Particle-Based Simulation of Ionic Charge Transport through Biological Ion Channels: Numerical Issues

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Abstract: The authors are Shela Aboud, Department of Molecular Biophysics and Physiology Rush University Chicago, IL Marco Saraniti Department of Electrical and Computer Engineering Illinois Institute of Technology Chicago, IL Bob Eisenberg Department of Molecular Biophysics and Physiology Rush University Chicago, IL Ion channels are an important class of proteins responsible for controlling the ion flux into and out of biological cells. Recent advances in experimental techniques have triggered the study of ion channels both in vivo and in vitro, making readily available to theoreticians a large amount of extremely reliable data. However, besides the molecular structure of the protein itself, several components define the physical environment that must be accounted for to realistically model the channel functionality. In particular, the lipid membrane structure, together with the water-ion interaction must be realistically modeled. Furthermore, an adequate set of electrostatic boundary conditions should be implemented on the computational box in order to properly model the basic interactions of the ion-channel-solvent system. This talk will introduce a discussion on the numerical and modeling challenges related to the implementation of efficient and realistic particle-based simulation tools for charge transport in biological ion channels. Simulation results will be shown as well.