MECHANICAL ENGINEERING

Effect of surface roughness on slip flows in nanoscale polymer films
Molecular dynamics simulations versus continuum predictions

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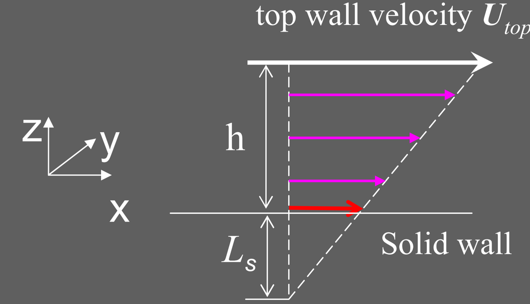
Motivation to investigate the slip phenomena at interfaces

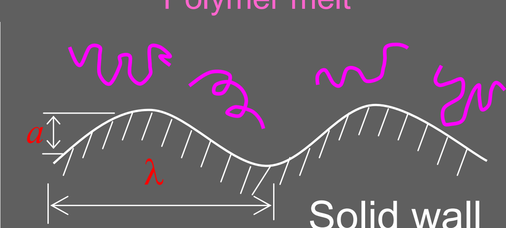
- What is *THE* boundary condition for liquid on solid flow in the presence of slip? Still *no fundamental understanding* of slip or what is proper BC for continuum studies.
- Navier slip boundary condition (1827) assumes constant slip length. *Is this always true?*
- How does surface roughness affect slip flow and conformation of a polymer chains?
- How does molecular dynamics simulations compare with continuum results?



Navier slip law

$$U_s = L_s\dot{\gamma}$$

$$\dot{\gamma} = \frac{dU_x(z)}{dz}$$



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

Details of molecular dynamics (MD) simulations

Equations of motion

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

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

f_i = Gaussian random force

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

Langevin thermostat: $T = 1.1\varepsilon/k_B$

Lennard-Jones potential

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

σ - molecular length scale

ε - energy scale

$\tau = \sqrt{\frac{m\sigma^2}{\varepsilon}}$ LJ time scale

Nonlinear elastic spring

$$V_{FENE}(r) = -\frac{1}{2}kr_o^2\ln\left(1-\frac{r^2}{r_o^2}\right)$$

$k = 30\,\varepsilon\sigma^{-2}$ and $r_o = 1.5\sigma$

10^3–10^4 fluid molecules

$N = 20$ bead-spring polymer chains

Conformation of polymer chains near corrugated wall

- To study the conformation of polymer chains, *radius of gyration* is calculated:

$$R_{g\alpha}^2 = \frac{1}{N}\sum_{i=1}^{N}(R_{i\alpha} - R_{G\alpha})^2 \qquad R_{G\alpha} = \frac{1}{N}\sum_{i=1}^{N} R_{i\alpha} \qquad (\alpha \equiv x, y, z)$$

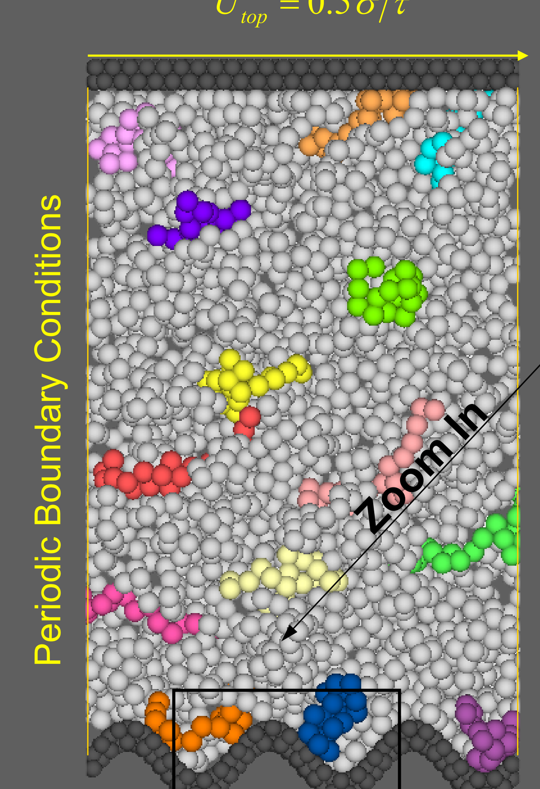
R_i = Position of *i*th bead of the polymer chain

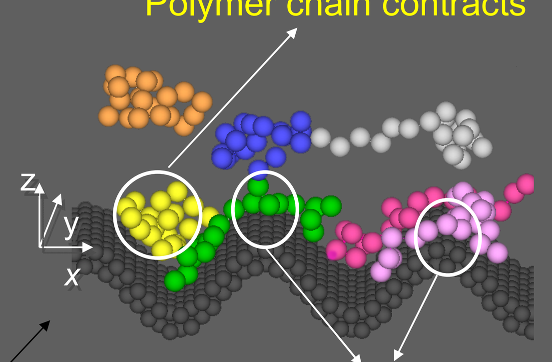
R_G = Position of *center of mass* of the polymer chain

$\lambda = 7.5\sigma$

a=0.2 σ	R_{gx}	R_{gy}	R_{gz}
bulk	1.70	1.11	1.03
top wall	1.64	1.25	0.73
peak	1.66	1.24	0.76
valley	1.53	1.28	0.73

a=1.4 σ	R_{gx}	R_{gy}	R_{gz}
bulk	1.79	1.10	1.01
top wall	1.69	1.24	0.73
peak	2.03	1.10	0.95
valley	0.83	1.57	0.70





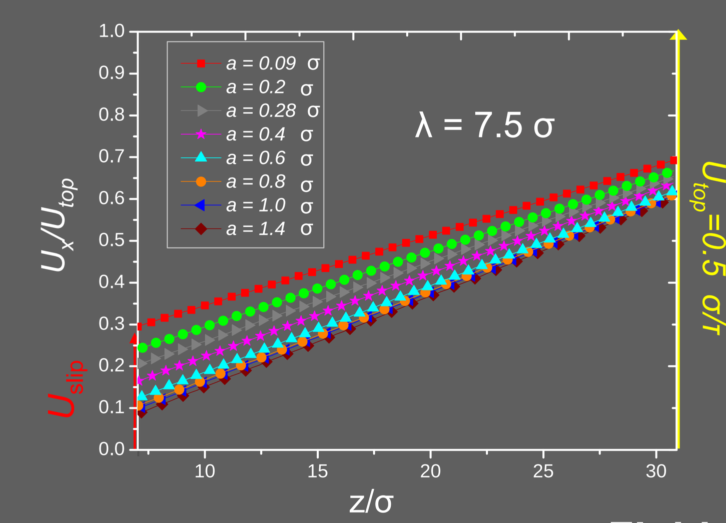
- Radius of gyration R_{gx} increases with the shear rate in the bulk

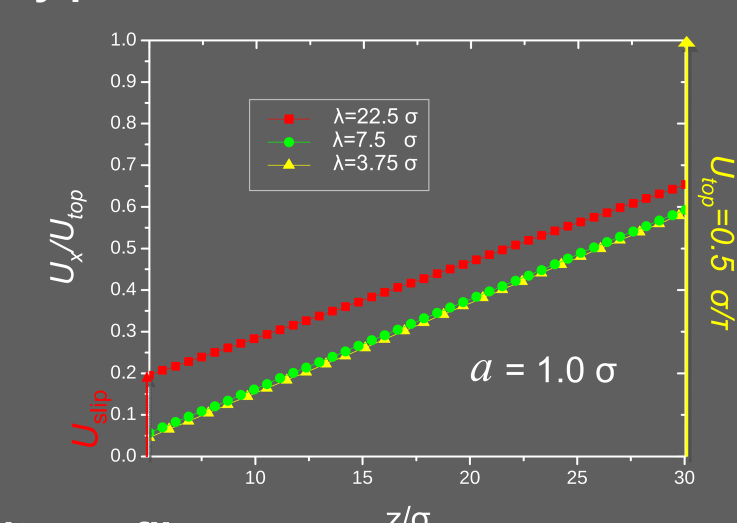
For a fixed amplitude *a* in a shear flow:

- R_{gx} *increases above peaks* and *decreases in valleys* in comparison with its value near top wall
- R_{gy} *increases in valleys*
- R_{gz} *decreases near top and bottom walls*

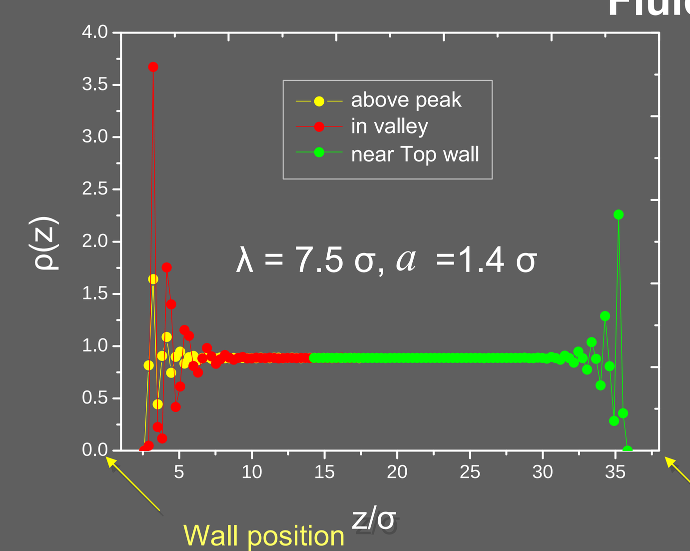
Rheology of a polymer melt near rough surfaces

Fluid velocity profiles





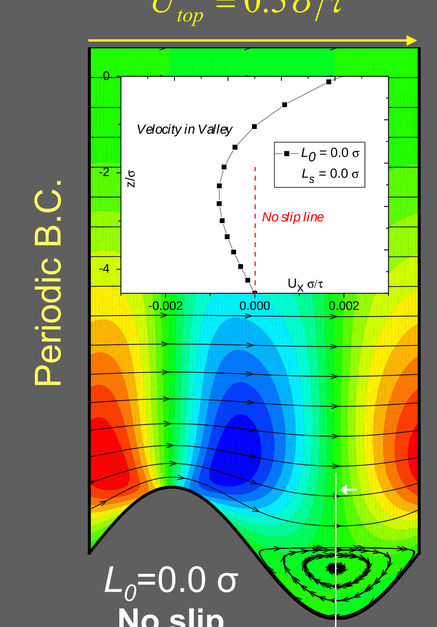
Fluid density profiles

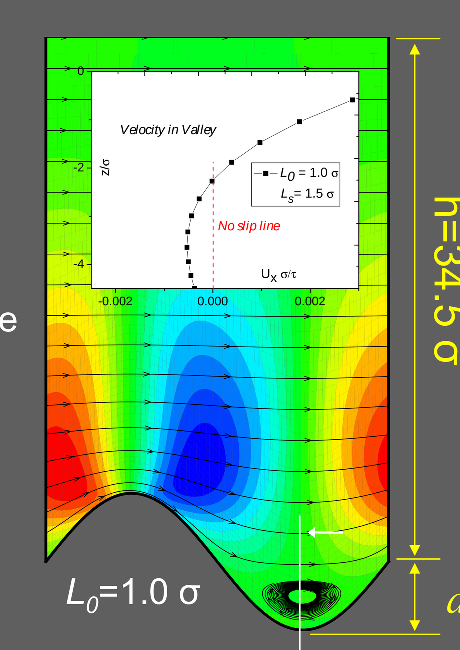


- For a fixed wavelength *λ*, slip velocity U_{slip} is reduced at larger amplitude *a*. R_{gx} increases with shear rate
- For a fixed amplitude *a*, more slip at larger wavelength *λ* and smaller shear rate
- The contact density inside the valley is larger than its value above the peak

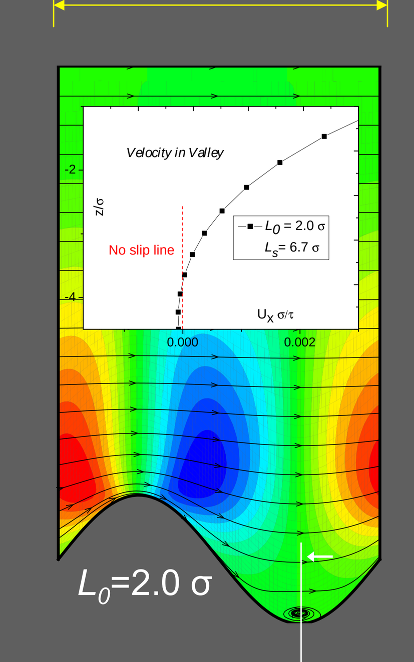
$$\text{Reynolds number} = \frac{\rho U_{top} h}{\mu} \approx O(1)$$

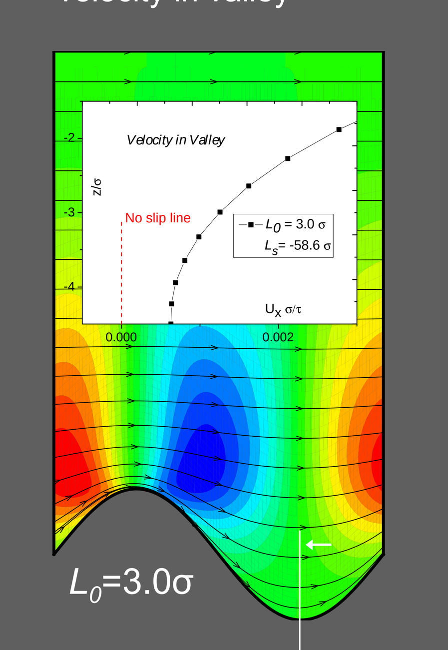
Continuum modeling of slip flow past a curved boundary





λ=22.5 σ





Method of solution

- Finite element penalty function with bilinear rectangular grid

Formulation

- 2D Stokes flow without body force

$$\mu\nabla^2 U = \nabla p$$

$$p = -\varphi\nabla\cdot U \qquad \varphi = 10^7$$

Boundary conditions

- Couette flow with constant slip length at the top wall

Local slip boundary conditions:

$$\frac{1}{L_s} = \frac{1}{L_0} - \frac{1}{R}$$

L_0 = slip length for flat wall

R = local radius of wall curvature

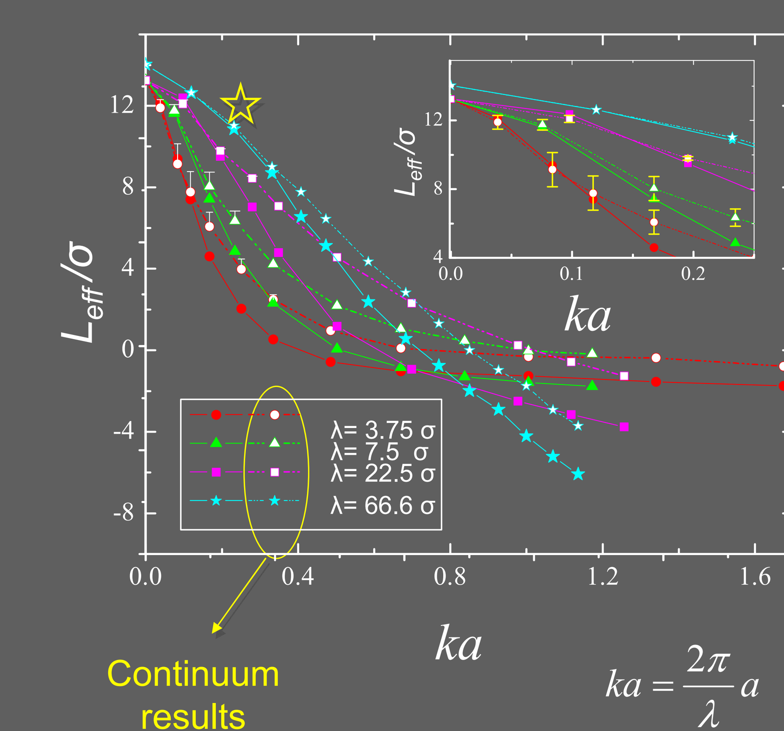
$$U_s = L_s\dot{\gamma} \qquad \dot{\gamma} = \left.\frac{dU}{dn}\right|_{@surface}$$

n = normal vector to the surface

Vorticity vanishes in valleys with increasing slip length

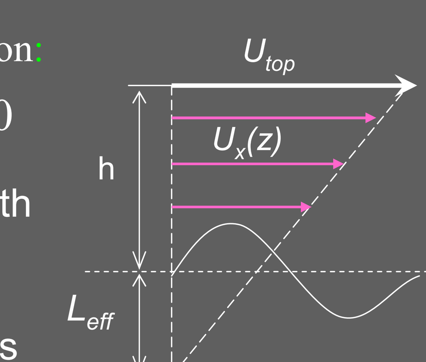
Pressure increases

Slip length: comparison between MD and continuum



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

- Continuum resolution: $90\times 50 - 130\times 40$

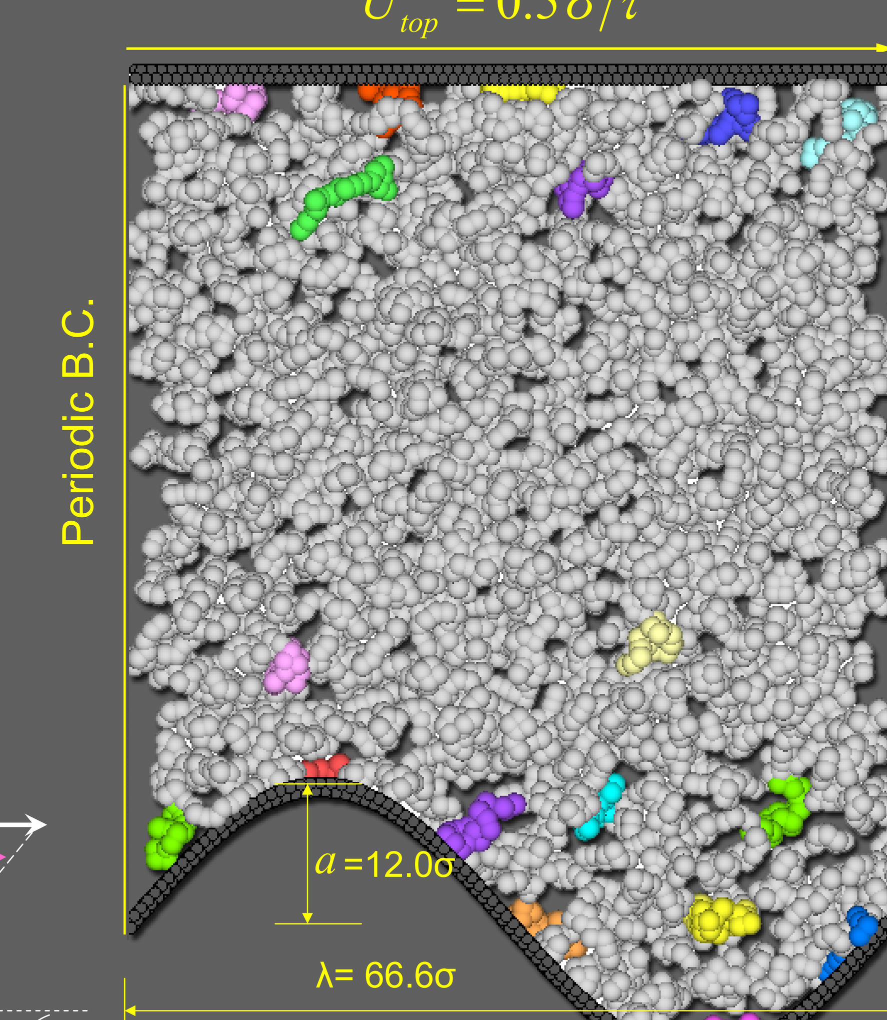


- Effective slip length L_{eff} decreases with increasing surface roughness parameter *ka*

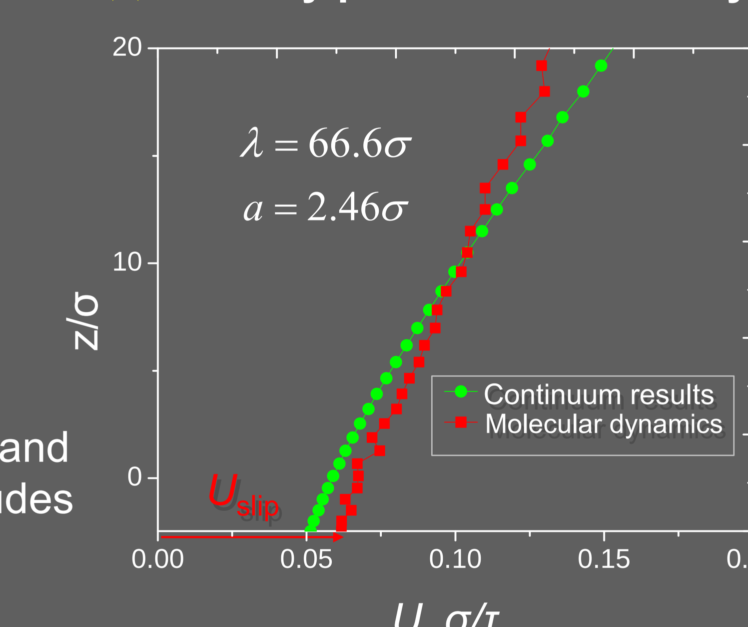
$$\longrightarrow ka = \frac{2\pi}{\lambda}\cdot a \text{ increase} \longrightarrow$$

Positive slip → No slip → Negative slip

Each MD point takes ~400 hrs on High Performance Computing Center



☆ Velocity profiles in the valley



- Excellent agreement between continuum and MD results for λ=66.6 σ and small amplitudes

Conclusions

- At small wavelengths $\lambda \sim R_g$, polymer chains tend to stretch in the direction of the shear flow in the regions above peaks of sinusoidal corrugation and elongate inside valleys along the *y* direction.
- Molecular dynamics results recover the continuum solutions in the Stokes regime in the limit of small surface roughness *ka* and λ=66.6 σ.
- Effective slip length is reduced at small wavelengths *λ* and/or large amplitude *a* of the corrugated surface.

References

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