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Assessing the applicability of Brownian Dynamics to simulation of nanoparticle clustering in liquid suspensions SERGIY MARKUTSYA, SHANKAR SUBRAMANIAM, MONICA LAMM, DENNIS VIGIL, RODNEY FOX, Iowa State University — Brownian Dynamics (BD) is an attractive approach to simulate solute nanoparticles in a suspension of solvent molecules because it exploits the separation of time scales between solvent and solute dynamics to avoid explicit representation of the solvent molecules. In BD a nanoparticle's velocity evolves because of interaction with other nanoparticles through a systematic pairwise interaction force, while the effect of the solvent molecules on the nanoparticles is represented by a combination of frictional and random forces (Langevin part). This Langevin equation for the velocity is solved along with the nanoparticle position evolution, and we denote this the Position-Velocity Langevin (PVL) system. If the momentum relaxation time of the nanoparticles is itself rapid and long-time configurational dynamics are of interest, then Ermak and McCammon showed that it is possible to reduce PVL to a Position Langevin (PL) equation system. The reduction from PVL to PL gives a significant gain in computational time, however, it was not clear if PL approach describes clustering adequately. Preliminary analysis indicates that the clustering regime does not admit the time scale separation for latex nanoparticles in water. While BD has been used to study such phenomena as diffusion, the purpose of this study is to ascertain whether BD can be used to model the clustering of nanoparticles in liquid suspension.

Sergiy Markutsya

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