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Dynamic Monte Carlo in Hierarchical Modeling of Polymer Processing

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The use of on-lattice Monte Carlo simulation to predict melt rheological properties of polymers is explored. The methodology employed consists of the cooperative motion algorithm of Pakula and a derived biasing technique based on previous studies of Binder and Baushnagel. The biasing technique is derived to be suitable for the face centered cubic lattice used in the simulations. In shear flow, a uniform linear velocity profile is obtainable for low molecular weight chains for all values of the biasing parameter. However, for larger chain lengths the velocity profile becomes distorted; this distortion is reflective of cohesive failure and slip phenomena. Use of the Kramers form for entropic springs allows the calculation of stress in the simulation providing a means for exploring rheological properties including viscosity and normal stress differences. Results are in excellent agreement with well-established experimental facts; a shear thinning viscosity is obtained, the first normal stress difference increases with shear rate, and the first normal stress coefficient decreases with shear rate. A higher order scheme is suggested that iterates between the molecular and continuum scales for simulating polymer flow.