Event-Driven Brownian Dynamics

A. Scala[1], Th. Voigtmann[2]
[1]*Physics dept. and INFM-CNR SMC, Univ. di Roma "La Sapienza", P.le Aldo Moro 2, 00185 Roma, Italy*
[2]*Scottish Universities Physics Alliance, School of Physics, The University of Edinburgh, JCMB King's Buildings, Edinburgh EH9 3JZ, U.K.*

The blossoming of interest in colloids and nano-particles has given renewed impulse to the study of hard-body systems. In particular, hard spheres (HS) have become a real test system for theories and experiments. At the colloidal length scales objects can behave as hard bodies while being still small enough to exhibit thermal or Brownian motion in a solvent. Dynamical light scattering has already provided a rich collection of data for such systems, encouraging a considerable effort in understanding the dynamics; the possibility of following single particle trajectories via confocal microscopy of latex particles has allowed a direct view on an experimental realization of HS systems and their dynamics.

The simplest model of a suspension of neutral particles is to consider a system of HS in an ideal solvent with no hydrodynamic interactions; real suspensions are often described in terms of their deviations from such ideal system and many theoretical results have been derived especially at low and intermediate packing fractions. While hydrodynamic interactions (HI) are well understood at low particle densities, much less is known at high densities, and theories often proceed by claiming them irrelevant. Non-HI simulations therefore have their place in testing such theories, and in circumventing the huge effort needed to simulate HI, should the claim be true.

In order to validate non-HI theories it is necessary to use computer simulations, as only a qualitative agreement is to be expected among non-HI theories and data for real suspension. Standard simulation methods for Brownian dynamic require continuous potentials; to circumvent such problem several algorithms have been introduced (with various degrees of justification) for the overdamped dynamics only recently it has been recognized that in the case of hard interactions such simulations are better performed by event-driven (ED) codes [1,2,3].

Starting from an expansion of the stochastic propagator we introduce a new ED algorithm that allows the simulation of the full Brownian dynamics. To overcome the inefficiency at high viscosity of such algorithm, we introduce a more efficient ED algorithm based on a short time approximation of the stochastic two-body hard collision. In doing so, we extend the image method for a random walker in the presence of a reflecting wall to the case of full Brownian walker.

[1] P. Strating, PRE **59**, 2175 (1999).
[2] Yu-Guo Tao et al, J. Chem. Phys. **124**, 134906 (2006).
[3] A. Scala, C. De Michele and Th. Voigtmann, J. Chem. Phys. **126**, 134109 (2007).