Applied Numerical Mathematics 93 (2015) 69–86

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

High-order difference potentials methods for 1D elliptic type models

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ARTICLE INFO

Article history:
Available online 3 March 2014

Keywords:
Difference potentials
Boundary projections
Cauchy's type integral
Boundary value problems
Variable coefficients
Heterogeneous media
High-order finite difference schemes
Difference Potentials Method
Immersed Interface Method
Interface problems
Parallel algorithms

ABSTRACT

Numerical approximations and modeling of many physical, biological, and biomedical problems often deal with equations with highly varying coefficients, heterogeneous models (described by different types of partial differential equations (PDEs) in different domains), and/or have to take into consideration the complex structure of the computational subdomains. The major challenge here is to design an efficient numerical method that can capture certain properties of analytical solutions in different domains/subdomains (such as positivity, different regularity/smoothness of the solutions, etc.), while handling the arbitrary geometries and complex structures of the domains. In this work, we employ one-dimensional elliptic type models as the starting point to develop and numerically test high-order accurate Difference Potentials Method (DPM) for variable coefficient elliptic problems in heterogeneous media. While the method and analysis are simple in the one-dimensional settings, they illustrate and test several important ideas and capabilities of the developed approach.

1. Introduction

Numerical approximations and modeling of many physical, biological, and biomedical problems often deal with equations with highly varying coefficients, heterogeneous models, and/or have to take into consideration the complex structure of the computational subdomains. The major challenge here is to design an efficient and flexible numerical method (for example, multi-scale method) that can capture certain properties of analytical solutions in different domains/subdomains, while handling the arbitrary geometries and complex structures of the domains.

There is extensive literature that addresses problems in domains with irregular geometries and interface problems. Some established finite-difference based methods for such problems are the Immersed Boundary Method (IB) ([17,18], etc.), the Immersed Interface Method (IIM) ([9–11], etc.), the Ghost Fluid Method (GFM) ([5,13,12], etc.), the Matched Interface and Boundary Method (MIB) ([32,30,31], etc.), and the method based on the Integral Equations approach ([15], 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 [11].

We consider here an approach based on Difference Potentials Method (DPM) [22,23]. The DPM on its own, or in combination with other numerical methods, is an efficient tool for the numerical solution of interior and exterior boundary value problems in arbitrary domains (see for example [22,23,14,24,28,16,25,26,3,4]). Viktor S. Ryaben'kii originally introduced DPM in his Doctor of Science thesis (Habilitation thesis) in 1969. The DPM allows one to reduce uniquely solvable and well-posed boundary value problems to pseudo-differential boundary equations with projections. Similar to the method in [15], methods based on Difference Potentials (see for example [23,26,25,4,16], etc.) introduce computationally simple

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http://dx.doi.org/10.1016/j.apnum.2014.02.005
0168-9274/

auxiliary domains. After that, the original domains/subdomains are embedded into simple auxiliary domains (and the auxiliary domains are discretized using Cartesian grids). However, compared to the integral equation approach in [15], 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 the methods based on Difference Potentials approach reduces to several solutions of simple auxiliary problems on structured Cartesian grids. Like the method in [15], and IIM, GFM and MIB, 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. But compared to [15], and to IIM and GFM, methods based on Difference Potentials are not restricted by the type of the boundary or interface conditions (as long as the continuous problems are well-posed), see [23] or some example of the recent works [2,25,26,4], etc. Furthermore, DPM is 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 (this property of the numerical method is crucial for computational and mathematical modeling of many applied problems). Finally, Difference Potentials approach is well-suited for the development of parallel algorithms, see [26,25,4] – examples of the second-order in space schemes based on Difference Potentials idea for 2D interface/composite domain problems. The reader can consult [23,22] and [19,20] for a detailed theoretical study of the methods based on Difference Potentials, and ([23,22,14,24,28,27,16,2,26,25,3,4], etc.) for the recent developments and applications of DPM.

In this work, we employ one-dimensional elliptic type models (second-order Boundary Value Problem (BVP)) as the starting point, to develop and numerically test high-order accurate methods based on Difference Potentials approach for variable coefficient elliptic type problems in heterogeneous media. Let us note that, previously in [26,25,4], we have developed efficient (second-order accurate in space) schemes based on Difference Potentials idea for 2D interface/composite domain problems. The method developed in [26,25,4] can handle non-matching interface conditions (as well as non-matching grids between each subdomain), and is well-suited for the design of parallel algorithms. However, these schemes were constructed and tested for the solution of Poisson's or heat equations (constant coefficient). Also, a different example of the efficient and high-order accurate method, based on Difference Potentials for the Helmholtz equation in homogeneous media with the variable wave number, was recently developed and numerically tested in [16] for a single 2D domain. *But to the best of our knowledge, this is the first application (at this point in the simple settings) of Difference Potentials approach for the construction of high-order accurate numerical schemes for problems with variable coefficients in heterogeneous media and non-matching interface conditions.* While the method and analysis are simple in the one-dimensional setting, they illustrate and test several important ideas and capabilities of Difference Potentials approach. Furthermore, to develop these methods, we employ here a more general viewpoint on Difference Potentials of being discrete potentials for the linear difference schemes (rather than approximation to the surface potentials [19,20]) – "Difference Potential plays the same role for the solution of a general system of linear difference equations (linear difference scheme), as the classical Cauchy's type integral for the solution of Cauchy–Riemann system, or in other words for the analytic functions" – see [22] or see Section 4.1 and Appendix A.

The paper is organized as follows. First, in Section 2 we give a brief summary of the main steps of the proposed algorithms. In Section 3 we introduce the formulation of our problem. *Next, to illustrate the framework for the construction of DPM with a different order of accuracy, we construct DPM with a second and with a fourth-order accuracy in Section 4.1 for a single domain 1D elliptic type model. In Section 5, we extend the second and the fourth-order DPM to one-dimensional elliptic type interface/composite domain model problem.* 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. Algorithm

In this section we will briefly summarize the main steps of our algorithm. We will give a detailed description of each step in the subsequent sections below.

- *Step 1:* Introduce a computationally simple auxiliary domain and formulate the auxiliary problem (AP).
- *Step 2:* Compute a *Particular solution*, $u_j := G^h f$, $x_j \in N^+$, as the solution of the *Auxiliary Problem* (AP). For the single domain method, see (4.12)–(4.13) in Section 4.1 (second-order and fourth-order method). For the straightforward extension of the algorithms to the interface and composite domains problems, see Section 5.
- *Step 3:* Next, compute the unknown *boundary values or densities* u_γ at the points of the *discrete grid boundary* γ (value of the unknown density u_γ on γ) by solving the system of linear equations derived from the system of *Boundary Equations with Projection*: see (4.31)–(4.32) (second-order method), or (4.35)–(4.36) (fourth-order method) in Section 4.1, and extension to the interface and composite domain problems (5.2)–(5.3) in Section 5.
- *Step 4:* Using the definition of the difference potential, Definition 4.2, Section 4.1, and Section 5 (algorithm for interface/composite domain problems), construct the *Difference Potential* $\mathbf{P}_{N^+\gamma} u_\gamma$ from the obtained density u_γ.
- *Step 5:* Finally, reconstruct the approximation to the continuous solution from u_γ using the generalized Green's formula $u(x) \approx \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$, see Theorem 4.4 in Section 4.1, and see Theorem 5.1 in Section 5.

3. Elliptic type interface models

We are concerned here with a 1D elliptic type interface problem of the form:

$$(k_1 u_x)_x - \sigma_1 u = f_1, \quad x \in I_1, \tag{3.1}$$

$$(k_2 u_x)_x - \sigma_2 u = f_2, \quad x \in I_2, \tag{3.2}$$

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

$$u(0) = a, \quad \text{and} \quad u(1) = b \tag{3.3}$$

and interface conditions at α:

$$l_{int}(u) = \phi, \qquad x = \alpha \tag{3.4}$$

where $I_1 := [0, \alpha) \subset I_1^0$ and $I_2 := (\alpha, 1] \subset I_2^0$ are two subdomains of the domain $I := [0, 1]$, $0 < \alpha < 1$ is the interface point, 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 $k_1(x) \geqslant 1$, $k_2(x) \geqslant 1$, $\sigma_1(x) \geqslant 0$, $\sigma_2(x) \geqslant 0$ are sufficiently smooth functions defined in a larger auxiliary subdomains I_1^0 and I_2^0, respectively. $f_1(x)$ and $f_2(x)$ 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. (3.1) is well-defined on some larger auxiliary domain $\overline{I_1^0}$, and the operator on the left-hand side of Eq. (3.2) is well-defined on some larger auxiliary domain $\overline{I_2^0}$. More precisely, we assume that for any sufficiently smooth functions on the right-hand side of (3.1)–(3.2), Eqs. (3.1) and (3.2) have a unique solution on I_1^0 and I_2^0, that satisfy the given boundary conditions on ∂I_1^0 and ∂I_2^0, respectively.*

Remark. The Dirichlet boundary conditions (3.3) are chosen only for the purpose of illustration and the method (DPM) is not restricted by any type of boundary conditions.

4. Single domain

Our goal is to develop high-order methods based on Difference Potentials idea for the problem (3.1)–(3.4). To simplify the presentation (*and to illustrate the unified framework for the construction of DPM with different orders of accuracy for the problems in single domain, and/or for the interface/composite domain problems*), we will first state the second and the fourth-order methods for the single domain problem:

$$(ku_x)_x - \sigma u = f, \quad x \in I \tag{4.1}$$

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

$$u(0) = a, \quad \text{and} \quad u(1) = b, \tag{4.2}$$

and then extend the developed ideas in a straightforward way to the interface/composite domain problem (3.1)–(3.4) in Section 5. As before, $I = [0, 1]$, the functions $k(x) \geqslant 1$, $\sigma(x) \geqslant 0$ are sufficiently smooth functions defined in some auxiliary domain I^0, such that $I \subset I^0$ and $f(x)$ is sufficiently smooth function defined in I. We also assume that the model problem (4.1)–(4.2) is well-posed, as well as that the operator on the left-hand side of Eq. (4.1) is well-defined on some larger auxiliary domain $\overline{I^0}$. Similar to [23,26,25,22], let us now introduce and define the main steps of the DPM for this problem.

4.1. Difference potentials approach for construction of high-order methods

We will present below (at this point, using simple one-dimensional settings) a framework based on Difference Potentials approach to construct high-order methods for problems with variable coefficients in heterogeneous media, and non-matching interface conditions. However, major principles of this framework will stay the same when applied to the numerical approximation of the models in arbitrary domains in 2D and 3D, and subject to general boundary conditions. Also, it is important to note that the presented approach based on Difference Potentials is general, and can be employed in similar ways with any (most suitable) underlying high-order discretization of the given continuous problem. In this work, the particular choices of the second-order discretization (4.6) and the fourth-order discretization (4.7) were only employed for purpose of the efficient illustration and implementation of the ideas.

We will present our ideas below by designing the second-order and the fourth-order methods together, and will only comment on the technical differences.

Introduction of the auxiliary domain

Let us place the original domain I in the auxiliary domain $I^0 := [c, d] \subset \mathbb{R}$. Next, we 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

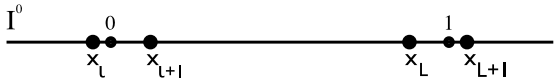

Fig. 1. Example (a sketch) of the auxiliary domain I^0, original domain $I=[0,1]$, and the example of points in set $\gamma=\{x_l, x_{l+1}, x_L, x_{L+1}\}$ for the 3-point second-order scheme.

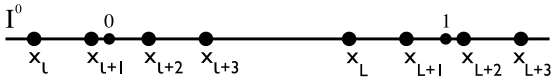

Fig. 2. Example (a sketch) of the auxiliary domain I^0, original domain $I=[0,1]$, and the example of points in set $\gamma=\{x_l, x_{l+1}, x_{l+2}, x_{l+3}, x_L, x_{L+1}, x_{L+2}, x_{L+3}\}$ for the 5-point fourth-order scheme.

$x=0$ and $x=1$ will typically fall between grid points, say $x_l \leqslant 0 \leqslant x_{l+1}$ and $x_L \leqslant 1 \leqslant x_{L+1}$ (for the 3-point second-order scheme); and between grid points $x_l < x_{l+1} \leqslant 0 \leqslant x_{l+2} < x_{l+3}$ and $x_L < x_{L+1} \leqslant 1 \leqslant x_{L+2} < x_{L+3}$ (for the 5-point fourth-order scheme), see Fig. 1 and Fig. 2.

Now, we define a finite-difference 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:

$$N_j^\kappa := \{j-1, j, j+1\}, \quad \kappa = 3, \quad \text{or} \tag{4.3}$$

$$N_j^\kappa := \{j-2, j-1, j, j+1, j+2\}, \quad \kappa = 5. \tag{4.4}$$

Next, we introduce 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 $N^+ := \{\bigcup_j N_j^\kappa \mid x_j \in M^+\}$, 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 $N^- := \{\bigcup_j N_j^\kappa \mid x_j \in M^-\}$, 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^-.

Now we can introduce the set $\gamma := N^+ \cap N^-$. The set γ is called the *discrete grid boundary*. The mesh nodes from set γ straddle the boundary $\partial I \equiv \{0, 1\}$. In case of the second-order method (with 3-point stencil), the set γ will contain four mesh nodes $\gamma = \{l, l+1, L, L+1\}$, see Fig. 1. In case of the fourth-order method (with 5-point stencil), the set γ will contain eight mesh nodes $\gamma = \{l, l+1, l+2, l+3, L, L+1, L+2, L+3\}$, see Fig. 2. Finally, define $N^0 := \{\bigcup_j N_j^\kappa \mid x_j \in M^0\} \subset \overline{I^0}$.

Once again, let us emphasize, that κ either takes here the value 3 *(if the* 3*-point stencil is used to construct the second-order method), or* 5 *(if the* 5*-point stencil is used to construct the fourth-order method).*

The point sets N^0, M^0, N^+, N^-, M^+, M^-, γ will be used to develop high-order methods based on the Difference Potentials idea.

Construction of difference equations

The discrete version of the problem (4.1) is to find $u_j \in N^+$ such that

$$L_h[u_j] = f_j, \quad x_j \in M^+ \tag{4.5}$$

The discrete system of Eqs. (4.5) is obtained here by discretizing (4.1) with the standard second-order 3-point central finite difference scheme (4.6) (if the second-order accuracy is desired), or with the fourth-order 5-point central finite difference scheme in space (4.7) (if the fourth-order accuracy is desired). *Here and below, by L_h we understand the discrete linear operator obtained using either the second-order approximation to (4.1), or the fourth-order approximation to (4.1), and with f_j as the discrete right-hand side.*

Second-order scheme

$$L_h[u_j] := \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(u_{j+1}-u_j) - k_{j-\frac{1}{2}}(u_j - u_{j-1})\right) - \sigma_j u_j, \tag{4.6}$$

the right-hand side $f_j := f(x_j)$, and the coefficients $k_{j+\frac{1}{2}} := k(x_{j+\frac{1}{2}}), \sigma_j := \sigma(x_j)$, and $x_{j+\frac{1}{2}}$ is the middle point of the interval $[x_j, x_{j+1}]$.

Fourth-order scheme

$$L_h[u_j] := k_j \frac{-u_{j-2} + 16u_{j-1} - 30u_j + 16u_{j+1} - u_{j+2}}{12h^2} + (k_x)_j \frac{u_{j-2} - 8u_{j-1} + 8u_{j+1} - u_{j+2}}{12h} - \sigma_j u_j, \tag{4.7}$$

the right-hand side $f_j := f(x_j)$, and the coefficients $k_j := k(x_j)$, $(k_x)_j := k_x(x_j)$, $\sigma_j := \sigma(x_j)$. In (4.7), we have used the following fourth-order approximation for

$$u_{xx} \approx \frac{-u_{j-2} + 16u_{j-1} - 30u_j + 16u_{j+1} - u_{j+2}}{12h^2} \tag{4.8}$$

$$u_x \approx \frac{u_{j-2} - 8u_{j-1} + 8u_{j+1} - u_{j+2}}{12h}. \tag{4.9}$$

Remark. Let us note that the scheme in the form of (4.7) is obtained by rewriting equation $(ku_x)_x - \sigma u = f$ in the form of $ku_{xx} + k_x u_x - \sigma u = f$ (in other words, we assume that this continuous problem (and a nearby problem) is well-posed as well). However, this is not always the best choice, for instance due to some properties of the coefficient k, or due to the physics of the problems. In some cases, it is better to discretize the model $(ku_x)_x - \sigma u = f$ directly (as we did in (4.6) for the second-order scheme). However, the main ideas of the DPM presented below will not change. Here, we illustrate the ideas using scheme (4.7) for the construction of the fourth-order method, especially since we develop a multi-domain approach in Section 5 (also, the same scheme applies to an equation of the form $k_1 u_{xx} + k_2 u_x - \sigma u = f$). If needed, derivatives of the coefficients, like $k_x, \ldots$, can be evaluated by the appropriate finite difference schemes to avoid analytic differentiation.

In general, the linear system of difference equations (4.5) will have multiple solutions since we did not impose any discrete boundary conditions. Once we complete the system (4.5) with the appropriate choice of the numerical boundary conditions, the scheme will result in an accurate approximation of the continuous problem in domain I. *To do so here, we will develop an approach based on the idea of the Difference Potentials [23,22].*

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 will give definition below.

Definition 4.1. For the given grid function $q \in M^0$, find the solution $v \in N^0$ of the discrete (AP) such that it satisfies the following system of equations:

$$L_h[v_j] = q_j, \quad x_j \in M^0, \tag{4.10}$$

$$v_j = 0, \quad x_j \in N^0 \backslash M^0. \tag{4.11}$$

Here, L_h is the same linear discrete operator as in (4.5), but now it is defined on the larger auxiliary domain $\overline{I^0}$ (note that, we assumed before in Section 4 that the operator on the left-hand side of Eq. (4.1) is well-defined on the entire domain $\overline{I^0}$). It is applied in (4.10) to the function $v \in N^0$. We note that (for small enough h (for (4.7)) and under the above assumptions on the continuous problem) the (AP) (4.10)–(4.11) is well-defined for any right hand side q_j: it has a unique solution $v \in N^0$. In this work we supplemented the discrete (AP) (4.10) by the zero boundary conditions (4.11). *In general, the boundary conditions for (AP) are selected to guarantee that the discrete equation $L_h[v_j] = q_j$ has a unique solution $v \in N^0$ for any discrete right-hand side q.*

Remark. The solution of the (AP) (4.10)–(4.11) defines a discrete Green's operator G^h (or the inverse operator to L_h). Although the choice of boundary conditions (4.11) will affect the operator G^h, and hence the difference potentials and the projections defined below, it will not affect the final approximate solution to (4.1)–(4.2), as long as the (AP) is uniquely solvable and well-posed.

Construction of a particular solution

Let us denote by $u_j := G^h f_j$, $u_j \in N^+$ the particular solution of the discrete problem (4.5), which we will construct as the solution (restricted to set N^+) of the auxiliary problem (AP) (4.10)–(4.11) of the following form:

$$L_h[u_j] = \begin{cases} f_j, & x_j \in M^+, \\ 0, & x_j \in M^-, \end{cases} \tag{4.12}$$

$$u_j = 0, \quad x_j \in N^0 \backslash M^0. \tag{4.13}$$

Remark. The right-hand side of (4.10) in (AP) for the construction of a particular solution, is set to

$$q_j = \begin{cases} f_j, & x_j \in M^+, \\ 0, & x_j \in M^-. \end{cases} \tag{4.14}$$

Difference potential

We now introduce a linear space $\mathbf{V}_\gamma$ of all the grid functions denoted by v_γ defined on γ [23,26,25,4], etc. We will extend the value v_γ by zero to other points of the grid N^0.

Definition 4.2. The Difference Potential with any given density $v_\gamma \in \mathbf{V}_\gamma$ is the grid function $u_j := \mathbf{P}_{N^+\gamma} v_\gamma$, defined on N^+, and coincides on N^+ with the solution u_j of the auxiliary problem (AP) (4.10)–(4.11) of the following form:

$$L_h[u_j] = \begin{cases} 0, & x_j \in M^+, \\ L_h[v_\gamma], & x_j \in M^-, \end{cases} \tag{4.15}$$

$$u_j = 0, \quad x_j \in N^0 \backslash M^0. \tag{4.16}$$

Remark. The right-hand side of (4.10) in (AP) for constructing a difference potential with density v_γ is set to

$$q_j = \begin{cases} 0, & x_j \in M^+, \\ L_h[v_\gamma], & x_j \in M^-. \end{cases} \tag{4.17}$$

The Difference Potential with density $v_\gamma \in \mathbf{V}_\gamma$ is the discrete inverse operator. Here, $\mathbf{P}_{N^+\gamma}$ denotes the operator which constructs the difference potential $u_j = \mathbf{P}_{N^+\gamma} v_\gamma$ from the given density $v_\gamma \in V_\gamma$. The operator $\mathbf{P}_{N^+\gamma}$ is the linear operator of the density v_γ. Hence, it can be easily constructed, as illustrated below:

$$u_m = \sum_{j\in\gamma} A_{jm} v_j, \quad x_m \in N^+,$$

with $\sum_{j\in\gamma} A_{jm} v_j$ being:

for the second-order method

$$\sum_{j\in\gamma} A_{jm} v_j \equiv A_{lm} v_l + A_{l+1m} v_{l+1} + A_{Lm} v_L + A_{L+1m} v_{L+1}, \quad x_m \in N^+, \tag{4.18}$$

and for the fourth-order method

$$\begin{aligned} \sum_{j\in\gamma} A_{jm} v_j \equiv{}& A_{lm} v_l + A_{l+1m} v_{l+1} + A_{l+2m} v_{l+2} + A_{l+3m} v_{l+3} \\ &+ A_{Lm} v_L + A_{L+1m} v_{L+1} + A_{L+2m} v_{L+2} + A_{L+3m} v_{L+3}, \quad x_m \in N^+. \end{aligned} \tag{4.19}$$

Here, by u_m we denote the value at the grid point x_m of the Difference Potential $P_{N_\gamma^+} v_\gamma$ with the density v_γ, and by $\{A_{jm}\}$ the coefficients of the difference potentials operator. The coefficients $\{A_{jm}\}$ can be computed by solving an auxiliary problem (AP) (4.15)–(4.16) (or by constructing a Difference Potential operator) with the unit density v_γ at points $x_{j^\star} \in \gamma$. Here, *for the second-order method*, $x_{j^\star} \in \gamma \equiv \{x_l, x_{l+1}, x_L, x_{L+1}\}$, and *for the fourth-order method*, $x_{j^\star} \in \gamma \equiv \{x_l, x_{l+1}, x_{l+2}, x_{l+3}, x_L, x_{L+1}, x_{L+2}, x_{L+3}\}$. Density v_γ is defined as the unit density at point $x_{j^\star} \in \gamma$:

$$v_\gamma = \begin{cases} 1, & \text{if } j = j^\star, \\ 0, & \forall j \neq j^\star. \end{cases} \tag{4.20}$$

Therefore, A_{jm} is the value at a point $x_m \in N^+$ of the solution of the auxiliary problem (AP) (4.15)–(4.16) with the unit density (or the value at a point $x_m \in N^+$ of the Difference Potential with the unit density (4.20)).

Next, similarly to ([23,3], 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 $\mathbf{P}_{N^+\gamma} v_\gamma$ on the grid boundary γ:

$$\mathbf{P}_\gamma v_\gamma := \mathrm{Tr}_\gamma(\mathbf{P}_{N^+\gamma} v_\gamma) = (\mathbf{P}_{N^+\gamma} v_\gamma)|_\gamma \tag{4.21}$$

We will now formulate the crucial theorem of the method (see [23] for the general result).

Theorem 4.3. *Density u_γ is the trace of some solution u to the Difference Equations (4.5): $u_\gamma \equiv \mathrm{Tr}_\gamma u$, if and only if, the following equality holds*

$$u_\gamma = \mathbf{P}_\gamma u_\gamma + G^h f_\gamma, \tag{4.22}$$

where $G^h f_\gamma := \mathrm{Tr}_\gamma (G^h f)$ is the trace (or restriction) of the particular solution $G^h f \in N^+$ constructed in (4.12)–(4.13) on the grid boundary γ.

Proof. The proof follows the argument from [23] and for the reader's convenience we will present it below.

First, let us assume that u_γ is the trace of some solution to the difference equations (4.5): $u_\gamma = \mathrm{Tr}_\gamma u$, where $u \in N^+$ is the solution to the difference equations $L_h[u_j] = f_j$, $x_j \in M^+$. Construct the grid function: $w := \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$ on N^0 (*not restricted to* N^+). From the definition of the difference potentials $\mathbf{P}_{N^+\gamma} u_\gamma$ (4.15), and the particular solution $G^h f$ (see (4.12)–(4.13)), the grid function $w \in N^0$ coincides with the solution of (AP) (4.10)–(4.11) of the form:

$$L_h[w_j] = \begin{cases} f_j, & x_j \in M^+, \\ L_h[u_\gamma], & x_j \in M^-, \end{cases} \tag{4.23}$$

$$w_j = 0, \quad x_j \in N^0 \backslash M^0. \tag{4.24}$$

At the same time, $u \in N^+$ is the solution of $L_h[u_j] = f_j$, $x_j \in M^+$, hence $f_j \equiv L_h[u_j]$ in (4.23), and u_γ is the trace of the solution u. Hence we have that:

$$L_h[w_j] = L_h[u_j], \quad x_j \in M^0 \tag{4.25}$$

Note that solution u is extended by 0 to the points of the set $N^0 \backslash N^+$. Due to the uniqueness argument, $w \equiv u$, on N^+. Hence, we can reconstruct solution u to the difference equations (4.5) using the formula: $u = \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$. Let us apply the trace operator to both sides of this formula to obtain the desired equality: $u_\gamma = \mathbf{P}_\gamma u_\gamma + G^h f_\gamma$.

Next, assume that the equality (4.22) holds true for some grid function $u_\gamma \in \mathbf{V}_\gamma$. Again, let us construct the grid function: $w := \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$ on N^0. Thus, w is the solution to (AP) (4.23)–(4.24), and therefore it coincides on M^+ with a solution u of the difference equations (4.5): $w \equiv u$ on M^+. Hence, due to equality (4.22), u_γ coincides with the trace w_γ of w, and thus coincides with the trace u_γ of a solution u of the difference equations (4.5): $u_\gamma \equiv \mathrm{Tr}_\gamma u$ (note that for any density $u_\gamma \in \mathbf{V}_\gamma$, grid function $\mathbf{P}_{N^+\gamma} u_\gamma + G^h f \in N^+$ is some solution to the difference equations (4.5)). □

Remark. Note that the difference potential $\mathbf{P}_{N^+\gamma} u_\gamma$ is the solution to the homogeneous difference equation $L_h[u_j] = 0$, $x_j \in M^+$, and is uniquely defined once we know the value of the density u_γ at the points of the boundary γ.

Also, note that density u_γ has to satisfy *Boundary Equations* $u_\gamma - \mathbf{P}_\gamma u_\gamma = G^h f_\gamma$ *in order to be a trace of the solution to the difference equation* $L_h[u_j] = f_j$.

Remark. In the case of a constant coefficient model problem (4.1) (assume, $k(x) \equiv 1$), using the technique from [21] let us show a direct connection of the difference potential $\mathbf{P}_{N^+\gamma} u_\gamma$ to the Cauchy-type integral (see [23,22] for more general discussion on the subject). We also assume $\sigma(x) = 0$ for simplicity of illustration and will consider the example of the second-order method here (4.6) (for reader's convenience we present similar calculations for the fourth-order method (4.7) in Appendix A).

Thus, the homogeneous difference equation $L_h[u_j] = 0$, $j = l+1, \ldots, L$ for the second order scheme is

$$\frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} = 0, \quad j = l+1, \ldots, L. \tag{4.26}$$

Consider a difference equation of the form

$$z_{j-1} - 2z_j + z_{j+1} = 0. \tag{4.27}$$

Denote, $z := (z_l, z_{l+1}, \ldots, z_L, z_{L+1})$ to be a solution of the difference equation (4.27). Next, define the generating polynomial

$$Z(g) = \sum_{j=l}^{L+1} z_j g^j,$$

where the coefficients of the polynomial z_j are the values of the solution z at the grid points. Multiply (4.27) by g^j, and sum from $l+1, \ldots, L$, thus we will have:

$$\sum_{j=l+1}^{L} z_{j-1}g^j - 2\sum_{j=l+1}^{L} z_j g^j + \sum_{j=l+1}^{L} z_{j+1}g^j = 0. \tag{4.28}$$

For example, we can rewrite the first term as:

$$g\sum_{j=l+1}^{L} z_{j-1}g^{j-1} = gZ(g) - z_L g^{L+1} - z_{L+1}g^{L+2}.$$

Similarly, the second and the third term in (4.28) can be rewritten as

$$\sum_{j=l+1}^{L} z_j g^j = Z(g) - z_l g^l - z_{L+1}g^{L+1}$$

and

$$\frac{1}{g}\sum_{j=l+1}^{L} z_{j+1}g^{j+1} = \frac{1}{g}Z(g) - z_l g^{l-1} - z_{l+1}g^l.$$

This way, (4.27) becomes

$$\left(gZ(g) - z_L g^{L+1} - z_{L+1}g^{L+2}\right) - 2\left(Z(g) - z_l g^l - z_{L+1}g^{L+1}\right) + \left(\frac{Z(g)}{g} - z_l g^{l-1} - z_{l+1}g^l\right) = 0. \tag{4.29}$$

Finally, let us recall Cauchy's residue Theorem, and represent

$$z_j = \frac{1}{2\pi i}\oint\limits_{|g|=2} \frac{Z(g)}{g^{j+1}}dg.$$

Solving (4.29) for $Z(g)$ we obtain

$$z_j = \frac{1}{2\pi i}\oint\limits_{|g|=2} \frac{g^l(1-2g)z_l + g^{l+1}z_{l+1} + g^{L+2}z_L + (g-2)g^{L+2}z_{L+1}}{(1-g)^2 g^{j+1}}dg, \quad j = l,\dots,L+1. \tag{4.30}$$

The Cauchy-type integral (4.30) plays the role of the discrete potential for the linear difference equations (4.27) (each z_j, $j = l,\dots,L+1$ is determined by values z_γ), as the difference potential $\mathbf{P}_{N^+\gamma}u_\gamma$ for the linear difference equations (4.26).

Coupling of Boundary Equations with boundary conditions

We will present below the details for the second-order scheme and for the fourth-order scheme separately since there are differences in the technical details (*however, the main strategy is the same for any high-order scheme*).

Case of the second-order method

The *Boundary Equations:* $u_\gamma - \mathbf{P}_\gamma u_\gamma = G^h f_\gamma$ for the unknown density u_γ is the linear system of equations:

$$(I - A)\mathbf{u} = \mathbf{G^h f}, \tag{4.31}$$

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

$$\begin{pmatrix} A_{ll} & A_{l+1l} & A_{Ll} & A_{L+1l} \\ A_{ll+1} & A_{l+1l+1} & A_{Ll+1} & A_{L+1l+1} \\ A_{lL} & A_{l+1L} & A_{LL} & A_{L+1L} \\ A_{lL+1} & A_{l+1L+1} & A_{LL+1} & A_{L+1L+1} \end{pmatrix}.$$

The column vector of the unknown densities is

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

and the column vector of the right-hand side is

$$\mathbf{G^h f} := \left(G^h f_l, G^h f_{l+1}, G^h f_L, G^h f_{L+1}\right)^T.$$

The above system of *Boundary Equations* (4.31) will have multiple solutions without boundary conditions (4.2), since it is equivalent to the difference equations $L_h[u_j] = f_j$, $x_j \in M^+$. We need to supplement it by the boundary conditions (4.2) to construct the unique u_γ.

Remark. It can be shown (see for example, [23] or [3]) that the rank of the linear system will be $|\gamma^{in}|$ (here, $|\gamma^{in}|$ is the cardinality of a set γ^{in} – the interior layer of the grid boundary $\gamma = \gamma^{in} \cup \gamma^{ex}$. Similarly, γ^{ex} denotes the exterior layer). For the second order method here, the rank is 2.

Therefore, we will consider the following approach to solve for the unknown densities u_γ from the *Boundary Equations* (4.31). Here, using the idea of the Taylor expansion, one can represent the unknown densities u_γ with the values of the continuous solution and its derivatives at the 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 (4.1). 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.* For example, in case of 3 terms, the extension operator is:

$$u_j := u|_{\partial I} \pm d u_x|_{\partial I} + \frac{d^2}{2} u_{xx}\Big|_{\partial I}, \quad x_j \in \gamma, \tag{4.32}$$

where

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

and

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

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

The value $u|_{\partial I}$ is given due to the boundary conditions (4.2). Let us denote the unknown value of $C_1 := u_x(0)$ and $C_2 := u_x(1)$. We can obtain the values of higher-order derivatives using the given differential equation (4.1). In case of the second-order derivatives, this is simply

$$u_{xx}(0) = \frac{f(0) + \sigma(0)a}{k(0)} - \frac{k_x(0)}{k(0)} C_1, \tag{4.33}$$

and

$$u_{xx}(1) = \frac{f(1) + \sigma(1)b}{k(1)} - \frac{k_x(1)}{k(1)} C_2. \tag{4.34}$$

Hence, the only unknowns that we need to solve for are C_1 and C_2. We will use expansion (4.32) for u_γ in the *Boundary Equations* (4.31) and obtain the overdetermined linear system for C_1 and C_2. This system is solved uniquely using the least square method. After that, we can obtain the value of the density u_γ at the points of the grid boundary γ using formula (4.32).

Case of the fourth-order method

Similarly to the second-order case above, the *Boundary Equations*: $u_\gamma - \mathbf{P}_\gamma u_\gamma = G^h f_\gamma$ for the unknown density u_γ is the linear system of equations:

$$(I - A)\mathbf{u} = \mathbf{G^h f}, \tag{4.35}$$

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

$$\begin{pmatrix}
A_{ll} & A_{l+1l} & A_{l+2l} & A_{l+3l} & A_{Ll} & A_{L+1l} & A_{L+2l} & A_{L+3l} \\
A_{ll+1} & A_{l+1l+1} & A_{l+2l+1} & A_{l+3l+1} & A_{Ll+1} & A_{L+1l+1} & A_{L+2l+1} & A_{L+3l+1} \\
A_{ll+2} & A_{l+1l+2} & A_{l+2l+2} & A_{l+3l+2} & A_{Ll+2} & A_{L+1l+2} & A_{L+2l+2} & A_{L+3l+2} \\
A_{ll+3} & A_{l+1l+3} & A_{l+2l+3} & A_{l+3l+3} & A_{Ll+3} & A_{L+1l+3} & A_{L+2l+3} & A_{L+3l+3} \\
A_{lL} & A_{l+1L} & A_{l+2L} & A_{l+3L} & A_{LL} & A_{L+1L} & A_{L+2L} & A_{L+3L} \\
A_{lL+1} & A_{l+1L+1} & A_{l+2L+1} & A_{l+3L+1} & A_{LL+1} & A_{L+1L+1} & A_{L+2L+1} & A_{L+3L+1} \\
A_{lL+2} & A_{l+1L+2} & A_{l+2L+2} & A_{l+3L+2} & A_{LL+2} & A_{L+1L+2} & A_{L+2L+2} & A_{L+3L+2} \\
A_{lL+3} & A_{l+1L+3} & A_{l+2L+3} & A_{l+3L+3} & A_{LL+3} & A_{L+1L+3} & A_{L+2L+3} & A_{L+3L+3}
\end{pmatrix}.$$

The column vector of the unknown densities is

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

and the column vector of the right-hand side is

$$\mathbf{G^h f} := \left(G^h f_l, G^h f_{l+1}, G^h f_{l+2}, G^h f_{l+3}, G^h f_L, G^h f_{L+1}, G^h f_{L+2}, G^h f_{L+3}\right)^T.$$

As before, the above system of *Boundary Equations* (4.35) without boundary conditions (4.2) will have multiple solutions, since it is equivalent to the difference equations $L_h[u_j] = f_j$, $x_j \in M^+$. To construct the unique u_γ we need to supplement it by the boundary conditions (4.2).

Remark. The rank of the system here is 4 for the fourth order scheme.

Therefore, similarly to the second-order case, we will consider the following approach to solve for the unknown densities u_γ from the *Boundary Equations* (4.35). Again, using the idea of Taylor expansion, we will construct the extension from the continuous boundary ∂I to the discrete boundary γ of the solution to (4.1). For example, in case of 5-terms, extension operator is:

$$u_j := u|_{\partial I} \pm d u_x|_{\partial I} + \frac{d^2}{2!}u_{xx}\Big|_{\partial I} \pm \frac{d^3}{3!}u_{xxx}\Big|_{\partial I} + \frac{d^4}{4!}u_{xxxx}\Big|_{\partial I} \quad x_j \in \gamma, \tag{4.36}$$

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

$$u|_{\partial I} := u(0), \qquad u_x|_{\partial I} := u_x(0), \qquad u_{xx}|_{\partial I} := u_{xx}(0), \qquad u_{xxx}|_{\partial I} := u_{xxx}(0), \qquad u_{xxxx}|_{\partial I} := u_{xxxx}(0),$$

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

$$u|_{\partial I} := u(1), \qquad u_x|_{\partial I} := u_x(1), \qquad u_{xx}|_{\partial I} := u_{xx}(1), \qquad u_{xxx}|_{\partial I} := u_{xxx}(1), \qquad u_{xxxx}|_{\partial I} := u_{xxxx}(1).$$

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

$u|_{\partial I}$ are given due to the boundary conditions (4.2). Let us denote the unknown value of $C_1 := u_x(0)$ and $C_2 := u_x(1)$. We can obtain the values of higher-order derivatives using the given differential equation (4.1). In case of the second-order derivatives, this is simply

$$u_{xx}(0) = \frac{f(0) + \sigma(0)a}{k(0)} - \frac{k_x(0)}{k(0)}C_1, \tag{4.37}$$

and

$$u_{xx}(1) = \frac{f(1) + \sigma(1)b}{k(1)} - \frac{k_x(1)}{k(1)}C_2. \tag{4.38}$$

For the third order derivatives we have:

$$u_{xxx}(0) = \frac{f_x(0) - \frac{2k_x(0)}{k(0)}f(0)}{k(0)} + \frac{\sigma_x(0) - \frac{2k_x(0)}{k(0)}\sigma(0)}{k(0)}a + \frac{\sigma(0) + 2\frac{k_x^2(0)}{k(0)} - k_{xx}(0)}{k(0)}C_1, \tag{4.39}$$

$$u_{xxx}(1) = \frac{f_x(1) - \frac{2k_x(1)}{k(1)}f(1)}{k(1)} + \frac{\sigma_x(1) - \frac{2k_x(1)}{k(1)}\sigma(1)}{k(1)}b + \frac{\sigma(1) + 2\frac{k_x^2(1)}{k(1)} - k_{xx}(1)}{k(1)}C_2. \tag{4.40}$$

And for the fourth order derivatives we have:

$$\begin{aligned} u_{xxxx}(0) = &-\frac{3k_{xx}(0) - \frac{6k_x^2(0)}{k(0)} - \sigma(0)}{k^2(0)}f(0) - \frac{3k_x(0)}{k^2(0)}f_x(0) + \frac{f_{xx}(0)}{k(0)} \\ &- \left(\frac{3k_{xx}(0) - \sigma(0)}{k^2(0)}\sigma(0) + \frac{3k_x(0)(\sigma_x(0) - \frac{2k_x(0)}{k(0)}\sigma(0))}{k^2(0)} - \frac{\sigma_{xx}(0)}{k(0)}\right)a \\ &+ \left(\frac{3k_{xx}(0) - \sigma(0)}{k^2(0)}k_x(0) - 3k_x\frac{\sigma(0) + 2\frac{k_x^2(0)}{k(0)} - k_{xx}(0)}{k^2(0)} - \frac{k_{xxx}(0) - 2\sigma_x(0)}{k(0)}\right)C_1, \end{aligned} \tag{4.41}$$

$$\begin{aligned} u_{xxxx}(1) = &-\frac{3k_{xx}(1) - \frac{6k_x^2(1)}{k(1)} - \sigma(1)}{k^2(1)}f(1) - \frac{3k_x(1)}{k^2(1)}f_x(1) + \frac{f_{xx}(1)}{k(1)} \\ &- \left(\frac{3k_{xx}(1) - \sigma(1)}{k^2(1)}\sigma(1) + \frac{3k_x(1)(\sigma_x(1) - \frac{2k_x(1)}{k(1)}\sigma(1))}{k^2(1)} - \frac{\sigma_{xx}(1)}{k(1)}\right)b \\ &+ \left(\frac{3k_{xx}(1) - \sigma(1)}{k^2(1)}k_x(1) - 3k_x\frac{\sigma(1) + 2\frac{k_x^2(1)}{k(1)} - k_{xx}(1)}{k^2(1)} - \frac{k_{xxx}(1) - 2\sigma_x(1)}{k(1)}\right)C_2. \end{aligned} \tag{4.42}$$

Hence, again, the only unknowns that we need to solve for are C_1 and C_2. We will use expansion (4.36) for u_γ in the *Boundary Equations* (4.35), and obtain the overdetermined linear system for C_1 and C_2. This system is solved uniquely for C_1 and C_2 using the least square method. After that, we can obtain the value of the density u_γ at the points of the grid boundary γ using formula (4.36).

Finally, the last step of the DPM is to use the obtained density u_γ to reconstruct the approximation to the solution (4.1)–(4.2) inside the domain I.

Generalized Green's formula

Theorem 4.4. *Discrete solution* $u_j := \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$ *is the approximation to the solution* $u_j \approx u(x_j)$, $x_j \in N^+ \cap I$ *of the continuous problem (4.1)–(4.2).*

Discussion: The result is the consequence of the sufficient regularity (smoothness) of the exact solution, Theorem 4.3, extension operator (4.32) (for the second-order method) or the extension operator (4.36) (for the fourth-order method), and the second-order accuracy of the scheme (4.6) (for the second-order method) and the fourth-order accuracy of the scheme (4.7) (for the fourth-order method). Therefore, we expect that the discrete solution $u_j := \mathbf{P}_{N^+\gamma} u_\gamma + G^h f$ will approximate the solution $u_j \approx u(x_j)$, $x_j \in N^+ \cap I$ of the continuous problem (4.1)–(4.2) with $O(h^2)$ (for the second-order method) and with $O(h^4)$ (for the fourth-order method) in the maximum norm. *In Section 6 we illustrate the capabilities and the consistence of the developed approach with several numerical experiments for the interface/composite domain problems.*

Let us remark, that in higher-dimensions ($\geqslant 2$), in [19,20] it was shown (under sufficient regularity of the exact solution), that the Difference Potentials approximate surface potentials of the elliptic operators (and, hence DPM approximates the solution to the elliptic boundary value problem) with the accuracy of $O(h^{\mathcal{P}-\varepsilon})$ in the discrete Hölder norm of order $\mathcal{Q}+\varepsilon$. Here, $0 < \varepsilon < 1$ is arbitrary number, $\mathcal{Q}$ is the order of the considered elliptic operator, and $\mathcal{P} = 2$ – if the second-order scheme is employed for the approximation of the elliptic operator, or $\mathcal{P} = 4$ – if the fourth-order scheme is employed for the approximation of the elliptic operator (see [19,20] or [23] for the details and proof of the general result. Also, see [16] for the brief discussion of the accuracy of DPM). *However, the rigorous theoretical analysis (accuracy, etc.) of more general concept of the Difference Potentials for arbitrary linear difference scheme still needs to be investigated [22].*

Remark.

- The formula $\mathbf{P}_{N^+\gamma} u_\gamma + G^h f$ is known as the *discrete generalized Green's formula.*
- Note that after density u_γ is obtained from the *Boundary Equations*, the difference potential is easily constructed as the solution of a simple (AP) using Definition 4.2.

5. Difference potentials approach for interface and composite domains problems

In Section 4.1 we formulated second and fourth-order methods based on Difference Potentials approach, for problems in the single domain I. In this section we will show how to extend these methods to interface/composite domains problems (3.1)–(3.4).

First, as we have done in Section 4 for the single domain I, we will introduce the auxiliary domains. 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 in a similar way as we did in Section 4.1. Also, for each I_s^0 we will introduce, for example 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 the considerations of the properties of the model and solution in each subdomain (3.1)–(3.3), as well as the efficiency and simplicity of the resulting discrete problems). After that, all the definitions, notations, and properties introduced in Section 4.1 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 (3.1)–(3.2) for each subdomain as:

$$L_h^s[u_j] = f_{sj}, \quad x_j \in M_s^+. \tag{5.1}$$

The difference problem (5.1) is obtained using either the second-order (4.6) or the fourth-order scheme (4.7).

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

Theorem 5.1. *Density* $u_\gamma := (u_{\gamma_1}, u_{\gamma_2})$ *is the trace of some solution* $u \in I_1 \cup I_2$ *to the Difference Equations (5.1):* $u_\gamma \equiv \mathrm{Tr}_\gamma u$, *if and only if, the following equality holds*

$$u_{\gamma_1} = \mathbf{P}_{\mathbf{1}_{\gamma_1}} u_{\gamma_1} + G_1^h f_{\gamma_1}, \quad x_j \in \gamma_1, \tag{5.2}$$

$$u_{\gamma_2} = \mathbf{P}_{\mathbf{2}_{\gamma_2}} u_{\gamma_2} + G_2^h f_{\gamma_2}, \quad x_j \in \gamma_2. \tag{5.3}$$

The obtained discrete solution $u_j := \mathbf{P}_{\mathbf{s}_{N_s^+\gamma_s}} u_{\gamma_s} + G_s^h f_s$ *is the approximation to the solution* $u_j \approx u(x_j) \in I_1 \cup I_2$, $x_j \in N_s^+ \cap I_s$, $s = 1, 2$ *of the continuous problem (3.1)–(3.4).*

Discussion: The result is a consequence of the results in Section 4.1. We expect that the solution $u_j := \mathbf{P}_{\mathbf{s}_{N_s^+\gamma_s}} u_{\gamma_s} + G_s^h f_s$ will approximate the exact solution $u(x_j) \in I_1 \cup I_2$, $x_j \in N_s^+ \cap I_s$, $s = 1, 2$ with the accuracy $O(h^2)$ for the second-order scheme,

and with the accuracy $O(h^4)$ for the fourth-order scheme in the maximum norm. See also Section 6 for the numerical results.

Remark. Similar to the discussion in Section 4.1, the *Boundary Equations* (5.2)–(5.3) alone will have multiple solutions and have to be coupled with boundary (3.3) and interface conditions (3.4) to obtain the unique densities u_{γ_1} and u_{γ_2}. We use the extension formula (4.32) (second-order scheme) or (4.36) (fourth-order scheme) to construct $u_{\gamma_s}, s = 1, 2$ in each subdomain/domain. The unknowns are $u|_{\partial I_1}, u_x|_{\partial I_1}$ and $u|_{\partial I_2}, u_x|_{\partial I_2}$. Here, $\partial I_1 := \{0, \alpha\}$ and $\partial I_2 := \{\alpha, 1\}$ (total 8 unknowns without imposed boundary and interface conditions (3.3)–(3.4)).

Note that we constructed the algorithm here based on the inhomogeneous *Boundary Equations* (5.2)–(5.3) instead of the homogeneous *Boundary Equations* $u_{\gamma_s} - \mathbf{P}_{\mathbf{s}\gamma_s} u_{\gamma_s} = 0$ like in [26,25,4]. *We do not see too many advantages of one approach over the other one in* 1*D, but in* 2*D and in* 3*D we expect that the algorithms based on homogeneous Boundary Equations will be more efficient and will have more flexibility, such as the ability to consider different auxiliary problems for the construction of the difference potentials and the particular solutions, etc. (see for more details in our work [26,25,4]). This will be part of our future research for problems with variable coefficients in* 2*D and in* 3*D.*

6. Numerical examples

In this section, we will consider two test problems. We will first compare the performance of the second-order Difference Potentials Method (DPM) with the second-order Immersed Interface Method (IIM) [9–11], as well as with the standard second-order central difference method in Section 6.1. Moreover, we will present the result of the fourth-order DPM for the same test problem. Next, in Section 6.2 we will test and compare the second and the fourth-order DPM on the variable coefficient problem in heterogeneous media as well. In all numerical experiments below, we compute the maximum error

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

Moreover, in Tables 3, 4 and in Table 8 to further illustrate the potential of the developed approach to capture the discontinuities at the interface, we also compute the maximum error between the discrete gradient (derivative) of the exact solution and the numerical solution

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

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

6.1. Second and fourth order difference potentials method and comparison with other methods

To test and compare second and fourth order DPM, second-order IIM and the standard central second-order finite difference method we consider the following problems in this section (which is the modification of a problem in [11]).

$$(\beta u_x)_x = 56x^6, \quad \beta = \begin{cases} 1, & \text{if } 0 \leqslant x \leqslant 0.5 \\ 2, & \text{if } 0.5 < x \leqslant 1 \end{cases} \tag{6.1}$$

subject to the boundary and interface conditions:

$$u(0) \equiv u_1(0) = 0, \qquad u(1) \equiv u_2(1) = \frac{257}{512} \tag{6.2}$$

$$u_1(0.5) = u_2(0.5), \tag{6.3}$$

$$u_{1x}(0.5) = 2u_{2x}(0.5). \tag{6.4}$$

The exact solution to (6.1)–(6.4) is given as:

$$u(x) = \begin{cases} u_1(x) = x^8, & \text{if } x \leqslant 0.5 \\ u_2(x) = \frac{1}{2}(x^8 + \frac{1}{256}), & \text{if } x > 0.5. \end{cases} \tag{6.5}$$

In the tables below, DPM 2 stands for second-order DPM, DPM 4 stands for the fourth-order DPM, and IIM 2 stands for the second-order IIM. For DPM 2 and DPM 4, we implement the algorithm from Section 5. We consider auxiliary domain $[-0.25, 0.75]$ in Tables 1–4, and auxiliary domain $[-0.667, 0.833]$ in Tables 5–6 to discretize the problem using DPM in subdomain $I_1 := [0, 0.5]$. We consider auxiliary domain $[0.25, 1.25]$ in Tables 1–4, and auxiliary domain $[-0.167, 1.33]$ in Tables 5–6 to discretize the problem using DPM in subdomain $I_2 := [0.5, 1.0]$. Each auxiliary domain is subdivided by N intervals, and in Tables 1–6 we use the same number of intervals (the same grids) for each subdomain. The results presented in Tables 1–4 show that the errors of the second-order DPM 2 and the second-order IIM 2 are similar (there is difference

Table 1
Errors in the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider auxiliary domains $[-0.25, 0.75]$ for $0 \leqslant x \leqslant 0.5$, and $[0.25, 1.25]$ for $0.5 < x \leqslant 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. Problem (6.1).

N	Error (DPM 2)	Conv. rate	Error (IIM 2)	Conv. rate	Error (DPM 4)	Conv. rate
20	0.003998		0.003998		7.361e−05	
40	0.001002	1.996	0.001002	1.996	2.346e−06	4.972
80	0.0002506	1.999	0.0002506	1.999	8.688e−08	4.755
160	6.267e−05	2.000	6.267e−05	2.000	6.92e−09	3.650
320	1.567e−05	2.000	1.567e−05	2.000	4.756e−10	3.863
640	3.917e−06	2.000	3.917e−06	2.000	1.119e−10	2.088

Table 2
Errors in the solution as functions of the number of intervals: for DPM 2 and DPM 4 we consider auxiliary domains $[-0.25, 0.75]$ for $0 \leqslant x \leqslant 0.5$, and $[0.25, 1.25]$ for $0.5 < x \leqslant 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. Problem (6.1).

N	Error (DPM 2)	Conv. rate	Error (IIM 2)	Conv. rate	Error (DPM 4)	Conv. rate
24	0.002775		0.002775		2.996e−05	
48	0.000696	1.995	0.000696	1.995	9.408e−07	4.993
96	0.0001741	1.999	0.0001741	1.999	4.579e−08	4.361
192	4.352e−05	2.000	4.352e−05	2.000	3.453e−09	3.729
384	1.088e−05	2.000	1.088e−05	2.000	2.141e−10	4.012
768	2.72e−06	2.000	2.72e−06	2.000	2.641e−10	−0.303

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 auxiliary domains $[-0.25, 0.75]$ for $0 \leqslant x \leqslant 0.5$, and $[0.25, 1.25]$ for $0.5 < x \leqslant 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. Problem (6.1).

N	Error (DPM 2)	Conv. rate	Error (IIM 2)	Conv. rate	Error (DPM 4)	Conv. rate
20	0.019756		0.019756		4.629e−04	
40	0.006241	1.663	0.006241	1.663	3.579e−05	3.693
80	0.001743	1.840	0.001743	1.840	2.412e−06	3.891
160	4.600e−04	1.922	4.600e−04	1.922	1.555e−07	3.955
320	1.181e−04	1.961	1.181e−04	1.961	9.846e−09	3.981
640	2.992e−05	1.981	2.992e−05	1.981	4.044e−10	4.606

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 auxiliary domains $[-0.25, 0.75]$ for $0 \leqslant x \leqslant 0.5$, and $[0.25, 1.25]$ for $0.5 < x \leqslant 1$. The mesh size h is the same for DPM and IIM due to the choice of the auxiliary domains. Problem (6.1).

N	Error (DPM 2)	Conv. rate	Error (IIM 2)	Conv. rate	Error (DPM 4)	Conv. rate
24	0.014861		0.014861		2.421e−04	
48	0.004499	1.724	0.004499	1.724	1.773e−05	3.771
96	0.001233	1.868	0.001233	1.868	1.176e−06	3.915
192	3.223e−04	1.935	3.223e−04	1.935	7.534e−08	3.964
384	8.239e−05	1.968	8.239e−05	1.968	4.731e−09	3.993
768	2.083e−05	1.984	2.083e−05	1.984	6.565e−10	2.849

Table 5
Errors in the solution as functions of the number of intervals for DPM 2: we consider auxiliary domains $[-0.667, 0.833]$ for $0 \leqslant x \leqslant 0.5$, and $[-0.167, 1.33]$ for $0.5 < x \leqslant 1$. Problem (6.1).

N	Error (DPM 2)	Conv. rate	N	Error (DPM 2)	Conv. rate
20	0.009871		24	0.006677	
40	0.002115	2.223	48	0.001521	2.134
80	0.0005357	1.981	96	0.0003978	1.935
160	0.0001488	1.848	192	9.719e−05	2.033
320	3.441e−05	2.113	384	2.458e−05	1.983
640	8.59e−06	2.002	768	6.109e−06	2.009

in 6th–8th digits when small enough h is considered and we believe that this is due to different effect of round off errors in DPM and IIM). Moreover, the results presented in Tables 3–4 show the ability of the Difference Potentials approach to capture very accurately discontinuities at the interface.

We believe that these results are expected. The proposed method here is based on the idea of the difference potentials, which allows to construct *Boundary Equations with Projection* for the trace of the solution at the points near a continuous

Table 6
Errors in the solution as functions of the number of intervals for DPM 4: we consider auxiliary domains $[-0.667, 0.833]$ for $0 \leqslant x \leqslant 0.5$, and $[-0.167, 1.33]$ for $0.5 < x \leqslant 1$. Problem (6.1).

N	Error (DPM 4)	Conv. rate	N	Error (DPM 4)	Conv. rate
20	0.0001759		24	9.473e−05	
40	9.466e−06	4.216	48	4.397e−06	4.429
80	6.124e−07	3.950	96	2.746e−07	4.001
160	4.202e−08	3.865	192	1.972e−08	3.800
320	2.361e−09	4.154	384	1.231e−09	4.002
640	1.117e−10	4.402	768	1.286e−10	3.259

Table 7
Errors in the solution as functions of the number of intervals. Problem (6.1).

N	Error (Standard Central FD)	N	Error (Standard Central FD)
20	0.006789	24	0.007191
40	0.009214	48	0.009633
80	0.01037	96	0.01053
160	0.01083	192	0.01089
320	0.01103	384	0.01106
640	0.01112	768	0.01113

Table 8
Errors in the solution and in the discrete derivative of the solution as functions of the number of intervals for DPM 4: we consider auxiliary domains $[-0.667, 0.833]$ for $0 \leqslant x \leqslant 0.5$, and $[-0.167, 1.33]$ for $0.5 < x \leqslant 1$. Problem (6.6).

N	Solution error (DPM 4)	Gradient (derivative) error (DPM 4)
24	3.809e−15	1.466e−14
48	8.59e−15	2.145e−13
96	3.819e−13	1.266e−12
192	1.618e−12	1.032e−11
384	2.404e−12	5.165e−11
768	4.71e−11	1.999e−10

boundary (at the points of the discrete grid boundary). Therefore, the accuracy of DPM is only limited by the accuracy of the scheme employed to construct the difference potentials and the particular solutions (see a more detailed exposition of the theory in [23]). Hence, the accuracy of the DPM 2 in this case is limited only by the second-order scheme. At the same time, IIM is derived from the idea of minimizing the magnitude of local truncation error near the irregular points (near interface) using the explicit information about jump conditions on the solution and the flux across the interface. This allows to obtain a numerical scheme that achieves second-order accuracy (for a second-order scheme; note, that extension of IIM to higher than second order is not straightforward) on the interface problems [11]. Thus, the accuracy of the second-order IIM and the accuracy of the second-order DPM is very close to each other. Similar results are observed in 2D when DPM is compared with the second order finite difference scheme [25,4] (when classical solution exists).

At the same time, as expected, and illustrated in Table 7, the standard centered second-order finite-differences scheme failed to converge on the interface problem (6.1)–(6.2). Furthermore, the results in Tables 1–6 confirm second-order convergence for DPM 2 and fourth-order convergence for DPM 4 in the solution, as well as in the discrete derivative of the solution – Tables 3–4 (we consider different choice of auxiliary problems for DPM in Tables 1–4 and in Tables 5–6). Let us remark that the breakdown of convergence of 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.

Finally, we use the test problem below (6.6)–(6.9) to illustrate that the fourth-order DPM captures the solution and the discrete derivative with almost machine-accuracy (again, the observed breakdown of accuracy of the fourth-order scheme on finer grids is due to the loss of significant digits); see results in Table 8.

$$(\beta u_x)_x = 12x^2, \quad \beta = \begin{cases} 1, & \text{if } 0 \leqslant x \leqslant 0.5, \\ 2, & \text{if } 0.5 \leqslant x \leqslant 1 \end{cases} \tag{6.6}$$

subject to the boundary and interface conditions:

$$u(0) \equiv u_1(0) = 0, \qquad u(1) \equiv u_2(1) = \frac{17}{32}, \tag{6.7}$$

$$u_1(0.5) = u_2(0.5), \tag{6.8}$$

$$u_{1x}(0.5) = 2u_{2x}(0.5). \tag{6.9}$$

Table 9
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
40	40	0.00018		4.187e−06	
80	80	4.512e−05	1.996	1.817e−07	4.526
160	160	1.133e−05	1.994	2.417e−08	2.910
320	320	2.837e−06	1.998	1.466e−09	4.043
640	640	7.091e−07	2.000	9.334e−11	3.973

Table 10
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
48	48	0.0001253		2.106e−06	
96	96	3.159e−05	1.988	1.345e−07	3.969
192	192	7.862e−06	2.007	2.617e−09	5.684
384	384	1.97e−06	1.997	1.238e−09	1.080
768	768	4.918e−07	2.002	1.079e−10	3.520

The exact solution is:

$$u(x) = \begin{cases} u_1(x) = x^4 & \text{if } 0 \leqslant x \leqslant 0.5, \\ u_2(x) = \frac{1}{2}(x^4 + \frac{1}{16}), & \text{if } 0.5 \leqslant x \leqslant 1. \end{cases}$$

6.2. Second and fourth order difference potentials method for problem in heterogeneous media

In this section we consider the following test problem with variable coefficients:

$$(k_s u_{s_x})_x - \sigma_s u_s = f_s, \quad s = 1, 2 \tag{6.10}$$

with

$$k_1(x) = 3e^{-10(x-0.5)^4 x^4},$$
$$k_2(x) = 3,$$
$$\sigma_1(x) = 2,$$
$$\sigma_2(x) = 1$$

subject to the boundary and interface conditions:

$$u(0) \equiv u_1(0) = 0, \qquad u(1) \equiv u_2(1) = 1.0156, \tag{6.11}$$
$$u_1(0.5) = u_2(0.5), \tag{6.12}$$
$$u_{1x}(0.5) = u_{2x}(0.5) \tag{6.13}$$

and

$$u(x) = \begin{cases} u_1(x), & \text{if } 0 \leqslant x \leqslant 0.5, \\ u_2(x), & \text{if } 0.5 \leqslant x \leqslant 1 \end{cases} \tag{6.14}$$

where the exact solution is given below

$$u_1(x) = \sin(\pi x),$$
$$u_2(x) = 2(x - 0.5)^7 + 1.$$

The f_s are computed from the above equation. We have a variable coefficient $k_1(x)$ in subdomain I_1 and a constant coefficient k_2 in subdomain I_2. In Tables 9–14, we demonstrate overall second-order convergence for DPM 2 and fourth-order convergence for DPM 4 (6.10)–(6.13). However, the error does not converge monotonically, but rather oscillates for the variable coefficient problem. Again, we note that the breakdown of convergence of 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. In Tables 11–14, we select different grids for each subdomain. Results in Tables 11 and 13 show that we can take a coarser mesh in the subdomain with less oscillatory solution, while the error remains almost the same as in Tables 9 and 10. Similar results with the use

Table 11
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
80	40	7.242e−05		9.375e−08	
160	80	1.78e−05	2.025	1.649e−08	2.507
320	160	4.467e−06	1.995	9.082e−10	4.182
640	320	1.122e−06	1.993	1.184e−10	2.939

Table 12
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
40	80	0.0001571		4.275e−06	
80	160	3.959e−05	1.989	1.894e−07	4.496
160	320	9.941e−06	1.994	2.473e−08	2.937
320	640	2.487e−06	1.990	1.655e−09	3.901

Table 13
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
96	48	5.085e−05		9.327e−08	
192	96	1.237e−05	2.039	6.243e−09	3.901
384	192	3.134e−06	1.981	1.111e−09	2.490
768	384	7.784e−07	2.009	1.363e−10	3.027

Table 14
Errors in the solution as functions of the number of intervals for DPM 2 and DPM 4: we consider auxiliary domains $[-0.167, 0.583]$ with N_1 subintervals for $0 \leqslant x \leqslant 0.5$, and $[0.333, 1.08]$ with N_2 subintervals for $0.5 < x \leqslant 1$. Problem (6.10).

N_1	N_2	Error (DPM 2)	Conv. rate	Error (DPM 4)	Conv. rate
48	96	0.000109		2.147e−06	
96	192	2.776e−05	1.973	1.393e−07	3.946
192	384	6.879e−06	2.013	2.491e−09	5.805
384	768	1.727e−06	1.994	1.476e−09	0.755

of different grids in different subdomains are observed in 2D for the constant coefficient problem [25,4]. This illustrates the important flexibility of the method for the future development of the proposed ideas (multigrid/multiscale approach) for variable coefficient problems in 2D and 3D.

7. Concluding remarks

In this work, we used the one-dimensional elliptic type model with variable coefficients as the starting point, to develop and numerically test high-order methods based on Difference Potentials approach for the variable coefficient elliptic problems in heterogeneous media. We also illustrated the unified framework (principles) for the construction of Difference Potentials Methods with high-order accuracy for the single domain, and for the interface/composite domain problems with non-matching interface conditions. While the methods and analysis are simple for these one-dimensional problems, they allow us to illustrate and test several ideas and capabilities of high-order methods based on 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 the 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 in the one-dimensional settings (as well as preliminary 2D numerical tests in [26, 25,4,3]) indicate the capability of Difference Potentials approach to resolve discontinuities very accurately at the interface. Therefore, we expect that the proposed approach will be well-suited for the general heterogeneous models and interface problems.

For future research, we plan to extend and further develop the proposed approach (as well as methods that we developed in [26, 25,4,3]) to high-order methods for variable coefficient problems in arbitrary domains in 2D and 3D, including the time-dependent problems. The high-order Difference Potentials methods for time-dependent problems will be developed by considering the time-discrete version of the continuous problems (employing Backward Euler, Crank–Nicolson or high-order IMEX, etc. time discretizations; see some examples of 2D second order in space and first order in time DPM schemes in [3,4]). We also plan to develop iterative solvers, for

example a multigrid iterative solver for the efficient solution of the auxiliary problems in each subdomain/domain, see some references on multigrid [6,7,1,8,29] and other references. We expect that the developed approach will be well-suited for multi-physics/multi-scale problems with general boundary conditions, as well as for the development of parallel algorithms.

Acknowledgements

The authors are grateful to the anonymous referees for the valuable suggestions and questions that helped to improve the manuscript.

The research of Yekaterina Epshteyn is supported in part by the National Science Foundation Grant # DMS-1112984 and the research of Spencer Phippen is supported in part by the National Science Foundation Grant # DMS-1112984 and by the REU research at the Mathematics Department at the University of Utah.

Appendix A

For the reader's convenience, similar to the second-order method in the case of a constant coefficient model problem (4.1) (assume, $k(x) \equiv 1$), let us show a direct connection of the difference potential $\mathbf{P}_{N^+\gamma} u_\gamma$ to the Cauchy-type integral. Again, we will assume $\sigma(x) = 0$.

The homogeneous difference equation $L_h[u_j] = 0$, $j = l+2, \dots, L+1$ for the fourth order scheme is

$$\frac{-u_{j-2} + 16u_{j-1} - 30u_j + 16u_{j+1} - u_{j+2}}{12h^2} = 0, \quad j = l+2, \dots, L+1. \tag{A.1}$$

Consider the difference equation of the form

$$-z_{j-2} + 16z_{j-1} - 30z_j + 16z_{j+1} - z_{j+2} = 0. \tag{A.2}$$

Denote, $z := (z_l, z_{l+1}, \dots, z_{L+2}, z_{L+3})$ to be a solution of the difference equation (A.2). Next, define the generating polynomial

$$Z(g) = \sum_{j=l}^{L+3} z_j g^j,$$

where the coefficients of the polynomial z_j are the values of the solution z at the grid points. Multiply (A.2) by g^j, and sum from $l+2, \dots, L+1$ to obtain:

$$\sum_{j=l+2}^{L+1} z_{j-2} g^j - 16 \sum_{j=l+2}^{L+1} z_{j-1} g^j + 30 \sum_{j=l+2}^{L+1} z_j g^j - 16 \sum_{j=l+2}^{L+1} z_{j+1} g^j + \sum_{j=l+2}^{L+1} z_{j+2} g^j = 0. \tag{A.3}$$

As for the second-order method in Section 4.1, we can rewrite each term. For example, we can rewrite the first term as:

$$g^2 \sum_{j=l+2}^{L+1} z_{j-2} g^{j-2} = g^2 Z(g) - z_L g^{L+2} - z_{L+1} g^{L+3} - z_{L+2} g^{L+4} - z_{L+3} g^{L+5}.$$

Similarly, the other terms in (A.3) can be rewritten as well. Again, let us recall Cauchy's residue theorem, and represent

$$z_j = \frac{1}{2\pi i} \oint_{|g|=2} \frac{Z(g)}{g^{j+1}} dg.$$

Thus, we obtain

$$\begin{aligned} z_j = {} & \frac{1}{2\pi i} \oint_{|g|=2} \frac{(1 - 16g + 30g^2 - 16g^3) g^l z_l + (1 - 16g + 30g^2) g^{l+1} z_{l+1} + (1 - 16g) g^{l+2} z_{l+2}}{(g-1)^2 (g^2 - 14g + 1) g^{j+1}} dg \\ & + \frac{1}{2\pi i} \oint_{|g|=2} \frac{g^{l+3} z_{l+3} + g^{L+4} z_L + (-16 + g) g^{L+4} z_{L+1} + (30 - 16g + g^2) g^{L+4} z_{L+2}}{(g-1)^2 (g^2 - 14g + 1) g^{j+1}} dg \\ & + \frac{1}{2\pi i} \oint_{|g|=2} \frac{(-16 + 30g - 16g^2 + g^3) g^{L+4} z_{L+3}}{(g-1)^2 (g^2 - 14g + 1) g^{j+1}} dg, \quad j = l, \dots, L+3. \end{aligned} \tag{A.4}$$

The Cauchy-type integral (A.4) plays the role of the discrete potential for the difference equation (A.2) (each z_j, $j = l, \dots, L+3$ is determined by values z_γ), similar to the difference potential $\mathbf{P}_{N^+\gamma} u_\gamma$ for (A.1).

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