Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts HENDRIK MEYER, JEAN FARAGO, A.N. SEMENOV, Institut Charles Sadron, CNRS and Universite de Strasbourg, France — We have recently discovered that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and simulation is found. The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time; it is generally active in melts of any topology. Surprisingly, the effects are relevant for both, momentum-conserving and Langevin dynamics [1,2] and this presentation will focus on the differences: The commonly employed Langevin thermostat significantly changes the CM motion on short and intermediate time scales, but approaching the Rouse time, the melt behavior is close to momentum-conserving simulations. On the other hand, if momentum-conserving simulations are run in too small a simulation box, the result looks as if a Langevin thermostat was used.

[1] PRL 107, 178301 (2011); PRE 85, 051807 (2012).
[2] PRL 109, 248304 (2012); Soft Matter 9, 4249 (2013).

Hendrik Meyer
Institut Charles Sadron, CNRS and Universite de Strasbourg

Date submitted: 15 Nov 2013 Electronic form version 1.4