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

Anoosheh Niavarani and Nikolai V. Priezjev

Motivation to investigate the slip phenomena at interfaces:
- What is the boundary condition for liquid on solid flow in the presence of slip?
- Is the boundary condition (planar) always true?
- Does surface roughness affect slip flow and deformation of a polymer chain?
- How do molecular dynamics simulations compare with continuum results?

Details of molecular dynamics (MD) simulations:
- Equations of motion:
  \[ m \ddot{r} = -\nabla \phi(r) + f_c \]

- Leonard-Jones potential:
  \[ V_c(r) = 4 \varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \]

- Nonlinear elastic spring:
  \[ V_{es}(r) = \frac{1}{2} k (r - r_0)^2 \]

Conformation of polymer chains near corrugated wall:
- To study the conformation of polymer chains, radius of gyration is calculated:
  \[ \lambda = \frac{1}{2\pi} \left( \sum_{i=1}^{N} \left( r_i - R_e \right) \cdot \lambda = 7.5 \sigma \right) \]

Continuous modeling of slip flow past a curved boundary:
- Method of solution:
  - Finite element penalty function with bilinear rectangular grid
  - 2D Stokes flow without body force
  - \[ \frac{\partial}{\partial t} \vec{U} = \nabla \cdot \vec{p} \]
  - \[ \vec{p} = -\nabla \vec{P} \]
  - \[ \phi \ni \sigma \]

- Boundary conditions:
  - Couette flow with constant slip length at the top wall
  - \[ L_s = \text{slip length for flat wall} \]
  - \[ Z = L_s \hat{y} = \frac{dU}{dz} \]

- Velocity in valley:
  - Vorticity vanishes in valleys with increasing slip length
  - Pressure increases

- Slip length: comparison between MD and continuum:
  - Fluid velocity profiles
  - Fluid density profiles

Conclusions:
- At small wavelengths \( \lambda < R_w \), 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 Stokes regime in the limit of small surface roughness \( \xi_a \) and \( \lambda = 66.5 \sigma \).
- Effective slip length is reduced at small wavelengths \( \lambda \) and for large amplitude \( a \) of the corrugated surface.

References: