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LINEARIZATION OF A NONLINEAR PERIODIC BOUNDARY CONDITION RELATED TO CORROSION MODELING*

Y. S. Bhat
(*Institute for Mathematics and its Applications, Univ. of Minnesota, Minneapolis, MN 55455, USA*
Email: bhat@ima.umn.edu)
S. Moskow
(*Department of Mathematics, Drexel University, Philadelphia, PA 19104, USA*
Email: moskow@math.drexel.edu)

Abstract

We study galvanic currents on a heterogeneous surface. In electrochemistry, the oxidation-reduction reaction producing the current is commonly modeled by a nonlinear elliptic boundary value problem. The boundary condition is of exponential type with periodically varying parameters. We construct an approximation by first homogenizing the problem, and then linearizing about the homogenized solution. This approximation is far more accurate than both previous approximations or direct linearization. We establish convergence estimates for both the two and three-dimensional case and provide two-dimensional numerical experiments.

Mathematics subject classification: 35J65, 35Q72.
Key words: Galvanic corrosion, Homogenization, Nonlinear elliptic boundary value problem, Butler-Volmer boundary condition, Robin boundary condition.

1. Introduction

A galvanic current is an electron transport process that occurs between anode and cathode. When anode and cathode are placed in electrical contact, the difference in electrolytic voltage rest potential results in an electron flow from anode to cathode. The anode undergoes oxidation, *i.e.*, the anode loses an electron, while the cathode undergoes reduction, *i.e.*, the cathode gains an electron. The anode is said to be corroded and the electron flow is known as a corrosion current, or galvanic current. Rust is the result of a similar type of oxidation-reduction reaction that occurs between different parts of the *same* surface. In fact, rust-causing current is very similar to a galvanic current on a heterogeneous surface. See [14] for further discussion of the subject.

Mathematically, such galvanic interactions can be modeled by the so-called Butler-Volmer boundary conditions of exponential type. The potential is represented by a function ϕ over a Euclidean domain Ω where a portion of its boundary, Γ, is electrochemically active and composed of anodic and cathodic regions. The potential satisfies the Butler-Volmer boundary conditions over both these regions, but with different material parameters in each region. More specifically, we consider Ω to be a cylindrical domain with base some two-dimensional region. The bottom base of the cylinder is a cathodic plane in which anodic islands are periodically distributed throughout. We denote the anodic part of the bottom base of the cylinder as $\partial\Omega_A$ and the cathodic part as $\partial\Omega_C$, see Fig. 1.1. If we define the bottom base of the cylinder to be

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Γ, then the inert portion of the boundary is $\partial\Omega \setminus \Gamma$. Furthermore, $\Gamma = \overline{\partial\Omega_A \cup \partial\Omega_C}$, where $\partial\Omega_A$ and $\partial\Omega_C$ are open sets such that $\partial\Omega_A \cap \partial\Omega_C = \emptyset$. The electrolytic voltage potential, ϕ, satisfies the following nonlinear problem,

$$\begin{aligned}
&\Delta\phi = 0 \quad \text{in } \Omega,\\
&-\frac{\partial\phi}{\partial n} = J_A[e^{\alpha_{aa}(\phi - V_A)} - e^{-\alpha_{ac}(\phi - V_A)}] \quad \text{on } \partial\Omega_A,\\
&-\frac{\partial\phi}{\partial n} = J_C[e^{\alpha_{ca}(\phi - V_C)} - e^{-\alpha_{cc}(\phi - V_C)}] \quad \text{on } \partial\Omega_C,\\
&-\frac{\partial\phi}{\partial n} = 0 \text{ on } \partial\Omega \setminus \{\partial\Omega_A \cup \partial\Omega_C\},
\end{aligned} \tag{1.1}$$

where the transfer coefficients $\alpha_{aa},\ \alpha_{ac},\ \alpha_{ca},\ \alpha_{cc}$ are such that

$$\alpha_{aa} + \alpha_{ac} = 1, \quad \alpha_{ca} + \alpha_{cc} = 1.$$

The anodic and cathodic polarization parameters J_A and J_C are positive constants and $V_A,\ V_C$ are the anodic and cathodic rest potentials respectively.

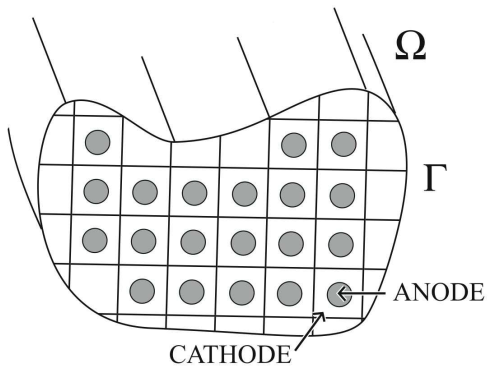

Fig. 1.1. The cylindrical domain, Ω, has a two-dimensional base, Γ, that is made up of anodic islands periodically distributed in a cathodic plane.

This problem has been studied quite a bit in the electrochemistry community. For example, in [12, 13] the authors compute finite element numerical solutions to (1.1). They observe resulting currents for various anodic shapes. Within the applied mathematics community, several aspects of the two dimensional homogeneous problem, including optimal control [9], and singular solutions for negative polarization parameters [7, 11, 15] have been investigated. In [6] we analyzed the periodically heterogeneous problem in two and three dimensions, and suggested a linear correction term. Although the approximations were reasonable and could be shown to converge in various norms, significant error remained in the approximation of the boundary current.

In this paper we suggest a new approximation to (1.1) that consists of the constant solution to the homogenized problem plus a linear correction that is essentially a linearization of (1.1) about the homogenized solution. This approximation, while no more expensive to compute than that of [6], is far more accurate. We demonstrate this both analytically and numerically.

The approximation we present here differs from [6] in that the correction satisfies a Robin boundary condition which more accurately models the microstructure than the previous Neumann correction. Robin boundary conditions are known to be a good way to accurately model periodic rough boundaries, see for example [1, 2, 10], where some difficult flow problems are analyzed. Here the nonlinearity and the periodicity are together in the boundary condition, and the Robin condition in the correction is obtained by a linearization of the model about the homogenized solution.

We should also remark that while the correction is easier to compute since it is linear, it is still inhomogeneous. So, for very small scales, it may be desirable to homogenize or otherwise analytically approximate the correction term itself. See the techniques in [2, 5], for example.

The paper is organized as follows. In Section 2, we present the periodic model and its homogenized limit as the periodic size $\epsilon \to 0$. Since direct linearization is common [12, 13, 15], we also discuss what happens if one linearizes (1.1) directly. In Section 3, we briefly present the results established in [6]. Section 4 contains the presentation of our new proposed approximation and convergence estimates. Numerical experiments are presented in Section 5, and in Section 6 we discuss the results.

2. The Analytic Model, Homogenization and Direct Linearization

Mathematically, we study a periodic structure with period approaching zero. To model this periodic structure, define

$$f(y,v) = \lambda(y)[e^{\alpha(y)(v-V(y))} - e^{-(1-\alpha(y))(v-V(y))}],$$

where $v \in \mathbb{R}$ and $y \in Y$, the boundary period cell, which for simplicity we take to be the unit square; $Y = [0,1] \times [0,1]$. We assume that λ, α, and V are all piecewise smooth Y-periodic functions and that there exist constants λ_0, Λ_0, α_0, A_0 and V_0 such that:

$$0 < \lambda_0 \leq \lambda(y) \leq \Lambda_0, \tag{2.1}$$

$$0 < \alpha_0 \leq \alpha(y) \leq A_0 < 1, \tag{2.2}$$

$$|V(y)| \leq V_0. \tag{2.3}$$

Consider the problem

$$\begin{aligned} &\Delta u_\epsilon = 0 \quad \text{in } \Omega, \\ &-\frac{\partial u_\epsilon}{\partial n} = f(x/\epsilon, u_\epsilon) \quad \text{on } \Gamma, \\ &-\frac{\partial u_\epsilon}{\partial n} = 0 \quad \text{on } \partial\Omega \setminus \Gamma. \end{aligned} \tag{2.4}$$

One expects that as $\epsilon \to 0$ the solutions will converge to a solution of a problem with an averaged boundary condition. In [6] we showed that u_ϵ converges to the solution of the homogenized problem

$$\begin{aligned} &\Delta u_0 = 0 \quad \text{in } \Omega, \\ &-\frac{\partial u_0}{\partial n} = f_0(u_0) \quad \text{on } \Gamma, \\ &-\frac{\partial u_0}{\partial n} = 0 \quad \text{on } \partial\Omega \setminus \Gamma, \end{aligned} \tag{2.5}$$

where $f_0(v)$ is the cell average of $f(y,v)$, that is,

$$f_0(v) = \int_Y f(y,v)dy. \tag{2.6}$$

Note that this problem is still nonlinear but now homogenous. We will look for a correction that is linear. Linearization of (1.1) is commonly used [12], so we briefly discuss this before proceeding. If one were to linearize the problem (2.4) directly we get

$$\begin{aligned} &\Delta u_\epsilon^L = 0 \ \text{ in } \Omega, \\ &-\frac{\partial u_\epsilon^L}{\partial n} = \lambda(x/\epsilon)(u_\epsilon^L - V(x/\epsilon)) \ \text{ on } \Gamma, \\ &-\frac{\partial u_\epsilon^L}{\partial n} = 0 \ \text{ on } \partial\Omega \setminus \Gamma. \end{aligned} \tag{2.7}$$

For large ϵ, this can yield a decent approximation, however as $\epsilon \to 0$ the direct linearization converges to the wrong limit. One can show that the solution to (2.7) converges at least weakly in $L^2(\Omega)$ to u_0^L which satisfies

$$\begin{aligned} &\Delta u_0^L = 0 \ \text{ in } \Omega, \\ &-\frac{\partial u_0^L}{\partial n} = \overline{\lambda} u_0^L - \overline{b} \ \text{ on } \Gamma, \\ &-\frac{\partial u_0^L}{\partial n} = 0 \ \text{ on } \partial\Omega \setminus \Gamma, \end{aligned}$$

where $\overline{\lambda}$ and $\overline{b}$ are the averages

$$\overline{\lambda} = \int_Y \lambda(y)\ d\sigma_y \text{ and } \overline{b} = \int_Y \lambda(y)V(y)\ d\sigma_y.$$

Clearly then

$$u_0^L = \overline{b}/\overline{\lambda}$$

and in general $\overline{b}/\overline{\lambda} \neq u_0$. So, for small scale problems, the direct linearization approximation is highly inaccurate, for example see Fig. 2.1. We discuss the precise parameters used here in Section 5. One can see here that the linearized problem is converging to the wrong limit potential as $\epsilon \to 0$.

3. Previously Established Estimates

We briefly discuss the existence and uniqueness of solutions to (2.4) and (2.5) and present results from [6] which we will use in Section 4. Consider the energy functional

$$E_\epsilon(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 \ \ dx + \int_\Gamma F(\frac{x}{\epsilon}, v)d\sigma_x, \tag{3.1}$$

where

$$F(y,v) = \frac{\lambda(y)}{\alpha(y)} e^{\alpha(y)(v-V(y))} + \frac{\lambda(y)}{1-\alpha(y)} e^{-(1-\alpha(y))(v-V(y))}.$$

In [6] the following result is established in arbitrary dimension. For $n = 2$, this result had been previously established for the homogeneous case in [9, 15].

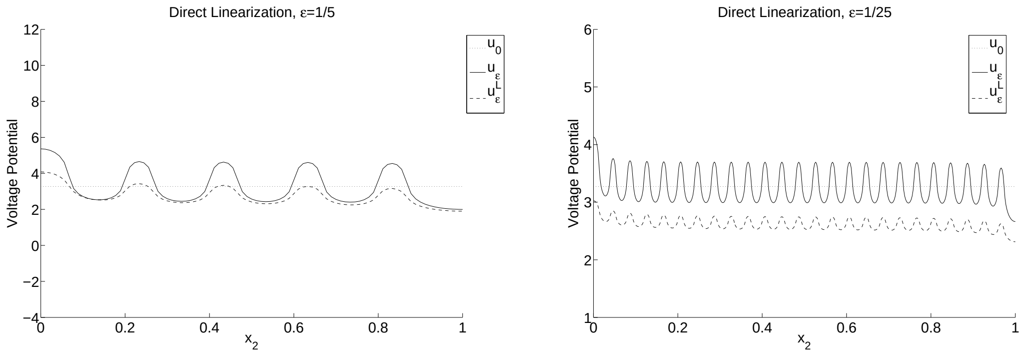

Fig. 2.1. The direct linearization approximation and the original on the boundary Γ, $\epsilon = 1/5$, $\epsilon = 1/25$ respectively.

Theorem 3.1 (Existence and Uniqueness of the Minimizer) *Let* E_ϵ *be defined by* (3.1), *where* λ, α, *and* V *satisfy* (2.1)-(2.3). *Then there exists a unique function* $u_\epsilon \in H^1(\Omega)$ *satisfying*

$$E_\epsilon(u_\epsilon) = \min_{u \in H^1(\Omega)} E_\epsilon(u).$$

Similarly, if we define the energy functional

$$E_0(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 \; dx + \int_\Gamma F_0(v) \; d\sigma_x, \tag{3.2}$$

where

$$F_0(v) = \int_Y F(y,v)dy,$$

then we are able to conclude a similar result about u_0 using techniques similar to those used in the proof of Theorem 3.1. Furthermore, the solution u_0 is a constant. Note that (2.1), (2.2), (2.3) and (2.6) imply that if $v > V_0$ then $f_0(v) > 0$ and if $v < -V_0$ then $f_0(v) < 0$. Since $f_0(v)$ is continuous, by the Intermediate Value Theorem there exists a constant $K \in (-V_0, V_0)$ such that $f_0(K) = 0$. Now note that clearly $u_0 = K$ is a classical solution of (2.5), and so we see that u_0 is a constant. Note that this argument holds in any dimension.

In [6] we defined a correction, which we call w_ϵ here, to satisfy

$$\begin{aligned} &\Delta w_\epsilon = 0 \;\text{ in } \Omega, \\ &-\frac{\partial w_\epsilon}{\partial n} = \frac{1}{\epsilon}(f(\frac{x}{\epsilon}, u_0) - f_0(u_0)) + e_\epsilon \;\text{ on } \Gamma, && (3.3)\\ &-\frac{\partial w_\epsilon}{\partial n} = 0 \;\text{ on } \partial\Omega \setminus \Gamma, \\ &\int_\Gamma w_\epsilon \; d\sigma_x = 0, && (3.4)\end{aligned}$$

where

$$e_\epsilon = \frac{1}{\epsilon}\int_\Gamma (f_0(u_0) - f(x/\epsilon, u_0))d\sigma_x.$$

The constant e_ϵ is added to ensure the existence of the solution. Additionally, if u_ϵ and u_0 are in $L^\infty(\Gamma)$, define

$$D_\epsilon = \max\left\{ \|u_\epsilon\|_{L^\infty(\Gamma)}, \|u_0\|_{L^\infty(\Gamma)} \right\} \tag{3.5}$$

and

$$M_\epsilon = \sup_{(y,w)\in Y\times[-D_\epsilon,D_\epsilon]} \frac{\partial f}{\partial v}(y,w). \tag{3.6}$$

Note that by definition $0 < M_\epsilon < 2\Lambda_0 e^{V_0} e^{D_\epsilon}$. Then assuming D_ϵ is finite, the following convergence result can be established.

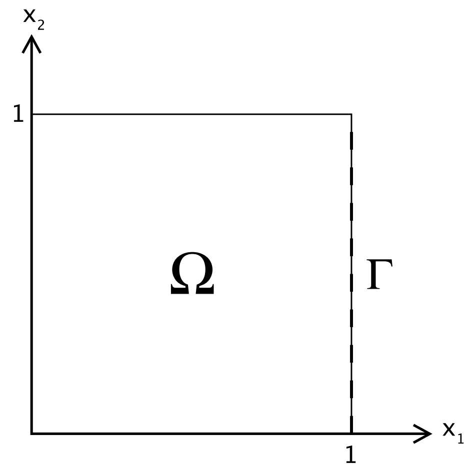

Fig. 3.1. Two-dimensional analogue.

Proposition 3.1. *Let* $n = 2$ *or* 3 *and let* u_ϵ, u_0 *be minimizers of* (3.1), (3.2) *respectively, and let* w_ϵ *be the solution to* (3.3). *Assume also that* $u_\epsilon \in C^0(\bar{\Omega})$. *Then there exist constants* C_1 *and* C_2 *independent of* ϵ *such that*

$$\|u_\epsilon - u_0 - \epsilon w_\epsilon\|_{H^1(\Omega)} \le \mathrm{C}_1 \epsilon (M_\epsilon + \mathrm{C}_2),$$

where M_ϵ *is defined by* (3.6). *Furthermore, there exists a constant* D_1 *independent of* ϵ *such that,*

$$\|w_\epsilon\|_{L^2(\Gamma)} \le \mathrm{D}_1.$$

Remark 3.1. We do not know that D_ϵ is finite in general for $n = 3$ but seems to be a physically reasonable assumption to make. When the material is layered, *i.e.*, when the dependence of f on y is only in one direction, the problem reduces to one in two dimensions. In the two-dimensional case the domain Ω is a unit square and Γ is the right side of the square, that is $\Gamma = \{(x_1, x_2) \in \Omega : x_1 = 1\}$, (see Fig. 3.1). When $n = 2$, using an Orlicz estimate, we have $f(x/\epsilon, u_\epsilon) \in L^2(\Omega)$ if $u_\epsilon \in H^1(\Omega)$. Then problem (2.4) and standard regularity theory imply $u_\epsilon \in H^{3/2}(\Omega)$. Thus, by the Trace Theorem , we have $u_\epsilon \in H^1(\Gamma)$ independent of ϵ. Finally, using the Sobolev Imbedding Theorem we have $u_\epsilon \in C^0(\Gamma)$. Thus, we can show D_ϵ is bounded independently of ϵ when $n = 2$. See [6] for more details.

4. A Robin Boundary Condition

In Fig. 5.1 we plot for certain sample parameters our approximations from [6]. Note that this previously developed approximation is slightly shifted away from u_ϵ. In this section we present an alternative correction term to w_ϵ. Define $u_\epsilon^{(1)}$ to satisfy the Robin boundary condition problem

$$\begin{aligned} &\Delta u_\epsilon^{(1)} = 0 \quad \text{in } \Omega, \\ &-\frac{\partial u_\epsilon^{(1)}}{\partial n} = \frac{1}{\epsilon}(f(\frac{x}{\epsilon}, u_0) - f_0(u_0)) + u_\epsilon^{(1)} \frac{\partial f}{\partial v}(x/\epsilon, u_0) \quad \text{on } \Gamma, \\ &-\frac{\partial u_\epsilon^{(1)}}{\partial n} = 0 \quad \text{on } \partial\Omega \setminus \Gamma. \end{aligned} \tag{4.1}$$

Before we develop rigorous estimates or provide numerical data, let us give some motivation for (4.1). Assuming

$$u_\epsilon \approx u_0 + \epsilon u_\epsilon^{(1)},$$

we have

$$u_\epsilon^{(1)} \approx \frac{1}{\epsilon}(u_\epsilon - u_0),$$

which motivates the ideal boundary condition

$$-\frac{\partial u_\epsilon^{(1)}}{\partial n} = \frac{1}{\epsilon}(f(x/\epsilon, u_\epsilon) - f_0(u_0)). \tag{4.2}$$

So, by using

$$f(x/\epsilon, u_\epsilon) \approx f(x/\epsilon, u_0) \tag{4.3}$$

we obtain the Neumann boundary condition

$$-\frac{\partial w_\epsilon}{\partial n} = (f(x/\epsilon, u_0) - f_0(u_0))/\epsilon,$$

which was used in [6]. Here we take (4.3) a step further by using the next term in the Taylor approximation of f in the second variable:

$$f(x/\epsilon, u_\epsilon) \approx f(x/\epsilon, u_0) + \frac{\partial f}{\partial v}(x/\epsilon, u_0)(u_\epsilon - u_0).$$

Now, since

$$\epsilon u_\epsilon^{(1)} \approx (u_\epsilon - u_0),$$

we get

$$f(x/\epsilon, u_\epsilon) \approx f(x/\epsilon, u_0) + \epsilon \frac{\partial f}{\partial v}(x/\epsilon, u_0) u_\epsilon^{(1)}$$

which if we substitute into (4.2) yields the Robin boundary condition (4.1). One can obtain improved convergence estimates using the new correction. In particular, we show that we have $\mathcal{O}(\epsilon^{3/2})$ convergence when $n = 3$, where just as in [6], the constant depends on D_ϵ (recall that by definition there exists a constant C such that $0 < M_\epsilon < Ce^{D_\epsilon}$). We also show that we have $\mathcal{O}(\epsilon^{2-\delta})$ for any $\delta > 0$ convergence when $n = 2$, without any additional assumptions. Before we present the proposition, for the sake of notation, let us define

$$C_\epsilon = \max\Big\{D_\epsilon, M_\epsilon\Big\}, \tag{4.4}$$

where D_ϵ and M_ϵ are defined by (3.5) and (3.6).

Proposition 4.1. *Let $n = 3$ and let u_ϵ, u_0 be minimizers of* (3.1), (3.2) *respectively, and let $u_\epsilon^{(1)}$ be the solution to* (4.1)*. Assume also that $u_\epsilon \in C^0(\bar{\Omega})$. Then there exists constants C and D independent of ϵ such that*

$$\|u_\epsilon - u_0 - \epsilon u_\epsilon^{(1)}\|_{H^1(\Omega)} \le \epsilon^{3/2} C\tilde{C}_\epsilon,$$

where $\tilde{C}_\epsilon = [C_\epsilon + D]^3$ and C_ϵ is defined by (4.4)*.*

Proof. Let

$$z_\epsilon = u_\epsilon - u_0 - \epsilon u_\epsilon^{(1)},$$

since u_ϵ is continuous, by the variational form of (2.4) and (2.5), we have that for any $v \in H^1(\Omega)$,

$$\begin{aligned}\int_\Omega \nabla z_\epsilon \cdot \nabla v \; dx &= \int_\Omega \nabla u_\epsilon \cdot \nabla v \; dx - \int_\Omega \nabla u_0 \cdot \nabla v \; dx - \epsilon \int_\Omega \nabla u_\epsilon^{(1)} \cdot \nabla v \; dx \\ &= -\int_\Gamma f(x/\epsilon, u_\epsilon) v d\sigma_x + \int_\Gamma f(x/\epsilon, u_0) v d\sigma_x + \epsilon \int_\Gamma \frac{\partial f}{\partial v}(x/\epsilon, u_0) u_\epsilon^{(1)} v d\sigma_x.\end{aligned}$$

Consequently,

$$\int_\Omega \nabla z_\epsilon \cdot \nabla v \; dx + \int_\Gamma [f(x/\epsilon, u_\epsilon) - f(x/\epsilon, u_0)] v d\sigma_x - \epsilon \int_\Gamma \frac{\partial f}{\partial v}(x/\epsilon, u_0) u_\epsilon^{(1)} v d\sigma_x = 0. \quad (4.5)$$

Now note that u_0 and u_ϵ are defined pointwise on Γ. So, by Taylor's Theorem, using Lagrange's form of the remainder term we have that for each fixed ϵ and $x \in \Gamma$ there exists ξ_ϵ^x between $u_0(x)$ and $u_\epsilon(x)$ such that

$$f(\frac{x}{\epsilon}, u_\epsilon) - f(\frac{x}{\epsilon}, u_0) = \frac{\partial f}{\partial v}(\frac{x}{\epsilon}, u_0)(u_\epsilon - u_0) + \frac{1}{2}\frac{\partial^2 f}{\partial v^2}(\frac{x}{\epsilon}, \xi_\epsilon^x)(u_\epsilon - u_0)^2.$$

By subtracting and adding $\epsilon u_\epsilon^{(1)}$ within the parentheses of the first term on the right hand side we have

$$f(\frac{x}{\epsilon}, u_\epsilon) - f(\frac{x}{\epsilon}, u_0) = \frac{\partial f}{\partial v}(\frac{x}{\epsilon}, u_0) z_\epsilon + \epsilon \frac{\partial f}{\partial v}(\frac{x}{\epsilon}, u_0) u_\epsilon^{(1)} + \frac{1}{2}\frac{\partial^2 f}{\partial v^2}(\frac{x}{\epsilon}, \xi_\epsilon^x)(u_\epsilon - u_0)^2. \quad (4.6)$$

Thus substituting (4.6) into (4.5) yields

$$\int_\Omega \nabla z_\epsilon \cdot \nabla v \; dx + \int_\Gamma \frac{\partial f}{\partial v}(x/\epsilon, u_0) z_\epsilon v d\sigma_x = -\frac{1}{2}\int_\Gamma \frac{\partial^2 f}{\partial v^2}(x/\epsilon, \xi_\epsilon^x)(u_\epsilon - u_0)^2 v d\sigma_x. \quad (4.7)$$

Now, if we pick $v = z_\epsilon$, we have

$$\int_\Omega |\nabla z_\epsilon|^2 \; dx + \int_\Gamma \frac{\partial f}{\partial v}(\frac{x}{\epsilon}, u_0) z_\epsilon^2 d\sigma_x = -\frac{1}{2}\int_\Gamma \frac{\partial^2 f}{\partial v^2}(\frac{x}{\epsilon}, \xi_\epsilon^x)(u_\epsilon - u_0)^2 z_\epsilon d\sigma_x.$$

One can check that there exists a constant $c_0 > 0$ such that $\frac{\partial f}{\partial v}(y, v) \ge c_0 > 0$ for all $(y, v) \in Y \times \mathbb{R}$. Using a variant of the Poincaré inequality (*e.g.* see [9]) yields

$$\begin{aligned}\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} &\le \int_\Omega |\nabla z_\epsilon|^2 \; dx + \int_\Gamma \frac{\partial f}{\partial v}(\frac{x}{\epsilon}, u_0) z_\epsilon^2 d\sigma_x \\ &= -\frac{1}{2}\int_\Gamma \frac{\partial^2 f}{\partial v^2}(\frac{x}{\epsilon}, \xi_\epsilon^x)(u_\epsilon - u_0)^2 z_\epsilon d\sigma_x\end{aligned}$$

for some $\tilde{c_0} > 0$. Now note that

$$\begin{aligned}\left|\frac{\partial^2 f}{\partial v^2}(y,v)\right| &= \left|\lambda(y)[\alpha(y)^2 e^{\alpha(y)(v-V(y))} - (1-\alpha(y))^2 e^{-(1-\alpha(y))(v-V(y))}]\right| \\ &\leq \lambda(y)\left[\alpha(y)^2 e^{\alpha(y)(v-V(y))} + (1-\alpha(y))^2 e^{-(1-\alpha(y))(v-V(y))}\right] \\ &\leq \frac{\partial f}{\partial v}(y,v),\end{aligned}$$

where the last inequality follows from the fact that $0 < \alpha(y) < 1$ for all $y \in Y$. So

$$\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} \leq \frac{1}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \int_\Gamma (u_\epsilon - u_0)^2 |z_\epsilon| d\sigma_x. \tag{4.8}$$

Now note that by Hölder's Inequality we have

$$\begin{aligned}\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} &\leq \frac{1}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \int_\Gamma (u_\epsilon - u_0)^2 |z_\epsilon| d\sigma_x \\ &\leq \frac{C}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \|u_\epsilon - u_0\|_{L^2(\Gamma)} \|(u_\epsilon - u_0)|z_\epsilon|\|_{L^2(\Gamma)}.\end{aligned}$$

Note that since we assume D_ϵ is finite, by a variant of Hölder's Inequality, see [4], p.25, we have

$$\|(u_\epsilon - u_0)|z_\epsilon|\|_{L^2(\Gamma)} \leq \|u_\epsilon - u_0\|_{L^4(\Gamma)} \|z_\epsilon\|_{L^4(\Gamma)}$$

and then using an interpolation inequality, see [4], p.27, yields

$$\|u_\epsilon - u_0\|_{L^4(\Gamma)} \leq \|u_\epsilon - u_0\|^{1/2}_{L^2(\Gamma)} \|u_\epsilon - u_0\|^{1/2}_{L^\infty(\Gamma)}.$$

Note that by Theorem 7.58(i) in [3] we have the imbedding

$$H^{1/2}(\Gamma) \to L^4(\Gamma),$$

thus we have

$$\|z_\epsilon\|_{L^4(\Gamma)} \leq C\|z_\epsilon\|_{H^{1/2}(\Gamma)}.$$

So,

$$\begin{aligned}\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} &\leq \frac{C}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \|u_\epsilon - u_0\|_{L^2(\Gamma)} \|u_\epsilon - u_0\|^{1/2}_{L^2(\Gamma)} \|u_\epsilon - u_0\|^{1/2}_{L^\infty(\Gamma)} \|z_\epsilon\|_{H^{1/2}(\Gamma)} \\ &\leq \tilde{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \|u_\epsilon - u_0\|^{3/2}_{L^2(\Gamma)} \|u_\epsilon - u_0\|^{1/2}_{L^\infty(\Gamma)} \|z_\epsilon\|_{H^1(\Omega)},\end{aligned}$$

where the last inequality follows by the Trace Theorem. Thus

$$\|z_\epsilon\|_{H^1(\Omega)} \leq \hat{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi^x_\epsilon)\|_{L^\infty(\Gamma)} \|u_\epsilon - u_0\|^{3/2}_{L^2(\Gamma)} \|u_\epsilon - u_0\|^{1/2}_{L^\infty(\Gamma)}.$$

Now if w_ϵ is a weak solution to (3.3) then by the Triangle Inequality and Proposition 3.1 we have

$$\begin{aligned}\|u_\epsilon - u_0\|_{L^2(\Gamma)} &= \|u_\epsilon - u_0 - \epsilon w_\epsilon + \epsilon w_\epsilon\|_{L^2(\Gamma)} \\ &\leq \|u_\epsilon - u_0 - \epsilon w_\epsilon\|_{L^2(\Gamma)} + \epsilon\|w_\epsilon\|_{L^2(\Gamma)} \\ &\leq C_1\epsilon(M_\epsilon + C_2) + \epsilon D_1 \\ &\leq C_1\epsilon[M_\epsilon + C_3],\end{aligned} \tag{4.9}$$

where C_3 is a constant independent of ϵ such that $C_2 + D_1/C_1 \leq C_3$. Thus, we have that

$$\begin{aligned}
\|z_\epsilon\|_{H^1(\Omega)} &\leq \hat{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon},\xi_\epsilon^x)\|_{L^\infty(\Gamma)}\|u_\epsilon - u_0\|^{3/2}_{L^2(\Gamma)}\|u_\epsilon - u_0\|^{1/2}_{L^\infty(\Gamma)} \\
&\leq \epsilon^{3/2}\sqrt{2}\hat{C}C_1^{3/2}M_\epsilon D_\epsilon^{1/2}[M_\epsilon + C_3]^{3/2} \\
&\leq \epsilon^{3/2}\sqrt{2}\hat{C}C_1^{3/2}C_\epsilon^{3/2}[C_\epsilon + C_3]^{3/2} \\
&\leq \epsilon^{3/2}K\tilde{C}_\epsilon,
\end{aligned}$$

where K is a constant independent of ϵ and $\tilde{C}_\epsilon = [C_\epsilon + C_3]^3$.

For the two-dimensional case we can prove a stronger result. In this case, recall in [6] we saw that u_ϵ is continuous and bounded independent of ϵ and so Proposition 3.1 implies

$$\|u_\epsilon - u_0\|_{L^2(\Gamma)} \leq \tilde{C}\epsilon \tag{4.10}$$

for some constant $\tilde{C}$ independent of ϵ.

Proposition 4.2. *Let $n = 2$ and let u_ϵ, u_0 be minimizers of* (3.1), (3.2) *respectively, and let $u_\epsilon^{(1)}$ be the solution to* (4.1). *Then for any $\delta > 0$ there exists a constant C independent of ϵ such that*

$$\|u_\epsilon - u_0 - \epsilon u_\epsilon^{(1)}\|_{H^1(\Omega)} \leq C\epsilon^{2-\delta}.$$

Proof. As in Proposition 4.1, if we let

$$z_\epsilon = u_\epsilon - u_0 - \epsilon u_\epsilon^{(1)},$$

since u_ϵ is continuous, by the variational form of (2.4) and (2.5), we can establish that

$$\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} \leq \frac{1}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon},\xi_\epsilon^x)\|_{L^\infty(\Gamma)}\int_\Gamma (u_\epsilon - u_0)^2|z_\epsilon|d\sigma_x. \tag{4.11}$$

By Hölder's Inequality we have

$$\int_\Gamma (u_\epsilon - u_0)^2|z_\epsilon|d\sigma_x \leq ||u_\epsilon - u_0||_{L^2(\Gamma)}||(u_\epsilon - u_0)|z_\epsilon|||_{L^2(\Gamma)}.$$

Now by a variant of Hölder's Inequality, p.25 [4], we have

$$\|(u_\epsilon - u_0)|z_\epsilon|\|_{L^2(\Gamma)} \leq \|u_\epsilon - u_0\|_{L^{2/\alpha}(\Gamma)}\|z_\epsilon\|_{L^{2/1-\alpha}(\Gamma)}$$

for $0 < \alpha < 1$ and then using an interpolation inequality, p.27 [4], yields

$$\|u_\epsilon - u_0\|_{L^{2/\alpha}(\Gamma)} \leq \|u_\epsilon - u_0\|^\alpha_{L^2(\Gamma)}\|u_\epsilon - u_0\|^{1-\alpha}_{L^\infty(\Gamma)}.$$

Note that by Theorem 7.58(ii) in [3] we have the imbedding

$$H^{1/2}(\Gamma) \to L^q(\Gamma), \quad \text{for } 2 \leq q < \infty,$$

thus we have

$$\|z_\epsilon\|_{L^{2/1-\alpha}(\Gamma)} \leq C\|z_\epsilon\|_{H^{1/2}(\Gamma)} \quad \text{for } 0 < \alpha < 1.$$

So,

$$\begin{aligned}
\tilde{c_0}\|z_\epsilon\|^2_{H^1(\Omega)} &\leq \frac{C}{2}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon},\xi_\epsilon^x)\|_{L^\infty(\Gamma)}\|u_\epsilon - u_0\|_{L^2(\Gamma)}\|u_\epsilon - u_0\|^\alpha_{L^2(\Gamma)}\|u_\epsilon - u_0\|^{1-\alpha}_{L^\infty(\Gamma)}\|z_\epsilon\|_{H^{1/2}(\Gamma)} \\
&\leq \tilde{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon},\xi_\epsilon^x)\|_{L^\infty(\Gamma)}\|u_\epsilon - u_0\|^{1+\alpha}_{L^2(\Gamma)}\|u_\epsilon - u_0\|^{1-\alpha}_{L^\infty(\Gamma)}\|z_\epsilon\|_{H^1(\Omega)},
\end{aligned}$$

where the last inequality follows by the Trace Theorem. Thus

$$\|z_\epsilon\|_{H^1(\Omega)} \le \hat{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi_\epsilon^x)\|_{L^\infty(\Gamma)}\|u_\epsilon - u_0\|_{L^2(\Gamma)}^{1+\alpha}\|u_\epsilon - u_0\|_{L^\infty(\Gamma)}^{1-\alpha}.$$

Now recalling (4.9) we have

$$\|u_\epsilon - u_0\|_{L^2(\Gamma)} \le C_1\epsilon[M_\epsilon + C_3],$$

where C_1 and C_3 are constants independent of ϵ. Note that when $n = 2$ we have that D_ϵ is bounded independently of ϵ, thus there exists a positive constant K, bounded independently of ϵ, such that

$$\begin{aligned}\|z_\epsilon\|_{H^1(\Omega)} &\le \hat{C}\|\frac{\partial f}{\partial v}(\frac{x}{\epsilon}, \xi_\epsilon^x)\|_{L^\infty(\Gamma)}\|u_\epsilon - u_0\|_{L^2(\Gamma)}^{1+\alpha}\|u_\epsilon - u_0\|_{L^\infty(\Gamma)}^{1-\alpha} \\ &\le \epsilon^{1+\alpha}KD_\epsilon^{1-\alpha} \quad \text{for } 0 < \alpha < 1.\end{aligned}$$

So, for any $\delta > 0$ we have

$$\|z_\epsilon\|_{H^1(\Omega)} \le C\epsilon^{2-\delta},$$

where C can be picked independently of ϵ.

5. Numerical Experiments

We now demonstrate the accuracy of this approximation with numerical experiments when $n = 2$. We begin by using the same parameters as in [6]: $J_A = 1$, $J_C = 10$, $V_A = 0.5$, $V_C = 1.0$, $\alpha_{aa} = 0.5$, $\alpha_{ca} = 0.85$, and $Y = Y_A \cup Y_C$ where $Y_A = [0, 1/3]$ and $Y_C = [1/3, 1]$. For the parameter values used here, we have $u_0 = 0.9758$. Recall that in the two-dimensional case the domain Ω is a unit square, see Fig. 3.1.

To compute u_ϵ, u_0, and $u_\epsilon^{(1)}$, we use piecewise linear finite elements on a regular mesh, and choose a grid which conforms to the medium to avoid singularities within elements. We compute the correction, $u_\epsilon^{(1)}$, using standard finite elements (conforming to the media) for a linear problem. When solving for u_ϵ we use a conjugate gradient descent based algorithm developed by Hager and Zhang [8] to perform the nonlinear minimization.

Our previous approximations [6] are shown in Fig. 5.1, where we see the slight shift in the approximation away from the solution to the nonlinear problem (2.4). In Fig. 5.2 we graph the new approximation and the solution to the nonlinear problem (2.4) using the same parameter values used in [6]. Note the high accuracy of this approximation. Since the curves seem to be overlapping, by plotting node values, we demonstrate in Fig. 5.3 that the two curves are indeed slightly different. In Fig. 5.4 we provide surface plots of the full solution on Ω.

In Table 5.1 we present the computed norm errors and empirical values for the convergence rate α using the parameter values from [6]. Since piecewise linear finite elements yield only $\mathcal{O}(h)$ approximations for the gradient, the error of our finite element approximation (using about 1 million elements) is on the order of our observed errors ($h \approx 6.5 \times 10^{-4}$). So calculations of convergence rates for the H^1-norm are meaningless.

In order to get better empirical convergence rates, we choose our second set of parameter values to contain a much higher contrast in rest potentials. We expect this will lead to larger errors in all approximations. The second set of parameter values are $J_A = 3$, $J_C = 7$, $V_A = 10$,

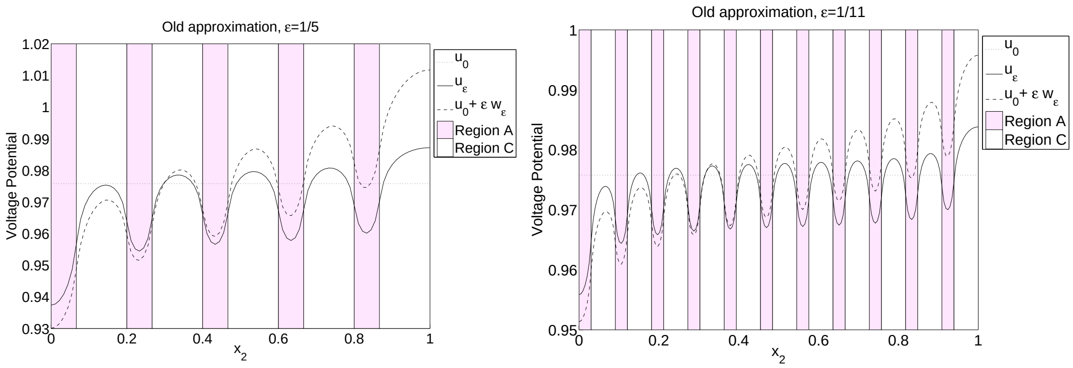

Fig. 5.1. Previous approximation and the brute force solution on the boundary Γ, $\epsilon = 1/5$, $\epsilon = 1/11$ respectively.

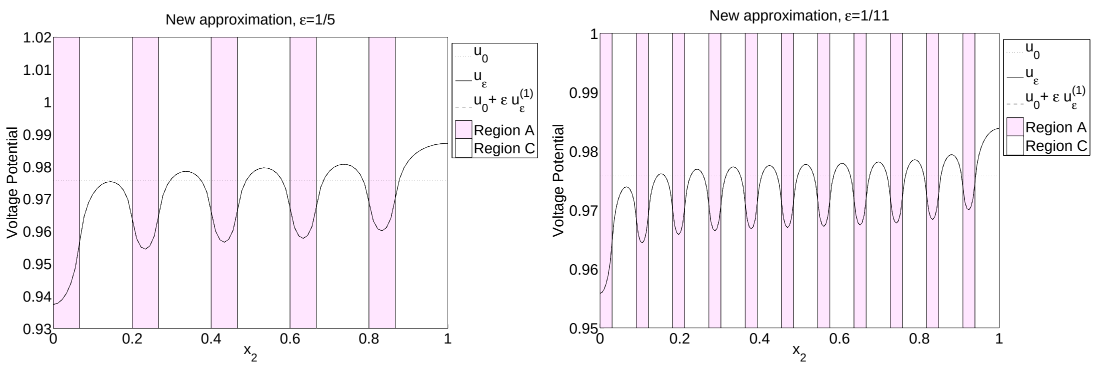

Fig. 5.2. New approximation and the brute force solution on the boundary Γ, $\epsilon = 1/5$, $\epsilon = 1/11$ respectively.

Table 5.1: Table of estimates and convergence rates.

ϵ	1/2	1/3	1/4	1/5	1/6	α			
$\\|u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\\|_{H^1(\Omega)}$	.8406e-4	.4420e-4	.2877e-4	.2124e-4	.2104e-4	n.a.	n.a.	n.a.	n.a.
$\\|u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\\|_{L^\infty(\Omega)}$	.0019	.0013	.0009	.0007	.0004	1.4183	1.7004	2	3.0694
$\\|u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\\|_{L^2(\Omega)}$	.5254e-4	.2427e-4	.1290e-4	.0720e-4	.0417e -4	2.3062	2.5411	2.7852	2.9956
$\\|u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\\|_{L^2(\Gamma)}$	.5729e-4	.2908e-4	.1791e-4	.1212e-4	.0736e -4	1.8679	1.9822	2.1933	2.7358

$V_C = 1.0$, $\alpha_{aa} = 0.5$, $\alpha_{ca} = 0.85$ and $Y = Y_A \cup Y_C$ where $Y_A = [0, 1/3]$ and $Y_C = [1/3, 1]$. Here we have $u_0 = 3.272$.

Figs. 5.5 and 5.6 show the surface plots of the brute force solution and our approximation for $\epsilon = 1/5$ and $\epsilon = 1/11$ respectively. The errors are indeed larger in this case, as we can see from the plot of the potentials on Γ in Fig. 5.7 for $\epsilon = 1/5$. The approximation is still very accurate, and one sees that for smaller ϵ (Fig. 5.7) the plots are almost indistinguishable.

In Table 5.2 we measure the accuracy of our approximation in various norms and calculate the convergence rate. In the L^2-norm the error is low and, as one expects, the H^1 error is larger. Although approximating the gradient of the solution of the heterogeneous, nonlinear problem (2.4) is difficult, the solution of the problem with Robin boundary data (4.1) yields a correction term which has a gradient that is an accurate and numerically efficient approximation. In Table 5.3 we examine the accuracy of all the approximation strategies discussed here. Note

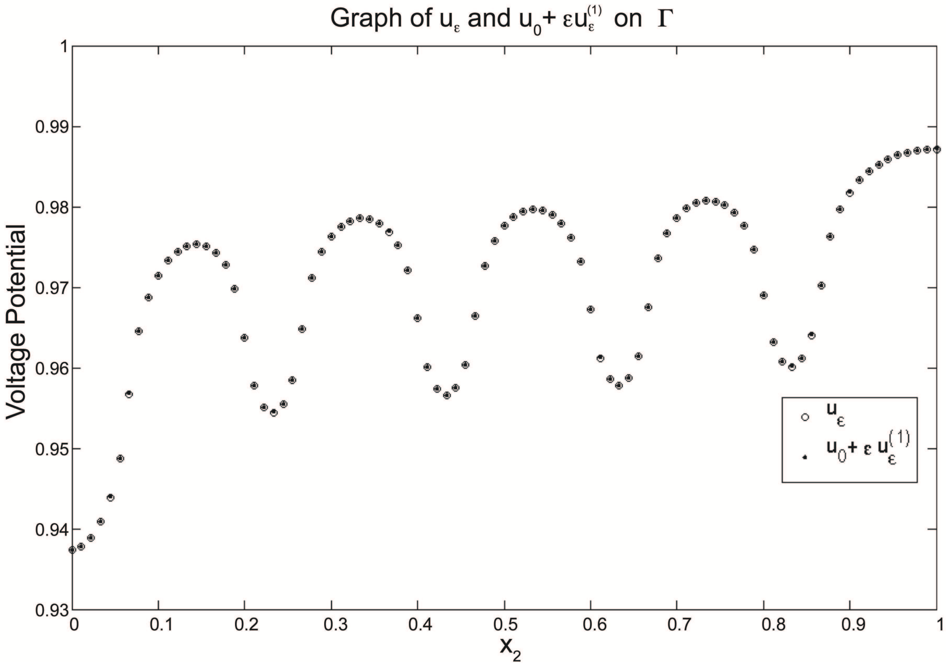

Fig. 5.3. New approximation and the brute force solution on the boundary Γ, $\epsilon = 1/5$.

Table 5.2: Table of norms over Ω and Γ and convergence rates.

ϵ	1/5	1/11	1/25	1/40	α		
$\Vert u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\Vert_{H^1(\Omega)}$	.8080	.3150	.0859	.0366	1.4884	1.6677	1.8164
$\Vert u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\Vert_{L^2(\Omega)}$	.0486	.0149	.0039	.0015	1.6726	1.7784	2.033
$\Vert u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\Vert_{L^2(\Gamma)}$	.1888	.0561	.0132	.0054	1.7093	1.8131	1.9017
$\Vert u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\Vert_{L^\infty(\Gamma)}$	.5756	.2225	.0692	.0347	1.3507	1.4394	1.4686

Table 5.3: Comparison of approximations over Ω and convergence rates.

ϵ	1/5	1/11	1/25	1/40	α		
$\Vert u_\epsilon - (u_0 + \epsilon u_\epsilon^{(1)})\Vert_{H^1(\Omega)}$	.8080	.3150	.0859	.0366	1.4884	1.6677	1.8164
$\Vert u_\epsilon - (u_0 + \epsilon w_\epsilon)\Vert_{H^1(\Omega)}$	6.8550	3.1770	1.3441	.8108	1.0266	1.0579	1.0756
$\Vert u_\epsilon - u_\epsilon^L\Vert_{H^1(\Omega)}$	2.8178	2.8821	2.5022	2.1940	.1203	.2113	.2797

that the direct linearization approximation is poor as ϵ decreases. While the approximation developed in [6] improves as $\epsilon \to 0$, the approximation presented in this paper is substantially more accurate.

6. Conclusion

We have constructed an accurate approximation to the solution to (2.4), a nonlinear, heterogeneous problem, by using its homogenized limit and a linear correction. This linear correction, while just as easy to compute, is far better than the correction proposed in [6], although both converge to the correct limit as $\epsilon \to 0$. If the period size ϵ were large, *i.e.*, the number of anodes is small, linearizing the problem directly also yields reasonable results. However, the approximation introduced in this paper appears to be even better, and the direct linearization

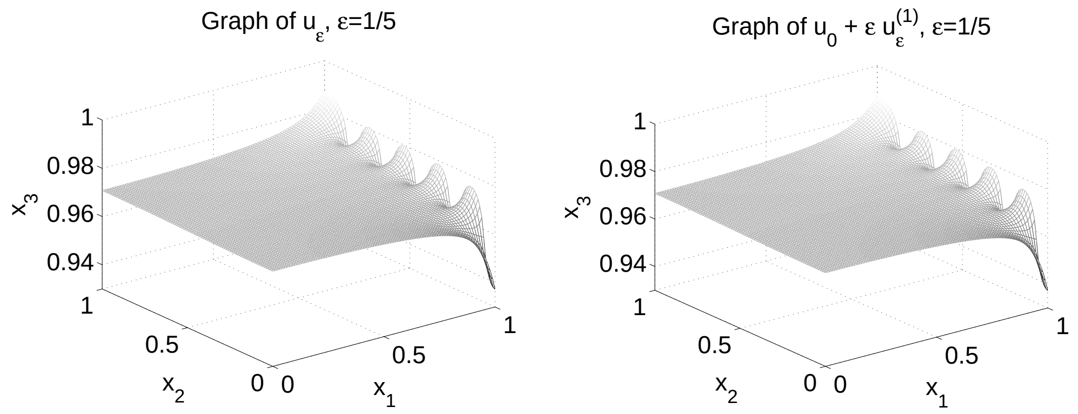

Fig. 5.4. Left: Brute force solution. Right: New approximation. $\epsilon = 1/5$.

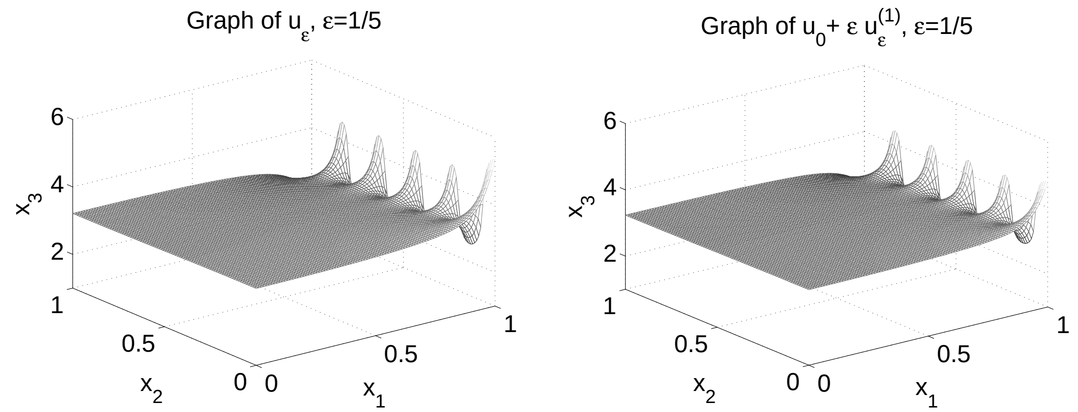

Fig. 5.5. Left: Brute force solution. Right: New approximation. $\epsilon = 1/5$.

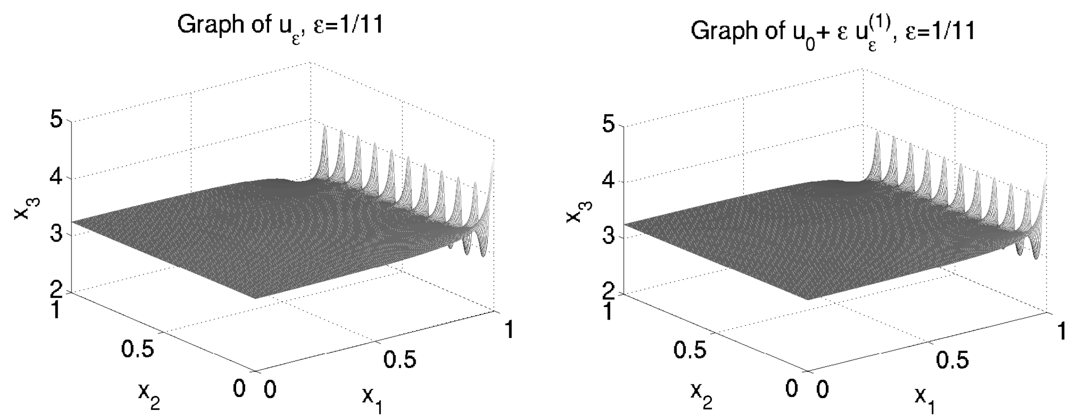

Fig. 5.6. Left: Brute force solution. Right: New approximation. $\epsilon = 1/11$.

can be very bad for a large number of anodes.

If one were to prescribe a nonzero current over the inactive part of the boundary in (1.1), the same results will hold. However, the homogenized solution u_0 in this case will no longer be constant and will solve a nonlinear problem. But, since this problem is homogeneous, u_0 will

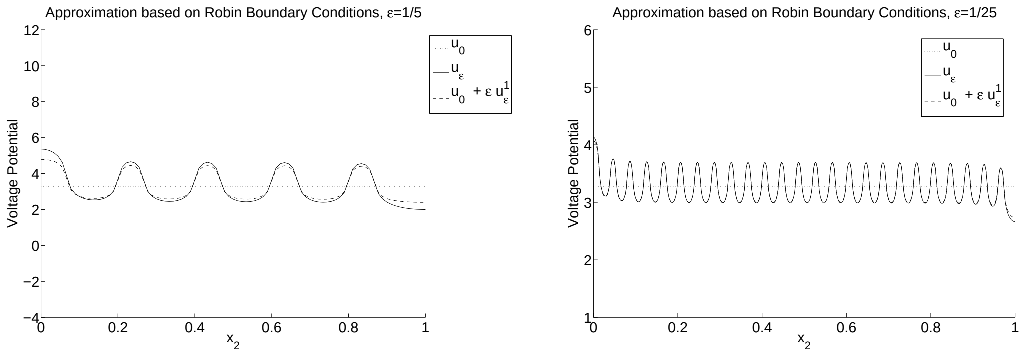

Fig. 5.7. The approximation and the original, $\epsilon = 1/5$, $\epsilon = 1/25$ respectively.

generally be much easier to compute than the original.

It seems that this technique of homogenizing and then linearizing about the homogenized solution could be extended to more complicated media, *e.g.*, with boundary conditions of the form

$$-\frac{\partial u_\epsilon}{\partial n} = f(x, x/\epsilon, u_\epsilon)$$

in problem (2.4) or other semilinear periodic problems. We also suspect that for $n = 3$, we can obtain convergence on the order of $\mathcal{O}(\epsilon^2)$. Further analysis must be done and certain issues regarding imbeddings must be resolved to obtain $\mathcal{O}(\epsilon^2)$ convergence. Another subject of future research is the study of related eigenvalue problems, as in [15], but with periodically varying parameters.

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