Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Extensions of an analytical coarse-grained description for polymer liquids: thermodynamic determinations and an intermediate length-scale description EDWARD SAMBRISKI, MARINA GUENZA, Department of Chemistry, Institute of Theoretical Science, University of Oregon, Eugene, Oregon 97403 — We extend our previous analytical coarse-graining (CG) procedure [1], which maps polymer liquids onto a system of interacting soft-colloidal particles. First, we present an optimized representation of the effective pair potential, $v_{cc}(r)$ [initially determined via the hypernetted-chain closure], by carrying out an interative predictor-corrector (PC) scheme. Then, we compare the thermodynamics obtained through the virial and compressibility routes, for which we observe an improvement in their consistency when using the PC result. Finally, we present an intermediate length-scale CG treatment for polymers by performing an analytical remapping of the chain onto "blobs" (monomer aggregates). The derived expression for the blob-blob total correlation function, $h_{bb}(r)$, is seen to be in agreement with data from united-atom molecular dynamics simulations.

[1]G. Yatsenko, E. J. Sambriski, and M. G. Guenza, J. Chem. Phys., **106,** 054907:1-12 (2005); G. Yatsenko, E. J. Sambriski, M. A. Nemirovskaya, and M. Guenza, Phys. Rev. Lett., **93,** 257803:1-4 (2004).

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Date submitted: 22 Nov 2005 Electronic form version 1.4