Particle-Based Simulation of Bio-Electronic Systems

Marco Saraniti – EE Department – Arizona State University

The talk will offer a review of the latest algorithmic work performed on particle-based methods for the simulation of both wild, i.e. naturally occurring, and man-made biological systems. Several needed improvements will be discussed, as well as the potential of the current algorithms for modeling systems of higher complexity with a minimal set of input parameters.
In particular, the crucial aspects and applications of a new algorithm will be discussed: the real-space Particle-Particle—Particle-Mesh (P^3M) force-field scheme for the selectively constrained Brownian Dynamics simulation of non-periodic biological systems.

Traditionally, both Brownian Dynamics (BD) and Molecular Dynamics (MD) simulations of biological systems are performed by imposing periodic boundary conditions on the computational domain. This negatively affected the capability of simulating systems with complex geometry, concentration gradients at the boundary, and embedded equipotential regions such as shaped electrodes. A new non-periodic force-field scheme based on the solution of Poisson's equation in the real rather than the reciprocal space will be discussed during the talk. Such scheme allowed the Brownian Dynamics simulation of nanoscale protein electrophoresis in electrolytic solutions over geometrically complex computational cells.