Some Studies on Finite Element Computing for the Poisson-Boltzmann Equation

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In this thesis, the finite element solution of the Poisson-Boltzmann equation (PBE) is studied. First, a local averaging type of a posteriori error estimators is established and analyzed for a nonlinear elliptic problem of second order in three dimensions. Based on this type of estimators, an adaptive algorithm is designed and applied to solving the Poisson-Boltzmann equation. Second, to deal with the point source type of singularities in PBE, a two-scale error analysis for the finite element solution of Green function of a three-dimensional second order linear elliptic problem is provided, which may be viewed as another type of analysis for adaptive computing. Finally, a defect correction scheme for improving approximation accuracy of discrete Green function is presented and analyzed. It is shown by a series of numerical examples that the efficiency of solving the Poisson-Boltzmann equation and related problems has been much improved by using our algorithms.

Keywords: Poisson-Boltzmann equation, Green function, a posteriori error estimator, adaptive algorithm, defect correction scheme, two-scale.