Adaptation of Computational Electronics approaches for Transport Simulation of Ionic Channels

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Abstract: Ionic channels are natural nanotubes that permeate the membrane of cells, performing a wide variety of sensing and actuating functions to control the cell environment. These structures have become of great interest to the solid-state community, because they might be utilized as devices in future applications, or show the way to realize artificial channels with similar properties.

Simulation of ionic channels is difficult because of a number of reasons. First, the nanopore consists of a protein structure, usually with a strong distribution of electrical charge. Only for a few channels the complete structure is known from measurements, and even then, it is difficult to know how the structure configuration might change in different operation states. Second, in most ionic channels a successful ion traversal event is a rare event. Conduction in channels is therefore a time-multiscale problem where detailed transport should be resolved perhaps on femtosecond scale, while the macroscopic behavior requires observation on typical biological time scales, on the order of milliseconds or more.

A number of simulation approaches have been pursued for ionic channels. The most detailed one involves molecular dynamics, where both ions and water molecules in the environment are simulated. Although this approach provides key information regarding the mechanisms of ion permeation, the computational cost makes it prohibitive for practical investigation of ionic channels as device structures. On the end of the spectrum, continuum models based on drift-diffusion flow provides a relatively fast solution of ionic flow so that complete current-voltage curves may be computed. However, a number of approximations are built in the standard continuum models. Following a similar path as in solid-state device simulation, there is great interest in the development of a reduce particle simulation model where the random nature of the transport and the finite size of ions is naturally included, while interaction between ions and water is introduced in a simplified way to reduce computational cost.

This talk will discuss the development of simulators for ionic channels, based on the drift-diffusion and on the particle Monte Carlo methods, which in many ways extend similar approaches used in semiconductor simulation. Examples will be given for simulation of gramicidin and ompF porin channels. Performance of the implementation and limitations of the models will also be discussed.