Abstract Submitted
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Stochastic Rotation Dynamics: generalizations and applications for non-ideal fluids, binary mixtures and colloids THOMAS IHLE, Department of Physics, North Dakota State University, ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, DANIEL KROLL, Department of Physics, North Dakota State University — A particle-based algorithm for the coarse-grained modeling of a fluctuating Solvent, namely Stochastic Rotation Dynamics (SRD), was recently introduced by Malevanets and Kapral[1]. This algorithm describes a fluid with an ideal gas equation of state and has been successfully applied to study polymers, colloids, and vesicles in flow. Here, we present generalizations of SRD for modeling fluids with non-trivial equations of state[2]. In particular, we show how to model a simple liquid with a non-ideal equation of state by incorporating excluded volume effects. We show the thermodynamic consistency of the model by independently measuring the pressure, density fluctuations and the speed of sound and compare with analytical results. This idea is extended to model binary mixtures with a miscibility gap; and the phase diagram of such a mixture will be presented. Furthermore, colloids are included in the SRD solvent and results for colloidal suspensions driven by external forces will be shown. [1] A. Malevanets, R. Kapral, J. Chem. Phys. 110, 8605 (1999). [2] T. Ihle, E. Tuzel, D. M. Kroll, cond-mat/0509631.

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