A particle-based simulation technique for fluid flow: applications to binary mixtures, microemulsions and colloids ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, THOMAS IHLE, GUOAI PAN, DANIEL KROLL, Department of Physics, North Dakota State University — Particle-based simulation techniques provide an attractive alternative to traditional methods for the coarse-grained modeling of a fluctuating solvent. A particularly appealing algorithm was introduced by Malevanets and Kapral[1]. The algorithm has been successfully applied to study the behavior of polymer solutions, colloids and vesicles in shear flow. We present generalizations of this algorithm to fluids with non-ideal equations of state and binary mixtures with a miscibility gap[2]. We show the thermodynamic consistency of the model by measuring the pressure and density fluctuations and compare with analytical results. Results for the demixing of a binary mixture are presented such as the phase diagram and measurements of interface fluctuations and the surface tension of a droplet as well as the coarsening of domains during spinodal decomposition. Preliminary results for the lowering of the surface tension in microemulsions and the onset of emulsification are presented. Furthermore, colloids are included in the 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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