

Abstract Submitted  
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**Stochastic Rotational Dynamics Simulations of Nanocolloid Suspensions**<sup>1</sup> JEREMY B. LECHMAN, MATT K. PETERSEN, STEVEN J. PLIMPTON, P. RANDALL SCHUNK, GARY S. GREY, Sandia National Laboratories, PIETER IN'T VELD, Polymer Research, BASF — The use of nanoparticle suspensions to potentially tailor the functionality of composite devices has broad applicability, but is limited in practice, in part, due to poor understanding of the phenomena at that scale. In order to address this we have implemented a mesoscale fluid technique called Stochastic Rotation Dynamics (SRD). Here, we discuss the use of this method to investigate the behavior of hard sphere like nanocolloids. In particular we will present a direct, “one-to-one” comparison of an SRD fluid with an explicit Lennard Jones solvent. For small colloids in this low viscosity fluid no “telescoping of timescales” is required for efficiency, which allows us to consider the accuracy of the base numerical scheme without complicating approximations. We present the diffusion and reduced viscosity as a function of volume fraction of colloids and compare to well known results. The efficiency of an SRD simulation relative to an explicit atom simulation is also discussed.

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