FAST FACTORIZATION UPDATE FOR GENERAL ELLIPTIC EQUATIONS UNDER MULTIPLE COEFFICIENT UPDATES

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Abstract. For discretized elliptic equations, we develop a new factorization update algorithm that is suitable for incorporating coefficient updates with large support and large magnitude in subdomains. When a large number of local updates are involved, in addition to the standard factors in various (interior) subdomains, we precompute some factors in the corresponding exterior subdomains. Exterior boundary maps are constructed hierarchically. The data dependencies among tree-based interior and exterior factors are exploited to enable extensive information reuse. For coefficient updates in a subdomain, *only the interior problem in that subdomain needs to be re-factorized and there is no need to propagate updates to other tree nodes*. The combination of the new interior factors with a chain of existing factors quickly provides the new global factor and thus an effective solution algorithm. The introduction of exterior factors avoids updating higher-level subdomains with large system sizes, and makes the idea suitable for handling multiple occurrences of updates. The method can also accommodate the case when the support of updates moves.

Key words. elliptic equations, coefficient update, fast factorization update, exterior boundary map, exterior factor, Schur complement domain decomposition

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1. Introduction.

In the solution of elliptic partial differential equations (PDEs) in practical fields such as inverse problems and computational biology, it often needs to update the coefficients associated with subdomains. For example, one key application in inverse problems is the iterative reconstruction of the wavespeed governed by the Helmholtz equation, which needs to incorporate modified coefficients into the following *reference problem*:

$$Lu = f \text{ in } D, \quad L = -\nabla \cdot p_2(x)\nabla + p_1(x) \cdot \nabla + p_0(x), \tag{1.1}$$

where D is the domain of interest, $p_0(x)$, $p_1(x)$, and $p_2(x)$ are coefficient functions of the partial differential operator L. After discretizations with continuous Galerkin or finite difference approaches, we get a system of linear equations with a sparse coefficient matrix.

1.1. Coefficient update problem.

Given the reference problem (1.1), the *coefficient update problem* is written as

$$\tilde{L}\tilde{u} = f \text{ in } D, \quad \tilde{L} = -\nabla \cdot \tilde{p}_2(x)\nabla + \tilde{p}_1(x) \cdot \nabla + \tilde{p}_0(x), \tag{1.2}$$

where $\tilde{p}_0(x)$, $\tilde{p}_1(x)$, and $\tilde{p}_2(x)$ are the modified coefficients and $\tilde{u}$ is the new solution. The modification is localized if the coefficient update $(\tilde{L} - L)$ has small support. Assuming that we know the reference solution u of (1.1), then (1.2) is equivalent to

$$\tilde{L}(\tilde{u} - u) = f - \tilde{L}u = (L - \tilde{L})u. \tag{1.3}$$

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Note that the right-hand side of (1.3) has the same local support as the coefficient update.

There are several strategies for solving either (1.2) or (1.3). For iterative solution, one can either reuse the preconditioner for L or perform additional changes for better convergence. For direct solution, if there is only a small amount of local updates, then the Sherman-Morrison-Woodbury (SMW) formula may be used. However, if there is a sequence of many local updates, then a *factorization update* from L to $\tilde{L}$ is preferred. The primary focus of this paper is to develop a fast factorization update algorithm in direct solution. Our algorithm has nearly optimal complexity for the update of the factorization, and is effective for handling modifications $(\tilde{L} - L)$ supported at various different locations.

Note that (1.2) can also be formulated as integral equations. Applying the solution operator G of (1.1) to both sides of (1.2), we get

$$(I + G(\tilde{L} - L))\tilde{u} = u. \tag{1.4}$$

Restricting to the support of $(\tilde{L} - L)$, we get the Lippmann-Schwinger integral equation. For direct solutions, (1.4) is not suitable since dense factorization in subdomains can be expensive. Boundary integral formulations may be more suitable because of the reduced system size, and are in fact related to our approach.

1.2. Existing work. Sparse direct solvers provide robust solutions to the fixed reference problem (1.1). After nested dissection reordering [10], the factorization of an $n \times n$ sparse discretized matrix generally costs $O(n^{3/2})$ in 2D, and $O(n^2)$ in 3D. Recent software packages provide the option of solving sparse right-hand sides, for example MUMPS [24, 27] and PARDISO [28, 25]. A similar factorization process can be derived from Schur-complement domain decomposition strategies [5, 13, 16, 22, 26].

In the recent years, rank-structured representations are developed to effectively compress fill-in and obtain fast factorizations of elliptic problems. Several such representations are $\mathcal{H}$ matrices [14], $\mathcal{H}^2$ matrices[15], and hierarchically semiseparable (HSS) matrices [3, 33]. Sparse factorization with HSS operations is proposed in [12, 30, 31, 32].

Updating LU factorizations of general matrices has been studied in [2, 4, 7, 11]. For sparse factorizations, these methods propagate updates from child nodes to ancestors in elimination trees. For integral operators, updates to local geometries and kernels are studied in [8, 23, 34]. In [8], the update of the structures and the values of hierarchical matrices under adaptive refinement is discussed. In [23], the changes are propagated bottom-up in a quadtree. The SMW formula is used in [34] to compute the action of the inverse. For all of these methods, the updates are typically restricted to a few entries or low-rank updates. If the updates have large support or move locations, these methods may become inefficient.

For updating the coefficients in the PDE problem (1.2), the amount of modifications can be large due to the volumetric change in the support of $(\tilde{L} - L)$. For such a situation, it is beneficial to decompose the problem into a modified interior problem and a fixed exterior problem. This idea traces back to [18, 19], where boundary integral equations are formulated for piecewise constant media. For inhomogeneous reference problems, related formulations are developed in [17, 29], where the fundamental solution is replaced by the inverse matrix of some finite difference stencil. In order to efficiently precompute selected parts of the inverse, the location of the updates usually needs to be fixed.

1.3. Overview of the proposed method. In this work, we design a fast factorization update algorithm that is suitable for handling multiple volumetric updates. The method has a precomputation step that factorizes the reference problem in various interior and exterior subdomains. When the problem changes, re-factorizations are done only for those subdomains containing the changes, and the solution is updated by solving (1.3) using the locality of the right-hand side.

The method starts from a domain partitioning governed by a binary tree (denoted by $\mathcal{T}$), similarly to related direct solvers. In the factorization of the reference problem, *interior boundary value problems* for adjacent subdomains are combined by eliminating their shared interface. The work flow is *bottom-up* in $\mathcal{T}$. That is, child nodes pass data to parents.

For solving coefficient update problems with a relatively large amount of updates, we precompute additional factors following a *top-down* traversal of $\mathcal{T}$ before knowing the specific region or value of perturbations. This top-down process constructs factors for *exterior boundary value problems*, which helps to bypass existing data dependencies. Then for the solution of (1.3), we only re-factorize the smallest subdomain containing the updates, and select existing factors of exterior problems which remain unchanged. For each subtree $\tilde{\mathcal{T}} \subset \mathcal{T}$ corresponding to the updates, the solution update algorithm treats the nodes inside and outside $\tilde{\mathcal{T}}$ separately. Inside $\tilde{\mathcal{T}}$, the solution algorithm is similar to the traditional one, but requires the factors of the updated system. Outside $\tilde{\mathcal{T}}$, a boundary value problem is solved using the factorization of the exterior problems.

The advantages of our method include:

- For the factorization update, the use of tree-based interior and exterior factors enables us to change only the factors inside the region of coefficient updates, namely, only the nodes in $\tilde{\mathcal{T}}$. There is *no propagation of updates to other nodes*. Thus, *the factorization update cost only depends on the size of the updates* instead of the total number of unknowns.
- The method is suitable for incorporating coefficient updates with *large support and large magnitude in subdomains.*
- Because the precomputation prepares for coefficient updates in *any subtree* of $\mathcal{T}$, *the supports of updates are allowed to move.*
- Regarding the discretized Green's function, the explicit precomputation and storage of relevant dense matrices are replaced by fast and flexible matrix-vector products. The matrix-vector products support local applications inside certain subdomains.

The method is tested on the transmission problem for the Helmholtz equation. The precomputation has the same scaling as related direct factorizations. The method is especially suitable for large number of changes (e.g. 10^5 nodals), because the re-factorization cost is *independent of the total number of unknowns.*

The remaining sections are organized as follows. We formulate the interior and exterior problems in Section 2. Hierarchical factorization algorithms are developed in Section 3 for the coefficient update problems. The algorithm complexity is estimated in Section 4 and is supported by the performance tests in Section 5. Some conclusions are drawn in Section 6.

2. Interior and exterior problems and basic solution update methods.

Factorization update problems can be complicated in general because there are many different scenarios regarding the locations and sizes of the updates. We first present our method for the simplest case and then generalize it to more advanced forms. In

Section 2.1, updates in fixed locations are solved by a one-level relation between an interior and an exterior problem. In Section 2.2, a two-level method gives additional flexibility to change the locations and sizes of the updates.

The problem of changing the coefficient in the interior of a subdomain is originally formulated and solved using potential theories, see for example [19, Theorem 4.1]. Note that the fundamental solution (free-space Green's function) is challenging to compute or to store in inhomogeneous media. We choose instead a Schur-complement domain decomposition formulation, which focuses on solving sub-problems on the boundaries of subdomains.

For a certain subdomain $\Omega \subset D$, we start by introducing unknowns on the boundary $\partial\Omega$ and in the interior Ω. Consider an auxiliary local PDE problem

$$\begin{cases} Lu^{(\Omega)} = f^{(\Omega)} & \text{in } \Omega, \\ \alpha u^{(\Omega)} + \beta\nu \cdot \left(p_2 \nabla u^{(\Omega)}\right) = g^{(\Omega)} & \text{on } \partial\Omega, \end{cases} \tag{2.1}$$

where L is defined in (1.1) with leading-order coefficient function $p_2(x)$, $f^{(\Omega)}$ is the *interior source*, $g^{(\Omega)}$ is the *boundary source*, ν is the outward unit normal vector with respect to $\partial\Omega$, and α, β are two scalar coefficients. The solution $u^{(\Omega)}$ generates the *boundary data* $\hat{g}^{(\Omega)}$ on $\partial\Omega$ defined as

$$\hat{g}^{(\Omega)} = \hat{\alpha} u^{(\Omega)} + \hat{\beta}\nu \cdot \left(p_2 \nabla u^{(\Omega)}\right) \text{ on } \partial\Omega, \tag{2.2}$$

where $\hat{\alpha}, \hat{\beta}$ are scalar coefficients such that $\hat{g}^{(\Omega)}$ is not a scalar multiple of $g^{(\Omega)}$.

Next, we introduce solution operators of the local problem (2.1), and they involve the boundary-boundary, interior-boundary, boundary-interior, and interior-interior interactions for the subdomain Ω. For given $f^{(\Omega)}$ and $g^{(\Omega)}$, the solution of (2.1) is expressed as

$$u^{(\Omega)} = G^{(\Omega)} f^{(\Omega)} + K^{(\Omega)} g^{(\Omega)}, \tag{2.3}$$

where $G^{(\Omega)}$ is the interior solution operator, the kernel of which is the Green's function, and $K^{(\Omega)}$ is the solution operator of the corresponding boundary value problem. $\hat{g}^{(\Omega)}$ also has a linear relation with $f^{(\Omega)}$ and $g^{(\Omega)}$

$$\hat{g}^{(\Omega)} = T^{(\Omega)} g^{(\Omega)} + S^{(\Omega)} f^{(\Omega)}, \tag{2.4}$$

where $T^{(\Omega)}$ is the *boundary map* between the boundary source $g^{(\Omega)}$ and the boundary data $\hat{g}^{(\Omega)}$, and $S^{(\Omega)}$ is the linear map from the interior source $f^{(\Omega)}$ to $\hat{g}^{(\Omega)}$.

After discretizations, (2.3)–(2.4) become matrix-vector multiplications that can be combined as

$$\begin{pmatrix} \hat{g}^{(\Omega)} \\ u^{(\Omega)} \end{pmatrix} = \begin{pmatrix} T^{(\Omega)} & S^{(\Omega)} \\ K^{(\Omega)} & G^{(\Omega)} \end{pmatrix} \begin{pmatrix} g^{(\Omega)} \\ f^{(\Omega)} \end{pmatrix}. \tag{2.5}$$

The size of $T^{(\Omega)}$ is usually smaller than the other blocks ($S^{(\Omega)}$, $K^{(\Omega)}$, and $G^{(\Omega)}$), because $\partial\Omega$ is one dimension lower than Ω. In Section 2.1, we show how (2.5) is used to solve the coefficient update problem. Starting from Section 2.2, we improve the efficiency by considering the factorizations inside Ω and avoiding forming large matrices explicitly. For the rest of the paper, we use linear algebra notation for ease of exposition.

2.1. One-level method and interior and exterior problems. We show the basic idea of solving the coefficient update problem (1.3) by combining the information of interior and exterior subdomains. For coefficient updates supported in Ω, (2.5) is insufficient because $g^{(\Omega)}$ is unknown. To get the unknowns on $\partial\Omega$, we need to consider the *exterior subdomain* $\Omega^c := D\backslash\overline{\Omega}$, which is the relative complement of Ω's closure in D. There is one level of domain partitioning, where Ω and Ω^c are *level-one subdomains* of D.

Similar to (2.5), for the exterior subdomain Ω^c, we have

$$\begin{pmatrix} \hat{g}^{(\Omega^c)} \\ u^{(\Omega^c)} \end{pmatrix} = \begin{pmatrix} T^{(\Omega^c)} & S^{(\Omega^c)} \\ K^{(\Omega^c)} & G^{(\Omega^c)} \end{pmatrix} \begin{pmatrix} g^{(\Omega^c)} \\ f^{(\Omega^c)} \end{pmatrix}, \tag{2.6}$$

which contains the solution operators to the problem (2.1) with Ω replaced by Ω^c. Choosing a special case of *Robin-to-Robin map* such that $\alpha\beta \neq 0$ in (2.1) and $(\hat{\alpha}, \hat{\beta}) = (\alpha, -\beta)$ in (2.2), then the *transmission condition* on $\partial\Omega$ is

$$g^{(\Omega)} = \hat{g}^{(\Omega^c)}, \quad \hat{g}^{(\Omega)} = g^{(\Omega^c)}, \tag{2.7}$$

because the outward normal changes sign across $\partial\Omega$. By eliminating $\hat{g}^{(\Omega)}$ and $\hat{g}^{(\Omega^c)}$ in (2.5)–(2.6), we get

$$\begin{pmatrix} T^{(\Omega)} & -I & S^{(\Omega)} & 0 \\ -I & T^{(\Omega^c)} & 0 & S^{(\Omega^c)} \\ K^{(\Omega)} & 0 & G^{(\Omega)} & 0 \\ 0 & K^{(\Omega^c)} & 0 & G^{(\Omega^c)} \end{pmatrix} \begin{pmatrix} g^{(\Omega)} \\ g^{(\Omega^c)} \\ f^{(\Omega)} \\ f^{(\Omega^c)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ u^{(\Omega)} \\ u^{(\Omega^c)} \end{pmatrix}. \tag{2.8}$$

Let

$$M^{(\partial\Omega)} = \begin{pmatrix} T^{(\Omega)} & -I \\ -I & T^{(\Omega^c)} \end{pmatrix}. \tag{2.9}$$

The solution operator in D is the Schur complement of $M^{(\partial\Omega)}$ in (2.8) as follows:

$$G^{(D)} = \begin{pmatrix} G^{(\Omega)} & \\ & G^{(\Omega^c)} \end{pmatrix} - \begin{pmatrix} K^{(\Omega)} & \\ & K^{(\Omega^c)} \end{pmatrix} (M^{(\partial\Omega)})^{-1} \begin{pmatrix} S^{(\Omega)} & \\ & S^{(\Omega^c)} \end{pmatrix}. \tag{2.10}$$

The coefficient update problem (1.3) can be solved by computing matrix-vector products of $G^{(D)}$ using (2.10). The boundary map matrices need to be formed explicitly in order to factorize $M^{(\partial\Omega)}$, but the remaining ones can be implicit as long as matrix-vector products can be performed.

Based on the current formulation, we propose an algorithm for directly solving the simplest coefficient update problem in which the region of modifications Ω is known. The factorization operations related to the reference operator L include:

1. Factorize L in Ω so that the matrix-vector product (2.5) can be computed by direct solutions.
2. Factorize L in Ω^c similarly for (2.6).
3. Factorize $M^{(\partial\Omega)}$ in (2.9).

Then for each new problem $\tilde{L}\tilde{u} = f$, the solution process is:

1. Solve $Lu = f$ by multiplying (2.10) with f.
2. Update the factors of L to get those of $\tilde{L}$ in Ω.
3. Solve $\tilde{L}(\tilde{u} - u) = (L - \tilde{L})u$ by multiplying (2.10) with $(L - \tilde{L})u$.

If Ω is much smaller than D, the method is very effective because the factorization in Ω is much cheaper than that in D. The last step of solution does not involve $G^{(\Omega^c)}, S^{(\Omega^c)}$ because the right-hand side is supported in Ω.

REMARK 2.1. Before describing more sophisticated generalizations, we show that this method can already be beneficial for *coefficient updates in disjoint locations.* If the problem can be modified in at most J subdomains denoted by $\{\Omega_j : j = 1, 2, \ldots, J\}$ with disjoint closure, then we choose $\Omega = \bigcup_j \Omega_j$ as their union. The solution update method can be described as:

1. Factorize L in Ω^c, and $\tilde{L}$ in each Ω_j.
2. Compute $\tilde{u} - u$ by multiplying (2.10) with $(L - \tilde{L})u$. Note that each operator for Ω is decoupled, for example,

$$T^{(\Omega)} = \mathrm{diag}(T^{(\Omega_1)}, T^{(\Omega_2)}, \ldots, T^{(\Omega_J)}),$$

   where diag() is used to denote a block diagonal matrix.

Because of the decoupled forms, the method is essentially still a one-level method and the level-one subdomains are $\Omega_1, \Omega_2, \ldots, \Omega_J$, and Ω^c.

2.2. Two-level method.

If a level-one subdomain Ω is partitioned further into two non-overlapping subdomains Ω_1, Ω_2, and coefficient updates may be restricted to one of the subdomains, then based on (2.10), there are three equivalent representations of the solution kernel:

$$\begin{aligned}
(2.11)\quad G^{(D)} &= \begin{pmatrix} G^{(\Omega)} & \\ & G^{(\Omega^c)} \end{pmatrix} - \begin{pmatrix} K^{(\Omega)} & \\ & K^{(\Omega^c)} \end{pmatrix} (M^{(\partial\Omega)})^{-1} \begin{pmatrix} S^{(\Omega)} & \\ & S^{(\Omega^c)} \end{pmatrix} \\
&= \begin{pmatrix} G^{(\Omega_1)} & \\ & G^{(\Omega_1^c)} \end{pmatrix} - \begin{pmatrix} K^{(\Omega_1)} & \\ & K^{(\Omega_1^c)} \end{pmatrix} (M^{(\partial\Omega_1)})^{-1} \begin{pmatrix} S^{(\Omega_1)} & \\ & S^{(\Omega_1^c)} \end{pmatrix} \\
&= \begin{pmatrix} G^{(\Omega_2)} & \\ & G^{(\Omega_2^c)} \end{pmatrix} - \begin{pmatrix} K^{(\Omega_2)} & \\ & K^{(\Omega_2^c)} \end{pmatrix} (M^{(\partial\Omega_2)})^{-1} \begin{pmatrix} S^{(\Omega_2)} & \\ & S^{(\Omega_2^c)} \end{pmatrix}.
\end{aligned}$$

One can observe that these three representations select the interior subdomain as Ω, Ω_1, and Ω_2 respectively. Here, we discuss the procedure to generate all the components in (2.11), and how to solve the problem by fast matrix-vector products of (2.11).

The direct method is based on the inherent dependencies among different subdomains. The set of subdomains has a partial order governed by the subset relation "$\subseteq$". The graph in Figure 2.1 visualizes the partial order, each edge of which starts from a subset and points to a superset. Three tree structures can be extracted from the graph in Figure 2.1, which are illustrated separately in Figure 2.2. According to the support of coefficient modifications, one of the tree structure can be selected to solve the problem:

- For modifications in Ω, the interior subdomain is Ω which contains Ω_1 and Ω_2, and the exterior subdomain is Ω^c;
- For modifications in Ω_1, the interior subdomain is Ω_1, and the exterior subdomain is Ω_1^c which contains Ω_2 and Ω^c;
- For modifications in Ω_2, the interior subdomain is Ω_2, and the exterior subdomain is Ω_2^c which contains Ω_1 and Ω^c.

For Ω, Ω_1^c, and Ω_2^c, each one contains two subdomains. Here, it is important to effectively combine the results from smaller subdomains.

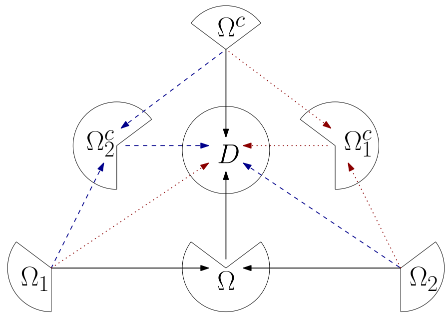


FIG. 2.1. *Graph structures of the two-level method in Section 2.2. The solid, dashed, and dotted edges give the three trees in Figure 2.2. The geometric relations are illustrated by the example of partitioning a disk into sectors.*

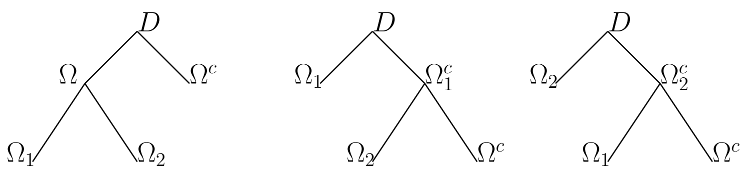


FIG. 2.2. *Tree structures extracted from Figure 2.1. The three trees have the same set of leaves:* $\Omega_1, \Omega_2, \Omega^c$.

We construct each component of (2.11) by factorizing the related interior and exterior problems. The three cases in (2.11) share a similar relation, but the formulas become more sophisticated because now Ω_1, Ω_2, and Ω^c have different shared boundaries. We define them as

$$\Gamma_0 = \partial\Omega_1 \cap \partial\Omega_2, \quad \Gamma_1 = \partial\Omega_1 \cap \partial\Omega, \quad \Gamma_2 = \partial\Omega_2 \cap \partial\Omega.$$

Similar to the derivation from (2.7) to (2.8), solution operators for Ω can be obtained from merging Ω_1 and Ω_2. The same transmission condition (2.7) is imposed on Γ_0, and we get

$$\begin{pmatrix} T_{0,0}^{(\Omega_1)} & -I & T_{0,1}^{(\Omega_1)} & 0 & S_{0,:}^{(\Omega_1)} & 0 \\ -I & T_{0,0}^{(\Omega_2)} & 0 & T_{0,2}^{(\Omega_2)} & 0 & S_{0,:}^{(\Omega_2)} \\ T_{1,0}^{(\Omega_1)} & 0 & T_{1,1}^{(\Omega_1)} & 0 & S_{1,:}^{(\Omega_1)} & 0 \\ 0 & T_{2,0}^{(\Omega_2)} & 0 & T_{2,2}^{(\Omega_2)} & 0 & S_{2,:}^{(\Omega_2)} \\ K_{:,0}^{(\Omega_1)} & 0 & K_{:,1}^{(\Omega_1)} & 0 & G^{(\Omega_1)} & 0 \\ 0 & K_{:,0}^{(\Omega_2)} & 0 & K_{:,2}^{(\Omega_2)} & 0 & G^{(\Omega_2)} \end{pmatrix} \begin{pmatrix} g_0^{(\Omega_1)} \\ g_0^{(\Omega_2)} \\ g_1^{(\Omega_1)} \\ g_2^{(\Omega_2)} \\ f^{(\Omega_1)} \\ f^{(\Omega_2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \hat{g}_1^{(\Omega_1)} \\ \hat{g}_2^{(\Omega_2)} \\ u^{(\Omega_1)} \\ u^{(\Omega_2)} \end{pmatrix}, \tag{2.12}$$

where $g_k^{(\Omega_m)}$ denotes the restriction of $g^{(\Omega_m)}$ on Γ_k, $T_{0,1}^{(\Omega_m)}$ denotes the restriction of $T^{(\Omega_m)}$ on $\Gamma_0 \times \Gamma_1$, the colon in the subscript means taking no restriction in the corresponding column or row set, and the other notation can be similarly understood. The first four block rows are rewritten from (2.4), and the transmission condition is substituted in the first two block rows. The last two block rows are from (2.3). The coupling between subdomains lies in the leading 2×2 block

$$M^{(\Gamma_0)} = \begin{pmatrix} T_{0,0}^{(\Omega_1)} & -I \\ -I & T_{0,0}^{(\Omega_2)} \end{pmatrix}. \tag{2.13}$$

The Schur complement of $M^{(\Gamma_0)}$ in (2.12) contains solution operators (2.5) for Ω, where

$$T^{(\Omega)} = \begin{pmatrix} T_{1,1}^{(\Omega_1)} & \\ & T_{2,2}^{(\Omega_2)} \end{pmatrix} - \begin{pmatrix} T_{1,0}^{(\Omega_1)} & \\ & T_{2,0}^{(\Omega_2)} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} T_{0,1}^{(\Omega_1)} & \\ & T_{0,2}^{(\Omega_2)} \end{pmatrix}, \tag{2.14}$$

$$S^{(\Omega)} = \begin{pmatrix} S_{1,:}^{(\Omega_1)} & \\ & S_{2,:}^{(\Omega_2)} \end{pmatrix} - \begin{pmatrix} T_{1,0}^{(\Omega_1)} & \\ & T_{2,0}^{(\Omega_2)} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} S_{0,:}^{(\Omega_1)} & \\ & S_{0,:}^{(\Omega_2)} \end{pmatrix}, \tag{2.15}$$

$$K^{(\Omega)} = \begin{pmatrix} K_{:,1}^{(\Omega_1)} & \\ & K_{:,2}^{(\Omega_2)} \end{pmatrix} - \begin{pmatrix} K_{:,0}^{(\Omega_1)} & \\ & K_{:,0}^{(\Omega_2)} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} T_{0,1}^{(\Omega_1)} & \\ & T_{0,2}^{(\Omega_2)} \end{pmatrix}, \tag{2.16}$$

$$G^{(\Omega)} = \begin{pmatrix} G^{(\Omega_1)} & \\ & G^{(\Omega_2)} \end{pmatrix} - \begin{pmatrix} K_{:,0}^{(\Omega_1)} & \\ & K_{:,0}^{(\Omega_2)} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} S_{0,:}^{(\Omega_1)} & \\ & S_{0,:}^{(\Omega_2)} \end{pmatrix}. \tag{2.17}$$

Again, we do not form $S^{(\Omega)}$, $K^{(\Omega)}$, and $G^{(\Omega)}$ explicitly because they can be much larger than the boundary map $T^{(\Omega)}$. (2.15)–(2.17) can be used to compute fast matrix-vector products instead.

For the exterior subdomain Ω_1^c, we merge Ω_2 and Ω^c with similar procedures. Using the transmission condition (2.7) on Γ_2, we have

$$T^{(\Omega_1^c)} = \begin{pmatrix} T_{0,0}^{(\Omega_2)} & \\ & T_{1,1}^{(\Omega^c)} \end{pmatrix} - \begin{pmatrix} T_{0,2}^{(\Omega_2)} & \\ & T_{1,2}^{(\Omega^c)} \end{pmatrix} (M^{(\Gamma_2)})^{-1} \begin{pmatrix} T_{2,0}^{(\Omega_2)} & \\ & T_{2,1}^{(\Omega^c)} \end{pmatrix}, \tag{2.18}$$

$$K^{(\Omega_1^c)} = \begin{pmatrix} K_{:,0}^{(\Omega_2)} & \\ & K_{:,1}^{(\Omega^c)} \end{pmatrix} - \begin{pmatrix} K_{:,2}^{(\Omega_2)} & \\ & K_{:,2}^{(\Omega^c)} \end{pmatrix} (M^{(\Gamma_2)})^{-1} \begin{pmatrix} T_{2,0}^{(\Omega_2)} & \\ & T_{2,1}^{(\Omega^c)} \end{pmatrix}, \tag{2.19}$$

where

$$M^{(\Gamma_2)} = \begin{pmatrix} T_{2,2}^{(\Omega_2)} & -I \\ -I & T_{2,2}^{(\Omega^c)} \end{pmatrix}. \tag{2.20}$$

Clearly, we can also merge Ω_1 and Ω^c by exchanging the role of Ω_1 and Ω_2 in (2.18)–(2.20).

Finally, for computing the solution, we develop tree-based algorithms built upon the leaf subdomains Ω_1, Ω_2, and Ω^c by substituting (2.13)–(2.20) into (2.11). For example, if the coefficient updates and the right-hand sides are supported in Ω_1, based on the second case of (2.11) the solution process is as follows.

1. Factorize the updated operator $\tilde{L}$ in Ω_1 for forming $\tilde{T}^{(\Omega_1)}$ and for computing matrix-vector products of $\tilde{S}^{(\Omega_1)}$, $\tilde{K}^{(\Omega_1)}$, and $\tilde{G}^{(\Omega_1)}$.
2. Solve the coupling system for $\partial\Omega_1$ using the second case of (2.11):
$$\begin{pmatrix} \tilde{T}^{(\Omega_1)} & -I \\ -I & T^{(\Omega_1^c)} \end{pmatrix} \begin{pmatrix} g^{(\Omega_1)} \\ g^{(\Omega_1^c)} \end{pmatrix} = \begin{pmatrix} -\tilde{S}^{(\Omega_1)} f^{(\Omega_1)} \\ 0 \end{pmatrix}.$$
3. Compute the solution in Ω_1 using (2.3):
$$u^{(\Omega_1)} = \tilde{G}^{(\Omega_1)} f^{(\Omega_1)} + \tilde{K}^{(\Omega_1)} g^{(\Omega_1)}.$$
4. Solve the coupling system for Γ_2:
$$M^{(\Gamma_2)} \begin{pmatrix} g_2^{(\Omega_2)} \\ g_2^{(\Omega^c)} \end{pmatrix} = \begin{pmatrix} -T_{2,0}^{(\Omega_2)} g_0^{(\Omega_1^c)} \\ -T_{2,1}^{(\Omega^c)} g_1^{(\Omega_1^c)} \end{pmatrix}.$$

5. Compute the solution in Ω_2 and Ω^c:

$$u^{(\Omega_2)} = K_{:,0}^{(\Omega_2)} g_0^{(\Omega_1^c)} + K_{:,2}^{(\Omega_2)} g_2^{(\Omega_2)},$$
$$u^{(\Omega^c)} = K_{:,1}^{(\Omega^c)} g_1^{(\Omega_1^c)} + K_{:,2}^{(\Omega^c)} g_2^{(\Omega^c)}.$$

In steps 4 and 5, $K^{(\Omega_1^c)} g^{(\Omega_1^c)}$ is computed using (2.19). This two-level process illustrates the capability of dealing with coefficient updates of different volumes. The results of this section provide key components of the general hierarchical algorithms in Section 3.

3. General hierarchical algorithms.

In this section, we write the complete hierarchical algorithms for solving coefficient update problems. In particular, we focus on generalizing the two-level method in Section 2.2 to a constructive multi-level method. The multi-level method involves the tree-based domain partitioning. Comparing with simpler alternatives in Section 2, the multi-level method is more flexible because it supports updates in any subdomain used in the domain partitioning, and is more efficient because the computational cost is minimized by isolating the smallest subdomains containing the coefficient updates. Besides a factorization update in subdomains, the major steps include: introduction of exterior subdomains in the domain partitioning, factorization of interior and exterior problems, and solution update with localized right-hand sides.

3.1. Transformation of binary domain partitioning.

First, we describe the structures of the domain partitioning when exterior subdomains are introduced. The computational domain D is partitioned hierarchically following a tree denoted by $\mathcal{T}$. For notational simplicity, we restrict the discussion to binary trees. If i is the parent node of c_1 and c_2 in the tree $\mathcal{T}$, then the open subdomain $\Omega_i \subset D$ is partitioned into two open subdomains Ω_{c_1} and Ω_{c_2} such that

$$\Omega_{c_1} \cap \Omega_{c_2} = \emptyset, \quad \overline{\Omega_i} = \overline{\Omega_{c_1} \cup \Omega_{c_2}}. \tag{3.1}$$

According to Figure 2.1, for the interior problems, each parent i depends on the children c_1 and c_2; for the exterior domains, $\Omega_{c_1}^c$ can be partitioned into Ω_i^c and Ω_{c_2}, and $\Omega_{c_2}^c$ can be partitioned into Ω_i^c and Ω_{c_1}. The partitioning of exterior subdomains is well defined in the sense of (3.1) because of the following lemma.

LEMMA 3.1. *If Ω_i, Ω_{c_1}, and Ω_{c_2} are open subdomains of D satisfying (3.1), then*

$$\Omega_i^c \cap \Omega_{c_2} = \emptyset, \quad \overline{\Omega_{c_1}^c} = \overline{\Omega_i^c \cup \Omega_{c_2}}, \tag{3.2}$$

where Ω_j^c represents $D \setminus \overline{\Omega_j}$ for each $j \in \{i, c_1, c_2\}$.

Proof. $\overline{\Omega_i} \supset \overline{\Omega_{c_2}}$ from (3.1), so

$$\Omega_i^c \cap \Omega_{c_2} = (D \setminus \overline{\Omega_i}) \cap \Omega_{c_2} \subset (D \setminus \overline{\Omega_{c_2}}) \cap \Omega_{c_2} = \emptyset.$$

The open sets Ω_{c_1} and Ω_{c_2} have empty intersection, so

$$\overline{\Omega_{c_1}} \cap \Omega_{c_2} = \emptyset, \quad \Omega_{c_2} \subset D \setminus \overline{\Omega_{c_1}} = \Omega_{c_1}^c.$$

$\overline{\Omega_i^c \cup \Omega_{c_2}} \subset \overline{\Omega_{c_1}^c}$ because $\Omega_i^c \subset \Omega_{c_1}^c$ and $\Omega_{c_2} \subset \Omega_{c_1}^c$. $\overline{\Omega_{c_1}^c} \subset \overline{\Omega_i^c \cup \Omega_{c_2}}$ because

$$\Omega_{c_1}^c = D \setminus \overline{\Omega_{c_1}} \subset D \setminus (\overline{\Omega_i} \setminus \overline{\Omega_{c_2}}) \subset (D \setminus \overline{\Omega_i}) \cup \overline{\Omega_{c_2}} = \Omega_i^c \cup \overline{\Omega_{c_2}}. \qquad \square$$

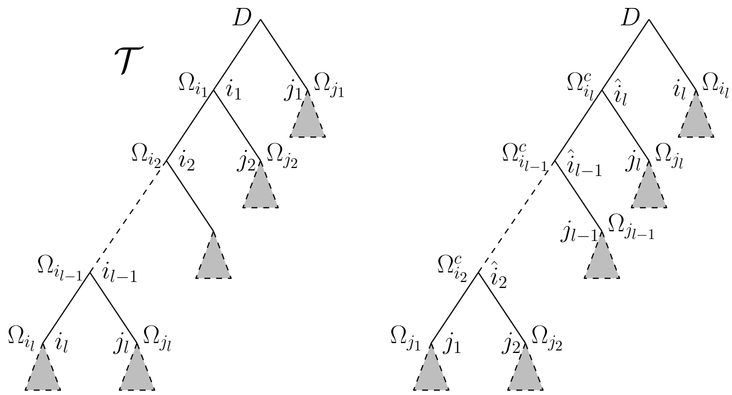


FIG. 3.1. *Transformation between trees of subdomains. Left panel: the original tree $\mathcal{T}$ with the associated subdomains; Right panel: the new tree for localized solution in Ω_{i_l}.*

Suppose the problem is modified in Ω_p for a level-l node p. Write the path from the root i_0 to p as $i_0 \to i_1 \to \cdots \to i_l = p$, so $\Omega_{i_0} \supset \Omega_{i_1} \supset \cdots \supset \Omega_{i_l} = \Omega_p$. Therefore, modifications in Ω_p not only lead to changes in the subtree generated by p, but also propagate along the path to the root. The goal here is to reorganize the domain partitioning such that p is a child of the root, then changes in Ω_p do not propagate to multiple larger subdomains. Denote i_k's sibling by j_k for $1 \le k \le l$. See the left panel of Figure 3.1 for the illustration of i_k, j_k in $\mathcal{T}$. Denote $\hat{i}_k$ the new node associated with the exterior subdomain

$$\Omega_{\hat{i}_k} = \Omega^c_{i_k}, \quad 1 < k \le l. \tag{3.3}$$

We construct the new binary domain partitioning step by step:

1. For the root node i_0, let i_l, $\hat{i}_l$ be its children. From (3.3), one can check that
$$\Omega_{i_l} \cap \Omega^c_{i_l} = \emptyset, \quad \overline{\Omega_{i_0}} = \overline{\Omega_{i_l} \cup \Omega^c_{i_l}}.$$
We preserve the partitioning in Ω_{i_l}, and continue with the new node $\hat{i}_l$.
2. For the node $\hat{i}_k$ with $k \in \{l, l-1, \ldots, 3\}$, let j_k, $\hat{i}_{k-1}$ be $\hat{i}_k$'s children. Since i_{k-1} is the parent of i_k, j_k in $\mathcal{T}$, we have from (3.2)–(3.3) that
$$\Omega^c_{i_{k-1}} \cap \Omega_{j_k} = \emptyset, \quad \overline{\Omega^c_{i_k}} = \overline{\Omega^c_{i_{k-1}} \cup \Omega_{j_k}},$$
which means the partitioning from $\hat{i}_k$ to j_k, $\hat{i}_{k-1}$ is well defined. We preserve the partitioning in Ω_{j_k} and continue with the new node $\hat{i}_{k-1}$.
3. For the node $\hat{i}_2$, let j_1, j_2 be its children. From (3.2) and noticing that $\Omega_{j_1} = \Omega^c_{i_1}$, we have
$$\Omega_{j_1} \cap \Omega_{j_2} = \emptyset, \quad \overline{\Omega^c_{i_2}} = \overline{\Omega_{j_1} \cup \Omega_{j_2}}.$$
The partitioning in Ω_{j_1} or Ω_{j_2} is preserved.

The new binary tree is visualized in the right panel of Figure 3.1. The new tree can be constructed in $O(l)$ operations, because $l-1$ nodes are removed and $l-1$ nodes are introduced. From the construction process, we see that the new elements $\{\hat{i}_k\}$ are not leaf nodes. That is to say, every exterior subdomain introduced here is a union of existing interior subdomains. The key results are summarized into the following theorem.

THEOREM 3.2. *Given a binary tree $\mathcal{T}$, let $\{\Omega_i : i \in \mathcal{T}\}$ be a binary domain partitioning satisfying* (3.1)*. For a non-root level-l node $p \in \mathcal{T}$, there exists a well-defined binary domain partitioning such that*

1. *Ω_p is a child subdomain of D,*
2. *the elements of $\{\Omega_i : i$ is an ancestor of p in $\mathcal{T}, 1 \leq \text{level}(i) < l\}$ are removed,*
3. *the elements of $\{\Omega_i^c : i$ is an ancestor of p in $\mathcal{T}, 1 < \text{level}(i) \leq l\}$ are inserted,*
4. *every new element cannot be a leaf in the new binary partitioning.*

The new domain partitioning is used to isolate the perturbations in Ω_p, because the level-one subdomains are precisely Ω_p and Ω_p^c. Then, according to the solution operator (2.10), the interior problem in Ω_p needs to be re-factorized, but the exterior problem in Ω_p^c remains the same.

3.2. Hierarchical factorization and solution update. Inspired by the two-level example in Section 2.2, we describe the family of hierarchical algorithms needed for solving coefficient update problems, including the factorization and solution of interior and exterior problems. The major novelties are the hierarchical algorithms of exterior problems.

The factorization of interior problems follows a bottom-up (postordered) traversal of the tree $\mathcal{T}$. If the node i is a leaf, we factorize the discretized PDE (2.1) in Ω_i to obtain the matrices defined in (2.3)–(2.4). If i has children, then the boundary map $T^{(\Omega_i)}$ can be constructed from those at its children using (2.14). The construction of interior boundary maps has been developed in [13, 21]. Since the process is the foundation of exterior problems and factorization update, we review this result in Algorithm 3.1, FACINT, using the notation in this paper.

The construction of exterior boundary maps follows a top-down (reverse postordered) traversal of $\mathcal{T}$. The major difference from computing interior boundary maps is that the *data dependency is reversed*. For the node i with children c_1, c_2, we have $\Omega_{c_1}, \Omega_{c_2} \subset \Omega_i$ for the interior problems, but $\Omega_{c_1}^c, \Omega_{c_2}^c \supset \Omega_i^c$ for the exterior ones. Based on (2.18), we construct $T^{(\Omega_{c_1}^c)}$ from $T^{(\Omega_i^c)}, T^{(\Omega_{c_2})}$ and construct $T^{(\Omega_{c_2}^c)}$ from $T^{(\Omega_i^c)}, T^{(\Omega_{c_1})}$. This process is described in Algorithm 3.2, FACEXT.

For the coefficient update problem (1.3), recall that the coefficient update and the right-hand side are supported in the same subdomain Ω_p for some $p \in \mathcal{T}$. According to the solution process at the end of Section 2.2, the major steps include: re-factorization in Ω_p, computing boundary sources on the boundary $\partial\Omega_p$, and extracting the solution inside and outside Ω_p. This is Algorithm 3.4, SOLINT–SOLEXT.

In SOLINT, the modified operator $\tilde{L}$ in Ω_p is factorized and the solution in Ω_p is computed via (2.3). It is essentially a local version of the solution algorithm presented in [21]. The matrix-vector products governed by (2.15)–(2.17) are carefully combined based on the superposition principle. Inside Ω_p, each subdomain is visited twice by a postordered and a reverse postordered traversal.

SOLEXT extends the solution to the exterior subdomain Ω_p^c by solving a boundary value problem using $K^{(\Omega_p^c)} g^{(\Omega_p^c)}$. It has a top-down traversal of the new domain partitioning inside Ω_p^c defined in Theorem 3.2. For the matrix-vector product of $K^{(\Omega_p^c)}$, (2.19) replaces (2.16) if there are exterior subdomains involved. At each step, we get the solution of a subdomain along the path from p to the root of $\mathcal{T}$, and the cost increases for high-level problems. The algorithm can be terminated in the middle once the desired part of the solution is computed.

In general, it *does not need to know which subdomain is going to be changed* in FACEXT, and its output can handle coefficient updates in any subdomain of the domain partitioning. If we have additional information about p, the cost and storage can be further reduced by only calculating the exterior factors related to p. As can be seen in Theorem 3.2 and SOLEXT, the related nodes correspond to the ancestors of p. Table 3.1 lists the roles and properties of the routines.

TABLE 3.1
Major properties of the hierarchical factorization and solution algorithms.

Name	Description	Type of traversal	Equation
FACINT	Factorize interior problems	Postorder	(2.14)
FACEXT	Factorize exterior problems	Reverse postorder	(2.18)
SOLINT	Solve interior problems	Postorder, reverse postorder	(2.15)–(2.17)
SOLEXT	Solve exterior problems	Reverse postorder of new tree	(2.19)

Algorithm 3.1 Factorization of interior problems (review of the result in [21])

procedure FACINT($\mathcal{T}, L$)
  for each $i \in \mathcal{T}$ following the postordered traversal **do**
    if i is a leaf **then**
      Factorize L in Ω_i for $T^{(\Omega_i)}, S^{(\Omega_i)}$ in (2.4) and $K^{(\Omega_i)}, G^{(\Omega_i)}$ in (2.3)
    else
      $(c_1, c_2) \leftarrow i$'s children
      $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
      Factorize $M^{(\Gamma_0)} = \begin{pmatrix} T_{0,0}^{(\Omega_{c_1})} & -I \\ -I & T_{0,0}^{(\Omega_{c_2})} \end{pmatrix}$ where $T_{j,k}^{(\Omega_m)} := T^{(\Omega_m)}|_{\Gamma_j \times \Gamma_k}$
      Based on (2.14), compute $T^{(\Omega_i)}$ via

$$\begin{pmatrix} T_{1,1}^{(\Omega_{c_1})} & \\ & T_{2,2}^{(\Omega_{c_2})} \end{pmatrix} - \begin{pmatrix} T_{1,0}^{(\Omega_{c_1})} & \\ & T_{2,0}^{(\Omega_{c_2})} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} T_{0,1}^{(\Omega_{c_1})} & \\ & T_{0,2}^{(\Omega_{c_2})} \end{pmatrix}$$

    end if
  end for
  return $T^{(\Omega_i)}$, factors of $M^{(\Omega_i)}$, and for leaf nodes i, $S^{(\Omega_i)}, K^{(\Omega_i)}, G^{(\Omega_i)}$
end procedure

In summary, we suggest the following calling sequence for solving coefficient update problems:

1. SOLINT($\mathcal{T}, i_0, L, f, \dots$) for factorizing L and solving $Lu = f$, where i_0 is the root of $\mathcal{T}$;
2. FACEXT($\mathcal{T}, \dots$) for factorizing exterior problems;
3. SOLINT($\mathcal{T}, p, \tilde{L}, (L - \tilde{L})u, \dots$) for the solution update $\tilde{u} - u$ in Ω_p and the exterior boundary source $g^{(\Omega_p^c)}$;
4. SOLEXT($\mathcal{T}, p, g^{(\Omega_p^c)}, \dots$) for the solution update $\tilde{u} - u$ in Ω_p^c.

Note that the solution steps (1, 3, and 4) can be trivially extended for solving multiple right-hand sides. Before giving the complexity estimates in Section 4, there are several qualitative arguments about the cost effectiveness of this family of algorithms. The factorization of exterior problems does not increase the order of factorization

Algorithm 3.2 Factorization of exterior problems

procedure FACEXT($\mathcal{T}, T^{(*)}$)
  for each $i \in \mathcal{T}$ following a reverse postordered traversal **do**
    if i is not a leaf **then**
      $(c_1, c_2) \leftarrow i$'s children
      $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
      Factorize $M^{(\Gamma_j)} = \begin{pmatrix} T_{j,j}^{(\Omega_{c_j})} & -I \\ -I & T_{j,j}^{(\Omega_i^c)} \end{pmatrix}$, $j \in \{1, 2\}$
      Based on (2.18), compute $T^{(\Omega_{c_1}^c)}$ via

$$\begin{pmatrix} T_{0,0}^{(\Omega_{c_2})} & \\ & T_{1,1}^{(\Omega_i^c)} \end{pmatrix} - \begin{pmatrix} T_{0,2}^{(\Omega_{c_2})} & \\ & T_{1,2}^{(\Omega_i^c)} \end{pmatrix} (M^{(\Gamma_2)})^{-1} \begin{pmatrix} T_{2,0}^{(\Omega_{c_2})} & \\ & T_{2,1}^{(\Omega_i^c)} \end{pmatrix}$$

      Compute $T^{(\Omega_{c_2}^c)}$ via

$$\begin{pmatrix} T_{0,0}^{(\Omega_{c_1})} & \\ & T_{2,2}^{(\Omega_i^c)} \end{pmatrix} - \begin{pmatrix} T_{0,1}^{(\Omega_{c_1})} & \\ & T_{2,1}^{(\Omega_i^c)} \end{pmatrix} (M^{(\Gamma_1)})^{-1} \begin{pmatrix} T_{1,0}^{(\Omega_{c_1})} & \\ & T_{1,2}^{(\Omega_i^c)} \end{pmatrix}$$

    end if
  end for
  return $T^{(*)}$ and factors of $M^{(*)}$
end procedure

complexity, because the cost depends on the sizes of boundaries $\{\partial\Omega_i\}$ in the same way as existing factorization of interior problems. The cost of the re-factorization step is low because it only depends on the local problem size in Ω_p. The cost of solution is low if terminated early because Algorithm 3.4 visits smaller subdomains first.

4. Algorithmic complexity.

4. Algorithmic complexity. In this section, we estimate the complexity of the algorithms presented in Section 3. The major components of our method includes: a precomputation step that constructs interior and exterior boundary maps of the reference problem, a factorization update step that modifies the factors of an interior problem, and a solution update step to get the final solution.

The complexity of the solution algorithms relies on the quality of the domain partitioning. For an $n \times n$ discretized linear system from a d-dimensional elliptic problem ($d = 2$ or 3). The following assumption is used to obtain an optimal complexity.

ASSUMPTION 4.1. Let $\mathcal{T}$ be a complete binary tree containing $\mathbf{l}$ levels. Each level-k subdomain of the domain partitioning $\{\Omega_i : i \in \mathcal{T}\}$ contains $O(n_k)$ interior unknowns and $O(m_k)$ boundary unknowns, where

$$n_k = 2^{-k} n, \quad m_k = n_k^{(d-1)/d}.$$

Furthermore, let $n_{\mathbf{l}} = O(1)$. Here, the constants in the big O notation are assumed to be uniformly bounded.

REMARK 4.1. The condition on n_k and m_k requires that the domain partitioning is balanced. The fractional power in m_k comes from the dimension reduction from a d-dimensional domain to a $(d-1)$-dimensional boundary.

Algorithm 3.3 Matrix-vector multiplications of $S^{(\Omega)}$ and $K^{(\Omega)}$ in (2.5)

procedure SMVINT$(\mathcal{T}, f, S^{(*)}, T^{(*)}, M^{(*)})$ ▷ Compute $\hat{g}^{(\Omega_i)} = S^{(\Omega_i)} f^{(\Omega_i)}$
  for each $i \in \mathcal{T}$ following the postordered traversal **do**
    if i is a leaf **then**
      $\hat{g}^{(\Omega_i)} \leftarrow S^{(\Omega_i)} f^{(\Omega_i)}$
    else
      $(c_1, c_2) \leftarrow i$'s children
      $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
      Based on (2.15), compute

$$\hat{g}^{(\Omega_i)} \leftarrow \begin{pmatrix} \hat{g}_1^{(\Omega_{c_1})} \\ \hat{g}_2^{(\Omega_{c_2})} \end{pmatrix} - \begin{pmatrix} T_{1,0}^{(\Omega_{c_1})} & \\ & T_{2,0}^{(\Omega_{c_2})} \end{pmatrix} (M^{(\Gamma_0)})^{-1} \begin{pmatrix} \hat{g}_0^{(\Omega_{c_1})} \\ \hat{g}_0^{(\Omega_{c_2})} \end{pmatrix}$$

    end if
  end for
  return $\hat{g}^{(*)}$
end procedure

procedure KMVINT$(\mathcal{T}, g, K^{(*)}, T^{(*)}, M^{(*)})$ ▷ Compute $K^{(\Omega_i)} g^{(\Omega_i)}$
  for each $i \in \mathcal{T}$ following a reverse postordered traversal **do**
    if i is a leaf **then**
      $u|_{\Omega_i} \leftarrow K^{(\Omega_i)} g^{(\Omega_i)}$
    else
      $(c_1, c_2) \leftarrow i$'s children
      $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
      Based on (2.16), compute

$$\begin{pmatrix} g_0^{(\Omega_{c_1})} \\ g_0^{(\Omega_{c_2})} \end{pmatrix} \leftarrow (M^{(\Gamma_0)})^{-1} \begin{pmatrix} -T_{0,1}^{(\Omega_{c_1})} g_1^{(\Omega_i)} \\ -T_{0,2}^{(\Omega_{c_2})} g_2^{(\Omega_i)} \end{pmatrix}$$

      $g_1^{(\Omega_{c_1})} \leftarrow g_1^{(\Omega_i)}, \quad g_2^{(\Omega_{c_2})} \leftarrow g_2^{(\Omega_i)}$
    end if
  end for
  return u
end procedure

If boundary maps are stored as dense matrices, then according to (2.14) and (2.18), the precomputation of interior and exterior boundary maps has dense factorizations and multiplications at every node. The complexity $\mathcal{C}_{\text{pre}}$ and the storage $\mathcal{S}_{\text{pre}}$ are respectively

$$\begin{aligned} \mathcal{C}_{\text{pre}} &= \sum_{k=0}^{1} 2^k O\left(m_k^3\right) = \begin{cases} O(n^{3/2}) & \text{in 2D}, \\ O(n^2) & \text{in 3D}, \end{cases} \\ \mathcal{S}_{\text{pre}} &= \sum_{k=0}^{1} 2^k O\left(m_k^2\right) = \begin{cases} O(n \log n) & \text{in 2D}, \\ O(n^{4/3}) & \text{in 3D}. \end{cases} \end{aligned} \tag{4.1}$$

The results are in the same orders as those in the direct factorization of sparse matrices

Algorithm 3.4 Solution update with modified coefficients in Ω_p

procedure $\mathsf{SOLINT}(\mathcal{T}, p, \tilde{L}, f, T^{(\Omega_p^c)})$ ▷ *Solution in* $\overline{\Omega_p}$
    $\tilde{\mathcal{T}} \leftarrow \text{subtree}(p)$ ▷ *Subtree of* $\mathcal{T}$ *with root* p
    $\mathsf{FACINT}(\tilde{\mathcal{T}}, \tilde{L})$ for $\tilde{T}^{(*)}, \tilde{S}^{(*)}, \tilde{K}^{(*)}, \tilde{G}^{(*)}, \tilde{M}^{(*)}$ in Ω_p
    $\hat{g}^{(*)} \leftarrow \mathsf{SMVINT}(\tilde{\mathcal{T}}, f, \tilde{S}^{(*)}, \tilde{T}^{(*)}, \tilde{M}^{(*)})$ ▷ $\tilde{S}^{(\Omega_p)} f^{(\Omega_p)}$ via Algorithm 3.3
    Based on (2.10), solve

$$\begin{pmatrix} \tilde{T}^{(\Omega_p)} & -I \\ -I & T^{(\Omega_p^c)} \end{pmatrix} \begin{pmatrix} g^{(\Omega_p)} \\ g^{(\Omega_p^c)} \end{pmatrix} = \begin{pmatrix} -\hat{g}^{(\Omega_p)} \\ 0 \end{pmatrix}$$

    for each $i \in \tilde{\mathcal{T}}$ following a reverse postordered traversal **do**
    ▷ $u^{(\Omega_p)} = \tilde{G}^{(\Omega_p)} f^{(\Omega_p)} + \tilde{K}^{(\Omega_p)} g^{(\Omega_p)}$
        if i is a leaf **then**
            $u^{(\Omega_p)}|_{\Omega_i} \leftarrow \tilde{G}^{(\Omega_i)} f^{(\Omega_i)} + \tilde{K}^{(\Omega_i)} g^{(\Omega_i)}$
        else
            $(c_1, c_2) \leftarrow i$'s children
            $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
            Based on (2.16)–(2.17), compute

$$\begin{pmatrix} g_0^{(\Omega_{c_1})} \\ g_0^{(\Omega_{c_2})} \end{pmatrix} \leftarrow -(\tilde{M}^{(\Gamma_0)})^{-1} \begin{pmatrix} \hat{g}_0^{(\Omega_{c_1})} + \tilde{T}_{0,1}^{(\Omega_{c_1})} g_1^{(\Omega_i)} \\ \hat{g}_0^{(\Omega_{c_2})} + \tilde{T}_{0,2}^{(\Omega_{c_2})} g_2^{(\Omega_i)} \end{pmatrix}$$

            $g_1^{(\Omega_{c_1})} \leftarrow g_1^{(\Omega_i)}, \quad g_2^{(\Omega_{c_2})} \leftarrow g_2^{(\Omega_i)}$
        end if
    end for
    return $u^{(\Omega_p)}, g^{(\Omega_p^c)}$
end procedure

procedure $\mathsf{SOLEXT}(\mathcal{T}, p, g^{(\Omega_p^c)}, K^{(*)}, T^{(*)}, M^{(*)})$
▷ Solution in Ω_p^c via $K^{(\Omega_p^c)} g^{(\Omega_p^c)}$
    $c_1 \leftarrow p$
    while c_1 is not the root **do**
        $c_2 \leftarrow c_1$'s sibling, $i \leftarrow c_1$'s parent
        $\Gamma_0 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_{c_2}$, $\Gamma_1 \leftarrow \partial\Omega_{c_1} \cap \partial\Omega_i$, $\Gamma_2 \leftarrow \partial\Omega_{c_2} \cap \partial\Omega_i$
        Based on (2.19), compute

$$\begin{pmatrix} g_2^{(\Omega_{c_2})} \\ g_2^{(\Omega_i^c)} \end{pmatrix} \leftarrow -(M^{(\Gamma_2)})^{-1} \begin{pmatrix} T_{2,0}^{(\Omega_{c_2})} & \\ & T_{2,1}^{(\Omega_i^c)} \end{pmatrix} g^{(\Omega_{c_1}^c)}$$

        $\tilde{\mathcal{T}} \leftarrow \text{subtree}(c_2)$
        $u^{(\Omega_p^c)}|_{\Omega_{c_2}} = \mathsf{KMVINT}(\tilde{\mathcal{T}}, g^{(\Omega_{c_2})}, K^{(*)}, T^{(*)}, M^{(*)})$
        ▷ $K^{(\Omega_{c_2})} g^{(\Omega_{c_2})}$ via Algorithm 3.3
        $c_1 \leftarrow i$
    end while
    return $u^{(\Omega_p^c)}$
end procedure

with nested dissection reordering.

Consider modifying the problem in some level-l subdomain Ω_p containing $O(n_l)$ interior unknowns. The subtree corresponding to Ω_p has $(\mathbf{l}-l)$ levels. The complexity $\mathcal{C}_{\text{upd}}$ and storage $\mathcal{S}_{\text{upd}}$ of local factorization update are respectively

$$\begin{aligned} \mathcal{C}_{\text{upd}} &= \sum_{k=0}^{\mathbf{l}-l} 2^k O\left(m_{k+l}^3\right) = \begin{cases} O(n_l^{3/2}) & \text{in 2D,} \\ O(n_l^2) & \text{in 3D,} \end{cases} \\ \mathcal{S}_{\text{upd}} &= \sum_{k=0}^{\mathbf{l}-l} 2^k O\left(m_{k+l}^2\right) = \begin{cases} O(n_l \log n_l) & \text{in 2D,} \\ O(n_l^{4/3}) & \text{in 3D.} \end{cases} \end{aligned} \tag{4.2}$$

Observe that $\mathcal{C}_{\text{upd}}$ and $\mathcal{S}_{\text{upd}}$ only depend on the number of interior unknowns in Ω_p.

In comparison, we consider the naive factorization update method which changes the factors following the original data dependencies in $\mathcal{T}$. In addition to the refactorization in Ω_p that has complexity $\mathcal{C}_{\text{upd}}$ in (4.2), the naive method has an additional step which updates every ancestor of p. This additional step costs

$$\begin{aligned} \mathcal{C}_{\text{anc}} &= \sum_{k=0}^{l-1} O\left(m_k^3\right) = \begin{cases} O(n^{3/2}) & \text{in 2D,} \\ O(n^2) & \text{in 3D,} \end{cases} \\ \mathcal{S}_{\text{anc}} &= \sum_{k=0}^{l-1} O\left(m_k^2\right) = \begin{cases} O(n) & \text{in 2D,} \\ O(n^{4/3}) & \text{in 3D.} \end{cases} \end{aligned} \tag{4.3}$$

This additional cost, on the contrary, is primarily determined by n because the ancestors of p have larger and larger matrix sizes. The proposed new method reduces the cost from $\mathcal{C}_{\text{anc}} + \mathcal{C}_{\text{upd}}$ to $\mathcal{C}_{\text{upd}}$. *If $n_l \ll n$, then the new method avoided the dominant cost (4.3) that is comparable to the cost (4.1) for re-factorizing the entire problem.*

The solution update in Algorithm 3.4 has the solution in Ω_p and Ω_p^c, and the computational cost is proportional to the memory access. The solution complexity is $\mathcal{S}_{\text{upd}}$ in Ω_p, and is $\mathcal{S}_{\text{pre}}$ in Ω_p^c. If the exterior solution is terminated early, then the total cost can be as low as $\mathcal{S}_{\text{upd}}$.

As a summary, the following theorem describes the complexity of the proposed algorithms.

THEOREM 4.1. *Let the domain partitioning satisfy Assumption 4.1. The cost of precomputation in Algorithm 3.1 (*FACINT*) and Algorithm 3.2 (*FACEXT*) is governed by the matrix size via (4.1). The cost of factorization update is (4.2), which only depends on the size of the updated subdomain.*

5. Numerical tests.

In this section, we check how the cost of our direct method scales with respect to the size of the computational domain and the support of the coefficient update. The method is able to solve general elliptic problems with coefficient updates. A particular problem of interest is the variable-coefficient Helmholtz equation

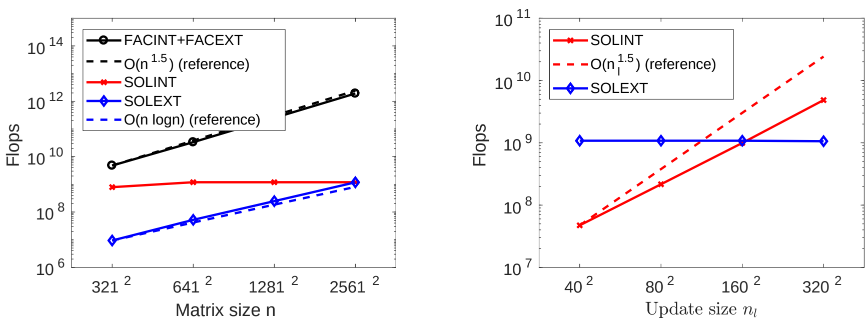
$$-\Delta u(x) - k^2(x)u(x) = f(x),$$

where $k(x)$ is the wavenumber that may be updated in various applications. The solution algorithms are implemented in MATLAB, and are run in serial on a Linux workstation with 3.5GHz CPU and 64GB RAM.

In two dimensional space, we discretize the Helmholtz equation by a continuous Galerkin method with fourth-order nodal bases. The performance of the direct method is mostly determined by the matrix size and sparsity pattern. The matrix size equals the number of nodals in the domain, and high-order schemes usually lead to more nonzeros. We update the wavenumber in a subdomain close to the center of the computational domain, and the magnitude of the update is as large as 1/2 of the original wavenumber.

If we enlarge the computational domain and increase n while fixing the size of the modified subdomain, the test results are listed in Table 5.1 and plotted in Figure 5.1(a). As estimated by (4.1), the factorizations of the interior problems (Algorithm 3.1) and the exterior problems (Algorithm 3.2) share the same order of complexity. Direct factorizations contribute to the major computational cost and storage of the method. Algorithm 3.4 (SOLINT) contains the re-factorization and solution in the modified subdomain, and the cost does not depend on the matrix n. Algorithm 3.4 (SOLEXT) is the solution in the exterior subdomain, and the cost depends approximately linearly on n. Such complexity is consistent with our estimate.

For the largest computational domain with n fixed, we also vary the size n_l of the modified subdomain. The results are listed in Table 5.2 and plotted in Figure 5.1(b). The cost of SOLINT is dominated by the direct factorization in the modified subdomain. The dependence on n_l as illustrated in Figure 5.1(b) is a little better than the estimate in (4.2). The cost of SOLEXT does not increase because n is fixed.



(a) *Flops of Table 5.1* (b) *Flops of Table 5.2*

FIG. 5.1. *Scaling plots.*

These test results demonstrate that the proposed algorithms are capable of solving the challenging cases where the coefficient updates have large magnitude and support. The algorithms can accommodate large amounts of modifications fairly easily. In addition, the solution update algorithms produce high accuracies as in stand-alone direct solvers and no approximation is made.

We would also like to mention that, the large magnitude and support of the updates make the modified problems no longer close to the reference problem. This situation is handled efficiently with our algorithms, but causes troubles to standard methods such as iterative solvers using the factorization of the reference problem as a preconditioner. To verify this, we reuse the factorization of the reference problem as a preconditioner to solve the four matrices considered in Table 5.2. This preconditioner quickly losses effectiveness when the modified subdomain increases its size. It takes 32, 180, 717, and 2585 preconditioned GMRES iterations respectively to reach the relative residual accuracy 10^{-5}.

TABLE 5.1

Test for increasing matrix sizes n with a fixed modified subdomain size ($n_l = 160^2$). The updated solution u is compared with a stand-alone direct solution v, and the relative ℓ_p-distance is $\|u - v\|_p / \|v\|_p$.

(a) *Problem setup*

#nodals	321^2	641^2	1281^2	2561^2
Matrix size	103,041	410,881	1,640,961	6,558,721
#non-zeros	2,437,184	9,748,736	38,994,944	155,979,776

(b) *Factorization of interior problems*

Time	1.77s	7.70s	33.10s	156.30s
Flops	$3.11E9$	$1.58E10$	$8.93E10$	$5.62E11$
Factor storage	$9.03E6$	$4.65E7$	$2.31E8$	$1.11E9$

(c) *Factorization of exterior problems*

Time	0.52s	3.75s	25.02s	170.29s
Flops	$1.66E9$	$1.75E10$	$1.62E11$	$1.35E12$
Factor storage	$3.87E6$	$2.56E7$	$1.46E8$	$7.66E8$

(d) *Solution of the reference problem*

Time	0.08s	0.32s	1.39s	7.08s
Flops	$2.52E7$	$1.11E8$	$4.83E8$	$2.10E9$

(e) *Solution update after modifying* 160^2 *nodals*

SOLINT time	0.46s	0.56s	0.58s	0.67s
SOLINT flops	$7.90E8$	$1.19E9$	$1.19E9$	$1.19E9$
SOLEXT time	0.03s	0.14s	0.63s	2.89s
SOLEXT flops	$9.34E6$	$5.21E7$	$2.47E8$	$1.18E9$
Relative ℓ_2-distance	$4.74E-16$	$5.95E-16$	$6.88E-16$	$6.75E-16$
Relative ℓ_∞-distance	$1.20E-15$	$1.34E-15$	$9.89E-16$	$7.81E-16$

TABLE 5.2

Test for a fixed matrix size (2561^2) and increasing modified subdomain sizes.

Modified nodals	40^2	80^2	160^2	320^2
SOLINT time	0.12s	0.14s	0.47s	1.86s
SOLINT flops	$4.73E7$	$2.16E8$	$9.94E8$	$4.85E9$
SOLEXT time	2.93s	2.52s	2.50s	2.47s
SOLEXT flops	$1.08E9$	$1.08E9$	$1.08E9$	$1.06E9$
Relative ℓ_2-distance	$3.76E-16$	$5.06E-16$	$6.75E-16$	$8.02E-16$
Relative ℓ_∞-distance	$7.31E-16$	$6.40E-16$	$7.81E-16$	$8.78E-16$

6. Conclusions. We developed a new framework for updating the factorization of discretized elliptic operators. A major significance is the hierarchical construction of exterior boundary maps. For each modified operator, we only need to update the factorization for locations where the coefficients are updated, and the locations of coefficient update are allowed to change to different subdomains. Tree-based algorithms were given for solving the interior and exterior problems. The complexity estimates and the scaling test based on the Helmholtz equation show that the cost of factorization update only depends on the size of the modified subdomain and that the solution update cost is much faster than the standard direct solution algorithms. The solution update algorithms produce high accuracies as in expensive stand-alone direct solvers The method is suitable for solving the challenging cases where the updates have large magnitude and support.

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