

Continuum Modeling of Electrostatic Induced Macromolecular Deformation

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Abstract

The conformational change in large spatial and temporal scale is essential for the proper functions of macromolecules such as ion channel gating, membrane transport and molecular motors; These large deformations usually involve the electrostatic force as the major driving force. This study is focused on the continuum modeling and computation of the electrostatic force and its coupling with the large macromolecular deformation modeled as nonlinear elastic displacement. We will study the regularity and the solvability of these electro-elasticity equations, efficient and accurate evaluation of electrostatic forces from the Poisson-Boltzmann equation, and demonstrate the applications of our model to an important biological process: the BAR domain-induced membrane curvature. Mathematical problems related to the refinement of our model will be highlighted.