Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Stretching wormlike chain: interplay between chain stiffness and excluded volume in the long chain limit XIAOLAN LI, ABHIRAM MURALIDHAR, Chemical Engineering and Materials Science, University of Minnesota, CHARLES SCHROEDER, Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, KEVIN DORFMAN, Chemical Engineering and Materials Science, University of Minnesota — Nearly 20 years ago, Marko and Siggia (*Macromolecules* **1995**, 8759-8770) proposed an approximate interpolation formula for the force-extension (f-z) behavior of a wormlike chain that has found widespread use in biophysics and polymer physics. We have extended their result to account for excluded volume interactions. Our analysis takes advantage of Pruned-Enriched-Rosenbluth Method (PERM) simulations of wormlike chains of varying monomer anisotropy. Our simulations use up to 80,000 hard beads, allowing us to reach the long chain limit with sub-persistence length resolution. The simulations produce the Pincus scaling $z \sim f^{2/3}$, followed by a crossover to the linear behavior $z \sim f$, and subsequent saturation approaching the fully stretched limit. We also developed an approximate interpolation formula that captures these three regimes. This interpolation formula is in good agreement with PERM simulation results and can be reduced to the Marko-Siggia interpolation formula when the excluded volume effect is eliminated. Practically, our work provides a handy description of force-extension behavior for real wormlike chain, which will be useful for coarse-grained simulations and interpreting experiment results.

Xiaolan Li
Chemical Engineering and Materials Science, University of Minnesota

Date submitted: 12 Nov 2014 Electronic form version 1.4