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High-order accurate difference potentials methods for parabolic problems

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ABSTRACT

Highly-accurate numerical methods that can efficiently handle problems with interfaces and/or problems in domains with complex geometry are crucial for the resolution of different temporal and spatial scales in many problems from physics and biology. In this paper we continue the work started in [8], and we use modest one-dimensional parabolic problems as the initial step towards the development of high-order accurate methods based on the Difference Potentials approach. The designed methods are well-suited for variable coefficient parabolic models in heterogeneous media and/or models with non-matching interfaces and with non-matching grids. Numerical experiments are provided to illustrate high-order accuracy and efficiency of the developed schemes. While the method and analysis are simpler in the one-dimensional settings, they illustrate and test several important ideas and capabilities of the developed approach.

1. Introduction

Designing numerical methods with high-order accuracy for problems with interfaces (for example, models for composite materials or fluids, etc.), as well as models in domains with complex geometry is crucial to many physical and biological applications. Moreover, interface problems result in non-smooth solutions (or even discontinuous solutions) at the interfaces, and therefore standard numerical methods (finite-difference, finite-element methods, etc.) in any dimension (including 1D) will very often fail to produce accurate approximation of the solutions to the interface problems, and thus special numerical algorithms have to be developed for the approximation of such problems (for instance, see simplified 1D example of interface problem in [8], page 12 and Table 7 on page 14).

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) ([24,25], etc.), the Immersed Interface Method (IIM) ([14–16,1,12], etc.), the Ghost Fluid Method (GFM) ([9,17,18,10], etc.), the Matched Interface and Boundary Method (MIB) ([42,39,41,40], etc.), and the method based on the Integral Equations approach ([20], etc.). Among the finite-element methods for interface problems are ([2,4,35,22,38,37], etc.). These methods are robust sharp interface methods that have been applied to solve many problems in science and engineering. For a detailed review of the subject the reader can consult, for example, [16]. *However, in spite of great advances in the numerical methods (finite-difference, finite-element, etc.) for interface problems it is still a challenge to design high-order accurate methods for such problems. To the best of our knowledge, there are currently only a few high order (higher than second order in space) schemes for parabolic interface problems*

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[10]. In [10], the high-order (fourth-order in space) GFM is constructed for the 2D heat equation under the assumption of the Dirichlet boundary conditions at the interfaces, and extended (as the third-order method) to the Stefan problem as well. Note, that the method in [10] is developed for the piecewise constant coefficients problems.

We develop here an approach based on the Difference Potentials Method (DPM) [28,31] (see about DPM for example in, [28,31,11,19,32,36,21,23,29,34,6–8], etc.). The DPM allows one to reduce uniquely solvable and well-posed boundary value problems to pseudo-differential boundary equations with projections. Methods based on Difference Potentials ([28, 29,34,7,8,21,30], etc.) introduce computationally simple auxiliary domains. After that, the original domains/subdomains are embedded into simple auxiliary domains (and the auxiliary domains are discretized using Cartesian grids). Next, methods based on Difference Potentials construct discrete pseudo-differential *Boundary Equations with Projections* to obtain the values of the solutions at the points near the continuous boundaries of the original domains (at the points of the discrete grid boundaries which approximate the continuous boundaries from the inside and outside of the domains). Using the obtained values of the solutions at the discrete grid boundaries, the approximation to the solution in each domain/subdomain is constructed through the discrete generalized Green's formulas.

The main complexity of methods based on Difference Potentials reduces to several solutions of simple auxiliary problems on structured Cartesian grids. Methods based on Difference Potentials approach are not restricted by the type of the boundary or interface conditions (as long as the continuous problems are well-posed), and are also computationally efficient since any change of the boundary/interface conditions affects only a particular component of the overall algorithm, and does not affect most of the numerical algorithm (see [28], or some example of the recent works [3,29,34,7,8], etc.). Finally, unlike many existing finite-difference based methods for interface problems, the Difference Potentials approach is well-suited for the development of parallel algorithms for such problems, see [29,34,7] – examples of the second-order in space schemes based on the Difference Potentials for 2D interface/composite domain problems and see Section 4 below. The reader can consult [28,31] and [26,27] for a detailed theoretical study of the methods based on Difference Potentials, and ([28,31,19, 32,36,33,21,3,13,11,30,23,29,34,6–8], etc.) for the recent developments and applications of DPM.

In this paper, we extend the work on high-order methods started in [8] *to variable coefficient parabolic models.* We begin here with the modest consideration of one-dimensional variable coefficient parabolic interface models, and we develop and numerically test high-order accurate methods based on Difference Potentials methodology. *At this point we are not aware of any other high-order (higher than second-order in space) method for the parabolic interface problems in heterogeneous media. Moreover, numerical experiments in Section 6 indicate that the developed method preserves high-order accuracy on the interface problems (including problems with discontinuous diffusion coefficients at the interface and jump conditions in the solution at the interface), not only in the solution, but also in the discrete gradient of the solution. To the best of our knowledge, the present work is also the first extension (at this point, in modest 1D settings) of the Difference Potentials approach for the construction of high-order accurate numerical schemes for parabolic problems.* Although, the method and analysis are simpler in the current one-dimensional settings, they illustrate and test several important ideas and abilities of the Difference Potentials approach with application to interface problems. Let us note that, previously in [7], we have developed an efficient (second-order accurate in space and first-order accurate in time) scheme based on Difference Potentials approach for 2D interface/composite domain constant coefficient parabolic problems. The second-order in space method developed in [7] can handle non-matching interface conditions on the solution (as well as non-matching grids between each subdomain), and is well-suited for the design of parallel algorithms. However, it was constructed and tested for the solution of the heat equation in irregular domains and/or with interfaces.

The paper is organized as follows. In Section 2, we introduce the formulation of the problem. Next, to illustrate the unified approach behind the construction of DPM with different orders of accuracy, we construct DPM with second and with fourth-order accuracy in space in Section 3.1 for a single domain 1D parabolic model. In Section 4, we extend the developed methods to one-dimensional parabolic interface/composite domain model problems. In Section 5 for the reader's convenience we give a brief summary of the main steps of the presented algorithms. Finally, we illustrate the performance of the proposed Difference Potentials Methods, as well as compare Difference Potentials Methods with the Immersed Interface Method, in several numerical experiments in Section 6. Some concluding remarks are given in Section 7.

2. Parabolic interface models

We are concerned in this work with a 1D parabolic interface (with fixed interface at this point) problem of the form: denote, $u_t - L_1[u] \equiv u_t - (k_1 u_x)_x$, and $u_t - L_2[u] \equiv u_t - (k_2 u_x)_x$, thus

$$u_t - L_1[u] = f_1, \quad x \in I_1, \tag{2.1}$$

$$u_t - L_2[u] = f_2, \quad x \in I_2, \tag{2.2}$$

subject to the Dirichlet boundary conditions specified at the points $x = 0$ and $x = 1$:

$$u(0,t) = a(t), \quad \text{and} \quad u(1,t) = b(t), \tag{2.3}$$

interface conditions at α:

$$\beta_1 u_1(\alpha,t) - \beta_2 u_2(\alpha,t) = \phi(t), \qquad \tilde{\beta}_1 u_{1x}(\alpha,t) - \tilde{\beta}_2 u_{2x}(\alpha,t) = \tilde{\phi}(t) \tag{2.4}$$

and an initial condition

$$u(x,0) = u^0(x), \tag{2.5}$$

where $u(x,t) \equiv u_1(x,t), x \in I_1 := [0,\alpha) \subset I_1^0$ and $u(x,t) \equiv u_2(x,t), x \in I_2 := (\alpha,1] \subset I_2^0$. $I_1 \subset I_1^0$ and $I_2 \subset I_2^0$ are two subdomains of the domain $I := [0,1]$, $0 < \alpha < 1$ is the interface point, $\beta_1, \beta_2, \tilde{\beta}_1, \tilde{\beta}_2$ are the coefficients independent of time, and I_1^0 and I_2^0 are some auxiliary subdomains that contain the original subdomains I_1 and I_2, respectively. The functions $k_1(x) \geq 1$ and $k_2(x) \geq 1$ are sufficiently smooth functions defined in a larger auxiliary subdomains I_1^0 and I_2^0, respectively. We assume here that the coefficients $k_1(x)$ and $k_2(x)$ depend only on the space variable, but the presented ideas below can be directly extended to time-dependent coefficients as well. $f_1(x,t)$ and $f_2(x,t)$ are sufficiently smooth functions defined in each subdomain I_1 and I_2, respectively. Note, we assume that the operator on the left-hand side of Eq. (2.1) and the operator on the left-hand side of Eq. (2.2) are well-defined on some larger auxiliary domains $\overline{I_1^0}$ and $\overline{I_2^0}$, respectively. More precisely, we assume that for any sufficiently smooth functions on the right-hand side of (2.1)–(2.2), Eqs. (2.1) and (2.2) have a unique solution on I_1^0 and I_2^0, which satisfies the given boundary and initial conditions on ∂I_1^0 and ∂I_2^0, respectively.

Remark. The Dirichlet boundary conditions (2.3) are chosen only for the purpose of illustration and the developed methods based on Difference Potentials are not restricted by any type of boundary conditions (as long as the problem is well-posed).

3. Single domain

Our goal is to construct a high order approximation based on the Difference Potentials idea for the parabolic interface/composite domain problem (2.1)–(2.5). To simplify the presentation, similar to work [8], we will first state the high-order methods for the single domain problem. Denote, $u_t - L[u] \equiv u_t - (ku_x)_x$, then

$$u_t - L[u] = f, \quad x \in I \tag{3.1}$$

subject to the Dirichlet boundary conditions specified at the points $x = 0$ and $x = 1$:

$$u(0,t) = a(t), \quad \text{and} \quad u(1,t) = b(t), \tag{3.2}$$

and the initial conditions

$$u(x,0) = u^0(x) \tag{3.3}$$

and then extend the developed ideas in a straightforward way, to the interface/composite domain problem (2.1)–(2.5) in Section 4, and comment only on the technical differences.

As before, $I = [0,1]$, the function $k(x) \geq 1$ is a sufficiently smooth function defined in some auxiliary domain I^0, such that $I \subset I^0$ and $f(x,t)$ is sufficiently smooth function defined in I. We also assume that the model problem (3.1)–(3.3) is well-posed, and that the operator on the left-hand side of Eq. (3.1) is well-defined on some larger auxiliary domain $\overline{I^0}$. Let us now introduce and define the main steps of the Difference Potentials approach [31,28].

3.1. High-order accurate methods based on difference potentials for parabolic problems in heterogeneous media

We will present below (at this point, using simple one-dimensional settings), a methodology based on Difference Potentials approach to construct high-order methods for time-dependent problems with variable coefficients in heterogeneous media, as well as non-matching interface conditions and non-matching grids. However, major principles of this framework will stay the same when applied to the numerical approximation of the models in domains with complex geometry in 2D and 3D, and subject to general boundary conditions.

To develop the methods in this paper, we will consider a time-discrete version of the continuous model (3.1) and we will employ the elliptic structure of the time-discrete reformulation of the problem. Furthermore, to illustrate and implement the ideas in an efficient way, we will apply below a trapezoidal second-order in time scheme along with the second and fourth-order finite-difference methods for the space discretization. However, the approach based on Difference Potentials which will be developed below is general, and can be employed in a similar way with any (most suitable) underlying high-order discretization of the given continuous problem in space, as well as time discretizations (such as high order IMEX methods, etc.).

Introduction of the Auxiliary Domain in Space:

Place the original domain I in the auxiliary domain $I^0 := [c,d] \subset \mathbb{R}$. Next, introduce a Cartesian mesh for I^0, with points $x_j = c + j\Delta x$, $(j = 0,1,\ldots,N^0)$. Let us assume for simplicity that $\Delta x := h = \frac{d-c}{N^0}$. Note that the boundary points $x = 0$ and $x = 1$ will typically fall between grid points, say $x_l \leq 0 \leq x_{l+1}$ and $x_L \leq 1 \leq x_{L+1}$ (for the 3-point second order scheme); and between grid points $x_l < x_{l+1} \leq 0 \leq x_{l+2} < x_{l+3}$ and $x_L < x_{L+1} \leq 1 \leq x_{L+2} < x_{L+3}$ (for the 5-point fourth order scheme), see Fig. 1 and Fig. 2 (from [8]).

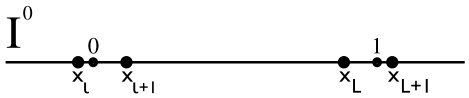

Fig. 1. Example of the auxiliary domain I^0, original domain $I = [0, 1]$, and the example of points in set $\gamma = \{x_l, x_{l+1}, x_L, x_{L+1}\}$ for the 3-point second-order method.

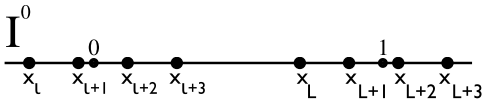

Fig. 2. Example of the auxiliary domain I^0, original domain $I = [0, 1]$, and the example of points in set $\gamma = \{x_l, x_{l+1}, x_{l+2}, x_{l+3}, x_L, x_{L+1}, x_{L+2}, x_{L+3}\}$ for the 5-point fourth-order method.

Define a stencil $N_j^\kappa := N_j^3$ or $N_j^\kappa := N_j^5$ with its center placed at x_j, to be a 3-point central finite-difference stencil of the second-order method, or a 5-point central finite-difference stencil of the fourth-order method, respectively:

$$N_j^\kappa := \{j-1, j, j+1\}, \quad \kappa = 3, \quad \text{or} \tag{3.4}$$

$$N_j^\kappa := \{j-2, j-1, j, j+1, j+2\}, \quad \kappa = 5 \tag{3.5}$$

Next, define a point set M^0, the set of all the grid nodes x_j that belong to the interior of the auxiliary domain I^0; $M^+ := M^0 \cap I$, the set of all the grid nodes x_j that belong to the interior of the original domain I; and $M^- := M^0 \backslash M^+$, the set of all the grid nodes x_j that are inside of the auxiliary domain I^0, but belong to the exterior of the original domain I. Define $N^+ := \{\bigcup_j N_j^\kappa | x_j \in M^+\}$, the set of all points covered by the stencil N_j^κ when the center point x_j of the stencil goes through all the points of the set $M^+ \subset I$. Similarly, define $N^- := \{\bigcup_j N_j^\kappa | x_j \in M^-\}$, the set of all points covered by the stencil N_j^κ when the center point x_j of the stencil goes through all the points of the set M^-.

After that, define the *discrete grid boundary* set $\gamma := N^+ \cap N^-$. The mesh nodes from set γ straddle the boundary $\partial I \equiv \{0, 1\}$. In case of the second-order method, the set γ contains four mesh nodes $\gamma = \{l, l+1, L, L+1\}$, see Fig. 1. In case of the fourth-order method, the set γ contains eight mesh nodes $\gamma = \{l, l+1, l+2, l+3, L, L+1, L+2, L+3\}$, see Fig. 2. Finally, define $N^0 := \{\bigcup_j N_j^\kappa | x_j \in M^0\} \subset \overline{I^0}$.

As in [8], the point sets N^0, M^0, N^+, N^-, M^+, M^-, γ are used to develop high-order methods based on the Difference Potentials idea.

Construction of the difference equations:

The time discrete reformulation of the parabolic problem (3.1) using the trapezoidal scheme in time is:

Given solution u^i at the previous time level, find u^{i+1} such that

$$L_{\Delta t}\left[u^{i+1}\right] = F^{i+1}, \tag{3.6}$$

here, the operator $L_{\Delta t}[u^{i+1}]$ denotes the linear elliptic operator applied to $u^{i+1} \approx u(x, t^{i+1})$ which can be written in one of the forms:

$$L_{\Delta t}\left[u^{i+1}\right] := \left(k u_x^{i+1}\right)_x - m u^{i+1}, \quad \text{or} \tag{3.7}$$

$$L_{\Delta t}\left[u^{i+1}\right] := \left(k_x u_x^{i+1} + k u_{xx}^{i+1}\right) - m u^{i+1}, \tag{3.8}$$

where $m := \frac{2}{\Delta t}$ and Δt is the time step. For the development of the second-order in space scheme, we will employ the linear operator, $L_{\Delta t}[u^{i+1}]$ in the form of (3.7), and (3.8) for the fourth-order space discretization. The right-hand side in (3.6) is

$$F^{i+1} := -\left(f\left(x, t^i\right) + f\left(x, t^{i+1}\right)\right) - L_{\Delta t}^+\left[u^i\right], \tag{3.9}$$

here

$$L_{\Delta t}^+\left[u^i\right] := \left(k u_x^i\right)_x + m u^i$$

which corresponds to $L_{\Delta t}[u^{i+1}]$ in the form of (3.7), or

$$L_{\Delta t}^+\left[u^i\right] := \left(k_x u_x^i + k u_{xx}^i\right) + m u^i$$

which corresponds to $L_{\Delta t}[u^{i+1}]$ in the form of (3.8).

The fully discrete version of the problem (3.6) is: find $u_j^{i+1} \in N^+$ such that

$$L_{\Delta t,h}\left[u_j^{i+1}\right] = F_j^{i+1}, \quad x_j \in M^+ \tag{3.10}$$

Similarly to the work [8], the fully discrete system of Eqs. (3.10) is obtained here by discretizing (3.6) with the standard second-order 3-point central finite difference scheme (3.11) (if second-order accuracy is desired), or with the fourth-order 5-point central finite difference scheme in space (3.12) (if fourth-order accuracy is desired).

Here and below, by $L_{\Delta t,h}$ we denote the discrete linear operator obtained using either the second, or the fourth-order approximation to (3.6), and by F_j^{i+1}, the corresponding discrete version of the right-hand side F^{i+1}.

Second-order scheme:

$$L_{\Delta t,h}\left[u_j^{i+1}\right] := \frac{1}{h^2}\left(k_{j+\frac{1}{2}}u_{j+1}^{i+1} - (k_{j+\frac{1}{2}} + k_{j-\frac{1}{2}})u_j^{i+1} + k_{j-\frac{1}{2}}u_{j-1}^{i+1}\right) - mu_j^{i+1}. \tag{3.11}$$

The coefficients $k_{j+\frac{1}{2}} := k(x_{j+\frac{1}{2}})$ and $x_{j+\frac{1}{2}}$ is the middle point of the interval $[x_j, x_{j+1}]$.

Fourth-order scheme:

$$\begin{aligned} L_{\Delta t,h}\left[u_j^{i+1}\right] := {} & k_j \frac{-u_{j-2}^{i+1} + 16u_{j-1}^{i+1} - 30u_j^{i+1} + 16u_{j+1}^{i+1} - u_{j+2}^{i+1}}{12h^2} \\ & + (k_x)_j \frac{u_{j-2}^{i+1} - 8u_{j-1}^{i+1} + 8u_{j+1}^{i+1} - u_{j+2}^{i+1}}{12h} - mu_j^{i+1}, \end{aligned} \tag{3.12}$$

and the coefficients $k_j := k(x_j)$, $(k_x)_j := k_x(x_j)$. The right-hand side for the second-order and for the fourth-order is given as

$$F_j^{i+1} := -\left(f\left(x_j, t^i\right) + f\left(x_j, t^{i+1}\right)\right) - L_{\Delta t,h}^+\left[u_j^i\right], \tag{3.13}$$

where for the second-order scheme:

$$L_{\Delta t,h}^+\left[u_j^i\right] := \frac{1}{h^2}\left(k_{j+\frac{1}{2}}u_{j+1}^i - (k_{j+\frac{1}{2}} + k_{j-\frac{1}{2}})u_j^i + k_{j-\frac{1}{2}}u_{j-1}^i\right) + mu_j^i, \quad \text{and}$$

for the fourth-order scheme:

$$\begin{aligned} L_{\Delta t,h}^+\left[u_j^i\right] := {} & k_j \frac{-u_{j-2}^i + 16u_{j-1}^i - 30u_j^i + 16u_{j+1}^i - u_{j+2}^i}{12h^2} \\ & + (k_x)_j \frac{u_{j-2}^i - 8u_{j-1}^i + 8u_{j+1}^i - u_{j+2}^i}{12h} + mu_j^i. \end{aligned}$$

See [8] for more details on the space discretization.

In general, at each time level t^{i+1}, the linear system of difference equations (3.10) will have multiple solutions since we did not impose any discrete boundary or initial conditions. Once we complete the system (3.10) with the appropriate choice of the numerical boundary and initial conditions, the scheme will result in an accurate approximation of the continuous problem in domain I. Similar to the work [8], we will develop here an approach based on the idea of Difference Potentials [28,31].

General discrete auxiliary problem:

One of the major steps of the DPM is the introduction of the auxiliary problem, which we will denote as (AP) and define as follows:

Definition 3.1. The problem of solving (3.14)–(3.15) is referred to as the discrete *auxiliary problem (AP):* at each time level t^{i+1}, for the given grid function $q^{i+1} \in M^0$, find the solution $v^{i+1} \in N^0$ of the following system of equations:

$$L_{\Delta t,h}\left[v_j^{i+1}\right] = q_j^{i+1}, \quad x_j \in M^0, \tag{3.14}$$

$$v_j^{i+1} = 0, \quad x_j \in N^0 \backslash M^0. \tag{3.15}$$

Here, $L_{\Delta t,h}$ is the same linear discrete operator as in (3.10), but now it is defined on the larger auxiliary domain $\overline{I^0}$. It is applied in (3.14) to the function $v^{i+1} \in N^0$. We note that for small enough h and Δt (and under the above assumptions on the continuous problem), the (AP) (3.14)–(3.15) is well defined for any right hand side q_j^{i+1}: it has a unique solution $v^{i+1} \in N^0$. In this work, we supplemented the discrete (AP) (3.14) by the zero boundary conditions (3.15). In general, the boundary conditions for (AP) are selected to guarantee that the discrete equation $L_{\Delta t,h}[v_j^{i+1}] = q_j^{i+1}$ has a unique solution $v^{i+1} \in N^0$ for any discrete right-hand side, q^{i+1}.

Remark. The solution of the (AP) (3.14)–(3.15) defines a discrete operator, $G^h_{\Delta t}$ (the inverse operator to $L_{\Delta t,h}$). Although the choice of boundary conditions (3.15) will affect the operator, $G^h_{\Delta t}$, and hence the difference potentials and the projections defined below, it will not affect the final approximation to the solution of (3.1)–(3.3), as long as the (AP) is uniquely solvable and well-posed.

Construction of a particular solution:

Let us denote by $u^{i+1}_j := G^h_{\Delta t} F^{i+1}_j$, $u^{i+1}_j \in N^+$, the particular solution (restricted to set N^+) of the discrete problem (3.10), which is constructed at each time level t^{i+1} as the solution of the auxiliary problem (AP) (3.14)–(3.15) of the following form:

$$L_{\Delta t,h}\big[u^{i+1}_j\big] = \begin{cases} F^{i+1}_j, & x_j \in M^+, \\ 0, & x_j \in M^-, \end{cases} \tag{3.16}$$

$$u^{i+1}_j = 0, \quad x_j \in N^0 \backslash M^0 \tag{3.17}$$

Remark. The right-hand side of (3.14) in (AP) for the construction of a particular solution is set to

$$q^{i+1}_j = \begin{cases} F^{i+1}_j, & x_j \in M^+, \\ 0, & x_j \in M^-, \end{cases} \tag{3.18}$$

with F^{i+1}_j given in (3.13).

Construction of the boundary equations with projections:

i. Difference potential:

Introduce a linear space, $\mathbf{V}_\gamma$ of all the grid functions denoted by v^{i+1}_γ defined on γ ([28], see also [8,29,34,7], etc.). We will extend the value v^{i+1}_γ by zero to other points of the grid N^0.

Definition 3.2. The Difference Potential at time level t^{i+1} with any given density $v^{i+1}_\gamma \in \mathbf{V}_\gamma$ is the grid function $u^{i+1}_j := \mathbf{P}_{N^+\gamma} v^{i+1}_\gamma$, defined on N^+, and coincides on N^+ with the solution u^{i+1}_j of the auxiliary problem (AP) (3.14)–(3.15) of the following form:

$$L_{\Delta t,h}\big[u^{i+1}_j\big] = \begin{cases} 0, & x_j \in M^+, \\ L_{\Delta t,h}[v^{i+1}_\gamma], & x_j \in M^-, \end{cases} \tag{3.19}$$

$$u^{i+1}_j = 0, \quad x_j \in N^0 \backslash M^0 \tag{3.20}$$

Remark. The right-hand side of (3.14) in (AP) for constructing a difference potential with density v^{i+1}_γ is set to

$$q_j = \begin{cases} 0, & x_j \in M^+, \\ L_{\Delta t,h}[v^{i+1}_\gamma], & x_j \in M^-. \end{cases} \tag{3.21}$$

The Difference Potential with density $v^{i+1}_\gamma \in \mathbf{V}_\gamma$ is the discrete inverse operator. Here, $\mathbf{P}_{N^+\gamma}$ denotes the operator that constructs the difference potential, $u^{i+1}_j = \mathbf{P}_{N^+\gamma} v^{i+1}_\gamma$ from the given density $v^{i+1}_\gamma \in V_\gamma$. The operator $\mathbf{P}_{N^+\gamma}$ is the linear operator of the density v^{i+1}_γ, and it can be easily constructed as in [8]:

$$u^{i+1}_p = \sum_{j\in\gamma} A_{jp} v^{i+1}_j, \quad x_p \in N^+$$

Here, by u^{i+1}_p we denote the value at the grid point x_p of the Difference Potential $P_{N^+\gamma} v^{i+1}_\gamma$ with the density v^{i+1}_γ, and by $\{A_{jp}\}$ the coefficients of the difference potentials operator. The coefficients $\{A_{jp}\}$ can be computed by solving an auxiliary problem (AP) (3.19)–(3.20) (or by constructing a Difference Potential operator) with the unit density v_γ at points $x_{j^\star} \in \gamma$. See [8] for more details.

Remark. Note that if the time step Δt stays fixed during simulations, then the coefficients A_{jp} of the Difference Potentials operator $\mathbf{P}_{N^+\gamma}$ can be computed only once and stored.

Next, similarly to [28] (see also [8,6,7], etc.), we can define another operator $\mathbf{P}_\gamma : V_\gamma \to V_\gamma$ that is defined as the trace (or restriction/projection) of the Difference Potential $\mathbf{P}_{N^+\gamma} v_\gamma^{i+1}$ on the grid boundary γ:

$$\mathbf{P}_\gamma v_\gamma^{i+1} := \mathrm{Tr}_\gamma \left(\mathbf{P}_{N^+\gamma} v_\gamma^{i+1}\right) = \left(\mathbf{P}_{N^+\gamma} v_\gamma^{i+1}\right)\big|_\gamma \tag{3.22}$$

We will now formulate the crucial theorem of the method.

Theorem 3.3. *At each time level t^{i+1}, density u_γ^{i+1} is the trace of some solution, $u^{i+1} \in N^+$ to the Difference Equations (3.10): $u_\gamma^{i+1} \equiv \mathrm{Tr}_\gamma u^{i+1}$ if and only if the following equality holds*

$$u_\gamma^{i+1} = \mathbf{P}_\gamma u_\gamma^{i+1} + G_{\Delta t}^h F_\gamma^{i+1}, \tag{3.23}$$

where $G_{\Delta t}^h F_\gamma^{i+1} := \mathrm{Tr}_\gamma (G_{\Delta t}^h F^{i+1})$ is the trace (or restriction) of the particular solution, $G_{\Delta t}^h F^{i+1} \in N^+$ constructed in (3.16)–(3.17) on the grid boundary γ.

Proof. The proof follows closely the argument of the theory from [28] and for the reader's convenience we will briefly review it in Appendix A. □

Lemma 3.4. *At each time level t^{i+1} the rank r of the system (3.23) is equal to $|\gamma^{in}|$. Here, $|\gamma^{in}|$ is the cardinality of the set γ^{in} – the interior layer of the grid boundary, $\gamma = \gamma^{in} \cup \gamma^{ex}$. Similarly, γ^{ex} denotes the exterior layer.*

Proof. The system of difference equations (3.10), $L_{\Delta t,h}[u_j^{i+1}] = F_j^{i+1}, \quad x_j \in M^+$, will have a unique solution once the component of the solution $u_j^{i+1}, \quad x_j \in \gamma^{ex}$ to (3.10) is given at the exterior layer γ^{ex} of the grid boundary γ (the matrix for the system of difference equations (3.10) is strictly diagonally dominant (and hence non-singular) for any $\Delta t > 0$ for the second-order scheme (3.11), and for any $\Delta t < \min_{x_j \in M^+} \frac{12h^2}{2k_j + 9h|(k_x)_j|}$ for the fourth-order scheme (3.12)). Also, note that the linear system of *Boundary Equations* (3.23) is equivalent to the linear system of the difference equations (3.10) due to Theorem 3.3.

Therefore, the rank, r of the matrix for the linear system of *Boundary Equations*,

$$u_\gamma^{i+1} - \mathbf{P}_\gamma u_\gamma^{i+1} = G_{\Delta t}^h F_\gamma^{i+1}$$

is equal to $r = |\gamma| - |\gamma^{ex}| = |\gamma^{in}|$. □

Remark.

1. The restriction on the time step Δt for the fourth-order scheme in the proof of the Lemma 3.4 can be relaxed if one does not use strictly diagonally dominant property of the matrix of the obtained linear system to show the existence (or uniqueness) of the solution.
2. Note that for any density, $u_\gamma^{i+1} \in \mathbf{V}_\gamma$, the grid function, $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G_{\Delta t}^h F^{i+1} \in N^+$ is some solution to the difference equations (3.10) (consequence of Theorem 3.3).
3. The difference potential, $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1}$ is the solution to the homogeneous difference equation, $L_{\Delta t,h}[u_j^{i+1}] = 0, x_j \in M^+$, and is uniquely defined once we know the value of the density u_γ^{i+1} at the points of the boundary γ (see Definition 3.2).
4. Also, note that density u_γ^{i+1} has to satisfy *Boundary Equations*, $u_\gamma^{i+1} - P_\gamma u_\gamma^{i+1} = G_{\Delta t}^h F_\gamma^{i+1}$ *in order to be a trace of the solution to the difference equation*, $L_{\Delta t,h}[u_j^{i+1}] = F_j^{i+1}$ (consequence of Theorem 3.3).
5. In the case of a constant coefficient model problem (3.1) (assume, $k(x) \equiv 1$), using a technique as in [8], one can show a direct connection of the difference potential $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1}$ to the Cauchy-type integral (see [28,31] for a more general discussion on the subject).

ii. Coupling of the boundary equations with the boundary conditions:

Below, we will present the details for the second and for the fourth-order schemes in space (3.11) and (3.12) (*however, the main strategy presented below is the same for any high-order method in space and time*).

The *Boundary Equations:* $u_\gamma^{i+1} = \mathbf{P}_\gamma u_\gamma^{i+1} + G_{\Delta t}^h F_\gamma^{i+1}$ for the unknown density u_γ^{i+1} are a linear system of equations:

$$(I - A)\mathbf{u}^{i+1} = \mathbf{G}_{\Delta \mathbf{t}}^{\mathbf{h}} \mathbf{F}^{i+1}, \tag{3.24}$$

where I is the identity matrix and A is the matrix of the coefficients of the difference potentials with unit densities.

In case of the second-order method in space:

Matrix A is

$$A := \{A_{rs}\}, \quad \text{with } r,s = l, l+1, L, L+1 \tag{3.25}$$

The column vector of the unknown densities is

$$\mathbf{u} := \left(u_l^{i+1}, u_{l+1}^{i+1}, u_L^{i+1}, u_{L+1}^{i+1}\right)^T,$$

and the column vector of the right-hand side is

$$\mathbf{G}^{\mathbf{h}}_{\Delta \mathbf{t}}\mathbf{F}^{i+1} := \left(G^h_{\Delta t}F_l^{i+1}, G^h_{\Delta t}F_{l+1}^{i+1}, G^h_{\Delta t}F_L^{i+1}, G^h_{\Delta t}F_{L+1}^{i+1}\right)^T.$$

In case of the fourth-order method in space:
Matrix A is

$$A := \{A_{rs}\}, \quad \text{with } r,s = l, l+1, l+2, l+3, L, L+1, L+2, L+3 \tag{3.26}$$

The column vector of the unknown densities is

$$\mathbf{u}^{i+1} := \left(u_l^{i+1}, u_{l+1}^{i+1}, u_{l+2}^{i+1}, u_{l+3}^{i+1}, u_L^{i+1}, u_{L+1}^{i+1}, u_{L+2}^{i+1}, u_{L+3}^{i+1}\right)^T,$$

and the column vector of the right-hand side is

$$\mathbf{G}^{\mathbf{h}}\mathbf{F}^{i+1} := \left(G^h_{\Delta t}F_l^{i+1}, G^h_{\Delta t}F_{l+1}^{i+1}, G^h_{\Delta t}F_{l+2}^{i+1}, G^h_{\Delta t}F_{l+3}^{i+1}, G^h_{\Delta t}F_L^{i+1}, G^h_{\Delta t}F_{L+1}^{i+1}, G^h_{\Delta t}F_{L+2}^{i+1}, G^h_{\Delta t}F_{L+3}^{i+1}\right)^T.$$

Remark. The matrix A (3.25) or the matrix A (3.26) of the coefficients of the difference potentials with unit densities, and hence, also the matrix $I - A$, are the same at each time-step, provided that Δt is constant. Thus, it can be computed once at the beginning of the simulations and stored.

Under the assumption that u_γ^i is given from the previous time level t^i, the above system of *Boundary Equations* (3.24) will have multiple solutions without boundary conditions (3.2), since it is equivalent to the difference equations $L_{\Delta t,h}[u_j^{i+1}] = F_j^{i+1}, x_j \in M^+$. Thus, we need to supplement the system (3.24) with the boundary conditions (3.2) to construct the unique density u_γ^{i+1}.

We will consider the following approach to solve for the unknown densities u_γ^{i+1} from the *Boundary Equations* (3.24). Here, using the idea of the Taylor expansion, one can construct the unknown densities u_γ^{i+1} with the values of the continuous solution and its derivatives at the continuous boundary of the domain with the desired accuracy: in other words, one can define the extension operator from the continuous boundary ∂I to the discrete boundary γ for the solution of (3.1). Note that the extension operator (the way it is constructed below) depends only on the properties of the given model at the continuous boundary ∂I.

1. For example, for the second-order method, in case of 3*-terms, the extension operator is:*

$$u_j^{i+1} := u|_{\partial I} \pm du_x|_{\partial I} + \frac{d^2}{2!}u_{xx}|_{\partial I}, \quad x_j \in \gamma, \tag{3.27}$$

where

$$u|_{\partial I} := u\left(0, t^{i+1}\right), \qquad u_x|_{\partial I} := u_x\left(0, t^{i+1}\right), \qquad u_{xx}|_{\partial I} := u_{xx}\left(0, t^{i+1}\right), \quad \text{if } j = \{l, l+1\},$$

and

$$u|_{\partial I} := u\left(1, t^{i+1}\right), \qquad u_x|_{\partial I} := u_x\left(1, t^{i+1}\right), \qquad u_{xx}|_{\partial I} := u_{xx}\left(1, t^{i+1}\right), \quad \text{if } j = \{L, L+1\}.$$

2. For example, for the fourth-order method in space, in case of 5*-terms, extension operator is*:

$$u_j^{i+1} := u|_{\partial I} \pm du_x|_{\partial I} + \frac{d^2}{2!}u_{xx}\Big|_{\partial I} \pm \frac{d^3}{3!}u_{xxx}\Big|_{\partial I} + \frac{d^4}{4!}u_{xxxx}\Big|_{\partial I} \quad x_j \in \gamma, \tag{3.28}$$

where, if $j = \{l, l+1, l+2, l+3\}$, we have that:

$$u|_{\partial I} := u\left(0, t^{i+1}\right), \qquad u_x|_{\partial I} := u_x\left(0, t^{i+1}\right), \qquad u_{xx}|_{\partial I} := u_{xx}\left(0, t^{i+1}\right),$$
$$u_{xxx}|_{\partial I} := u_{xxx}\left(0, t^{i+1}\right), \qquad u_{xxxx}|_{\partial I} := u_{xxxx}\left(0, t^{i+1}\right),$$

and if $j = \{L, L+1, L+2, L+3\}$, we denote:

$$u|_{\partial I} := u\left(1, t^{i+1}\right), \qquad u_x|_{\partial I} := u_x\left(1, t^{i+1}\right), \qquad u_{xx}|_{\partial I} := u_{xx}\left(1, t^{i+1}\right),$$
$$u_{xxx}|_{\partial I} := u_{xxx}\left(1, t^{i+1}\right), \qquad u_{xxxx}|_{\partial I} := u_{xxxx}\left(1, t^{i+1}\right).$$

d Denotes the distance from point $x_j \in \gamma$ to the boundary point. We take it with either the sign "+", or with the sign "−".

Under the assumption of sufficient regularity of the continuous model (3.1) and its solution, we can express all the higher-order derivatives (higher than first-order) in the extension operators (3.27) (second-order scheme) or in (3.28) (fourth-order scheme) in terms of the lower-order ones, more precisely, in terms of u and u_x only, using consecutive differentiation of the model equation (3.1) with respect to the space variable. In the case of the second-order derivatives, this is simply

$$u_{xx}\big(0,t^{i+1}\big) = \frac{u_t(0,t^{i+1}) - f(0,t^{i+1})}{k(0)} - \frac{k_x(0)}{k(0)} u_x\big(0,t^{i+1}\big), \tag{3.29}$$

and

$$u_{xx}\big(1,t^{i+1}\big) = \frac{u_t(1,t^{i+1}) - f(1,t^{i+1})}{k(1)} - \frac{k_x(1)}{k(1)} u_x\big(1,t^{i+1}\big). \tag{3.30}$$

The third-order derivative at the boundary points can be expressed as:

$$\begin{aligned} u_{xxx}\big(0,t^{i+1}\big) = {} & -2\frac{k_x(0)}{k(0)^2}\big(u_t\big(0,t^{i+1}\big) - f\big(0,t^{i+1}\big)\big) - \frac{f_x(0,t^{i+1})}{k(0)} + \left(2\frac{k_x(0)^2}{k(0)^2} - \frac{k_{xx}(0)}{k(0)}\right) u_x\big(0,t^{i+1}\big) \\ & + \frac{u_{xt}(0,t^{i+1})}{k(0)} \end{aligned} \tag{3.31}$$

$$\begin{aligned} u_{xxx}\big(1,t^{i+1}\big) = {} & -2\frac{k_x(1)}{k(1)^2}\big(u_t\big(1,t^{i+1}\big) - f\big(1,t^{i+1}\big)\big) - \frac{f_x(1,t^{i+1})}{k(1)} + \left(2\frac{k_x(1)^2}{k(1)^2} - \frac{k_{xx}(1)}{k(1)}\right) u_x\big(1,t^{i+1}\big) \\ & + \frac{u_{xt}(1,t^{i+1})}{k(1)} \end{aligned} \tag{3.32}$$

And the fourth-order derivative has the following expression at the boundary points:

$$\begin{aligned} u_{xxxx}\big(0,t^{i+1}\big) = {} & \left(6\frac{k_x(0)^2}{k(0)^3} - 3\frac{k_{xx}(0)}{k(0)^2}\right)\big(u_t\big(0,t^{i+1}\big) - f\big(0,t^{i+1}\big)\big) + 3\frac{k_x(0)}{k(0)^2} f_x\big(0,t^{i+1}\big) - \frac{f_{xx}(0,t^{i+1})}{k(0)} \\ & + \frac{u_{tt}(0,t^{i+1}) - f_t(0,t^{i+1})}{k(0)^2} + \left(6\frac{k_x(0)}{k(0)^2}\left[k_{xx}(0) - \frac{k_x(0)^2}{k(0)}\right] - \frac{k_{xxx}(0)}{k(0)}\right) u_x\big(0,t^{i+1}\big) \\ & - 4\frac{k_x(0)}{k(0)^2} u_{xt}\big(0,t^{i+1}\big) \end{aligned} \tag{3.33}$$

$$\begin{aligned} u_{xxxx}\big(1,t^{i+1}\big) = {} & \left(6\frac{k_x(1)^2}{k(1)^3} - 3\frac{k_{xx}(1)}{k(1)^2}\right)\big(u_t\big(1,t^{i+1}\big) - f\big(1,t^{i+1}\big)\big) + 3\frac{k_x(1)}{k(1)^2} f_x\big(1,t^{i+1}\big) - \frac{f_{xx}(1,t^{i+1})}{k(1)} \\ & + \frac{u_{tt}(1,t^{i+1}) - f_t(1,t^{i+1})}{k(1)^2} + \left(6\frac{k_x(1)}{k(1)^2}\left[k_{xx}(1) - \frac{k_x(1)^2}{k(1)}\right] - \frac{k_{xxx}(1)}{k(1)}\right) u_x\big(1,t^{i+1}\big) \\ & - 4\frac{k_x(1)}{k(1)^2} u_{xt}\big(1,t^{i+1}\big) \end{aligned} \tag{3.34}$$

Note that in the above formulas for higher order derivatives, the terms u_t and u_{tt} can be calculated explicitly at the boundary nodes from the boundary conditions (3.2). However, the term u_{xt} will be replaced, for example, by a second-order backward finite difference approximation in time:

$$u_{xt}\big(0,t^{i+1}\big) \approx \frac{3u_x(0,t^{i+1}) - 4u_x(0,t^i) + u_x(0,t^{i-1})}{2\Delta t}. \tag{3.35}$$

$$u_{xt}\big(1,t^{i+1}\big) \approx \frac{3u_x(1,t^{i+1}) - 4u_x(1,t^i) + u_x(1,t^{i-1})}{2\Delta t}. \tag{3.36}$$

The value $u|_{\partial I}$ is given due to the boundary conditions (3.2). Let us denote the unknown values $C_1^{i+1} := u_x(0,t^{i+1})$ and $C_2^{i+1} := u_x(1,t^{i+1})$. Therefore, at each time level t^{i+1}, the only unknowns that we need to solve for are C_1^{i+1} and C_2^{i+1}. We will use expansion (3.27) (second-order in space method) or (3.28) (fourth-order in space method) for u_γ^{i+1} in the boundary equations (3.24) and obtain an overdetermined linear system for C_1^{i+1} and C_2^{i+1}. This system is solved uniquely using the least square method. After that, we can obtain the value of the density u_γ^{i+1} at the points of the grid boundary γ using formula (3.27) or (3.28).

Finally, the last step of the proposed approach based on Difference Potentials is to use the obtained density u_γ^{i+1} to reconstruct the approximation to the solution (3.1)–(3.3) inside the domain I.

Generalized Green's formula:

Statement 3.5. *At each time level t^{i+1}, the discrete solution, $u_j^{i+1} := \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G^h_{\Delta t} F_j^{i+1}$ is the approximation to the solution, $u_j^{i+1} \approx u(x_j, t^{i+1})$, $x_j \in N^+ \cap I$ of the continuous problem (3.1)–(3.3).*

Discussion. The result is a consequence of sufficient regularity (smoothness) of the exact solution, Theorem 3.3, the extension operator (3.27) (for the second-order method) or the extension operator (3.28) (for the fourth-order method), the second-order accuracy of the trapezoidal time scheme, and the second-order accuracy in space of the scheme (3.11) (for the second-order method) or the fourth-order accuracy in space of the scheme (3.12) (for the fourth-order method).

More precisely, consider the trapezoidal scheme in time, and rewrite the continuous model (3.1) in a time-discrete version as presented below:

$$L_{\Delta t}\big[u\big(x, t^{i+1}\big)\big] = F\big[u\big(x, t^i\big), f\big] + O\big(\Delta t^2\big), \tag{3.37}$$

here, as before, the operator $L_{\Delta t}$ is defined as in (3.7) (if the second-order in space scheme will be considered) or as in (3.8) (if the fourth-order in space scheme will be considered), $F[u(x,t^i), f] := -L^+_{\Delta t}[u(x,t^i)] - (f(x,t^{i+1}) + f(x,t^i))$, (see Section 3.1, formulas (3.6)–(3.9)), and here $u(x,t^i)$ is the exact solution at time t^i. Error $O(\Delta t^2)$ is due to the local truncation error of the trapezoidal scheme in time. The equation (3.37) is subject to the boundary conditions (3.2) and the initial condition (3.3). Define $\mathcal{E}u$ to be some extension of the solution u to the auxiliary domain I^0, which satisfies

$$\mathcal{E}u|_{\bar{I}} = u, \quad \forall x \in \bar{I}$$

and the zero Dirichlet boundary conditions on the boundary of the auxiliary domain I^0:

$$\mathcal{E}u|_{\partial I^0} = 0$$

(for example, in higher dimensions, one can investigate a Whitney extension of u to construct $\mathcal{E}u$ near the boundary of the original domain, [26,27]). Hence, we can define on the entire auxiliary domain $\bar{I^0}$,

$$L_{\Delta t}\big[\mathcal{E}u\big(x, t^{i+1}\big)\big] = \begin{cases} F[u(x,t^i), f] + O(\Delta t^2), & \forall x \in I, \\ L_{\Delta t}[\mathcal{E}u(x, t^{i+1})], & \forall x \in I^0 \backslash I, \\ \mathcal{E}u|_{\partial I^0} = 0. \end{cases} \tag{3.38}$$

Next, approximate the linear elliptic operator $L_{\Delta t}$ on the left and right-hand sides of (3.38) by the discrete (in space) linear operator $L_{\Delta t,h}$. Similarly, approximate the right-hand side function $F[u(x,t^i), f]$ with accuracy $O(h^\nu)$ in space ($\nu = 2$ or $\nu = 4$ in this work, see Section 3.1). Therefore, obtain

$$L_{\Delta t,h}\big[\mathcal{E}u\big(x_j, t^{i+1}\big)\big] = \begin{cases} F[u(x_j,t^i), f_j] + O(h^\nu) + O(\Delta t^2), & \forall x_j \in M^+, \\ L_{\Delta t,h}[\mathcal{E}u(x_j, t^{i+1})], & \forall x_j \in M^-, \\ \mathcal{E}u|_{I^0} = 0. \end{cases} \tag{3.39}$$

After that, omit the truncation error terms $O(h^\nu) + O(\Delta t^2)$, obtaining the following numerical scheme:

At every time level t^{i+1}, find the approximate solution $w^{i+1} \approx \mathcal{E}u(x_j, t^{i+1})$, $x_j \in N^+$, where w^{i+1} is

$$w_j^{i+1} = \begin{cases} \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G^h_{\Delta t} F_j^{i+1}, & \forall x_j \in N^+, \\ 0, & \forall x_j \in N^0 \backslash N^+, \end{cases} \tag{3.40}$$

which coincides on N^+ with the solution of the numerical scheme (see Section 3.1):

$$L_{\Delta t,h}\big[\tilde{w}^{i+1}\big] = \begin{cases} F_j^{i+1}, & \forall x_j \in M^+, \\ L_{\Delta t,h}[u_\gamma^{i+1}], & \forall x_j \in M^-, \\ 0, & \forall x_j \in N^0 \backslash M^0. \end{cases} \tag{3.41}$$

The extension $\tilde{w}^{i+1}$ of the discrete solution employs the trace $u_\gamma^{i+1} \equiv \tilde{w}_\gamma^{i+1}$, which is defined in (3.27 and 3.29–3.30) (second-order in space scheme) and in (3.28)–(3.34) (fourth-order in space scheme).

Thus, for sufficiently small enough h and Δt (and under sufficient regularity of the exact solution), we expect that at every time level t^{i+1} the constructed discrete solution $u_j^{i+1} := \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G^h_{\Delta t} F_j^{i+1}$ will approximate the solution $u_j \approx u(x_j, t^{i+1})$, $x_j \in N^+ \cap I$ of the continuous problem (3.1)–(3.3), with $O(h^2 + \Delta t^2)$ (for the second-order method in space) and with $O(h^4 + \Delta t^2)$ (for the fourth-order method in space) in the 2-norm or the maximum norm.

- The developed Difference Potentials based scheme of the second-order accuracy in space can be viewed as a modified Crank–Nicolson scheme.

- In Section 6, we illustrate the capabilities and the consistence of the developed approach with several numerical experiments for the interface/composite domain problems. In the conducted numerical experiments, we considered time step $dt \approx O(\frac{h}{\max k(x)})$ for the second-order in space scheme and $dt \approx O(\frac{h^2}{\max k(x)})$ for the fourth-order in space scheme.

Remark.

- The formula $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G^h_{\Delta t} F_j^{i+1}$ is known as the *discrete generalized Green's formula.*
- Note that after density u_γ^{i+1} is obtained from the *Boundary Equations*, the difference potential is easily constructed as the solution of a simple (AP) using Definition 3.2.

4. Application to interface and composite domains problems

In Section 3.1, we formulated second and fourth-order methods in space based on the Difference Potentials approach, for problems in the single domain I. In this section, similar to the elliptic work [8], we will show how to extend these methods in a direct and a straightforward way to interface/composite domains problems (2.1)–(2.5).

First, we will introduce the auxiliary domains, as in Section 3 for the single domain I. We will place each of the original subdomains I_s in the auxiliary domains $I_s^0 \subset \mathbb{R}$ $(s = 1, 2)$, and will formulate the auxiliary difference problems in each subdomain I_s $(s = 1, 2)$. The choice of these auxiliary domains I_1^0 and I_2^0 does not need to depend on each other. Again, for each subdomain, we will proceed as we did in Section 3.1. Also, for each I_s^0 we will introduce a Cartesian grid (the choice of the grids for the auxiliary problems in each subdomain will be independent. The choice for each subdomain is based on considerations of the properties of the model and solution in each subdomain (2.1)–(2.5), as well as the efficiency and simplicity of the resulting discrete problems). After that, all the definitions, notations, and properties introduced in Section 3.1 extend to each subdomain I_s in a direct and straightforward way: we will use index s $(s = 1, 2)$ to distinguish each subdomain. Let us denote the difference problem of (2.1)–(2.2) for each subdomain as:

$$L^s_{\Delta t,h}\left[u_j^{i+1}\right] = F_{sj}^{i+1}, \quad x_j \in M_s^+. \tag{4.1}$$

The difference problem (4.1) is obtained using a trapezoidal scheme in time, and either the second (3.11) or the fourth-order scheme (3.12) in space.

The cornerstone of the Difference Potentials approach for the composite domains and interface problems is the following proposition.

Statement 4.1. *Density* $u_\gamma^{i+1} := (u_{\gamma_1}^{i+1}, u_{\gamma_2}^{i+1})$ *is the trace of some solution* $u^{i+1} \in N_1^+ \cup N_2^+$ *to the Difference Equations (4.1):* $u_\gamma^{i+1} \equiv \mathrm{Tr}_\gamma u^{i+1}$ *if and only if the following equality holds*

$$u_{\gamma_1}^{i+1} = \mathbf{P_1}_{\gamma_1} u_{\gamma_1}^{i+1} + G^h_{1\Delta t} F_{1\gamma_1}^{i+1}, \quad x_j \in \gamma_1 \tag{4.2}$$

$$u_{\gamma_2}^{i+1} = \mathbf{P_2}_{\gamma_2} u_{\gamma_2}^{i+1} + G^h_{2\Delta t} F_{2\gamma_2}^{i+1}, \quad x_j \in \gamma_2 \tag{4.3}$$

At each time level t^{i+1}*, the obtained discrete solution,* $u_j^{i+1} := \mathbf{P_s}_{N_s^+\gamma_s} u_{\gamma_s}^{i+1} + G^h_{s\Delta t} F_{sj}^{i+1}$ *is the approximation to the solution* $u_j^{i+1} \approx u(x_j, t^{i+1}) \in I_1 \cup I_2$, $x_j \in N_s^+ \cap I_s$, $s = 1, 2$ *of the continuous problem (2.1)–(2.5).*

Discussion. The result is a consequence of the results in Section 3.1. We expect that the solution $u_j^{i+1} := \mathbf{P_s}_{N_s^+\gamma_s} u_{\gamma_s}^{i+1} + G^h_{s\Delta t} F_{sj}^{i+1}$ will approximate the exact solution $u(x_j, t^{i+1}) \in I_1 \cup I_2$, $x_j \in N_s^+ \cap I_s$, $s = 1, 2$ with the accuracy $O(h^2 + \Delta t^2)$ for the second-order scheme in space, and with the accuracy $O(h^4 + \Delta t^2)$ for the fourth-order scheme in space in the maximum norm. See also Section 6 for the numerical validation.

Remark. Similar to the discussion in Section 3.1, at every time level t^{i+1} the *Boundary Equations* (4.2)–(4.3) alone will have multiple solutions and have to be coupled with the initial conditions (solutions at the previous time level t^i), boundary (2.3) and interface conditions (2.4) to obtain the unique densities $u_{\gamma_1}^{i+1}$ and $u_{\gamma_2}^{i+1}$.

We use the extension formula (3.27) (second-order scheme) or (3.28) (fourth-order scheme) to construct $u_{\gamma_s}^{i+1}$, $s = 1, 2$ in each subdomain/domain. The unknowns are $u^{i+1}|_{\partial I_1}, u_x^{i+1}|_{\partial I_1}$ and $u^{i+1}|_{\partial I_2}, u_x^{i+1}|_{\partial I_2}$. Here, $\partial I_1 := \{0, \alpha\}$ and $\partial I_2 := \{\alpha, 1\}$ (total 8 unknowns without imposed boundary and interface conditions (2.3)–(2.4)).

Note, that at the interface, the time derivatives: u_t, u_{tt}, u_{xt}, in formulas (3.29)–(3.34) are obtained using second-order backward difference approximations in time.

Remark. In the numerical tests that we conducted, we explored both first and second-order backward finite difference approximations in time for the time derivatives terms in (3.29)–(3.34). In most numerical tests, they both preserved second-order accuracy for the second-order scheme in space, and fourth-order accuracy for the fourth-order scheme in space (we

used time step $dt = 0.5h$ for the second-order method and $dt = 0.5h^2$ for the fourth-order method). However, in more intricate test problems, we observed a slight improvement using the more accurate second-order backward finite difference approximation, and hence in the numerical examples in Section 6 we will present results using only this approximation (when needed) for the time derivatives terms in (3.29)–(3.34).

5. Algorithm

In this section for the reader's convenience we will briefly summarize the main steps of the algorithm.

- *Step 1:* Introduce a computationally simple auxiliary domain and formulate the auxiliary problem (AP).
- *Step 2:* At each new time level t^{i+1} compute a *Particular solution*, $u_j^{i+1} := G^h_{\Delta t} F_j^{i+1}, x_j \in N^+$, as the solution of the *Auxiliary Problem* (AP). For the single domain method, see (3.16)–(3.17) in Section 3.1 (second-order and fourth-order method in space). For the direct extension of the algorithms to interface and composite domains problems, see Section 4.
- *Step 3:* Next, at each time level t^{i+1} compute the unknown *boundary values or densities*, u_γ^{i+1} at the points of the *discrete grid boundary* γ by solving the system of linear equations derived from the system of *Boundary Equations with Projection*: see (3.24), (3.25) and (3.27) (second-order method in space), or (3.24), (3.26) and (3.28) (fourth-order method in space) in Section 3.1, and extension to interface and composite domain problems (4.2)–(4.3) in Section 4.

  Remark. Note, that computation of the matrix for the system of *Boundary Equations with Projection* (3.24) is the key contribution to the overall computational complexity of the algorithm. However, if the time step Δt is kept constant, then the matrix associated with the system of *Boundary Equations with Projection* (3.24) can be computed only once at initial time step and stored. Thus, only the right-hand side will be updated at each time level t^{i+1} in the linear system of *Boundary Equations with Projection* (3.24). This is a consequence of the definition of the difference potential Definition 3.2, property that Difference Potential is a linear operator of u_γ^{i+1}, and the definition of the extension operator (3.27) and (3.28), (3.29)–(3.34). Therefore, the computations at each time level t^{i+1} will be performed very efficiently.

  Moreover, in higher-dimensions, for example in 2D, the *Auxiliary Problem* (AP) can be solved very efficiently as well. Let us briefly mention a few examples. In the case of constant coefficients problems and compact finite-difference schemes as the underlying discretizations of the continuous problem, it can be solved by a sine Fast Fourier Transform (FFT) in the y direction, together with tri-diagonal elimination in the x direction. The complexity of this solution is log-linear with respect to the grid dimension in the y direction, and linear with respect to the grid dimension in the x direction. The grid dimension in the y direction should be 2^p, where p is a positive integer. In the case of a "classical" finite-difference scheme (dimension by dimension) or variable coefficients problems, either a sparse LU decomposition or iterative methods can be developed for the solution of the *Auxiliary Problem (AP)*.
- *Step 4:* Using the definition of the difference potential, Definition 3.2, Section 3.1, and Section 4 (algorithm for interface/composite domain problems), construct the *Difference Potential*, $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1}$ from the obtained density, u_γ^{i+1}.
- *Step 5:* Finally, at each new time level t^{i+1} reconstruct the approximation to the continuous solution from u_γ^{i+1} using the generalized Green's formula $u(x, t^{i+1}) \approx \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G^h_{\Delta t} F^{i+1}$, see Statement 3.5 in Section 3.1, and see Statement 4.1 in Section 4 (algorithm for interface/composite domain problems).

6. Numerical examples

In this section we will consider several test problems. First, we compare the performance of the second-order Difference Potentials Method (DPM) with the second-order Immersed Interface Method (IIM) [14–16]. Moreover, we present the result of the fourth-order DPM for the same test problem. After that, in Section 6.2 we test and compare the second and the fourth-order DPM in space on several variable coefficient problems in heterogeneous media. In all numerical experiments below, we compute the maximum error in the solution

$$\max_{t^i \in [0,1]} \max_{x_j \in [0,1]} \left| u(x_j, t^i) - u_j^i \right|,$$

as well as the maximum error in the discrete gradient of the solution using either this formula below (results in Tables 3–6)

$$\max_{t^i \in [0,1]} \max_{(x_j, x_{j+1}) \in (0,1)} \left| \frac{u(x_{j+1}, t^i) - u(x_j, t^i)}{h} - \frac{u_{j+1}^i - u_j^i}{h} \right|,$$

or using the following formula (results in Tables 8, 10, 12, 14 and 16): denote,

$$E^i := \max \left\{ \max_{(x_j, x_{j+1}) \in I_1} \left| \frac{u(x_{j+1}, t^i) - u(x_j, t^i)}{h} - \frac{u_{j+1}^i - u_j^i}{h} \right|, \max_{(x_j, x_{j+1}) \in I_2} \left| \frac{u(x_{j+1}, t^i) - u(x_j, t^i)}{h} - \frac{u_{j+1}^i - u_j^i}{h} \right| \right\},$$

Table 1
Errors in the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider the auxiliary domains $[-0.23, 0.77]$ for $0 \le x \le 0.5$ and $[0.23, 1.23]$ for $0.5 < x \le 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. $dt = 0.5h$ for DPM 2 and IIM and $dt = 0.5h^2$ for DPM 4. Problem (6.1).

N	DPM2	Conv Rate	IIM	Conv Rate	DPM4	Conv Rate
20	3.20889 E–03		3.30746 E–03		1.69012 E–05	
40	8.58076 E–04	1.90290	8.27528 E–04	1.99884	1.20118 E–06	3.81460
80	2.08901 E–04	2.03828	2.06941 E–04	1.99959	1.00956 E–07	3.57266
160	5.12743 E–05	2.02651	5.17390 E–05	1.99989	8.14846 E–09	3.63105
320	1.29065 E–05	1.99013	1.29354 E–05	1.99993	4.75048 E–10	4.10038

hence, the error is computed in Tables 8, 10, 12, 14 and 16 as:

$$\max_{t^i \in [0,1]} E^i.$$

Here, $u(x_j, t^i)$ is the exact solution at the grid points and time t^i, u_j^i is the numerical solution at the grid points and time t^i, and h is the mesh size.

6.1. Second and fourth order difference potentials method and comparison with the second order immersed interface method

In this section we consider first the following problem (which is the modification of a problem in [16]):

$$u_t - (ku_x)_x = f, \quad k = \begin{cases} 1, & \text{if } 0 \le x \le 0.5 \\ 2, & \text{if } 0.5 < x \le 1. \end{cases} \tag{6.1}$$

The exact solution is

$$u(x,t) = \begin{cases} u_1(x,t) = x^8 e^{-t}, & 0 \le x \le 0.5 \\ u_2(x,t) = \frac{1}{2}(\frac{1}{256} + x^8)e^{-t}, & 0.5 < x \le 1. \end{cases} \tag{6.2}$$

The initial conditions are

$$u(x,0) = \begin{cases} u_1(x,0) = x^8, & 0 \le x \le 0.5 \\ u_2(x,0) = \frac{1}{2}(\frac{1}{256} + x^8), & 0.5 < x \le 1. \end{cases} \tag{6.3}$$

The boundary conditions are

$$u_1(0,t) = 0 \quad \text{and} \quad u_2(1,t) = \frac{257}{512} e^{-t}. \tag{6.4}$$

And the interface conditions are

$$u_1(0.5,t) = u_2(0.5,t) \quad \text{and} \quad u_{1x}(0.5,t) = 2u_{2x}(0.5,t). \tag{6.5}$$

The right-hand side in the model (6.1) is computed in each subdomain using the exact solution (6.2).

In the tables below, DPM 2 stands for second-order in space DPM with an extension operator as in (3.27), DPM 4 stands for the fourth-order in space DPM with an extension operator as in (3.28). IIM 2 stands for the second-order in space IIM with the trapezoidal scheme for the time discretization as in [16] ("modified version of Cranck–Nicolson scheme"). For DPM 2 and DPM 4, we implement the algorithm from Section 4. We consider the auxiliary domain $[-0.23, 0.77]$ to discretize the problem using DPM in subdomain $I_1 := [0, 0.5]$ and we consider the auxiliary domain $[0.23, 1.23]$ to discretize the problem using DPM in subdomain $I_2 := [0.5, 1.0]$, see Tables 1–4. Each auxiliary domain is subdivided by N intervals, and in Tables 1–4 we use the same number of intervals (the same grids) for each subdomain. The time-step is set to $dt = 0.5h^2$ for DPM 4, and to $dt = 0.5h$ for DPM 2 and IIM. The time-interval $[0, 1]$ was used for all the tests. Note, that h is the same for DPM and IIM tests in Tables 1–4 due to the choice of the auxiliary domains for DPM.

The results presented in Tables 1–4 show that the errors of the second-order DPM 2 and the second-order IIM 2 are very close in the solution. For the discrete gradient, the error is better in magnitude by about a factor of 3 for IIM 2 than for DPM 2. However, DPM 4 shows much better accuracy than IIM 2 or DPM 2 in both the solution and the discrete gradient. Note, that the extension of IIM to higher than second order is not straightforward, and in some cases, may not be possible (see [16]).

As can be seen from the Tables 1–4, DPM 2 and DPM 4 confirm second-order $O(h^2)$ and fourth-order accuracy $O(h^4)$ in space, respectively, in both the approximation of the solution and in the discrete gradient.

To conclude Section 6.1, we use the test problem below (6.6)–(6.10) to illustrate that the fourth-order DPM 4 captures the solution and the discrete derivative with almost machine-accuracy, see results in Tables 5–6. The time step was again set to $dt = 0.5h^2$ over the time interval $[0, 1]$.

Table 2
Errors in the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider the auxiliary domains $[-0.23, 0.77]$ for $0 \le x \le 0.5$ and $[0.23, 1.23]$ for $0.5 < x \le 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. $dt = 0.5h$ for DPM 2 and IIM and $dt = 0.5h^2$ for DPM 4. Problem (6.1).

N	DPM2	Conv Rate	IIM	Conv Rate	DPM4	Conv Rate
27	1.89425 E–03		1.70518 E–03		6.01061 E–06	
54	4.59529 E–04	2.04340	4.54095 E–04	1.90886	4.51690 E–07	3.73411
108	1.12109 E–04	2.03525	1.13548 E–04	1.99969	3.89478 E–08	3.53572
216	2.82364 E–05	1.98928	2.83904 E–05	1.99983	2.33761 E–09	4.05843
432	7.11373 E–06	1.98888	7.09767 E–06	1.99998	1.33932 E–10	4.12547

Table 3
Errors in the discrete gradient (derivative) of the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider the auxiliary domains $[-0.23, 0.77]$ for $0 \le x \le 0.5$ and $[0.23, 1.23]$ for $0.5 < x \le 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. $dt = 0.5h$ for DPM 2 and IIM and $dt = 0.5h^2$ for DPM 4. Problem (6.1).

N	DPM2	Conv Rate	IIM	Conv Rate	DPM4	Conv Rate
20	2.05400 E–02		7.60408 E–03		6.26046 E–05	
40	5.48004 E–03	1.90618	1.73872 E–03	2.12875	6.14695 E–06	3.34833
80	1.52702 E–03	1.84347	4.36646 E–04	1.99349	2.83496 E–07	4.43847
160	4.03691 E–04	1.91940	1.09240 E–04	1.99896	1.87820 E–08	3.91591
320	1.01516 E–04	1.99154	2.73321 E–05	1.99883	1.15657 E–09	4.02143

Table 4
Errors in the discrete gradient (derivative) of the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider the auxiliary domains $[-0.23, 0.77]$ for $0 \le x \le 0.5$ and $[0.23, 1.23]$ for $0.5 < x \le 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. $dt = 0.5h$ for DPM 2 and IIM and $dt = 0.5h^2$ for DPM 4. Problem (6.1).

N	DPM2	Conv Rate	IIM	Conv Rate	DPM4	Conv Rate
27	1.09645 E–02		3.50021 E–03		2.03922 E–05	
54	3.23580 E–03	1.76064	9.56794 E–04	1.87116	1.32410 E–06	3.94493
108	8.79987 E–04	1.87857	2.39492 E–04	1.99823	8.93245 E–08	3.88981
216	2.21609 E–04	1.98946	5.99580 E–05	1.99795	5.58354 E–09	3.99980
432	5.57632 E–05	1.99063	1.50022 E–05	1.99878	3.61838 E–10	3.94776

Table 5
Errors in the solution and in the discrete gradient as functions of the number of intervals for DPM 4: we consider the auxiliary domains $[-0.230, 0.770]$ for $0 \le x \le 0.5$ and $[0.230, 1.230]$ for $0.5 < x \le 1$. The time step is set $dt = 0.5h^2$. Problem (6.6).

N	DPM4: Error in the Solution	DPM4: Error in the Discrete Gradient
20	9.54608 E–10	2.18486 E–09
40	5.07710 E–11	1.36601 E–10
80	3.17950 E–12	9.24372 E–12
160	1.74680 E–13	1.02585 E–12
320	1.63564 E–13	3.99680 E–13

$$u_t - (ku_x)_x = f, \quad k = \begin{cases} 1, & \text{if } 0 \le x \le 0.5 \\ 2, & \text{if } 0.5 < x \le 1, \end{cases} \tag{6.6}$$

The exact solution is

$$u(x,t) = \begin{cases} u_1(x,t) = x^4 e^{-t}, & 0 \le x \le 0.5 \\ u_2(x,t) = \frac{1}{2}(\frac{1}{16} + x^4)e^{-t}, & 0.5 < x \le 1. \end{cases} \tag{6.7}$$

The initial conditions are

$$u(x,0) = \begin{cases} u_1(x,0) = x^4, & 0 \le x \le 0.5 \\ u_2(x,0) = \frac{1}{2}(\frac{1}{16} + x^4), & 0.5 < x \le 1. \end{cases} \tag{6.8}$$

The boundary conditions are

$$u_1(0,t) = 0 \quad \text{and} \quad u_2(1,t) = \frac{17}{32}e^{-t}. \tag{6.9}$$

The interface conditions are

$$u_1(0.5,t) = u_2(0.5,t) \quad \text{and} \quad u_{1x}(0.5,t) = 2u_{2x}(0.5,t) \tag{6.10}$$

The right-hand side in the model (6.6) is computed in each subdomain using the exact solution (6.7).

Table 6
Errors in the solution and in the discrete gradient as functions of the number of intervals for DPM 4: we consider the auxiliary domains $[-0.230, 0.770]$ for $0 \le x \le 0.5$ and $[0.230, 1.230]$ for $0.5 < x \le 1$. The time step is set $dt = 0.5h^2$. Problem (6.6).

N	DPM4: Error in the Solution	DPM4: Error in the Discrete Gradient
27	2.78599 E–10	6.45468 E–10
54	1.55945 E–11	4.41681 E–11
108	9.73041 E–13	3.13549 E–12
216	6.30607 E–14	3.95683 E–13
432	1.44199 E–12	5.76739 E–12

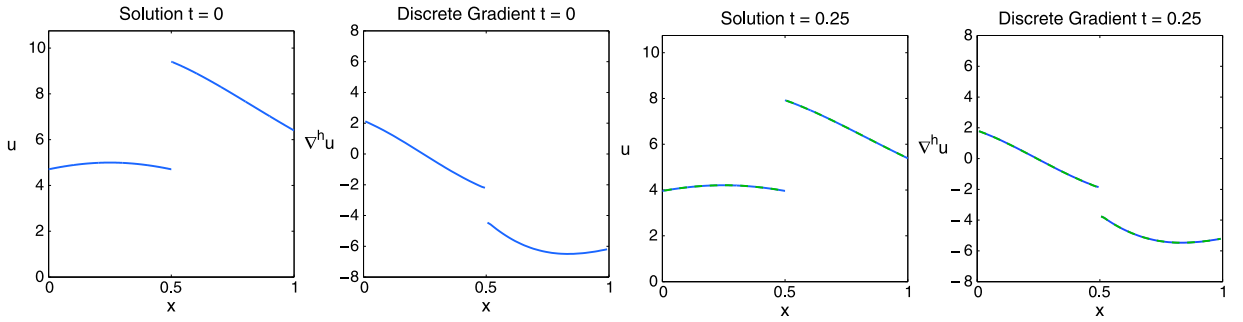

Fig. 3. Plot of the exact solution and the discrete gradient of the exact solution at time $t = 0$ (left figure), and plot of the exact solution and the discrete gradient of the exact solution versus the numerical solution and the discrete gradient of the numerical solution (DPM 4) at time $t = 0.25$ (right figure). Problem (6.11).

6.2. Second and fourth order difference potentials methods for parabolic interface problems in heterogeneous media

In this section, we first consider the following interface/composite domain test problem with variable coefficients:

$$u_{st} - (k_s u_{s_x})_x = f_s, \quad s = 1, 2 \tag{6.11}$$

with

$$k(x) = \begin{cases} k_1(x) = 1 + x^2, & 0 \le x \le 0.5 \\ k_2(x) = 1 + (x - \frac{1}{4})^2, & 0.5 < x \le 1. \end{cases} \tag{6.12}$$

The exact solution is

$$u(x,t) = \begin{cases} u_1(x,t) = \frac{1}{1+3t^2}\frac{5}{1+(x-\frac{1}{4})^2}, & 0 \le x \le 0.5 \\ u_2(x,t) = \frac{1}{1+3t^2}\frac{10}{1+(x-\frac{1}{4})^2}, & 0.5 < x \le 1. \end{cases} \tag{6.13}$$

The initial conditions are

$$u(x,0) = \begin{cases} u_1(x,0) = \frac{5}{1+(x-\frac{1}{4})^2}, & 0 \le x \le 0.5 \\ u_2(x,0) = \frac{10}{1+(x-\frac{1}{4})^2}, & 0.5 < x \le 1. \end{cases} \tag{6.14}$$

The boundary conditions are

$$u_1(0,t) = \frac{80}{17(1+3t^2)} \quad \text{and} \quad u_2(1,t) = \frac{32}{5(1+3t^2)}. \tag{6.15}$$

The interface conditions are

$$2u_1(0.5,t) = u_2(0.5,t) \quad \text{and} \quad 2u_{1x}(0.5,t) = u_{2x}(0.5,t) \tag{6.16}$$

Again, the right-hand side in this model (6.11) is computed in each subdomain using the exact solution (6.13). Here, the exact solution (6.13) has a jump in both the solution and the derivative at the interface, see Fig. 3. Moreover, we have a variable coefficient $k_1(x)$ in subdomain I_1, and a variable coefficient $k_2(x)$ in subdomain I_2 with a discontinuity in the coefficient at the interface. In Tables 7–8, we consider auxiliary domains $[-0.23, 0.77]$ and $[0.23, 1.23]$ to construct difference potentials approximation in I_1 and I_2 respectively. In Tables 9–10, we consider auxiliary domains $[-0.667, 0.833]$ and $[-0.167, 1.333]$ to construct the Difference Potentials approximation in I_1 and I_2 respectively. Each auxiliary domain is

Table 7
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider the auxiliary domains $[-0.230, 0.770]$ for $0 \le x \le 0.5$ and $[0.230, 1.230]$ for $0.5 < x \le 1$. The time step is $dt = 0.5h$ for DPM 2 and $dt = 0.5h^2$ for DPM 4. Problem (6.11).

N	DPM2	Conv Rate	DPM4	Conv Rate
27	1.39101 E–03		3.17450 E–06	
54	3.49728 E–04	1.99183	2.30391 E–07	3.78438
108	8.80409 E–05	1.98999	9.16988 E–09	4.65104
216	2.20121 E–05	1.99987	7.30761 E–10	3.64943
432	5.52320 E–06	1.99472	5.90488 E–11	3.62942

Table 8
Errors in the discrete gradient (derivative) of the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider the auxiliary domains $[-0.230, 0.770]$ for $0 \le x \le 0.5$ and $[0.230, 1.230]$ for $0.5 < x \le 1$. The time step is $dt = 0.5h$ for DPM 2 and $dt = 0.5h^2$ for DPM 4. Problem (6.11).

N	DPM2	Conv Rate	DPM4	Conv Rate
27	3.84544 E–03		1.34950 E–05	
54	9.20733 E–04	2.06229	1.08108 E–06	3.64188
108	2.37836 E–04	1.95282	4.42891 E–08	4.60938
216	5.92558 E–05	2.00494	3.35365 E–09	3.72315
432	1.47789 E–05	2.00342	2.93632 E–10	3.51365

Table 9
Errors in the solution as functions of the number of intervals for DPM 2, and DPM 4: we consider the auxiliary domains $[-0.667, 0.833]$ for $0 \le x \le 0.5$ and $[-0.167, 1.333]$ for $0.5 < x \le 1$. The time step is $dt = 0.5h$ for DPM 2 and $dt = 0.5h^2$ for DPM 4. Problem (6.11).

N	DPM2	Conv Rate	DPM4	Conv Rate
27	2.90206 E–03		1.99710 E–04	
54	7.64170 E–04	1.92511	1.31170 E–05	3.92840
108	1.95309 E–04	1.96813	8.12292 E–07	4.01329
216	4.93374 E–05	1.98501	4.74572 E–08	4.09730
432	1.23948 E–05	1.99294	2.51220 E–09	4.23960

Table 10
Errors in the discrete gradient (derivative) of the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider the auxiliary domains $[-0.667, 0.833]$ for $0 \le x \le 0.5$ and $[-0.167, 1.333]$ for $0.5 < x \le 1$. The time step is $dt = 0.5h$ for DPM 2 and $dt = 0.5h^2$ for DPM 4. Problem (6.11).

N	DPM2	Conv Rate	DPM4	Conv Rate
27	8.93270 E–03		1.74080 E–03	
54	2.36855 E–03	1.91509	4.64187 E–05	5.22890
108	6.01715 E–04	1.97685	1.19060 E–06	5.28494
216	1.43762 E–04	2.06540	4.55888 E–08	4.70687
432	3.31913 E–05	2.11480	2.62572 E–09	4.11789

Table 11
Errors as functions of the number of intervals for solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
20	20	5.91034 E–02		5.67412 E–03	
40	40	1.22885 E–02	2.26593	1.68164 E–04	5.07645
80	80	2.38617 E–03	2.36454	7.48936 E–06	4.48889
160	160	5.65604 E–04	2.07683	4.50653 E–07	4.05475
320	320	1.41801 E–04	1.99593	2.82018 E–08	3.99816

subdivided by N intervals, and we use the same number of intervals (the same grids) for each subdomain in Tables 7–10. The time-step is given by $dt = 0.5h^2$ for DPM 4 and $dt = 0.5h$ for DPM 2. The time-interval $[0, 1]$ was used for all tests.

As can be seen from the Tables 7–10, DPM 2 and DPM 4 again confirm the second-order $O(h^2)$ and fourth-order accuracy $O(h^4)$ in space, respectively, in both the approximation of the solution and in the discrete gradient. However, the convergence is not as strictly monotone as in Tables 1–4 for the model (6.1). Similar (but more noticeable) non-monotone behavior of the error was observed for the elliptic variable coefficient problem in [8]. Let us remark that the slowdown of convergence of the fourth-order scheme on finer grids is due to the loss of significant digits as the absolute levels of error get very close to machine zero. Again, DPM 4 yields superior accuracy compared to DPM 2.

As a final example, we consider in Tables 11–16 (see Fig. 4) the following test problem with variable coefficients:

$$(u_s)_t - (k_s u_{s_x})_x = f_s, \quad s = 1, 2 \tag{6.17}$$

Table 12
Errors as functions of the number of intervals for discrete gradient (derivative) of the solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
20	20	8.10172 E–01		2.89043 E–02	
40	40	1.78616 E–01	2.18137	1.42670 E–03	4.34053
80	80	3.61706 E–02	2.30398	8.39558 E–05	4.08690
160	160	7.37614 E–03	2.29388	5.28580 E–06	3.98944
320	320	1.84976 E–03	1.99553	3.55334 E–07	3.89487

Table 13
Errors as functions of the number of intervals for solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
40	20	1.22889 E–02		1.69078 E–04	
80	40	2.39104 E–03	2.36164	7.53575 E–06	4.48780
160	80	5.64233 E–04	2.08328	4.53707 E–07	4.05392
320	160	1.41434 E–04	1.99616	2.83975 E–08	3.99792

Table 14
Errors as functions of the number of intervals for discrete gradient (derivative) of the solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
40	20	1.78735 E–01		1.42918 E–03	
80	40	3.62203 E–02	2.30295	8.40339 E–05	4.08807
160	80	7.37497 E–03	2.29609	5.29015 E–06	3.98959
320	160	1.84934 E–03	1.99562	3.56265 E–07	3.89229

Table 15
Errors as functions of the number of intervals for solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
20	40	4.88790 E–02		7.26540 E–03	
40	80	9.59556 E–03	2.34877	1.88898 E–04	5.26536
80	160	2.26402 E–03	2.08348	7.61359 E–06	4.63289
160	320	5.65992 E–04	2.00003	4.54727 E–07	4.06551

Table 16
Errors as functions of the number of intervals for discrete gradient (derivative) of the solution over [0,1]: we consider the auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \le x \le 0.5$, and $[0.333, 1.080]$ with N_2 subintervals for $0.5 < x \le 1$. DPM2 and DPM4. Problem (6.17).

N_1	N_2	DPM2	Conv Rate	DPM4	Conv Rate
20	40	7.08038 E–01		7.06176 E–02	
40	80	1.44413 E–01	2.29362	1.48784 E–03	5.56874
80	160	2.93694 E–02	2.29782	8.43808 E–05	4.14016
160	320	7.37527 E–03	1.99355	5.30915 E–06	3.99036

with

$$k(x) = \begin{cases} k_1(x) = 3e^{-10(x-0.5)^4 x^4}, & 0 \le x \le 0.5 \\ k_2(x) = 3, & 0.5 < x \le 1 \end{cases} \tag{6.18}$$

The exact solution is given below

$$u(x,t) = \begin{cases} u_1(x,t) = e^{-t}\sin(5\pi x), & 0 \le x \le 0.5 \\ u_2(x,t) = e^{-t}(2(x-0.5)^7 + 1), & 0.5 < x \le 1 \end{cases} \tag{6.19}$$

subject to the initial conditions

$$u(x,0) = \begin{cases} u_1(x,0) = \sin(5\pi x), & 0 \le x \le 0.5 \\ u_2(x,0) = 2(x - \frac{1}{2})^7 + 1, & 0.5 < x \le 1 \end{cases} \tag{6.20}$$

subject to the boundary and interface conditions:

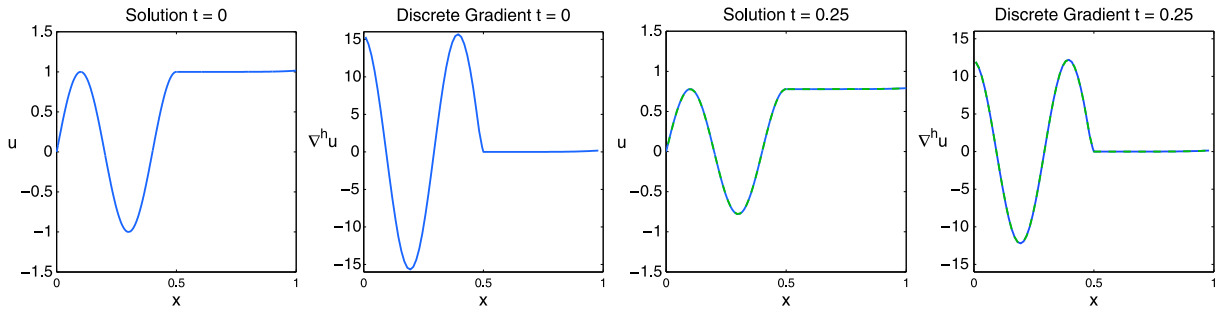

Fig. 4. Plot of the exact solution and the discrete gradient of the exact solution at time $t = 0$ (left figure), and plot of the exact solution and the discrete gradient of the exact solution versus the numerical solution and the discrete gradient of the numerical solution (DPM 4) at time $t = 0.25$ (right figure). Problem (6.17).

$$u_1(0,t) = 0, \qquad u_2(1,t) = 1.0156e^{-t}, \tag{6.21}$$

$$u_1(0.5,t) = u_2(0.5,t), \tag{6.22}$$

$$u_{1x}(0.5,t) = u_{2x}(0.5,t). \tag{6.23}$$

The f_s are computed from the above equation and the exact solution (6.19). We have a variable coefficient $k_1(x)$ in subdomain I_1 and a constant coefficient k_2 in subdomain I_2. Note that the solution given by (6.19) is more oscillatory in subdomain I_1 than in the subdomain I_2, see Fig. 4. The time-step is given by $dt = 0.5\min\{h_{I_1}^2, h_{I_2}^2\}$ for DPM 4, and $dt = 0.5\min\{h_{I_1}, h_{I_2}\}$ for DPM 2 (where h_{I_1} is the grid size for the domain I_1 and h_{I_2} is the grid size for the domain I_2).

In Tables 11–16, we demonstrate overall second-order convergence for DPM 2 and fourth-order convergence for DPM 4 in problem (6.19).

In Tables 13–16 we select different grids for each subdomain. Results in Tables 13–14 show that we can take a coarser mesh in the subdomain with less oscillatory solution (subdomain I_2), while the error remains almost the same as in Tables 11–12. Similar results with the use of different grids in different subdomains are observed in 2D for the constant coefficient problem [34,7]. This illustrates the important flexibility of the method for the future development and applications of the proposed ideas (multigrid/multi-scale approach), for variable coefficient problems in 2D and 3D.

7. Concluding remarks

In this paper, we employed one-dimensional parabolic models with variable coefficients as a starting point, to design high-order methods based on Difference Potentials approach for variable coefficient parabolic problems in heterogeneous media. We presented the construction of Difference Potentials Methods with high-order accuracy for single domain, and for the interface/composite domain problems with non-matching interface conditions. While the methods and analysis are simpler for these one-dimensional problems, they allow us to show and test several ideas and capabilities of high-order methods based on the Difference Potentials approach. The numerical schemes, as well as meshes can be chosen totally independently for each subdomain/domain; in higher-dimensions the boundaries of the subdomains and interfaces do not need to conform/align with the grids. We expect that high-order schemes can be constructed for problems with general boundary conditions, and the main complexity of the developed algorithm reduces to the several solutions of simple auxiliary problems on structured Cartesian grids. Also, the preliminary tests that we conducted here and in [8] in one-dimensional settings, as well as preliminary 2D numerical tests in irregular domains in [29,34,7,6] indicate the capability of Difference Potentials approach to resolve discontinuities very accurately at interfaces. Therefore, we expect that in higher-dimensions, the developed method will be well-suited for the elliptic and parabolic problems in arbitrary domains and with non-matching interface conditions.

For future research, we plan to develop numerical analysis, as well as extend and further develop the proposed approach (as well as methods that we developed in [29,34,7,6]) to high-order methods for variable coefficient problems in complex 2D and 3D domains. Finally, we also plan to investigate the possibility of designing an Alternating Direction Implicit Method (ADI) [5] in higher dimensions, within the Difference Potentials methodology proposed here.

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Appendix A

For the reader's convenience, we will briefly review here the proof of the Theorem 3.3. The proof follows the argument from [28].

First, let us assume that at time, t^{i+1}, u_γ^{i+1} is the trace of some solution to the difference equations (3.10): $u_\gamma^{i+1} = Tr_\gamma u^{i+1}$, where $u^{i+1} \in N^+$ is the solution to the difference equations $L_{\Delta t,h}[u_j^{i+1}] = F_j^{i+1}, \quad x_j \in M^+$. Now, construct the grid function $w^{i+1} \in N^0$ as the solution of the following problem:

$$L_{\Delta t,h}\big[w_j^{i+1}\big] = \begin{cases} F_j^{i+1}, & x_j \in M^+, \\ L_{\Delta t,h}[u_\gamma^{i+1}], & x_j \in M^-, \end{cases} \tag{A.1}$$

$$w_j^{i+1} = 0, \quad x_j \in N^0 \backslash M^0. \tag{A.2}$$

Note that the restriction of this function w^{i+1} to the set N^+ is $w^{i+1}|_{N^+} := \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G_{\Delta t}^h F^{i+1}$ (this is a consequence of the definition of the difference potentials $\mathbf{P}_{N^+\gamma} u_\gamma^{i+1}$, (3.19)–(3.20)) and the particular solution $G_{\Delta t}^h F^{i+1}$, (3.16)–(3.17). At the same time, $u^{i+1} \in N^+$ is the solution of $L_{\Delta t,h}[u_j^{i+1}] = F_j^{i+1}, x_j \in M^+$, and thus $F_j^{i+1} \equiv L_h[u_j^{i+1}]$ in (A.1). Also, u_γ^{i+1} is the trace of the solution u^{i+1}. Hence we have that:

$$\begin{aligned} &L_{\Delta t,h}\big[w_j^{i+1} - u_j^{i+1}\big] = 0, \quad x_j \in M^0, \\ &w_j^{i+1} - u_j^{i+1} = 0, \quad x_j \in N^0 \backslash M^0. \end{aligned} \tag{A.3}$$

Note that the solution u^{i+1} is extended by zero to the points of the set $N^0 \backslash N^+$. Due to the uniqueness argument, $w^{i+1} \equiv u^{i+1}$, on N^+. Hence, we can reconstruct the solution, u^{i+1} to the difference equations (3.10) using the formula: $u^{i+1} = \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G_{\Delta t}^h F^{i+1}$. Let us apply the trace operator to both sides of this formula to obtain the desired equality: $u_\gamma^{i+1} = \mathbf{P}_\gamma u_\gamma^{i+1} + G_{\Delta t}^h F_\gamma^{i+1}$.

Next, assume that at time t^{i+1} the equality (3.23) holds true for some grid function, $u_\gamma^{i+1} \in \mathbf{V}_\gamma$. Again, let us construct the grid function: $w^{i+1} := \mathbf{P}_{N^+\gamma} u_\gamma^{i+1} + G_{\Delta t}^h F^{i+1}$ on N^+. Thus, w^{i+1} is the solution (restricted to N^+) of (AP) (A.1)–(A.2), and therefore, it coincides on M^+ with a solution u^{i+1} of the difference equations (3.10): $w^{i+1} \equiv u^{i+1}$ on M^+. Hence, due to equality (3.23), u_γ^{i+1} coincides with the trace w_γ^{i+1} of w^{i+1}, and thus coincides with the trace, u_γ^{i+1} of a solution, u^{i+1} of the difference equations (3.10): $u_\gamma^{i+1} \equiv \mathrm{Tr}_\gamma u^{i+1}$. □

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