

Dynamical picture of ion permeation

Ion channels are natural nanotubes in cellular membranes that control a vast range of biological functions in health and disease. They are highly selective with respect to the charge and/or size of the ions passing through them. They are a primary target of the pharmaceutical industry. Analogous to nano-scale transistors, they are present in the membranes of all biological cells. Accordingly, their main properties - structure, conformational changes, selectivity, conductivity, and gating - are subject to intensive, ever-growing, fundamental and applied research.

The molecular structures of some channels have been determined by crystallographic analysis, including the KcsA channel that discriminates (selects) between Na⁺ and K⁺. These structures provide the experimental information needed for molecular modelling (molecular dynamics) of the dynamical features of the observed selectivity. However this molecular dynamics modelling is very time consuming and a simpler description is desirable. Such description can be formed by considering ions as particles moving in potential fields under stochastic forces and it is called Brownian dynamics.

In this project it is suggested to develop Brownian (stochastic) dynamics models of ion permeation (conduction) on the base of analysis of ion trajectories coming from molecular dynamics simulations. The project is based on the outgoing research project in CSC. The key feature of the developing model is the introduction of explicit coupling between ions and water molecules inside and outside of ion channel. Preliminary results show that dynamics of a single ion is characterized by long-range correlation (1/f spectrum). The challenge is to characterize the coupling of ions having long-range correlation properties.

Please contact [\[redacted\]](#) to discuss the details of the project.