Development and implementation of hybrid atomistic / coarse grained modelling applied to interfaces

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Multiscale simulations combine different levels of detail to understand the behaviour of a system across various time and length scales and in different environments. The term “system” includes, but is not limited to, soft matter, polymers, electrolytes, colloids, and biomolecules. To thoroughly study the physical, kinetic and thermodynamic properties of these systems, several scales need to be sampled, and this requires a compromise between the resolution and computational cost. Along with the advent of modern computers and high-performing facilities, different strategies were developed to improve the model in terms of both accuracy and computational efficiency. In my PhD work, I am working on the development and implementation of a hybrid coupling scheme that combines atomistic and coarse-grained resolutions in the same simulation box, allowing the particles in the system to change their resolution “on the fly” during the course of the simulation, and this method is being implemented in LAMMPS 2023 [1]. One such method has already been developed for bulk liquids [2][3], but never for solids or solid/liquid or solid/gas interfaces. We started with studying the metal-organic framework ZIF-8 [4] in dual resolution as a proof of concept. We also studied ZIF-8/PVDF and ZIF-8/CO_2 systems. Along with the method and implementations, we will evaluate how the application of this method affects the quality of the estimated radial distribution functions, cell characteristics, and dipole orientations.

Keywords : Multiscale simulation; All atom/ Coarse graining; ZIF-8; Interfaces;MOF/polymer; MOF/gas;

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