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A framework for embedding molecular-level information in continuum-scale simulations of interfacial flows

APS 2015

11:01 AM–11:14 AM

By

Edward Smith,

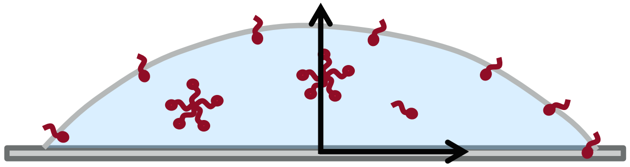
In collaboration with Panagiotis Theodorakis, Erich Muller, Richard Craster and Omar Matar

Computational Fluid Dynamics (CFD)

1) G. Karapetsas, R. Craster & O. Matar, JFM, 2011

- Incompressible Navier Stokes with the thin-film approximation.

$$\frac{\partial P}{\partial x} = \frac{\partial^2 u}{\partial z^2} \qquad \frac{\partial P}{\partial z} = 0 \qquad \frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0$$



- With boundary conditions

$$P = -\left(\frac{H}{L}\right)^2 \frac{\partial^2 h}{\partial x^2}\left(\sigma_l + \frac{1}{\Sigma_l}\right) \qquad \frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x} = w \qquad \frac{\partial u}{\partial z} = \frac{\partial \sigma_l}{\partial x} \qquad z = h$$

$$u = \beta\frac{\partial u}{\partial z} \qquad w = 0 \qquad z = 0$$

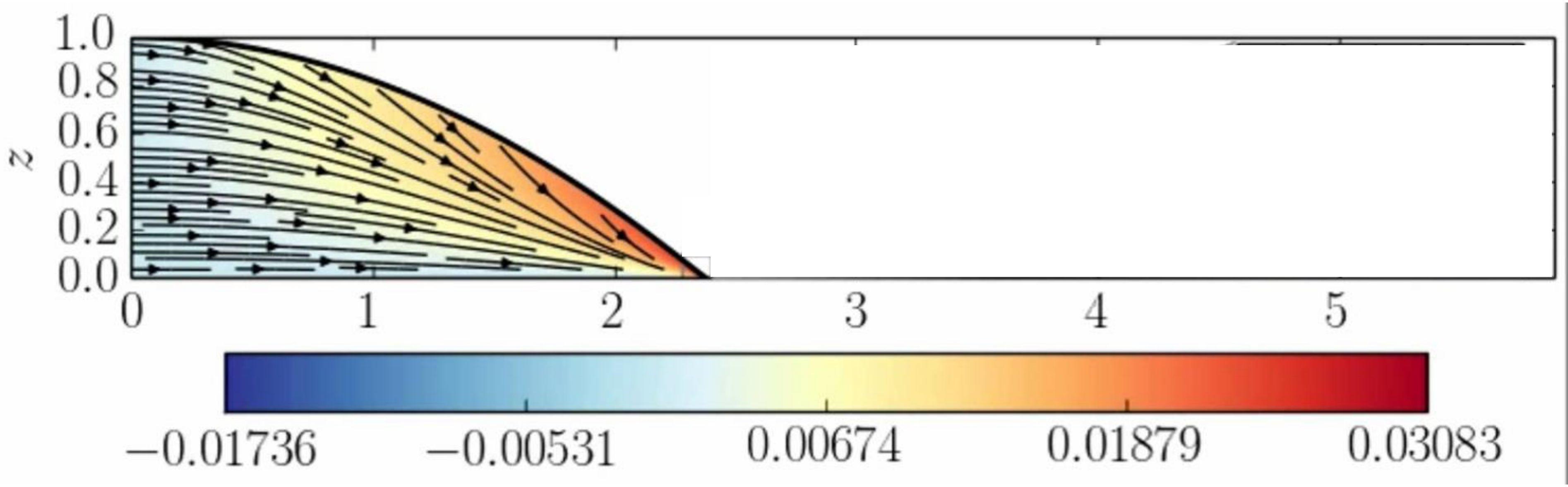
- *Surfactant modelled by advection-diffusion equations with empirical sorption processes - coupled to the dynamics through surface tension*
- *Contact line evolution is modelled by an empirical law*

$$\frac{dx_c}{dt} = k(\theta - \theta_a)^n$$

- *The angle coupled to surfactant absorption at the contact line is essential*[1)]

1) Thompson and Robbins (1989)

Coupled Droplet Spreading and MD



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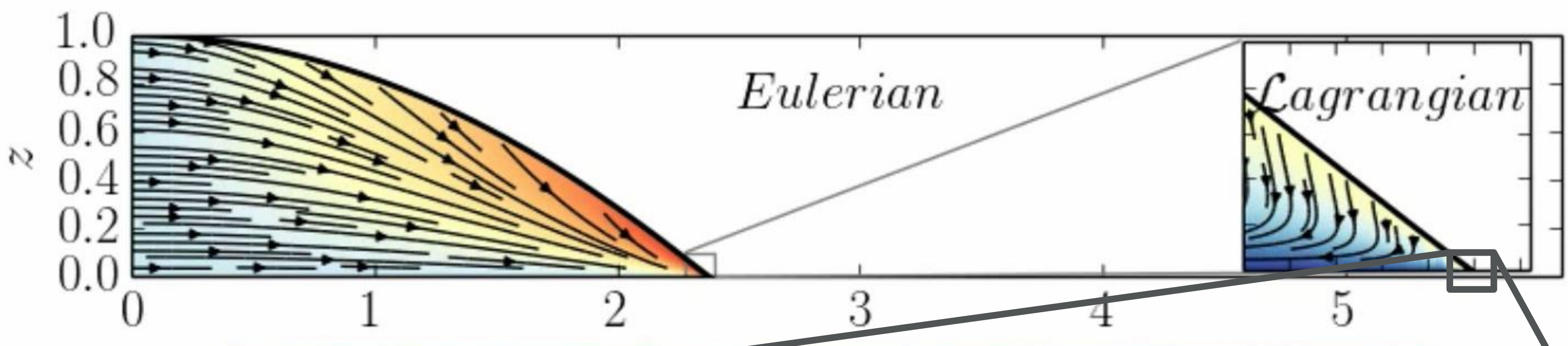
Coupled Droplet Spreading and MD

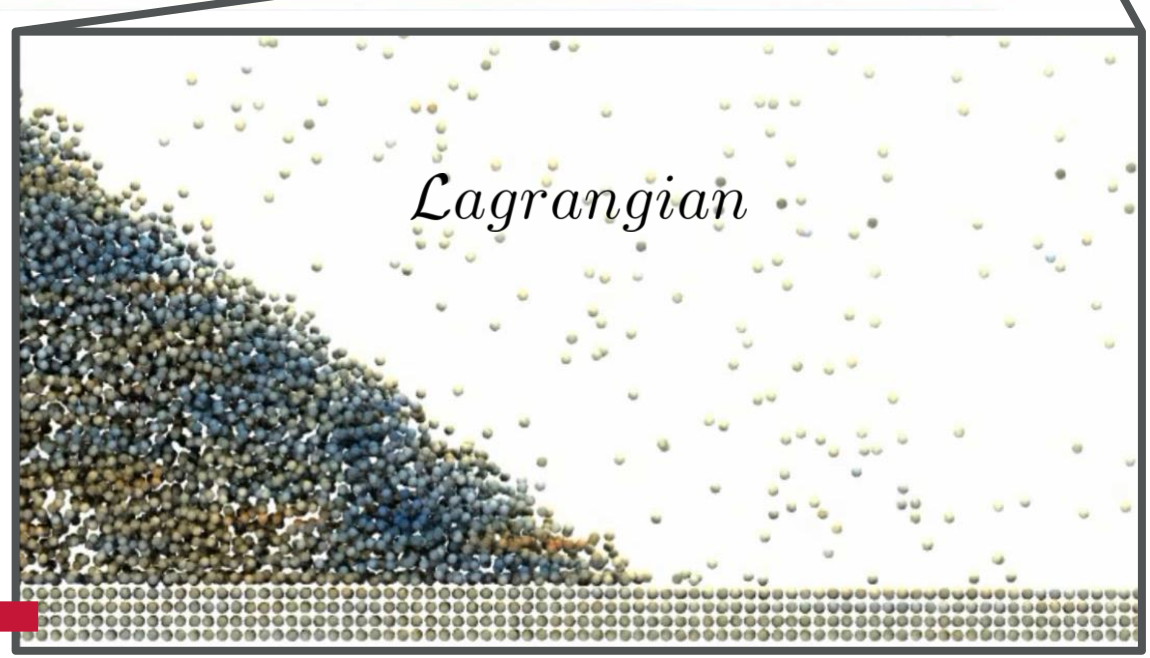
1) Thompson and Robbins (1989)



- Model the moving contact line with MD

- We want contact line speed as a function of continuum contact angle

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

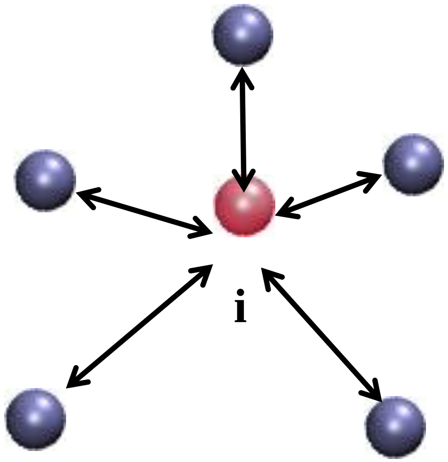


Molecular Dynamics

Discrete molecules in continuous space

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

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



Acceleration obtained from forces

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

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

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

- SAFT[1)] using the γ-Mie[2)] potential

$$\Phi(r_{ij}) = 4C\epsilon_{ij} \left[\left(\frac{\ell_{ij}}{r_{ij}} \right)^{\lambda_r} - \left(\frac{\ell_{ij}}{r_{ij}} \right)^{\lambda_a} \right]$$

1) *Statistical Associated Field Theory*
2) *Müller & Jackson (2014)*

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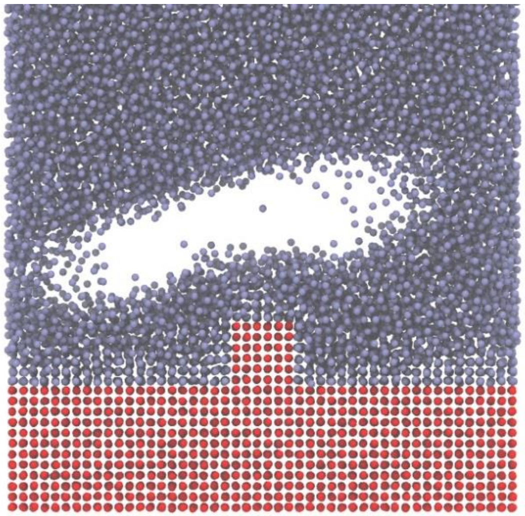
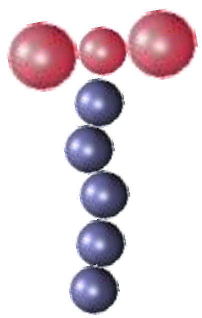
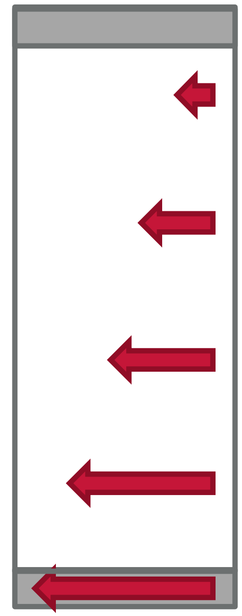
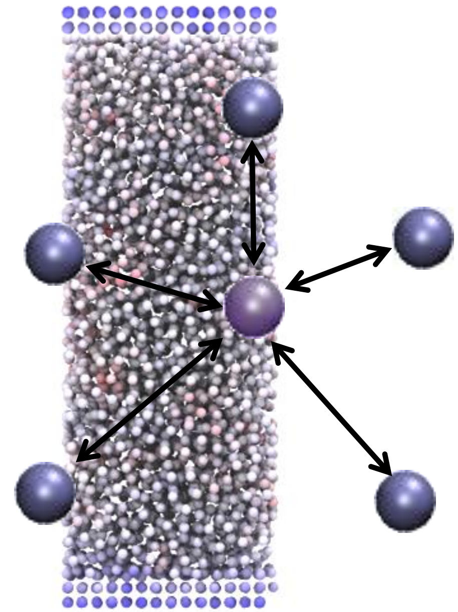
Molecular Dynamics

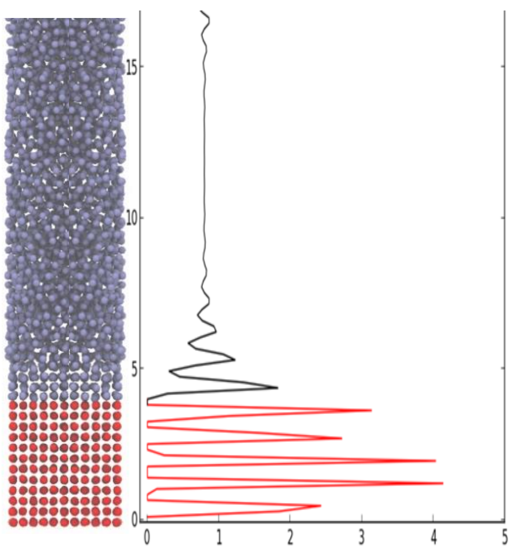


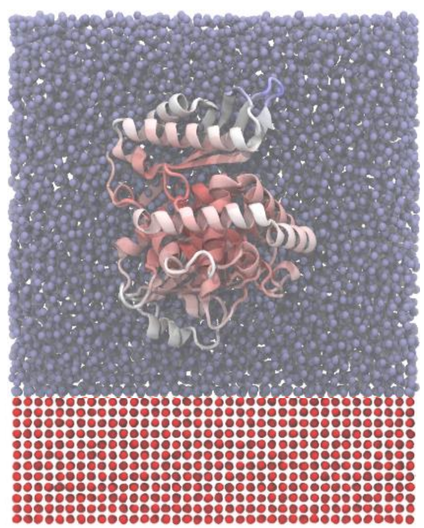
Superspreading Surfactant, e.g. Silwet-L77



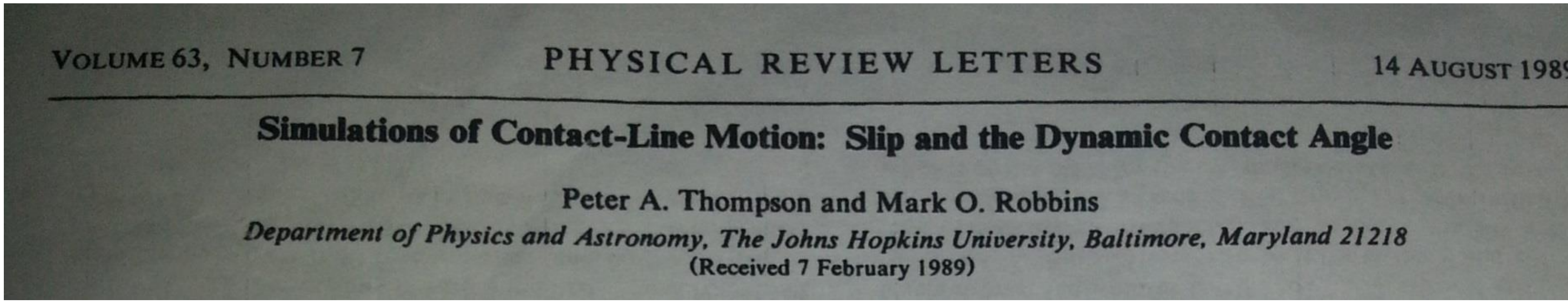








A Better way of Getting the Contact Angle



VOLUME 63, NUMBER 7 — PHYSICAL REVIEW LETTERS — 14 AUGUST 1989

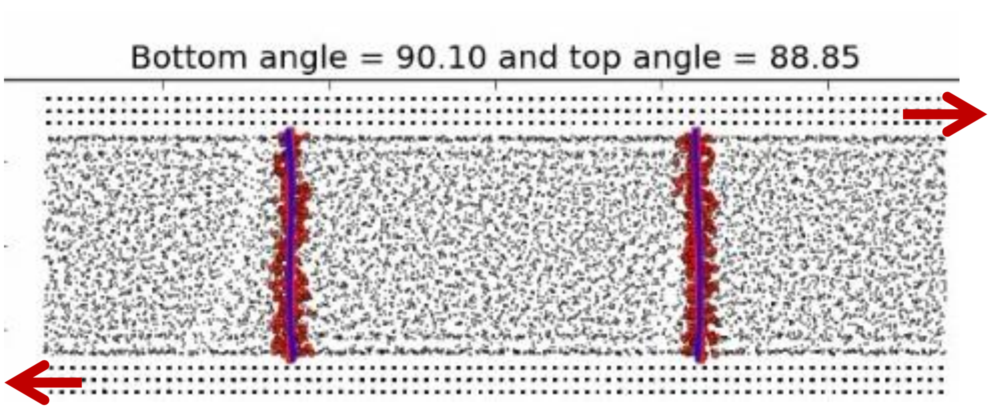
Simulations of Contact-Line Motion: Slip and the Dynamic Contact Angle

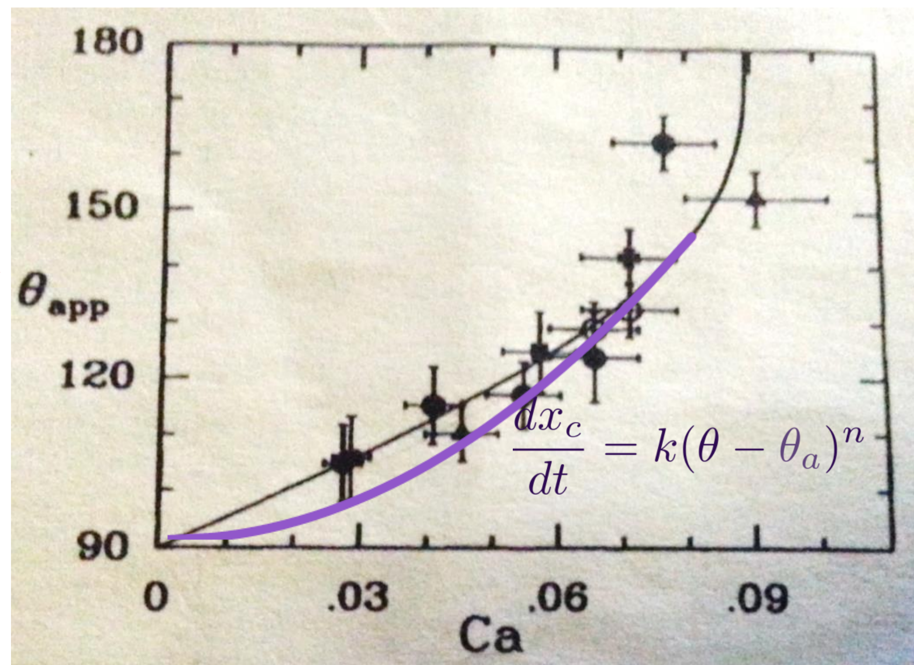
Peter A. Thompson and Mark O. Robbins

Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218

(Received 7 February 1989)

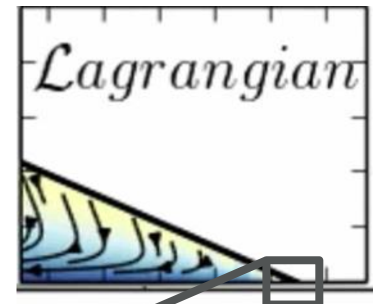
- Reproduces Cox's Law

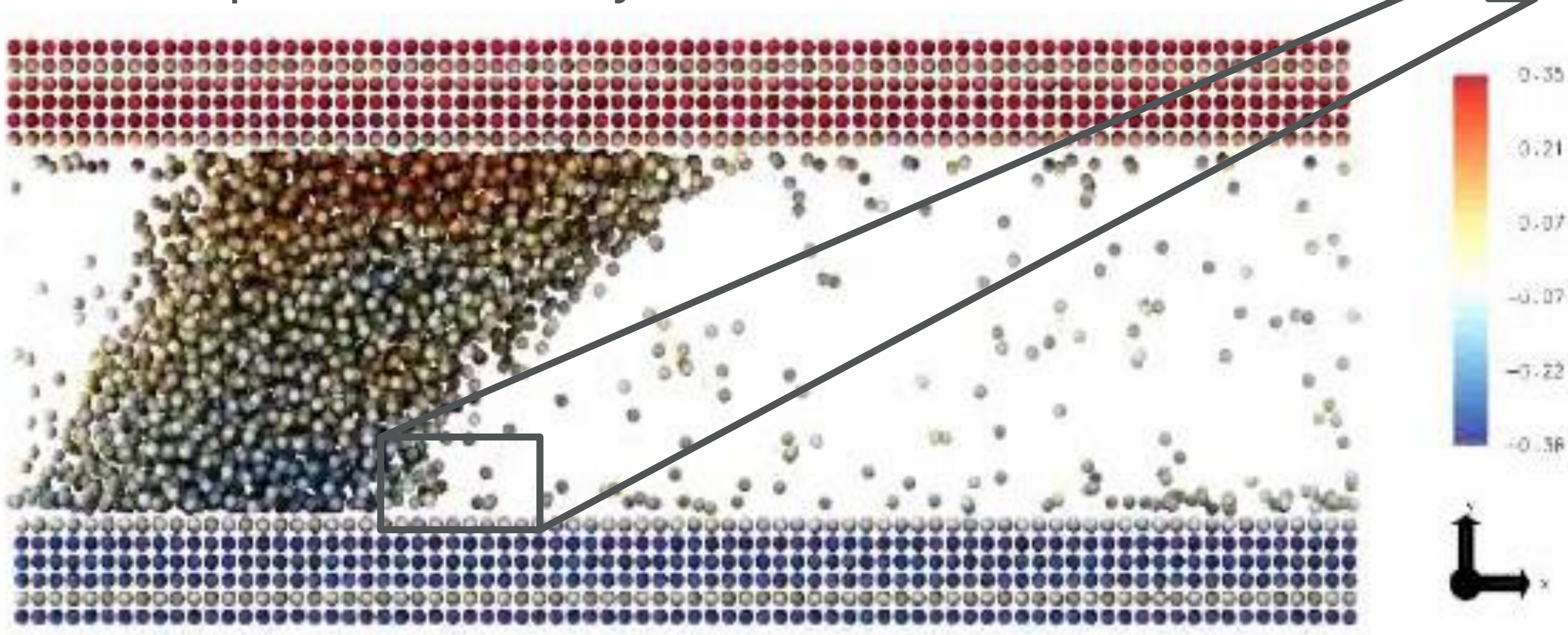




Two phase version closer to experimental reality

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





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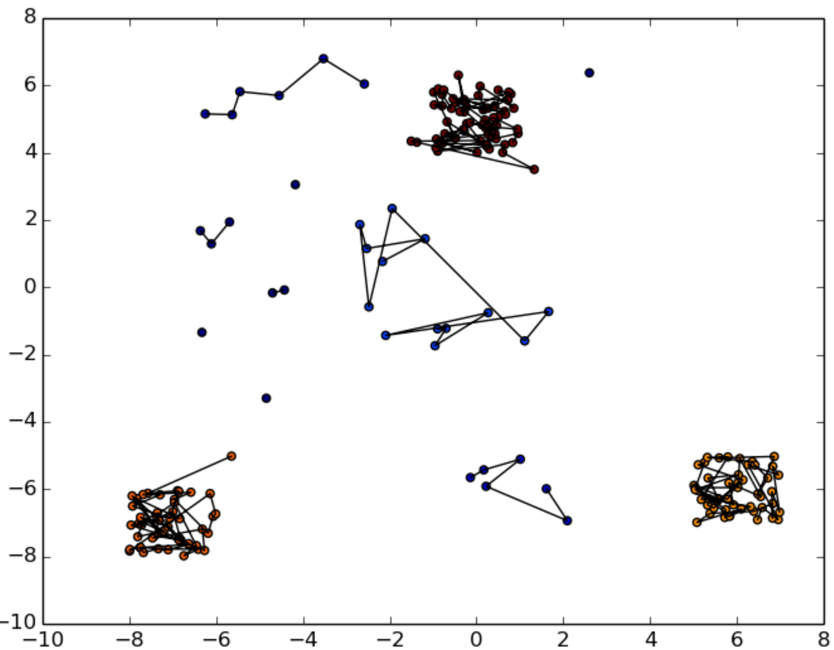
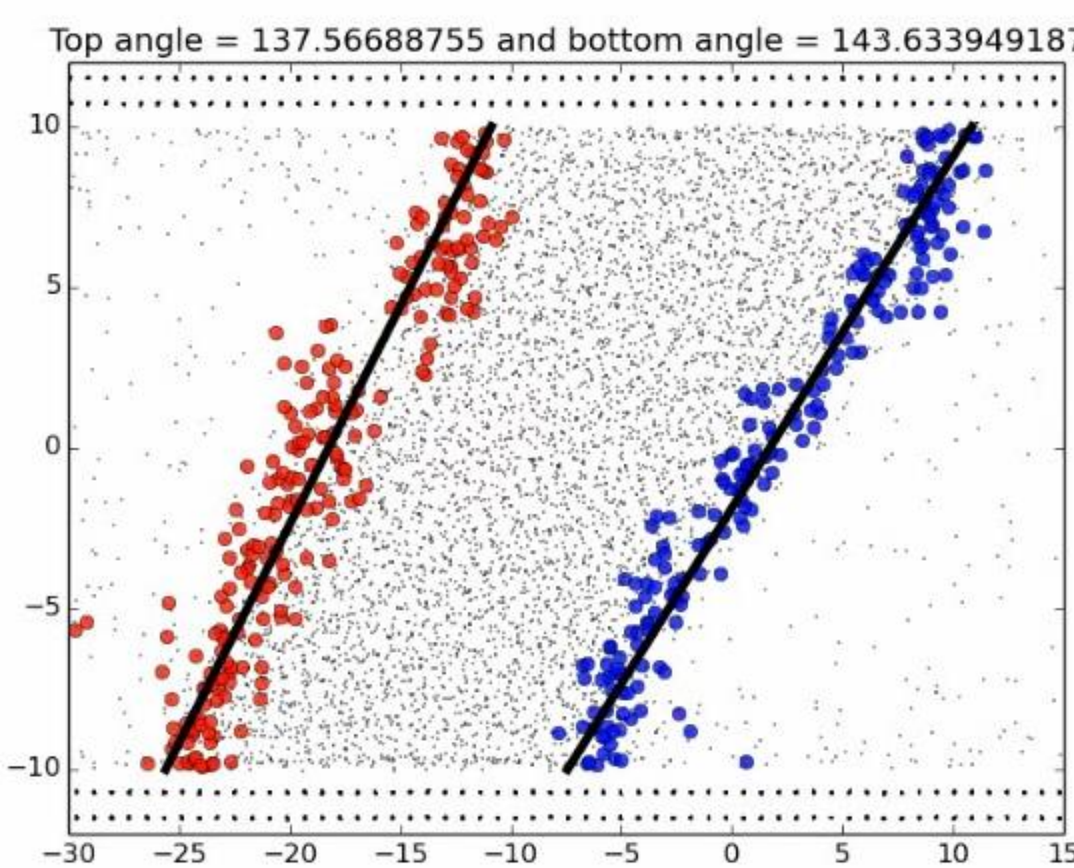
Cluster analysis and surface fitting



- Cluster analysis

- Finding the fluid-liquid interface



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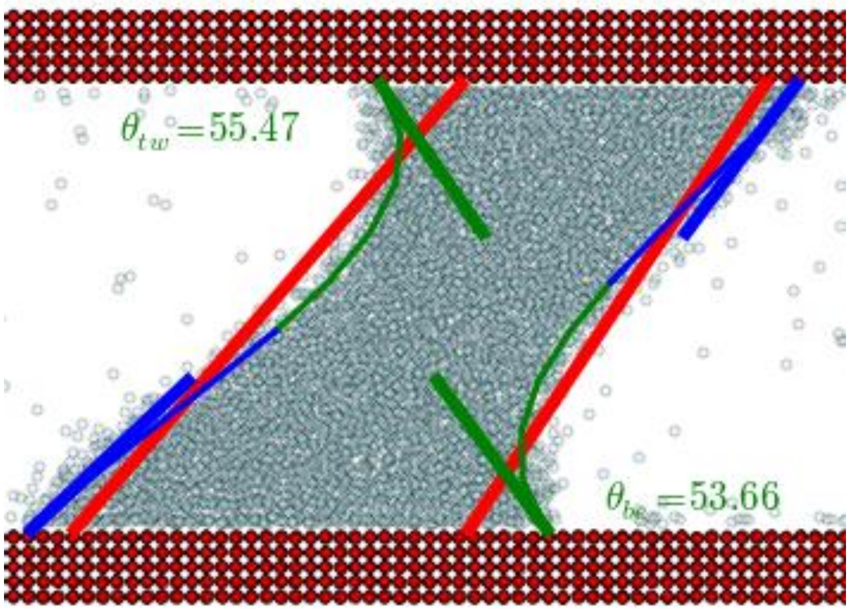
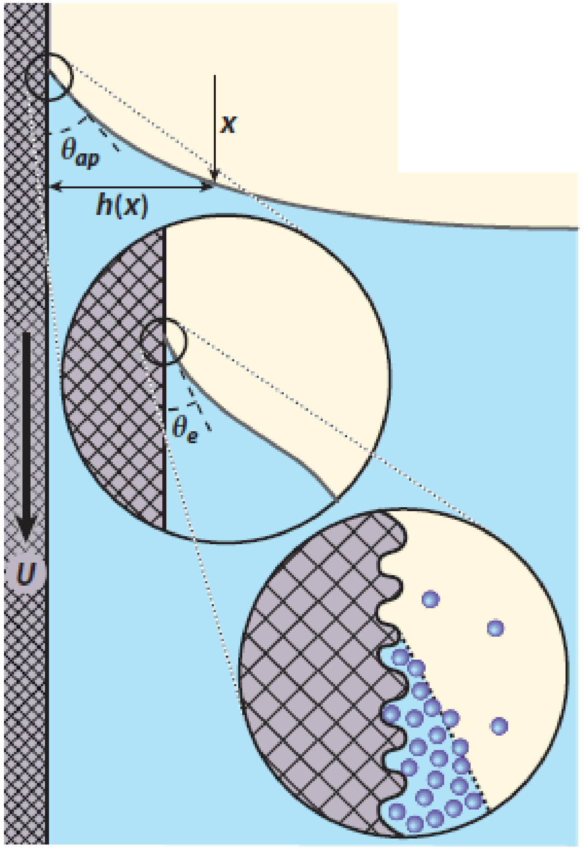
Determining the Contact angle

1) Snoeijer, Andreotti (2013) Annual Rev Fluid Mech 45:269–92

- Linear, Advancing and Receding angles



1)



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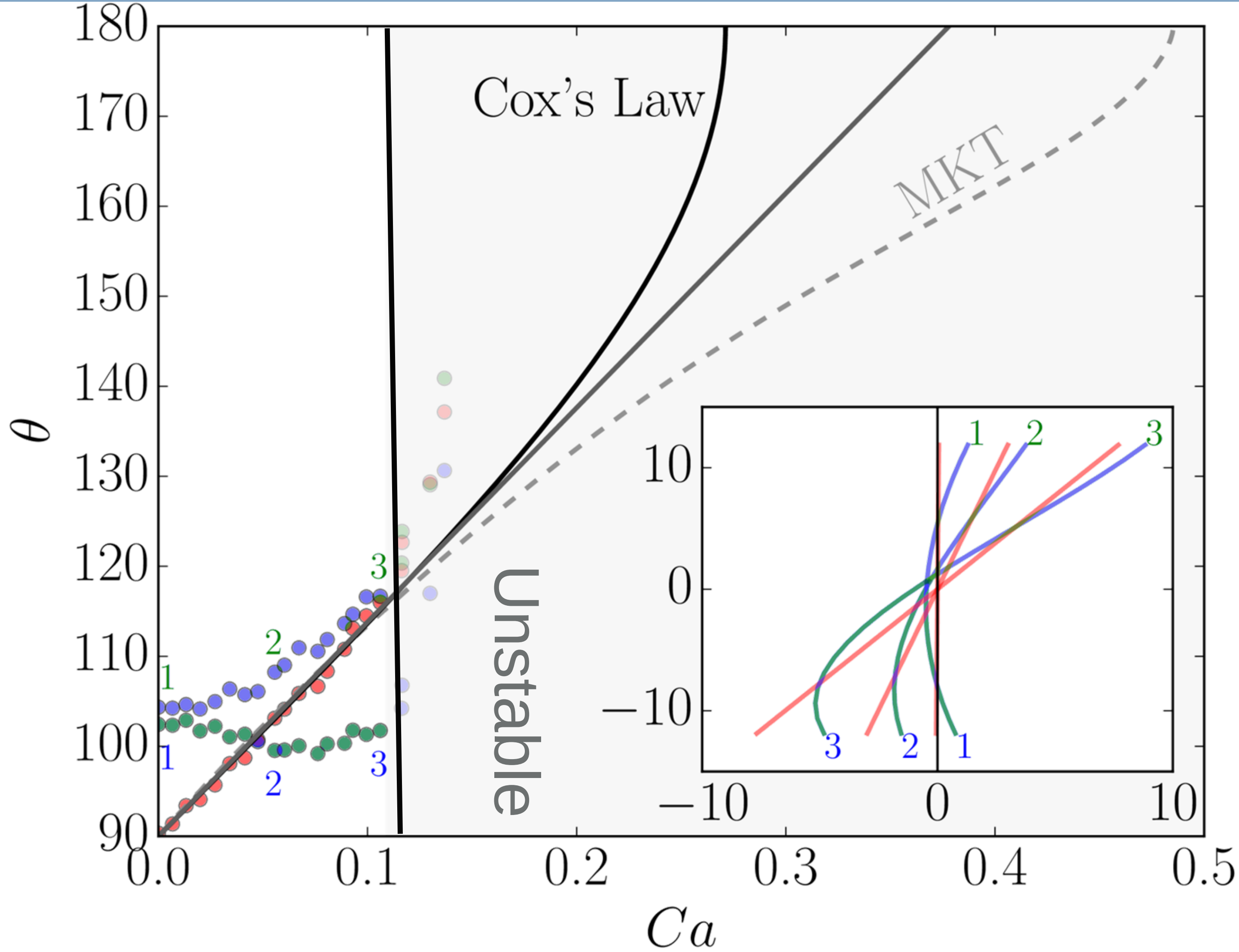
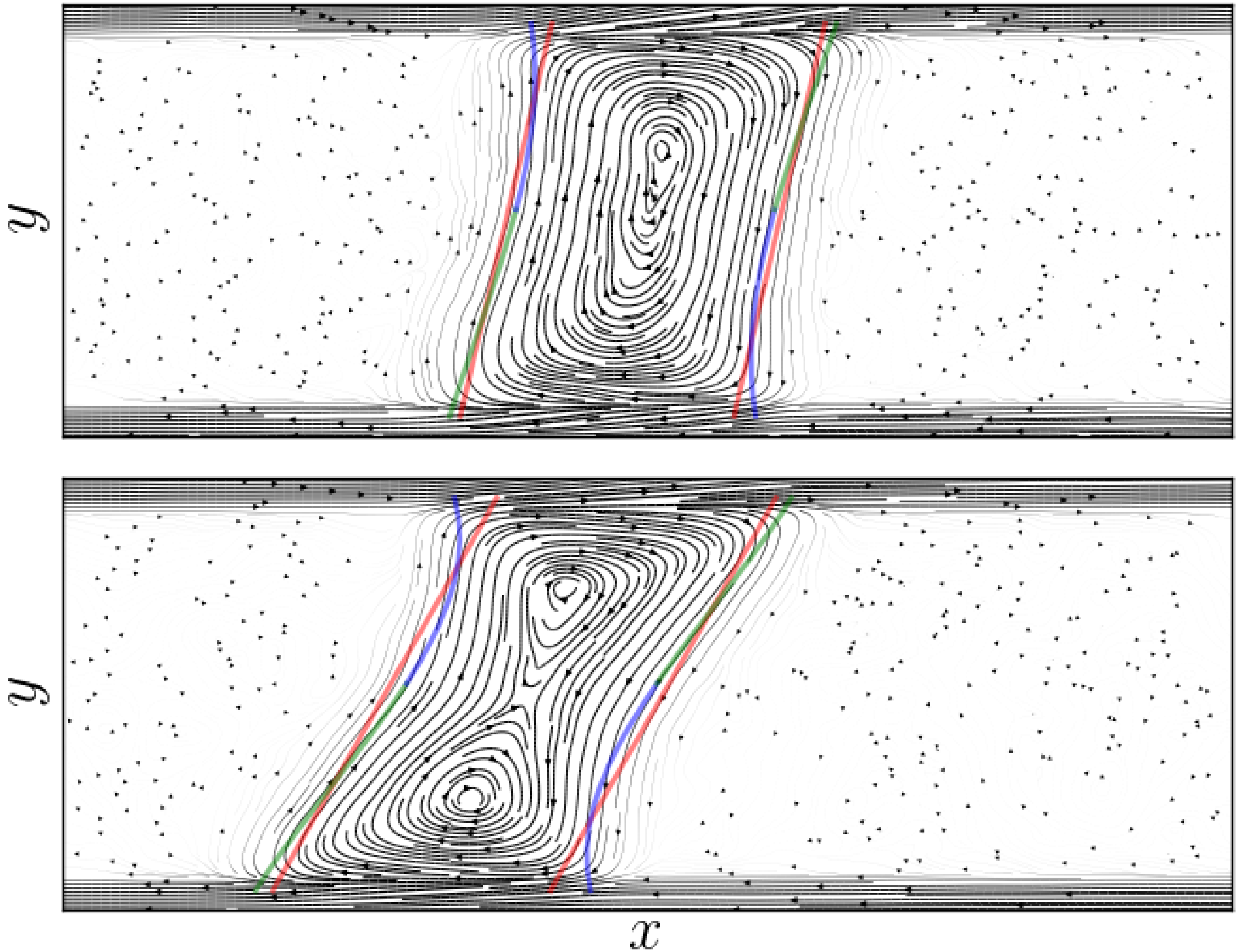
Contact angles vs sliding velocity



- Linear
- Advancing
- Receding

Streamlines



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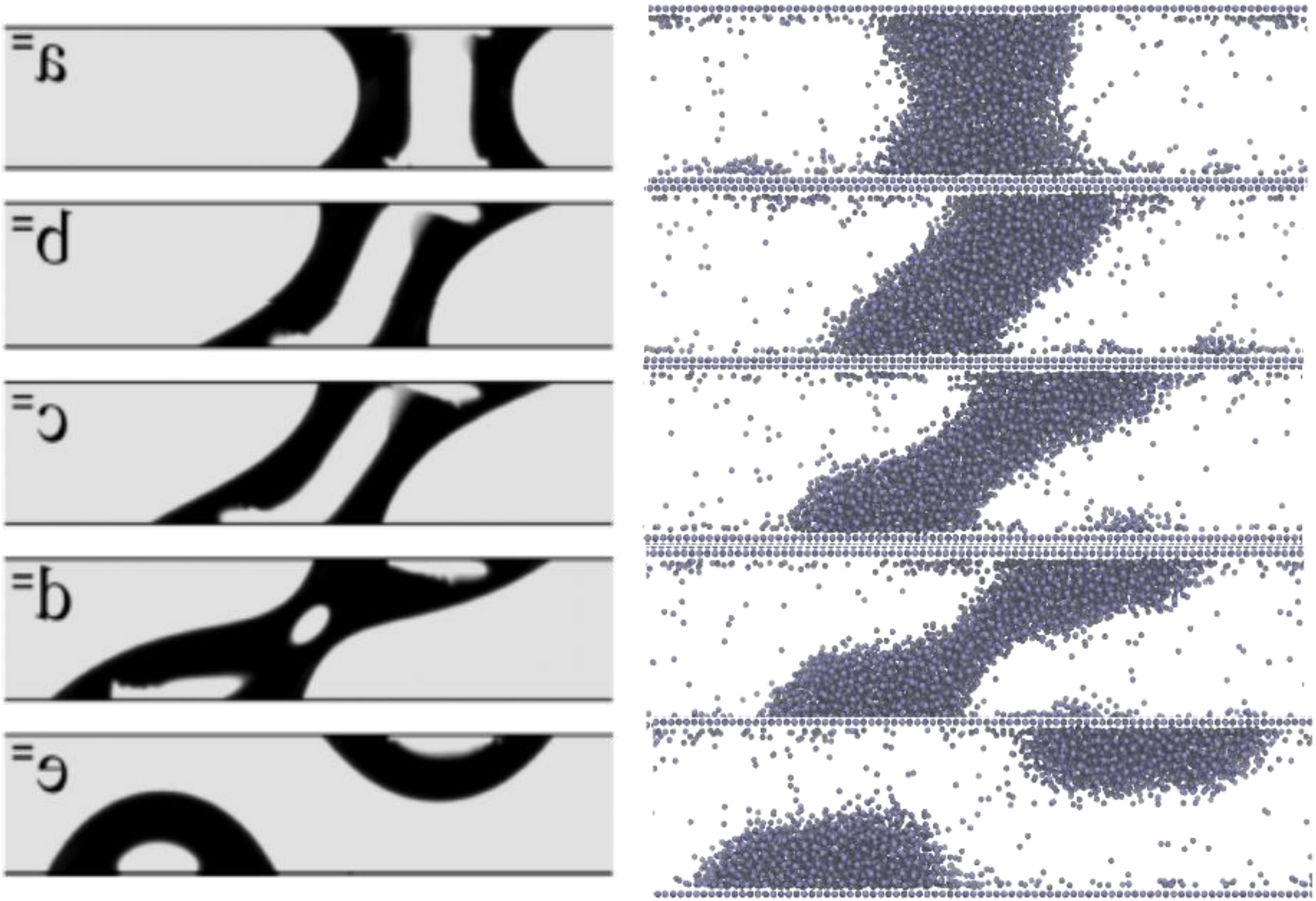
Droplet Breakdown

L. Wang, T. J. McCarthy (2013) Shear Distortion and Failure of Capillary Bridges. Wetting Information Beyond Contact Angle Analysis Langmuir 29, 7776−7781



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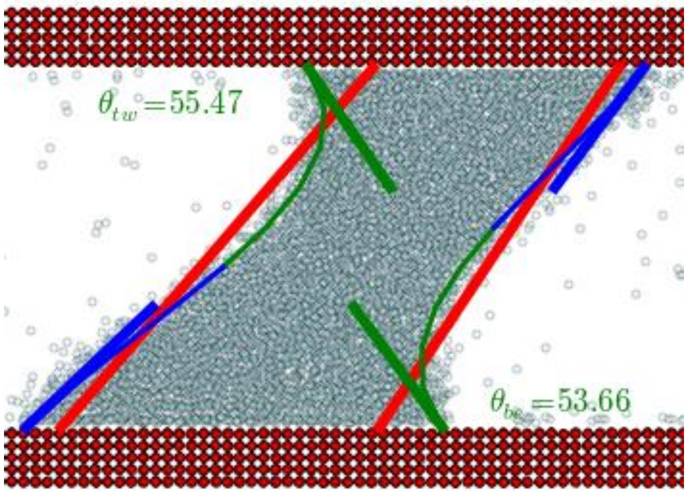
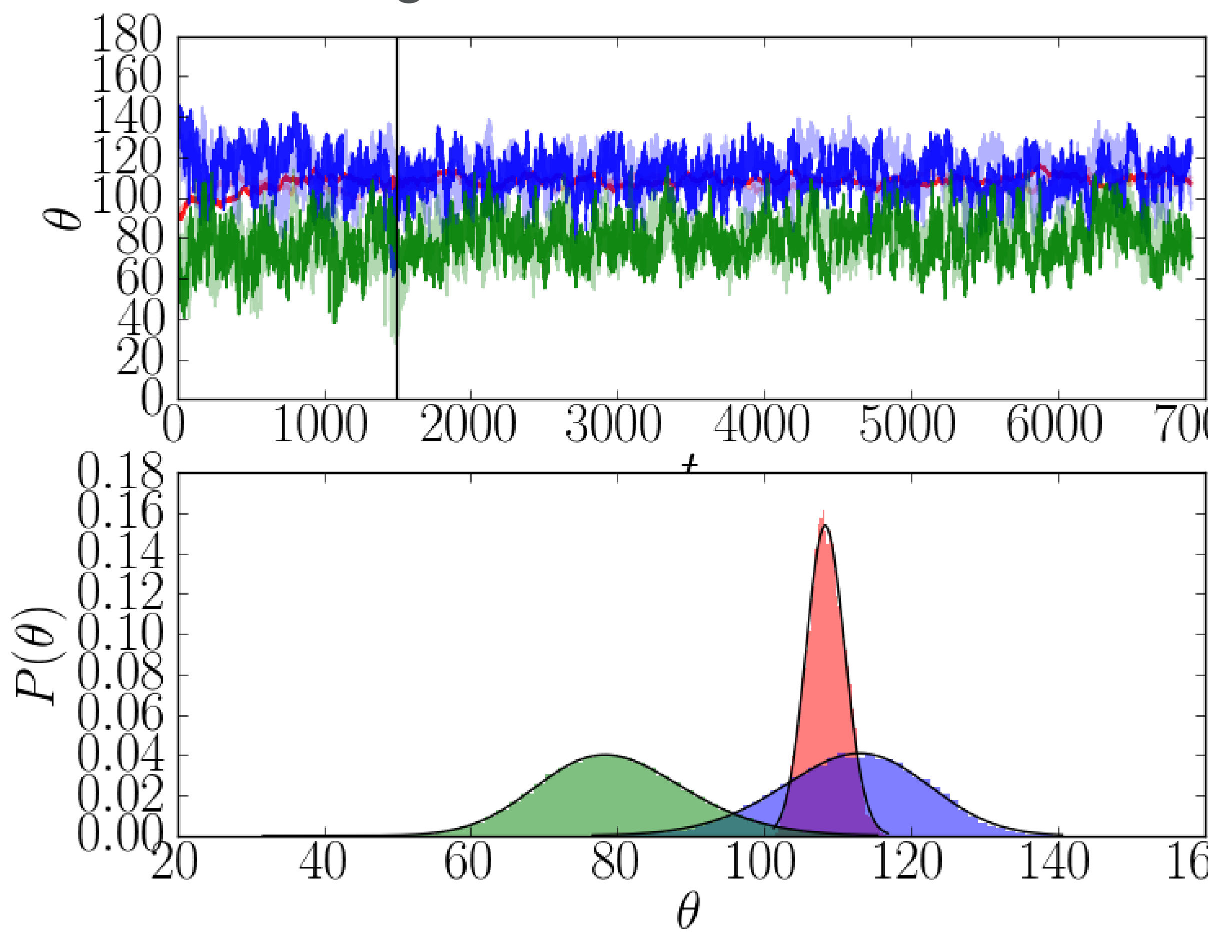
Time Evolution of Contact Angle

- Plot evolution of various contact angles as a function of time

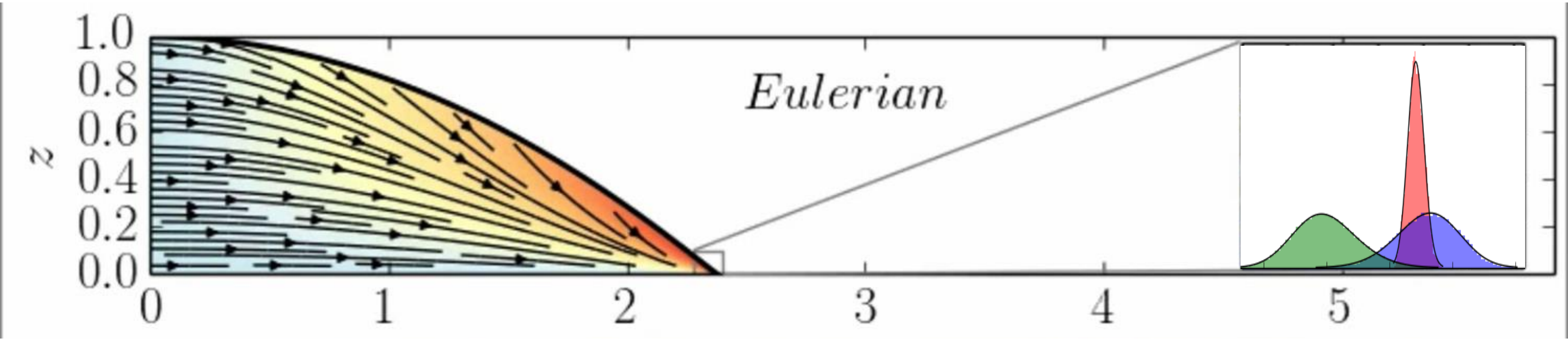




- Probability density function of angle shows range of micro-scale behaviour

- Linear, Advancing and Receding angles

Building this into the Continuum Model



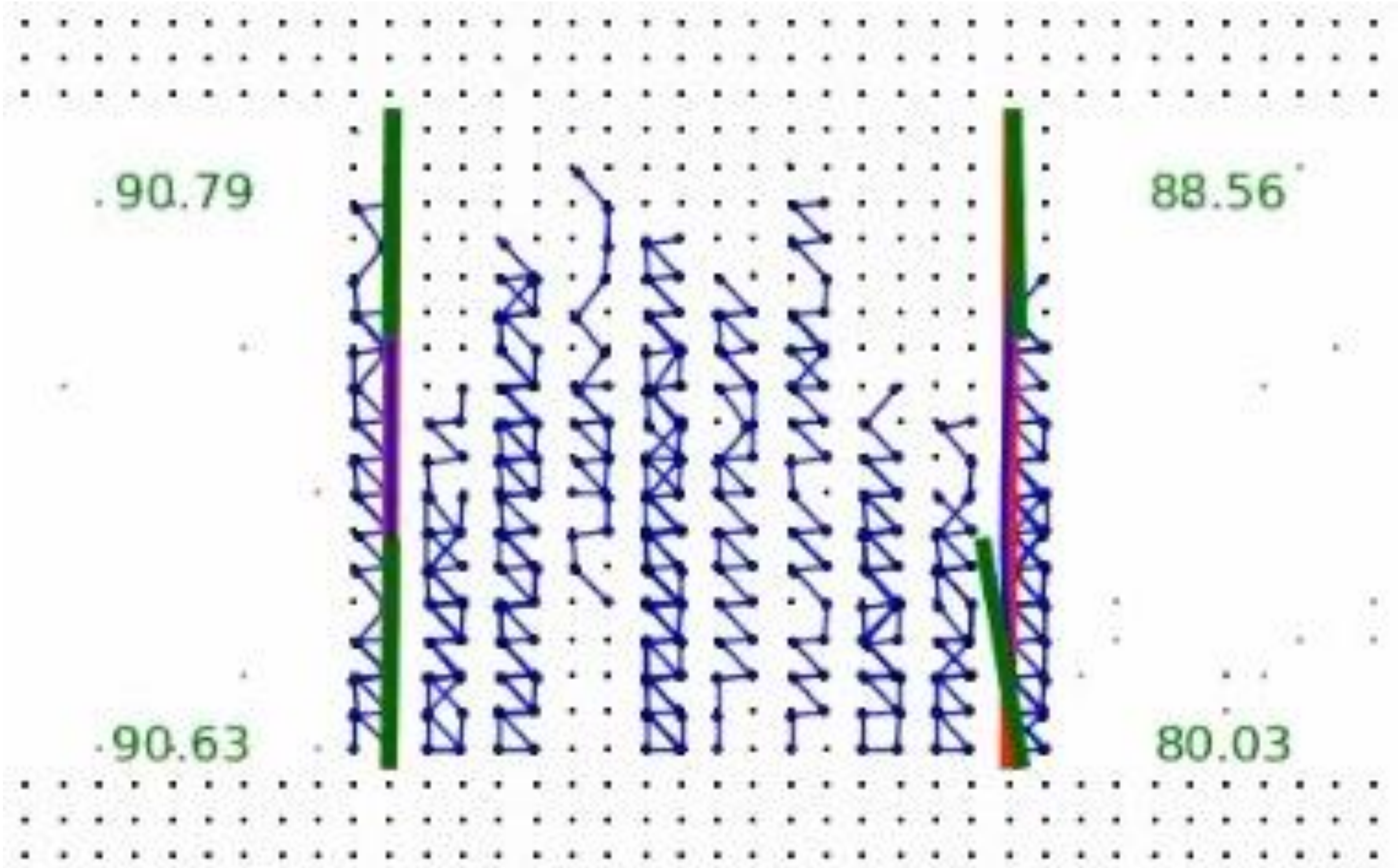
- Speed of contact line can be chosen from the molecular PDF with the appropriate speed in a simple fluid model

$$\frac{dx_c}{dt} = k(\theta - \theta_a)^n$$

- The more complex surfactant case requires simulations to be run dynamically for current surfactant concentration

Surfactant Spreading More Complex

- Surfactant concentration impacts contact angle
  - Includes mechanism for absorption at contact line



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Conclusions and Future Aims

- Molecular dynamics provides a more detailed model of the contact line, multiple phases and wall-fluid interactions

- We want to combine both in a single model
  - For simple cases, probability density functions of molecular detail
  - For surfactant simulations the references solutions could be run on the fly based on surfactant concentration
  - Longer term domain decomposition using a detailed continuum model

- Choice of methodology depends on phenomenon of interest
  - But any molecular modelling represents an improvement on empirical models.

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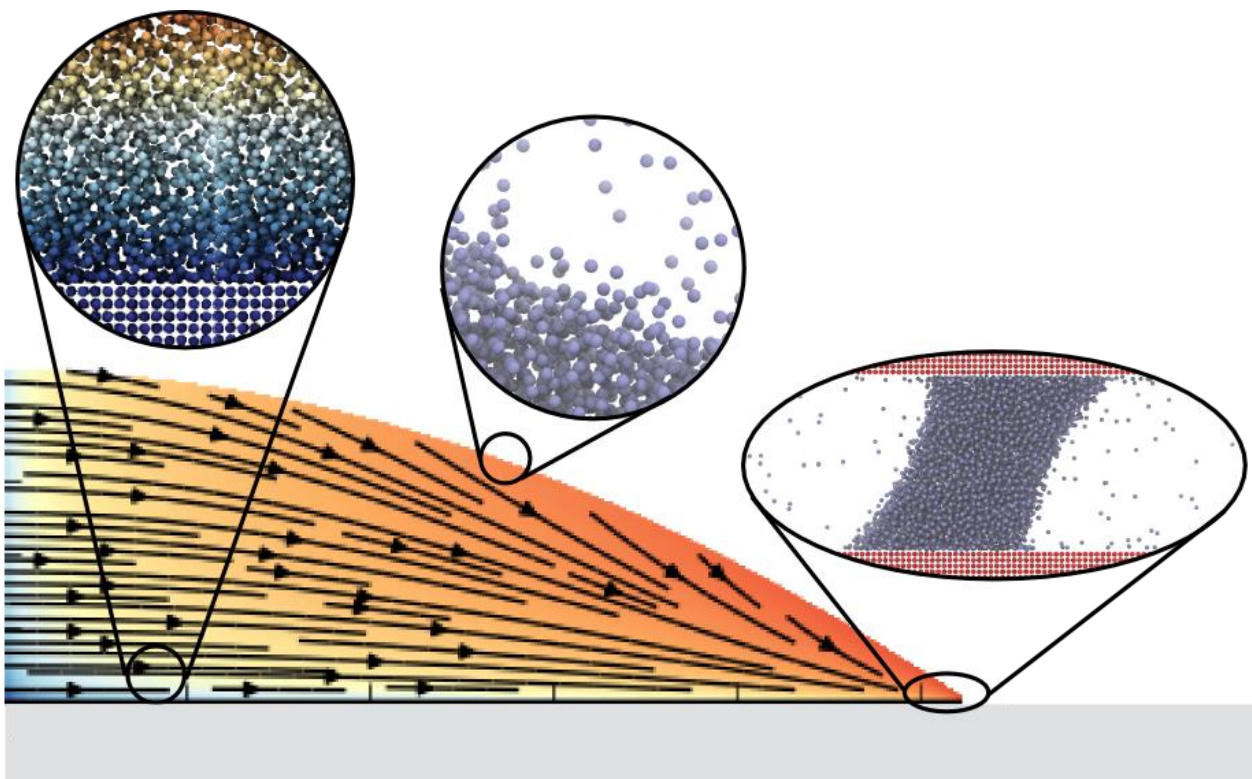
Acknowledgements

- Current work funded by EPSRC Grant number EP/J010502/1
- Working with Erich Muller, Richard Craster and Omar Matar



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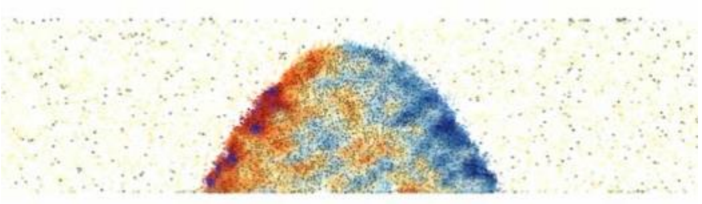
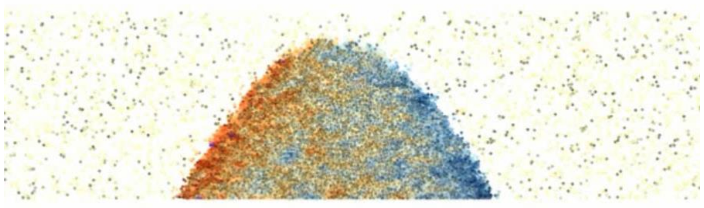
MD Simulation of Droplets

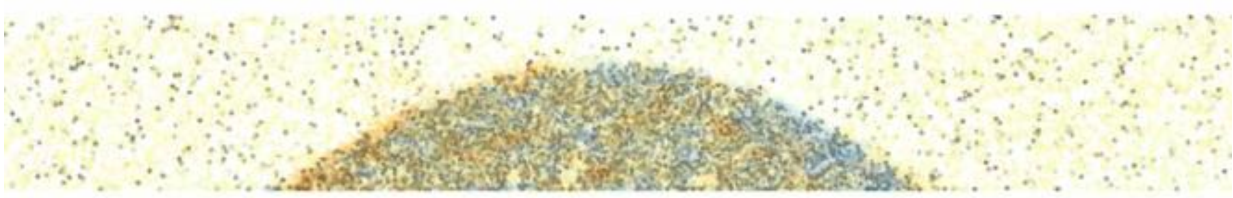
- Low Wettability



- Intermediate Wettability



- High Wettability



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Coupling Overview

1) Ren (2007), E et al (2003), Borg et al (2013)
2) O'Connell and Thompson (1995), Flekkøy at al (2000), Nie et al (2004), Hadjiconstantinou et al (1999), Delgado-Buscalioni and Coveney, (2003)

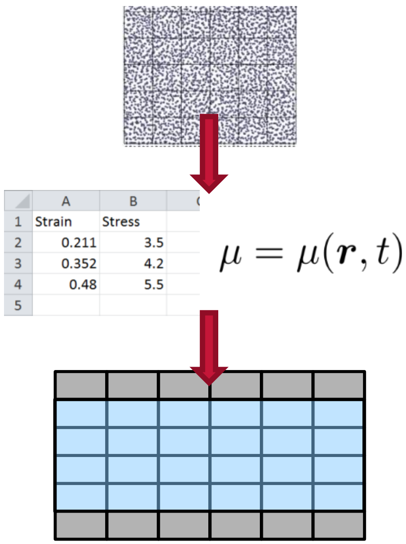
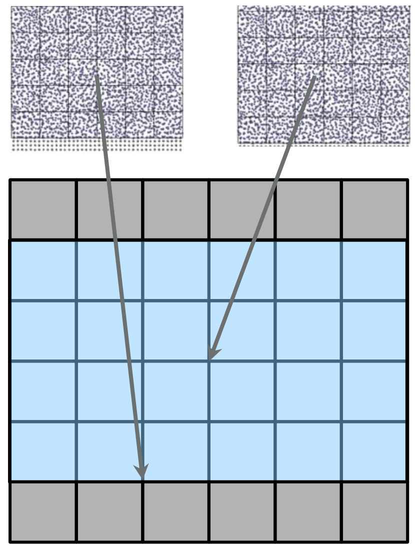


Table Lookup or Coefficients

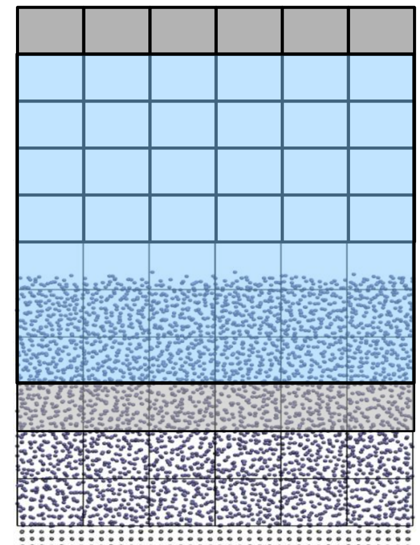
MD parameter study stored in table and CFD uses data



Embedded Models

MD – embedded in a CFD simulation

Used for Non-Newtonian effects [1)]



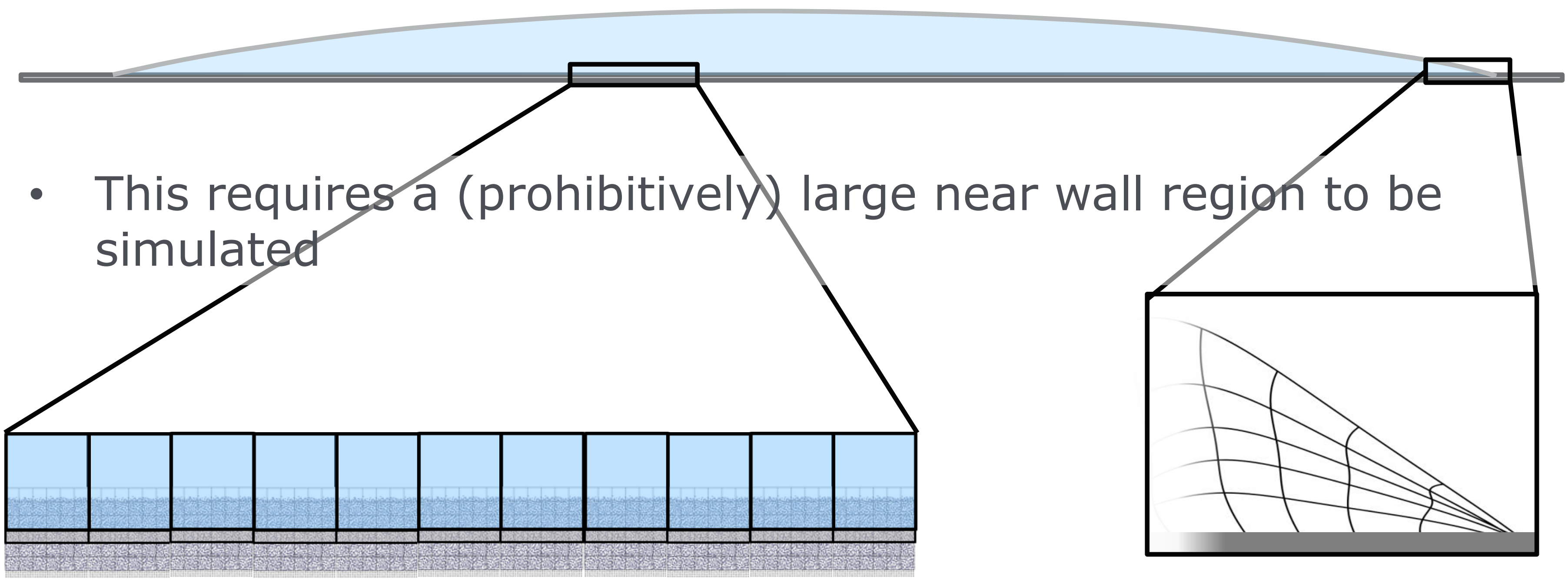
Domain Decomposition

MD –CFD linked along an interface

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

Droplet Modelling

- Thin film equations assumes a large length to height ratio



- This requires a (prohibitively) large near wall region to be simulated

- Especially when only the contact line dynamics are of interest
  - Stretched grid and moving interface are complex to model

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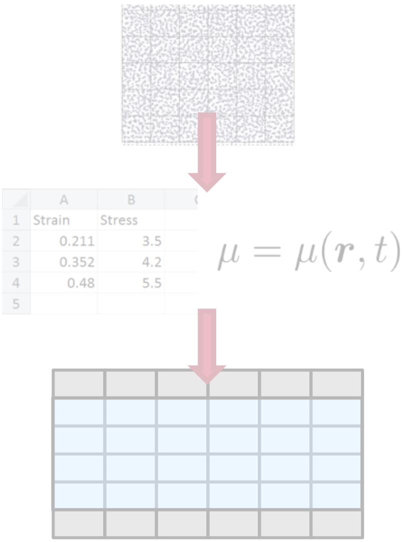

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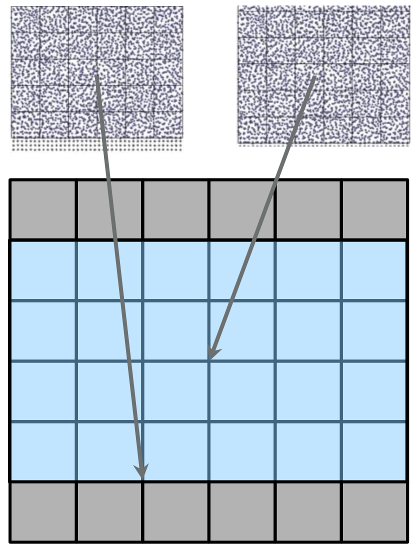

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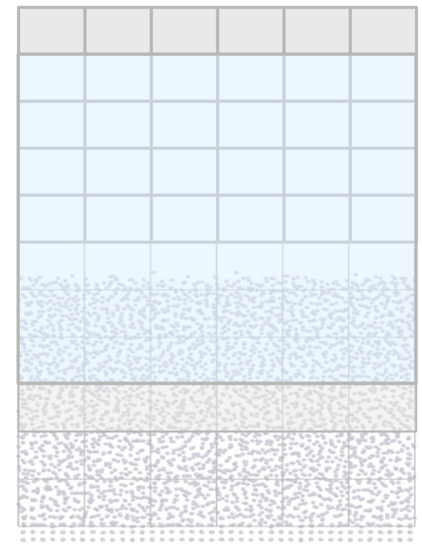

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