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High-order numerical schemes based on difference potentials for 2D elliptic problems with material interfaces

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A B S T R A C T

Numerical approximations and computational modeling of problems from Biology and Materials Science often deal with partial differential equations with varying coefficients and domains with irregular geometry. The challenge here is to design an efficient and accurate numerical method that can resolve properties of solutions in different domains/subdomains, while handling the arbitrary geometries of the domains. In this work, we consider 2D elliptic models with material interfaces and develop efficient high-order accurate methods based on Difference Potentials for such problems.

1. Introduction

Highly-accurate numerical methods (see [38], etc.) that can efficiently handle irregular geometry and interface problems (usually described by mathematical models that have input data and solutions with discontinuities/non-smoothness across the interfaces), are crucial for the resolution of different temporal and spatial scales of physical, biological, biomedical problems, and problems from material sciences (models for composite materials, fluids, chemotaxis models, biofilms), to name a few. The major challenge here is to design a robust method that accurately captures certain properties of the solutions in different domains/subdomains (different regularity of the solutions in the domains, positivity, etc.), while handling the arbitrary geometries of the domains/subdomains. Moreover, any standard numerical method designed for smooth solutions, in general and in any dimension, will fail to produce accurate solutions to interface problems due to discontinuities in the model's parameters/solutions.

There is extensive literature that addresses problems in domains with irregular geometries and interface problems. Among finite-difference based methods for such problems are the Immersed Boundary Method (IB) [25,26], etc., the Immersed Interface Method (IIM) [15–17], etc., the Ghost Fluid Method (GFM) [12,19,18], etc., the Matched Interface and Boundary Method (MIB) [45,43,46], etc., and the method based on the Integral Equations approach, [21], etc. Among the

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finite-element methods for interface problems are [3,6,37,24,44,42,13], etc. These methods are sharp interface methods that have been employed to solve problems in science and engineering. For a detailed review of the subject the reader can consult [17]. However, in spite of great advances in the past 40 years in the numerical methods for problems in arbitrary domains and/or interface problems, it is still a challenge to develop efficient numerical algorithms that can deliver high-order accuracy in space (higher than second-order), and that can handle general boundary/interface conditions.

Therefore, we consider here an approach based on Difference Potentials Method (DPM) [31,32]. The DPM on its own, or in combination with other numerical methods, is an efficient technique for the numerical solution, as well as for the discrete modeling of interior and exterior boundary value problems in domains with arbitrary geometry (see for example, [31,32,20,33,39,22,34,35,7,8,10,1,2]). The main idea of DPM is to reduce uniquely solvable and well-posed boundary value problems to pseudo-differential boundary equations with projections. Methods based on Difference Potentials introduce computationally simple auxiliary domains (see for example [31,34,35,8,10,1,2,22], etc.). After that, the original domains are embedded into auxiliary domains (and the auxiliary domains are discretized using regular structured grids). Next, DPM constructs discrete pseudo-differential *Boundary Equations with Projections* to obtain the value of the solution at the points near the continuous boundary of the original domain (at the points of the discrete grid boundary which straddles the continuous boundary from the inside and outside of the domain). Using the reconstructed values of the solution at the discrete grid boundary, the approximation to the solution in each domain/subdomain is obtained through the discrete generalized Green's formula. *DPM offers geometric flexibility (without the use of unstructured meshes or "body-fitted" meshes), but does not require explicit knowledge of the fundamental solution. Furthermore, DPM is not limited to constant coefficient problems, does not involve singular integrals, and can handle general boundary and/or interface conditions*.

The major computational cost of methods based on the Difference Potentials approach reduces to several solutions of simple auxiliary problems on regular structured grids. Methods based on Difference Potentials preserve the underlying accuracy of the schemes being used for the space discretization of the continuous PDEs in each domain/subdomain and at the same time are not restricted by the type of the boundary or interface conditions (as long as the continuous problems are well-posed). Moreover, numerical schemes based on Difference Potentials are well-suited for the development of parallel algorithms (see [34,35,8], etc.). The reader can consult [31,32] and [28,29] for a detailed theoretical study of the methods based on Difference Potentials, and [31,32,11,20,33,39,36,22,5,34,35,7,8,10,1,2], etc. for the recent developments and applications of DPM.

In this work, we consider 2D elliptic models with material interfaces and develop efficient, high-order accurate (second-order and fourth-order) methods based on the Difference Potentials approach for such problems. This paper is an extension of the work in [10] to 2D models, and extension of the work in [34,35,8,9] to higher orders. The main contributions of the current work are 1) The development and validation of high-order methods based on Difference Potentials using central-difference discretization as the underlying approximation of the PDE (rather than compact schemes). Note that the employed central-difference stencils result in a multi-layer discrete grid boundary set for the BEP, and hence different BEP are constructed at the boundaries/interfaces in comparison to Difference Potentials schemes based on compact stencils (compact stencils [22,23] generate standard two-layer discrete grid boundary for BEP similar to the second-order central-difference stencil); 2) Consideration of the general interface conditions without assumptions of the continuity of the solution or/and continuity of the flux at the interface; 3) The conducted numerical experiments corroborate high-order accuracy and stability of the proposed numerical methods for interface problems with general interface conditions.

Let us also mention that a different example of an efficient and high-order accurate method, based on Difference Potentials and compact schemes for the Helmholtz equation in homogeneous media with the variable wave number in 2D, was recently developed and numerically tested in [22] and extended to the numerical simulation of the transmission and scattering of waves in [23].

The paper is organized as follows. First, in Section 2 we introduce the formulation of our problem. Next, to simplify the presentation of the ideas for the construction of DPM with different orders of accuracy, we construct DPM with second and with fourth-order accuracy together in Section 3.2 for elliptic type models in a single domain. In Section 4, we extend the second and the fourth-order DPM to interface/composite domain model problems. After that, in Section 5 we give a brief summary of the main steps of the proposed numerical algorithms. Finally, we illustrate the performance of the designed numerical algorithms based on Difference Potentials, as well as compare these algorithms with the Immersed Interface Method [15,4], Mayo's method [21,4] and recently developed Edge-Based Correction Finite Element Interface method (EBC-FEI) [13] in several numerical experiments in Section 6. We also present application of the developed methods based on Difference Potentials to the simulation of the linear static model of biological cell electropermeabilization (this model arises in Biological/Biomedical applications). Moreover, we illustrate in Section 6 that for DPM, the underlying numerical discretization (for example, numerical schemes with different orders of the approximation in different subdomains/domains), as well as meshes can be chosen totally independently for each subdomain/domain and the boundaries of the subdomains/interfaces do not need to conform/align with the grids. The constructed DPM based numerical algorithms are not restricted by the choice of boundary conditions, and the main computational complexity of the designed algorithms reduces to the several solutions of simple auxiliary problems on regular structured grids. Some concluding remarks are given in Section 7.

2. Elliptic problem with material interface

In this work we consider the interface/composite domain problem defined in some bounded domain $\Omega^0 \subset \mathbb{R}^2$: