

Towards a deterministic kinetic theory approach of colloidal suspensions

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Usual models of colloidal suspensions proceed within the Brownian dynamics (BD) framework. Thus, suspended particles are subjected to different kind of forces coming from the fluid drag, inter-particles potentials, particles-solvent interaction, Brownian forces describing the bombardment that colloidal particles suffer from other solvent and colloidal particles, As soon as the position and eventually the momentum of all the colloidal particles are known the virial stress could be computed without any major difficulty. However, the tracking of all the particles in the population implies significant time computing in order to limit the inherent statistical noise that stochastic simulations induce.

An alternative to the BD simulations lies in deriving a continuum and deterministic kinetic theory description. This formulation leads to the so called Fokker-Planck equation that instead of describing the position (and momentum) of all the particles, it gives the evolution of the probability distribution function that in the general case represents the fraction of particles that at certain point and time have a certain momentum. The Fokker-Planck equation is an advection-diffusion equation defined in both the physical and the conformation space. In colloidal systems the physical space consists of the usual 3D space and time, and the conformational space reduces in general to the velocity, but richer descriptions could be stated. If the velocity is ignored as a model conformational coordinate the resulting equation reduces to the usual advection-diffusion equation (fully defined in the usual physical space).

The main difficulty in deriving the deterministic counterpart of Brownian dynamics models for colloidal suspensions lies in the consideration of general potentials, others than the electrostatic one. The effects of general potentials could be taken into account explicitly in the drift term or it could be approximated and included in the diffusion one, as in usual LCP models.

This work presents some first attempts for elaborating deterministic descriptions of colloidal systems.