Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0226

Vol. **23**, No. 1, pp. 168-197
January 2018

Error Estimates for the Iterative Discontinuous Galerkin Method to the Nonlinear Poisson-Boltzmann Equation

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Communicated by Chi-Wang Shu

Received 28 November 2016; Accepted (in revised version) 29 March 2017

Abstract. This paper is devoted to the error estimate for the iterative discontinuous Galerkin (IDG) method introduced in [P. Yin, Y. Huang and H. Liu. *Commun. Comput. Phys.* 16: 491–515, 2014] to the nonlinear Poisson-Boltzmann equation. The total error includes both the iteration error and the discretization error of the direct DG method to linear elliptic equations. For the DDG method, the energy error is obtained by a constructive approach through an explicit global projection satisfying interface conditions dictated by the choice of numerical fluxes. The L^2 error of order $\mathcal{O}(h^{m+1})$ for polynomials of degree m is further recovered. The bounding constant is also shown to be independent of the iteration times. Numerical tests are given to validate the established convergence theory.

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

Key words: Poisson-Boltzmann equation, DG methods, global projection, energy error estimates, L^2 error estimates.

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1 Introduction

This paper is devoted to the error estimate for the iterative discontinuous Galerkin (IDG) schemes, introduced in [36] to solve the boundary value problem for the nonlinear Poisson-Boltzmann (PB) equation,

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

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

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In this model equation, u is the unknown in the bounded domain Ω, with f and g given; $\lambda > 0$ is a physical parameter, called scaled Debye length. In many physically relevant settings, this parameter is very small [16]. This PB equation appears in many applications, including semiconductor modeling [13,30] and charged particles in solutions [15,17].

There are two main challenges in numerically solving the PB problem (1.1), one is nonlinearity of the model, another is smallness of the parameter $\lambda \ll 1$. Resolution of the former requires some iteration techniques, instead of a direct discretization by standard methods; for the latter, one needs to properly choose initial guess for the iteration to converge. These two issues have been properly resolved by the IDG algorithm introduced in [36]. Such an algorithm involves two steps: (i) the nonlinear PB equation is iteratively approximated by a series of linear PB equations, and (ii) each linear PB equation is solved by the direct Discontinuous Galerkin (DDG) method following [23,24]. As illustrated in [36], the iterative DG method has linear complexity in terms of the degree of freedom even for small λ. Also, $(m+1)$th order of accuracy for P^m polynomials was numerically observed in [36]. This work aims to obtain the optimal L^2 error for the IDG method rigorously.

Our main result may be stated as follows: for smooth solution u to the nonlinear PB equation (1.1), let u_h^n be the numerical solution to the linearized PB equation at step n, generated by the DDG method using polynomials of degree m over computational cells of size h. For some appropriate iterative step and initial guess u^0 for the iteration, there exists $0 < \mu < 1$ such that the following estimate holds,

$$\|u_h^n - u\|_{L^2(\Omega)} \leq \mu^n \|u^0 - u\|_{L^2(\Omega)} + Ch^{m+1},$$

for some constant C independent of h and n. The idea to obtain this estimate is to split the error into iteration error $\|u^n - u\|$ and discretization error $\|u^n - u_h^n\|$ of the DDG method for the linearized PB equation with solution u^n at $n-$th step. The iteration error

$$\|u^n - u\|_{L^2(\Omega)} \leq \mu^n \|u^0 - u\|_{L^2(\Omega)}$$

was already obtained in [36], hence the main task of this work is to estimate $\|u^n - u_h^n\| \leq Ch^{m+1}|u^n|_{m+1}$ for each linearized PB equation, and uniform boundedness of $|u^n|_{m+1}$ in terms of n.

Due to the nonlinearity of the problem, bounding $|u^n|_{m+1}$ uniformly in n is more involved. There are three key ingredients in our analysis: (i) the elliptic regularity gives $\|u^{n+1}\|_{s+1} \leq \|F\|_s$ with F involving u^n, f and the nonlinear term e^{-u^n}, see Lemma 3.1; (ii) the Moser-type estimate is used to bound $|e^{-u^n}|_s$ by $|u^n|_s$ and $\|e^{-u^n}\|_{L^\infty}$, see Lemma 3.2; and (iii) the point-wise bound in (2.7) for the iterative solutions is used to bound $\|u^n\|_{L^\infty}$ by $\max\{\|u^0\|_{L^\infty}, \|u\|_{L^\infty}\}$ as shown in (3.10). These together suffice to deduce the desired uniform bound of $|u^n|_{m+1}$.

Obtaining error estimates for various DG methods has been a main subject of research. For the linear Poisson equation with the Dirichlet boundary condition, a unified analysis was presented in [1] to obtain the best possible error estimates for a class of existing DG methods, including the optimal L^2 estimates for the method of Babuska [5], the