Modeling the combined effect of surface roughness and shear rate on slip flow of simple fluids

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Introduction

- The no-slip boundary condition works well for macro- flows, however, in micro and nanoflows molecular dynamics simulations and experiments report the existence of a boundary slip.

- MD simulations have shown that at the interface between simple[1] and polymeric[2] liquids and flat walls the slip length is a function of shear rate.

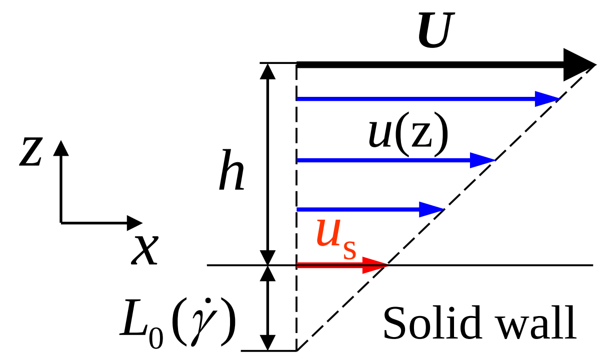
[1] P. A. Thompson and S. M. Troian, Nature (1997)
[2] N. V. Priezjev and S. M. Troian, Phys. Rev. Lett. (2004)

- Surface roughness reduces effective slip length.

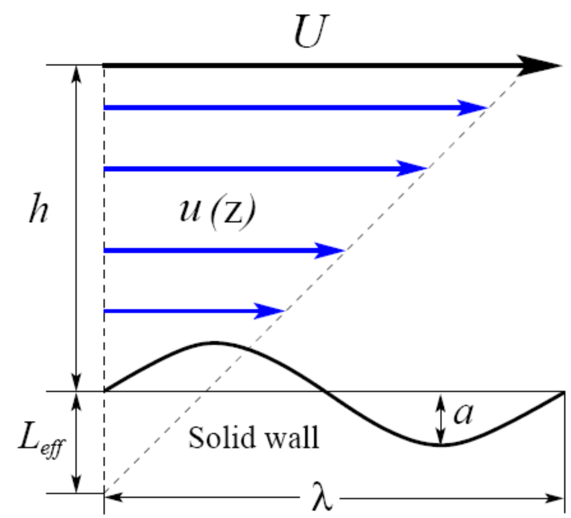
- For flow of simple[1] and polymeric[2] liquids past periodically corrugated surface there is an excellent agreement between MD and continuum results for the effective slip length (if $\lambda \geq 30\sigma$).

  Constant local slip length from MD was used as a boundary condition for continuum simulation.

[1] N. V. Priezjev and S. M. Troian, J. Fluid Mech. (2006)
[2] A. Niavarani and N. V. Priezjev, J. Chem. Phys. (2008)

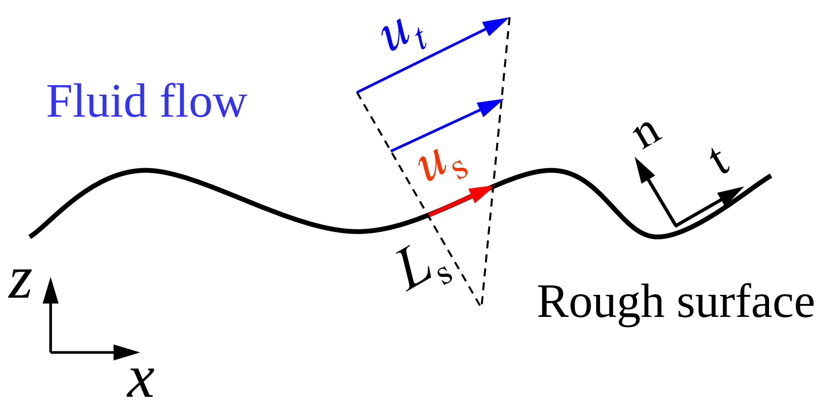


$$u_s = L_0(\dot{\gamma})\dot{\gamma} \qquad \dot{\gamma} = \frac{du(z)}{dz}$$



Introduction

Question: How to model the combined effect of surface roughness and shear rate?



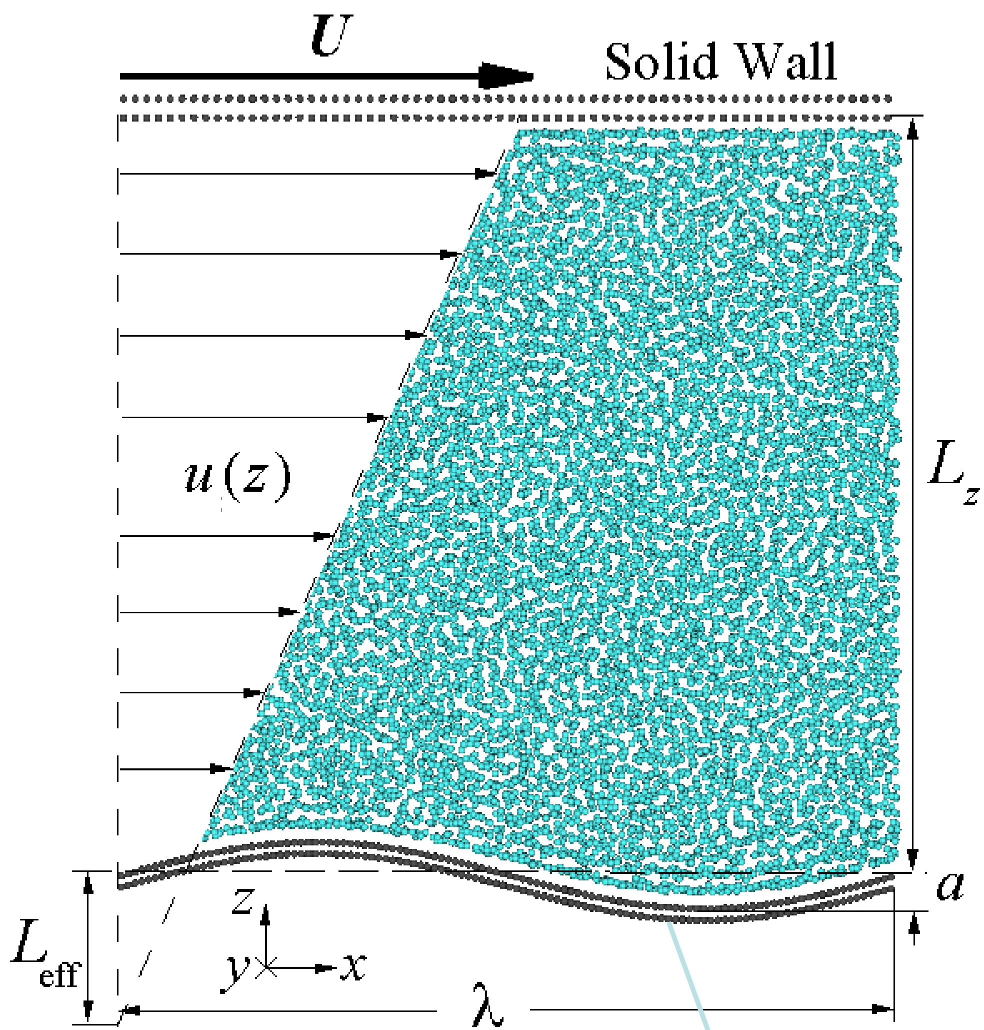
$$u_s(x) = L_s(\dot{\gamma}) \frac{\partial u_t(n)}{\partial n}$$

Solution 1: Perform full MD simulation of the flow past rough surface (very expensive computationally!!!).

Solution 2: From MD simulation extract *only* slip length as a function of shear rate $L_s(\dot{\gamma})$ for flat walls. And then, use $L_s(\dot{\gamma})$ as a local boundary condition for the flow over rough surface in the Navier-Stokes equation. (Is it possible?)

In this study we compare Solution 1 and Solution 2

Details of molecular dynamics (MD) simulations



$L_z = \lambda \approx 42\sigma$

$ka = \frac{2\pi a}{\lambda} = 0.27$

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:

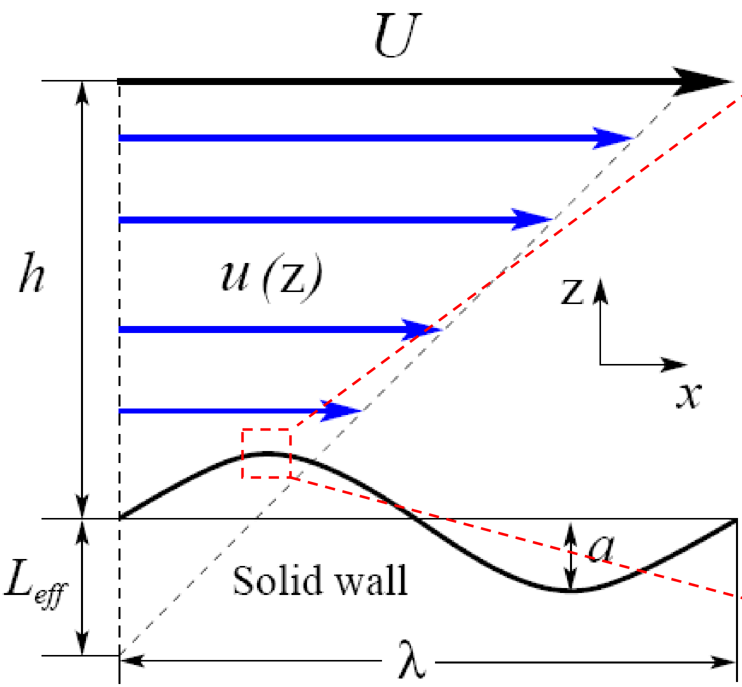
$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6}\right]$$

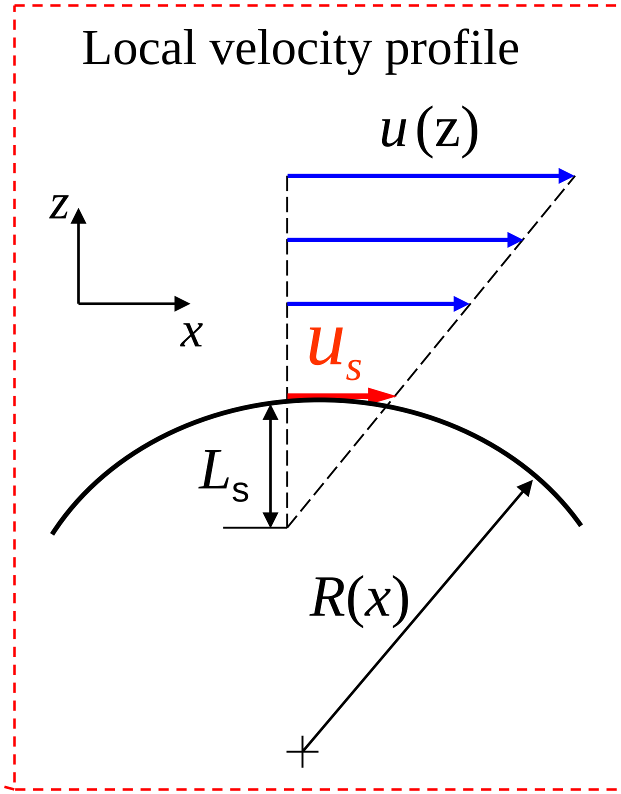
σ LJ molecular length scale

ε LJ energy scale

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

The effective slip length L_{eff} and intrinsic slip length L_0





$$z(x) = a\sin(2\pi x/\lambda)$$

$$u_s(x) = L_s \frac{\partial u(z)}{\partial n} \qquad \frac{1}{L_s} = \frac{1}{L_0} - \frac{1}{R(x)}$$

L_{eff} is the effective slip length, which characterizes the flow over macroscopically rough surface

L_s : local slip length

L_0 : intrinsic slip length extracted from MD simulation

$R(x)$: local radius of curvature

Details of continuum simulations (Finite Element Method)

Equations of motion (penalty formulation):

$$\nabla \cdot \mathbf{u} = -\frac{p}{\Lambda}$$

$$\rho\,(\mathbf{u} \cdot \nabla u) = \Lambda \nabla (\nabla \cdot \mathbf{u}) + \mu \nabla^2 u$$

$$\rho\,(\mathbf{u} \cdot \nabla v) = \Lambda \nabla (\nabla \cdot \mathbf{u}) + \mu \nabla^2 v$$

Boundary condition:

$$u_s = L_0(\dot{\gamma})[(\vec{n} \cdot \nabla) u_s + u_s / R(x)]$$

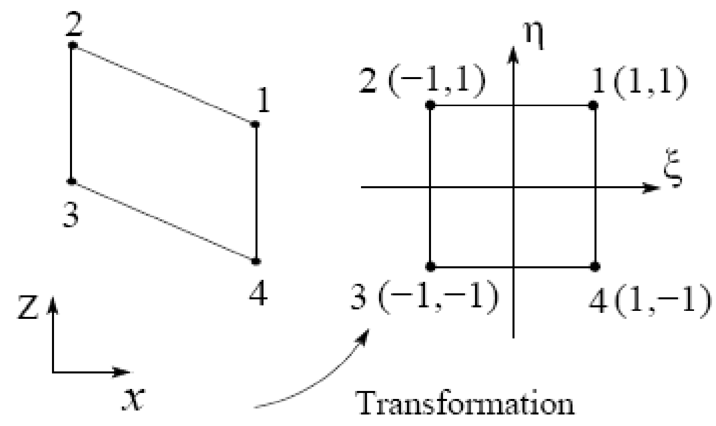
$R(x)$: local radius of curvature

(+) concave, (–) convex

L_0: intrinsic slip length as a function of

Shear rate: $\dot{\gamma} = (\vec{n}.\nabla) u_s + u_s / R(x)$

Bilinear quadrilateral elements



shape function $N_i = \dfrac{(1+\xi_i \xi)(1+\eta_i \eta)}{4}$

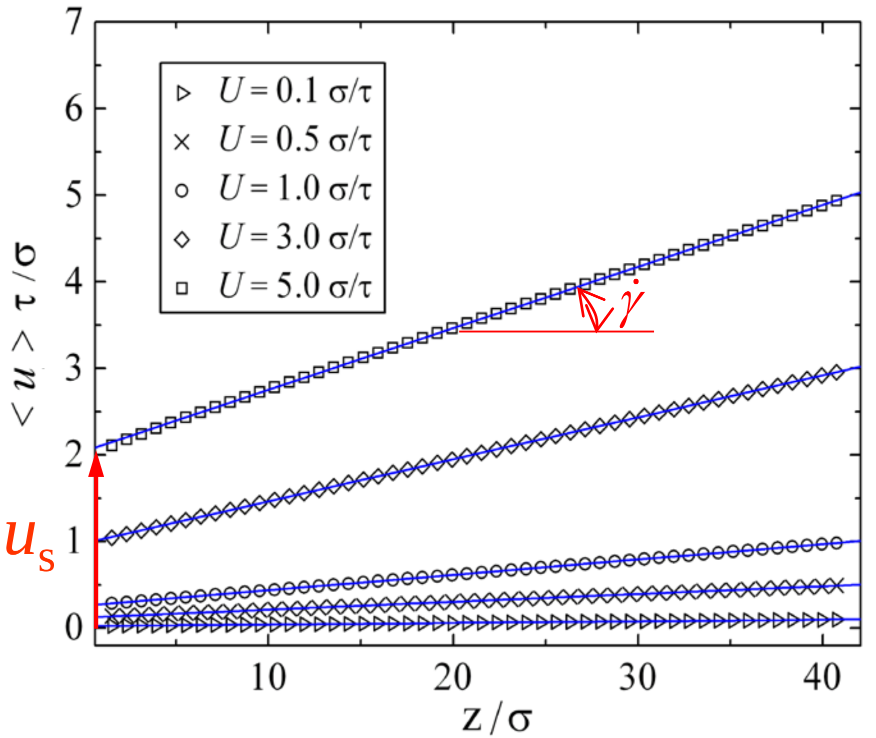
Galerkin formulation:

$$\Big[\int_\Omega \rho N_i \Big(\bar{u}_i v_j \frac{\partial N_j}{\partial x} + \bar{v}_i v_j \frac{\partial N_j}{\partial z}\Big)\Big] + \Big[\int_\Omega \Lambda \frac{\partial N_i}{\partial z}\Big(\frac{\partial N_j}{\partial x} u_j + \frac{\partial N_j}{\partial z} v_j\Big) d\Omega\Big] +$$

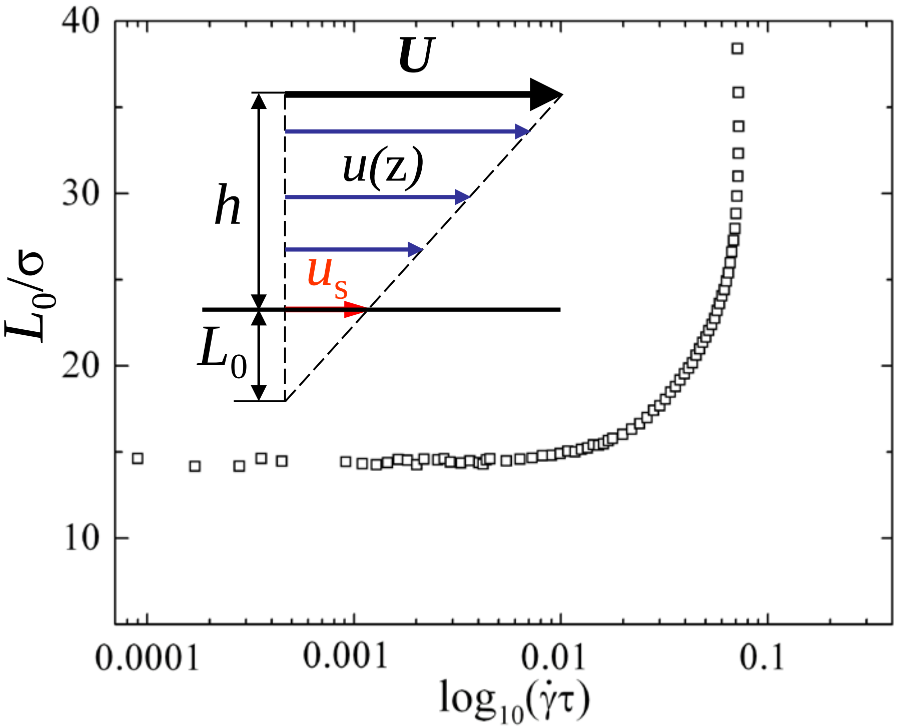
$$\Big[\int_\Omega \mu \Big(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\Big) v_j d\Omega\Big] = RHS_z$$

MD simulations: Velocity profiles and slip length for flat walls

Velocity profiles



Slip length vs. shear rate

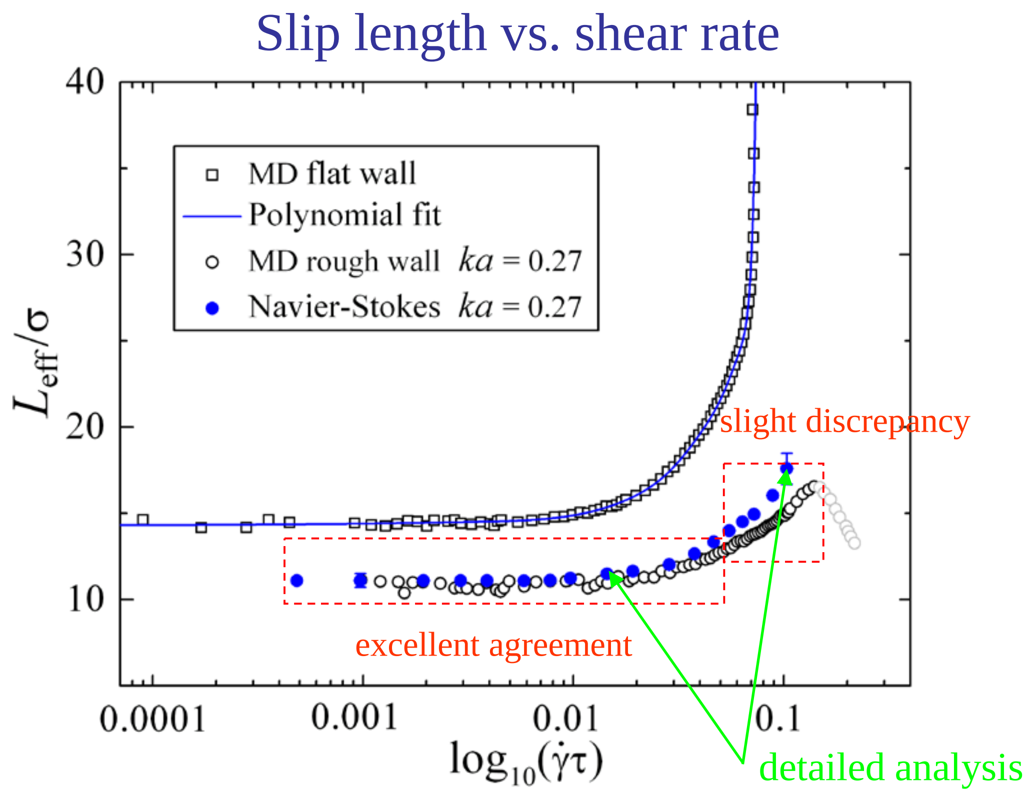


- Velocity profiles are linear across the channel
- Shear rate is extracted from a linear fit to velocity profiles
- No-slip at the upper wall (commensurable wall/fluid densities)

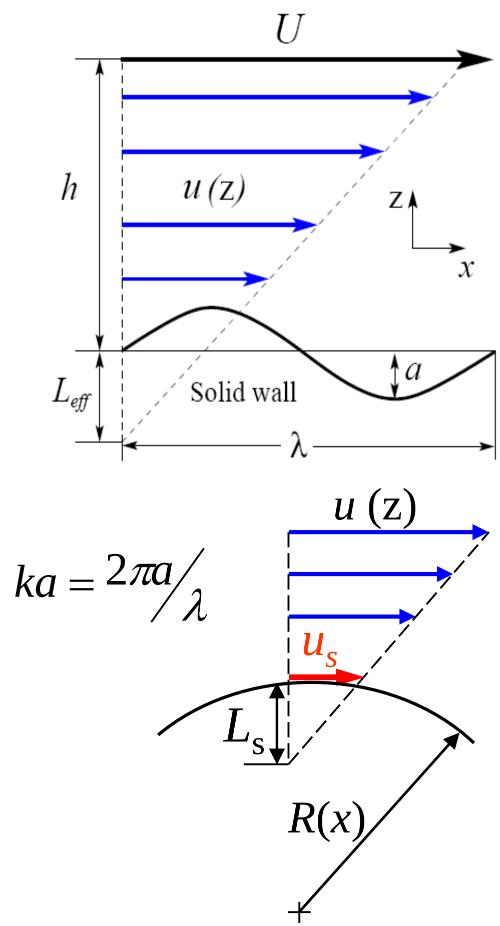
- Slip length is a highly nonlinear function of shear rate

$$u_s = L_0(\dot{\gamma})\dot{\gamma} \qquad \dot{\gamma} = \frac{du(z)}{dz}$$

Effective slip length as a function of shear rate for a rough surface



- Constant slip length at low shear rate, highly nonlinear function of shear rate at high shear rates
- Blue line is a polynomial fit used in Navier-Stokes solution
- Surface roughness reduces the effective slip length and its shear rate dependence
- Excellent agreement between MD and NS at low shear rates but continuum results slightly overestimate MD at high shear rates

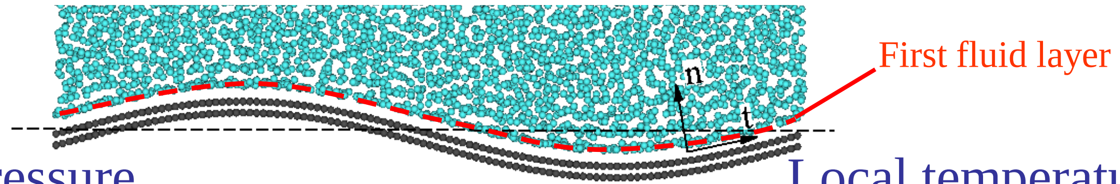


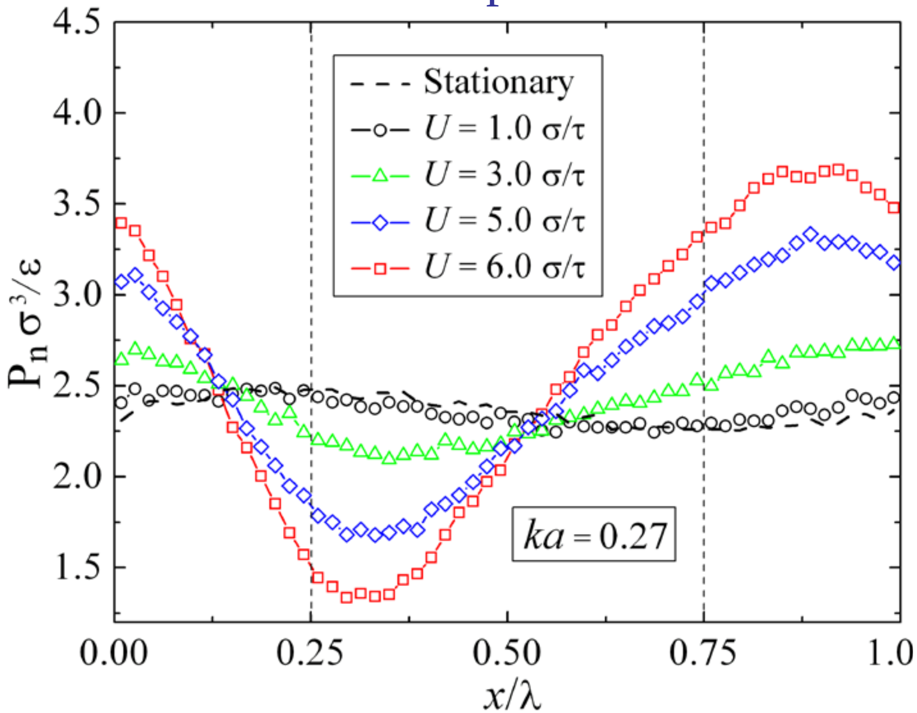
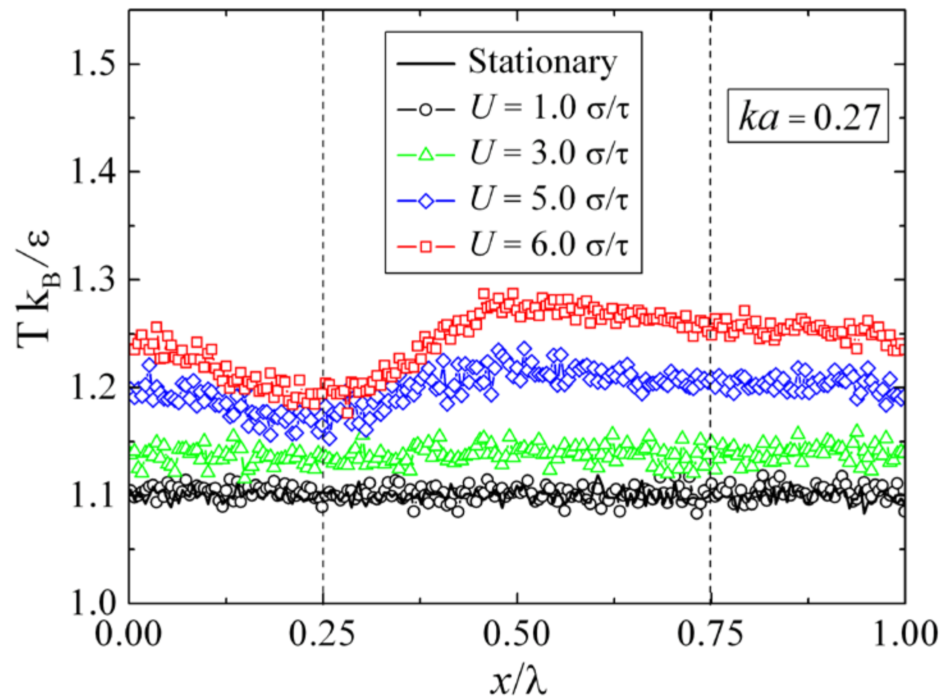
$$u_s = L_0(\dot{\gamma})\left[\frac{\partial u_s}{\partial n} + \frac{u_s}{R(x)}\right]$$

$$\dot{\gamma} = \left[\frac{\partial u_s}{\partial n} + \frac{u_s}{R(x)}\right]$$

$L_0(\dot{\gamma})$: polynomial fit

Detailed analysis of the flow near the curved boundary



Local pressure	Local temperature
	

- Pressure: average normal force on wall atoms from fluids monomers within the cutoff radius
- For $U \leq 1.0\sigma/\tau$ pressure is similar to equilibrium case and is mostly affected by the wall shape
- For $U > 1.0\sigma/\tau$ pressure increase when $x/\lambda < 0.12$ and $x/\lambda > 0.54$

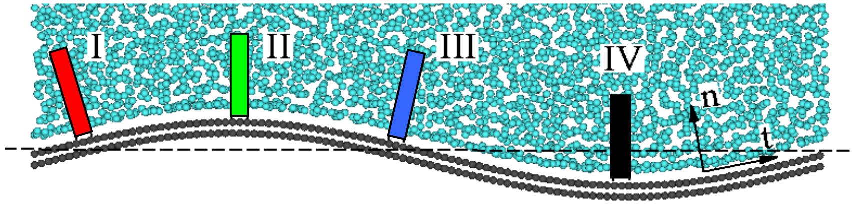
$$x/\lambda = 0.5 \qquad P = P_{flat} = 2.36\varepsilon/\sigma^3$$

- Average temperature is calculated in the first fluid layer
- At small upper wall speeds, temperature is equal to equilibrium temperature
- With increasing upper wall speed the temperature also increases and eventually becomes non-uniformly distributed

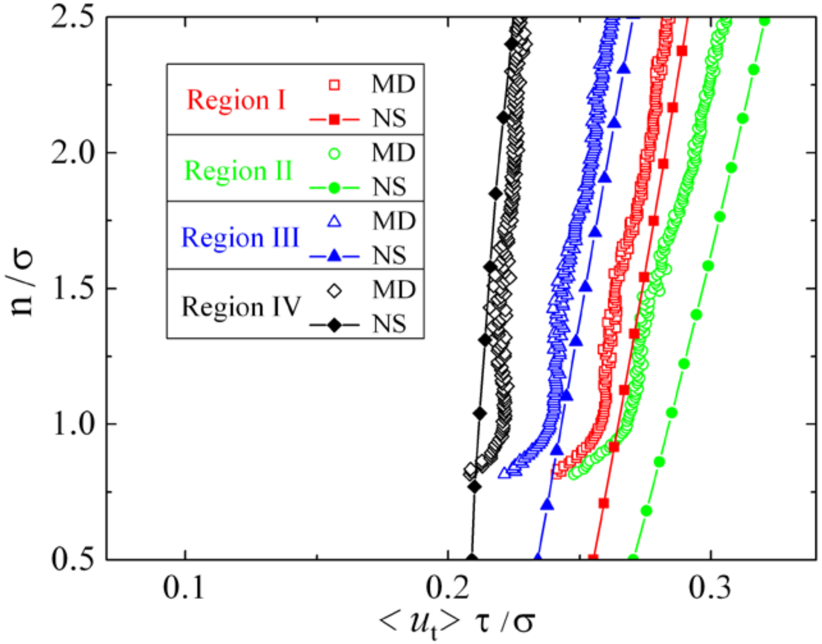
Local velocity profiles in four region (I-IV) along the stationary lower wall

Small upper wall speed

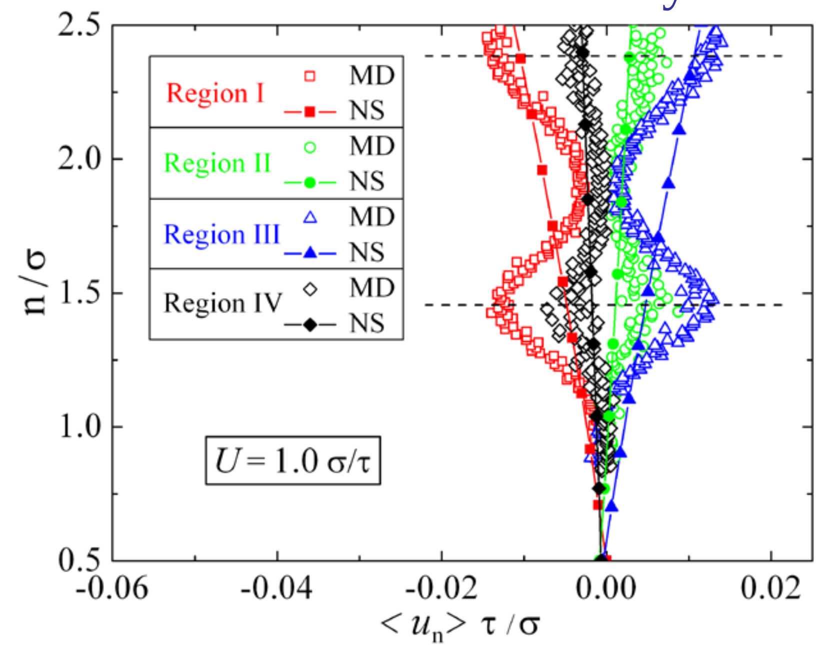
$U = 1.0\sigma/\tau \quad \mathrm{Re} \approx 17$



Local tangential velocity



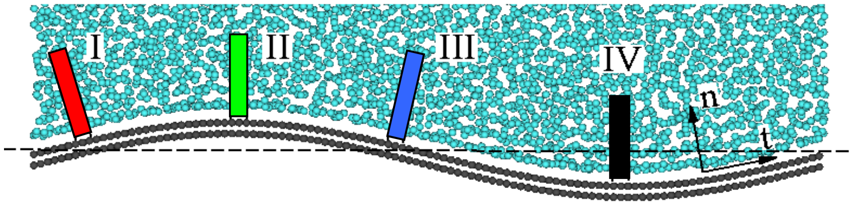
Local normal velocity



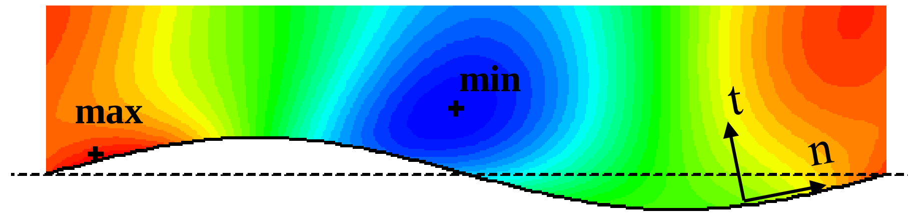
- At small ***U***, excellent agreement between NS and MD especially inside the valley (IV)
- The slip velocity above the peak (II) is larger than other regions
- Even at low Re, the inertia term in the NS equation breaks the symmetry of the flow with respect to the peak => u_t (I) > u_t (III)

- In regions I and III, negative and positive normal velocities are due to high pressure and low pressure regions
- The oscillation of the MD velocity profiles correlates well with the layering of the fluid density normal to the wall

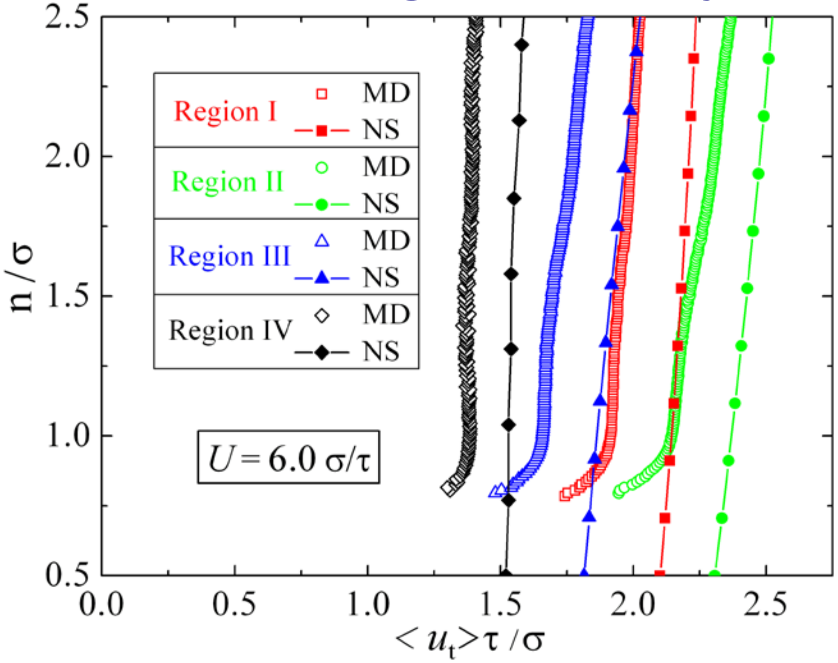
Large upper wall speed $U = 6.0\sigma/\tau$ $\quad Re \approx 100$



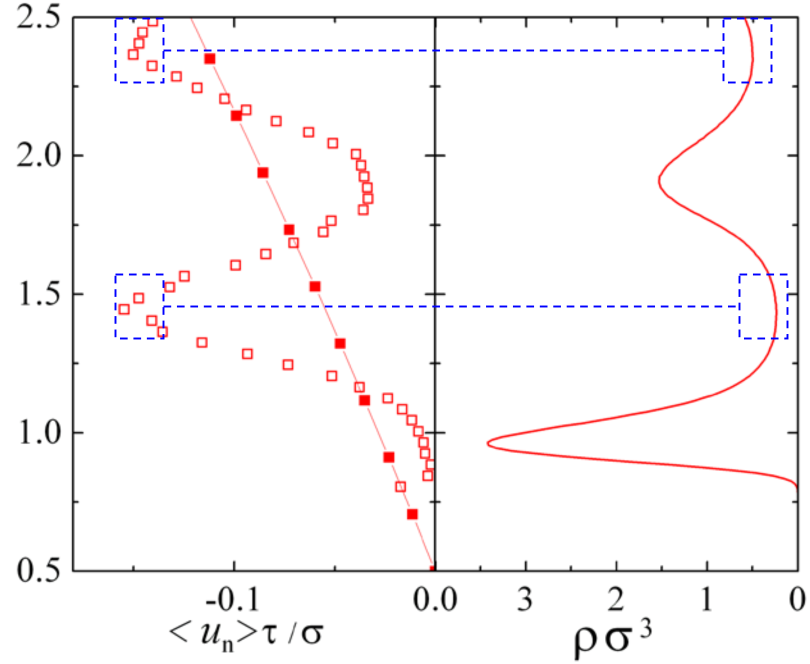
Pressure Contours from Navier-Stokes



Local tangential velocity



Normal velocity   Density

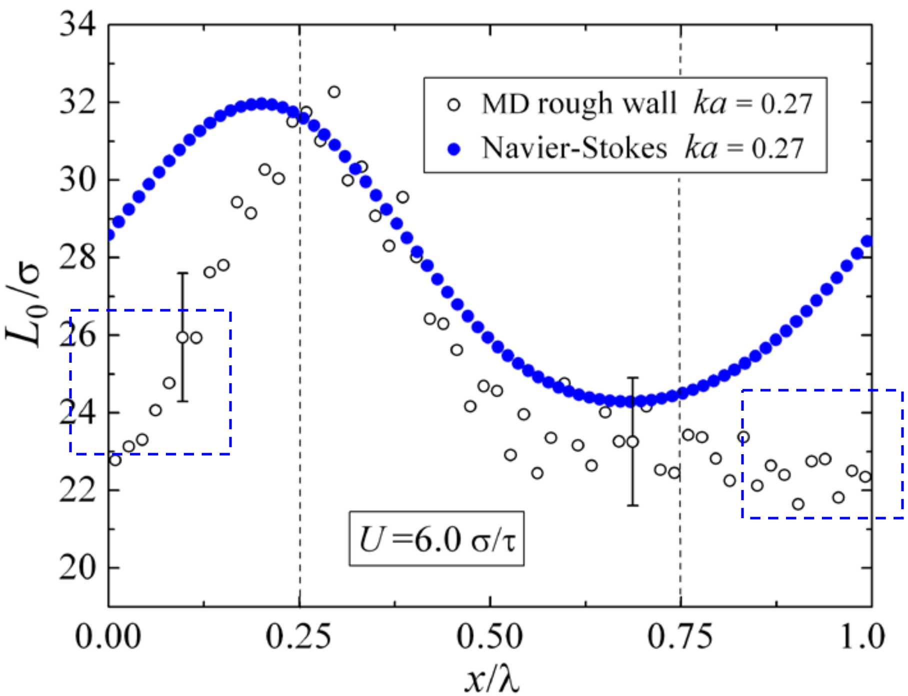


- For large ***U***, the tangential velocity from NS is larger than from MD
- MD velocity profiles are curved close to the surface, and, therefore, shear rate is subject to uncertainty

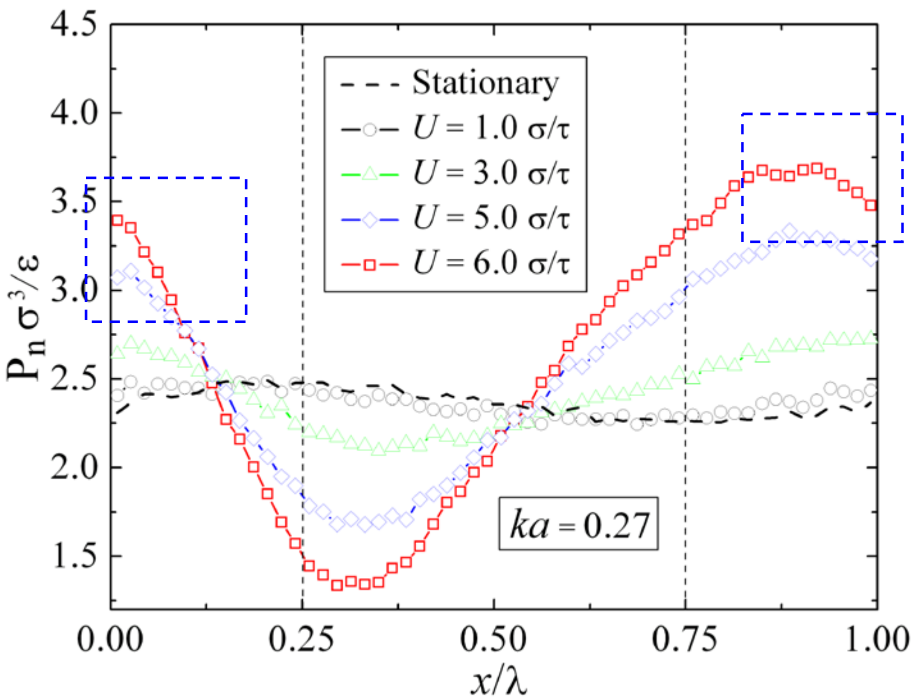
- The oscillations in the normal velocity profiles are more pronounced in MD simulations
- The location of maximum in the normal velocity profile correlates with the minimum in the density profile

Intrinsic slip length and the effect of local pressure along a rough surface

Local intrinsic slip length



Local pressure



- L_0 in MD is calculated from friction coefficient k_f due to uncertainty in estimating local shear rate
- L_0 in MD and NS is shear rate dependent
- L_0 in NS solution is calculated from 9th order polynomial fit and is not pressure dependent
- The viscosity is constant within the error bars

- Good agreement between L_0 from MD and continuum on the right side of the peak
- The L_0 from MD is about 3-4 σ smaller than NS due to higher pressure regions

$$L_0 = \frac{\mu}{k_f} \quad k_f = \frac{P_t}{u_s}$$

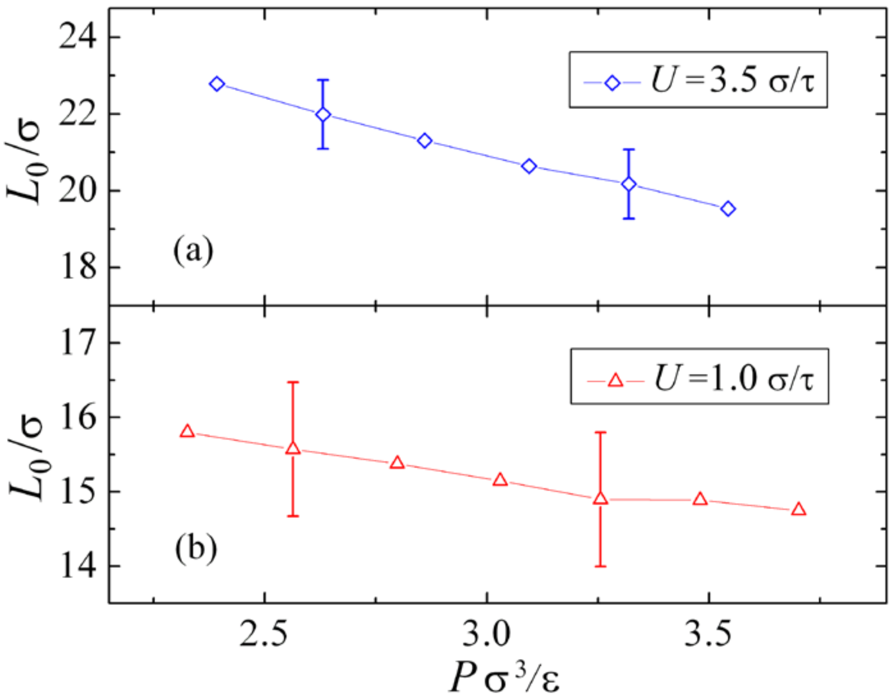
$$\mu = 2.15 \pm 0.15 \varepsilon\tau\sigma^{-3}$$

P_t: tangential stress

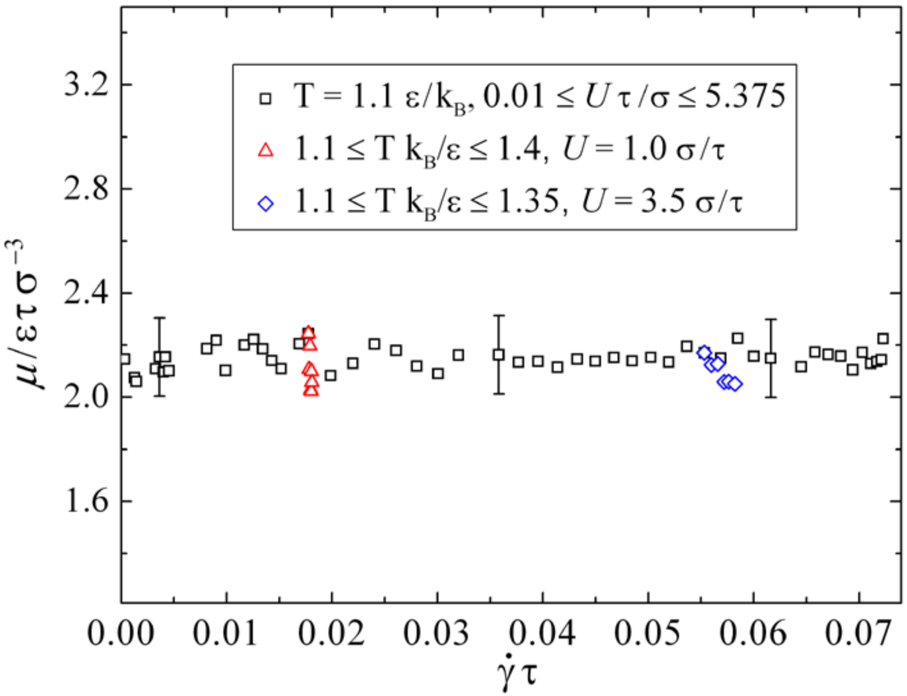
u_s: slip velocity

Intrinsic slip length and the effect of local pressure

Intrinsic slip length vs. pressure for flat wall



Bulk viscosity

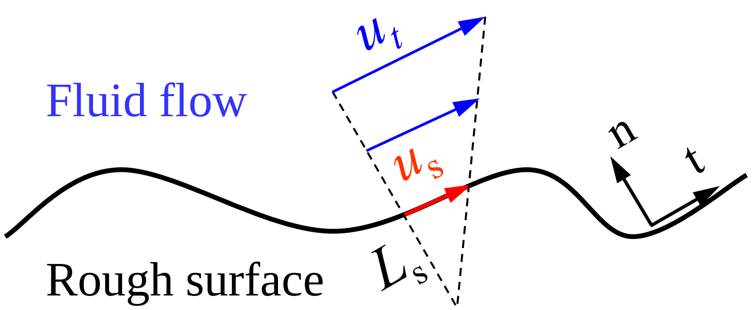


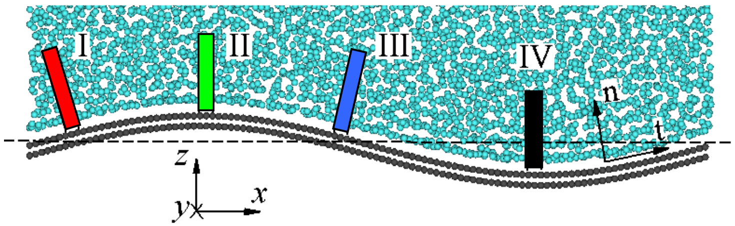
- By increasing the temperature of the Langevin thermostat the effect of pressure on L_0 is studied
- The bulk density and viscosity are independent of the temperature
- The friction coefficient only depends on the L_0
- L_0 is reduced about 3 σ as a function of pressure at higher ***U***
- The discrepancy between L_{eff} from MD and continuum is caused by high pressure region on the left side of the peak

Important conclusions

- The flow over a rough surface with local slip boundary condition was investigated numerically.
- The <u>local</u> slip boundary condition $L_s(\dot{\gamma})$ can not be determined from continuum analysis. Instead, MD simulations of <u>flow over flat walls</u> give $L_s(\dot{\gamma})$ which is a highly nonlinear function of shear rate.
- Navier-Stokes equation for flow over rough surface is solved using $L_s(\dot{\gamma})$ as a <u>local</u> boundary condition.
- The continuum solution reproduced MD results for the rate-dependent slip length in the flow over a rough surface.
- The main cause of discrepancy between MD and continuum at higher shear rates is due to reduction in the local intrinsic slip length in high pressure regions.

$$u_s(x) = L_s(\dot{\gamma}) \frac{\partial u_t(n)}{\partial n}$$





- The oscillatory pattern of the normal velocity profiles correlates well with the fluid layering near the wall in Regions I and III.