Continuum modeling of biomolecular electrostatics and diffusion using FEM/BEM

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Abstract

Continuum models are commonly used to combine with molecular model in order to bridge different scales and to take into account the average influence of solvent environment on molecular processes. Nano-sclae and macromolecular electrostatics and ion transport in ion channel/nanopores are our focused interests. The governing equations of these phenomena are the Poisson-Boltzmann/Poisson-Nernst-Planck equations and their improved forms. We developed a complete simulation tool chain. They include fast boundary element solution and stabilized finite element simulation packages, molecular meshing tool TMSmesh and visualization software VCMM. We are also making effort to provide a web-based simulation service. The methods are applied to calculate macromolecular electrostatics, current-voltage curve of ion channels (physiological property) with wide pores, nanotube simulations with time-dependent (varying) boundary conditions (voltage scanning), as well as to predict the current signals of a DNA-nanopore system for gen sequencing.

Keywords: Biomolecular electrostatics and diffusion, Nanopore, BEM/FEM, Fast algorithm, Meshing, Visualization.

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