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

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Multi-scale Modeling

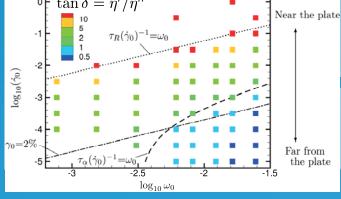
http://multiscale.jp

Multiscale Simulations for Softmatters

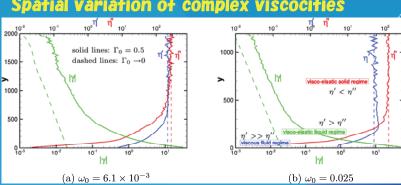
Difficulties in soft-matter simulations Constitutive relations are unknown in general

•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 Bench mark for parallel computation Schematic of system K-G Model Polymer Stress relaxation □: T2K (MPI) △: PQ(MPI/OMP) $(=t_1/t_{N_{ m CPU}})$ Streach exponentia K-G chains (N=10) 2H in severely jammed Rouse relaxation condition Ideal parallelization ø ong-time memory $T^* = 0.2$ 10² $v_x = \underline{\pm v_0} \cos(\omega_0 t) \quad v_0 = \Gamma_0 \omega_0 H$ Number of CPUs (N_{CPU}) Simulation scheme Velocity profiles NEMD (SLLOD): CFD (1D) MD (3D) bottom plate (non-slip b.c.) $\omega_0 = 0.0061$ CFD: 1000 beads in a box σ_{xy} ∂v_x $1 \partial \sigma_{xy}$ (N=10 x 100 chains) ∂t $\rho \ \partial y$ $\sigma(t, \vec{x}) = f[\dot{\gamma}(t', \vec{x})]$ (a) $\Gamma_0 \to 0$ (b) $\Gamma_0 = 0.005$ (c) $\Gamma_0 = 0.1$ $(0 \le t' \le t)$ $\omega_0 = 0.025$ History of previous strain rates bottom plate (non-slip b.c.) Slow dynamics of polymer configuration MD: Polymer Dynamics **CFD:** momentum Transport Rheological properties in oscillating plates v_x/v_0 v_x/v_0 v_x/v_0 o $tan <math>\delta = \eta'/\eta$



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 guite suitable for HPC architecture.