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Event-driven simulation of nearly hard spheres at low temperature

Event-driven molecular dynamics (EDMD) simulations have proven to be particularly robust for simulating hard sphere systems. They offer insights into a variety of self-assembly processes, among which crystal nucleation remains a topic of interest. Experimentally, colloidal hard spheres have been achieved with great success, but open questions remain regarding discrepancies in nucleation rates estimates. As a result, it is interesting to consider slightly softer interactions, that are expected to shift the solid-fluid coexistence region and lower the solid-fluid surface free energy, thus playing a role in speeding up the nucleation process. In this work, we investigate the approach introduced by Peters and de With [1] to simulate sharp continuous pair-wise interaction potentials by combining EDMD and Monte-Carlo methods. More specifically, this approach is applied here to the purely repulsive Weeks-Chandler-Andersen potential at very low temperatures. We focus on comparing this approach with conventional molecular dynamics (MD) simulations in terms of both system dynamics and efficiency. This is of particular interest as conventional time-driven MD simulations require increasingly smaller time-steps to accurately describe sharper interactions, while event-driven simulations can be highly efficient even in the limit of perfectly hard spheres. Hence, this approach opens the door to more efficient and detailed studies of the effects of softness on the spontaneous nucleation of nearly hard spheres.

[1] E. A. J. F. Peters and G. de With, Phys. Rev. E 85, 026703 (2012)

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