DOCTORAL THESIS

Numerical solution for nonlinear Poisson-Boltzmann equations and numerical simulations for spike dynamics

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Numerical Solution for Nonlinear Poisson-Boltzmann Equations and Numerical Simulations for Spike Dynamics

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Abstract

This thesis consists of two independent parts. The first part is concerned with the numerical solutions of the nonlinear Poisson-Boltzmann equations posed on some irregular solution domains. Since the solution domains are not of regular shape, it is difficult to design high-order and efficient approximation methods using the standard finite difference methods on a uniform Cartesian grid. To fix this problem, two numerical schemes based on finite difference approach are proposed in this thesis. The nonlinear Poisson-Boltzmann equations are linearized and then solved by certain monotone iterative methods. The linearized equations are discretized by a modified central finite difference scheme and an immerse interface method, respectively. One of the most important advantages for these approaches is that it enables us to use the fast Poisson solvers with multigrid and FFT techniques to speed up the computational process. The proposed numerical schemes are employed to solve the Poisson-Boltzmann equation for two charged spherical particles and for two charged parallel cylinders.

In the second part of this thesis, numerical schemes based on adaptive grid methods are designed for simulating the spike dynamics governed by the two-dimensional Gierer-Meinhardt Model. The moving mesh finite element method is employed in the numerical simulations. Numerically, we verify some stability properties of the spike dynamics following some recent asymptotic analysis results. Moreover, some spike oscillation and splitting phenomenon observed in one-dimensional analysis and computations are discussed using our two-dimensional computational results. On the computational side, it is observed that we can obtain accurate numerical results with much less grid resolution if the moving mesh methods are employed.

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