# A MESHLESS COLLOCATION METHOD BASED ON HIERARCHICAL MATRICES FOR EFFICIENT NUMERICAL ANALYSIS OF LARGE-SCALE LINEAR SYSTEMS

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ABSTRACT
This paper presents a novel approach to solving large-scale linear algebra problems by integrating hierarchical matrices (H-matrices) with a semi-analytic meshless collocation method (singular boundary method). The singular boundary method eliminates the need for mesh generation by using a set of discrete nodes to approximate the solution of partial differential equations. However, this approach often leads to dense linear systems that are computationally expensive and memory-intensive. To address this challenge, we employ H-matrices, which decompose these dense matrices into hierarchical sub-blocks that can often be approximated by low-rank matrices. This decomposition significantly reduces computational complexity from the conventional to or lower, depending on the matrix structure. The implementation of these data-sparse representations significantly enhances the efficiency of numerical computations by reducing both complexity and storage requirements traditionally associated with matrix operations. Our results demonstrate that the combination of H-matrices with the singular boundary method not only reduces memory requirements but also accelerates matrix operations, such as matrix-vector multiplication and inversion. The validity of the proposed method for solving the Laplace equation and the Helmholtz equation is verified by benchmark examples, highlighting its potential for large-scale engineering problems.
*Keywords: meshless collocation method, singular boundary method, hierarchical matrices, large-scale linear algebra, low-rank approximation.*

## 1 INTRODUCTION

Over the past few decades, various numerical methods have been developed to solve partial differential equations (PDEs) [1], [2], thereby enabling a deeper understanding of their physical and mathematical properties. Among these, semi-analytic meshless collocation methods have been widely employed to solve a range of complex problems. The singular boundary method (SBM) [3]–[5], which is derived from the boundary element method [6], [7] and the method of fundamental solutions (MFS) [8], is a boundary-type meshless collocation method. SBM introduces the concept of source intensity factors, effectively overcoming the fictitious boundary issues inherent in the MFS while retaining key advantages of boundary-type numerical methods, such as the elimination of numerical integration and ease of implementation. These characteristics have led to the widespread application of SBM across various fields.

Despite the numerous advantages of the SBM, the method typically produces dense and non-symmetric coefficient matrices, resulting in significant computational costs and high memory demands. This makes the efficient solution of large-scale problems using SBM a substantial challenge. To address these issues, this paper proposes a novel approach to solving large-scale linear algebra problems by integrating hierarchical matrices (H-matrices) [9]–[11] with a semi-analytic meshless collocation method (singular boundary method). H-matrices represent a state-of-the-art technique designed to efficiently handle large, dense matrices that arise during the discretisation of PDEs. They offer a data-sparse representation

WIT Transactions on Engineering Sciences, Vol 136, 
www.witpress.com, ISSN 1743-3533 (on-line)
doi:10.2495/BE470071

that is particularly effective in capturing non-local interactions within complex problems. Traditional matrix representations are computationally expensive and memory-intensive, but H-matrices differ by approximating distant matrix blocks with low-rank matrices, thus reducing both computational complexity and storage requirements. The core idea behind H-matrices is to partition a potentially sparse large matrix into smaller sub-blocks, which can then be approximated by low-rank matrices. This hierarchical representation significantly reduces the computational cost associated with large-scale matrix operations while maintaining the desired level of accuracy.

The integration of H-matrices with SBM effectively addresses the challenges posed by dense matrices in large-scale systems. As the scale of the problem increases, the computational burden associated with solving these systems also rises. By reducing the data complexity involved in matrix storage and operations, H-matrices enable SBM to solve more complex problems efficiently. The computational results presented in this paper demonstrate that this combined approach offers a promising solution for the efficient numerical analysis of large-scale linear systems, with broad applicability to problems such as the Laplace and Helmholtz equations.

## 2 METHODOLOGY

The SBM is a meshless collocation technique that eliminates the need for traditional mesh generation by using discrete collocation nodes to approximate the solution of PDEs. However, SBM often results in dense, non-symmetric matrices, which present significant challenges in terms of computational cost and memory requirements. To address these challenges, H-matrices are integrated with SBM, offering a data-sparse representation that mitigates the computational and storage demands associated with these dense systems.

### 2.1 Formulation of the SBM

To illustrate the methodology, consider the 3D Helmholtz equation in a bounded, homogeneous, isotropic domain $\Omega$:

$$(\Delta + \lambda^2)u = 0, \quad \text{in } \Omega, \tag{1}$$

subject to the boundary conditions:

$$u(x) = u_0(x), \quad x \in \Gamma_D, \tag{2}$$

$$\frac{\partial u(x)}{\partial n} = q(x), \quad x \in \Gamma_N, \tag{3}$$

where $u$ is the unknown function, $x$ represents the spatial coordinates, $\Omega$ and $\Gamma$ represent the computational domain and its boundary, with $\Gamma_D$ and $\Gamma_N$ representing Dirichlet and Neumann boundary conditions, respectively.

The SBM leads to the following linear system:

$$A_{ij}\alpha = b, \; A \in R^{n\times n}, x, b \in R^n, \tag{4}$$

where $A$ is a dense matrix,

$$A_{ij} = \begin{cases} \frac{exp(\sqrt{-1}\lambda r_{ij})}{4\pi r_{ij}}, & \text{if } i \neq j \\ \text{OIFs}, & \text{if } i = j \end{cases}, \tag{5}$$

with $r_{ij} = \|x_i - y_j\|$. The right-hand side vector $b$ corresponds to the boundary condition $u_0$.

When the collocation nodes $x_i$ coincide with the source nodes $y_j$, singularities arise in the fundamental solutions. SBM addresses these singularities by introducing origin intensity factors (OIFs) [12] to regularise the solution. OIFs can be determined by inverse interpolation techniques [13], subtraction and addition back techniques [14], [15] and integral mean values [16].

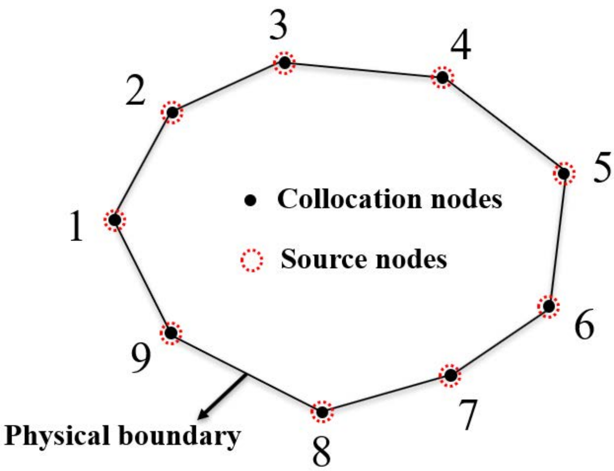


Figure 1: Schematic of the singular boundary method.

## 2.2 H-matrices for collocation method (SBM)

In the dense asymmetric matrix $A$ generated by SBM, directly solving the dense matrix $A \in R^{n\times n}$ requires $O(N^2)$ in storage and $O(N^3)$ in computational complexity. However, by leveraging H-matrices, the matrix can be divided into chunks where far-field interactions are represented by low-rank approximations.

Assuming the matrix $A$ has dimension $N$ and it consists of the following structure:

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix}, \tag{6}$$

where certain sub-blocks (e.g., $A_{1N}$ $A_{N1}$ $A_{2N}$ $A_{N2}$ ...) away from the diagonal can usually be approximated by low-rank matrices.

In the context of the 3D Helmholtz equation, the hierarchical decomposition provided by the H-matrix reduces the computational complexity from $O(N^2)$ to $O(Nk\log N)$, where $k$ is the rank of the approximation. This reduction significantly decreases both computational complexity and storage requirements, making the SBM method more efficient and scalable for large-scale problems.

By integrating H-matrices with SBM, the dense matrices resulting from the collocation process are decomposed into hierarchical sub-blocks, allowing far-field interactions to be approximated by low-rank matrices. This approach not only reduces computational and storage demands but also enhances the efficiency of matrix operations such as matrix-vector multiplication and inversion, which are critical in solving large-scale linear systems.

## 3 NUMERICAL RESULTS

This section presents three numerical examples to demonstrate the applicability and effectiveness of the proposed meshless collocation method based on H-matrices for solving the Laplace and Helmholtz equations. To quantify the accuracy of the numerical solutions, we introduce the $L_2$ norm relative error $L_{2err}(u)$ and the compression ratio. The $L_2$ norm relative error is defined as:

$$L_{2err}(u) = max\left(\frac{\sqrt{\sum_{i=1}^{N}|\hat{u}_i - u_i|^2}}{\sqrt{\sum_{i=1}^{N}|u_i|^2}}\right). \tag{7}$$

The compression ratio is given by:

$$\text{Compression ratio } = \frac{\text{size of the original matrix}}{\text{size of the compressed matrix}}. \tag{8}$$

### 3.1 Laplace equation in a unit circle domain (2D)

The first example considers the Laplace equation within a 2D unit circle domain:

$$\begin{cases} \Delta u = 0, & \text{in } \Omega \\ u = x^2 - y^2, & \text{on } \partial\Omega \end{cases}$$

The numerical results are shown in Table 1, which indicates that $L_2$ error increases with the increase of the number of nodes. However, it is important to note that the $L_2$ error remains within acceptable limits. The compression rate increases significantly with the increase of the number of nodes, indicating that the method effectively reduces the storage requirement while maintaining acceptable accuracy.

Table 1: H-matrix for the solution of the 2D Laplace equation with different node numbers (*N*).

| ***N*** | **Time (sec.)** | **$L_2$ error** | **Compression ratio** | **Size of the compressed matrix (MB)** |
|---|---|---|---|---|
| 100,000 | 79.68 | 2.07E-07 | 147.72 | 1,044.26 |
| 500,000 | 356.33 | 3.36E-06 | 703.07 | 5,497.76 |
| 1,000,000 | 670.74 | 5.95E-06 | 1,324.74 | 11,662.28 |
| 1,500,000 | 1,106.58 | 3.98E-05 | 1,766.98 | 19,604.49 |
| 2,000,000 | 2,475.09 | 3.99E-05 | 2,493.87 | 24,762.15 |

### 3.2 Laplace equation in a unit sphere domain (3D)

The second example considers the Laplace equation within a 3D unit sphere domain:

$$\begin{cases} \Delta u = 0, & \text{in } \Omega \\ u = e^x \cos(\frac{\sqrt{2}}{2}y)\cos(\frac{\sqrt{2}}{2}z), & \text{on } \partial\Omega \end{cases}$$

Fig. 2 illustrates the relationship between the number of nodes $N$, the $L_2$ error, and the compression ratio for the 3D Laplace equation. The graph demonstrates that the $L_2$ error decreases with an increasing number of nodes, but beyond a certain threshold, the error slightly increases. However, it is important to note that the $L_2$ error remains within acceptable limits. Nonetheless, the compression ratio continues to improve, emphasising the method's capability to handle large-scale problems efficiently.

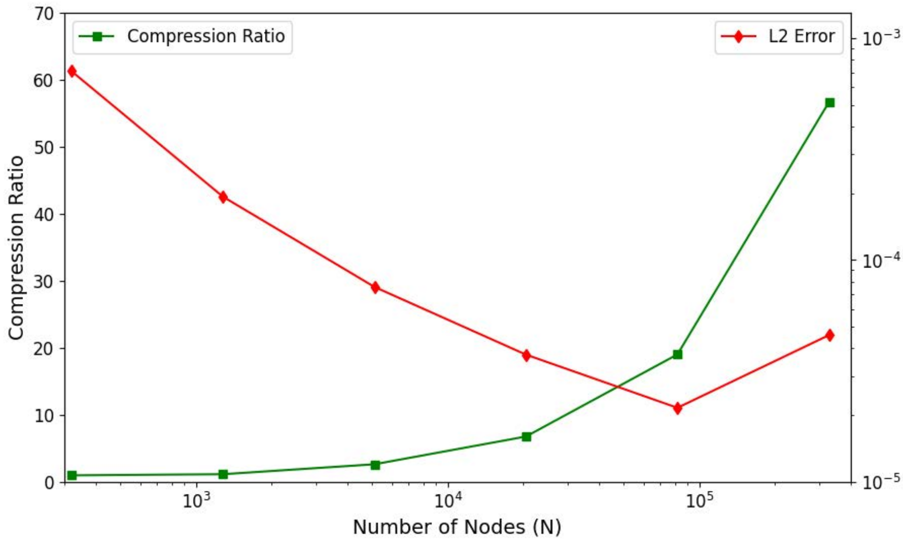


Figure 2: The numerical error of the compression rate varies with the number of collocation nodes in the 3D Laplace equation.

### 3.3 Helmholtz equation in a unit sphere domain (3D)

The third example addresses the Helmholtz equation in the same 3D unit sphere domain with a wave number $\lambda$ =1:

$$\begin{cases} (\Delta + \lambda^2)u = 0, & \text{in } \Omega \\ u = \exp(i\lambda r)/r, & \text{on } \partial\Omega \end{cases}$$

Fig. 3 presents a plot of the $L_2$ error and compression ratio against the number of nodes $N$ for this problem. The results for the Helmholtz equation are similar to those observed for the Laplace equation. The $L_2$ error decreases as the number of nodes increases, although it eventually increases slightly. However, it is important to note that the $L_2$ error remains within acceptable limits. The compression ratio improves with more nodes, reflecting the method's capability to efficiently compress the system matrix while solving the Helmholtz equation.

Next, we examine the performance of the H-matrix method for solving the 3D Helmholtz equation across various wave numbers ($\lambda$). Table 2 presents the computational time, $L_2$ error, compression ratio, and the size of the compressed matrix for different values of $\lambda$.

The results show that the computational accuracy tends to decrease significantly as the wave number λ increases. The decrease in accuracy can be attributed to the inherent oscillatory nature of the fundamental solution of the Helmholtz equation, which is particularly evident at higher wave numbers. Similarly, the compression ratio decreases with increasing wave number. This decrease suggests that the effectiveness of the method in compressing the matrix decreases as the wave number increases. In conclusion, while higher wave numbers pose a greater numerical challenge.

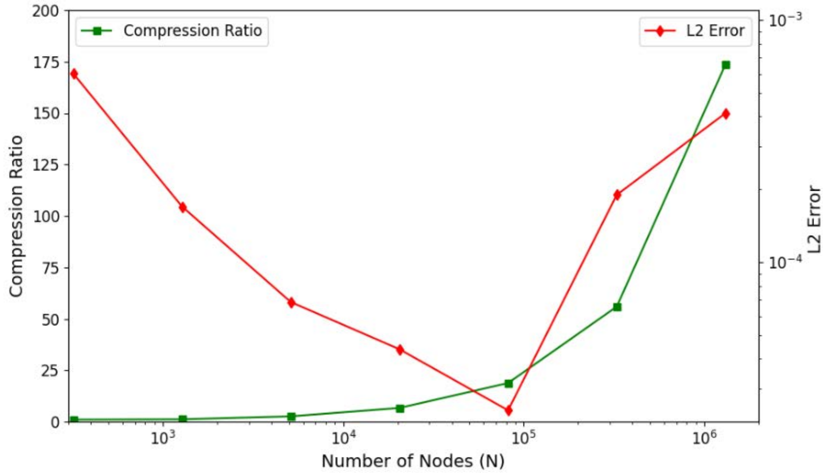


Figure 3: The numerical error of the compression rate varies with the number of collocation nodes in the 3D Helmholtz equation.

Table 2: H-matrix for the solution of the 3D Helmholtz equation with different wave numbers ($N$ = 327,680).

| $\lambda$ | Time (sec.) | $L_2$ error | Compression ratio | Size of the compressed matrix (MB) |
|---|---|---|---|---|
| 1 | 27.99 | 4.38E-05 | 6.79 | 966.16 |
| 5 | 32.58 | 1.37E-04 | 5.86 | 1,094.23 |
| 10 | 36.55 | 2.71E-04 | 5.09 | 1,259.61 |
| 20 | 46.58 | 7.59E-04 | 4.09 | 1,567.14 |
| 30 | 63.58 | 3.43E-03 | 3.44 | 1,862.79 |
| 40 | 78.29 | 1.22E-02 | 2.97 | 2,155.63 |

## 4 CONCLUSIONS

The results of this study demonstrate that the combination of H-matrices with the SBM provides an efficient numerical approach for solving large-scale linear systems. The numerical examples, particularly those involving the Laplace and Helmholtz equations, reveal that this method significantly reduces computational complexity and memory usage while maintaining a high degree of accuracy. Its capability to handle dense asymmetric matrices without sacrificing precision establishes it as a promising alternative to traditional numerical methods. However, challenges remain in addressing high wave number problems, indicating a need for further refinement of the method. Overall, this work underscores the effectiveness of the combined H-matrix and SBM approach, laying a strong foundation for future research aimed at expanding its applicability and optimising the H-matrix algorithm to enhance computational efficiency.

## ACKNOWLEDGEMENTS

The work described in this paper was supported by the National Natural Science Foundation of China (grant no. 12122205, 12372196).

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