

ABSTRACTS

25: D. Boda, D. Gillespie: Steady state electrodiffusion from the Nernst-Planck equation coupled to Local Equilibrium Monte Carlo simulations. *J. Chem. Theory Comp.*, 8 (2012) 824-829

We propose a procedure to compute the steady-state transport of charged particles based on the Nernst–Planck (NP) equation of electrodiffusion. To close the NP equation and to establish a relation between the concentration and electrochemical potential profiles, we introduce the Local Equilibrium Monte Carlo (LEMC) method. In this method, Grand Canonical Monte Carlo simulations are performed using the electrochemical potential specified for the distinct volume elements. An iteration procedure that self-consistently solves the NP and flux continuity equations with LEMC is shown to converge quickly. This NP+LEMC technique can be used in systems with diffusion of charged or uncharged particles in complex three-dimensional geometries, including systems with low concentrations and small applied voltages that are difficult for other particle simulation techniques.