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Adaptive Finite Element Modeling Techniques for the Poisson-Boltzmann Equation

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Abstract. We consider the design of an effective and reliable adaptive finite element method (AFEM) for the nonlinear Poisson-Boltzmann equation (PBE). We first examine the two-term regularization technique for the continuous problem recently proposed by Chen, Holst and Xu based on the removal of the singular electrostatic potential inside biomolecules; this technique made possible the development of the first complete solution and approximation theory for the Poisson-Boltzmann equation, the first provably convergent discretization and also allowed for the development of a provably convergent AFEM. However, in practical implementation, this two-term regularization exhibits numerical instability. Therefore, we examine a variation of this regularization technique which can be shown to be less susceptible to such instability. We establish *a priori* estimates and other basic results for the continuous regularized problem, as well as for Galerkin finite element approximations. We show that the new approach produces regularized continuous and discrete problems with the same mathematical advantages of the original regularization. We then design an AFEM scheme for the new regularized problem and show that the resulting AFEM scheme is accurate and reliable, by proving a contraction result for the error. This result, which is one of the first results of this type for nonlinear elliptic problems, is based on using

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continuous and discrete *a priori* L^∞ estimates. To provide a high-quality geometric model as input to the AFEM algorithm, we also describe a class of feature-preserving adaptive mesh generation algorithms designed specifically for constructing meshes of biomolecular structures, based on the intrinsic local structure tensor of the molecular surface. All of the algorithms described in the article are implemented in the Finite Element Toolkit (FETK), developed and maintained at UCSD. The stability advantages of the new regularization scheme are demonstrated with FETK through comparisons with the original regularization approach for a model problem. The convergence and accuracy of the overall AFEM algorithm is also illustrated by numerical approximation of electrostatic solvation energy for an insulin protein.

AMS subject classifications: 92-08, 65N06, 65N30, 65N38, 65N50, 92C05

Key words: Poisson-Boltzmann equation, semi-linear partial differential equations, supercritical nonlinearity, singularity, *a priori* L^∞ estimates, existence, uniqueness, well-posedness, Galerkin methods, discrete *a priori* L^∞ estimates, quasi-optimal *a priori* error estimates, adaptive finite methods, contraction, convergence, optimality, surface and volume mesh generation, mesh improvement and decimation.

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1 Introduction

The Poisson-Boltzmann Equation (PBE) has been widely used for modeling the electrostatic interactions of charged bodies in dielectric media, such as molecules, ions and colloids and thus is of importance in many areas of sciences and engineering, including biochemistry, biophysics and medicine. The PBE provides a high fidelity mean-field description of the electrostatic interactions and ionic distribution of a solvated biomolecular system at the equilibrium state and entails singularities of different orders at the position of the singular permanent charges and dielectric interface. The popularity of the PBE model is clearly evidenced by the success of software packages such as APBS, CHARMM, DelPhi and UHBD. We summarize the mathematical PBE model in some detail in Section 2, referring to the classical texts [36, 48] for more physical discussions.

While tremendous advances have been made in fast numerical solution of the PBE over the last twenty years (cf. [25, 26, 35] for surveys of some of this work), mathematical results for the PBE (basic understanding of the solution theory of the PBE, as well as a basic understanding of approximation theory for PBE numerical methods) were fundamentally unsatisfying, due to the following questions about the PBE and its numerical solution which remained open until 2007:

1. Is the PBE well-posed for the dimensionless potential $\tilde{u}$?
2. What function space does the solution $\tilde{u}$ lie in?
3. Can one derive *a priori* (energy and/or pointwise) estimates for the solution $\tilde{u}$?