Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Multiscale Simulation of Polymeric Liquids with Heat Transportation TAKAHIRO MURASHIMA, TOSHIHIRO KAWAKATSU, Department of Physics, Tohoku University — Polymeric liquids show complex flow behaviors coming from the complex microscopic molecular dynamics and structures. We usually assume a constitutive equation to represent a nonlinear relationship between strain and stress in polymeric liquids. In the multiscale simulation, we use a molecular dynamics simulation to describe the relationship between strain and stress at each fluid element instead of using the constitutive equation. The multiscale simulation consists of the macroscopic fluid particle simulation and the microscopic polymer dynamics simulation. The macroscopic fluid particle simulation represent the macroscopic flow of polymeric liquids and the microscopic polymer simulation represent the local dynamics of polymeric liquids. Since each polymer dynamics simulation is independent of the other simulators, the multiscale simulation is suitable for the massively parallel super computer. We have succeeded in describing the isothermal flow problem at the present framework. We develop the multiscale simulation framework to more general flow problem with heat transfer. In this talk, we use a dumbbell model as a microscopic simulator for the multiscale simulation. We discuss a heat transportation problem using the preliminary polymer model.

Takahiro Murashima
Department of Physics, Tohoku University

Date submitted: 28 Dec 2016 Electronic form version 1.4