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Brownian Simulations and Uni-Directional Flux in Diffusion

AMIT SINGER, ZEEV SCHUSS, Department of Mathematics, Tel Aviv University

— Brownian dynamics simulations of ion permeation in protein channels require the connection of a small discrete simulation volume to large baths that are maintained at fixed concentrations and voltages. Average boundary concentrations have to be maintained at their values in the baths by injecting and removing particles at the boundary of the simulation volume. The particles injected into the simulation volume represent a unidirectional diffusion flux. The classical diffusion equation defines net diffusion flux, but not unidirectional fluxes. The stochastic formulation of classical diffusion in terms of the Wiener process leads to a Wiener path integral, which can split the net flux into unidirectional fluxes. These unidirectional fluxes are infinite, though the net flux is finite and agrees with classical theory. We find that the infinite unidirectional flux is an artifact caused by replacing the Langevin dynamics with its Smoluchowski approximation, which is classical diffusion. We find that the probability of Brownian trajectories that cross an interface in one direction in unit time Δt equals that of the probability of the corresponding Langevin trajectories if $\gamma\Delta t = 2$. This unidirectional flux is proportional to the concentration and inversely proportional to $\sqrt{\Delta t}$ to leading order. We develop a BD simulation that maintains fixed average boundary concentrations in a manner consistent with the actual physics of the interface and without creating spurious boundary layers.

Amit Singer
Department of Mathematics, Tel Aviv University

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