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DISCONTINUOUS GALERKIN METHOD FOR THE LINEAR POISSON-BOLTZMANN EQUATION

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Abstract: We consider a boundary value problem for the linear Poisson-Boltzmann equation. A regularization method is introduced to solve the problem using the discontinuous Galerkin method with interior penalization. Numerical results that corroborate the theoretical results are presented.

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1. Introduction

Boundary value problems for the linearized Poisson-Boltzmann equation arise in several biological applications like in the simulation of the electrostatics properties of charged macromolecules in aqueous environments [4]. Due to the very nature of dielectric constants and charge distributions, this equation has discontinuous coefficients and singular source terms. Moreover, in realistic situations, the domain occupied by the macromolecule is non-smooth. As a consequence, the solution of the problem is singular and, even if we separate out its singularity, the remaining function can have unbounded derivatives [6]. These prevent the use of numerical methods like the traditional discontinuous Galerkin method, once the jumps of derivatives must be well defined on the internal boundaries [7]. On the other hand, the discontinuous Galerkin (dG) methods have advantages as: can handle problems with complicated geometries; facili-

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tate parallelization; conserve physical quantities and facilitate the handling of elements of various shape and types.

Taking into account these issues, the aim of this paper is to introduce a numerical approximation based on the discontinuous Galerkin method to solve a Dirichlet problem for the linearized Poisson-Boltzmann equation in polygonal regions. Following [2], we introduce a suitable decomposition of the solution in order to reduce the problem to a boundary value problem without singular terms. Then, to avoid the lack of the regularity in the new problem, we consider a regularization scheme: the discontinuous coefficient in the equation is replaced for a suitable Lipschitz approximation such that the approximate solution converges to the original solution in the H^1 norm. This allows us to use a discontinuous Galerkin formulation with interior penalization for the regularized problem. We establish error estimates and present some numerical results to illustrate the theoretical approach.

2. The Linear Poisson-Boltzmann Equation

Let us consider a charged macromolecule occupying the region $\overline{\mathcal{O}} \subset \Omega \subset \mathbb{R}^2$, where Ω and $\mathcal{O}$ are open connected sets whose boundaries are polygons. We suppose that Ω is convex and bounded and that $\overline{\mathcal{O}}$ is sufficiently far from the boundary Γ of Ω such that the boundary effects can be neglect. Also we assume that the solvent occupies the whole region $\overline{\mathcal{O}}^c := \Omega\backslash\overline{\mathcal{O}}$ and contains a 1:1 symmetric electrolyte. In the case of small salt concentration, the electrostatic potential $\widetilde{\phi}$ satisfies the linearized Poisson-Boltzmann equation [4]

$$\nabla \cdot (\mu \nabla \widetilde{\phi}) - \overline{\kappa}^2 \widetilde{\phi} = -2\pi e_c \sum_{i=1}^{J} z_i \delta_i \quad \text{in} \quad \Omega, \tag{1}$$

subject to the boundary condition $\widetilde{\phi}_\Gamma = g_*$. Usually, g_* is obtained through a far field condition from the analytical solution of the linearized Poisson-Boltzmann equation in the case of the complete ionic penetration [2]. Here, and throughout this paper, $\mu : \Omega \to \mathbb{R}$ and $\overline{\kappa} : \Omega \to \mathbb{R}$ are given by

$$\mu(\mathbf{x}) = \begin{cases} \mu_1 & \text{if } \mathbf{x} \in \mathcal{O} \\ \mu_2 & \text{if } \mathbf{x} \in \overline{\mathcal{O}}^c \end{cases} \quad \text{and } \overline{\kappa}(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} \in \mathcal{O} \\ \kappa\sqrt{\mu_2} & \text{if } \mathbf{x} \in \overline{\mathcal{O}}^c \end{cases}, \tag{2}$$

where $\mu_1 > 0$ and $\mu_2 > 0$ denote the dielectric constants of the particle and the solvent, respectively; $\kappa = \left(\frac{8\pi e_c^2 n_0}{\mu_2 \kappa_B \theta}\right)^{1/2}$ is the modified Debye-Hückel parameter,

e_c is the proton charge, n_0 is the bulk ionic concentration of the solvent, κ_B is the Boltzmann constant and θ is the temperature. Also, δ_i stands for the Dirac functional concentrated in $\mathbf{x}_i$, where $A := \{\mathbf{x}_i \in \mathcal{O},\ i = 1, \dots, J\}$ are the positions of the fixed charges and z_i is the amount of charge in the position $\mathbf{x}_i$.

Let us consider $G(\mathbf{x}) = \frac{e_c}{\mu_1}\sum_{i=1}^{J} z_i \ln|\mathbf{x} - \mathbf{x}_i|$ for each $\mathbf{x} \notin A$. It is well known that $G \in L^1_{loc}(\Omega)$, then we have $v_p(G) \in \mathcal{D}'(\Omega)$, where

$$\langle v_p(G), \vartheta\rangle := \frac{e_c}{\mu_1}\sum_{i=1}^{J} z_i \lim_{\epsilon \to 0} \int_{|\mathbf{x}-\mathbf{x}_i|>\epsilon} \vartheta \ \ln|\mathbf{x} - \mathbf{x}_i| \, d\mathbf{x}, \tag{3}$$

for all $\vartheta \in \mathcal{D}(\Omega)$. As $\Delta G(\mathbf{x}) = 0$ if $\mathbf{x} \notin A$, elementary calculations yield

$$\Delta v_p(G) = -2\pi \frac{e_c}{\mu_1}\sum_{i=1}^{J} z_i \delta_i \quad \text{in} \quad \mathcal{D}'(\Omega). \tag{4}$$

We denote $d = \operatorname{dist}(\partial\mathcal{O}, A)$ and $\mathcal{O}_d = \{\mathbf{x} \in \mathcal{O},\ \operatorname{dist}(\mathbf{x}, \partial\mathcal{O}) \geq d/2\}$. Take a cut-off function $\wp \in \mathcal{D}(\mathcal{O})$ such that $\wp = 1$ in $\mathcal{O}_d$ and recall that, for all $\Lambda \in \mathcal{D}'(\Omega)$ and $\vartheta \in \mathcal{D}(\Omega)$, $\langle \wp\Lambda, \vartheta\rangle = \langle \Lambda, \wp\vartheta\rangle$ (see [8], Section 6.15). As a consequence, from Leibniz formula, (3) and (4),

$$\Delta(\wp \, v_p(G)) = -2\pi \frac{e_c}{\mu_1}\sum_{i=1}^{J} z_i \delta_i + 2\nabla\wp \cdot \nabla v_p(G) + \Delta\wp \, v_p(G) \tag{5}$$

in $\mathcal{D}'(\Omega)$. Then, defining $\phi = \widetilde{\phi} - \wp \, v_p(G)$, we can write

$$\begin{aligned} &\nabla \cdot (\mu_1 \nabla(\wp \, v_p(G))) + \nabla \cdot ((\mu - \mu_1)\nabla(\wp \, v_p(G))) + \nabla \cdot (\mu\nabla\phi) \\ &- \overline{\kappa}^2(\phi + \wp \, v_p(G)) = -2\pi e_c \sum_{i=1}^{J} z_i \delta_i \quad \text{in} \quad \mathcal{D}'(\Omega). \end{aligned} \tag{6}$$

From the definition of μ, $\overline{\kappa}^2$ and $\wp$, it is clear that $(\mu - \mu_1)\nabla(\wp \, v_p(G)) = 0$ and $\overline{\kappa}^2 \wp \, v_p(G) = 0$ in $\mathcal{D}'(\Omega)$. Consequently, from (6) and (5), we obtain (in the distributional sense)

$$\begin{aligned} \nabla \cdot (\mu\nabla\phi) - \overline{\kappa}^2\phi &= \mathfrak{f} \quad \text{in} \quad \Omega, \\ \phi &= g_* \quad \text{on} \quad \Gamma, \end{aligned} \tag{7}$$

where $\mathfrak{f} := -2\mu_1 \nabla\wp \cdot \nabla v_p(G) - \mu_1 \Delta\wp \, v_p(G)$. Note that $\mathfrak{f}$ corresponds to a smooth function. In what follows, we consider the more general problem

$$\begin{aligned} \nabla \cdot (\mu\nabla\phi) - \overline{\kappa}^2\phi &= f \quad \text{in} \quad \Omega \\ \phi &= g \quad \text{on} \quad \Gamma, \end{aligned} \tag{8}$$

where $f \in L^2(\Omega)$ and we assume the existence of $\widehat{g} \in H^2(\mathcal{O})$ such that $\widehat{g}|_\Gamma = g$.

3. Weak Formulation

Let us define the functional space $V = \{v \in H^1(\Omega),\ v|_\Gamma = g\}$.

Definition 1. The function $\phi \in V$ is a weak solution of (8) if

$$a(\phi, \vartheta) = L(\vartheta), \qquad \forall \vartheta \in H_0^1(\Omega), \tag{9}$$

where

$$a(\phi, \vartheta) = \int_\Omega \mu\, \nabla\phi \cdot \nabla\vartheta d\mathbf{x} + \int_\Omega \overline{\kappa}^2\, \phi\, \vartheta d\mathbf{x}, \text{ and } L(\vartheta) = -\int_\Omega f\vartheta d\mathbf{x}.$$

It is a routine to check the existence and uniqueness of solutions of (9). Now, let us to denote ϕ_1 and ϕ_2 as the restrictions of ϕ to $\mathcal{O}$ and $\overline{\mathcal{O}}^c$, respectively. It is well known that, in general, $\phi_2 \notin H^2(\overline{\mathcal{O}}^c)$ and $\phi_1 \notin H^2(\mathcal{O})$ as μ is discontinuous [6]. However, the following regularity result holds.

Theorem 1. *There exists $\lambda \geq 1/2$ such that $\phi_1 \in H^{1+\lambda}(\mathcal{O})$ and $\phi_2 \in H^{1+\lambda}(\overline{\mathcal{O}}^c)$.*

Proof. Choose $\epsilon > 0$ sufficiently small such that $\Omega_\epsilon \cap \mathcal{O} = \emptyset$, where $\Omega_\epsilon = \{\mathbf{x} \in \Omega, \mathrm{dist}(\mathbf{x}, \Gamma) < \epsilon\}$. Taking a cut-off function $\xi \in C^\infty(\mathbb{R}^2)$ such that $\xi \equiv 1$ in $\Omega_{\epsilon/2}$ and $\mathrm{supp}(\xi) \subset\subset \Omega_\epsilon \cup (\mathbb{R}^2 \backslash \Omega)$, define $\widehat{\phi} = \phi - \xi\, \widehat{g}$. Then $\widehat{\phi}$ is the unique weak solution of the problem

$$\begin{aligned} \nabla \cdot (\mu \nabla \widehat{\phi}) &= F \quad \text{in} \quad \Omega, \\ \widehat{\phi} &= 0 \quad \text{on} \quad \Gamma, \end{aligned} \tag{10}$$

where $F = -\nabla \cdot (\mu \nabla(\xi\ \widehat{g}))$. According to Definitions 2.1 and 2.2 in [6], as Ω is convex, there is no homogeneous singular points $x \in \Gamma$ and the only heterogeneous singular points are the vertex of $\partial\mathcal{O}$. Then, as $F \in L^2(\Omega)$, we have $\widehat{\phi}_1 \in H^{3/2}(\mathcal{O})$ and $\widehat{\phi}_2 \in H^{3/2}(\overline{\mathcal{O}}^c)$, following Lemma 2.5 of [6]. □

4. Regularized Equations

As remarked before, the low regularity of ϕ prevents the use of methods like Galerkin discontinuous, as we need the existence of the normal derivatives at the interfaces (in the trace sense). In order to deal with these difficulties, we consider a sequence of functions $\{\mu_\epsilon\}_{\epsilon>0}$ that satisfy, for all $\epsilon > 0$,

H1. $\mu_\epsilon \in C^{0,1}(\overline{\Omega})$, $\|\mu_\epsilon\|_{C^{0,1}(\overline{\Omega})} \leq C_*\epsilon^{-1}$, where $C_* = C_*(\Omega, \mathcal{O}, \mu_1, \mu_2)$;

H2. For all $p \geq 1$, $\|\mu_\epsilon - \mu\|_{0,p,\Omega} \leq C_*\epsilon^{1/p}$;

H3. For all $\mathbf{x} \in \Omega$, $\mu_1 \leq \mu_\epsilon(\mathbf{x}) \leq \mu_2$;

H4. Set $B_\epsilon = \{\mathbf{x} \in \Omega,\ \mathrm{dist}(\mathbf{x}, \partial\mathcal{O}) \leq \epsilon\}$ and $\epsilon_0 = \sup\{\epsilon > 0;\ B_\epsilon \cap \mathcal{O}_d = \emptyset\}$. Then, if $0 < \epsilon < \epsilon_0$, $\mu_\epsilon|_{\mathcal{O}\setminus B_\epsilon} = \mu_1$, $\mu_\epsilon|_{\overline{\mathcal{O}}^c\setminus B_\epsilon} = \mu_2$.

Remark 1. We can assume, without loss of generality, that $0 < \epsilon_0 < 1$. Moreover, note that $|B_\epsilon| \leq C\epsilon$, where $C = C(\mathcal{O})$.

We present the regularized version of (8)

$$\begin{aligned} \nabla \cdot (\mu_\epsilon \nabla\phi_\epsilon) - \overline{\kappa}^2\phi_\epsilon = f \quad &\text{in} \quad \Omega \\ \phi_\epsilon|_\Gamma = g \quad &\text{on} \quad \Gamma, \end{aligned} \tag{11}$$

and the corresponding weak formulation:

Find $\phi_\epsilon \in V$ such that

$$a_\epsilon(\phi_\epsilon, \vartheta) = L(\vartheta), \qquad \forall\vartheta \in H_0^1(\Omega), \tag{12}$$

where

$$a_\epsilon(\phi_\epsilon, \vartheta) = \int_\Omega \mu_\epsilon\, \nabla\phi_\epsilon \cdot \nabla\vartheta d\mathbf{x} + \int_\Omega \overline{\kappa}^2\, \phi_\epsilon\, \vartheta d\mathbf{x}.$$

The fact that ϕ_ϵ is a good approximation for ϕ (in a suitable sense) is shown below.

Theorem 2. *Let us assume* **H1-H4**. *Then, the problem (12) has a unique solution $\phi_\epsilon \in V \cap H^2(\Omega)$ which satisfies (11) a. e. in Ω. Moreover, for each $0 < \epsilon < \epsilon_0$,*

$$\|\phi_\epsilon - \phi\|_{1,2,\Omega} \leq \frac{C_P C_*}{\mu_1}\epsilon^{\alpha/2}(\|\phi_1\|_{1+\lambda,2,\mathcal{O}} + \|\phi_2\|_{1+\lambda,2,\overline{\mathcal{O}}^c}), \tag{13}$$

where C_P is the constant in the standard Poincaré-Friedrichs inequality for Ω and, if $\lambda \neq 1$, $\alpha = \min\{1, \lambda\}$; if $\lambda = 1$, (13) is valid for any $0 < \alpha < 1$.

Proof. The existence and uniqueness are standard. The regularity $\phi_\epsilon \in H^2(\Omega)$ follows from Theorem 3.2.1.2 in [5], as Ω is convex. Defining $\eta_\epsilon = \phi - \phi_\epsilon$ and taking $\vartheta = \eta_\epsilon$ in (9) and (12) we obtain, after subtracting the resultant equations,

$$\int_\Omega (\mu \nabla \phi - \mu_\epsilon \nabla \phi_\epsilon) \cdot \nabla \eta_\epsilon d\mathbf{x} + \int_\Omega \overline{\kappa}^2 \, \eta_\epsilon^2 \, d\mathbf{x} = 0,$$

which gives us

$$\int_\Omega \mu_\epsilon |\nabla \eta_\epsilon|^2 \, d\mathbf{x} + \int_\Omega \overline{\kappa}^2 \, \eta_\epsilon^2 \, d\mathbf{x} = \int_\Omega (\mu_\epsilon - \mu) \nabla \phi \cdot \nabla \eta_\epsilon \, d\mathbf{x}.$$

Then, Young's inequality yields

$$\mu_1 \|\nabla \eta_\epsilon\|_{0,2,\Omega}^2 \leq \frac{1}{2\mu_1} \int_\Omega (\mu_\epsilon - \mu)^2 |\nabla \phi|^2 \, d\mathbf{x} + \frac{\mu_1}{2} \int_\Omega |\nabla \eta_\epsilon|^2 \, d\mathbf{x}.$$

Supposing that $\lambda \in [1/2, 1)$, from the standard Sobolev embedding, we have $|\nabla \phi_1| \in L^{\frac{2}{1-\lambda}}(\mathcal{O})$ and $|\nabla \phi_2| \in L^{\frac{2}{1-\lambda}}(\overline{\mathcal{O}}^c)$. As a consequence, using the Hölder's inequality we obtain

$$\frac{\mu_1}{2} \|\nabla \eta_\epsilon\|_{0,2,\Omega}^2 \leq \frac{1}{2\mu_1} \|\mu_\epsilon - \mu\|_{0,\frac{2}{\lambda},\Omega}^2 (\|\nabla \phi_1\|_{0,\frac{2}{1-\lambda},\mathcal{O}}^2 + \|\nabla \phi_2\|_{0,\frac{2}{1-\lambda},\overline{\mathcal{O}}^c}^2),$$

which implies in

$$\|\nabla \eta_\epsilon\|_{0,2,\Omega}^2 \leq \frac{C_*^2}{\mu_1^2} \epsilon^\lambda (\|\nabla \phi_1\|_{0,\frac{2}{1-\lambda},\mathcal{O}}^2 + \|\nabla \phi_2\|_{0,\frac{2}{1-\lambda},\overline{\mathcal{O}}^c}^2)$$

and the result follows from the Poincaré-Friedrichs inequality. In the case that $\phi_1 \in H^2(\mathcal{O})$ and $\phi_2 \in H^2(\overline{\mathcal{O}}^c)$ we have $|\nabla \phi_1| \in L^q(\mathcal{O})$ and $|\nabla \phi_2| \in L^q(\overline{\mathcal{O}}^c)$, for all $q \in [1, +\infty)$. Then, similarly as above we obtain, for all $q \in (1, +\infty)$,

$$\|\nabla \eta_\epsilon\|_{0,2,\Omega}^2 \leq \frac{C_*^2}{\mu_1^2} \epsilon^{\frac{q-1}{q}} (\|\nabla \phi_1\|_{0,2q,\mathcal{O}}^2 + \|\nabla \phi_2\|_{0,2q,\overline{\mathcal{O}}^c}^2).$$

Finally, in the case that $\lambda > 1$, we have $|\nabla \phi_1| \in L^\infty(\mathcal{O})$ and $|\nabla \phi_2| \in L^\infty(\overline{\mathcal{O}}^c)$ and it is easy to check that

$$\|\nabla \eta_\epsilon\|_{0,2,\Omega}^2 \leq \frac{C_*^2}{\mu_1^2} \epsilon (\|\nabla \phi_1\|_{0,\infty,\mathcal{O}}^2 + \|\nabla \phi_2\|_{0,\infty,\overline{\mathcal{O}}^c}^2).$$

□

Observing that $\mu_\epsilon \in W^{1,\infty}(\Omega)$, we are able to establish the following boundedness result.

Theorem 3. *Consider the assumptions of Theorem 2. Then, for each* $0 < \epsilon < \epsilon_0$,

$$\|\phi_\epsilon\|_{2,2,\Omega} \le C\epsilon^{\frac{\alpha-2}{2}}(\|\widehat{g}\|_{2,2,\Omega} + \|\phi_1\|_{1+\lambda,2,\mathcal{O}} + \|\phi_2\|_{1+\lambda,2,\overline{\mathcal{O}}^c}), \tag{14}$$

where $C = C(\mu_1, \mu_2, \kappa^2, \Omega)$; *if* $\lambda \ne 1$, $\alpha = \min\{1, \lambda\}$ *and if* $\lambda = 1$, *(14) is valid for any* $0 < \alpha < 1$.

Proof. Taking $\vartheta = \phi_\epsilon - \widehat{g}$ in (12), we obtain

$$\mu_1 \int_\Omega |\nabla(\phi_\epsilon - \widehat{g})|^2 d\mathbf{x} + \int_\Omega \overline{\kappa}^2\, (\phi_\epsilon - \widehat{g})^2 d\mathbf{x} \le \mu_2 \int_\Omega |\phi_\epsilon - \widehat{g}|\, |f|\, d\mathbf{x}$$
$$+ \int_\Omega \mu_2 |\nabla\widehat{g}||\nabla(\phi_\epsilon - \widehat{g})|\, d\mathbf{x} + \int_\Omega \overline{\kappa}^2\, |\widehat{g}|\, |\phi_\epsilon - \widehat{g}|\, d\mathbf{x}.$$

As a consequence, the Hölder, Young and Poincarè-Friedrichs inequalities yield

$$\|\phi_\epsilon\|^2_{1,2,\Omega} \le C(\|f\|^2_{0,2,\Omega} + \|\widehat{g}\|^2_{1,2,\Omega}), \tag{15}$$

where $C = C(\mu_1, \mu_2, \kappa^2, \Omega)$. Now, from (11),

$$\int_\Omega (\nabla \cdot (\mu_\epsilon \nabla(\phi_\epsilon - \widehat{g})) - \overline{\kappa}^2(\phi_\epsilon - \widehat{g}))^2\, d\mathbf{x} = \int_\Omega (f - \nabla \cdot (\mu_\epsilon \nabla\widehat{g}) + \overline{\kappa}^2\widehat{g})^2\, d\mathbf{x}.$$

Hence,

$$\int_\Omega (\nabla \cdot (\mu_\epsilon \nabla(\phi_\epsilon - \widehat{g})))^2\, d\mathbf{x} \le 2\int_\Omega \overline{\kappa}^2 |\nabla \cdot (\mu_\epsilon \nabla(\phi_\epsilon - \widehat{g}))|\, |\phi_\epsilon - \widehat{g}|\, d\mathbf{x}$$
$$+ 3\int_\Omega |\nabla \cdot (\mu_\epsilon \nabla\widehat{g})|^2 d\mathbf{x} + 3\int_\Omega \overline{\kappa}^4\, \widehat{g}^2 d\mathbf{x} + 3\int_\Omega f^2 d\mathbf{x},$$

which implies in

$$\int_\Omega (\nabla \cdot (\mu_\epsilon \nabla(\phi_\epsilon - \widehat{g})))^2\, d\mathbf{x}$$
$$\le C\int_\Omega \left(|\nabla\mu_\epsilon|^2 |\nabla\widehat{g}|^2 + (\Delta\widehat{g})^2 + \widehat{g}^2 + |\phi_\epsilon - \widehat{g}|^2 + f^2\right) d\mathbf{x},$$

where $C = C(\kappa^2)$. As $0 < \epsilon < \epsilon_0$ we have, from **H1-H4** and (15),

$$\begin{aligned}
&\int_\Omega (\Delta(\phi_\epsilon - \widehat{g}))^2 \, d\mathbf{x} \le C \int_\Omega |\nabla \mu_\epsilon| \, |\nabla(\phi_\epsilon - \widehat{g})| \, |\Delta(\phi_\epsilon - \widehat{g})| \, d\mathbf{x} \\
&+ C\epsilon^{-2} \int_{B_\epsilon} |\nabla \widehat{g}|^2 d\mathbf{x} + C(\|\phi_\epsilon\|^2_{1,2,\Omega} + \|\widehat{g}\|^2_{2,2,\Omega} + \|f\|^2_{0,2,\Omega}) \\
&\le \frac{1}{2} \int_\Omega |\Delta(\phi_\epsilon - \widehat{g})|^2 \, d\mathbf{x} + C\epsilon^{-2} \int_{B_\epsilon} |\nabla(\phi_\epsilon - \widehat{g})|^2 d\mathbf{x} \\
&+ C\epsilon^{-2} \int_{B_\epsilon} |\nabla \widehat{g}|^2 d\mathbf{x} + C(\|\widehat{g}\|^2_{2,2,\Omega} + \|f\|^2_{0,2,\Omega}),
\end{aligned}$$

where $C = C(\mu_1, \mu_2, \kappa^2, \Omega)$. As a consequence, we get

$$\begin{aligned}
\int_\Omega (\Delta(\phi_\epsilon - \widehat{g}))^2 \, d\mathbf{x} \le C\epsilon^{-2} \left(\int_{B_\epsilon} |\nabla \phi|^2 d\mathbf{x} + \int_{B_\epsilon} |\nabla \widehat{g}|^2 d\mathbf{x} \right) \\
+ C\epsilon^{-2} \int_{B_\epsilon} |\nabla(\phi_\epsilon - \phi)|^2 d\mathbf{x} + C(\|\widehat{g}\|^2_{2,2,\Omega} + \|f\|^2_{0,2,\Omega}).
\end{aligned} \tag{16}$$

From standard calculations we obtain, for all $q \in (1, +\infty)$,

$$\int_{B_\epsilon} |\nabla \widehat{g}|^2 d\mathbf{x} \le |B_\epsilon|^{\frac{q-1}{q}} \|\nabla \widehat{g}\|^2_{0,2q,B_\epsilon} \le C\epsilon^{\frac{q-1}{q}} \|\widehat{g}\|^2_{2,2,\Omega}. \tag{17}$$

If $\lambda \in [1/2, 1)$

$$\begin{aligned}
\int_{B_\epsilon} |\nabla \phi|^2 d\mathbf{x} &= \int_{B_\epsilon \cap \mathcal{O}} |\nabla \phi_1|^2 d\mathbf{x} + \int_{B_\epsilon \cap \overline{\mathcal{O}}^c} |\nabla \phi_2|^2 d\mathbf{x} \\
&\le |B_\epsilon|^\lambda (\|\nabla \phi_1\|^2_{0,\frac{2}{1-\lambda},\mathcal{O}} + \|\nabla \phi_2\|^2_{0,\frac{2}{1-\lambda},\overline{\mathcal{O}}^c}) \\
&\le C\epsilon^\lambda (\|\nabla \phi_1\|^2_{0,\frac{2}{1-\lambda},\mathcal{O}} + \|\nabla \phi_2\|^2_{0,\frac{2}{1-\lambda},\overline{\mathcal{O}}^c}).
\end{aligned}$$

For $\lambda = 1$ and any $q \in (1, +\infty)$,

$$\int_{B_\epsilon} |\nabla \phi|^2 d\mathbf{x} \le C\epsilon^{\frac{q-1}{q}} (\|\nabla \phi_1\|^2_{0,2q,\mathcal{O}} + \|\nabla \phi_2\|^2_{0,2q,\overline{\mathcal{O}}^c}).$$

Finally, if $\lambda > 1$ we get

$$\int_{B_\epsilon} |\nabla \phi|^2 d\mathbf{x} \le C\epsilon (\|\nabla \phi_1\|^2_{0,\infty,\mathcal{O}} + \|\nabla \phi_2\|^2_{0,\infty,\overline{\mathcal{O}}^c}).$$

Hence, recalling that $0 < \epsilon < \epsilon_0 < 1$ (see Remark 1), from the above estimates, (13), (16), (17) and standard Sobolev embedding theorems, we have

$$\int_\Omega (\Delta(\phi_\epsilon - \widehat{g}))^2 \, d\mathbf{x} \le$$
$$C\epsilon^{\alpha-2}(\|\widehat{g}\|^2_{2,2,\Omega} + \|f\|^2_{0,2,\Omega} + \|\phi_1\|^2_{1+\lambda,2,\mathcal{O}} + \|\phi_2\|^2_{1+\lambda,2,\overline{\mathcal{O}}^c}).$$

The bound (14) is a straightforward consequence of (15) and the calculations in the proof of Theorem 4.3.1.4 in [5]. □

5. Discontinuous Galerkin Formulation

Here and throughout this paper, we will use the traditional notation for the discontinuous Galerkin methods, see [1] for details. The general discontinuous formulation for the problem (12) reads:

Find $\phi_\epsilon \in H^2(\mathcal{T}_h)$ such that

$$\widetilde{a}_\epsilon(\phi_\epsilon, \vartheta) = \widetilde{L}_\epsilon(\vartheta), \qquad \forall \vartheta \in H^2(\mathcal{T}_h), \tag{18}$$

where

$$\widetilde{a}_\epsilon(\phi_\epsilon, \vartheta) = \sum_{K\in\mathcal{T}_h} \left(\int_K \mu_\epsilon \nabla\phi_\epsilon \cdot \nabla\vartheta \, d\mathbf{x} + \overline{\kappa}^2 \int_K \phi_\epsilon \, \vartheta \, d\mathbf{x} \right)$$
$$+ \sum_{e\in\mathcal{E}} \int_e \frac{\sigma_e}{h}[\phi_\epsilon] \cdot [\vartheta] ds - \sum_{e\subset\mathcal{E}} \int_e (\{\mu_\epsilon \nabla\phi_\epsilon\} \cdot [\vartheta] + \delta\{\mu_\epsilon \nabla\vartheta\} \cdot [\phi_\epsilon]) \, ds,$$
$$\widetilde{L}_\epsilon(\vartheta) = \sum_{e\subset\mathcal{E}^\partial_\Omega} \int_e g(\sigma_e h^{-1}\vartheta - \delta\mu_\epsilon \nabla\vartheta \cdot \mathbf{n}_K) \, ds - \sum_{K\in\mathcal{T}_h} \int_K f\vartheta \, d\mathbf{x},$$

$\delta \in \{-1, 1\}$ *and* $\sigma_e > 0$.

The obtaining of (18) from (12) is rather standard if we use (11) and the regularity result established in Theorem 3. In fact, the following equivalence result is a direct consequence of Proposition 2.9 in [7].

Theorem 4. *If $\phi_\epsilon \in V \cap H^2(\Omega)$ is the solution of (12), it is a solution of (18). Moreover, if $\phi_\epsilon \in H^1(\Omega) \cap H^2(\mathcal{T}_h)$ is a solution of (18), $\phi_\epsilon \in V$ and it is a solution of (12).*

Now, the discontinuous Galerkin formulation for (18) is:

Find $\phi_{h,\epsilon} \in \mathcal{P}_p(\mathcal{T}_h) = \left\{\vartheta \in L^2(\Omega): \ \forall\, K \ \in \mathcal{T}_h, \ \vartheta_{|K} \in \mathcal{P}_p(K)\right\}$, *such that*

$$\widetilde{a}_\epsilon(\phi_{h,\epsilon}, \vartheta) = \widetilde{L}_\epsilon(\vartheta), \quad \forall\, \vartheta \in \mathcal{P}_p(\mathcal{T}_h). \tag{19}$$

We define the energy norm

$$\|\!|\vartheta|\!\|^2_{\mathcal{T}_h,\epsilon} = \sum_{K\in\mathcal{T}_h} \left(\int_K \mu_\epsilon |\nabla\vartheta|^2 \ d\mathbf{x} + \overline{\kappa}^2 \int_K \vartheta^2 \ d\mathbf{x} \right) + \sum_{e\in\mathcal{E}} \int_e \frac{\sigma_e}{h} |[\vartheta]|^2 ds. \tag{20}$$

By slight modifications in the arguments in Section 2.7.1 and Lemma 2.12 in [7] we obtain the following result.

Theorem 5. *Suppose that* $\delta = 1$, $h \le 1$ *and*

$$\sigma_e \ge \frac{2C_t^2 \mu_2^2 n^*}{\mu_1}, \ \forall e \subset \mathcal{E}, \tag{21}$$

where n^* *is the maximum number of neighbors an element can have. Then, for any* $\epsilon > 0$, *the bilinear form* $\widetilde{a}_\epsilon$ *is coercive in* $\mathcal{P}_p(\mathcal{T}_h)$, *for all* p. *In particular, this implies that the problem (19) has a unique solution.*

As $\mu_1 \le \mu_\epsilon(\mathbf{x}) \le \mu_2$, for all $\mathbf{x} \in \Omega$ and $\epsilon > 0$, the following error estimates for the energy norm are a direct consequence of Theorems 2.13 and 2.14 in [7].

Theorem 6. *Consider the assumptions on* δ, h *and* σ_e *of Theorem 5. If* $p \ge 1$ *and* $\phi_\epsilon \in H^s(\Omega)$ $(s \ge 2)$, *there exists a constant* C *that does not depend on* ϵ *and* h *such that*

$$\|\!|\phi_{h,\epsilon} - \phi_\epsilon|\!\|_{\mathcal{T}_h,\epsilon} \le C\ h^{\min(p+1,s)-1} \left(\sum_{K\in\mathcal{T}_h} \|\phi_\epsilon\|^2_{s,2,K} \right)^{1/2}, \tag{22}$$

$$\|\phi_{h,\epsilon} - \phi_\epsilon\|_{0,2,\Omega} \le Ch^{\min(p+1,s)} \left(\sum_{K\in\mathcal{T}_h} \|\phi_\epsilon\|^2_{s,2,K} \right)^{1/2} \tag{23}$$

for each $0 < \epsilon < \epsilon_0$. *Moreover, (23) is optimal;* C *depends on* μ_1, μ_2, κ^2, Ω *and* $\mathcal{O}$.

Corollary 1. *If* $0 < \epsilon < \epsilon_0$,

$$\|\phi_{h,\epsilon} - \phi\|_{0,2,\Omega} \le C(\epsilon^{\frac{\alpha-2}{2}} h^{\min(p+1,s)} + \epsilon^{\alpha/2}) \, (\|f\|_{0,2,\Omega} + \|\widehat{g}\|_{2,2,\Omega} + \|\phi_1\|_{1+\lambda,2,\mathcal{O}} + \|\phi_2\|_{1+\lambda,2,\overline{\mathcal{O}}^c} \Big) \,, \tag{24}$$

where if $\lambda \neq 1$, $\alpha = \min\{1, \lambda\}$ *and if* $\lambda = 1$, *(24) is valid for any* $0 < \alpha < 1$.

Proof. We can write

$$\|\phi_{h,\epsilon} - \phi\|_{0,2,\Omega} \le \|\phi_{h,\epsilon} - \phi_\epsilon\|_{0,2,\Omega} + \|\phi_\epsilon - \phi\|_{0,2,\Omega},$$

then (24) follows from (13), (14) and (23). □

6. Numerical Results

In this section, we solve the problem (11) using the dG formulation (19) when the right hand side and the boundary condition were taken so that the problem have the exact solution given by:

$$\phi_\epsilon(x_1,\ x_2) = c_1 c_2 (x_1 - a)^3 (x_1 - b)(x_2 - c)(x_2 - d). \tag{25}$$

Here, $c_1 = \mu_1 \times \mu_2$ and the constant c_2 simply to stretch out the solution. In the numerical results we set $c_2 = 150$. In this case the domain is $\Omega = [0,\ 1] \times [0,\ 1]$ and the macromolecule occupy the region $\overline{\mathcal{O}} = [a,\ b] \times [c,\ d]$, where $a = c = 1/4$ and $b = d = 3/4$. With this choice, we can calculate the numerical order of convergence to confirm the theoretical results presented in Theorem 6 and Corollary 1.

The formulation described above was implemented in the PZ environment [3]. In order to check the convergence, we successively divide the domain using $2^L \times 2^L$ square elements. Thus, if e_L denotes the error at the level of refinement L, the rate of convergence for this level is given by $r_L = \log\left(e_L/e_{L-1}\right) / \log(0.5)$.

In our numerical simulations we set $\delta = 1$ and after some numerical tests we select $\sigma_e = 100$ for all cases.

As a first test, we set the parameters of the function μ defined by (2) as $\mu_1 = \mu_2 = 1$ and the function $\overline{\kappa}$ have the value one outside of macromolecule. Thus, we need to recovery the numerical order of convergence for the classic dG method (see [1]) applied to Poisson equation. Table 1 shows the results

	$L^2(\mathcal{T}_h)$		$H^1(\mathcal{T}_h)$		Energy	
L	e_L	r_L	e_L	r_L	e_L	r_L
3	9.1959e-4	2.8619	5.1708e-2	2.0183	5.1732e-2	2.0478
4	1.1892e-4	2.9510	1.2837e-2	2.0101	1.2837e-2	2.0107
5	1.5070e-5	2.9803	3.1991e-3	2.0046	3.1990e-3	2.0046

Table 1: Numerical convergence for $p = 2$ with $\mu_1 = \mu_2 = 1$.

for the energy, $H_1(\mathcal{T}_h)$ and $L_2(\mathcal{T}_h)$ norms, when $p = 2, \forall K \in \mathcal{T}_h$. Clearly, this numerical results confirm the theoretical results for this case.

In Table 2 we present the numerical results for $p = 2$ with $\mu_1 = 1$, $\mu_2 = 2$, $\epsilon = 1.e-4$ and the same function $\overline{\kappa}$ defined before. We can see that this results confirm Theorem 6, since for ϵ fixed and $p = 2$, the theorems shows that the order of convergence need to be $\mathcal{O}(h^3)$ for $L^2(\mathcal{T}_h)$ norm and $\mathcal{O}(h^2)$ for the energy norm. This was exactly what we get numerically for this example. We observe that very similar results of those of Table 2 were obtained for $\epsilon = 1.e-6$ and $\epsilon = 1.e-8$. However, if μ_2 is far greater than μ_1, we lost the order of convergence $\mathcal{O}(h^3)$ for $L^2(\mathcal{T}_h)$ norm and $\mathcal{O}(h^2)$ for the energy norm (when $p = 2$), although the method continues to be convergent. Analogous results were obtained for $p = 3$.

	$L^2(\mathcal{T}_h)$		$H^1(\mathcal{T}_h)$		Energy	
L	e_L	r_L	e_L	r_L	e_L	r_L
3	9.5756e-4	2.8640	7.4207e-2	2.0151	7.4225e-2	2.0307
4	1.2388e-4	2.9503	1.8437e-2	2.0089	1.8437e-2	2.0093
5	1.5750e-5	2.9755	4.5974e-3	2.0037	4.5974e-3	2.0037

Table 2: Numerical convergence for $p = 2$ with $\mu_1 = 1,\ \mu_2 = 2$ and $\epsilon = 1.e-4$.

In order to check the estimate (24), we choose the following sequence of ϵ, $1 > \epsilon_1 > \epsilon_2 > \ldots > \epsilon_8 > 0$, and we fix $h \leq \sqrt{\epsilon_4}$. Then, $\epsilon_i^{\frac{\alpha-2}{2}} h^2 \leq \epsilon_i^{\frac{\alpha-2}{2}} \epsilon_4 \leq \epsilon_i^{\frac{\alpha-2}{2}} \epsilon_i = \epsilon_i^{\alpha/2}$ and we obtain

$$\begin{aligned}\|\phi_{h,\epsilon} - \phi_{ad}\|_{0,2,\Omega} \leq C\epsilon_i^{\alpha/2} \big(&\|f\|_{0,2,\Omega} + \|\widehat{g}\|_{2,2,\Omega} \\ &+\|\phi_1\|_{1+\lambda,2,\mathcal{O}} + \|\phi_2\|_{1+\lambda,2,\overline{\mathcal{O}}^c}\big)\end{aligned}$$

for each $i = 1, 2, 3, 4$. We verify this inequality numerically by taking $L = 5$,

	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6
e_{ϵ_i}	1.892e-4	9.588e-5	5.506e-5	3.218e-5	2.219e-5	1.575e-5
r_{ϵ_i}		0.9810	0.8001	0.7749	0.5365	0.4942

Table 3: Numerical convergence for $p = 2$ with $\mu_1 = 1$, $\mu_2 = 2$, $L = 5$ and different values of ϵ.

$\epsilon_1 = 0.008$ and $\epsilon_j = 0.5\epsilon_{j-1}$ for $j = 2,\ 3,\ \ldots,\ 8$. For the first four values of ϵ_i, as we have $h \leq \sqrt{\epsilon_i}$ and the solution is smooth, we expect to get numerically the order of convergence $\mathcal{O}(\epsilon^{1/2})$. Moreover, we also expect that the numerically order of convergence vanishes for the last terms of this sequence. In Table 3 we present the numerical results obtained for the firsts six value of ϵ_i. In this table e_{ϵ_i} denotes the error in L^2 norm when $\epsilon = \epsilon_i$ and $r_{\epsilon_i} = \log\left(e_{\epsilon_i}/e_{\epsilon_{i-1}}\right)/\log(0.5)$ gives the rate of convergence in ϵ, when $\epsilon_i = 0.5\epsilon_{i-1}$ for $i = 2,\ 3,\ \ldots, 8$.

We can see clearly, that the numerical results for the firsts four values are better than the expected. And attained $\mathcal{O}(\epsilon^{1/2})$ in the fifth and sixth value. For the last two values of the sequence, the error was basically the same as the one obtained for ϵ_6, thereby the numerical order was practically equals to zero. These numerical results are in agreement with Corollary 1.

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