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Improving the Efficiency of BD Algorithms for Biological Systems Simulations

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ABSTRACT

The simulation of complex biological systems such as ion channels require very efficient and accu rate computer models. A Particle Particle Particle Mesh (P^3M) force field scheme for molecular and Brownian dynamics simulations was developed to improve the original approach proposed by Hock ney [1], allowing the simulation of non periodic systems by computing the Particle Mesh component in real space [2]. An assessment methodology for the error associated with the force computation within this framework was also developed in a previous work [3], together with the analysis of the accuracy and efficiency of the P^3M approach.

In this work, this error analysis methodology is applied to the study of various integration schemes used in Brownian Dynamics algorithms. The dura tion of the timestep between two successive inte grations of the particle motions governs the trade off between the accuracy of the particle trajectories and the time required for the simulation. Three algorithms have been compared for the integration of the full Langevin equation [4]. A first order Euler scheme [2], the Verlet like algorithm proposed by [5], and a novel Predictor Corrector scheme [6] have been implemented and analyzed using our assessment methodology. Our results, presented in Fig. 1 show the maximum value of the Radial Distribution Function (RDF) of K^+ and Cl^- ions as a function of the timestep duration for the three integration schemes and an analytical calculation based on the Hypernetted Chain approximation [3]. It can be seen that a significant increase in the integration timestep, and a subsequent reduction in computational cost, is obtained with the Predictor Corrector scheme, while maintaining an excellent accuracy for the description of both structure and dynamics of the electrolyte solution.

While the methodology discussed in [3] focuses on equilibrium properties of bulk electrolyte solu tions, this work extends the analysis to dynamic properties of the solution as well as the structural aspects of inhomogeneous systems such as a lipid membrane. The conductivity of bulk KCl electrolyte solutions is computed with the Predictor Corrector integration scheme and compared to published data. Furthermore, the simulation of a dielectric mem brane separating two electrolyte solutions and sub jected to an applied potential is performed as well. The ionic distribution in this non periodic system, such as the KCl solution in Fig. 2 shows the pre dicted accumulation of ions of opposite signs on the membrane surfaces. This distribution is compared to the theoretical prediction of the double layer theory of Gouy and Chapman [7] to validate the highly efficient modeling scheme proposed here.

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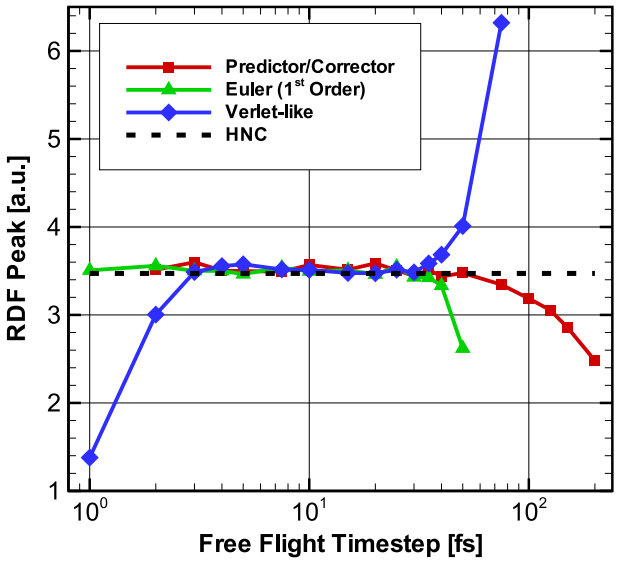

Fig. 1. Comparison of 3 different integration schemes for a range of integration timesteps. The RDF peak value for a bulk KCl solution of 0.30 M is used as a benchmark and compared to the analytical HNC result.

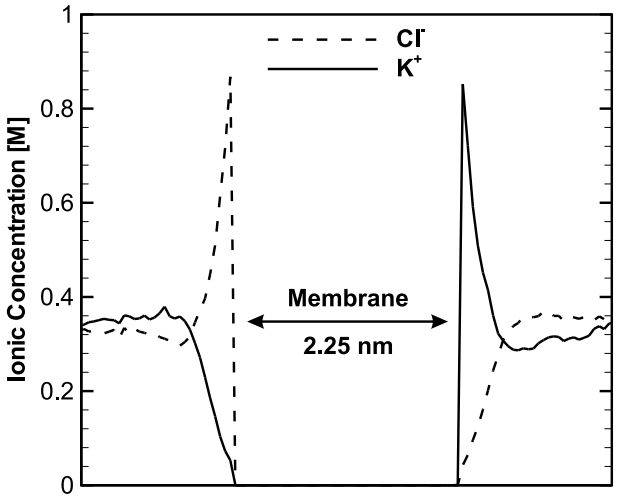

Fig. 2. Ionic distribution from a KCl 0.30 M solution in the vicinity of a dielectric membrane subjected to a potential of 1.0 V.