

Abstract for an Invited Paper
for the MAR10 Meeting of
The American Physical Society

Simulating the dynamics of a single polymer chain in solution: Lattice Boltzmann vs Brownian dynamics¹

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Two well-established and complementary methodologies to simulate the dynamics of polymers in solution are (i) Brownian Dynamics (BD), and (ii) Molecular Dynamics coupled dissipatively to a lattice Boltzmann background (MD/LB). The talk gives a brief introduction into both methods, and then presents results of a recent comparative study that applied both methods to the same model of a single chain that moves in a solvent under the influence of thermal noise. Emphasis is put on the question how to map the parameters onto each other, in particular those that are crucial for the dynamics. The agreement of static properties is perfect, as it must be. The dynamic properties agree very well, if for the MD/LB case the effects of finite box size are eliminated by extrapolation. We also find that proper thermalization of all MD/LB degrees of freedom (including the so-called “kinetic modes”) is necessary. Small deviations between BD and MD/LB remain as a result of the different simulation methodologies. Finally, the computational efficiency of the two methods is compared. For the single-chain system, BD is clearly much faster, while scaling estimates suggest that the opposite is true for semidilute solutions. References:

- Tri T. Pham, Ulf D. Schiller, J. Ravi Prakash, and B. Dünweg, *J. Chem. Phys.* **131**, 164114 (2009).
- B. Dünweg and A. J. C. Ladd, *Adv. Polym. Sci.* **221**, 89 (2009).

¹support by Volkswagen Foundation; collaboration with Monash University