Coarse-Grained Rheological Model of Entangled Polymers for Multiscale Simulations

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Polymeric fluids (melts or solutions) show various interesting rheological properties (especially for large molecular weight, entangled polymers) [1]. Macroscopic flows of a polymeric fluid strongly depend on its rheological properties. Therefore it is demanding to use an accurate rheological model when we perform macroscopic flow simulations for polymers. To directly take into account the microscopic/mesoscopic polymer dynamics information into macroscopic simulations, multiscale simulation methods which combine microscopic/mesoscopic simulations with macroscopic simulations have been developed [2, 3]. In these multiscale simulations, many microscopic/mesoscopic simulators are embedded to fluid elements, and calculation costs of microscopic/mesoscopic simulations become considerably large. The longest relaxation time of entangled polymers often becomes very long, which makes multiscale simulations inefficient. In this work, we propose a fast rheology simulation model for multiscale simulations of entangled polymers.

There are several requirements for simulators to be embedded to macroscopic fluid elements. For example, the simulation can be performed stably under any velocity gradient tensor (system deformation), if we consider flows of polymeric materials in complicated channels. The total calculation time is roughly proportional to the simulation time of an embedded simulator. Thus embedded simulators should be designed to be numerically efficient (especially for well entangled polymeric systems). To satisfy these requirements, in this work we employ the coarse-grained single chain model as a mesoscopic rheological model [4]. In this single chain model, the effect of entanglements is mimicked by virtual springs attached to the polymer chain (the slip-springs). We show that our model can reasonably reproduce linear and nonlinear rheological properties, and can be drastically accelerated by a graphic processor unit. We also show that we can design several different single chain slip-spring type models which have different characteristic time/length scales.

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