Multiscale hybrid simulation of MD and CFD for polymer melt flows in parallel plates

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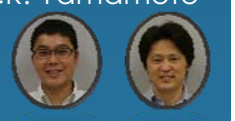
Multiscale Simulations for Softmatters
http://multiscale.jp



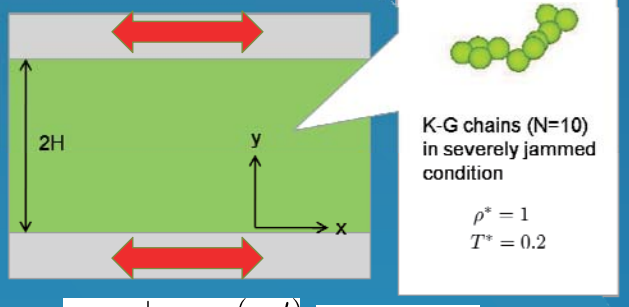
Multi-scale Modeling

Difficulties in soft-matter simulations — Constitutive relations are unknown in general

- Complex behaviors of fluids coupled with the dynamics of internal degrees of freedom .
- Macro-scale correlations far beyond molecular scales. — Out of Range for MD simulations

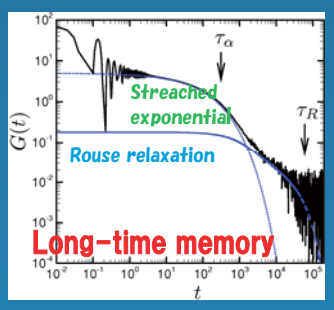
Schematic of system

K-G Model Polymer

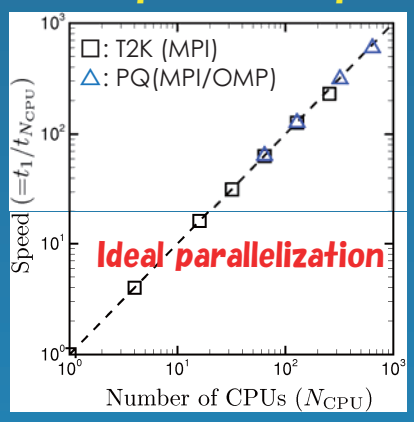


$v_x = \pm v_0 \cos(\omega_0 t)$ $v_0 = \Gamma_0 \omega_0 H$

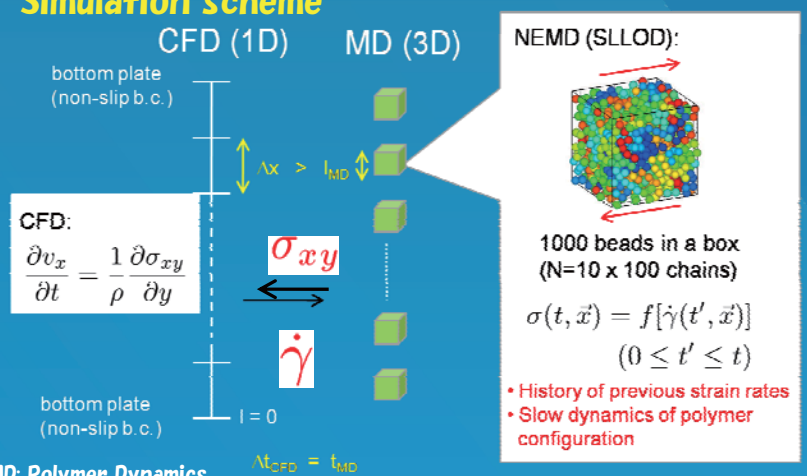
Stress relaxation



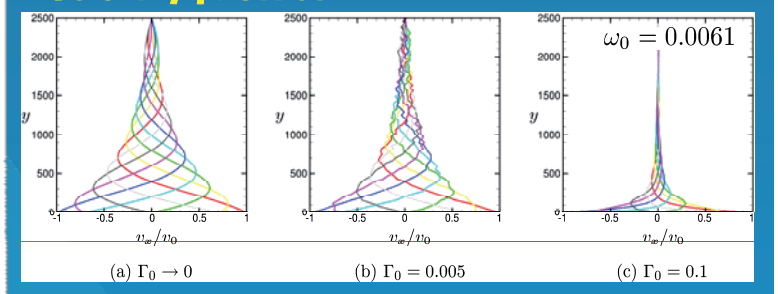
Bench mark for parallel computation

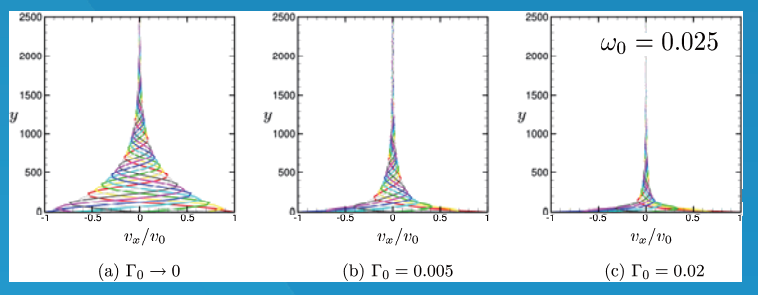


Simulation scheme

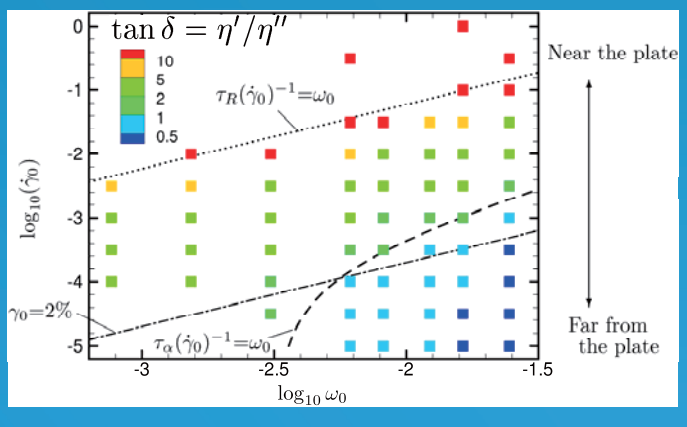


Velocity profiles

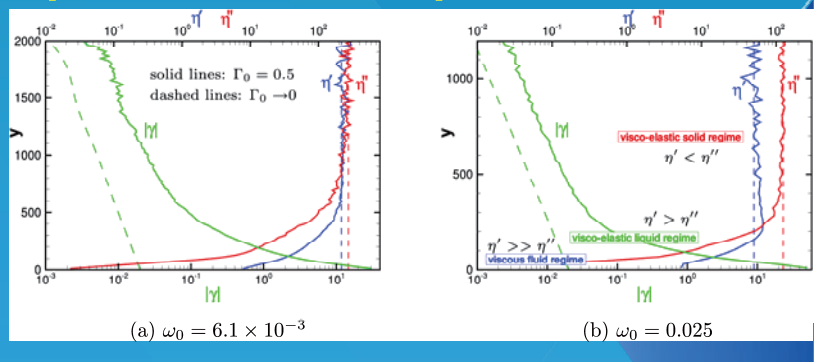




Rheological properties in oscillating plates



Spatial variation of complex viscocities



Summary

- We developed the multiscale hybrid simulation for polymer melt flows in parallel plate.
- Non-linear oscillating flows and complicated "local" rheological properties are analyzed.
- We found that three different rheological regimes, i.e., viscous fluid, visco-elastic liquid, visco-elastic solid regimes, form over the oscillating plate at high oscillation frequencies.
- Bench mark demonstrate that our hybrid scheme is quite suitable for HPC architecture.