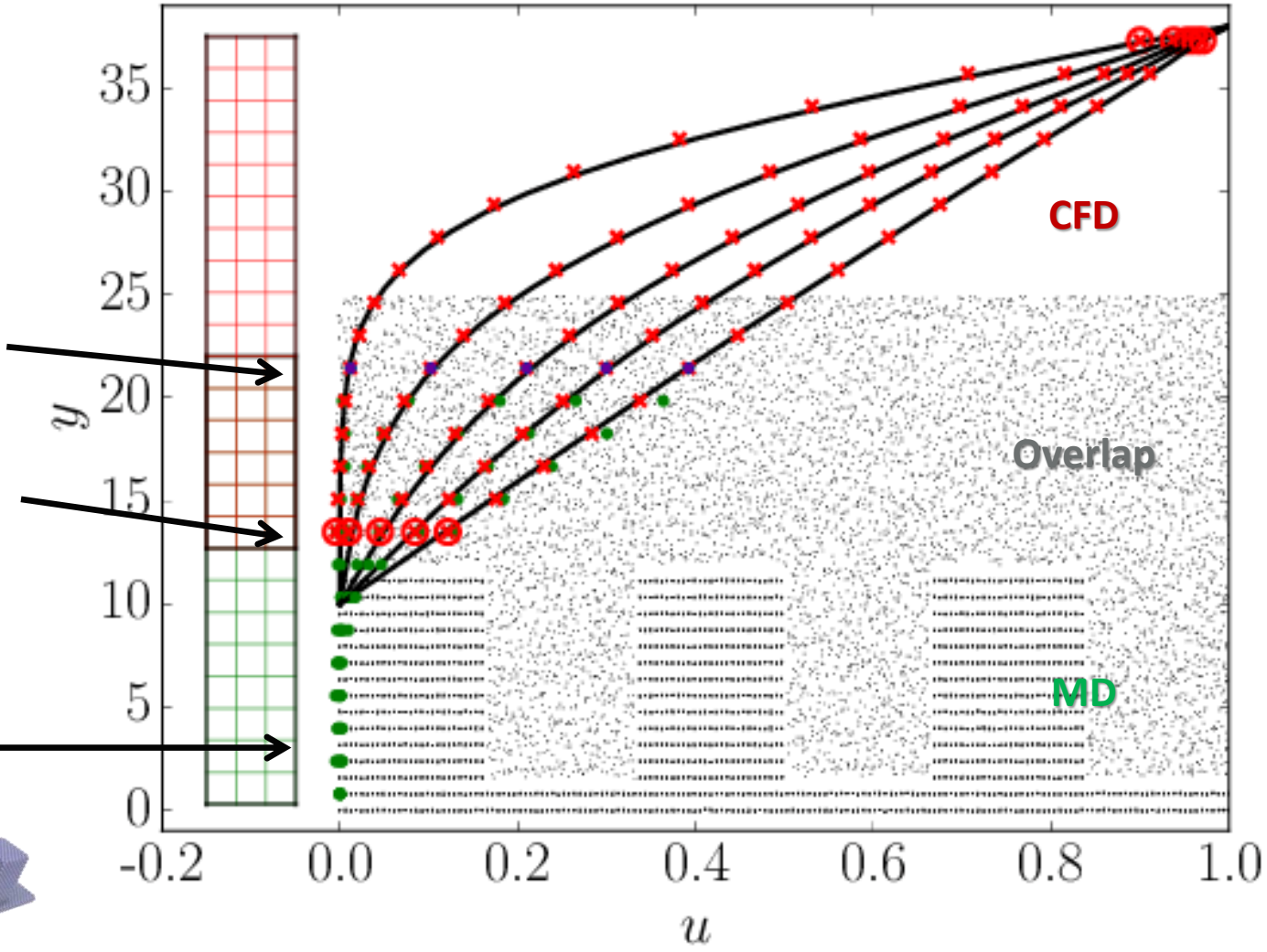


Coupling Results – Couette Flow

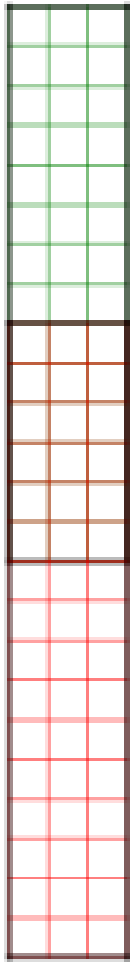


Posts shift zero location





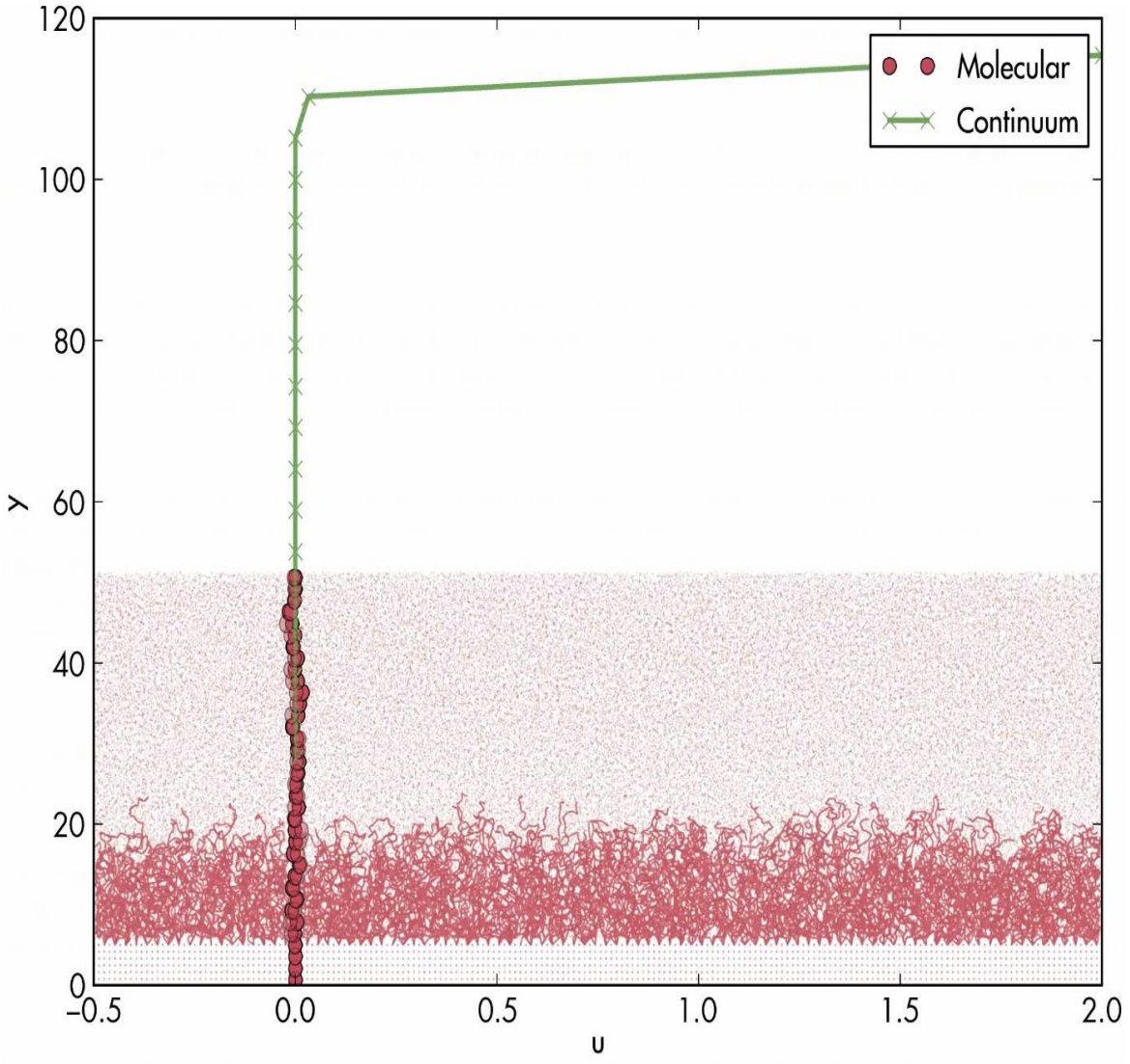
Coupling Results – Polymer Brushes



CFD Region

Overlap Region

MD Region



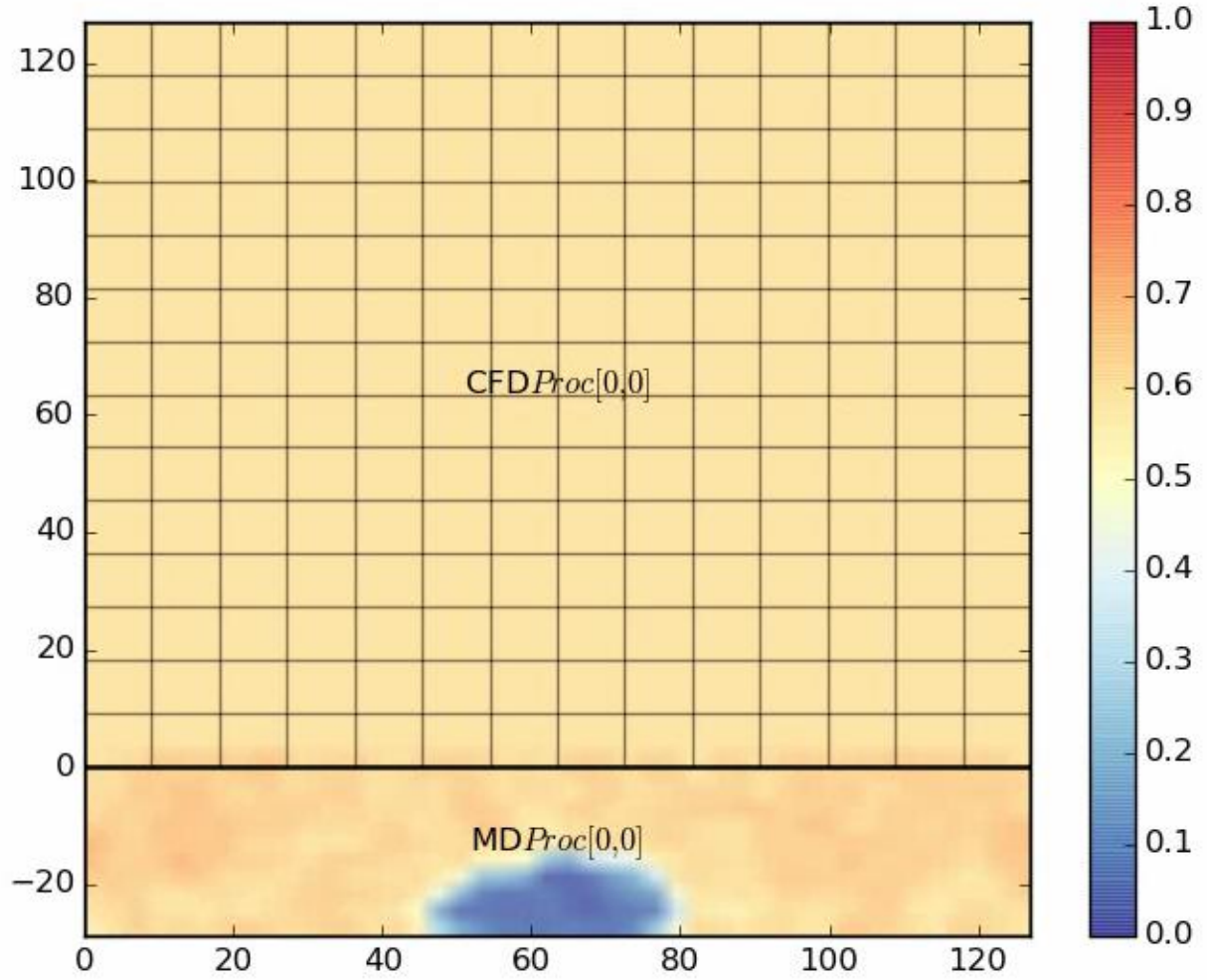
Coupling Results – Boiling

Brunel University London

CFD Region

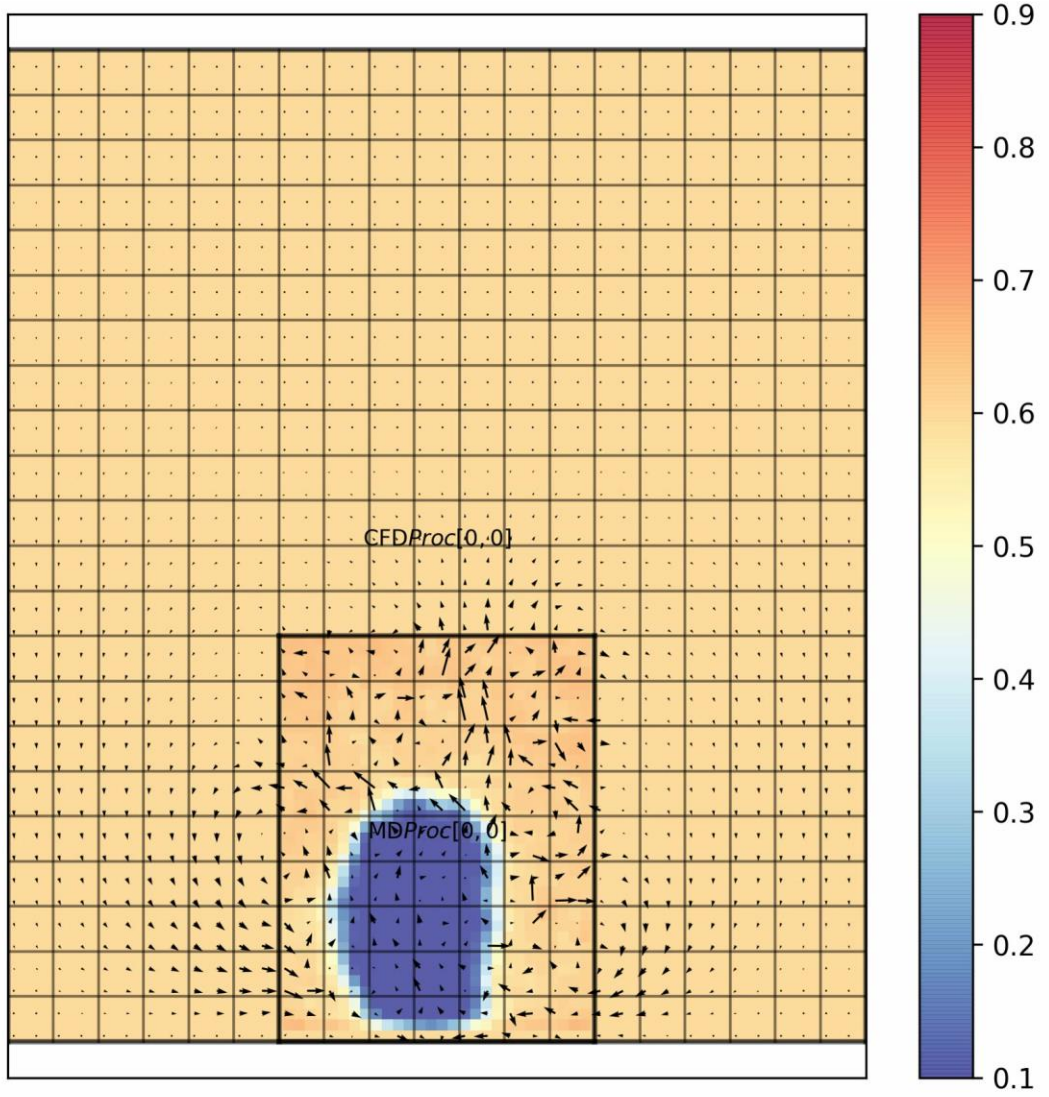
Overlap Region

MD Region

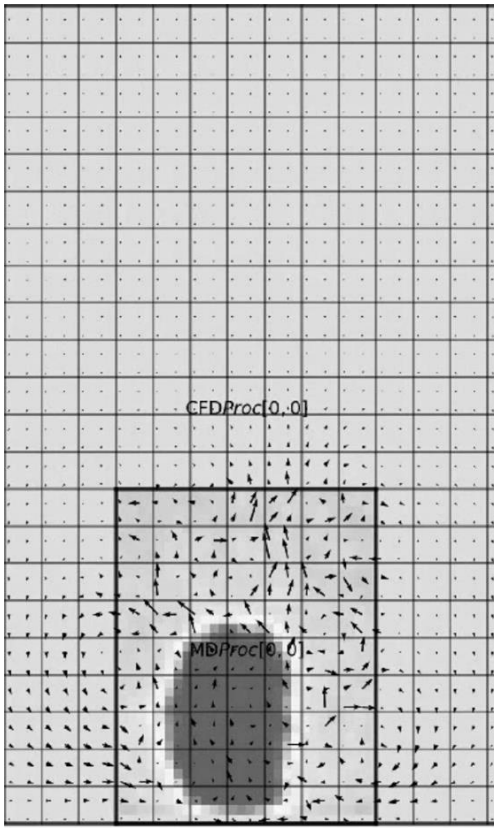


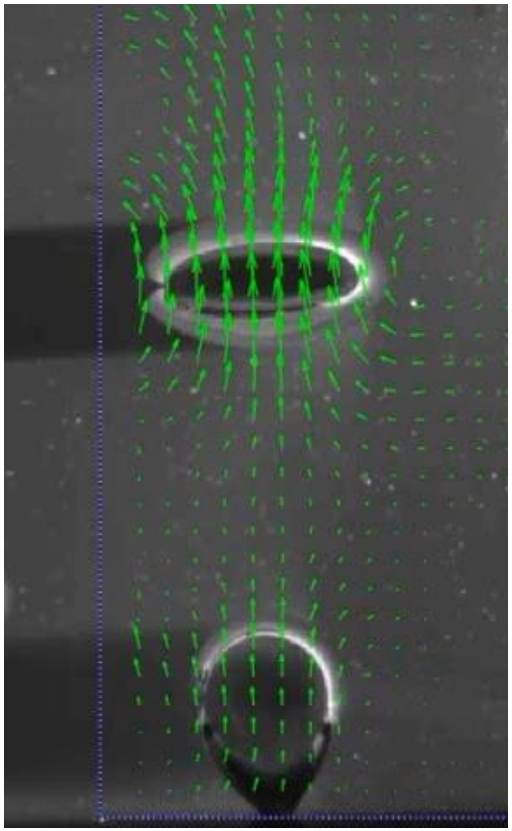
Coupled Simulation of Boiling

- CFD uses interface tracking to track MD bubble
- A minimal CFD in Python and MATLAB (written by Mirco)
- Density, velocity and temperature values passed to CFD



Compared To Experiments



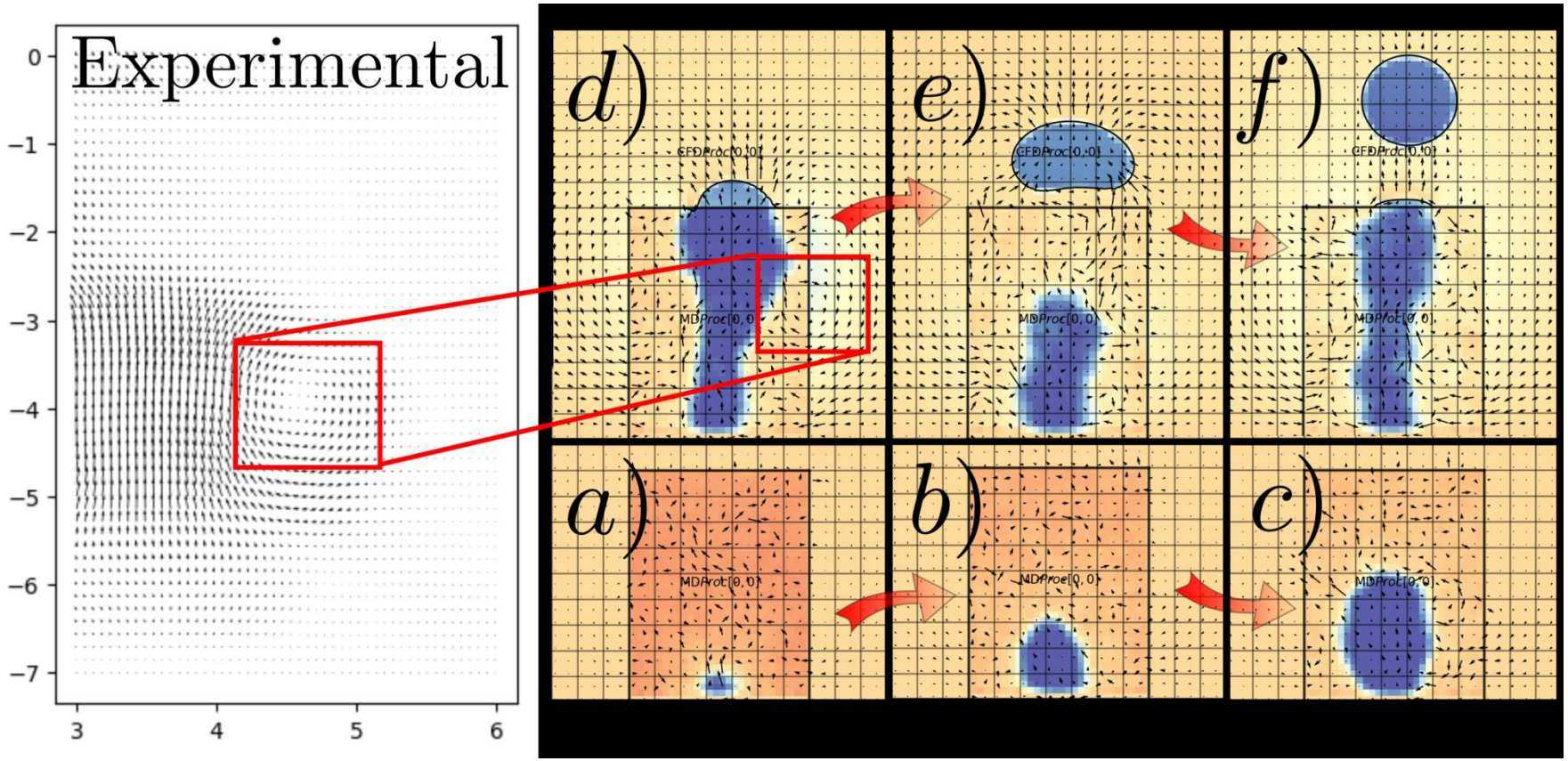


Experiments from Victor

$$Re = \frac{\rho u R}{\mu} \quad Eo = \frac{\Delta \rho g R^2}{\gamma}$$

$$Ca = \frac{\mu u}{\gamma} \quad Ma = -\frac{\partial \gamma}{\partial T} \frac{R \Delta T}{\mu \kappa}$$

Compared To Experiments

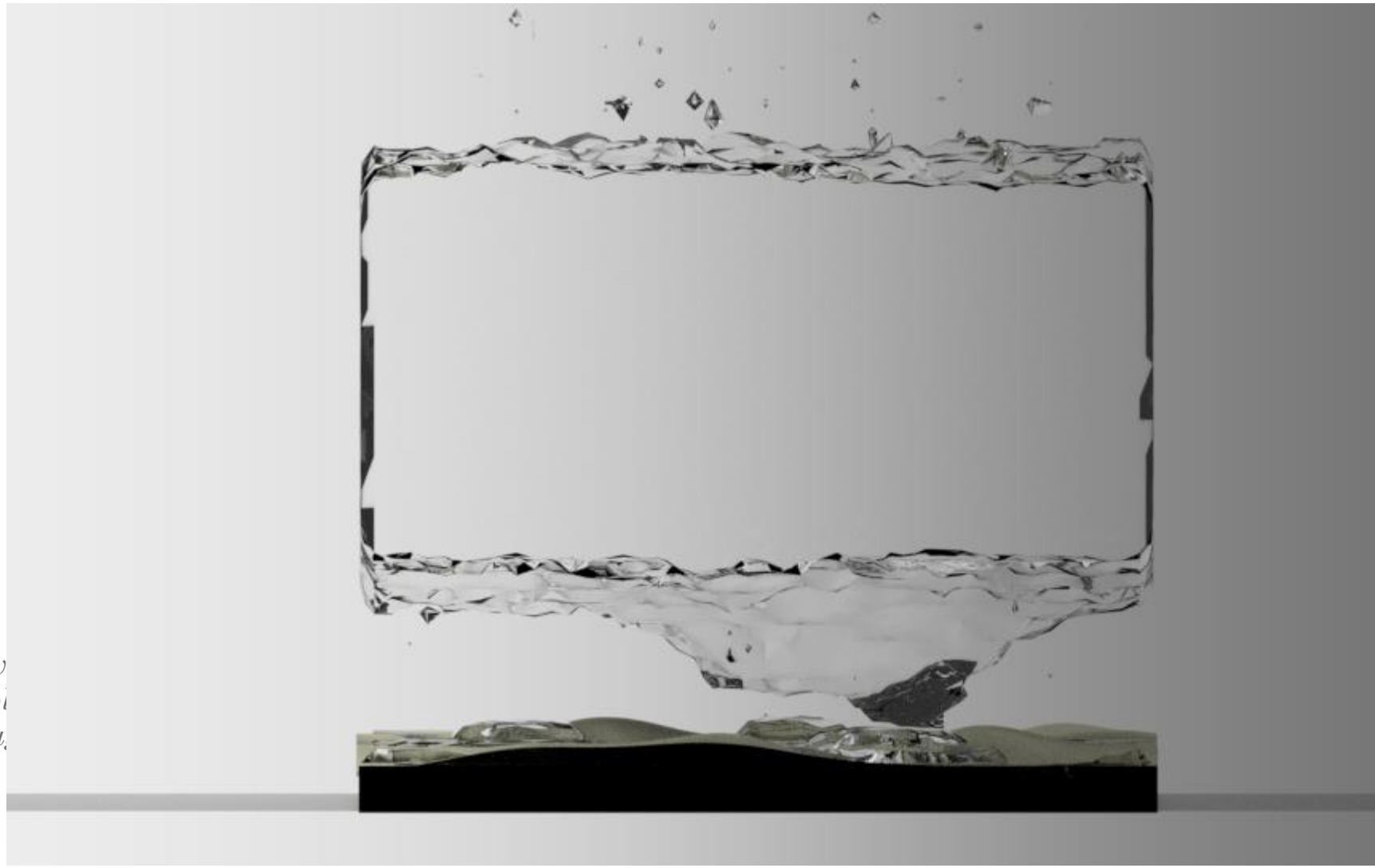


Summary

- Molecular dynamics (MD) provides nucleation, viscosity, heat flux, etc from Newton's law
- Coupled to computational fluid dynamics so only minimum MD computation required
- Experiments show some similarity once nucleated, relate by dimensionless numbers

Molecular Dynamics simulation of Nucleation

Brunel University London



Wall w
mo
rou