Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Finding the Missing Physics: Simulating Polydisperse Polymer Melts[1] NICHOALS RORRER, JOHN DORGAN, Colorado Sch of Mines — A Monte Carlo algorithm has been developed to model polydisperse polymer melts. For the first time, this enables the specification of a predetermined molecular weight distribution for lattice based simulations. It is demonstrated how to map an arbitrary probability distributions onto a discrete number of chains residing on an fcc lattice. The resulting algorithm is able to simulate a wide variety of behaviors for polydisperse systems including confinement effects, shear flow, and parabolic flow. The dynamic version of the algorithm accurately captures Rouse dynamics for short polymer chains, and reptation-like dynamics for longer chain lengths.[1] When polydispersity is introduced, smaller Rouse times and broadened the transition between different scaling regimes are observed. Rouse times also decrease under confinement for both polydisperse and monodisperse systems and chain length dependent migration effects are observed. The steady-state version of the algorithm enables the simulation of flow and when polydisperse systems are subject to parabolic (Poiseulle) flow, a migration phenomenon based on chain length is again present. These and other phenomena highlight the importance of including polydispersity in obtaining physically realistic simulations of polymeric melts. 1. Dorgan, J.R.; Rorrer, N.A.; Maupin, C.M., *Macromolecules* **2012**, *45* (21), 8833-8840.

[1]Work funded by the Fluid Dynamics program of the National Science Foundation under grant CBET-1067707

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Date submitted: 13 Nov 2013 Electronic form version 1.4