

PARTICLE DYNAMICS AND STRUCTURE OF SIMPLE COMPLEX MATTER

Ying Li¹, Martin Kröger² and Wing Kam Liu³

¹ Northwestern University, Department of Mechanical Engineering, Evanston, IL 60208, USA,
E-mail: yingli@u.northwestern.edu

² Polymer Physics, Department of Materials, ETH Zurich, Switzerland,
E-mail: mk@mat.ethz.ch, <http://www.complexfluids.ethz.ch>

³ Northwestern University, Department of Mechanical Engineering, Evanston, IL 60208, USA,
E-mail: w-liu@u.northwestern.edu

Key Words: *Hybrid simulation, Polymers, Nanoparticles, Entanglements.*

We present a particle based multiscale computational framework [1, 2] for the analysis of complex liquids at weak external fields, where classical nonequilibrium molecular dynamics tends to exceed its capabilities as an efficient solver. The multiscale computational method can be used to study liquids subject to arbitrary homogeneous flows as it is free of periodic boundary conditions by construction. In addition, we show a number of recent examples where we used particle methods to try to understand and interpret empirical observations: (i) entanglement network of uncrosslinked and crosslinked polymers [3], (ii) dynamics of polymer chains and their entanglement network in the presence of nanoparticles [4, 5, 6] and subjected to shear and elongational flow (iii) translocation of model particles through the cell membrane [7].

REFERENCES

- [1] Y. Li, S. Tang, B.C. Abberton, M. Kröger, C. Burkhart, B. Jiang, G.J. Papakonstantopoulos, M. Poldneff and W.K. Liu. *Polymer*, **53**, 5935-5952, 2012.
- [2] Y. Li, B.C. Abberton, M. Kröger and W.K. Liu. *Polymers*, **5**, 751-832, 2013.
- [3] Y. Li, M. Kröger and W.K. Liu. *Polymer*, **52**, 5867-5878, 2011.
- [4] Y. Li, M. Kröger and W.K. Liu. *Macromolecules* **45**, 2099–2112, 2012.
- [5] Y. Li, M. Kröger, W.K. Liu, *Phys. Rev. Lett.* **109**, 118001, 2012.
- [6] Y. Li, M. Kröger, W.K. Liu, *Soft Matter*, **10**, 1723-1737, 2014.
- [7] Y. Li, M. Kröger, W.K. Liu, *ACS Nano*, in preparation, 2014.