ABSTRACTS

23: Z. Ható, D. Boda, T. Kristóf: Simulation of Steady-State Diffusion: Driving Force Ensured by Dual Control Volumes or Local Equilibrium Monte Carlo. *J. Chem. Phys.*, 137 (2012) 054109 :1-14

We provide a systematic comparative analysis of various simulation methods for studying steady-state diffusive transport of molecular systems. The methods differ in two respects: (1) the actual method with which the dynamics of the system is handled can be a direct simulation technique [molecular dynamics (MD) and dynamic Monte Carlo (DMC)] or can be an indirect transport equation [the Nernst-Planck (NP) equation], while (2) the driving force of the steady-state transport can be maintained with control cells on the two sides of the transport region [dual control volume (DCV) technique] or it can be maintained in the whole simulation domain with the local equilibrium Monte Carlo (LEMC) technique, where the space is divided into small subvolumes, different chemical potentials are assigned to each, and grand canonical Monte Carlo simulations are performed for them separately. The various combinations of the transport-methods with the driving-force methods have advantages and disadvantages. The MD+DCV and DMC+DCV methods are widely used to study membrane transport. The LEMC method has been introduced with the NP+LEMC technique, which was proved to be a fast, but somewhat empirical method to study diffusion [D. Boda and D. Gillespie, J. Chem. Theor. Comput. 8, 824 (2012)]. In this paper, we introduce the DMC+LEMC method and show that the resulting DMC+LEMC technique has the advantage over the DMC+DCV method that it provides better sampling for the flux, while it has the advantage over the NP+LEMC method that it simulates dynamics directly instead of hiding it in an external adjustable parameter, the diffusion coefficient. The information gained from the DMC+LEMC simulation can be used to construct diffusion coefficient profiles for the NP+LEMC calculations, so a simultaneous application of the two methods is advantageous.