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A DIFFUSE DOMAIN APPROXIMATION WITH TRANSMISSION-TYPE BOUNDARY CONDITIONS I: ASYMPTOTIC ANALYSIS AND NUMERICS

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Abstract. Diffuse domain methods (DDMs) have garnered significant attention for approximating solutions to partial differential equations on complex geometries. These methods implicitly represent the geometry by replacing the sharp boundary interface with a diffuse layer of thickness ε, which scales with the minimum grid size. This approach reformulates the original equations on an extended regular domain, incorporating boundary conditions through singular source terms. In this work, we conduct a matched asymptotic analysis of a DDM for a two-sided problem with transmission-type Robin boundary conditions. Our results show that, in the one dimensional space, the solution of the diffuse domain approximation asymptotically converges to the solution of the original problem, with exactly first-order accuracy in ε. Furthermore, we provide numerical simulations that validate and illustrate the analytical result.

Key words. Partial differential equations, phase-field approximation, diffuse domain method, diffuse interface approximation, asymptotic analysis, numerical simulation, reaction-diffusion equation, transmission boundary conditions.

1. Introduction

Partial differential equations (PDEs) are foundational tools for modeling diverse phenomena across physical, biological, and engineering sciences, including fluid flow, material behavior, tissue dynamics, and phase transitions. In many practical scenarios, these problems arise within domains that are complex, irregular, or time-dependent, such as evolving interfaces in phase transitions or intricate geometries in biological systems. Traditional PDE solution methods often require domains with simple, specific geometric boundaries, posing challenges in mesh generation and driving up computational costs. To address these limitations, diffuse domain methods (DDMs) have emerged as versatile approaches for solving PDEs on irregular or dynamically evolving domains.

The fundamental principles of DDMs involve (i) embedding the original complex domain into a larger, simpler computational domain, like a square or a cube, (ii) creating a simple, structured mesh for the larger domain that resolves the shape of the complex domain without fitting it precisely, and (iii) solving an approximate PDE problem on the larger computational domain. This approach eliminates the need for intricate, boundary-conforming meshes that conventional methods typically require. This is especially important in the time-dependent setting where the shape of the complex domain is constantly changing, requiring expensive re-meshing. A smooth phase-field function is employed to approximate the characteristic function of the complex domain, while a parameter ε, typically related to the grid size, defines the width of the diffuse interfacial region, influencing the accuracy of the approximation. The original PDE is reformulated with additional source terms to enforce boundary conditions. For small values of ε, DDMs are especially efficient

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when paired with adaptive mesh refinement, which allows for fine grid cells in the narrow transition layer and coarser cells in the extended, non-physical regions of the domain. DDMs offer the advantage of flexible application to a broad range of equations and can be solved using standard discretization methods, both uniform and adaptive, along with fast iterative solvers based, for example, on geometric multigrid methods.

The concept of the DDM was first introduced by Kockelkoren and Levine [23] for studying diffusion within a cell with zero Neumann boundary conditions at the cell boundary. A related approach, known as the fictitious domain method, was earlier employed by Glowinski et al. [12, 22] to compute numerical solutions to Dirichlet problems for a class of elliptic operators. Since then, DDMs have been subsequently applied to model electrical waves in the heart [19] and membrane-bound Turing patterns [24]. More recent developments have expanded DDMs to solve PDEs on both stationary [30] and evolving surfaces (e.g., [11, 13, 14, 15, 16, 17]). The analysis of DDM approach to solving elliptic PDEs in domains with complex boundaries subject to Dirichlet, Neumann, and Robin boundary conditions is provided in [7, 6, 20, 26, 31]. DDMs have gained wide use in applications such as phase-field modeling, where they support simulations of complex phenomena in fields like biology (e.g., [8, 23, 19, 10, 28, 2]), fluid dynamics (e.g., [3, 34, 4, 1, 5, 33]), and materials science (e.g., [35, 28, 29, 9]).

1.1. The One-sided Diffuse Domain Problem. Let Ω_1 be a bounded open subset of $\mathbb{R}^n$. We consider the reaction-diffusion equation in Ω_1:

$$\begin{aligned} -\Delta u + u &= f, \quad \text{in } \Omega_1, \\ -\nabla u \cdot \boldsymbol{n}_1 &= \kappa u + g, \quad \text{on } \partial\Omega_1, \end{aligned} \tag{1}$$

where $\boldsymbol{n}_1$ denotes the outward-pointing unit normal vector on $\partial\Omega_1$. Here, $\kappa \geq 0$ is a given constant. Observe that Neumann boundary conditions hold when $\kappa = 0$, and Robin boundary conditions hold when $\kappa > 0$.

To approximate this problem using a diffuse domain approach, we define an extended domain Ω, a larger cuboidal region containing $\overline{\Omega_1}$ (see Figure 1). In this extended domain Ω, the diffuse domain approximation equation is

$$-\nabla \cdot (\phi_\varepsilon \nabla u_\varepsilon) + \phi_\varepsilon u_\varepsilon + \text{BC} = \phi_\varepsilon f, \tag{2}$$

where $\phi_\varepsilon(x)$ approximates the characteristic function $\chi_{\Omega_1}(x)$ of Ω_1, given by

$$\chi_{\Omega_1}(x) = \begin{cases} 1, & \text{if } x \in \Omega_1, \\ 0, & \text{if } x \notin \Omega_1. \end{cases}$$

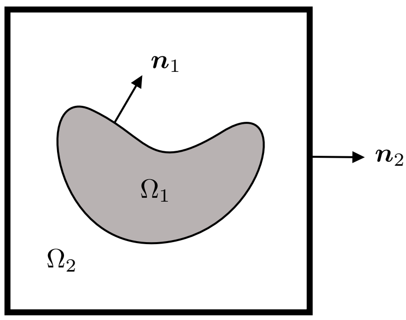

FIGURE 1. A domain Ω_1 is covered by a larger cuboidal domain Ω, with $\Omega_2 := \Omega \setminus \overline{\Omega}_1$.