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Abstract for an Invited Paper
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Calculating Ion Permeation through Biological Channel Proteins[1]

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We have developed methodology to simulate the current of ions (Na+, Cl-, etc.) through a general three-dimensional ion channel structure embedded in a lipid bilayer when an electric potential is applied across the membrane. These calculations are done at the level of Brownian dynamics, i.e., ions are treated as particles and their motion is computed using a stochastic algorithm which simulates Brownian motion. Water solvent is treated as a dielectric continuum, which both supplies the thermal agitation underlying the motion of the ions and influences the electrostatic forces on these ions by virtue of its dielectric constant (which differs substantially from that of the protein-membrane complex). Application is made to the Glycine Receptor channel, emphasizing physico-chemical influences on ion current, e.g., charges of critical pore-lining amino acids, channel geometry, etc.

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