Comparison of meshless MFS and CVBEM computational methods in analysis of groundwater flow pathways

Authors: Saleem Ali[1], Sebastian Neumann[1], T. V. Hromadka, II[2], B. Wilkins[3]

Cadet, Dept Mathematical Sciences, USMA, West Point, NY[1]

Distinguished Professor, USMA, West Point, NY[2]

Columbia University[3]

Introduction and Methodology

Computational methods to solve groundwater contamination problems continue to be of high interest to engineers and planners, among others. An important problem is identifying the source of contamination within a cluster of candidate sources. A key question is which candidate source(s) are the actual point source of the subject contamination. Using a node positioning algorithm approach [1], the modeled flow net can be computed with high accuracy, and the resulting streamline approximations can be traced to identify sources of contamination. This technique to locate sources of groundwater contamination has been tested in the finite element method and complex variable boundary element method (CVBEM), and it was concluded that CVBEM is more accurate [1].

The two methods compared in this study are CVBEM and the method of fundamental solutions (MFS) [2 and 3]. The general MFS approximation function is as follows: let $\Omega \subset \mathbb{R}$ such that $\hat{\phi}\,(x,y) = \sum_{j=1}^{n} a_j g_j(x,y),\;\; (x,y) \in \Omega$ where (x,y) is a point in the simply connected problem domain Ω, n is the number of nodes, a_j are real coefficients, and g_j are the real variable harmonic basis functions (nodes) [1]. In contrast, the general CVBEM approximation function is: let $\Omega \subset \mathbb{C}$ such that $\hat{\omega}(z) = \sum_{j=1}^{n} c_j g_j(z),\;\; z \in \Omega$ where *z* is the complex variable *x* + i*y* that is on simply connected problem domain Ω, *n* is the number of nodes, c_j are complex coefficients, and g_j are complex analytic basis functions (also nodes) [4]. By taking a linear combination of nodes equated to boundary data points (collocation points), the coefficients of the basis functions can be computed, and the model can be created. Furthermore, both methods are meshless, so only the boundary must be discretized into collocation points, which assists with computational efficiency. Another similarity is that the resulting models for ideal fluid flow potential are harmonic because the basis functions are harmonic. Thus, the Cauchy-Riemann equations can be used to find the conjugate streamline function. A key difference between MFS and CVBEM is that CVBEM nodes have 2 degrees of freedom (DOF) because the complex coefficients have a real and imaginary part. Thus, for *n* nodes, there are 2*n* DOF, and consequently, there are 2*n* collocation points [5]. As a result, a comparison of the computational error of the two models is best done based on DOF instead of number of nodes.

To compute error, since we are modeling harmonic functions with harmonic functions, the absolute error function is also harmonic. Therefore, by the maximum principle of harmonic functions, the approximation function's maximum error is located on the problem boundary [1]. For example, let ϕ be a harmonic function on domain Ω. $\hat{\phi}$ is a harmonic function that approximates ϕ. Thus, $\phi - \hat{\phi}$ is harmonic in Ω. Consequently, $max_{(x,y)\in\Omega}|\phi - \hat{\phi}| = max_{(x,y)\in\partial\Omega}|\phi - \hat{\phi}|$.

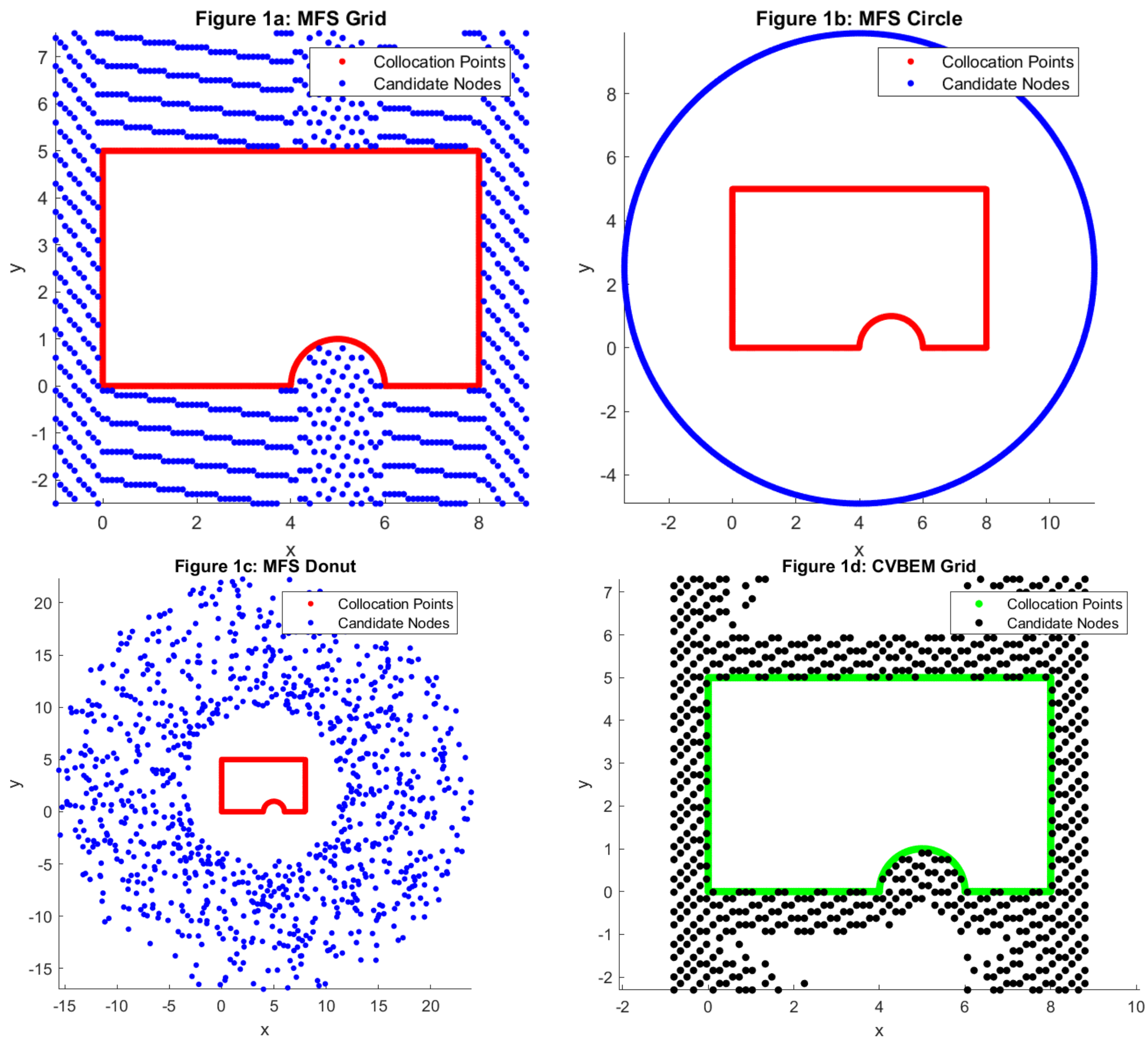
A recent development in treating computational node locations is utilizing another set of degrees of freedom known as the node positioning algorithm (NPA) [6]. NPA uses an initial set of candidate node locations as a baseline condition of determining the final set of node locations. The initial set of candidate node locations were developed using both a deterministic scheme and probabilistic approach to populate the study space with candidate nodes. While the NPA does not produce the optimal model, it has produced significant improvement in computational accuracy when compared with outcomes of these other techniques for node placement. The NPA for CVBEM works by selecting the best one node model, then the best two node model based on the selected node, then the best three node model based on the two selected nodes and so on, until the desired *n* node model based on *n*-1 selected nodes is built. In parallel, collocation points are placed at the two highest maxima of the error function [1 and 5].

This paper seeks to compare the accuracy of the NPA in CVBEM to the NPA in MFS and to determine the feasibility of using MFS to achieve the same task. Specifically, the NPA coupled with uniform, circular, and donut distributions of candidate nodes in MFS was compared to the previously used CVBEM method with the NPA.

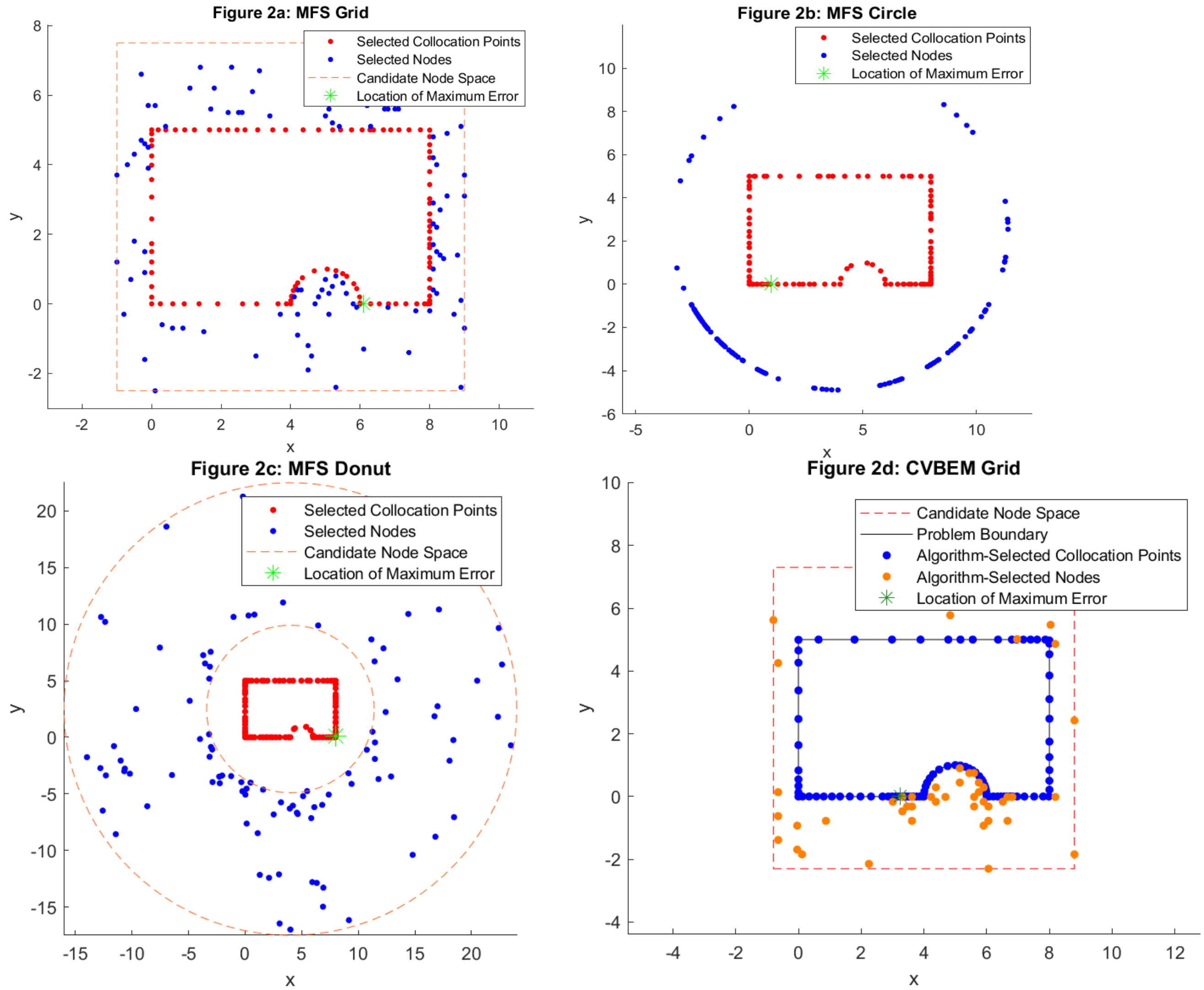
Results

Table 1: Definition of problem to be modeled.

Problem Definition	
Problem domain	$\Omega = f\{0 \leq x \leq 8, 0 \leq y \leq 5,$ and $(x-5)^2 + y^2 \geq 1\}$
Governing PDE	$\nabla^2 \psi = 0$
Boundary conditions	$\psi(\mathrm{x,y}) = \Re\left[z^2 + z + \frac{10}{z-5}\right] = x + x^2 - y^2 - \frac{50}{(x-5)^2+y^2} + \frac{10x}{(x-5)^2+y^2}, (x,y) \in \partial\Omega$
Number of candidate computational nodes	1000
Number of candidate collocation points	1000
MFS basis function	$g_{rv}(\boldsymbol{x}, \boldsymbol{x}') = -\frac{1}{2} log\lvert\boldsymbol{x} - \boldsymbol{x}'\rvert$ where $\boldsymbol{x} = \begin{bmatrix} x \\ y \end{bmatrix}$
CVBEM basis function	$g_{cv}(z, z') = (z - z')\ln(z - z')$, where $z = x + iy$
Degrees of freedom	100



Figures 1a-d: Pre NPA problem geometries. Figure 1a is MFS grid, figure 1b is MFS circle, figure 1c is MFS donut, and figure 1d is CVBEM grid.



Figures 2a-d: Post NPA problem geometries. Figure 2a is MFS grid, figure 2b is MFS circle, figure 2c is MFS donut, and figure 2d is CVBEM grid.

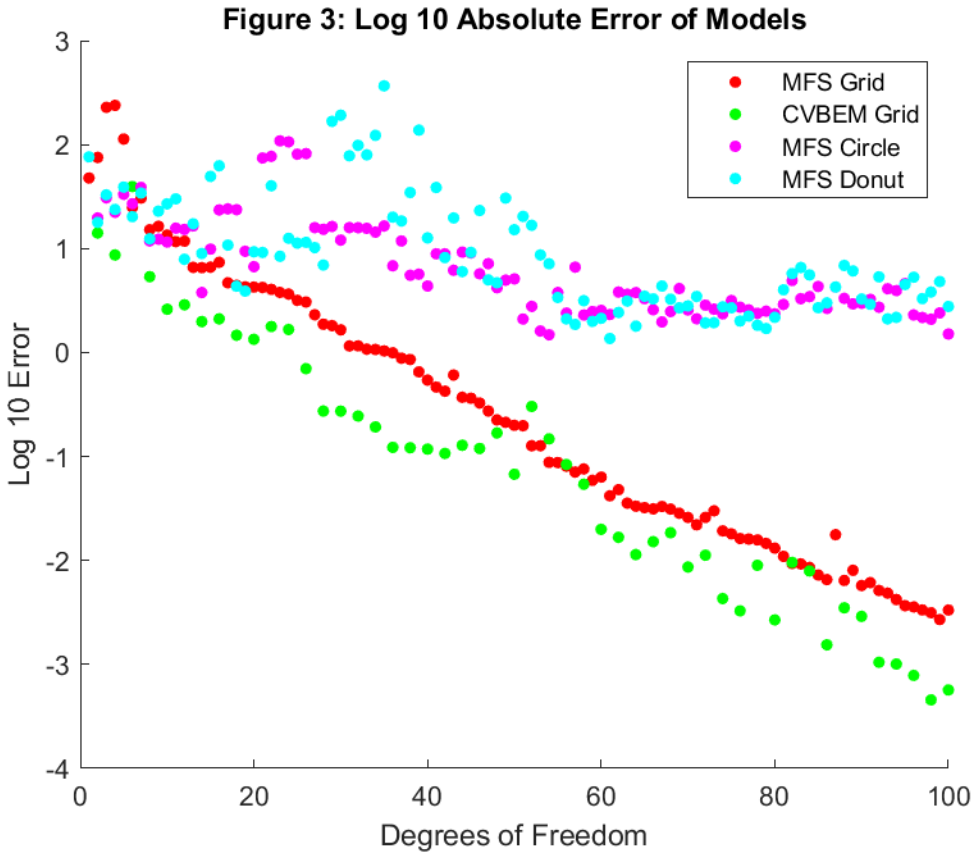
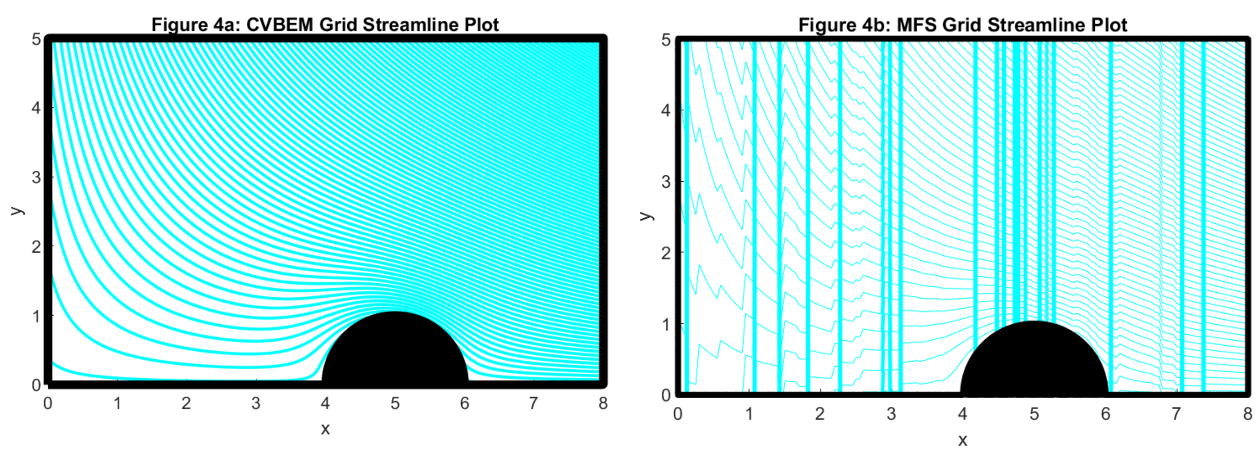


Figure 3: Each model's log10 absolute error plot for 100 degrees of freedom



Figures 4a-b: Streamline plots for CVBEM grid (figure 4a) and MFS grid (figure 4b). The CVBEM streamline plot exhibits smooth contours that can be used to track contamination, whereas the MFS streamline plot exhibits jagged behavior that hinders its efficacy in tracking contamination.

Three MFS models were selected to compare with the CVBEM model, and each model differed in their distribution of candidate nodes. The three models chosen were MFS grid (grid distribution), MFS circle (circle distribution), and MFS donut (donut distribution). The error for each model was plotted against degrees of freedom, so the MFS models used 100 nodes, whereas the CVBEM model used 50 nodes. The maximum absolute errors are as follows:

CVBEM: 5.6817e-04

MFS grid: 0.0033

MFS circle: 1.5061

MFS donut: 2.7732

Conclusions

CVBEM produced the most accurate model, outperforming the MFS grid by approximately 1 order of magnitude. However, at 52, 54, 56, and 84 degrees of freedom, the MFS grid performs slightly better than the CVBEM, which indicates that MFS can achieve errors at least as low as the CVBEM. The error of the MFS circle and donut models both appear to plateau after approximately 55 degrees of freedom, which suggests that their candidate node distribution is not conducive to computational accuracy. The streamline plots for groundwater flow analysis were only analyzed for the MFS grid and CVBEM grid candidate node distributions because only the MFS grid produced relatively similar computational error to the CVBEM grid. However, the streamline plot attained from the MFS grid through application of the Cauchy-Riemann equations contained jagged streamlines compared to the CVBEM streamline plot. Thus, groundwater contamination analysis cannot currently be performed as accurately utilizing the MFS. Further investigation should explore why this behavior occurs and compare the computational efficiency of the MFS in comparison to the CVBEM because MFS may perform faster due to only using real numbers.

References

[1] B.D. Wilkins, T.V. Hromadka II, AS-0020, W. Nevils, B. Siegel, and P. Yonzon, "Using a Node Positioning Algorithm to Improve Models of Groundwater Flow Based on Meshless Methods," *The Professional Geologist*, vol. 58, no. 2, 2021.

[2] T. V. Hromadka II and G.L. Guymon, "A complex variable boundary element method: development," *International Journal for Numerical Methods in Engineering*, vol. 20, pp. 25-27, 1984.

[3] C. S. Chen, A. Karageorghis, and Y. Li, "On choosing the location of the sources in the MFS", *Numerical Algorithms*, vol. 72, no. 1, pp. 107–130, May 2016.

[4] T.V. Hromadka II, "The complex variable boundary element method: Applications in determining approximative boundaries," *Engineering Analysis*, vol. 1, no. 4, 1984.

[5] B. D. Wilkins, T. V. Hromadka II, and J. McInvale, "Comparison of two algorithms for locating computational nodes in the complex variable boundary element method (CVBEM)," *International Journal of Computational Methods and Experimental Measurements*, vol. 8, no. 4, pp. 289-315, 2020.

[6] N.J. Demoes, G.T. Bann, B.D. Wilkins, K.E. Grubaugh, and T.V. Hromadka II, "Optimization algorithm for locating computational nodal points in the method of fundamental solutions to improve computational accuracy in geosciences modeling," *The Professional Geologist*, vol. 56, no. 1, 2019.

About the author

Saleem Ali is a mathematical sciences major at the United States Military Academy, who is majoring in mathematical sciences. His research experience includes the computational modeling of ideal fluid flow and studying the effects of time dilation in balloon satellite flight.

Contact Information

Saleem Ali: saleem.ali@westpoint.edu

Sebastian Neumann: sebastian.neumann@westpoint.edu

T. V. Hromadka II: tedhromadka@yahoo.com

Bryce D. Wilkins: bdwilkins95@gmail.com