Special

PHYSICAL MATHEMATICS SEMINAR

BROWNIAN SIMULATIONS AND UNI-DIRECTIONAL FLUX IN DIFFUSION

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ABSTRACT:

Existing continuum descriptions of ionic permeation through protein channels fail to capture the rich phenomenology of the permeation process, so it is therefore necessary to resort to particle simulations. Brownian dynamics (BD) simulations require the connection of a small discrete simulation volume to large baths that are maintained at fixed concentrations and voltages. The continuum baths are connected to the simulation through interfaces, located in the baths sufficiently far from the channel. Average boundary concentrations have to be maintained at their values in the baths by injecting and removing particles at the interfaces. The particles injected into the simulation volume represent a unidirectional diffusion flux, while the outgoing particles represent the unidirectional flux in the opposite direction. 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 (LD) with its Smoluchowski approximation, which is classical diffusion. The Smoluchowski approximation fails on time scales shorter than the relaxation time $1/\gamma$ of the Langevin equation. 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 BD and LD simulations that maintain fixed average boundary concentrations in a manner consistent with the actual physics of the interface and without creating spurious boundary layers.

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