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# THE PROFESSIONAL GEOLOGIST

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**Student Edition!**

**Classroom Earth**

*Peer Reviewed Articles:*

**Geoscience Modeling**

**Doppler Radar Estimates of  
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# The Professional Geologist

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On the Cover: Shirley Tsootsoo Mensah, SA-7566, from Eastern Illinois University at Yellowstone National Park's Upper Yellowstone Falls during summer field camp. Read about Shirley's experience at field camp on page 19 of this issue.

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# Optimization Algorithm for Locating Computational Nodal Points in the Method of Fundamental Solutions to Improve Computational Accuracy in Geosciences Modeling

## Authors

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## Abstract

Using the Complex Variable Boundary Element Method ("CVBEM") to model ideal fluid flow, a new algorithm is applied to an approximation method that reduces computational requirements while increasing matrix solution demands. Ideal fluid flow is examined by use of the algorithm with the CVBEM as a case study. Traditionally, the modeling nodes are placed on or close to the problem geometry boundary in a somewhat regular pattern. In the current paper, an algorithm is developed and demonstrated that optimizes node locations by examining the possible locations for nodes exterior of the problem domain and then measuring the computational accuracy of the corresponding approximation function with respect to the problem boundary conditions continuously specified on the problem geometry boundary surface. Application of the analysis approach to other similar problems in Geosciences is straight forward. A three-dimensional application towards modeling groundwater flow about a building foundation is examined as a case study. The methodology is gaining value within the Geosciences toolbox as experience with complex computational techniques continues to advance. The computational Method of Fundamental Solutions is also investigated with similar success.

**Keywords:** *Method of Fundamental Solutions, Optimization Algorithm, Complex Variable Boundary Element Method*

## Introduction

In this paper, the well-known three-dimensional source function is used as the basis function family from which specific basis functions are selected for an approximation function. The three-dimensional potential function approximation (real variable) examined is

$$\hat{u}(x, y, z) = \sum_{j=1}^n c_j \frac{1}{R_j}$$

where the  $c_j$ 's are constant real-valued coefficients determined by collocation of the approximation to candidate collocation points defined on the problem boundary; and the  $R_j$ 's are the usual non-zero radial distance measures between the nodal point locations ( $P_j$ 's) and arbitrary point  $P(x, y, z)$ . Other fundamental basis functions may be used that satisfy the governing partial differential equation (PDE) which in the current case, is the elliptic Laplace equation. Although variations on the PDE and additional sophistication may be readily included in the approximation, we only carry forward the basic formulation of the above equation. The focus of this paper is the description of the proposed nodal position optimization algorithm. As a case study, a three-dimensional brick-geometry problem domain is examined, representative of a high-rise building foundation element that is located in the midst of a highly urbanized area such as Los Angeles, California. The relevant soils are expansive clays and soil-water is abundant. At issue are the

solid-water pressures for purposes of designing dewatering system elements and protection against soil-water leakage in subterranean structures such as parking garages. In the problem, this geometry is positioned in the first octant of the usual three-dimensional coordinate system. The three dimensions are specified to be of different value. Figure 1 displays the problem setting.

The 3D geometry under detailed analysis has dimensions  $(x, y, z) = (8, 4, 2)$ . Several such elements are deployed in the building foundation, but only one such element is examined in this paper. For demonstration purposes, two three-dimensional (3D) potential functions are examined as case situations. These two 3D functions are defined by,

$$u_1(x, y, z) = \frac{1}{R}, R = \sqrt{x^2 + y^2 + z^2}, R \neq 0 \text{ and } u_2(x, y, z) = x^2 + y^2 - 2z^2.$$

Both of the above potential functions are entire functions defined throughout 3D space, and with values known continuously on the test problem boundary.

## Literature Review of MFS and BEM Nodal Point Positioning Techniques

The paper by C. S. Chen (2016) discusses a brief history of the Method of Fundamental Solutions (MFS) and the simplicity associated with this method that makes the method appealing [1]. In [1], Chen attempts to find the optimal node locations

for the MFS by utilizing two different search algorithms. Like many other computational methods, the origins of the MFS sprang from the convergent growth of computational thinking that coincides with the evolution of computational power as predicted by Gordon Moore [2]. The relationship between classic generalized Fourier Series theory [3] and the MFS, as well as many other computational approaches, including the more specialized Complex Variable Boundary Element Method (CVBEM) [4], is readily apparent. Many of these computational techniques can be shown to be generalized Fourier Series using specialized basis functions. For example, DeMoes (2018), in “35 Years of Advancements with the Complex Variable Boundary Element Method” (examines four different families of complex variable analytic basis functions [5]. In that paper, the computational approach is identical between schemes except that the basis function family is different. Yet, all these methods have the same underpinnings rooted in the generalized Fourier series approach to solving Partial Differential Equations (PDE). Additionally, the placement of both modeling node and collocation points were predetermined to be uniformly distributed without attempt to optimize the node and collocation point locations. In [1] and [6], among other papers [7–10], attention is paid to examining how to select locations for positioning computational nodes, among other issues, with no clear conclusion as to the best method for selecting computation node locations. For example, in [9] Carlos Alves uniformly distributes collocation points on the problem boundary and sources outside the boundary without determining which locations are best with use of the MFS. In 2015, Chen attempted to create an algorithm to find source locations that were “satisfactory” without proving the source locations to be the global maximum [10]. These papers indicate that there is significant variation in computational results depending on two key topics. The first is the choice of node locations. The second is the choice of collocation point locations. In the current paper, the focus is toward presenting a computational algorithm that addresses the computational node positioning problem by saturating a surrounding space of the problem domain with candidate node locations to be subsequently assessed in multiple node models based on the MFS, using the standard source function to generate basis functions. Of course, other PDE formulations and the choice of basis functions can be examined accordingly as long as they satisfy the Laplace equation and are analytic. Because collocation point locations are also subject to end-user preferences, the presented positioning algorithm used for selecting node locations is also applied to selecting collocation point locations on the problem boundary. Consequently, a set of ordered pairs of combinations of candidate locations of (node, collocation point) are developed and then examined as to computational model performance.

Thus, the approximation function includes node location and collocation location as variables as well as node and collocation point ordered pairs. The effectiveness of a particular model is measured, in this paper, by consideration of the usual RMS error (or  $E_2$  error) in matching problem boundary conditions and also examination of the maximum absolute value (or  $E_\infty$  error) in fitting to the problem boundary conditions. Obviously, other error norms can be examined. In the current paper, the effectiveness of the model is described by the dual measures of  $(E_2, E_\infty)$ .

The algorithm examined in this paper initiates by assessing the effectiveness of using a single node MFS model. This is the  $N=1$  situation of the algorithm. All candidate node locations are examined, in turn, in developing the respective single node

MFS model. Furthermore, the node positioning is cascaded with all candidate collocation point positions, producing a set of single node MFS models, each with a different node and collocation point combination. Once the entire space of said combinations are examined, the algorithm chooses the positioning ordered pair that has the minimum error measure outcome. This positioning order pair is then considered optimized and held fixed for further use in the evolving algorithm. The algorithm then continues to the  $N=2$  situation by developing all possible two-node and two-collocation point combinations. As with the  $N=1$  situation described above, all possible MFS models are developed and the corresponding error measures evaluated. However, in this situation the first node and the first collocation point optimized locations from the  $N=1$  situation described above are retained. As before, the algorithm chooses the second node and the second collocation point locations that minimize either of the error measures defined above. This completes the  $N=2$  situation. The algorithm continues to the  $N=3$  situation, and hence to larger  $N$  value situations, following the procedures described above. As the  $N$  value of the situation increases, the approximation computational error measure is reduced.

However, the use of the computational MFS involves issues such as the stability and accuracy of the underlying matrix solver. In our work, the matrix solver is a barrier that was not further examined. But because the algorithm results in a reduced error measure as  $N$  increases, the computational experiments indicate that fewer nodes and fewer collocation points can be used yet produce computational error measures that are as low as when using much larger but uniformly distributed node and collocation points. This means that with fewer nodes and collocation points involved in the MFS model, the matrix solver issue is generally more successful in producing a stable outcome.

## Optimization Algorithm Description

There are three types of modeling points that are used to determine the approximation function and its accuracy. The three types of points are candidate nodal points, candidate collocation points, and evaluation points. The candidate nodal points are points positioned exterior of the problem boundary that ultimately are the location of the basis function nodes used in the approximation function. The collocation points are points located on the problem domain that have known potential values and are used as the boundary conditions when determining the coefficients for each basis function in the approximation function. Lastly, the evaluation points are points on the problem boundary at different locations than the collocation points that enable the determination of error in the approximation function. Unlike the collocation and nodal points, evaluation points act independently of the other two model points. Nodal points and collocation points are related in that the pairing between one nodal point and one collocation point determines the coefficient of the basis function at that specific nodal point. Evaluation points exist solely to determine the error associated with the approximation function. Root means squared (RMS) error is used as the evaluation criteria for optimum node location, and also maximum absolute error (Max error).

To determine the optimum pairing between a specific node and a specific collocation point each node must be tested with each collocation point and the RMS error and Max error associated with that approximation function must be recorded. The following algorithm outlines the process by which nodal point and collocation point pairs are determined and optimized.

1. Create a pool of node points located exterior of the problem domain. This set should be in no particular pattern. Randomness in coordinates is beneficial.
2. Create a pool of collocation points located on the problem boundary. These are locations where the potential is known.
3. Create a one node approximation function for each combination of node and collocation point. Record the error for each.
4. Select the node and collocation pair that produced the least error.
5. Create a two node model, utilizing the selected pair from step 4 as one of the node pairs.
6. Test all two node approximations for error. The approximation function that results in the least error becomes the best two node model.
7. Repeat steps 4-6 until the number of nodes desired in the model is reached.

The following test problems are examined to demonstrate the validity of the algorithm.

## Example Problem: Pressure Source

To demonstrate the algorithm, a concerning soil-water pressure source, such as a longitudinal crack along the surface of a high pressure water pipeline, leads to detailed analysis, including forensic as well as remediation examination, involving complex computational modeling methods. The pipeline exerts pressure uniformly and can be modeled by the equation,

$$u_1(x, y, z) = \frac{h}{\sqrt{(x-x_j)^2 + (y-y_j)^2 + (z-z_j)^2}}$$

where  $h$  = the constant pressure source strength defined at source location  $(x_j, y_j, z_j)$ . The approximation function is defined by

$$\hat{u}_1(x, y, z) = \sum_{k=1}^n \alpha_k \frac{1}{R_k}$$

where  $\alpha_k$  is a real-valued coefficient, and

$$R_k = \sqrt{(x-x_k)^2 + (y-y_k)^2 + (z-z_k)^2}$$

where  $(x_k, y_k, z_k)$  is the  $k$ th node. To solve for the  $\alpha_k$ 's, pressures must be defined on the boundary. These locations  $P_l = (x_l, y_l, z_l)$ , points on the boundary become the collocation points where the pressure is known, by measuring the pressure at location  $P_l$ . Set  $k = l$  so there are an equal number of nodes and collocation points. The resulting collocation matrix equation results in the coefficients corresponding to each node, and produces an approximation function to approximate pressure on and within the problem domain.

The problem domain is located in the first octant. It is positioned so that the origin or bottom right corner is located at  $(1, 1, 1)$ , and has length = 8, depth = 2, and height = 4. The test problem is another source function with source point located at the origin  $(0, 0, 0)$  where  $h = 1$ .

Figure 1 depicts the problem domain and the location of the test pressure source as a star at  $(0, 0, 0)$ .

The solution to this boundary value problem is,

$$u(x, y, z) = \frac{1}{\sqrt{x^2 + y^2 + z^2}}, x, y, z \geq 0.$$

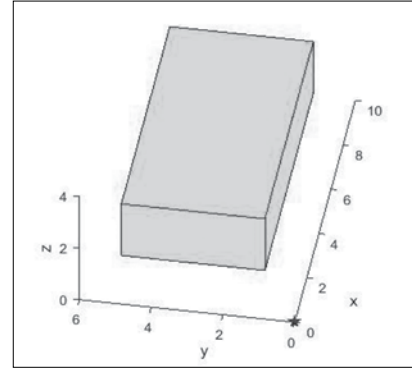


Figure 1 - Problem Domain

To create the space of candidate node locations for use in the basis function definition, an adequate amount of nodes must be assessed. To minimize the algorithm's run time, the number of node locations examined is limited to 512. Figure 2 depicts the location of each of the candidate nodes.

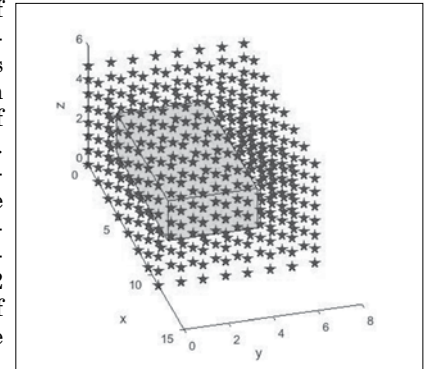


Figure 2 - Candidate node locations assessed.

Similar to the creation of the nodes, candidate collocation point locations must be positioned on the problem boundary. The number of collocation points need not be the same as the number of candidate node locations. For this example, there will be 1000 candidate collocation points. Figure 3 depicts the distribution of candidate collocation point locations.

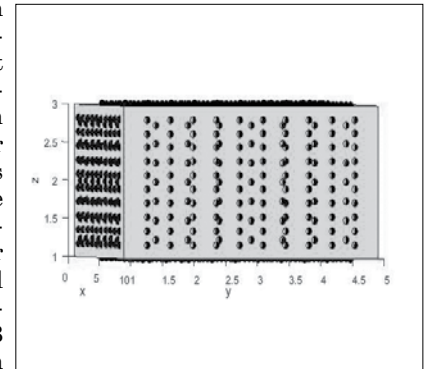


Figure 3 - Candidate collocation points in the problem domain.

The accuracy of each one node approximation function must be evaluated and compared. Let  $n$  = the number of candidate nodes and  $m$  = the number of candidate collocation points. To test accuracy, every combination of candidate nodes and candidate collocation points will be paired and used to create an approximation function. Thus, there will be  $n \times m$  approximation functions to be compared for computational error. The ordered pair with the least error is deemed the optimized node and collocation point location and combination for use in a one node model. Table 1 demonstrates the comparison of errors that occurs automatically within the algorithm for the one test node model and 5 test collocation locations.

Because the number of possible combinations of nodes and collocation points for the sample size that is used is large the first five error assessments are presented to give insight into the process that is occurring. Table 1 lists the possible ordered pairs for a one node model with five choices for col-

location point locations. If the ordered pairs listed in Table 1 were the only possible combinations that could be used for the approximation, then the algorithm would choose ordered pair 3 because it has the least error.

Utilizing a test pool of 1000 nodes and 729 collocation points, the best node to collocation point pair to approximate this pressure source is node (.01,.01,.01) and collocation point (3.18,5,1.36). The RMS error associated with this pair is .000164 and the max error was 0.00116. This result is expected because the approximation function picks the node that is closest to where the actual source function is located. Essentially, when using a one node model to model a single source the approximation function will simply attempt to "copy" the source.

Following the algorithm, the one node ordered pair is now held as the first node

**Table 1 - Record of Computational Error for the Single Node Models**

Ordered Pair	Node	Collocation Point	RMS Error
1	(11, 7, 5)	(5, 5, 2)	0.1085
2	(11, 7, 5)	(5, 1, 2)	0.2059
3	(11, 7, 5)	(9, 3, 2)	0.0836
4	(11, 7, 5)	(1, 3, 2)	0.4281
5	(11, 7, 5)	(5, 3, 3)	0.1317

selected in the next two node model and also is removed from the candidate ordered pairs for future selections. The algorithm now tests for the best two node solution keeping the optimum node and collocation pair from the one node model as one of the two nodes. This process is then repeated for each additional node until there are n basis functions in the approximation function.

Figures 4 - 9 are visualizations of the Approximate Solution using the Complex Variable Boundary Element Method optimization algorithm developed in this paper (left hand graphs), the analytical solution (center graphs) and the difference between them (right hand graphs) for representative orthogonal planar sections through the problem domain shown in Fig.1., using 10 nodes. The contours are unitless and display the

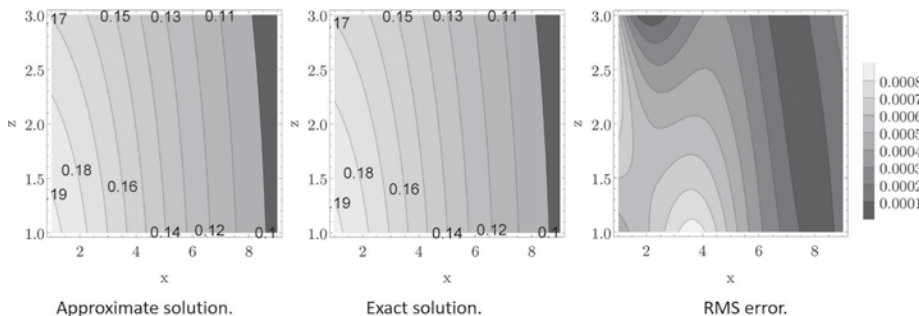


Figure 4: Computational results on the x-z plane where  $y=5$ .

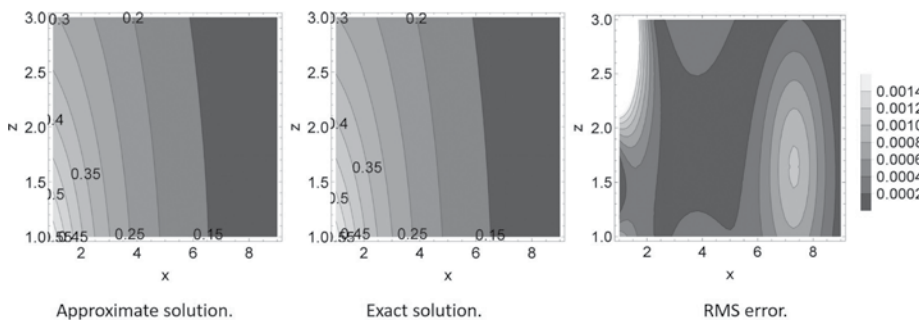


Figure 5: Computational results on the x-z plane where  $y=1$ .

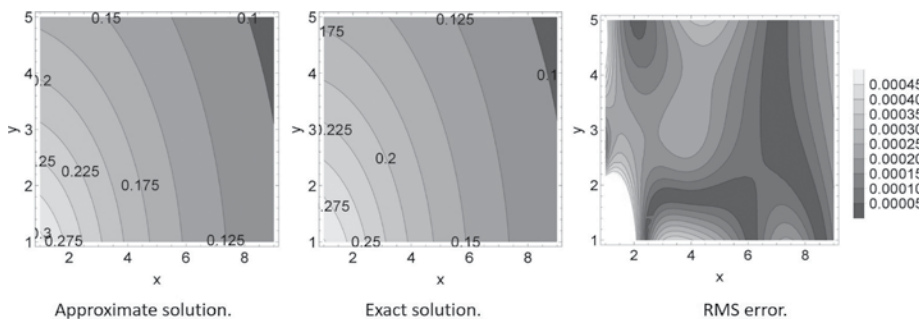


Figure 6: Computational results on the x-y plane where  $z=3$ .

## Two New Student Chapters Join AIPG!

Welcome,  
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and  
University of Alabama!



University of Alabama Student Chapter Group Photo: Marcella McIntyre-Redden, Geological Survey of Alabama and Alabama Geological Society; Richard Katz, Retired Mining Engineer/Geologist (Speakers on Left); Dr. Andrus University of Alabama Dept Chair, Geological Sciences; Student Officers, Caryl Orr AIPG Member Sponsor

# The Courses You Should Have Taken, but Did Not or Could Not

Lawrence Cerrillo, CPG-02763

The courses that may or may not be offered at your institution of higher learning are: conflict resolution and speech. Both are generally not within the earth sciences departments, but both are invaluable in your career. Regardless of the discipline you eventually specialize in - oil and gas, mineral exploration, hydrogeology, or environmental geology - all will require the knowledge and skills imparted by these two fields of study. Whether you are dealing with local, state, or federal agencies, conflicts are inevitable. Conflict within the workplace can also be unavoidable, add to that the almost inevitable dealings with the NIMBY members of the public, as well as with other anti-mineral or anti-fossil-energy organizations, and it is certain that you will be dealing with conflict. It is not practical to pursue the many facets of conflict resolution, but it is critical to know some of the basics that will make your job easier.

As regards a speech course, if you hope to advance in your profession, you will often be required to give presentations on the work you have done. This may be a presentation to upper management, a client, or at a professional meeting. Being able to present your work in a clear and timely speech will do wonders for career advancement.

The good news is that you may be able to obtain this knowledge after graduating. It is a bit more challenging and will require discipline and perseverance, but it is doable. Depending upon where you end up working, you may find adult education courses offered at a community college or a university college. Public speaking can be learned and practiced through a local chapter of Toastmasters. Toastmasters clubs are prevalent in many locations and can often even be found in small rural towns. With today's access to the internet, I suspect you may find numerous resources available to get proficient in both of these disciplines.

Give it a go, you will be glad you did!

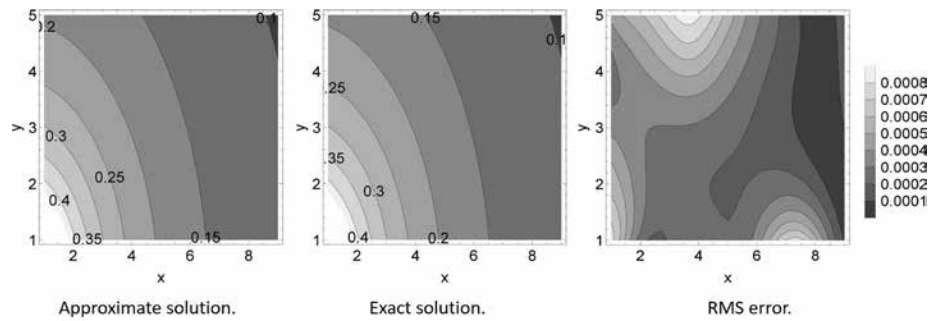


Figure 7: Computational results on the x-y plane where  $z=1$ .

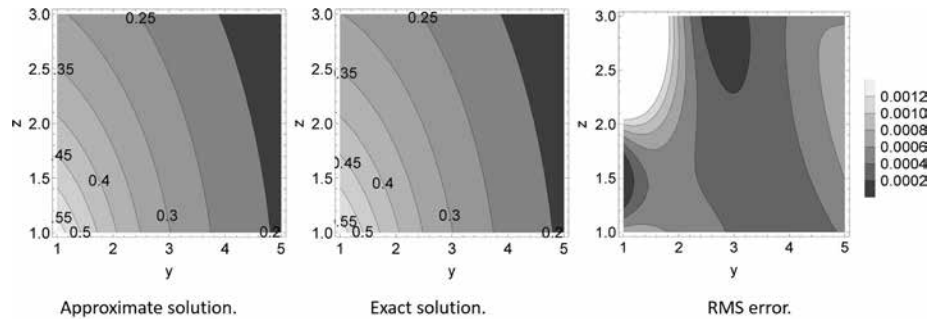


Figure 8: Computational results on the y-z plane where  $x=1$ .

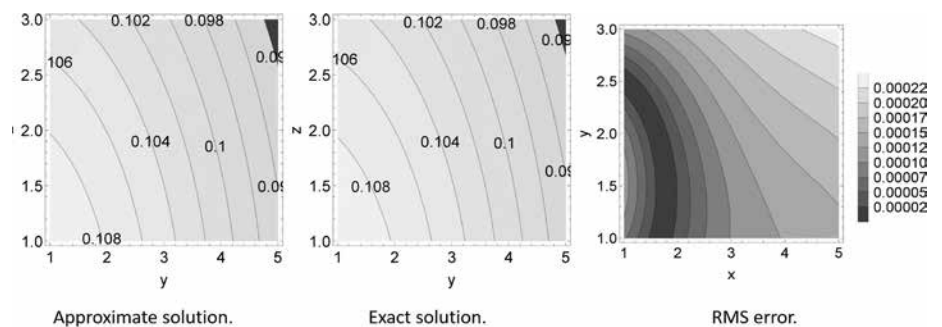


Figure 9: Computational results on the y-z plane where  $x=9$ .

error given the differing numerical solution methods. The results in Figure 16 demonstrate the error of 10 different approximation functions ranging from 1-10 nodes. The nodes were picked from a test pool of 64 candidate node and 125

candidate collocation point locations.

## Test Problem 2

A more computationally difficult problem is examined. The analytic solution to this boundary value problem is

$$u_2(x,y,z)=x^2+y^2-2z^2.$$

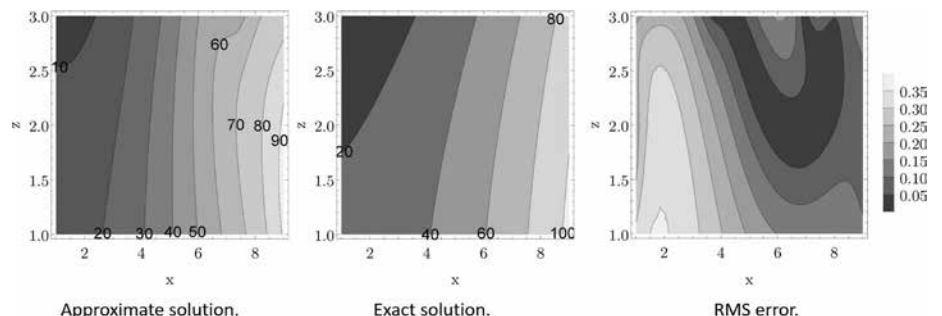


Figure 10: Computational results on x-z plane where  $y=5$ .

The same collocation and node candidate locations and problem domain as used in Problem 1 will be used to approximate the solution for this new test case.

Figs. 10 through 15 are visualizations of the solutions to Test Problem 2 constructed in the same way as were Figs. 4 through 9, for the case of 20 approximation functions.

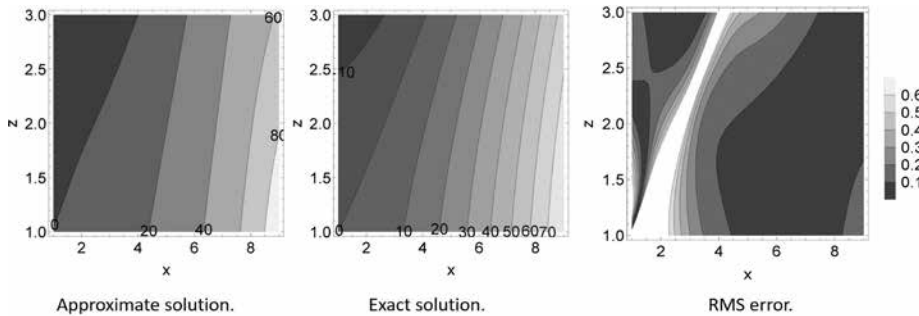


Figure 11: Computational results on x-z plane where  $y=1$ .

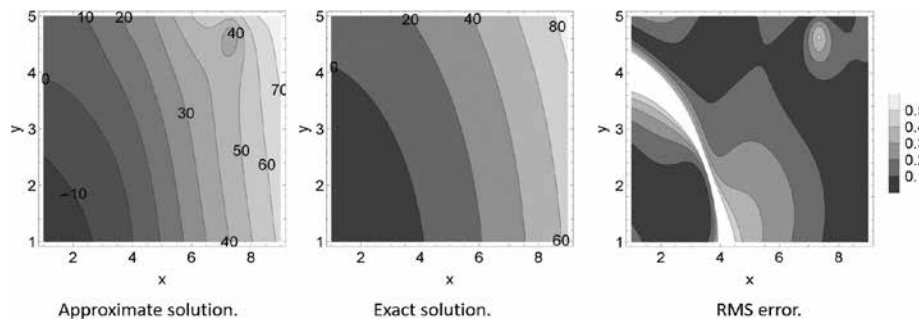


Figure 12: Computational results on x-y plane where  $z=3$ .

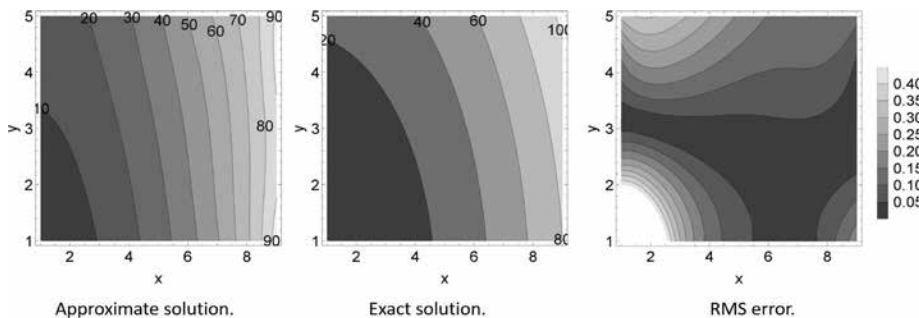


Figure 13: Computational results on x-y plane where  $z=1$ .

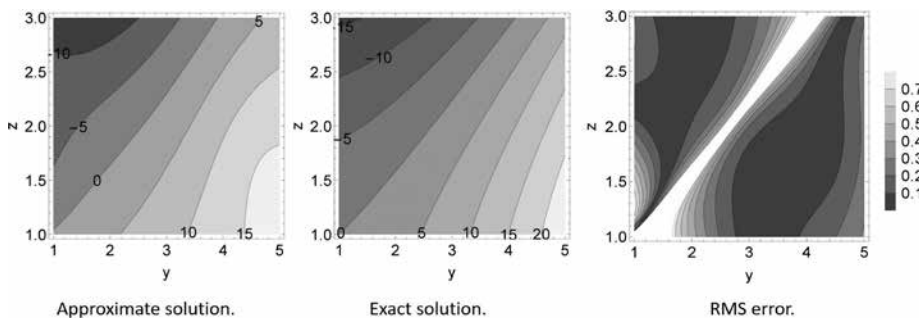


Figure 14: Computational results on y-z plane where  $x=1$ .



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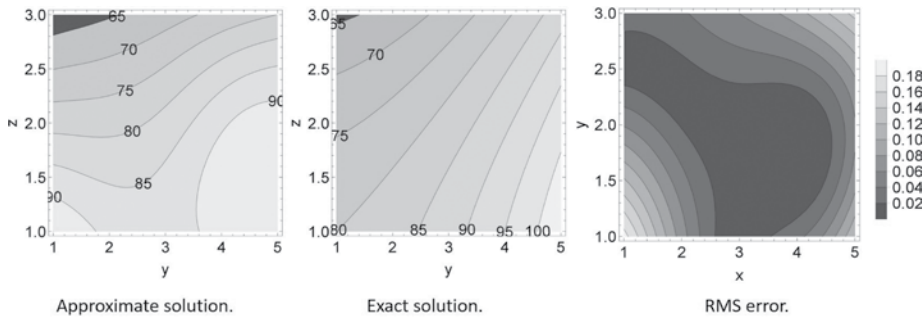


Figure 15: Computational results on y-z plane where x=9.

## Discussion of Computational Results

For Example 1, computational error decreases as the number of nodes used to approximate the exact solution increases. Remember that the analytic solution to this boundary value problem is

$$u(x, y, z) = \frac{1}{\sqrt{x^2 + y^2 + z^2}}, x, y, z \geq 0.$$

The basis functions used in the approximation are of the form

$$\frac{1}{\sqrt{(x-x_j)^2 + (y-y_j)^2 + (z-z_j)^2}}.$$

Thus, the one node approximation selects the node closest to the origin of the source function it attempts to model. When additional nodes are added in an attempt to better the approximation, error decreases, but the change in error between each additional error decreases. Figure 16 depicts the reduction in error that occurs when a higher n approximation function is used to approximate pressure.

Example problem 2 had similar error reduction patterns when more basis functions were introduced in the approximation function. Figure 17 depicts the

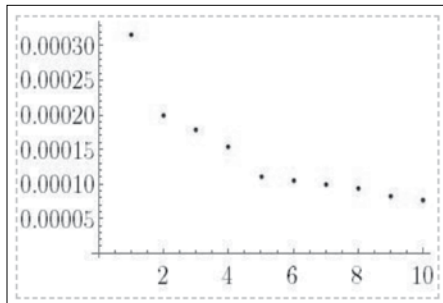


Figure 16: Error reduction depiction with increasing node use.

RMS error for 20 approximation basis functions with models developed for 1 to 20 basis functions for example problem 2.

The figure shows the error decreases, but takes longer than the first test problem and has more error than the first test

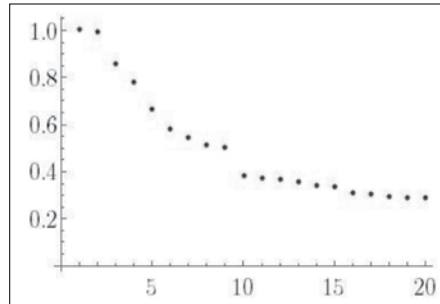


Figure 17: RMS error for twenty approximation functions.

problem. Because of the computational difficulty of this problem more nodes are necessary to gain a better approximation.

## Conclusions

Although there are some observations stated in the literature as to computational accuracy improvement by use of different nodal point location strategies, there is not a formalized procedure for identifying the optimum location of modeling nodes that minimize computational error goals. Such a formal procedure is presented in this paper in the form a new algorithm that enables such optimum node locations to be identified. The locations of modeling nodes are treated as additional degrees of freedom in the computational modeling effort to reduce computational error in achieving problem boundary conditions. As expected, the use of the presented algorithm improved computational modeling accuracy. The over-arching conclusion can be made that the associated increase in available degrees of freedom provides significant additional opportunities in reducing computational error. Additionally, the ability to optimize node locations enables the reduction in the number of basis functions required to create an approximation function with the same amount of computation error as previous approxima-

tion functions that required more basis functions. The reduction in the number of basis functions required to create an approximation function with error below tolerance reduces the likelihood of an ill-conditioned matrix when solving for the coefficients in the approximation function.

## Recommendations for Future Research

The algorithm explores a set of possible node locations, collocation point locations, and node, collocation order pairs. Because the algorithm is greedy the time to run the algorithm is expensive resulting in a restriction to the number of nodes and collocation points in the set of possible locations. Different problems will inherently result in different node locations. Future research into an algorithm that can reduce the set to only the most probable locations to offer the best approximation. This type of algorithm would use the gradient as criteria for deciding where to place more or less nodes.

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