Abstract Submitted for the MAR06 Meeting of The American Physical Society

Multiscale Modeling of Polymer Rheology SUBHRANIL DE, JA-COB FISH, MARK SHEPHARD, PAWEL KEBLINSKI, SANAT KUMAR — We propose a novel simulation method which can be used to readily parallelizesimulations on systems with a large spatial extent. We simulate small parts of thesystem with independent molecular dynamics simulations, and only occasionally passinformation between these simulations through a constitutive model free continuumapproach. We illustrate the power of this method in the case of a polymeric fluidundergoing rapid one dimensional shear flow. Since we show that this flow problemcannot be modeled by using a steady-state constitutive model, this method offersthe unique capability for accessing the non-linear viscoelasticity of complex fluids.

Daniel Sperber

Date submitted: 30 Nov 2005

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