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Multi-Scale Strategies for Dealing with Moving Contact Lines

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11:14AM–11:27AM

By

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EPSRC

Pioneering research and skills

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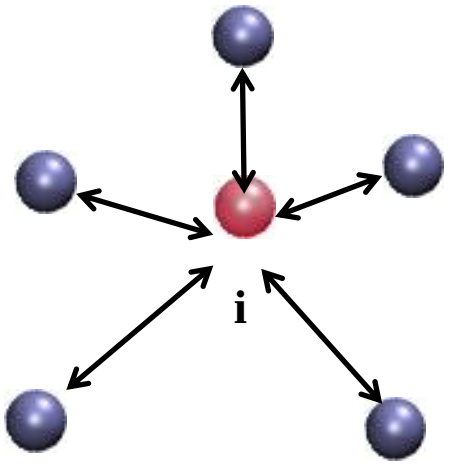
Molecular Dynamics

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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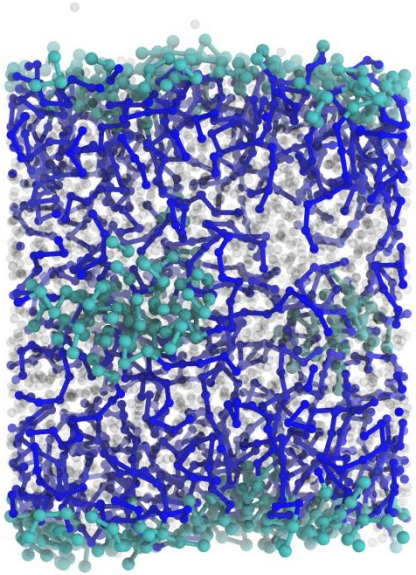
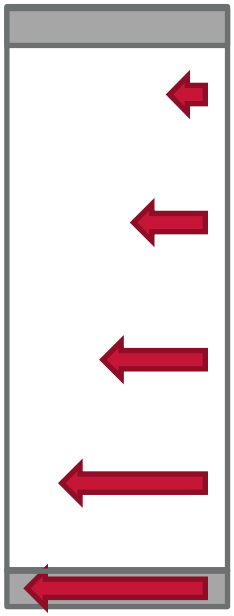
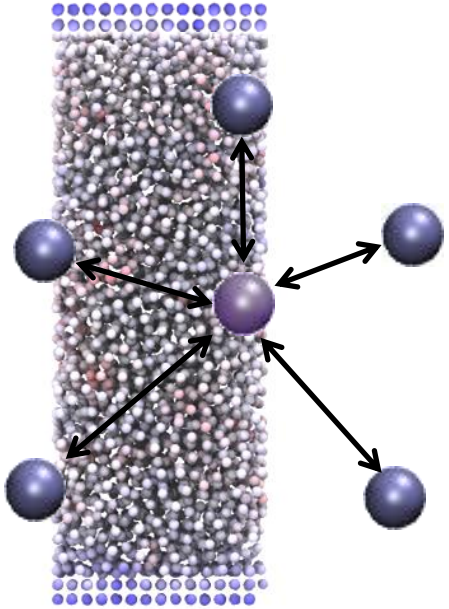
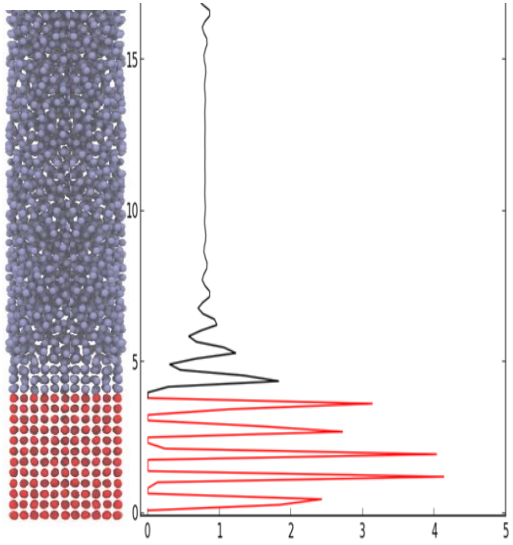
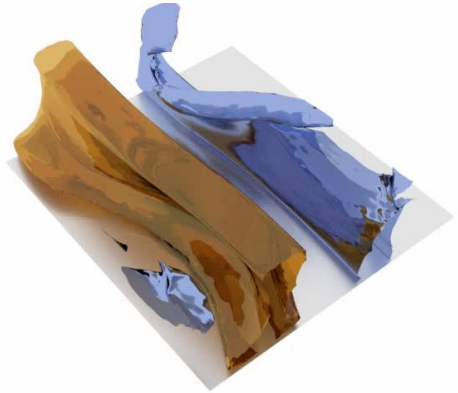
Molecular Dynamics





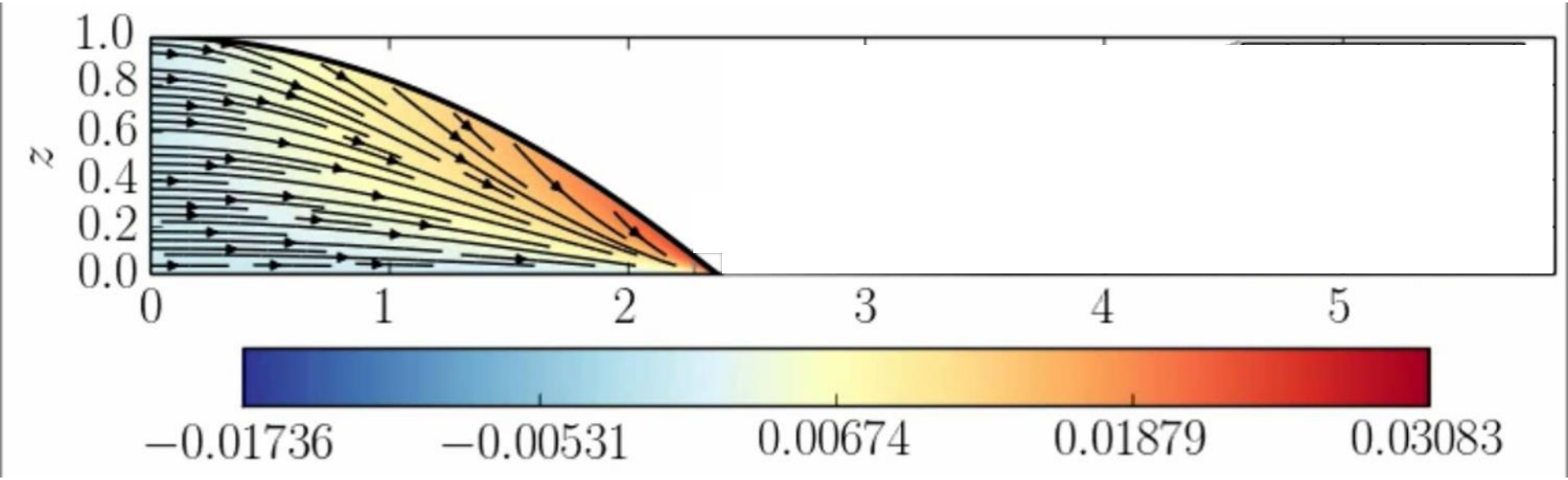






1) *Thompson and Robbins (1989)*

Coupled Droplet Spreading and MD



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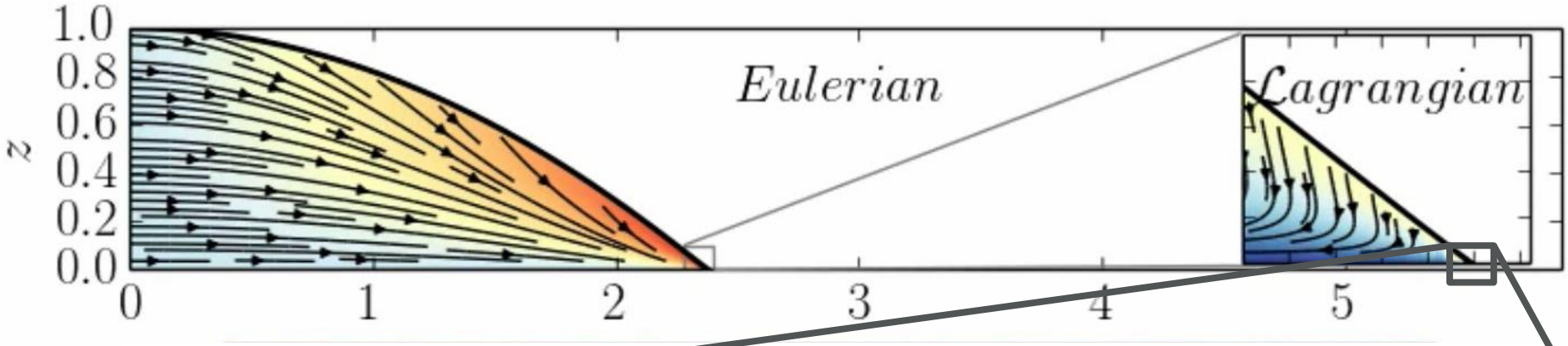
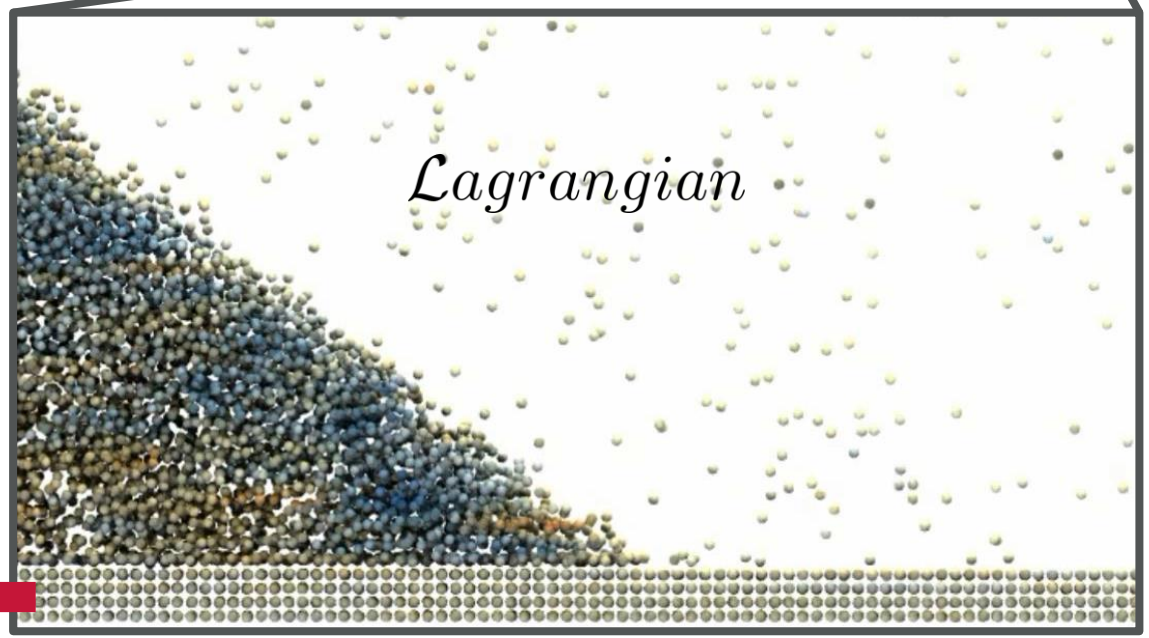
Coupled Droplet Spreading and MD



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



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

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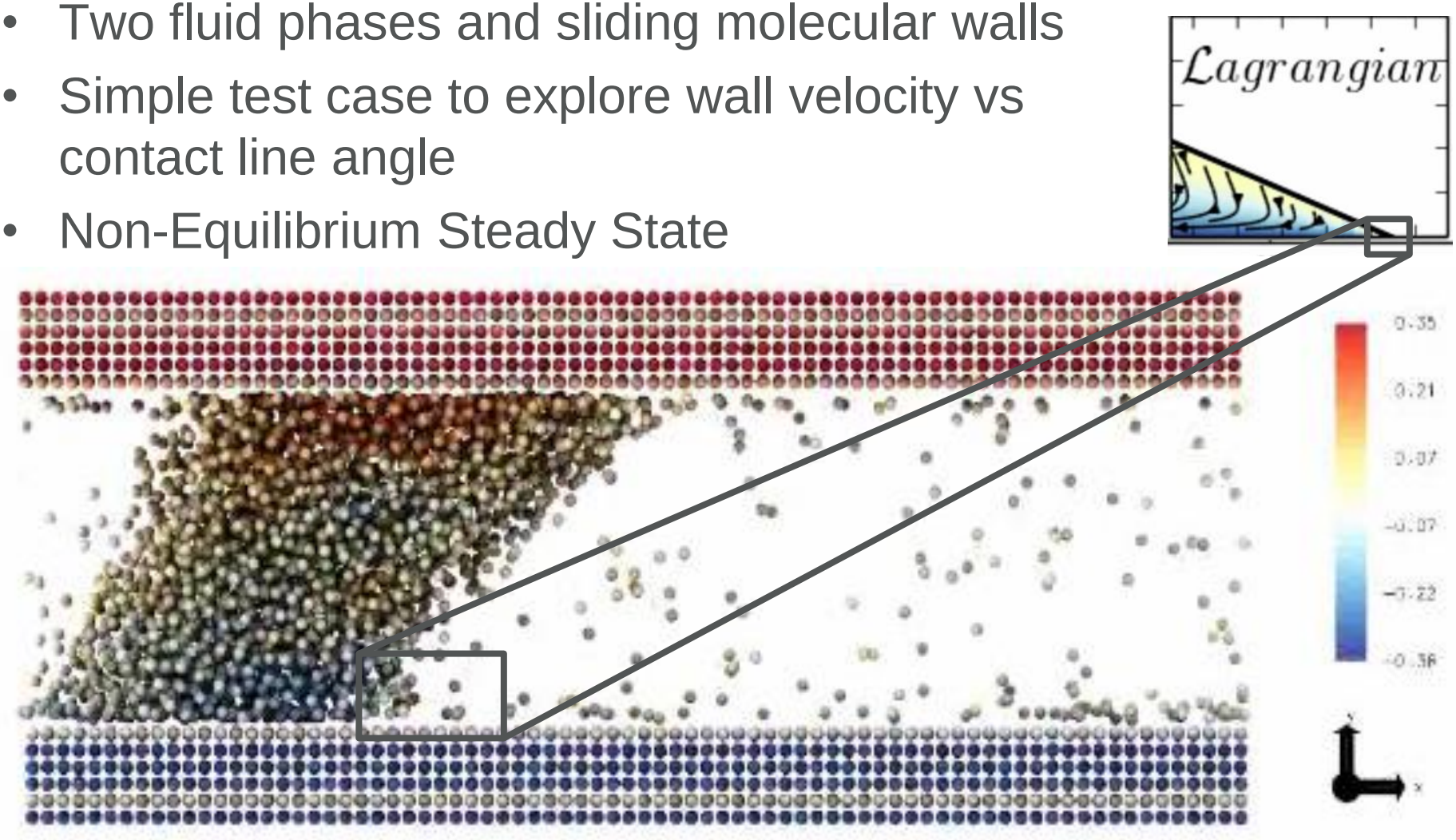
A Sheared Liquid Bridge

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



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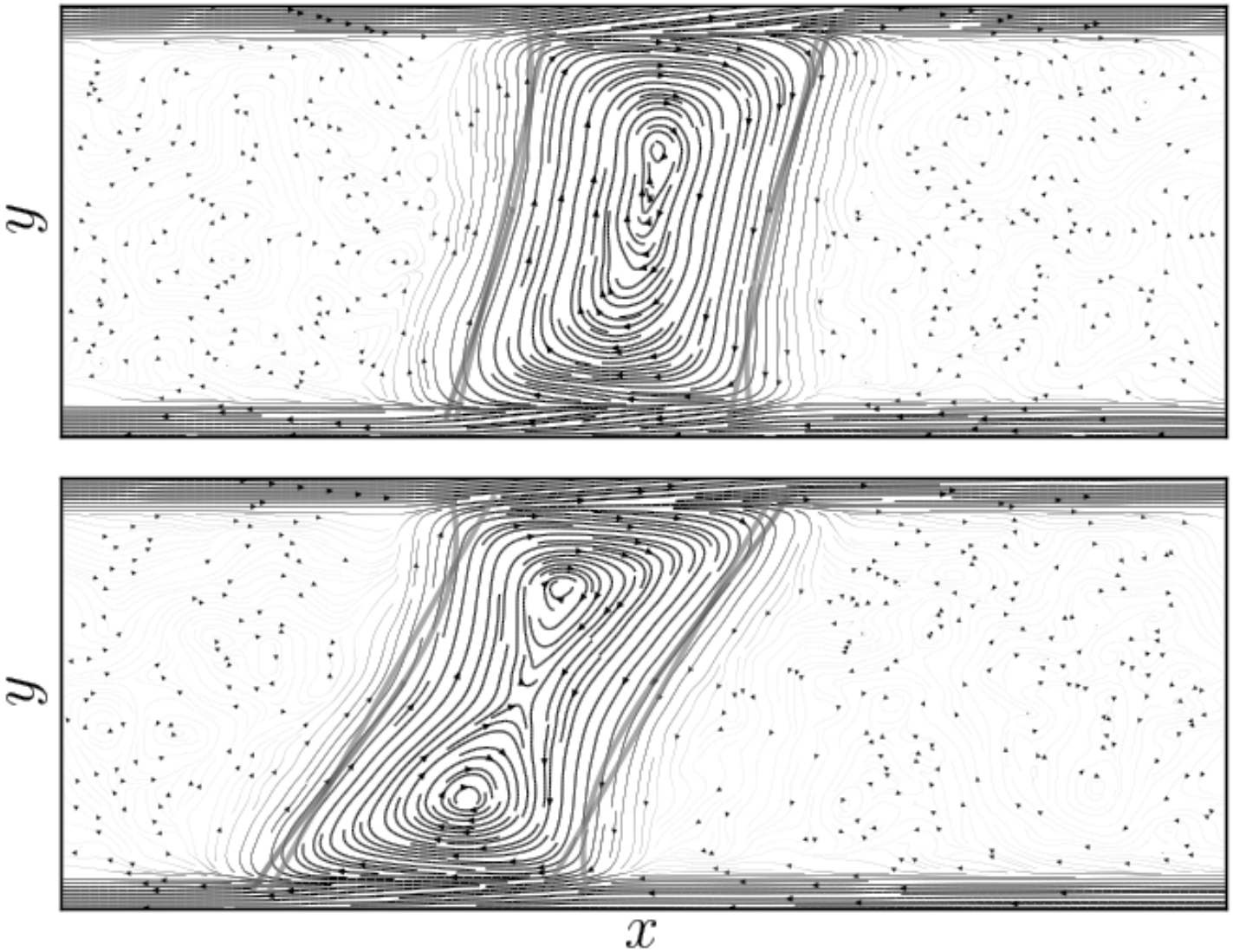
Streamlines



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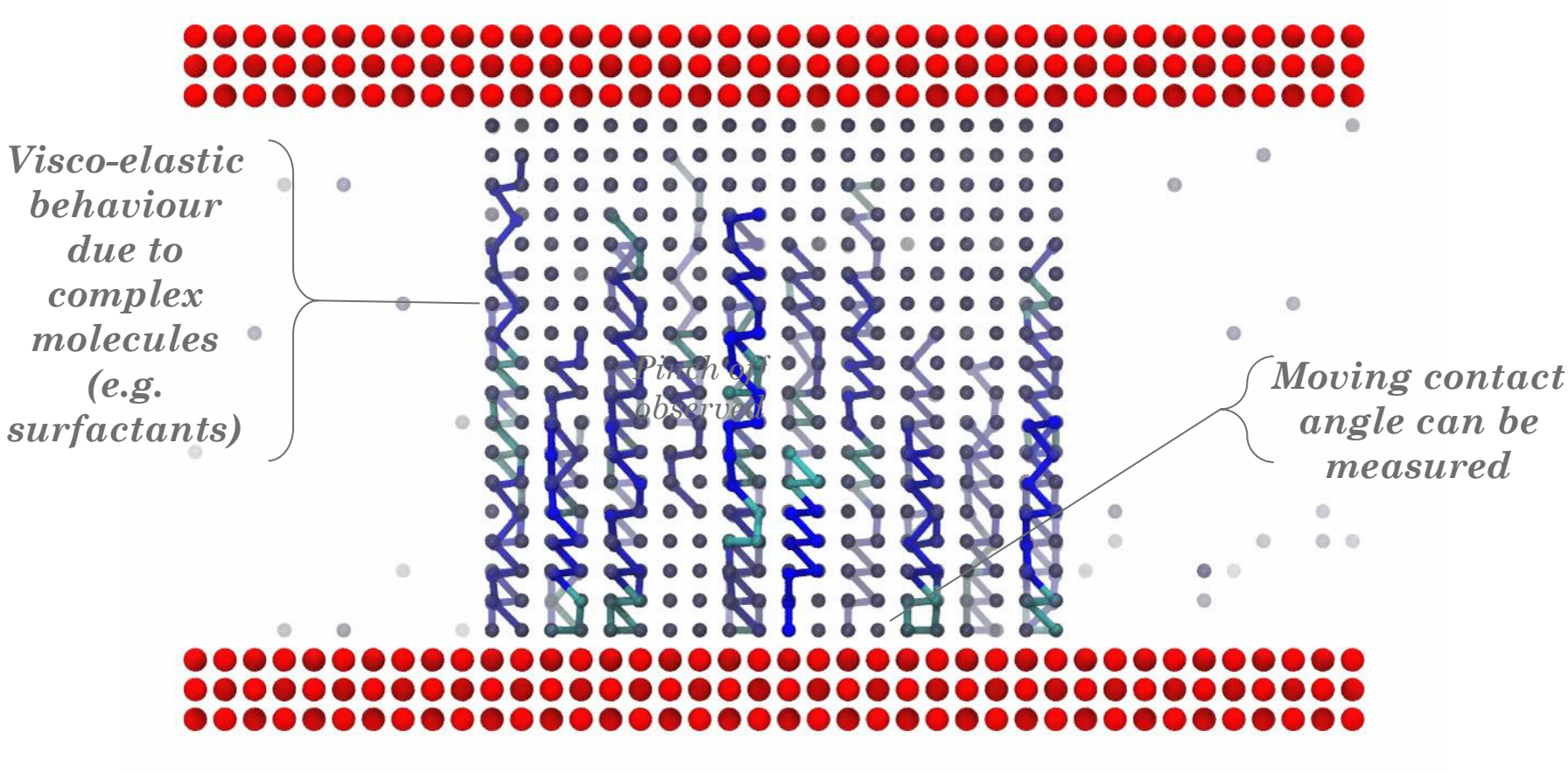
Pinch off in a Liquid Bridge



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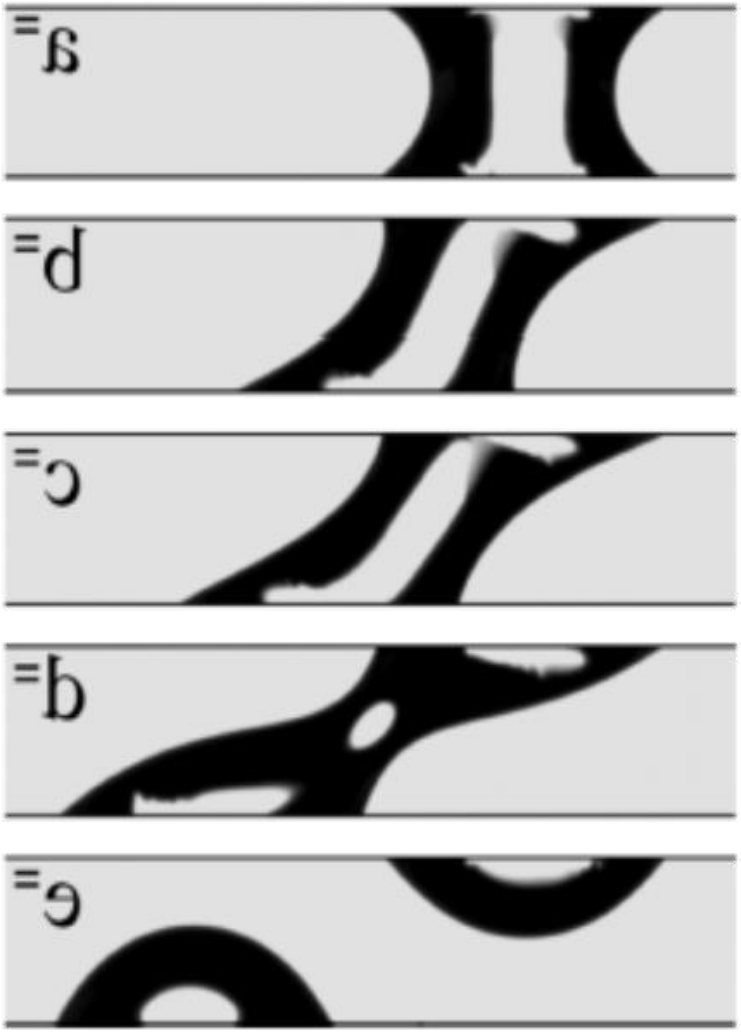
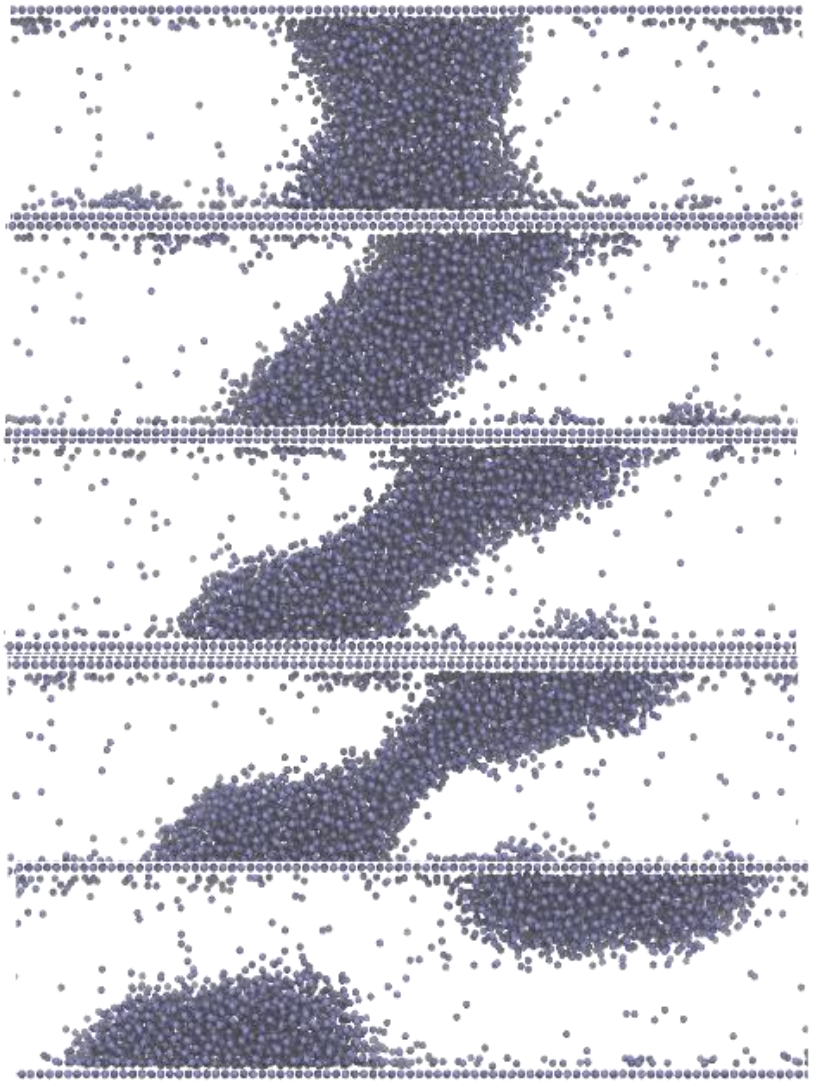
Droplet Breakdown

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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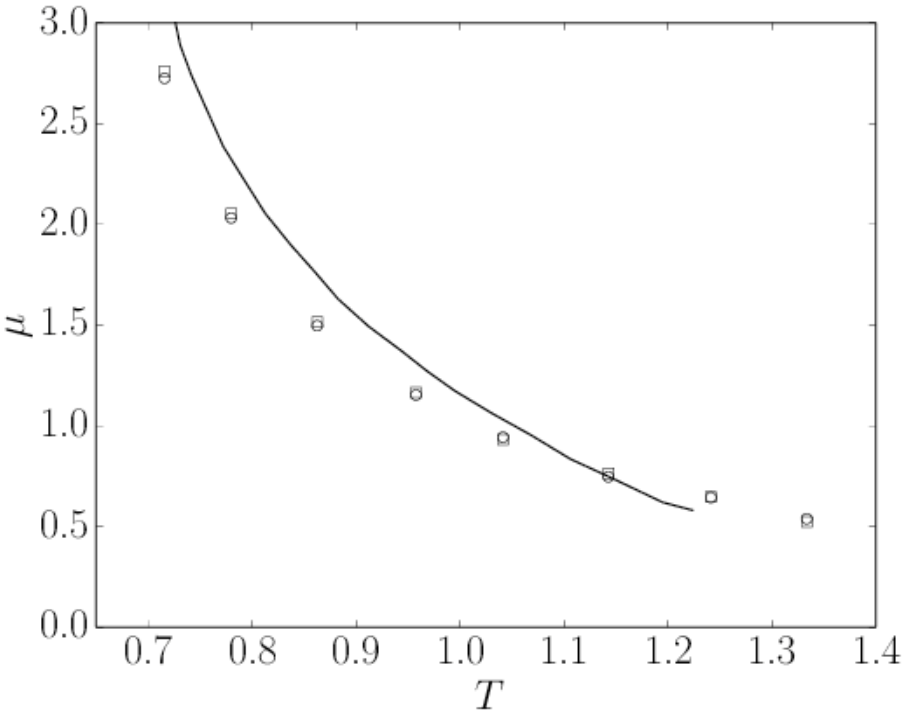
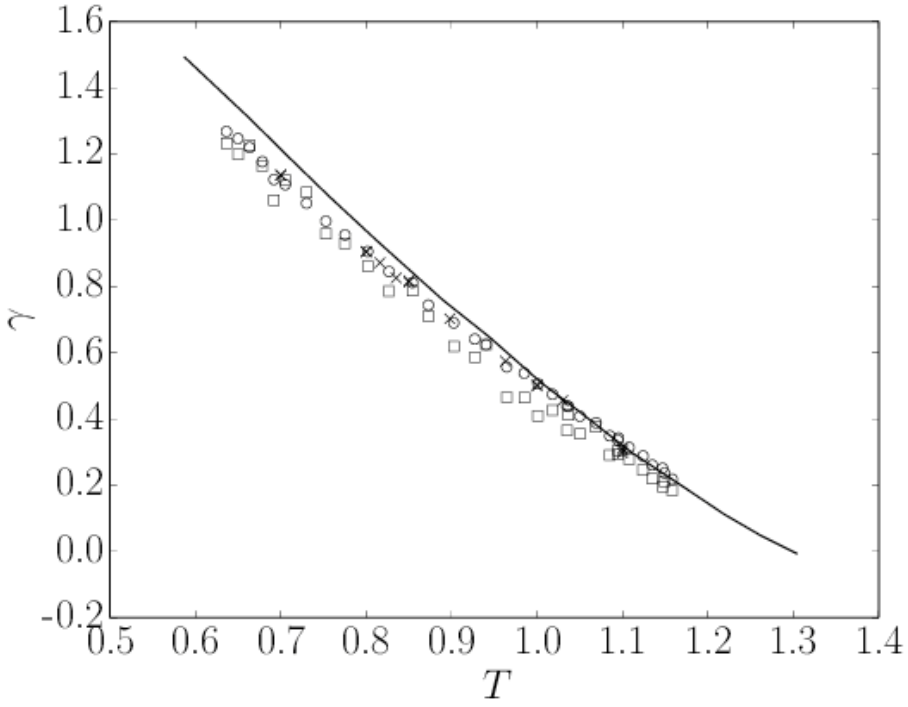
Quantitative Validation

- Molecular Dynamics can give a-priori values of viscosity, surface tension and models the near-wall slip



Viscosity vs Temperature



Surface Tension vs Temperature

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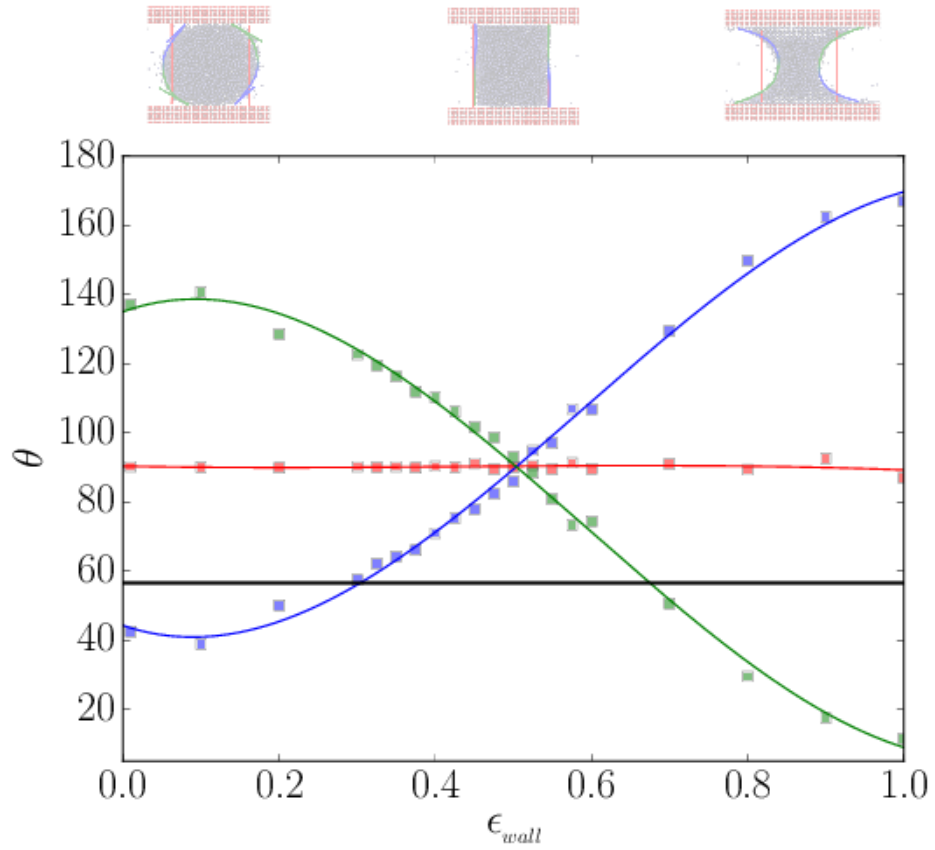
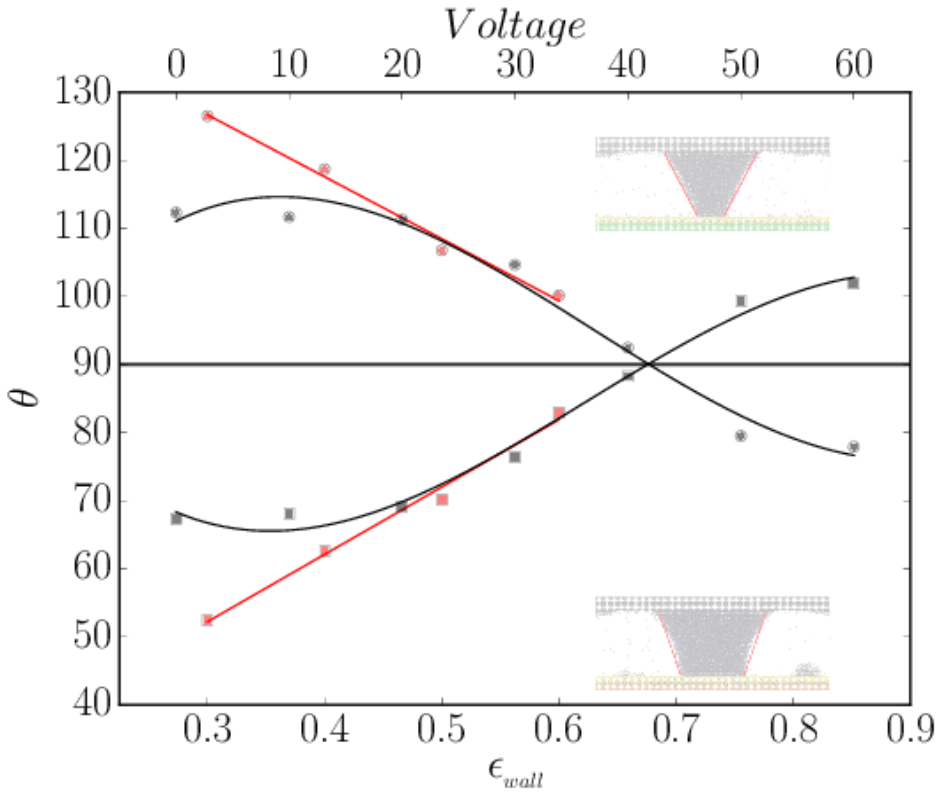
Tuning Wall-Fluid Interaction

W. C. Nelson, P. Sen and C. Kim, *Langmuir*, 2011, **27**, 10319–10326.

- A major source of MD modelling uncertainty is interaction strength between wall molecules and fluid molecules





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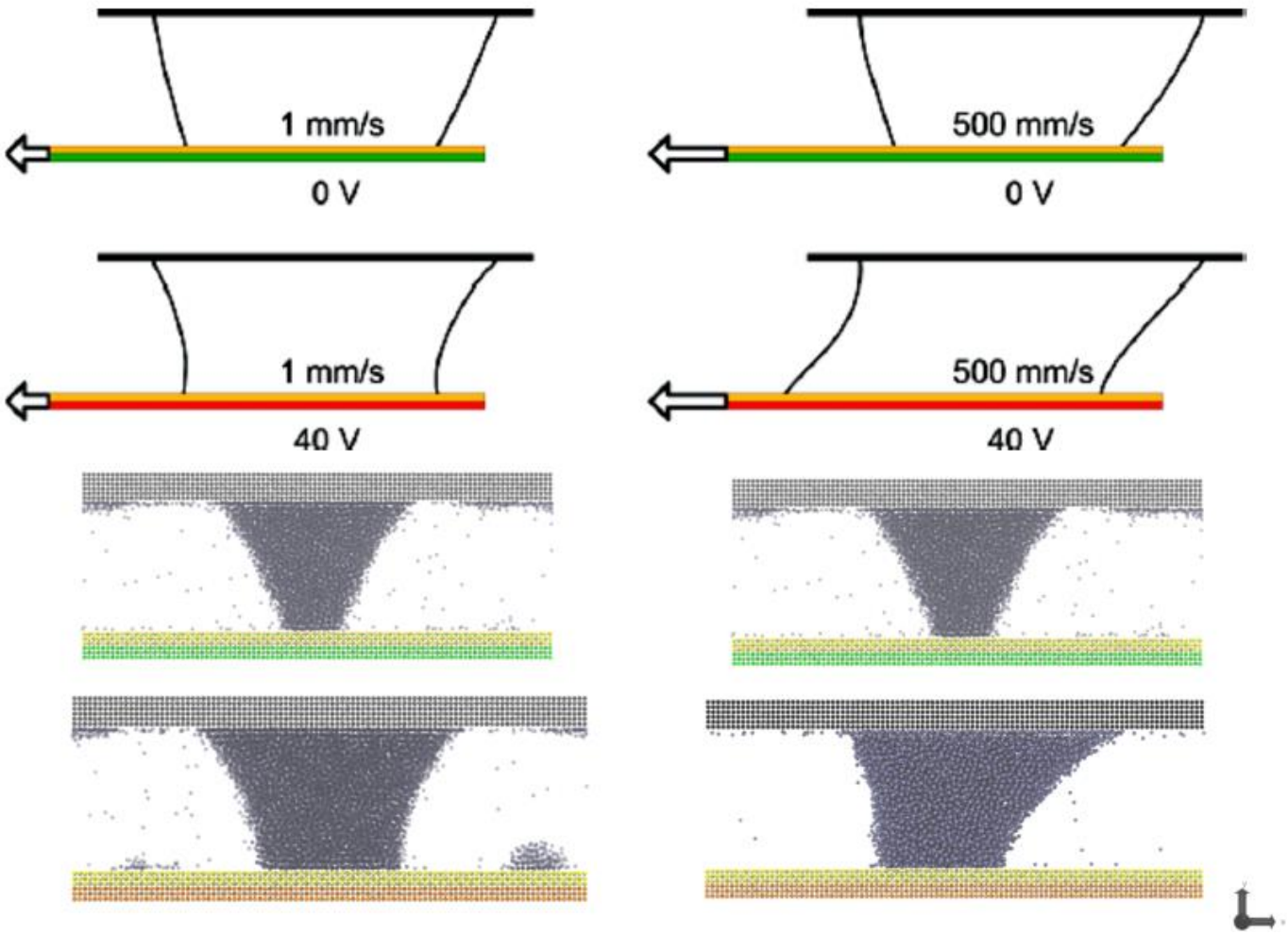
Studying Wall Sliding with Electrowetting

- Molecular compared to Experimental work by Nelson et al (2011)
- Sliding bottom wall for range of electro-wetting



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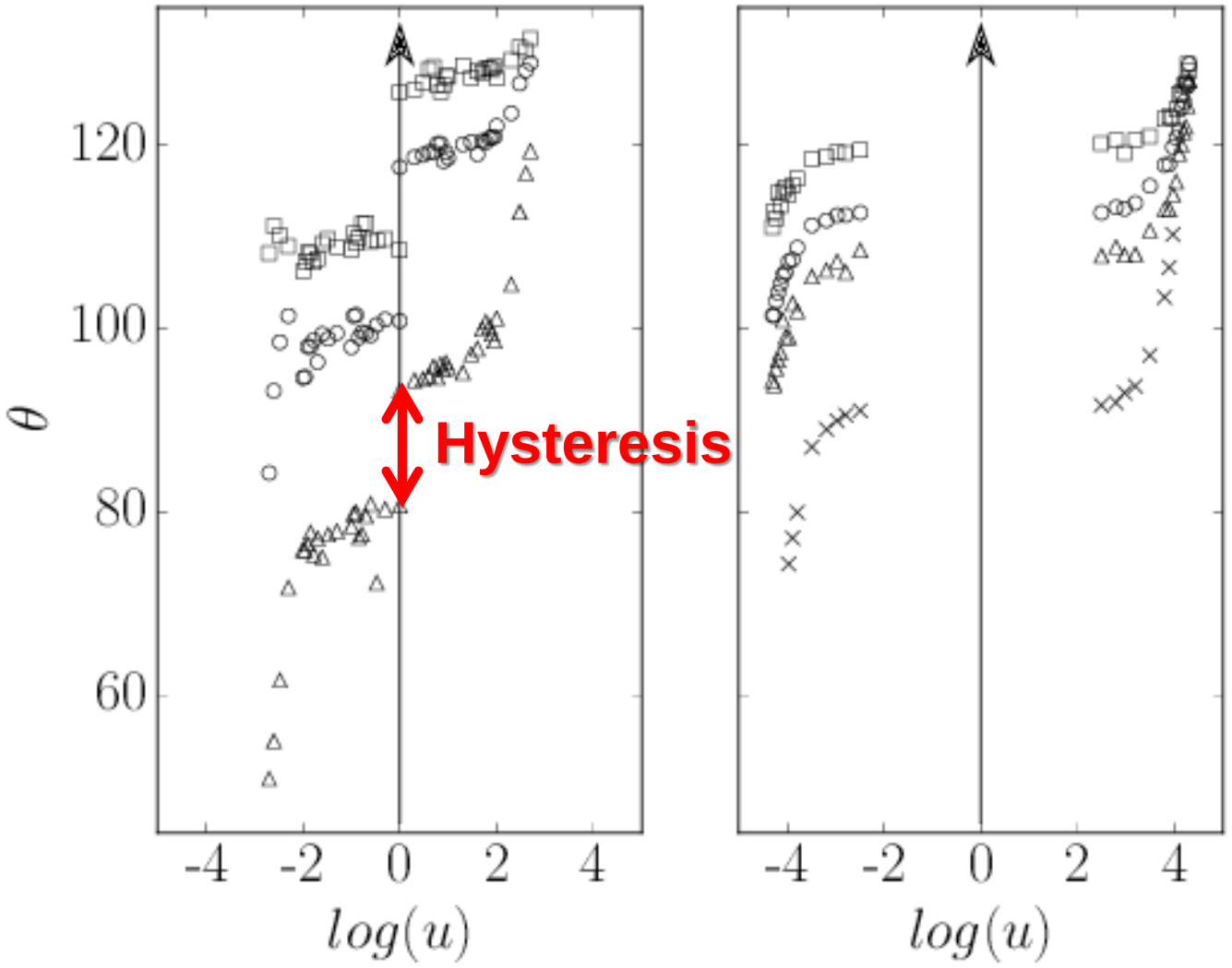

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Modelling Electrowetting

- Disagreement may be explained by
  - Lack of modelling of the rough wall
  - Over-simplified fluid model
  - Electrowetting modelled by simply adjusting interaction, electric field model could be used.
  - System size effects

Pinning may result in hysteresis

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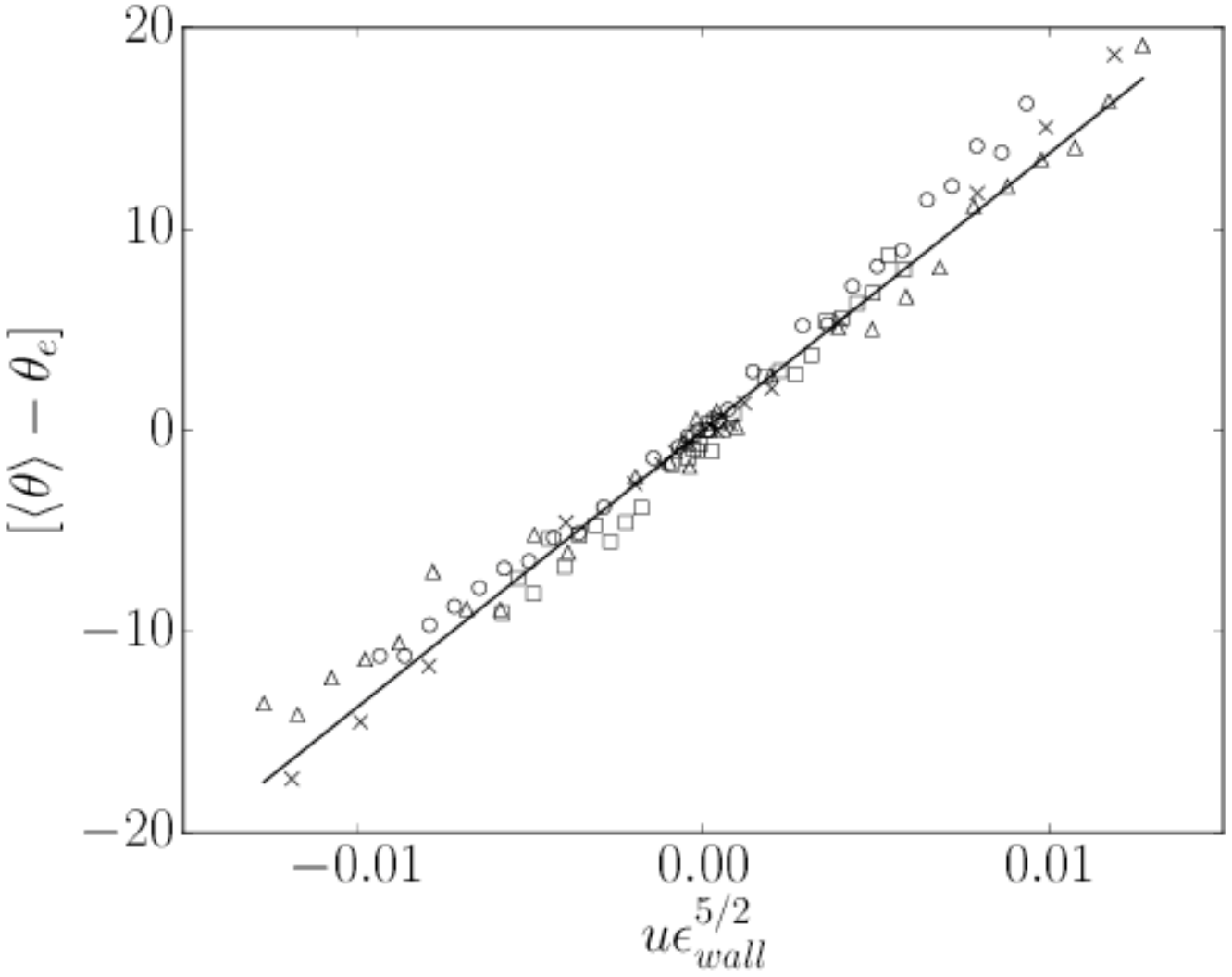
How to Use Wall Sliding with Electrowetting

- Introduce a quantity which combines wall velocity and electrowetting to collapse data onto a single curve
- This can then be used in a continuum model



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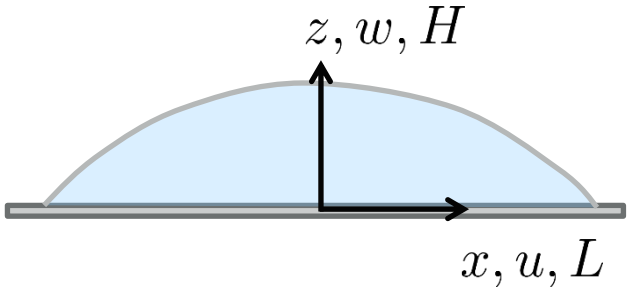
1) G. Karapetsas, R. Craster & O. Matar, JFM, 2011
2) E. Smith, E. Muller, R. Craster, O. Matar Soft Matter 2016

Integrating into a CFD model

- Incompressible Navier Stokes with the thin-film approximation (see 1).

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



- With boundary conditions

$$P = -\left(\frac{H}{L}\right)^2 \frac{\partial^2 h}{\partial x^2}\sigma_l \qquad \frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x} = w \qquad \frac{\partial u}{\partial z} = 0 \qquad z = h$$

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

- *Contact line evolution can be modelled by this reduced equation*

$$\frac{dx_c}{dt} = (\langle\theta\rangle - \theta_a)/E_{\text{wall}}^{5/2}$$

- *Evolution of contact line can include molecular fluctuations (see 2)*

$$\theta^{t+1} = \theta^t - \frac{k\Delta t}{\Gamma}\left[\theta^t - \langle\theta\rangle\right] + \xi\frac{\sqrt{C\Delta t}}{\Gamma}$$

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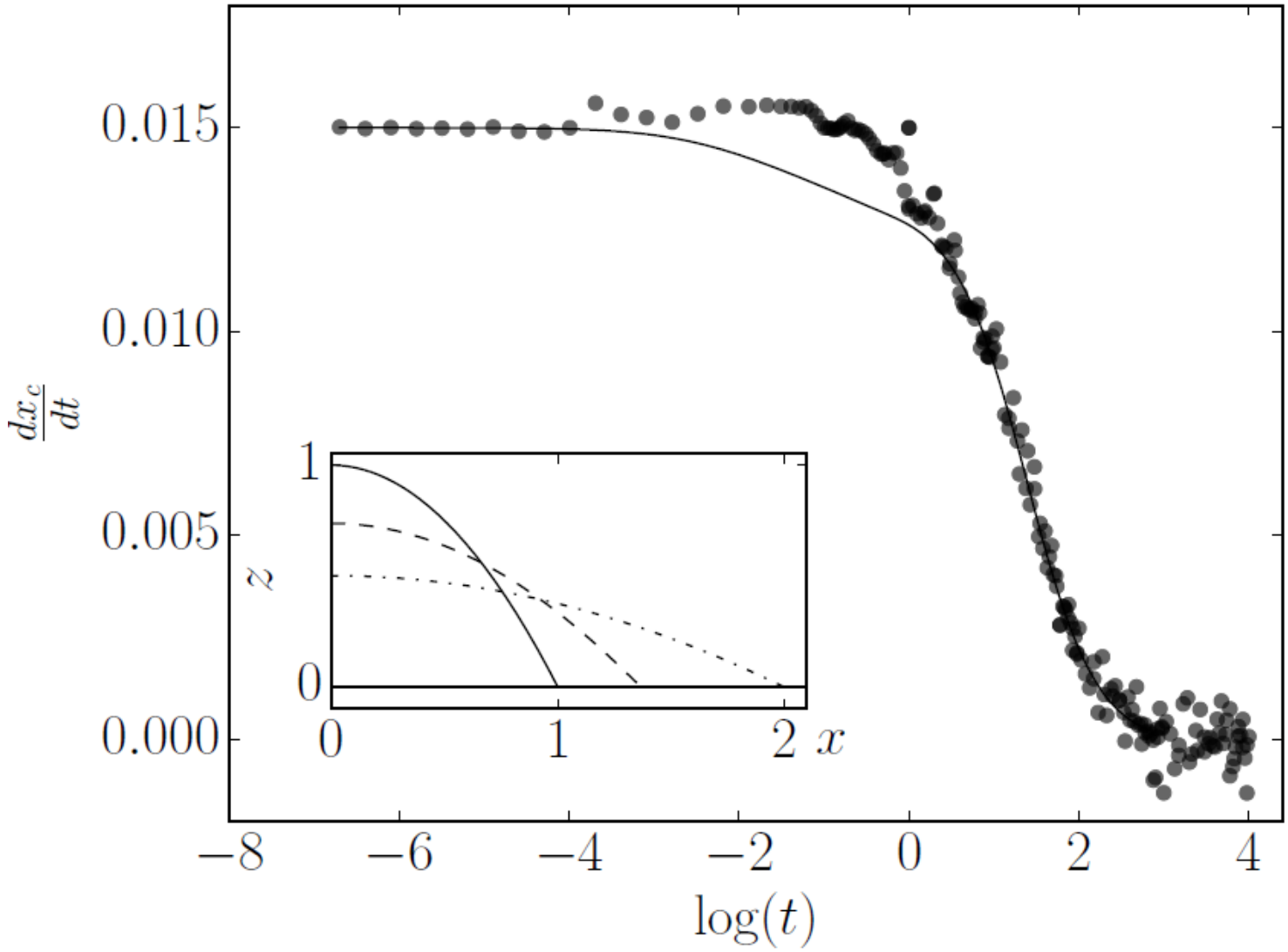
Molecular contact angle in continuum model



Summary

- Molecular Dynamics predicts a-priori viscosity, surface tension and qualitative behaviour in experiments.
- Seems ideal to model the contact line, dewetting and pinning as part of a multi-scale model (and has been used extensively in the literature)
- Choosing fluid-wall interaction is a problem
- Tuned using experiments for static contact angles, then applied to the dynamic case with poor results.
- Course grained behaviour with molecular fluctuations can be parameterised and included in a CFD model