

Hybrid Particle-Field Molecular Dynamics Under Constant Pressure

Sigbjørn Løland Bore^{1*}, Giuseppe Milano² and Michele Cascella¹

¹ Department of Chemistry, and Hylleraas Centre for Quantum Molecular Sciences University of Oslo, Norway

² Department of Organic Materials Science, Yamagata University, Japan

* s.l.bore@kjemi.uio.no

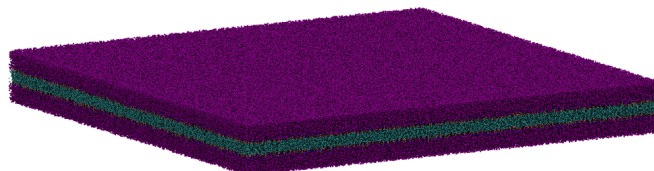


Figure 1: System setup for a coarse grained 130 nm \times 130 nm phospholipid-bilayer (DOPC).

Hybrid-particle-field molecular dynamics (hPF-MD) is becoming an established method for simulating large molecular systems at the coarse grained level [1]. In hPF-MD the non-bonded interactions, which computationally is the most expensive part of MD, are modelled in a density-functional approach. Instead of computing forces between pairs, particles are subject to forces due to the densities of the surrounding particles. This reduces significantly the communication needed for pair-lists in ordinary MD, allowing for applications on large systems with optimal scalability with the number of processors [2]. A particular success of this method has been its ability to model lipid bilayers, with electron density profiles and area per lipid in good agreement with experiments and simulations based on interacting particle potentials [3]. In fact, due to methodological limitations, so far applications have been run under constant volume conditions. For lipid-bilayers this is problematic as it does not ensure simulations under proper tensionless conditions obtained in constant pressure simulations. This talk presents the extension of hPF-MD to constant pressure simulations. Using the thermodynamic definition of pressure, pressure-contributions from the density-fields are derived. By systematic parameterization of constants in the density-field terms, we obtain the correct overall density of water and lipid-bilayers at 1 bar. The lipid-bilayers of previous NVT-simulations are found to have a net surface-tension, but by using an extra square-gradient term between the bilayer and water [4], tensionless lipid-bilayers at the correct area per lipid are obtained. Finally, using the parameters giving tensionless lipid-membranes, applications on lipid-bilayers up to 100s of nanometers are presented (Figure 1).

References

- [1] Milano, G. and Kawakatsu, T. *Hybrid particle-field molecular dynamics simulations for dense polymer systems*. J. Chem. Phys. **130** 214106 (2009).
- [2] Zhao, Y., De Nicola, A., Kawakatsu, T., and Milano G. *Hybrid particle-field molecular dynamics simulations: Parallelization and benchmarks*. J. Comput. Chem. **33**, 868–880 (2012)
- [3] Soares, T.A., Vanni, S., Milano, G. and Cascella, M. *Toward chemically resolved computer simulations of dynamics and remodeling of biological membranes*. J. Phys. Chem. Lett. **8**, 3586–3594 (2017)
- [4] Sgouros, A. P., Lakkas, A. T., Megariotis, G., and Theodorou, D. N. *Mesoscopic Simulations of Free Surfaces of Molten Polyethylene: Brownian Dynamics/Kinetic Monte Carlo Coupled with Square Gradient Theory and Compared to Atomistic Calculations and Experiment*. Macromolecules **51**, 9798-9815 (2018)