Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Systematic coarse-graining of the wormlike chain model for dynamic simulations ELENA KOSLOVER, ANDREW SPAKOWITZ, Stanford University — One of the key goals of macromolecular modeling is to elucidate how macroscale physical properties arise from the microscale behavior of the polymer constituents. For many biological and industrial applications, a direct simulation approach is impractical due to to the wide range of length and time scales that must be spanned by the model, necessitating physically sound and practically relevant procedures for coarse-graining polymer systems. We present a highly general systematic coarse-graining procedure that maps any detailed polymer model onto effective elastic-chain models at intermediate and large length scales, and we specifically focus on the wormlike chain model of semiflexible polymers. Our approach defines a continuous flow of coarse-grained models starting from the wormlike chain model, proceeding through an intermediate-scale stretchable, shearable wormlike chain, and finally resolving to a Gaussian chain at the longest lengths. Using Brownian dynamic simulations of our coarse grained polymer, we show that this approach to coarse graining the wormlike chain model captures analytical predictions for stress relaxation in a semiflexible polymer. Since we can arbitrarily coarse grain the polymer in these dynamic simulations, our approach greatly accelerates simulations.

Andrew Spakowitz
Stanford University

Date submitted: 18 Nov 2013 Electronic form version 1.4