Biological Ion Channels: Theory and Simulation

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Abstract

Ion channels are porous membrane proteins that control the flow of ions across cell membranes and play vital roles in various physiological processes in human body. Ion channel dysfunction can cause many diseases such as cardiac, neurological, renal, endocrine, and bone disorders. Single channel recordings are performed in thousands of laboratories worldwide on a daily basis using the patch clamp technique invented by the Nobel laureates Sakmann and Neher in 1970s. However, there are relatively very few simulation tools for calculating single ion currents under physiological or experimental conditions, which can assist experimentalists in the study of normal or mutated ion channels based on the crystal structures provided by the Protein Data Bank before experimentation. The Poisson-Nernst-Planck-Fermi theory we proposed in recent years is a Continuum-Molecular theory that can be used to simulate ion currents in biological ion channels under physiological or experimental conditions. PNPF treats ions and water as non-uniform hard spheres, and accounts for interstitial voids between spheres, as well as important physical properties such as water polarization and ion correlation. Numerical methods for solving the PNPF model includes an extended (optimal) Scharfetter-Gummel (SG) method to discretize the Nernst-Planck equation for ion and water transport in ion channels at atomic scale and a simplified matched interface and boundary method for treating molecular surfaces and singular charges of channel proteins. The extended SG method is shown to exhibit important features in flow simulations such as optimal convergence, efficient nonlinear iterations, and physical conservation.

Keywords: **Ion Channel Proteins, Continuum-Molecular Model, Numerical Methods**

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