ABSTRACTS

22: D. Boda, R. Kovács, D. Gillespie, T. Kristóf. Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernst-Planck equation. *J. Mol. Liq.*, 189 (2014) 100-112

We have recently introduced the Local Equilibrium Monte Carlo (LEMC) technique (Boda, Gillespie, J. Chem. Theor. Comput. 8 (2012) 824-829.) in which a non-equilibrium system is divided into small volume elements and separate Grand Canonical Monte Carlo simulations are performed for each using a local intensive parameter, which, as soon as local equilibrium is assumed, can be identified with the local electrochemical potential. The simulation provides the concentration profiles of the steady-state diffuse system, where ions are transported through a membrane from one bulk compartment to the other. The dynamics of the ions is described with the Nernst-Planck (NP) transport equation. The NP equation is coupled to the LEMC simulations via an iteration procedure that ensures that conservation of mass (the continuity equation) is satisfied. We apply the method to a simple calcium channel model and demonstrate its efficiency. The computer experiments are inspired by real electrophysiological experiments for the Ryanodine Receptor calcium channel. The diffusion coefficients in the channel are fitted to results of Dynamic Monte Carlo simulations.