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?
- Is the slip always true?
- How does surface roughness affect slip flow and conformation of a polymer chain?
- How do molecular dynamics simulations compare with continuum results?

Details of molecular dynamics (MD) simulations
- Equations of motion:
  \[ \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i \]
- Lennard-Jones potential:
  \[ V(r) = 4\epsilon \left( \frac{\sigma}{r} \right)^{12} - \frac{2\epsilon}{r} \] Nonlinear elastic spring
  \[ V_{es}(r) = -k_2(r - r_0)^2 \]
- Long-time scale:
  \( \lambda = 7.5 a \)
- Time scale:
  \( \lambda = 0.9 \) to \( \lambda = 1.4 a \)

Conformation of polymer chains near corrugated wall
- To study the conformation of polymer chains, the radius of gyration is calculated:
  \[ R_g^2 = \frac{1}{M} \sum_i \left( \mathbf{r}_i - \mathbf{r}_c \right)^2 \]
  \( R_c = 0.05 a \) for MD and continuum
  \( R_g = 0.05 a \) for MD

Rheology of a polymer melt near rough surfaces
- Fluid velocity profiles
- Fluid density profiles
- Continuum 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
- \( \mu \mathbf{v} \nabla \mathbf{v} = -\nabla p \)
- Attraction
- \( p = \nabla \cdot \nabla \mathbf{U} = -\phi \mathbf{U} \)
- \( \phi = 10^{-7} \)

Slip length: comparison between MD and continuum
- Continuum results
  - Continuum resolution
  - Effective slip length \( L_{sl} \) decreases with increasing surface roughness parameter \( k_a \)

Conclusions
- At small wavelengths \( \lambda \sim R_s \), polymer chains tend to stretch in the direction of the shear flow in the regions above peaks of sinuous 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 \( k_a \) and \( \lambda = 66.6 a \).
- Effective slip length is reduced at small wavelengths \( \lambda \) and/or large amplitude \( a \) of the corrugated surface.

References