A boundary collocation meshfree method for the treatment of Poisson problems with complex morphologies

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\section*{ABSTRACT}

A new meshfree method based on a discrete transformation of Green's basis functions is introduced to simulate Poisson problems with complex morphologies. The proposed Green's Discrete Transformation Method (GDTM) uses source points that are located along a virtual boundary outside the problem domain to construct the basis functions needed to approximate the field. The optimal number of Green's functions source points and their relative distances with respect to the problem boundaries are evaluated to obtain the best approximation of the partition of unity condition. A discrete transformation technique together with the boundary point collocation method is employed to evaluate the unknown coefficients of the solution series via satisfying the problem boundary conditions. A comprehensive convergence study is presented to investigate the accuracy and convergence rate of the GDTM. We will also demonstrate the application of this meshfree method for simulating the conductive heat transfer in a heterogeneous materials system and the dissolved aluminum ions concentration in the electrolyte solution formed near a passive corrosion pit.

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1. Introduction

Despite remarkable advances in both the computational science and computing resources in the past few decades, the analysis of engineering problems and physical phenomena with complex morphologies remains an ongoing challenge. Such complexities are not only due to the heterostructure and intricate morphology of the domain but also can emanate from the transient evolution of its geometry in problems such as the pitting corrosion [1]. In most cases, while conventional mesh-based techniques such as the standard finite element method (FEM) can accurately approximate the governing equations, the labor and computational costs associated with creating/updating the conforming (matching) mesh undermine the efficiency of such methods [2–4]. Furthermore, the quality of the resulting finite element (FE) mesh, i.e., the elements aspect ratio and the level of refinement, has a direct impact on the accuracy of the solution, which may not easily be assured for problems with complex morphologies [5–7]. In moving boundary problems, while adaptive mesh refinement techniques are

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often implemented to avoid the expensive re-meshing process, creating new elements with proper aspect ratios involves similar challenges \[8,9\].

Several numerical techniques have been proposed to mitigate the difficulties associated with the construction of conforming meshes needed in the standard FEM. Polygonal/polyhedral elements allow a more flexible algorithm for meshing complex geometries while providing a higher accuracy and less sensitivity on the element aspect ratio compared to Lagrangian elements \[10,11\]. The Virtual Element Method (VEM) \[12,13\] combines the advantages of polygonal/polyhedral elements with ideas from mimetic finite difference method \[14,15\] and has shown to yield satisfactory results using elements with bad aspect ratios. To allow the implementation of FE meshes that are completely independent of the problem morphology, mesh-independent techniques such as the Immersed FEM \[16\], eXtended/Generalized FEM \[17,18\], and the Hierarchical Interface-enriched FEM (HiFEM) \[19–21\] are also introduced. These methods can retrieve an optimal accuracy and convergence rate for problems discretized with non-matching meshes via incorporating appropriate enrichments along the problem boundaries and/or discontinuous phenomena in the domain.

The Boundary Element Method (BEM) \[22,23\] is another technique that can alleviate the difficulties associated with the implementation of the standard FEM for modeling problems with complex geometries. In BEM, the strong form of a boundary/initial value problem is converted into a boundary integral equation described in terms of Green’s basis functions. The approximation of the field thus requires constructing FE meshes that only discretize the domain boundaries, which considerably reduces the complexity of the mesh generation process by replacing a volume mesh with a surface mesh \[24\].

One of the key disadvantages of the classical BEM is the high computational cost associated with evaluating the boundary integrals in this method, which can be addressed by using more advanced techniques such as the fast multi-pole BEM \[24,25\] and the pre-corrected fast Fourier transformation method \[26\].

Meshfree Methods (MMs) completely eliminate the need for creating FE meshes by constructing a global field approximation over either a set of domain points \[27,28\] or (for linear problems) only along the boundary points \[29\]. Among widely used MMs, we can mention the smoothed particle hydrodynamics (SPH) \[30,31\], the method of fundamental solutions (MFS) \[32,33\] and the exponential basis functions (EBFs) method \[29,34,35\]. In SPH which is frequently used for simulating fluid problems, a set of kernel functions is transformed into motion equations to evaluate the governing equations \[36\]. The MFS approximation series is built on a set of boundary points (boundary collocation technique), using fundamental solutions with source points that are created outside the problem domain \[37\]. Similarly, the EBFs method only requires the discretization of the problem boundaries, but uses a discrete transformation technique to compute the unknown coefficients of the solution series \[38\]. Reviews of different MMs and their applications to simulate engineering problems are presented in \[31,39\].

In this manuscript, we introduce a new meshfree method that uses the same discrete transformation as the EBFs method \[29,40\] but employs Green’s basis functions to simulate the potential field in problems with complex morphologies. While the method is general and can be applied to any problem with existing Green’s functions, the current work focuses on Poisson problems. In the proposed Green’s Discrete Transformation Method (GDTM), the source points used for evaluating the basis functions are created along a virtual boundary outside the domain of interest. The discrete transformation technique introduced in \[29\] allows for using a larger number of basis functions than the number of boundary collocation points, which can improve accuracy of the method compared to conventional techniques such as the least squares approximation (LSA) \[33\]. By implementing Green’s functions in place of exponential bases used in the EBFs method, the GDTM provides more appropriate basis functions for simulating problems with complex geometries. However, in comparison with the EBFs method, this feature limits the application range of the GDTM to problems for which the Green’s functions can be computed analytically. A detailed numerical study is performed to identify the optimal number and location of the GDTM source points that yield the best approximation of a partition of unity while maintaining a reasonable computational cost. We show that the optimal source points evaluated via this approach can also accurately approximate other potential fields over complex domains with arbitrary domain shapes.

The remainder of this article is structured as follows. Section 2 presents the problem formulation together with describing the GDTM algorithm. In Sections 3 and 4, we study the impact of source points and boundary points on the accuracy and convergence rate of the GDTM. Finally, Section 5 presents the application of this method for simulating two Poisson problems with intricate geometries: the conductive heat transfer in a heterogeneous materials system and the ion concentration in an electrolyte solution formed by pitting corrosion.

2. Problem formulation and GDTM algorithm

Consider a two-dimensional open domain \(\Omega\) with closure \(\overline{\Omega}\) and boundaries \(\partial \Omega = \Gamma_D \cup \Gamma_N\) corresponding to the Dirichlet and Neumann boundaries, respectively (\(\Gamma_D \cap \Gamma_N = \emptyset\)). The strong form of the governing equations for the steady state diffusion of a potential field \(u(x)\) (Poisson equation) is expressed as: find \(u\) such that

\[
D V^2 u(x) = 0 \quad \text{in} \; \overline{\Omega} \\

u(x) = \bar{u} \quad \text{on} \; \Gamma_D \\

-\kappa V u(x) \cdot \mathbf{n}(x) = \bar{q} \quad \text{on} \; \Gamma_N,
\]

where \(D\) is the diffusivity, \(\kappa\) is a constant coefficient (e.g., thermal conductivity for heat transfer problems), \(\mathbf{n}\) is the unit normal vector to the boundary, \(\bar{u}\) is the fixed value of the species along \(\Gamma_D\), and \(\bar{q}\) is the applied flux along \(\Gamma_N\). Assuming a
Dirac delta function $\delta(\xi, x)$ defined at the source point $\xi$, the Green’s function $G(\xi, x)$ associated with (1) can be evaluated by solving the equation
\[
\nabla^2 G(\xi, x) = \delta(\xi, x) \quad \text{in } \Omega
\]
which can be computed as
\[
G(\xi, x) = \frac{1}{2\pi} \ln(\|\xi - x\|).
\]
The GDTM approximation of (1) is written as
\[
\hat{u} = \sum_{i=1}^{N} c_i G(\xi_i, x),
\]
where $N$ is the total number of Green’s functions used to approximate the field. Since the Green’s functions given in (3) satisfy the Poisson equation everywhere except at the source points $\xi_i$, the source points must be located outside $\Omega$ to allow the implementation of a point collocation method for approximating (1). Further details regarding the optimal number and location of the source points are presented in the following section.

To evaluate the unknown coefficients $c_i$ of the solution series given in (4), we first discretize the Dirichlet and Neumann boundaries using $M_D$ and $M_N$ points, with $M_D + M_N = M$. The $c_i$ coefficients are then computed using a discrete transformation similar to that given in [29], which is given by
\[
c_i = \mathbf{V}_i^T \mathbf{R} \hat{u},
\]
where $\hat{u}$ is a vector of size $M$ containing the boundary condition values,
\[
\hat{u} = \{ (\hat{u})_1, (\hat{u})_2, \ldots, (\hat{u})_{M_D}, (\hat{q})_{M_D+1}, (\hat{q})_{M_D+2}, \ldots, (\hat{q})_{M_D+M_N} \}^T.
\]
The $j$th component of $\mathbf{V}_i$ is obtained by applying the same differential operator as that used in (1) for evaluating the boundary condition value corresponding to the $j$th component of $\hat{u}$ to the Green’s basis function and computing that at $(\xi_i, x)$, i.e.,
\[
\mathbf{V}_i = \left\{ G(\xi_i, x_1), G(\xi_i, x_2), \ldots G(\xi_i, x_{M_D}), \ldots, -\kappa \nabla G(\xi_i, x_{M_D+1}) \cdot \mathbf{n}_{M_D+1}, \ldots, -\kappa \nabla G(\xi_i, x_{M_D+M_N}) \cdot \mathbf{n}_{M_D+M_N} \right\}^T.
\]
To evaluate the projection matrix $\mathbf{R}$, we substitute the coefficients $c_i$ in (4) with (5) and re-compute the boundary condition values at all boundary collocation points, which yields
\[
\hat{u} = \sum_{i=1}^{N} \mathbf{V}_i \mathbf{V}_i^T \mathbf{R} \hat{u}.
\]
By eliminating $\hat{u}$ from the above equation, the projection matrix $\mathbf{R}$ can be evaluated as
\[
\mathbf{R} = \left( \sum_{i=1}^{N} \mathbf{V}_i \mathbf{V}_i^T \right)^+ = \mathbf{G}^+,
\]
where the pseudo-inverse operator $(\cdot)^+$ is employed to resolve potential numerical problems associated with the rank deficiency of $\mathbf{G}$. At sharp corners of the domain, unless Dirichlet boundary conditions are assigned along both connected edges, two distinct boundary collocation points with the exact same coordinates are used to discretize the domain. Despite the use of similar coordinates for such nodes, according to (7), assigning Dirichlet and Neumann conditions to each point or Neumann conditions at both points but with different unit normal vectors yields two distinct components in $\mathbf{V}_i$, which leads to the construction of a non-singular matrix $\mathbf{G}$. The mathematical justification behind using the discrete transformation given in (5) is presented in [29].

The key advantage of using the Green’s functions in the GDTM in place of the exponential bases used in the EBFs is providing the ability to more accurately simulate problems with complex geometries using bases that are tailored to the problem morphology. The reason is that the exponential bases used in the EBFs method are oscillatory functions with increasing amplitudes with respect to the origin of the Cartesian coordinates axes and cannot be modified based on the morphology of the domain. As a result, the amplitudes of these fundamental solutions are exponentially increasing over the edges of the bounding box of the domain and they do not incorporate any information regarding the external morphology or internal geometry of the problem. Thus, depending on the shape and aspect ratio of the domain, the exceedingly high amplitude of the EBFs near the domain edges can hinder the accurate reconstruction of the solution field. For example, the EBFs method cannot accurately approximate the potential field over a square domain with a circular perforation very close to one of its edges or over a rectangular domain with a high aspect ratio. However, as will be discussed in more details...
in the following section, the flexibility to adjust the location of GDTM source points allows for creating appropriate bases with the radial function property that can be customized to the problem geometry and therefore yield a higher accuracy. It must be noted that the EBFs method allows for simulating a wider range of problems because unlike the GDTM it does not implement the Green’s basis functions, which cannot be analytically computed for all types of differential equations.

3. GDTM source points

As noted earlier, the source points used for evaluating the GDTM Green’s functions must be located outside the domain boundaries. However, the optimal number and location of these source points have a crucial impact on the accuracy of this method, which must be determined meticulously. A straightforward approach, which is also used in the MFS [41], is to create the source points on a circumscribing circle of the domain. However, despite its simplicity, this approach does not yield a satisfactory level of accuracy for problems with complex morphologies or sharp edges. As an alternative scheme, the source points can be placed along a virtual boundary constructed by mapping the boundary collocation points in the direction of the outward normal vector of the domain [42]. In this approach, the optimal location of the virtual boundary is determined via solving several least square systems of equations, which complicates its implementation.

In this work, the optimal number and location of source points are determined such that the GDTM yields the best approximation of a partition of unity, i.e., the ability to accurately reconstruct a constant field. Note that similarly to several other meshfree methods such as the SPH and MFS, the \( C_\infty \)-continuous basis functions used in the GDTM do not satisfy the partition of unity condition, which is one of the key features of the Lagrangian shape functions in the standard FEM. Thus, we propose a new approach for identifying the optimal GDTM source points such that the resulting basis functions yield the most accurate approximation of a partition of unity. We hypothesize that by implicitly imposing this condition in the GDTM, the \( C_\infty \)-continuous basis functions used in this method will also be able to accurately simulate more complex potential fields. This hypothesis will be verified with results of the numerical tests provided in the following section.

To simplify the explanation of the algorithm used for creating the GDTM source points, we focus on the quadrilateral domain shown in Fig. 1, which schematically shows the arrangements of both the boundary collocation and source points. In the proposed algorithm, the number and location of source points are assumed to be a function of the number and the relative distance between the boundary collocation points used for discretizing the problem boundaries. Similarly to [42], the first set of source points is created by moving each boundary collocation point \( x_j \) in the direction of its outward normal vector \( n_j \), i.e.,

\[
\xi_j = x_j + (\alpha d_j) n_j,
\]

where \( d_j \) is the average distance between \( x_j \) and the adjacent boundary points and \( \alpha \) is a constant scale factor, to be determined later. The larger blue circular nodes depicted in Fig. 1 correspond to this first set of source points. The distance between two adjacent nodes belonging to this first set of source points is then divided into \( \beta \) equally distanced subsections to create \( (\beta - 1) \) the second set of source points, which are shown as smaller blue circular points in Fig. 1. The red square source points shown in the vicinity of the sharp corners of the domain are also added to improve the accuracy of the GDTM approximation in those regions by extending the virtual boundaries on which the first and second set of source points are located. Few source points are also added in between the domain boundaries and the virtual boundaries in such regions. More details regarding the algorithm used for creating the additional source points are provided in Section 3.3.

The effects of \( \alpha \) and \( \beta \) values on the GDTM accuracy and the condition number of \( G \) for approximating the constant potential field \( u = 1 \) (a partition of unity) over a \( 5 \times 5 \) square domain are presented in Fig. 2. In this benchmark problem, the bottom edge of the domain has a fixed temperature of \( \bar{u} = 1 \) and the other edges have zero flux boundary condition, \( \bar{q} = 0 \). The problem boundaries are discretized using a total number of \( M = 300 \) collocation points, which ensures using...
sufficient number of boundary collocation points for approximating the field. The $l_2$-norm of the error and the maximum relative error values presented in Fig. 2 are then computed over a set of $n_d$ points inside the domain as follows

$$\|e\|_{l_2} = \sqrt{\frac{\sum_{i=1}^{n_d} (\hat{u}_i - u_i)^2}{\sum_{i=1}^{n_d} u_i^2}}, \quad \|e\|_{\text{max}} = \max\left(\frac{|\hat{u}_i - u_i|}{|u_i|}\right).$$

The optimal values of $\alpha$ and $\beta$ that provide a logical balance between the accuracy and computational cost of the GDTM can be evaluated by studying the plots presented in Fig. 2. However, the variations of the error and condition number of $G$ with respect to $\alpha$ and $\beta$ in that figure indicate that, except for the case of $\beta = 1$, they resemble a separable function of these two parameters. Thus, we take this opportunity to elaborate on the impact of each parameter on the accuracy and computational efficacy of the GDTM independently and determine their optimal values in the remainder of this section. Nevertheless, the optimal pair of $\alpha$ and $\beta$ that will be evaluated next would be similar to that one can directly determine by analyzing the results shown in Fig. 2.

3.1. Optimal location of source points

As indicated previously, the distance between the GDTM source points and boundary collocation points is controlled by the value of $\alpha$ defined in (10). In the context of the MFS, it has been shown that placing the source points far away from the domain boundary yields more appropriate bases for approximating the field, but simultaneously leads to highly ill-conditioned linear systems of equations that deteriorate the overall accuracy and stability of the solution [41]. Moving source points closer to the domain boundaries improves the condition number of the resulting matrices but reduces the accuracy of the numerical solution. Tsai et al. [43] reported a critical distance between the MFS source points and the problem boundaries, above which the condition number increases without a meaningful change in the accuracy.

The variations of the $l_2$-norm and maximum values of the error and the condition number of $G$ versus $\alpha$ for approximating the field $u = 1$ in the square domain of Fig. 1 are depicted in Fig. 3 ($\beta = 4$). According to this figure and also the results shown in Fig. 2, we adopt $\alpha = 2.5$ as the optimal value for determining the location of source points. Fig. 3(b) shows that reducing $\alpha$ below this optimal value improves the condition number of $G$ with a constant rate, although simultaneously deteriorates its accuracy according to Fig. 3(a). Furthermore, using $\alpha > 3.5$ initially leads to a plateau in the error and eventually deteriorates that, as the condition number of $G$ becomes exceedingly large (Fig. 3(b)). These observations are compatible with those reported by Tsai et al. in [43] for the MFS. Note that while using a different value for $M$ affects the accuracy of the GDTM, it does not affect the overall trend discussed above and the optimal value obtained for $\alpha$.

The proposed scheme for placing the source points on a virtual boundary created by mapping the boundary collocation points outside the actual boundaries of the domain can become problematic when dealing with slender cavities or sharp concave edges. In these cases, the virtual boundary containing the source points can potentially intersect with the domain boundaries, resulting in singularity in the GDTM approximation and thus poor accuracy in that region. The same limitation also exists for other MFS meshfree methods using the Green’s functions as fundamental solutions. The first approach for resolving this issue is to refine the boundary discretization in such regions to avoid the source points entering the problem domain. Note that the distance between source points and problem boundaries is a function of distance between the boundary collocation points and therefore by refining the discretization of the boundary, the source points will move closer
While performance partition in Section 3.3.

number and number shown of GDTM, of transformation 3.2.

instance, to the boundary. An alternative approach is to discretize the domain into smaller sub-regions to eliminate such cases. For instance, a concave polygon shape domain can be discretized into two convex polygons in which this problem no longer exists and each subdomain can be solved separately using the algorithm described in Section 5.1.

3.2. Optimal number of source points

While in the MFS, the number of source points is constrained by the number of collocation points [32], the discrete transformation technique used in the GDTM makes the choice for the number of source points independent of the number of boundary points. The ability to use more source points than the boundary points is one of the main advantages of the GDTM, which can improve the accuracy and stability of this method. However, it is evident that increasing the number of source points determined by \( \beta \) leads to a higher computational cost. Therefore, identifying the optimal value of \( \beta \) is crucial to both the accuracy and the efficacy of this method. The variations of the norms of the error and the condition number of \( \mathbf{G} \) versus different values of \( \beta \) for the square domain shown in Fig. 2(a) are presented in Fig. 4 (\( \alpha = 2.5 \)). As shown in Fig. 4(a), increasing \( \beta \) from 1 to 2 has a considerable impact on reducing the \( l_2 \)-norm and maximum value of the error. Moreover, as shown in Fig. 4(b), this increase in the value of \( \beta \) leads to significant improvement in the condition number of \( \mathbf{G} \). However, while using \( \beta > 2 \) will increase the computational cost, its effect on improving the GDTM accuracy and reducing the condition number of \( \mathbf{G} \) is negligible. According to these observations, we adopt \( \beta = 2 \) to determine the number of source points.

3.3. Effect of the domain geometry

The optimal values of \( \alpha \) and \( \beta \) given in Sections 3.1 and 3.2 were computed such that the GDTM yields the highest accuracy and simultaneously the lowest computational cost for approximating a constant field over the square domain shown in Fig. 2(a). We have also investigated the effect of these parameters on the performance of the GDTM for reconstructing a partition of unity over several other arbitrary shaped domains, revealing that using \( \alpha = 2.5 \) and \( \beta = 2 \) maintains the optimal performance regardless of the morphology of the problem. The results of this study for eight domains with different geometries are summarized in Table 1. In these problems, the edge shown in red has a Dirichlet boundary condition of \( \tilde{u} = 1 \) while a constant flux of \( \tilde{q} = 0 \) is assigned along the other edges. We have used Neumann boundary conditions along most
edges of the domain to demonstrate the ability of the GDTM in providing an accurate approximation of the field, even in the absence of essential boundary conditions. It must be noted that in GDTM, the type of the boundary condition (Dirichlet vs. Neumann) does not have a meaningful impact on the accuracy and this method can handle both equally well.

The values of the GDTM error presented in Table 1 are reported for two different types of simulations. In case 1, only the blue circular source points shown in Fig. 1 are employed for evaluating the field without any special treatment near $C^0$-continuous corners of the domain. In case 2, two layers of additional source points are created in the vicinity of the corners, which are illustrated as red squares in Fig. 1. One of these layers is simply created by expanding the virtual boundaries holding the circular-shaped source points and connecting them together. The second layer is formed by creating a new virtual boundary using $\alpha = 1.25$ (in the middle of the problem boundaries and the original virtual boundary) but only along 5% of the length of the domain edges on each side to still maintain a low computational cost. For both layers, $\beta = 2$ is used to determine the distance between the source points. These additional source points provide more support for approximating the field near sharp corners of the domain, where there are strong discontinuities in the boundary conditions and normal vectors to the boundaries to improve the accuracy of GDTM. The effectiveness of adding such source points is confirmed by the results presented in Table 1 for domains with different configurations. Fig. 5 illustrates the values of the error for the GDTM approximation of a partition of unity over the square domain of Fig. 2(a) with and without using the additional source points near the sharp corners of the domain, which clearly demonstrates the improved precision obtained via the former approach.

It must be noted that while the focus of the current manuscript is on the GDTM approximation of 2D Poisson problems, there is no intrinsic limitation for expanding this method to 3D and/or other types of problems with existing Green’s functions. A similar algorithm as that explained above can be used for selecting the number and location of source points and the proposed discrete transformation given in (5) can be implemented for modeling varying types of 3D problems, although a detailed convergence study must be conducted to assure the accuracy and stability of the solution.

<table>
<thead>
<tr>
<th>Shape</th>
<th>$l_2$-norm of error</th>
<th>Maximum error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>case 1</td>
<td>case 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.82E-07</td>
<td>3.61E-07</td>
</tr>
<tr>
<td></td>
<td>6.24E-06</td>
<td>2.79E-07</td>
</tr>
<tr>
<td></td>
<td>1.45E-06</td>
<td>8.68E-07</td>
</tr>
<tr>
<td></td>
<td>1.56E-06</td>
<td>1.55E-07</td>
</tr>
<tr>
<td></td>
<td>1.21E-05</td>
<td>8.15E-07</td>
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<td>8.71E-07</td>
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<tr>
<td></td>
<td>9.08E-07</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 5. Values of the error associated with the GDTM approximation of a partition of unity over the trapezoidal domain shown in the second row of Table 1 (a) without and (b) with additional source points in the vicinity of its sharp corners.
4. Convergence study

In this section, we study the accuracy and convergence rate of the GDTM for approximating two Poisson problems using \( \alpha = 2.5 \) and \( \beta = 2 \).

4.1. Example 1: Linear temperature field

As the first example problem, we implement the GDTM to simulate a linear temperature field over the square domain shown in Fig. 6. In this problem, a fixed temperature of \( \bar{u} = 100 \, ^\circ C \) is enforced along the bottom edge, a constant heat flux of \( \bar{q} = 100 \, \text{W/m} \) is applied along the top edge, and the side edges are insulated. While such a problem is often used as a patch test for the standard FEM, the implementation of logarithmic bases in the GDTM does not assure a super-convergent solution. However, the optimized \( \alpha \) and \( \beta \) values obtained in the previous section for approximating a constant field are also expected to yield a high precision for reconstructing a linear field. This hypothesis is confirmed by the results presented in Fig. 6(b), which shows the temperature profile along the y-axis of the domain using only \( M = 80 \) points for discretizing the domain boundaries (\( \|e\|_2 = 1.87 \times 10^{-7} \)).

4.2. Example 2: Complex domain morphology

In this example, we investigate the accuracy of the GDTM for approximating the potential field \( u_{\text{exact}} = 3x^2y - y^3 + 40 \) over the domain shown in Fig. 7. The boundary conditions for this problem are computed based on the function \( u_{\text{exact}} \) by assigning the Dirichlet condition along the right edge and Neumann boundary conditions along the other edges. Fig. 7(b) illustrates the GDTM approximation of the potential field in this problem using \( M = 124 \) collocation points for discretizing the boundaries. The variation of the \( l_2 \)-norm of the error versus \( M \) is depicted in Fig. 8(a). As shown in Fig. 8(a), the GDTM error initially decreases with a high rate when increasing \( M \) and then shows a reduced convergence rate. This behavior can be attributed to the error added to the numerical approximation due to the increasing condition number of \( G \), as depicted in Fig. 8(b). This error eventually takes over the improvement of the accuracy associated with increasing the number of boundary collocation points at \( M = 220 \), beyond which the \( l_2 \)-norm of the error shows an oscillatory behavior at \( 10^{-5} < \|e\|_2 < 5 \times 10^{-4} \).

Fig. 8(a) also illustrates the variation of the \( l_2 \)-norm of the error versus the number of finite elements for the standard FEM approximation of this problem using four-node quadrilateral elements. As shown in Fig. 8(a), compared to the FEM results and given the geometrical discretization error associated with the curved boundaries, the GDTM yields a high level of accuracy using relatively few boundary collocation points for discretizing the problem. For example, to achieve the same precision as that with \( M = 124 \) in the GDTM, one must implement approximately \( 10^4 \) quadrilateral elements in the standard FEM simulation.

The CPU times needed to perform the GDTM and FEM simulations presented in Fig. 8(a) are reported in Fig. 8(c), which indicates that the GDTM yields a lower computational cost than the standard FEM to achieve the same level of accuracy before the critical point \( M = 220 \). The reason is that, despite relying on logarithmic basis functions, GDTM simulations are conducted using significantly fewer degrees of freedom compared to the FEM analyses. It must be noted that the CPU times reported in Fig. 8(c) are highly in favor of the FEM results, which are obtained using the commercial software program Abaqus versus the GDTM simulations performed using a less efficient Mathematica code. Clearly, implementing a basic programming language such as C++ could have remarkably reduced the GDTM simulation times. Furthermore, while the CPU time required for the mesh generation process is not incorporated in evaluating the FEM computational cost, the GDTM solver provides a fully automated algorithm for discretizing the problem and creating the Green’s functions source points.
Fig. 7. Second example problem: (a) problem description; (b) GDTM approximation of the potential field $u = 3x^2y - y^3 + 40$ using $M = 124$ boundary collocation points to discretize the domain. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 8. Second example problem: variations of the (a) $l_2$-norm of error, (b) condition number, and (c) simulation time for the GDTM and the FEM approximation of the potential field versus the number of boundary collocation points and number of finite elements, respectively.

This automated approach is one of the key advantages of the GDTM for simulating problems with intricate morphologies, which can considerably reduce the labor cost associated with the modeling process.

5. Application problems

In this section, we implement the GDTM to simulate two Poisson problems with complex geometries: the conductive heat transfer in a heterogeneous materials system and the concentration of dissolved metal ions in the electrolyte solution formed in the vicinity of a passive corrosion pit.
5.1. Conductive heat transfer in a heterogeneous material

The geometry, materials properties, and boundary conditions of a representative volume element (RVE) of the heterogeneous materials system studied in this problem are shown in Fig. 9. The 5 cm × 5 cm domain is composed of alumina inclusions with a thermal conductivity of $\kappa_{\text{Al}} = 31$ W/m K embedded in a glass matrix with $\kappa_{\text{G}} = 1.4$ W/m K. The boundary conditions consist of a fixed temperature of $\bar{u} = 0$°C along the bottom edge, a constant heat flux of $\bar{q} = 500$ W/m along the top edge, and insulated along side edges. Due to the mismatch between thermal conductivities of the matrix and alumina inclusions, a weak (gradient) discontinuity occurs in the solution field along the interface between the two materials phases.

The GDTM approximation of the temperature field in this problem is depicted in Fig. 9(b), which clearly shows the ability of this method to capture weak discontinuities along the alumina/ glass interfaces. To implement the GDTM for modeling this problem, we first divided the domain into two subdomains: the matrix (in which inclusions are replaced with voids) and the alumina inclusions. We then approximated the temperature field in each sub-domain separately, although the boundary conditions along the edges associated with the matrix-inclusion interface in the original domain remain unknown. To resolve this issue, an unknown heat flux boundary condition is assigned along these edges in each subdomain and the zero net flux condition along the matrix-inclusion interfaces, i.e.,

$$\kappa_{\text{G}} (\nabla u \cdot \mathbf{n}_{\text{G}}) = \kappa_{\text{Al}} (\nabla u \cdot \mathbf{n}_{\text{Al}}),$$

is employed to eliminate the unknowns by relating the sub-domains to one another. By enforcing this continuity condition, the GDTM linear equations associated with each phase can be assembled into a single system of linear equations, in which the unknown heat flux boundary conditions vanish. The remainder of the computational procedure is similar to that described before for homogeneous domains.

5.2. Dissolved ions concentration in a corrosion pit

In this example, we implement the GDTM to evaluate the ions concentration in a passive corrosion pit, which is formed by the localized dissolution of the metal (in this example, aluminum) after the breakdown of its protective film due to the attack of aggressive anions [1]. Such corrosion pits often have complex geometries and can significantly accelerate the mechanical failure of the material by inducing stress concentrations and thus serving as sites of crack nucleation. During the stable growth stage of pits with medium size, which is often characterized by the formation of a saturated salt film over the pit surface, the dissolution of metal to the electrolyte solution can be formulated as a diffusion-controlled problem [44, 45]. After the re-passivation of the pit, one can implement the Poisson equation to simulate the concentration of ions in the electrolyte solution.

The problem description for the passive corrosion pit studied in this example is given in Fig. 10. A Dirichlet boundary condition of $\bar{u} = 0.5$ mol/L is enforced along the pit boundary, which corresponds to the formation of the saturated salt film on this surface. The electrolyte domain is composed of the pit solution and a semi-circular shape electrolyte outside the pit (bulk solution). The ions diffusion coefficient is assumed to be $D = 559$ $\mu$m$^2$/s. The GDTM approximation of the ions concentration in the electrolyte solution is illustrated in Fig. 10 using only $M = 320$ boundary collocation points to discretize the domain boundaries.
6. Conclusion

A new boundary collocation meshfree method was introduced for the treatment of Poisson problems with complex morphologies that relies on a discrete transformation of Green’s basis functions for approximating the field. The proposed Green’s Discrete Transformation Method (GDTM) allows for using more source points than boundary collocation points for approximating the field, which provides improved accuracy and stability. A detailed study was conducted to evaluate the optimal number and location of these source points such that the resulting Green’s basis functions yield the highest precision for reconstructing a partition of unity while maintaining a low computational cost. In the proposed algorithm, the number and location of source points are determined based on the number and relative distance between the boundary collocation points and created on a virtual boundary outside the problem domain. We investigated the accuracy and convergence rate of the GDTM for approximating non-constant potential fields over varying domains with intricate geometries, which showed the ability of the method to handle such cases accurately. We also presented the application of the GDTM for simulating the thermal response of a heterogeneous materials system and evaluating the ions concentration in a corrosion pit.

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References
