Slip boundary conditions for the moving contact line in molecular dynamics and continuum simulations

Anoosheh Niavarani and Nikolai V. Priezjev

Department of Mechanical Engineering

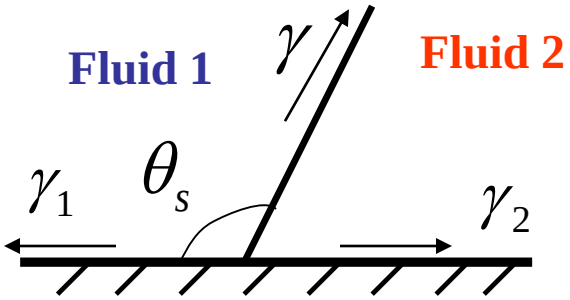
Michigan State University

Movies and preprints @ http://www.egr.msu.edu/~niavaran

- A. Niavarani and N. V. Priezjev, “Modeling the combined effect of surface roughness and shear rate on slip flow of simple fluids”, *Physical Review E* **81**, 011606 (2010).
- A. Niavarani and N. V. Priezjev, “The effective slip length and vortex formation in laminar flow over a rough surface”, *Physics of Fluids* **21**, 052105 (2009).

Introduction

Question: How to model the moving contact line problem in a shear flow using molecular dynamics and continuum methods?



Equilibrium:

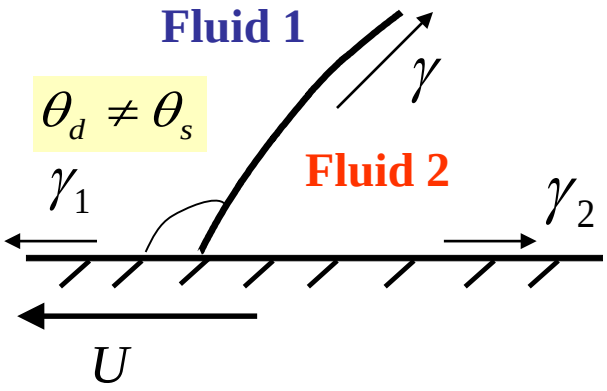
θ_s : Contact angle

γ : Surface tension

Young's equation

$$\gamma \cos\theta_s = \gamma_2 - \gamma_1$$

Moving contact line:



- No-slip boundary condition leads to divergence of energy dissipation (unphysical)

$$\tau_{r\theta} = \frac{2\mu}{r}(c\cos\theta - d\sin\theta)$$

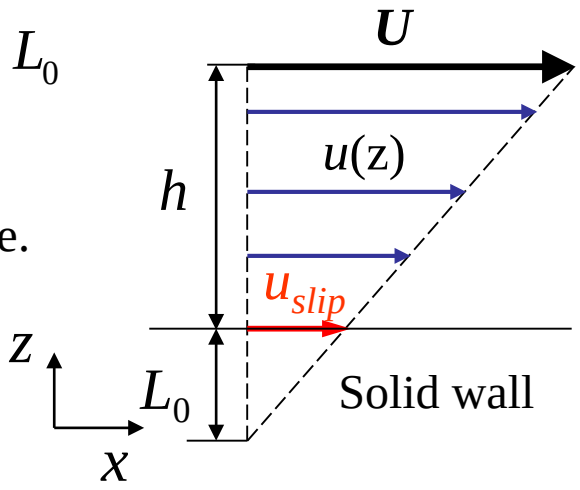
Huh and Scriven, J. Colloid Interface Sci. **35**, 85 (1971)

- Contact line singularity is regularized by introduction of the slip region near the contact line.

What is the boundary condition near the moving contact line?

- The Navier model describes the slip boundary condition at the solid/liquid interface:

Linear relation outside contact line: $\tau = \beta u_{slip}, \ \beta = \mu / L_0$



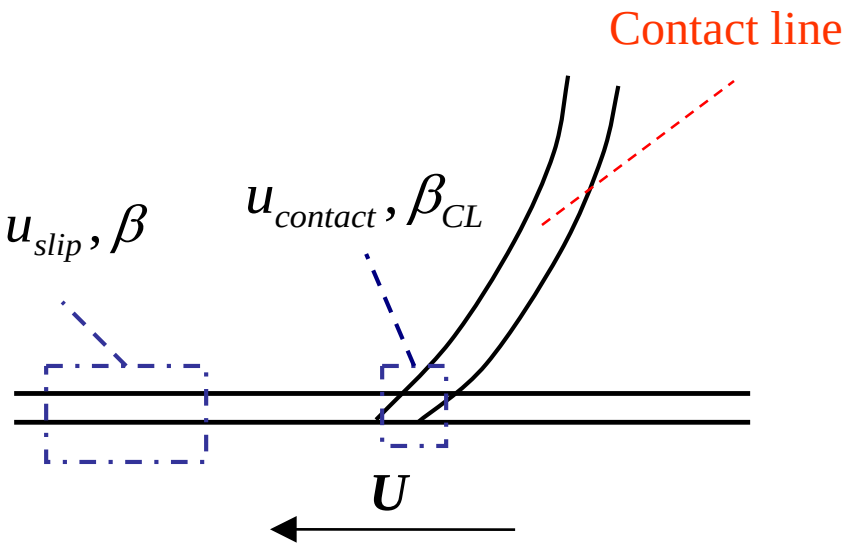
- The friction coefficients β can be estimated from the molecular dynamics simulation away from the contact line.

- At the contact line $\beta_{CL} u_{contact} = \gamma(\cos\theta_s - \cos\theta)$

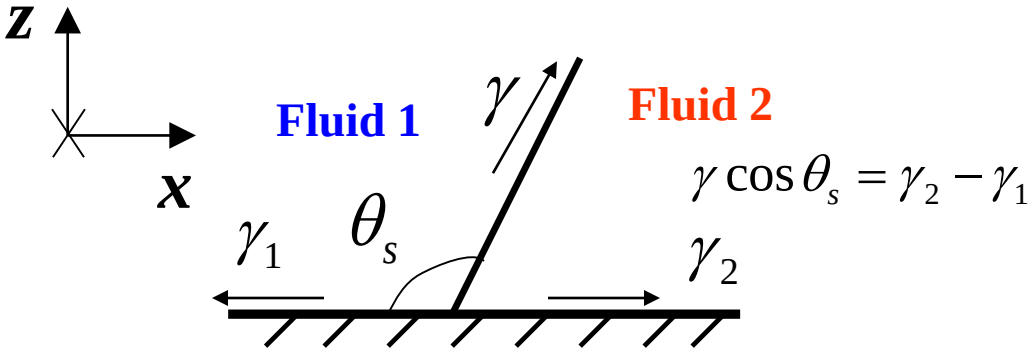
Qian, Wang, and Sheng, Phys. Rev. E **68**, 016306 (2003)

Ren and E, Physics of Fluids **19**, 022101 (2007)

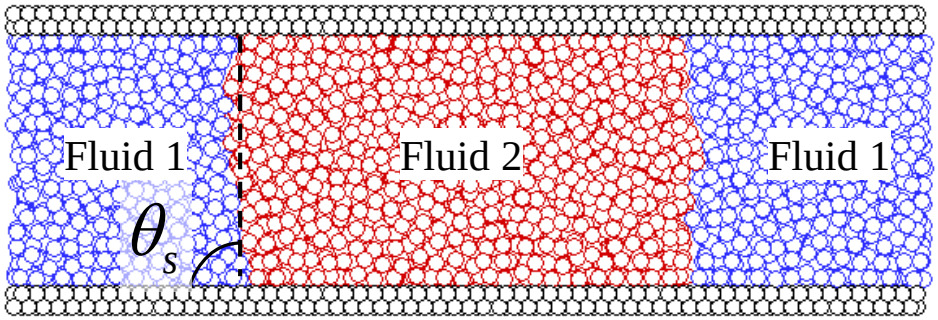
- Our goal is to use molecular dynamics simulations to estimate the stress tensors, friction coefficient, and flow profiles and determine the correct boundary condition for continuum modeling.



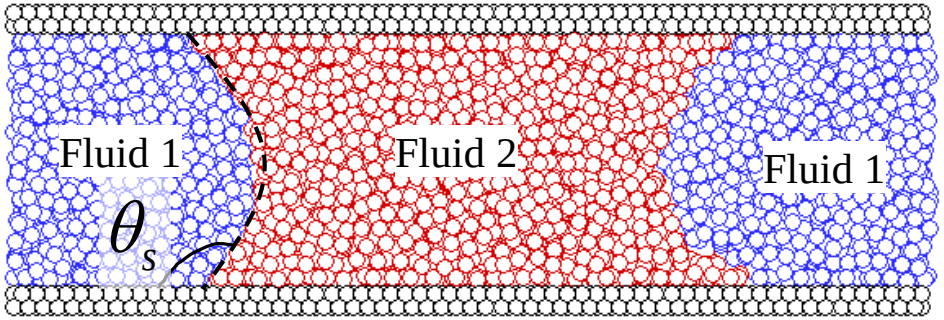
Details of the molecular dynamics simulations



$\varepsilon_{w2} = \varepsilon_{w1}$ $\gamma_1 = \gamma_2$ $\theta_s = 90$



$\varepsilon_{w2} = 2\varepsilon_{w1}$ $\gamma_1 > \gamma_2$ $\theta_s \approx 130$



Equation of motion:

$$m\ddot{y}_i + m\Gamma\dot{y}_i = -\sum_{i\neq j}\frac{\partial V_{ij}}{\partial y_i} + f_i$$

f_i Gaussian random force

$$\langle f_i(t)\, f_i(t')\rangle = 2mk_B T\Gamma\delta(t-t')$$

$\Gamma = \tau^{-1}$ Friction coefficient

Langevin Thermostat $T=1.1\varepsilon/k_B$

Fluid density $\rho = 0.81\sigma^{-3}$

Lennard-Jones potential:

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{r}{\sigma}\right)^{12} - \delta\left(\frac{r}{\sigma}\right)^{6}\right]$$

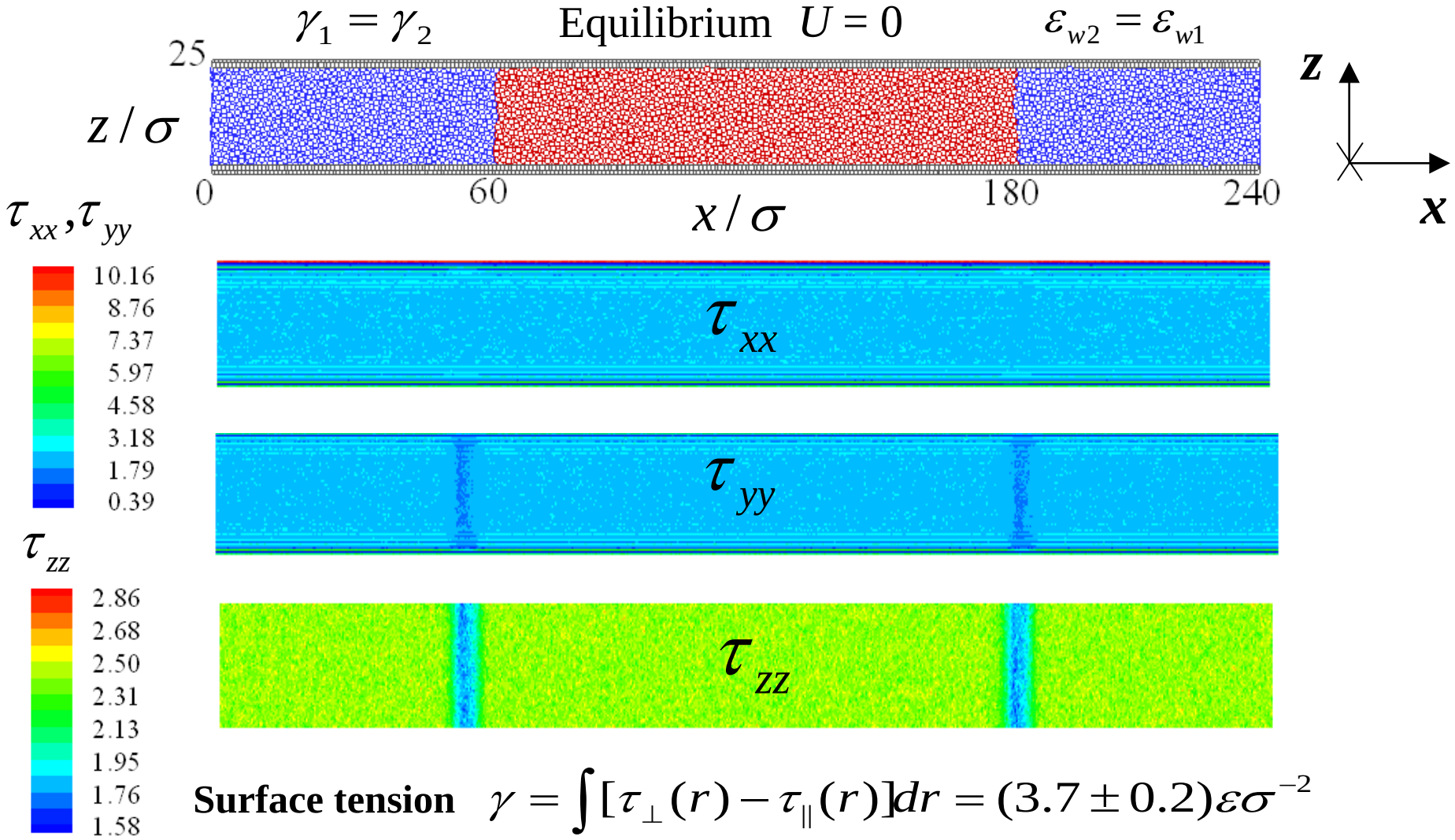
σ LJ molecular length scale

ε LJ energy scale

$\tau = (m\sigma^2/\varepsilon)^{1/2}$ LJ time scale

$\delta = -1$ Immiscible fluids

Extracting normal stresses from molecular dynamics

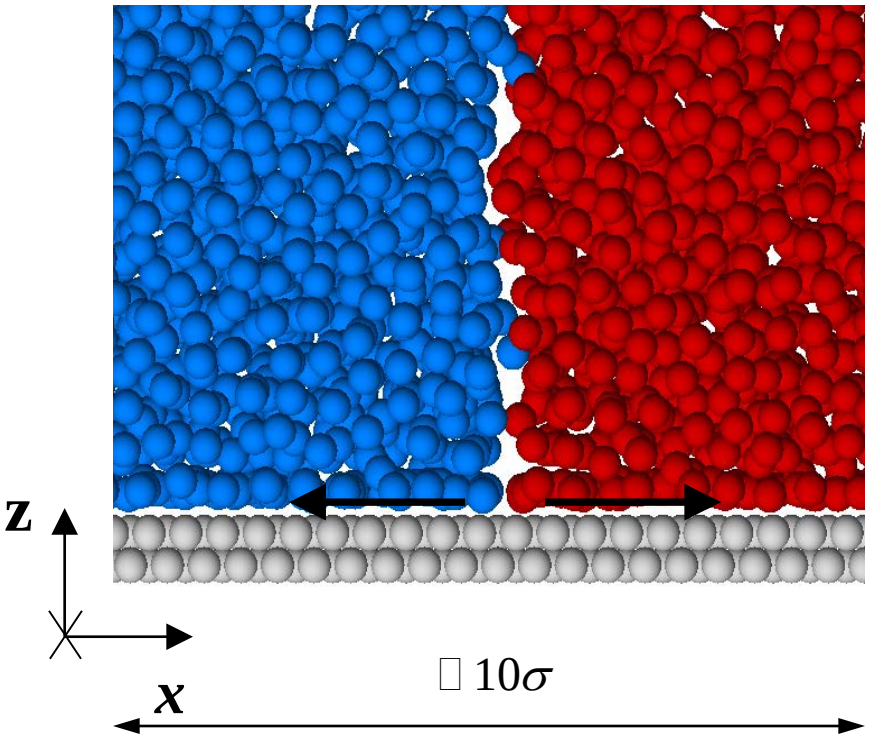


Surface tension $\gamma = \int [\tau_{\perp}(r) - \tau_{\parallel}(r)] dr = (3.7 \pm 0.2)\varepsilon\sigma^{-2}$

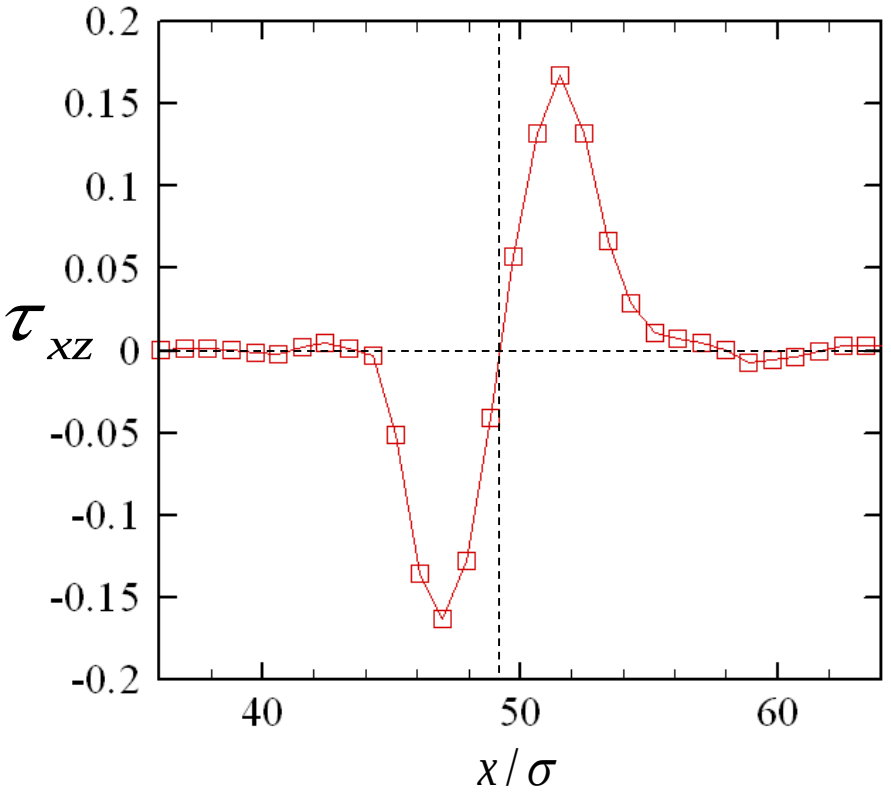
- To calculate the surface tension, the normal stresses are estimated accurately using a modified Irving-Kirkwood relation.
- The surface tension from molecular dynamics simulations is then used in continuum simulations.

Distribution of the shear stress along the lower wall in equilibrium (U=0)

Snapshot of the atoms near the contact line

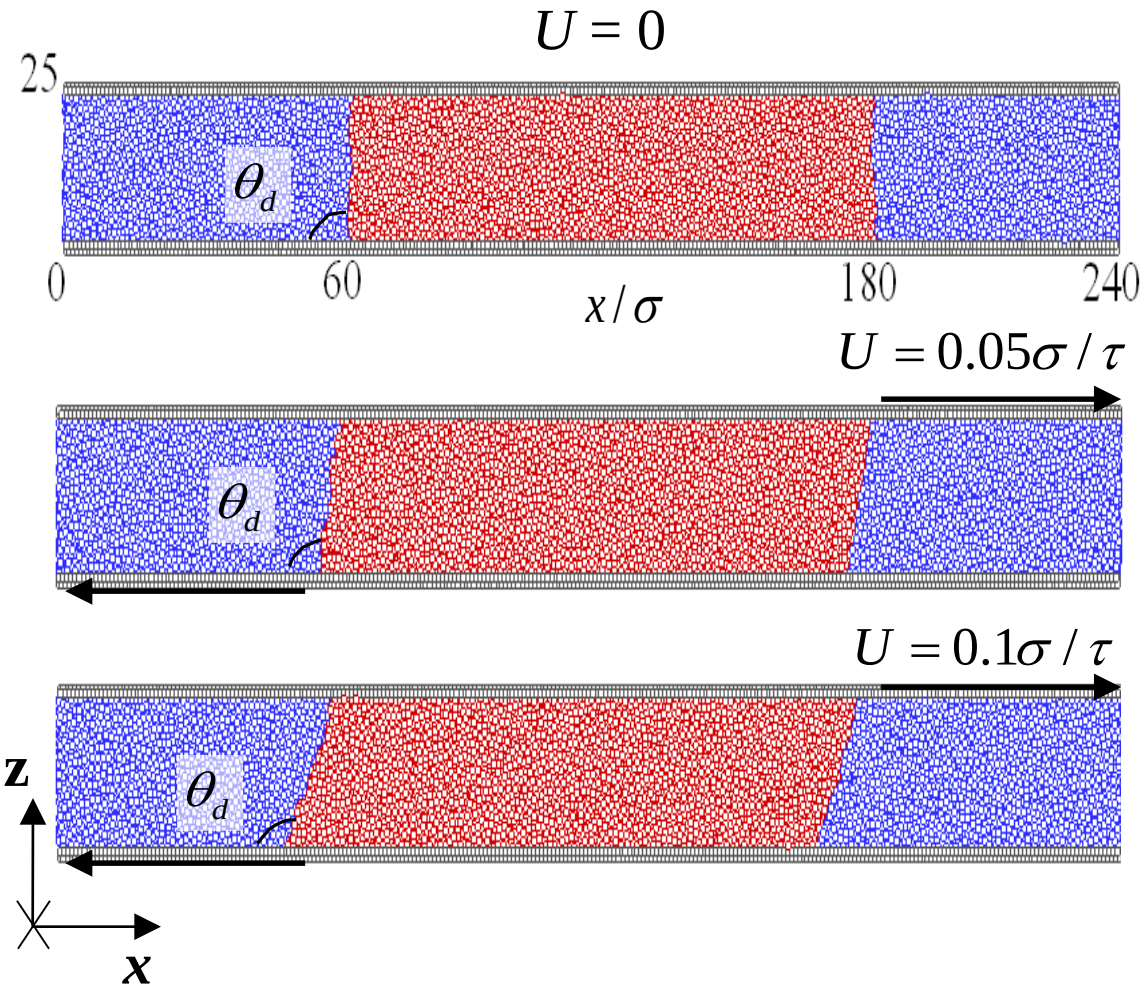


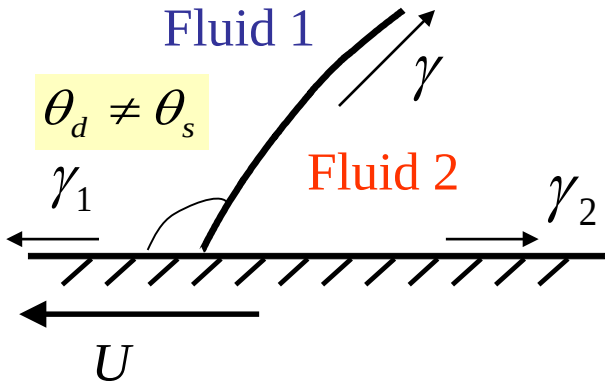
Tangential stress along the lower wall



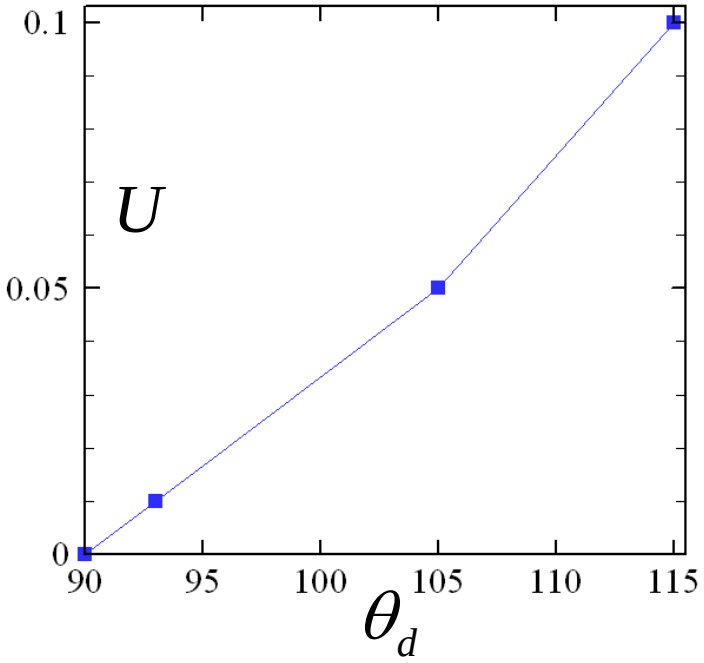
- The tangential stresses along the lower wall is calculated from *LJ* forces per unit area between wall atoms and fluids molecules.
- The negative and positive stresses, within 5σ from the contact line, are due to a reduced density in the fluid/fluid interfacial region.

Dynamic contact angle and shape of interface in steady-state shear flow



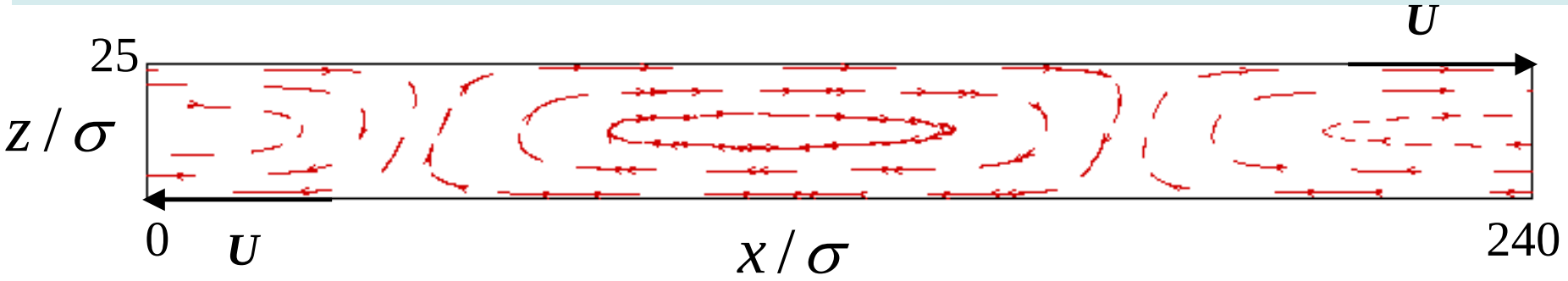


Dynamic contact angle vs wall speed

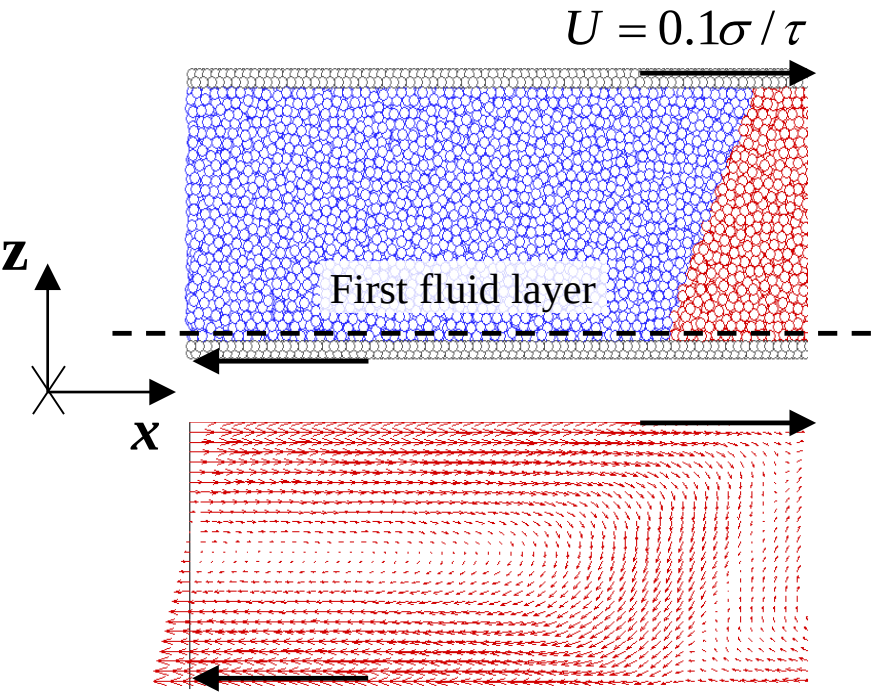


- The dynamic contact angle is $\theta_d > 90$.
- As the wall speed (Capillary number) increases, the contact angle becomes larger.

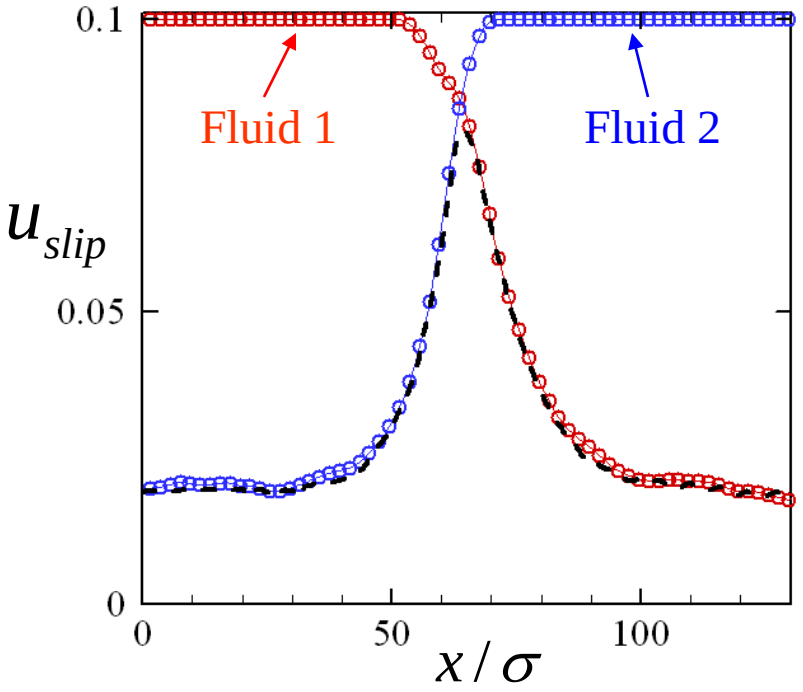
Extracting macroscopic velocities from molecular dynamics



- The flow velocities are computed from the time averaging of instantaneous molecule speeds in small spatial bins over a long period of time.

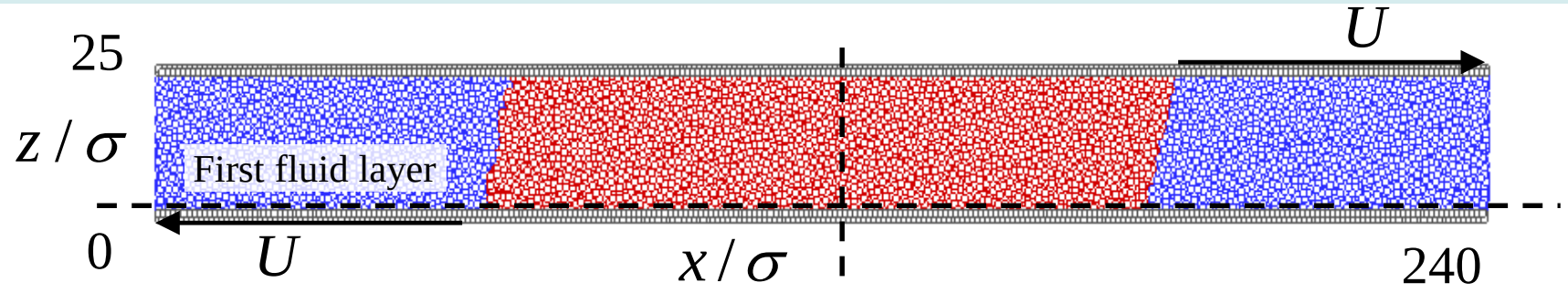


Velocity profiles in the first fluid layer

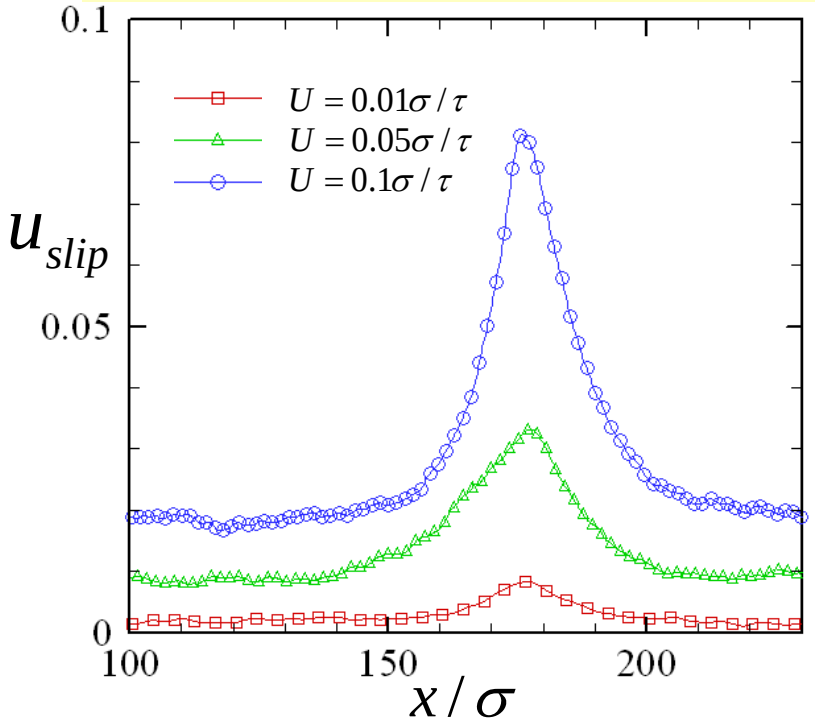


- In each fluid phase the slip velocity of the first fluid layer increases near the contact line (symbols), but the overall slip velocity is smaller than wall speed at the contact line (dashed line).

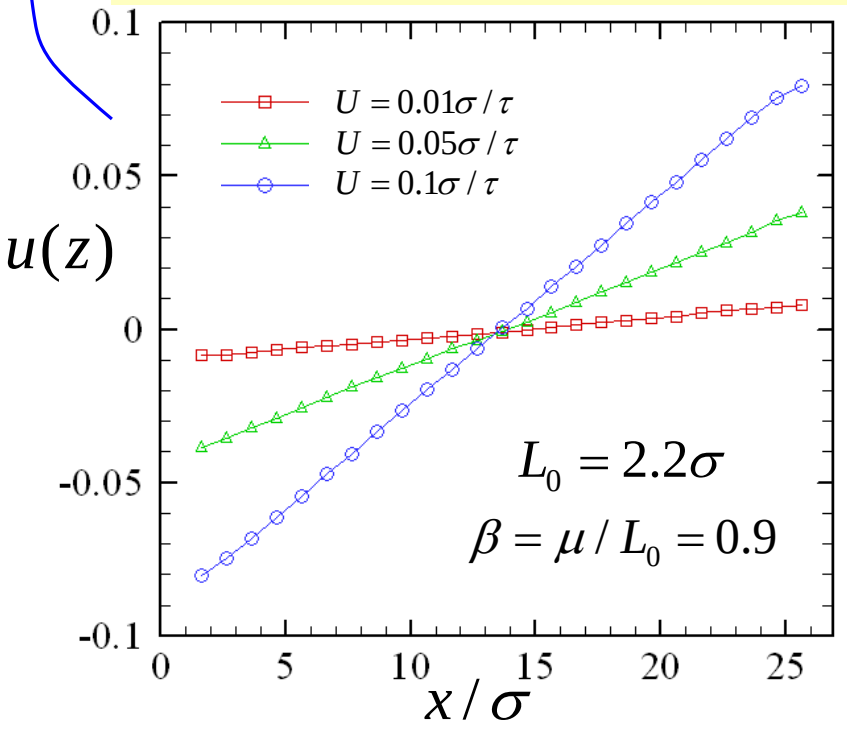
Slip velocity and the friction coefficient from molecular dynamics



Velocity profile in the first fluid layer



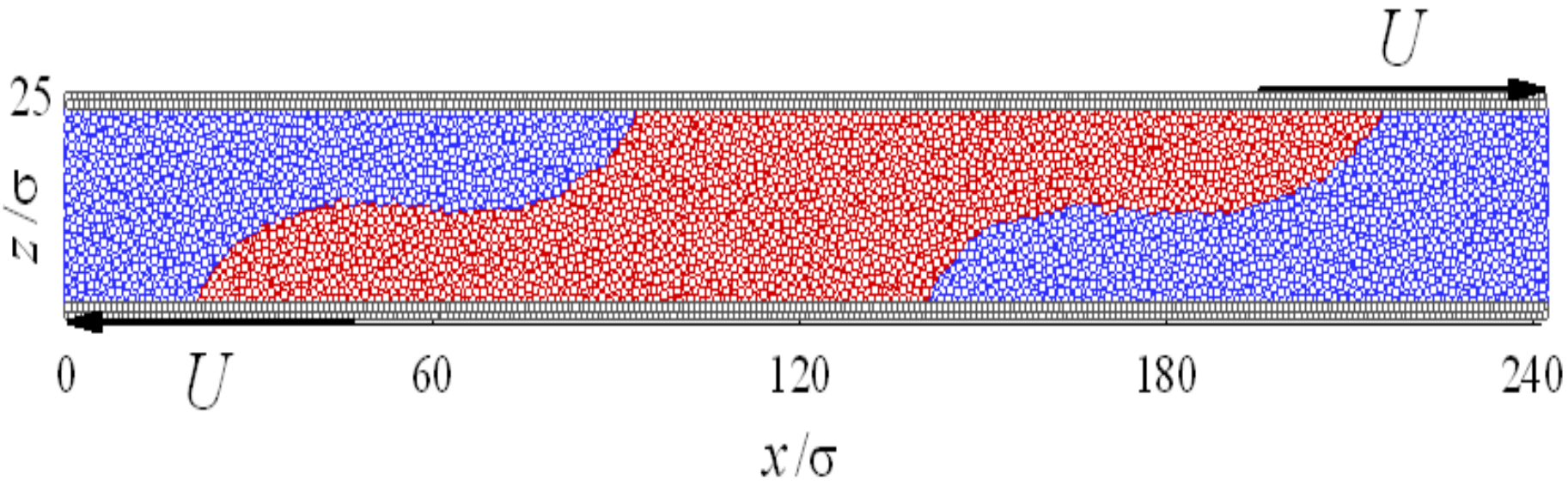
Velocity profile along the z direction



- The slip velocity near the contact line becomes larger with increasing the wall speed.
- The velocity profiles are linear and the slip length is calculated from a linear fit to the profiles.

Motion of the contact line at high shear rates

- At higher capillary numbers (higher ***U***) the contact line undergoes an unsteady motion.
- High stresses at the contact line lead to a pronounced curvature of the fluid-fluid interface and a breakup of a continuous fluid phase.



$U = 0.2\sigma / \tau$

http://www.egr.msu.edu/~niavaran

$\varepsilon_{w2} = \varepsilon_{w1}$

Movie length ~ 3000τ

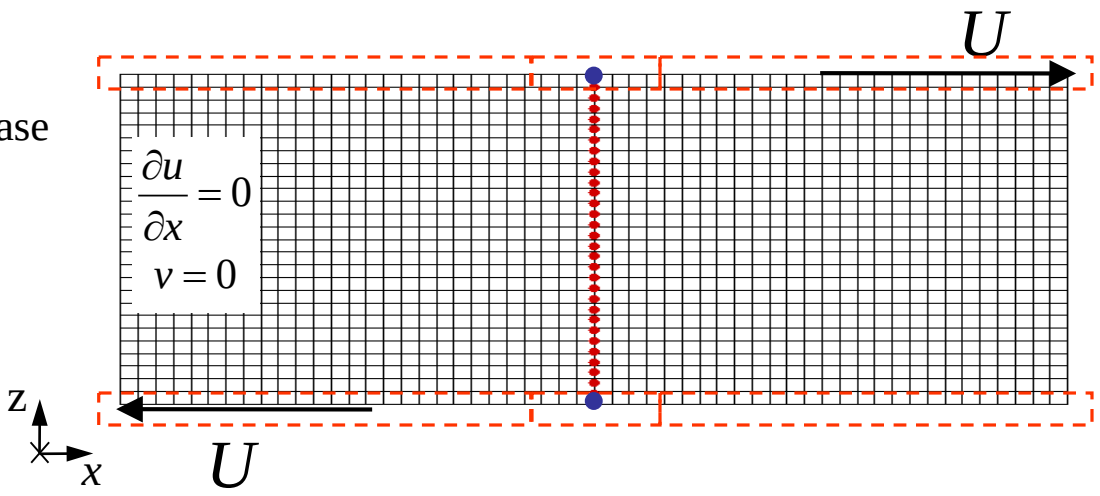
Details of the continuum modeling of the moving contact line

Boundary conditions

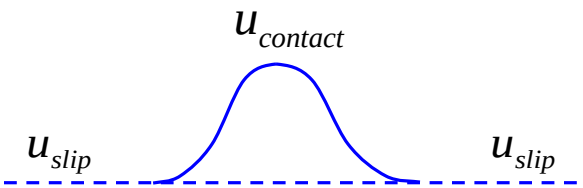
- Away from the contact point (single phase fluid): Navier Slip B.C.: $\tau_{xz} = \beta u_{slip}$
- At the contact point (the marker point):

$$\beta_{CL} u_{contact} = \gamma(\cos\theta_s - \cos\theta)$$

$\gamma, \beta, \beta_{CL}$ extracted from molecular dynamics simulations



- Near the contact point: a distribution function interpolates the velocities between the contact point and single phase fluid



$$\delta(\vec{x} - \vec{x}_k) = \prod_{m=1}^{\dim} \frac{1}{2d}\left(1 + \cos\frac{\pi(\vec{x}_m - (\vec{x}_m)_k)}{d}\right) \quad if\ |\vec{x} - \vec{x}_k| \le d$$

Navier-Stokes equation applied on the fixed grids

$$\nabla \cdot u = 0 \qquad \rho\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u\right) = -\nabla p + \mu \nabla^2 u + f$$

Interface location predicted by marker points

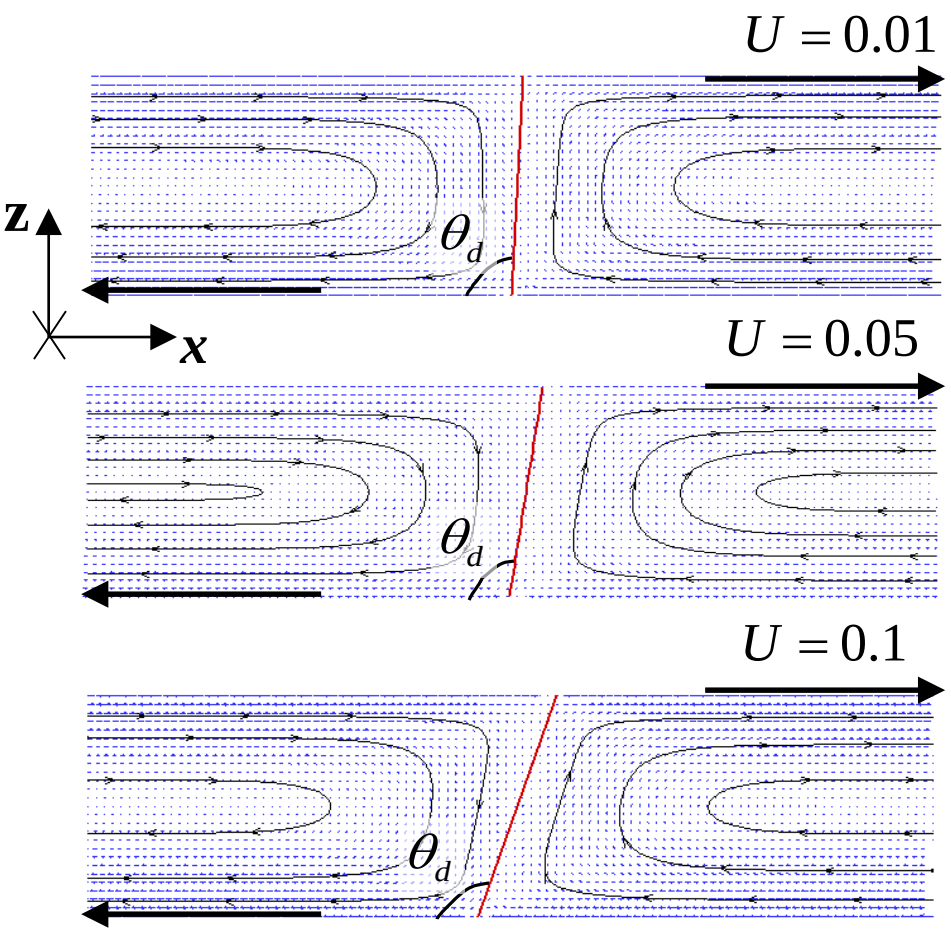
$$\vec{u}_k = \sum_{ij} \vec{u}_{ij} \delta(\vec{x} - \vec{x}_k)$$

$$\vec{x}_k^{\,t+1} = \vec{x}_k^{\,t} + \Delta t(\vec{u}_k^{\,t})$$

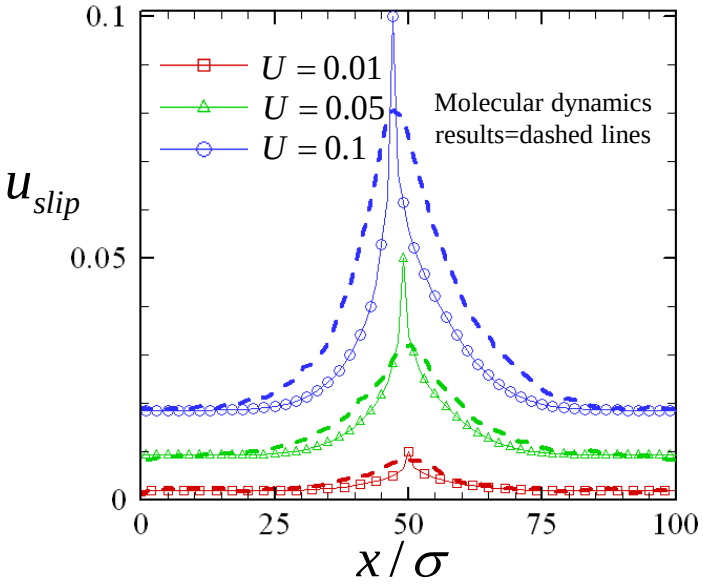
$$f = -\sum_k \gamma \kappa \vec{n}_k \delta(\vec{x} - \vec{x}_k) \Delta S_k$$

The system size and the flow properties are the same as in the molecular dynamics method

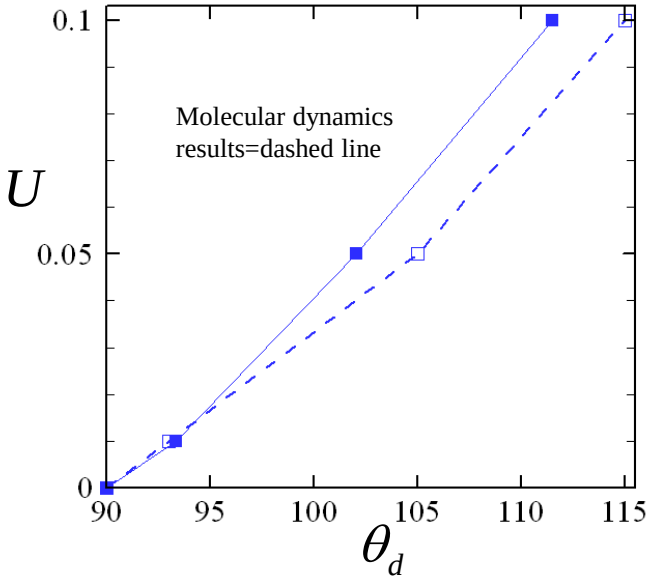
Dynamic contact angle and flow profiles near the moving contact line



Velocity profiles in the first fluid layer



Dynamic contact angle vs wall speed



- The slip velocity and the contact angle increase at higher wall speeds.
- The continuum results agree well with molecular dynamics simulations.

Important conclusions

- The slip boundary conditions near the moving contact line extracted from MD simulations were used in the continuum solution of the Navier-Stokes equation in the same geometry to reproduce velocity profiles and the shape of the fluid-fluid interface.

- The MD results show that both dynamic contact angle and slip velocity near the contact line increase with increasing the capillary number (Ca).

- At higher capillary numbers (higher *U*) the contact line undergoes an unsteady motion. High stresses at the contact line lead to a pronounced curvature of the fluid-fluid interface and a breakup of a continuous fluid phase.