Commun. Comput. Phys.
doi: 10.4208/cicp.270713.280214a

Vol. **16**, No. 2, pp. 491-515
August 2014

An Iterative Discontinuous Galerkin Method for Solving the Nonlinear Poisson Boltzmann Equation

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Received 27 July 2013; Accepted (in revised version) 28 February 2014

Available online 12 June 2014

Abstract. An iterative discontinuous Galerkin (DG) method is proposed to solve the nonlinear Poisson Boltzmann (PB) equation. We first identify a function space in which the solution of the nonlinear PB equation is iteratively approximated through a series of linear PB equations, while an appropriate initial guess and a suitable iterative parameter are selected so that the solutions of linear PB equations are monotone within the identified solution space. For the spatial discretization we apply the direct discontinuous Galerkin method to those linear PB equations. More precisely, we use one initial guess when the Debye parameter $\lambda=\mathcal{O}(1)$, and a special initial guess for $\lambda\ll 1$ to ensure convergence. The iterative parameter is carefully chosen to guarantee the existence, uniqueness, and convergence of the iteration. In particular, iteration steps can be reduced for a variable iterative parameter. Both one and two-dimensional numerical results are carried out to demonstrate both accuracy and capacity of the iterative DG method for both cases of $\lambda=\mathcal{O}(1)$ and $\lambda\ll 1$. The $(m+1)$th order of accuracy for L^2 and mth order of accuracy for H^1 for P^m elements are numerically obtained.

AMS subject classifications: 65D15, 65N30, 35J05, 35J25

Key words: Poisson-Boltzmann equation, nonlinear, existence, uniqueness, DDG methods, numerical flux.

1 Introduction

In this paper, we propose an iterative discontinuous Galerkin method to solve the nonlinear Poisson Boltzmann (PB, for short) equation, following the direct discontinuous

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Galerkin (DDG) method introduced by Liu and Yan [12] for parabolic equations, and then further developed by Huang et al. [13] for linear elliptic equations.

We restrict ourselves to the following nonlinear Poisson Boltzmann model,

$$-\lambda^2\Delta u = f(x) + e^{-u}, \quad \text{in } \Omega, \tag{1.1a}$$

$$u = g(x), \qquad \text{on } \partial\Omega, \tag{1.1b}$$

where Ω is a convex bounded domain in $\mathbb{R}^d(d=1,2)$ with smooth boundary $\partial\Omega$, $\lambda>0$ is a physical parameter, $f(x)$,$g(x)$ are given functions.

The PB equation (1.1a) arises in many applications in physics, biology and chemistry. It was first introduced by Debye and Hückel [2] almost a century ago and further developed by Kirkwood [3]. In past twenty years a growing interest in this model has been driven mainly by numerical and experimental advances. Two examples of applications are particularly worth mentioning: the PB continuum electrostatic model has been widely accepted as a tool in theoretical studies of interactions of biomolecules such as proteins and DNAs in aqueous solutions, see e.g., [9]. The PB equation has also been used as a standard tool in modeling the electrostatic potential in plasma physics, see e.g., [10], where an asymptotic preserving numerical method is proposed to compute the PB equation arising in plasma physics.

There are two main challenges in numerically solving the PB problem (1.1), one is the nonlinear term e^{-u}, which requires some iteration techniques, instead of a direct discretization by standard methods. The other is the smallness of the parameter $\lambda \ll 1$, which needs to be properly resolved to maintain the approximation accuracy. Several numerical techniques have been applied to solve the PB equation, such as finite difference methods [4,6,7,10,15,16], boundary element methods [9], multigrid methods [14] and finite element methods [1,8].

The discontinuous Galerkin (DG) method we discuss in this paper is a class of finite element methods, using a completely discontinuous piecewise polynomial space for the numerical solution and the test functions. The flexibility of the DG method is afforded by local approximation spaces combined with the suitable design of numerical fluxes crossing cell interfaces, leading to several obvious advantages such as high order accuracy, flexibility in hp-adaptation, capacity to handle the domain with complex geometry, over the usual continuous Galerkin method even for elliptic problems. Indeed our primary motivation of considering the PB equation is to extend the recent developed direct DG method [11,12] to nonlinear elliptic problems. Our strategy is to couple an iteration with the DDG spatial discretization. The iteration techniques have been exploited by many authors to prove the existence of solutions to nonlinear elliptic equations, see e.g., [17,18]. The monotone iteration can also be used as a numerical method to approximate the solution, see e.g., [19]. However, when the parameter $\lambda \ll 1$, solving (1.1) by a monotone iteration with a constant iterative parameter may be inappropriate, as evidenced by our numerical experiments.

The iterative DG method is based on a series of linear PB equations with a variable iterative parameter. Through a careful analysis we identify an appropriate iterative pa-