

SIAM Conference on
**Mathematical
& Computational Issues**
in the Geosciences



March 11 – March 14, 2019
Houston Marriott Westchase
Houston, Texas, U.S.

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Tuesday, March 12

PP1

Coffee Break and Poster Session **Posters will be on display during Tuesday coffee breaks**

continued

Development of a Numerical Framework for the Study of Solid Earth Tides

Mattia Penati, Edie Miglio, and Simone Carriero, Politecnico di Milano, Italy

Characterizing Volumetric Strain at Brady Hot Springs, Nevada, USA using InSAR, GPS, Numerical Models and Prior Information

Elena C. Reinisch, Michael Cardiff, and Kurt L. Feigl, University of Wisconsin, Madison, U.S.

Effective Models for Two-phase Flow in Porous Media with Evolving Interfaces at the Pore Scale

Sohely Sharmin and Iuliu Sorin Pop, Hasselt University, Belgium; Carina Bringedal, Universität Stuttgart, Germany

Novel Principles for Effective Earth Model Grid Management While Geosteering

Erich Suter and Helmer Andre Friis, NORCE Norwegian Research Centre, Norway; Terje Kårstad and Alejandro Escalona, University of Stavanger, Norway; Erlend Vefring, NORCE Norwegian Research Centre, Norway

Imaging of Densely Located Many Point-like Scatterers by the Application of the Pseudo Projection Method and Kirchhoff Migration

Terumi Touhei and Taizo Maruyama, Tokyo University of Science, Japan

Joint Inversion of Surface Wave Dispersion and Bouguer Gravity Anomalies using Constrained Optimization

Azucena Zamora, University of Texas at El Paso, U.S.; Anibal Sosa, Universidad Icesi, Colombia; Aaron Velasco, University of Texas at El Paso, U.S.

Generalized Approximate Static Condensation Method for a Heterogeneous Multi-material Diffusion Problem

Alexander Zhiliakov, University of Houston, U.S.

Performance and Cost Analysis of Single and Double U-Tube Ground Heat Exchangers

Paul Christodoulides, Cyprus University of Technology, Cyprus; Mateusz Zerun, Polish Geological Institute, National Research Institute, Poland; Lazaros Aresti, Soteris Kalogirou, and Georgios Florides, Cyprus University of Technology, Cyprus

Mathematical Modelling of the Removal of Micropollutants. I Linear Cometabolism Model

Rubayyi Alqahtani, Imam University, Saudi Arabia

Advances in use of Meshless Computational Methods in Geosciences and Related Topics

T.V. Hromadka II, United States Military Academy, U.S.; Kameron Grubaugh, Independent Researcher; Aidan Doyle and Anton Nelson, United States Military Academy, U.S.; Bryce Wilkins, Massachusetts Institute of Technology, U.S.

Tuesday, March 12

MS14

HPC Methods in the Geosciences - Part II of II

9:45 a.m.-11:50 a.m.

Room: Grand Ballroom EFGH

For Part 1 see MS6

Many phenomena in geophysics, such as mantle convection, seismic wave propagation, oceanic circulation, and the motion of land and sea ice are characterized by complex multiscale physical processes. Accurate computer simulations of these phenomena require suitable mathematical models, high spatial and temporal resolution and, thus, efficient parallel algorithms and implementations. The immense compute power on current and future supercomputers is indispensable for this research, but it brings along challenges for software development, mathematical modeling and the construction of efficient and scalable algorithms. This minisymposium is addressed at researchers working in the interdisciplinary field of complex modeling, mathematical algorithms and their implementation for grand-challenge applications in geophysics on state-of-the-art supercomputers. A special focus is on the reusability and the high-performance awareness of the presented approaches in different software packages.

Organizer: *Lorenzo Colli*
University of Houston, U.S.

Organizer: *Markus Huber*
Technische Universität München, Germany

Organizer: *Georg Stadler*
Courant Institute of Mathematical Sciences, New York University, U.S.

Organizer: *Barbara Wohlmuth*
Technische Universität München, Germany

9:45-10:05 Improved Newton Linearization for L^1 -Norm-type Minimization with Application to Viscoplastic Fluid Solvers

Johann Rudi, University of Texas at Austin, U.S.; *Georg Stadler*, Courant Institute of Mathematical Sciences, New York University, U.S.; *Omar Ghattas*, University of Texas at Austin, U.S.

Advances in the use of Meshless Computational Methods in Geosciences and Related Topics

Bryce D. Wilkins¹, T.V. Hromadka II², Aidan Doyle², Anton Nelson², Kameron Grubaugh³

¹ Massachusetts Institute of Technology ² United States Military Academy ³ Independent Researcher

Abstract

Many applied problems in geoscience involve the use of computer models to simulate phenomena of interest. These simulations often entail approximating the solution to a boundary value problem (BVP) of a partial differential equation (PDE). Research seeking to improve computational methods for approximating the solutions to these BVPs continues with advances providing increased computational accuracy and reduced computational burden. Of recent interest in numerical methods for PDEs are the techniques generally classified as mesh reduction methods. Many of these numerical methods require the user to locate computational nodes (alternatively, source points) as part of the modeling process. For these methods, the accuracy of the resulting BVP model depends on the selected locations of the computational nodes. Consequently, procedures for locating these computational nodes so that the resulting BVP model is sufficiently accurate are of great importance. This poster summarizes our group's recent progress in developing a procedure for locating the computational nodes that are commonly encountered in the computer implementation of mesh reduction numerical methods for PDEs.

Introduction

Since mesh creation is often the most time-consuming part of modeling PDEs when using the popular domain-based approaches such as the finite element and finite difference methods, increasing the viability of mesh reduction methods has been the subject of much recent research. However, many of the mesh reduction numerical methods that have been developed incorporate the use of computational nodes that must be located during the modeling process. Since, the accuracy of the resulting BVP model depends on the locations of the computational nodes it is important to have a procedure for determining suitable locations for the nodes. In this work we describe a Node Positioning Algorithm (NPA) that includes our new **refinement procedure**, which allows for the locations of previously-located nodes to be updated if there exists a new location for the node that would result in a BVP model with greater accuracy. Although the NPA that is proposed in this work could be applied to any of the PDE mesh reduction methods that require the modeler to specify the locations of computational nodes, we will demonstrate the NPA by applying it to a Complex Variable Boundary Element Method (CVBEM) model of potential flow over a half-cylinder.

The New Node Positioning Algorithm

The new refinement procedure is a useful addition to recent NPA efforts due to its monotonic improvement of the PDE method's approximation function since upon each application of the refinement procedure, either (i) the current model is kept so that there is no change in overall approximation error, or (ii) a previously-located node is exchanged for a node in a different location so as to reduce the overall approximation error. Therefore, with each application of the refinement procedure, the approximation error of the model either stays the same or decreases, but never increases.

NPA ALGORITHM APPLIED TO THE CVBEM:

1. Input n , which is the number of terms that will be used in the linear combination of the approximation function.
2. Create a set of candidate computational nodes and a set of candidate collocation points. The set of candidate computational nodes must include at least n nodes, and the set of candidate collocation points must include at least $2n$ points.
3. **Initialize:** search all combinations of 1 computational node and 2 collocation points for the 1-node model resulting in the least maximum error.
4. **Repeat (a)-(e) for $k = 2, \dots, n$:** construct the CVBEM model one node at a time by repeating the following steps.
 - (a) Use the current CVBEM model to compute the error function along the boundary.
 - (b) Determine the locations of the local maxima of the error function.
 - (c) Place one new collocation point at the each of the two maxima of the error function with greatest magnitude. The model now has $k - 1$ nodes and $2k$ collocation points. See Figure 1 for a depiction typical depiction of the error function mapped from the boundary of the problem domain onto a line segment. The two maxima of interest of the error are shown as blue dots in the figure.
 - (d) Test all of the candidate computational nodes to see which additional node will result in the CVBEM model of least maximum error. Add the new computational node to the model. The model now has k computational nodes and $2k$ collocation points.
 - (e) **Repeat for $j = 1, \dots, m_1 \times k$:** where m_1 is the number of iterations of refinement
 - i. Let $p = \text{mod}(j, k)$. If $p = 0$, then replace p with $p \leftarrow k$. p is the index of the computational node whose location is being refined.
 - ii. Remove the p^{th} -selected node from the CVBEM model. The model now has $k - 1$ nodes and $2k$ collocation points.
 - iii. Test all of the candidate computational nodes to see which node will result in the CVBEM model of least maximum error. Add the new computational node to the model replacing the p^{th} -selected node that was previously removed. The model now has k computational nodes and $2k$ collocation points.
5. **Repeat for $j = 1, \dots, m_2 \times k$:** where m_2 is the number of iterations of refinement
 - (a) Let $p = \text{mod}(j, k)$. If $p = 0$, then replace p with $p \leftarrow k$. p is the index of the computational node whose location is being refined.
 - (b) Remove the p^{th} -selected node from the CVBEM model. The model now has $k - 1$ nodes and $2k$ collocation points.
 - (c) Test all of the candidate computational nodes to see which node will result in the CVBEM model of least maximum error. Add the new computational node to the model replacing the p^{th} -selected node that was previously removed. The model now has k computational nodes and $2k$ collocation points.

In the algorithm above, the refinement procedure (written in green text) is implemented twice: once at Part (e) of Step 4, and a second time at Step 5. The implementation that occurs at Part (e) of Step 4 refines the locations of the computational nodes as each new node is added to the model. The implementation that occurs at Step 5 only refines the locations of the computational nodes after all of the nodes have been selected. For a faster implementation, it is possible to forgo the Refinement Procedure at Part (e) of Step 4 and only do the refinement after having selected all of the nodes without using the Refinement Procedure. When Part (e) of Step 4 is omitted, the BVP model is obtained more quickly, however, usually at a cost to the accuracy of the model. However, only applying the refinement procedure at Step 5 is better than not applying it at all.

Visualization of The Refinement Procedure

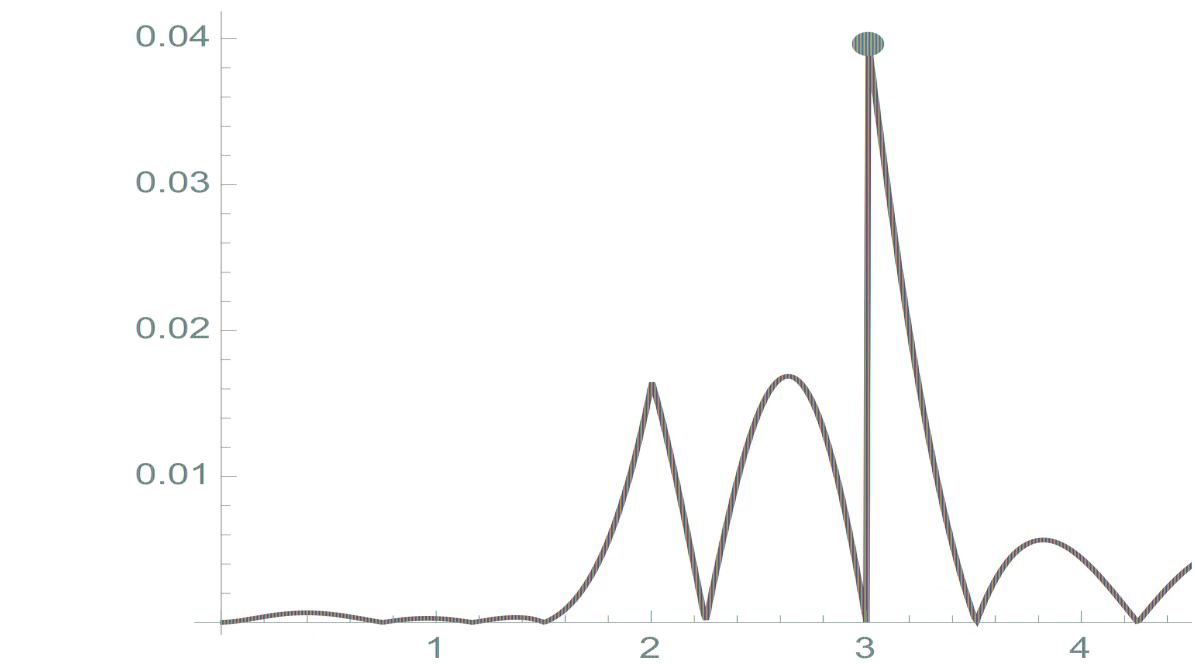
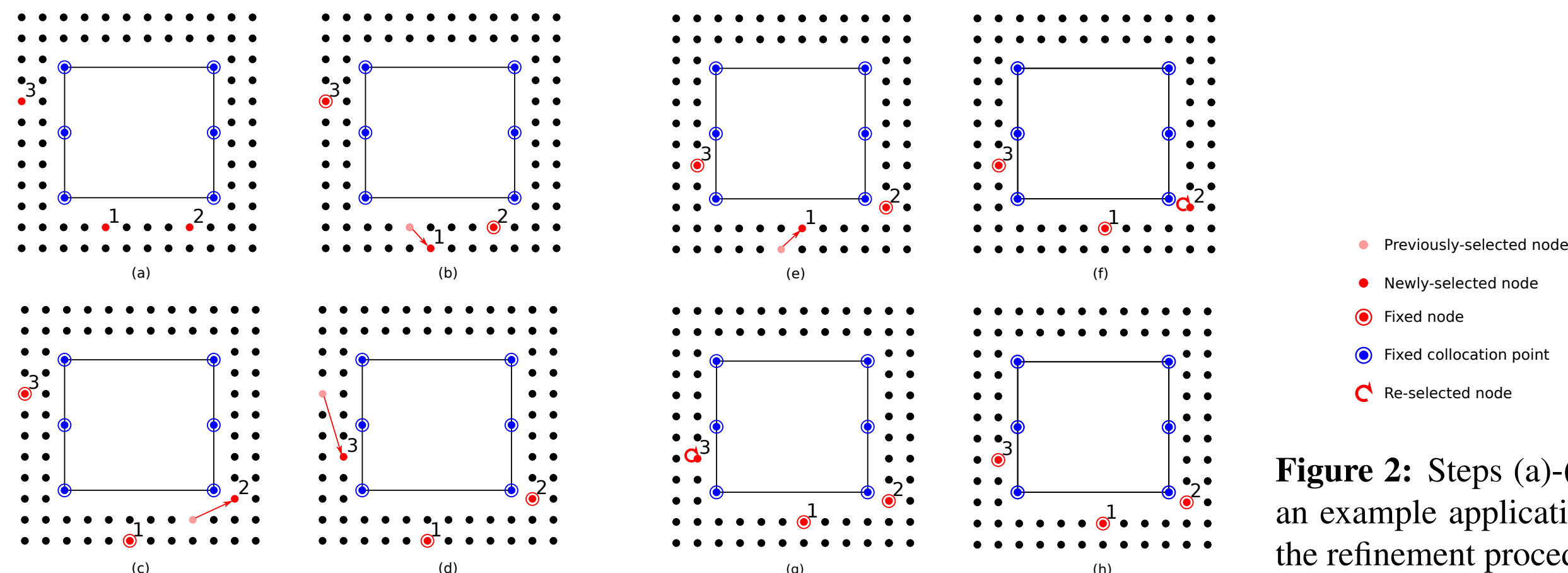


Figure 1: Typical plot of the CVBEM error function along the boundary of a sample problem domain. In this figure, the problem boundary has been mapped using a bijection onto the line $[0, 6]$. The two local maxima of the error function with greatest magnitude are depicted as blue dots. The two new collocation points would be located at the points on the problem boundary corresponding to the locations of these two maxima.

Example Problem: Potential Flow Over a Half-Cylinder

Problem Statement:

Domain: $\Omega = \{(x, y) : -10 \leq x \leq 10, 0 \leq y \leq 20, \text{ and } x^2 + y^2 \geq 1\}$
PDE: $\nabla^2 \psi = 0$
Boundary Conditions: $\psi(x, y) = \Im[\omega(z)], \quad (x, y) \in \partial\Omega$
Number of Candidate Computational Nodes: 1,500
Number of Candidate Collocation Points: 20,000

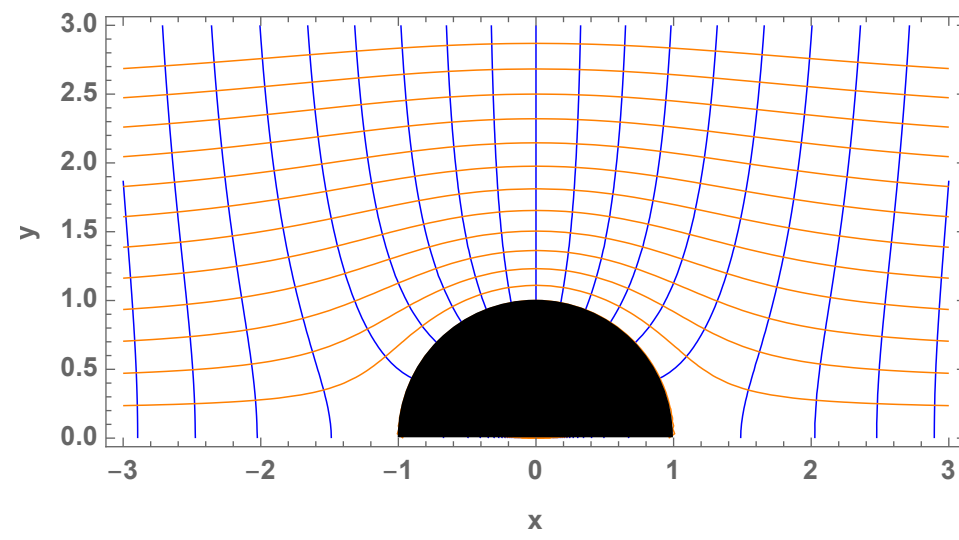


Figure 3: Contour plot of the analytic solution for potential flow over a half-cylinder. The exact solution is $\omega(z) = z + 1/z, \quad \Im[z] \geq 0$. The depicted flow net is obtained by plotting contours (level curves) of the real and imaginary parts of ω . This example problem contains two stagnation points, located at $(-1, 0)$ and $(1, 0)$, respectively, at which the curvature of the solution is most extreme.

The exact representation of the velocity potential for this problem is given by

$$\omega(z) = z + 1/z, \quad \Im[z] \geq 0. \quad (1)$$

Since the exact solution is analytic everywhere except for $z = 0$, the real and imaginary parts of ω are harmonic functions in $\mathbb{C} \setminus \{0\}$ and thus harmonic throughout Ω . Consequently, the CVBEM is well-suited for modeling the velocity potential of this example problem. Moreover, the availability of the exact solution for this flow situation, as given in Equation (1), allows for a precise description of the computational error of the CVBEM model, which is useful for the purpose of assessing the efficacy of the new NPA.

Graphical Results

In the figures below, emphasis is given to the north pole of the half-cylinder, which is located at $(0, 1)$, as well as to the two stagnation points, located at $(-1, 0)$ and $(1, 0)$, respectively, where the curvature of the local flow situations are most extreme. The high-precision computational modeling that is required in order to provide a satisfactory approximation of this flow is the reason that this problem has been selected to demonstrate the application of the NPA to the CVBEM.

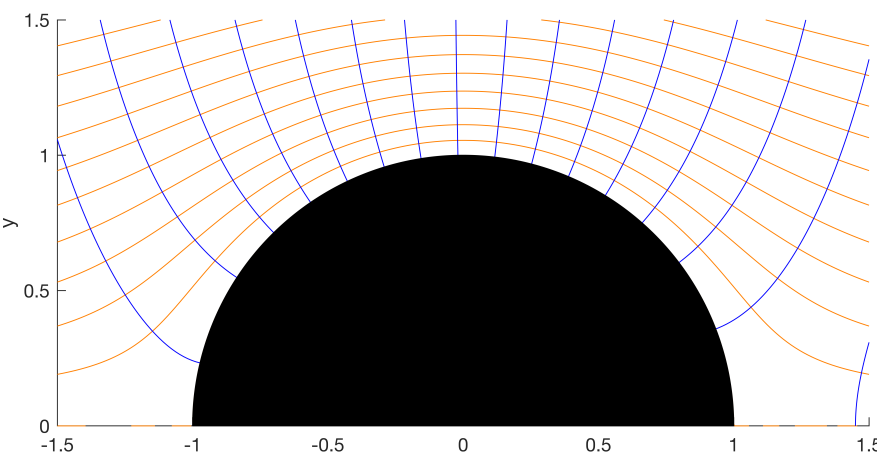


Figure 4: Magnified view of the CVBEM approximation of the flow regime depicted near the obstacle. The curvature of the solution increases near the north pole of the half-cylinder. Besides the stagnation points, the north pole is the location of greatest curvature in the exact solution, which makes it difficult to model.

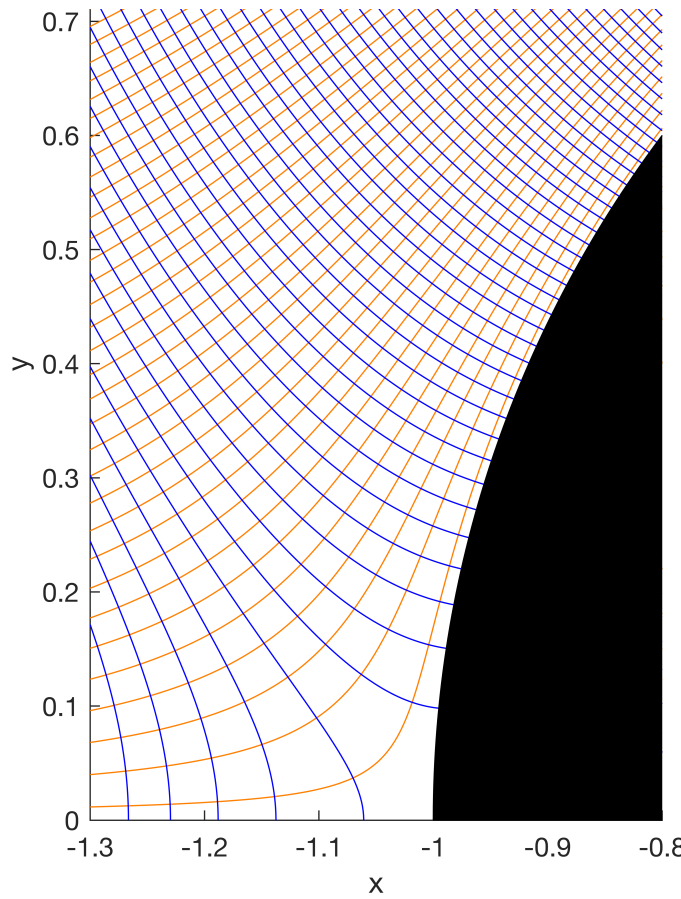


Figure 5: Left stagnation point

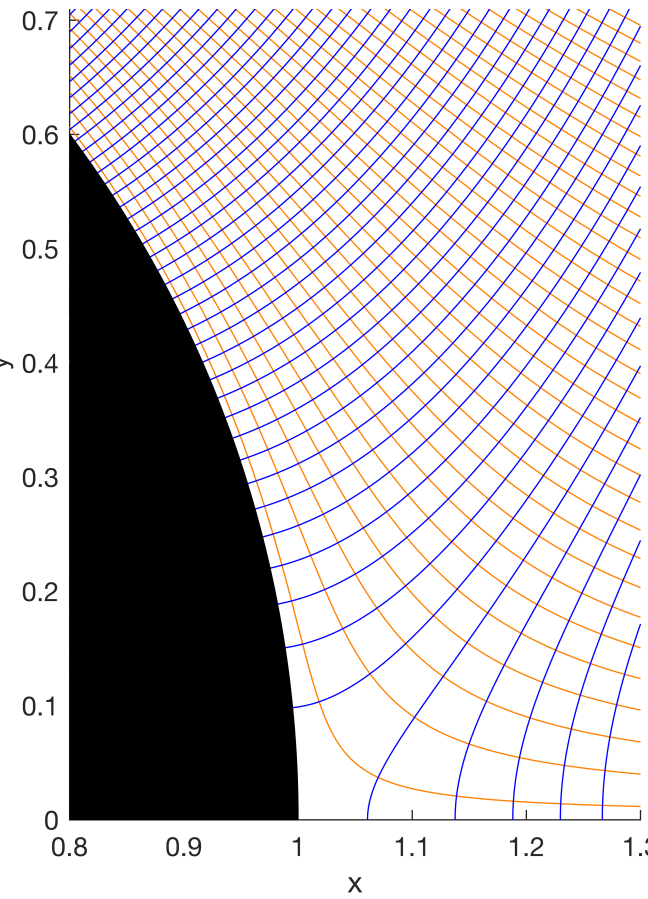
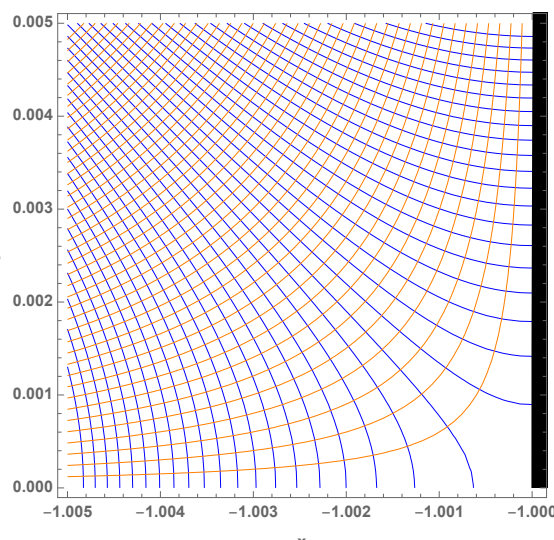
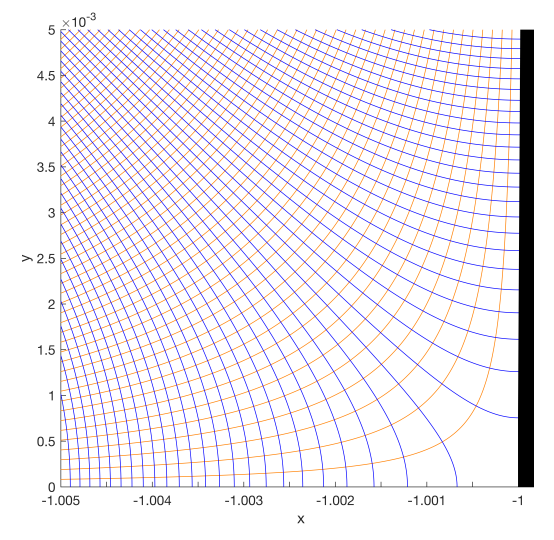


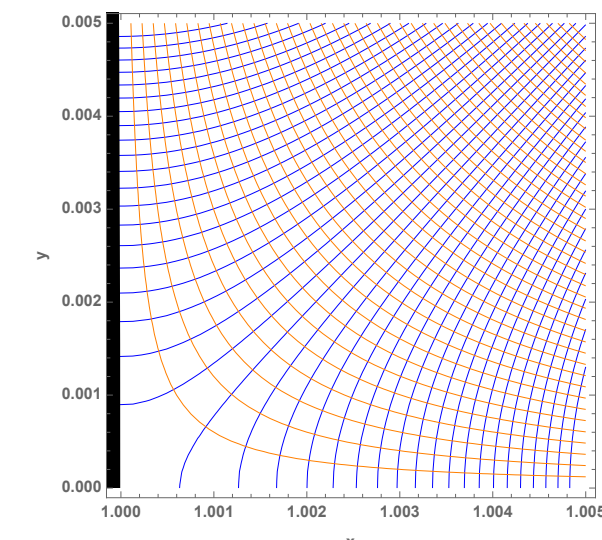
Figure 6: Right stagnation point



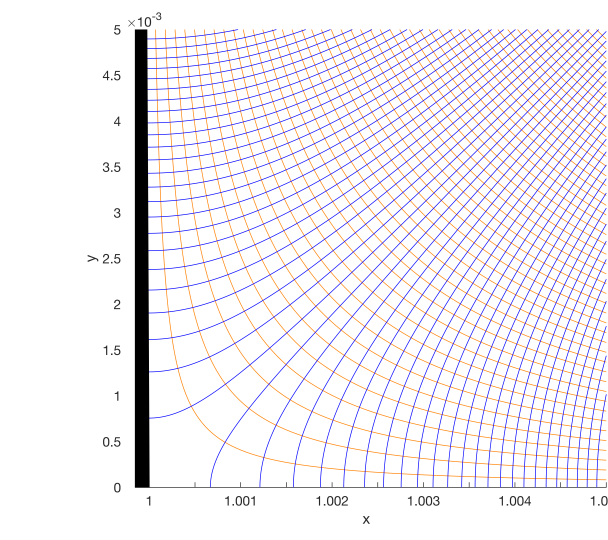
Exact (Left)



CVBEM Approx. (Left)



Exact (Right)



CVBEM Approx. (Right)

Figure 7: Exact and approximate flow nets near the stagnation points where the curvature of the solution is most extreme.

Comparison Between Unrefined and Refined Implementations

Table 1 contains the results from three different CVBEM implementations. For each of the three methods, maximum error results are reported for several different model sizes with respect to the number of degrees of freedom (dof) used in obtaining the CVBEM approximation function. The final column of Table 1 shows the order of magnitude of the improvement in the accuracy of the CVBEM approximation function obtained by applying the refinement procedure compared to when no refinement is used.

Number of Basis Functions (n)	Number of dof ($2n$)	Max. Error for Un-optimized Method	Max. Error for Optimized Method (No Refinement)	Max. Error for Optimized Method (with Refinement)	Order of Magnitude of Improvement
1	2	1.946105e+01	1.657752e+00	1.657752e+00	0
2	4	1.204797e+00	3.033696e+00	1.876661e+00	0
3	6	7.818511e-01	1.585200e+00	1.081110e+00	0
4	8	4.722863e+00	1.212144e+00	1.178229e+00	0
5	10	9.561156e-01	1.113585e+00	4.158998e-01	0
10	20	9.942122e-01	1.446775e-01	3.832625e-03	1
15	30	9.959928e-01	7.673386e-02	4.720970e-05	3
20	40	9.961047e-01	2.453100e-03	5.638322e-07	3
25	50	9.957117e-01	1.073772e-03	6.275395e-08	4
30	60	9.957136e-01	2.954499e-05	1.591035e-08	3
35	70	9.957140e-01	1.861172e-06	4.140663e-09	2

Table 1: Maximum error results for variously-sized CVBEM models. The CVBEM models that are considered are an un-optimized CVBEM model, an optimized CVBEM model without refinement, and an optimized CVBEM model with refinement. The word "optimized" means that an NPA was used to locate the computational nodes of the CVBEM model.

Conclusions

This poster reports on a new NPA for locating computational nodes in mesh reduction methods for PDEs. The novelty of this research is with respect to the development of the refinement procedure as described above, which allows for the relocation of already-located nodes if making a change would result in a BVP model with less error. This procedure is an important addition to recent NPA research due to its monotonic improvement of the BVP model to which it is applied.

To demonstrate this new algorithm, the NPA is applied to a CVBEM model of potential flow over a half-cylinder. This is a useful demonstration problem involving the computational difficulty of modeling the potential flow in the vicinity of two stagnation points. Additionally, the fact that the exact solution is known allows for the development of a precise description of the computational error resulting from the application of the NPA to the CVBEM model. Maximum error results are tabulated for three different node positioning schemes, including the NPA at hand.

Acknowledgements

This research was supported by the consulting firm Hromadka & Associates.