Full Brownian Dynamics simulation techniques for Hard Spheres

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Hard spheres, thanks to the blossoming fields of colloids and nano-particles, have become a real test system for theories and experiments. Several theoretical approaches, including Mode Coupling, often disregard hydrodynamic interactions when trying to study the dynamics of such systems in presence of a solvent.

Numerical integrations of the equation of motion are the ancillary techniques to such analytical theories; unfortunately,standard algorithms require that interactions are slowly varying during an integration timestep. This in not the case for hard-body systems, where there is no clearcut between the correlation time of the noise and the timescale of the interactions.

To leapfrog such issues, new event-driven techniques must be introduced.

First, we introduce a general algorithm based on the splitting of the Fokker-Plank operator associated with the Brownian dynamics and discuss its limitations.

We then revise a previously introduced event driven scheme for the overdamped Brownian dynamics by extending the algorithm to the case of inhomogeneous hard sphere systems.

Finally, we extend the algorithm to the case of the full Brownian dynamics.