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Application of Sobolev gradient method to Poisson–Boltzmann system

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ABSTRACT

The idea of a weighted Sobolev gradient, introduced and applied to singular differential equations in [1], is extended to a Poisson–Boltzmann system with discontinuous coefficients. The technique is demonstrated on fully nonlinear and linear forms of the Poisson– Boltzmann equation in one, two, and three dimensions in a finite difference setting. A comparison between the weighted gradient and FAS multigrid is given for large jump size in the coefficient function.

1. Introduction

In this article, a weighted Sobolev gradient is used as a preconditioner to solve the linear and nonlinear Poisson–Boltzmann equation (PBE) with discontinuous coefficient functions. The idea of a weighted gradient, was introduced by Mahavier in [1] who demonstrated its effectiveness in dealing with linear and nonlinear singular differential equations. Sobolev gradients were considered as preconditioners for solution of first order and second order differential equations in [2] in which a one dimensional PBE that arises in semiconductor modeling is considered. An example is also given in [2] of a problem for which the Sobolev gradient method converges but Newton's method does not. In this article, we combine the idea of preconditioning with a weighted Sobolev gradient and present its application to linear and nonlinear PBE. We investigate how well the weighted Sobolev gradient works for large discontinuities in linear and nonlinear PBE and compare to unweighted Sobolev gradient and FAS multigrid.

In [3] Neuberger has introduced and developed the Sobolev gradient technique for solutions of differential equations. This method has proven its usefulness for problems from many fields such as minimization related to Ginzburg–Landau free energy functionals [4,5], the nonlinear Schrodinger equation [6], superconductors [7,8], applications to Differential Algebraic Equations [9], image processing problems [10] and optimal control problems [11]. The underlying idea is to formulate problems in terms of minimizing a functional whose critical points are the desired solutions. The functional that is to be minimized could be a least square functional or energy functional related to the system. Steepest descent is used for the minimization process.

In Section 2, we discuss the PBE in some detail. In Section 3, we build on [1] and give explanations and justifications for a weighted gradient and its possible application to differential equations with discontinuous coefficients. In Section 4, we present problems in the finite difference setting. In Section 5, we give results for numerical test problems for both linear and nonlinear PBE in finite difference settings. In Section 6, we compare the weighted Sobolev gradient with a nonlinear

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multigrid method. In Section 7, details of the software used are given. Finally, in Section 8 we conclude our results and offer possible future improvements.

2. Poisson–Boltzmann equation

This section is an introduction to the PBE and its application in estimating the electric potential around biomolecules. The PBE is an elliptic partial differential equation that models many important phenomena such as charge distributions in semiconductor devices [2] and the protein-folding problem. The PBE is being extensively studied to analyze the properties of the biomolecules in physics and chemistry. Here we present an overview and background of the equation sufficient for this article, interested readers are referred to [12,13] for more analysis and the derivation of the equation. For material covered in this section, we heavily relied upon [12].

When a macromolecule such as a protein is immersed in an ionic solution, a thick layer is formed due to the penetration of solvent ions that prevents contact of the molecule with the ionic solvent. This molecule can be identified with a charged cluster of atoms. The extended Deybe–Hückle theory [12] is used to model this phenomenon. Fig. 1 shows a sketch of the Deybe–Hückle model.

The electrostatic potential anywhere in the region Ω, where Ω is a cubical region as shown in Fig. 1, is given by the PBE

$$-\nabla\cdot(a(x)\nabla u)+\bar{\kappa}^2(x)\sinh(u(x))=\frac{4\pi e_c^2}{\kappa_B T}\sum_{i=1}^{N_m} z_i\delta(x-x_i)\quad x\in\Omega\subset\mathbb{R}^3\quad\text{and } u(x)=g(x), x\in\Gamma \tag{1}$$

Our notation follows Holst's work in his thesis [12]. Here Γ denotes the boundary of the domain Ω and $g(x)$ is some boundary function. e_c denotes the charge of electron, T represents the temperature, k_B the Boltzmann constant. If $q_i=z_i e_c$ represents the charge at the location x_i in the molecular region, z_i is the fraction of charge at the location x_i. The dielectric ε and the modified Debye–Hückle parameter $\bar{\kappa}$ are piecewise constant functions. If Ω_1,Ω_2 and Ω_3 denote molecular region, exclusion layer and solvent respectively, the other two coefficients $\varepsilon,\bar{\kappa}$ and the force term f can be defined below.

i. $a:\Omega\mapsto L(\mathbb{R}^3,\mathbb{R}^3),\quad a_{ij}(x)=\delta_{ij}\varepsilon(x)$

$$\varepsilon(x)=\begin{cases}\varepsilon_1 & x\in\Omega_1\\ \varepsilon_2=\varepsilon_3 & x\in\Omega_2\cup\Omega_3\end{cases} \tag{2}$$

ii. $\bar{\kappa}:\Omega\mapsto\mathbb{R}$,

$$\bar{\kappa}(x)=\begin{cases}0 & x\in\Omega_1\cup\Omega_2\\ \sqrt{\varepsilon_3}\kappa & x\in\Omega_3\end{cases} \tag{3}$$

where κ is the Debye–Hückle parameter that depends on the ionic strength I_s of the solvent and is given by the formula $(\frac{8\pi N_A e_c^2}{1000\varepsilon_3 k_B T})^{1/2} I_s^{1/2}$, where N_A is Avogadro's number.

iii. $f:\Omega\to\mathbb{R}$,

$$f(x)=\frac{4\pi e_c^2}{\kappa_B T}\sum_{i=1}^{N_m} z_i\delta(x-x_i) \tag{4}$$

where $x_1,x_2,\ldots,x_{N_m}\in\Omega_1$ denote the charge locations and $z_1,z_2,\ldots,z_{N_m}$ are associated fractional charges respectively.

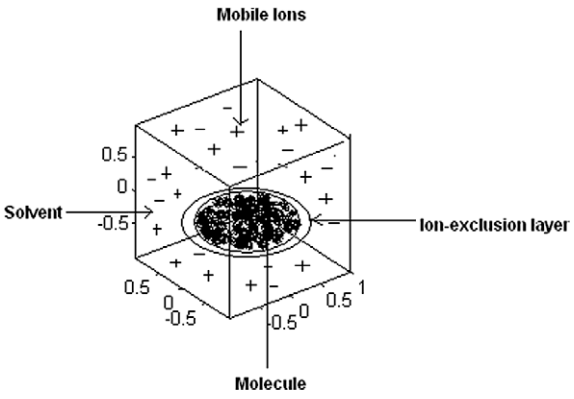

Fig. 1. A sketch of Debye–Hückle model in 3d.