

## POLYMER SEMINAR

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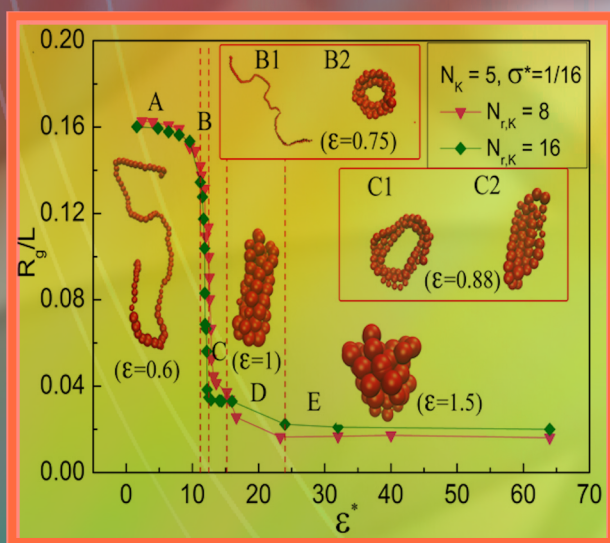
UNIVERSITY OF MICHIGAN



# "Accurate Modeling of Polymer Dynamics in Simple and Complex Flows"

## Summary

We assess the accuracy and efficiency of mesoscopic simulation methods, namely Brownian Dynamics (BD), Stochastic Rotation Dynamics (SRD) and Dissipative Particle Dynamics (DPD), for flows of polymer solutions in simple extensional and shear flows, and microfluidic geometries. Using systematic refinement of bead-spring and bead-rod models, the level of model resolution is determined for accurate results as a function



of shear rate, for both good or theta solvent and poor-solvent (collapsing-chain) conditions. We assess the speed and accuracy of predictions of SRD and DPD for computing flow through a periodic contraction. In the periodic contraction, we find that there is an elasto-hydrodynamic drift that allows polymers to be size segregated based on molecular weight, and that this mechanism can be most efficiently simulated by BD simulations, for dilute solutions and by SRD for non-dilute solutions. We also use similar methods to analyze the swimming and tumbling behavior of *E. coli* micro-swimmers. We show that it is now possible to solve coupled polymer dynamics and fluid flow that includes polymer-modified flow, hydrodynamic interactions among the polymers and with the wall, and flow-induced polymer migration. Accurate simulation of all these phenomena simultaneously would be very difficult to achieve with conventional continuum mechanical approaches.



WED. APRIL 9th, 2014 • ROOM 66-110

SEMINAR 3:30 - 5:00 PM • REFRESHMENTS 3:00 PM

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