Stokesian Dynamics of colloidal suspensions in extensional flow

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ABSTRACT

Molecular Dynamics methods have been applied to the study of Soft Matter systems in order to develop numerical simulations of dense hard-spheres suspensions in Newtonian fluids under several background flow conditions. Low Reynolds numbers induce important simplifications of the flow equations, therefore Stokesian Dynamics provides a computational study of suspensions rheology.

The principal aim of the work is to show the validity and versatility of the methodology based on a box-deformation scheme developed by **Andersen, Parrinello and Rahman (1981)**, as an efficient computational technique to describe the behavior of suspensions of particles under generic flow conditions.

First, the work has demonstrated the consistency of numerical results with the method developed by **Lees and Edwards (1972)** for simple shear flow conditions. Consequently, the computational technique has been adapted to describe planar and three-dimensional extensional flows.

The idea of the deformation of the computational box and the box-reinitialization strategy of **Kraynik and Reinelt (1992)** have provided unrestricted time numerical simulations for extensional flows. Perpetual simulations generated a computational study of quantities of rheological interest, such as the effective viscosity of suspensions. The stability of the code showed the robustness of numerically-computed macroscopical properties against the computationally-induced ordering effect of shear-flow simulations.

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