Volume 12, Number 4, 2002

Boundary Element Communications

An International Journal

WITPRESS Southampton & Boston

A NOTE ON APPROXIMATING THREE-DIMENSIONAL POTENTIAL PROBLEMS USING THE CVBEM AND DOMAIN ROTATIONS

T.V. HROMADKA II[1] & R.J. WHITLEY[2]
[1]Department of Mathematics, California State University, California, USA.
[2]University of California, California, USA.

ABSTRACT

In this note, the primary focus is to introduce an extension of the two-dimensional (2D) CVBEM to solve potential problems in a three-dimensional (3D) spherical geometry problem domain. This is achieved by (1) applying the CVBEM to three coupled projections of the 3D sphere, onto orthogonal 2D planes, and then superimposing the resulting corresponding 2D CVBEM solutions, and (2) rotating the problem domain and reapplying the previous step (1). Although the current paper only addresses a spherical geometry the resulting numerical approximations demonstrate the utility of using a 2D boundary element method, such as the CVBEM, towards solving 3D potential problems on other 3D geometries.

1 INTRODUCTION

The Complex Variable Boundary Element Method, or CVBEM, is a numerical technique for use in solving, in an approximation sense, two-dimensional (2D) potential problems or 2D Poisson problems. The considerations of multiply connected regions, i.e. problem domains that contain holes, and various types of boundary conditions, e.g. flux or Dirichlet type, has been examined in detail in various publications, including the recent book of Hromadka and Whitley (1998). Applications of the CVBEM to a wide variety of practical problems is also reported in the literature, see the cited reference. Ever since the introduction of the CVBEM, e.g. Hromadka and Guymon, 1984, the CVBEM has been limited to solving potential problems in 2D.

Recently, the 2D CVBEM has been extended to solve three-dimensional (3D) problems, see Hromadka, (2001) and Hromadka and Whitley (2001a.b). This is accomplished by applying the CVBEM to three coupled projections of the 3D problem domain, in orthogonal 2D planes, and then superimposing the resulting 2D CVBEM solutions. The cited references include several numerical applications that demonstrate the utility of using a 2D boundary element method, such as the CVBEM, towards solving 3D potential problems with Dirichlet boundary conditions. In the current research, the new 3D CVBEM is enhanced by considering application of the CVBEM to rotations of the problem domain, Ω, and adding the resulting approximations.

The use of two-dimensional (2D) basis functions to solve the Laplace equation in three dimensions (3D) provides some interesting theoretical and practical advantages. For example, 2D basis functions of the lnr type do not exhibit the singularity behavior demonstrated by the 3D basis functions of the 1/r type. Convergence properties are readily established such as given in the proofs provided by Whitley and Hromadka (2001). The use of complex variable functions to solve potential problems provides the benefits of conjugate functions that relates, in 2D, potentials to streamlines. Although this paper only deals with a spherical 3D geometry problem domain, this work provides the underpinning for extending the approach towards generalization to arbitrary 3D geometry problem domains.

2 MATHEMATICAL FORMULATION OF PROBLEM

The three-dimensional (3D) potential problem considered is to solve the PDE

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}=0 \text{ in } \Omega \tag{1}$$

with Dirichlet boundary conditions $\phi=\phi_b$ on Γ, where Ω is the 3D domain with boundary Γ; ϕ is the 3D potential function; and x,y,z are the usual Cartesian coordinates. For development purposes, Ω is assumed to be simply connected (no holes in the interior of Ω).

3 GRAMM-SCHMIDT APPROXIMATION SETTING (HILBERT SPACE)

The approximation technique being considered is to define a particular set of basis functions, and then to determine the best approximation in a least squares error minimization sense, i.e. a Hilbert space setting, see Hromadka and Whitley, (1993). In this case, the best approximation is determined by the usual Gramm-Schmidt process, with respect to the assembled set of basis functions in matching the value of the boundary conditions, ϕ_b, on Γ (again, see the above cited references). For the reader's convenience, a brief overview of the necessary steps is presented.

3.1Gramm-Schmidt Inner Product

The Gramm-Schmidt orthonormalization process involves the use of integrals of the form (f,g), known as an inner-product, given by

$$(f,g)=\int_\Gamma fg \; d\Gamma \tag{2}$$

where f and g are integrable on Γ. In general, expression (2) is solved numerically, and the approach used herein is as follows:

- Step 1. Define a set of "integration points", $\{p_i\}$, of uniform density, on the problem boundary Γ. Number the integration points from 1 to NI. The uniform density of the $\{p_i\}$ on Γ can be relaxed if the integral of expression (2) is extended to include a weighting function.
- Step 2. Develop a GEOMETRY vector, of dimension NI, composed of the coordinates of p_i, i=1,2,...,NI.
- Step 3. For any function used in expression (2), say f, develop a vector F, of dimension NI, composed of the values $F=\{f(p_i); i=1,2,...NI\}$, i.e. develop a column or row vector.
- Step 4. To approximate expression (2), use the vector dot product,

$$(f,g)>(F,G)=\sum_{i=1}^{NI} f(p_i)g(p_i)\Delta\Gamma \tag{3}$$

where $\Delta\Gamma$ is the measure of the incremental boundary associated to pi. It should be noted that as $NI\rightarrow\infty$ and $\Delta\Gamma\rightarrow 0$, then (F,G) $\rightarrow$ (f,g). Also, the requirement that the set of integration points be uniformly distributed on Γ can be readily relaxed by defining $\Delta\Gamma$, in expression (3), as a function of the p_i.

3.2 Gramm-Schmidt Orthonormalization Process

Given a set of m linearly independent basis functions, i.e. basis dimension m, noted as $\{f_j; j=1,2,...,m\}$, orthonormalization is achieved by using the Gramm-Schmidt process, except now we are in a vector representation of the set $\{f_j\}$, noted as $\{F_j\}$, and we use the vector dot product given in expression (3). The resulting orthonormalized vectors are $\{H_j; j=1,2,...,m\}$.

3.3 Determining the Best Approximation of ϕ_b on Γ

To approximate ϕ_b on Γ, another vector, ϕ_B, of dimension NI, is developed as $\phi_B = \{\phi_b(p_i);\ i = 1,2,\ldots,NI\}$. The best approximation of ϕ_b on Γ, noted as ϕ^*, is given by

$$\phi^* = \sum_{j=1}^{m} (H_j, \phi_B) H_j \tag{4}$$

By back-substitution, ϕ can be rewritten in terms of the original vectors, F_j, giving

$$\phi^* = \sum_{j=1}^{m} \alpha_j F_j \tag{5}$$

where α_j are the coefficients determined from the usual Gramm-Schmidt back-substitution process from the (H_j, ϕ_B) values, see Hromadka and Whitley, (1993). Note that as $NI \rightarrow \infty$ and $\Delta\Gamma \rightarrow 0$, then $\alpha_j \rightarrow \beta_j$, where β_j is the Gramm-Schmidt coefficient corresponding to the original basis function, f_j, and in the original space spanned by the $\{f_j\}$, we have

$$\phi^* = \sum_{j=1}^{m} \beta_j f_j \tag{6}$$

4 APPROXIMATING 3D POTENTIAL FUNCTIONS USING 3D BASIS FUNCTIONS FROM THE CVBEM

In the previous section, the focus of the Gramm-Schmidt procedure was to minimize $(\phi^* - \phi_b)$ on Γ. No attention was paid to how ϕ^* relates to the interior of Ω. In this section, the choice of basis functions will be addressed such that ϕ^* exactly solves the PDE operator equation, $L(\bullet) = 0$, where L is given by

$$L(\bullet) = \frac{\partial^2(\bullet)}{\partial x^2} + \frac{\partial^2(\bullet)}{\partial y^2} + \frac{\partial^2(\bullet)}{\partial z^2} \tag{7}$$

and where $(\bullet)$ is a function that is twice differentiable with respect to x, y, and z.

4.1 2D Geometry CVBEM Basis Functions

The Complex Variable Boundary Element Method, or CVBEM, will be utilized to generate 2D geometry basis functions to be used in the 3D problem setting of Eq. (7). Details regarding the CVBEM can be found in numerous papers and books, including Hromadka and Whitley, (1998), and consequently, these details will not be repeated here. For our purposes, it is sufficient to state the form of the CVBEM basis functions for the case of a linear global trial function used in the CVBEM.

The CVBEM involves the sum of products of complex coefficients multiplied by analytic functions of the form

$$\hat{\omega}(z) = \sum_{j=1}^{N} C_j (z - z_j) Ln_j (z - z_j) \tag{8}$$

where $\hat{\omega}(z)$ is the CVBEM approximation in the (x,y) plane; N is the number of CVBEM basis

functions; $C_j = (a_j - ib_j)$ are complex constants; z_j is $x_j + iy_j$, the (x,y) plane coordinate of node j; and Ln_j is the complex natural logarithm with branch cut oriented to lie exterior of Ω and not intersecting with other such branch cuts emanating from other CVBEM nodes. Again it should be noted that z is used for the third coordinate in a 3D geometry, and also it denotes the complex variable. From Euler's formula,

$$z - z_j = r_j e^{i\theta_j} \tag{9}$$

where r_j is the 2D radial distance from z to z_j, and θ_j is the radial angle measured counterclockwise from the branch cut defined at CVBEM node j. From equations (8) and (9), the associated 2D CVBEM basis functions are linear combinations of

$$a_j r_j\left(\cos\theta_j \ln r_j - \theta_j \sin\theta_j\right) \text{ or } b_j r_j\left(\sin\theta_j \ln r_j - \theta_j \cos\theta_j\right) \tag{10}$$

where the a_j and b_j are real constants. The choice of a_j and b_j is determined by minimizing the usual least squares residual difference in matching the boundary condition values on the problem boundary.

By rewriting the complex variable in terms of the other spatial coordinates, using x+iz or y+iz, the CVBEM basis functions (10) are readily extended into the other 2D (x,z) and (y,z) planes, resulting in another set of extended 2D basis functions.

The CVBEM formulation involves the use of three sets of 2D plane nodal points, one set of nodes being defined for each of the three orthogonal 2D planes. The approach used herein is described as follows:

- Step 1. Define the 3D problem domain (sphere) to have geometry coordinates all greater than zero, i.e. if necessary simply translate the 3D $\Omega \cup \Gamma$.
- Step 2. Project the 3D $\Omega \cup \Gamma$ onto the (x,y) 2D plane. The 2D projected domain is denoted by Ω_{xy} with boundary Γ_{xy}. Similarly, project $\Omega \cup \Gamma$ onto the 2D (x,z) and (y,z) planes, resulting in Ω_{xz} and Γ_{xz}, and Ω_{yz} and Γ_{yz}, respectively.
- Step 3. Define CVBEM nodes in the (x,y) 2D plane, all located exterior of Ω_{xy}, but arbitrarily close to or on Γ_{xy}. Similarly, define other CVBEM node sets corresponding to Γ_{xz} and Γ_{yz}, respectively.
- Step 4. Develop CVBEM basis functions of the form (12), with respect to each node, corresponding to the Γ_{xy}, Γ_{xz}, and Γ_{yz} surfaces, in the (x,y), (x,z), and (y,z) planes, respectively.

5 USING EXTENDED 2D CVBEM BASIS FUNCTIONS IN APPROXIMATING 3D POTENTIAL FUNCTIONS ON A SPHERE

The extended 2D CVBEM basis functions can be written in a more general form as

$$\phi_j^{\alpha\beta} = \left[r_j\left(\cos\theta_j \ln r_j - \theta_j \sin\theta_j\right)\right]^{\alpha\beta}$$

$$\psi_j^{\alpha\beta} = \left[r_j\left(\sin\theta_j \ln r_j + \theta_j \cos\theta_j\right)\right]^{\alpha\beta} \tag{11}$$

where the superscript $\alpha\beta$ refers to any of the (x,y), (x,z), or (y,z) 2D planar coordinates. That is ϕ_j^{xy},

and ψ_j^{xy} refer to CVBEM basis functions defined with respect to the jth CVBEM nodal point that is located exterior of the 2D projection, Ω_{xy} of the 3D problem domain, Ω, onto the (x,y) plane. Thus, for n_1, n_2, and n_3, CVBEM nodes are defined appropriately, i.e. exterior or on the 2D projected surfaces Γ_{xy}, Γ_{xz}, and Γ_{yz}, respectively, in each of the (x,y), (x,z), and (y,z) 2D planes, respectively, the 3D CVBEM approximation function is given by

$$\hat{\phi}(x,y,z) = \sum_{j=1}^{n_1}\left(a_j^{xy}\phi_j^{xy} + b_j^{xy}\psi_j^{xy}\right) + \sum_{j=1}^{n_2}\left(a_j^{xz}\phi_j^{xz} + b_j^{xz}\psi_j^{xz}\right) + \sum_{j=1}^{n_3}\left(a_j^{yz}\phi_j^{yz} + b_j^{yz}\psi_j^{yz}\right) \tag{12}$$

where $a_j^{\alpha\beta}$ and $b_j^{\alpha\beta}$ are constants to be determined by the Gramm-Schmidt process described previously. It is noted that, for simplicity, a 3D approximator can be readily developed in terms of only using the $\phi_j^{\alpha\beta}$ or the $\psi_j^{\alpha\beta}$ functions, rather than both forms of basis functions. It is also noted that, from expression (12),

$$L\left(\hat{\phi}(x,y,z)\right) = 0 \text{ in } \Omega \tag{13}$$

and the usual least squares residual norm $\left\|\hat{\phi}(x,y,z) - \phi_b\right\|$ is minimized on Γ by the Gramm-Schmidt procedure.

6 APPLICATION

To implement the CVBEM method, the n nodes ($n = n_1 + n_2 + n_3$ from Eq. 12) and their associated branch cuts must be defined. A branch cut is a ray which emanates from a node and does not intersect the 2D boundary except at the node itself. There is only one branch cut assigned to each node, from which all angles θ will be measured for that node.

To simplify the process, all CVBEM nodes are chosen at equally spaced intervals with the pattern of node points identical on each side of Γ. The branch cuts are selected to be at outward normal angles (i.e. orthogonal to the problem boundary). Note that CVBEM nodes do not need to lie on the problem boundary projections.

Integration points, used for the numerical integration of equation (2), must also be chosen on the boundary of the sphere, Γ. However, no integration point should coincide with a node used with the CVBEM approximator and if q represents the number of integration points chosen, then $q \geq n$.

Let C be the $q \times n$ matrix whose columns are the basis functions evaluated at all of the integration points. Figure 1 illustrates the quantities involved in the evaluation of a CVBEM basis function at an integration point.

The function f to be approximated on the sphere is defined discretely at the integration points on Γ, resulting in a $q \times 1$ column vector E. The system

$$Cy = E \tag{14}$$

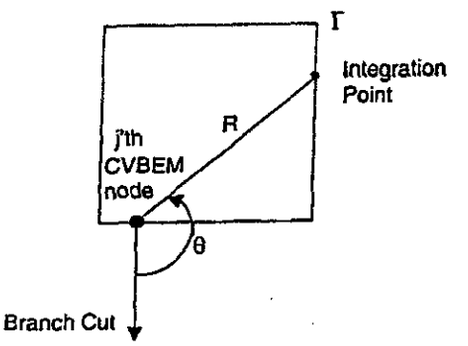
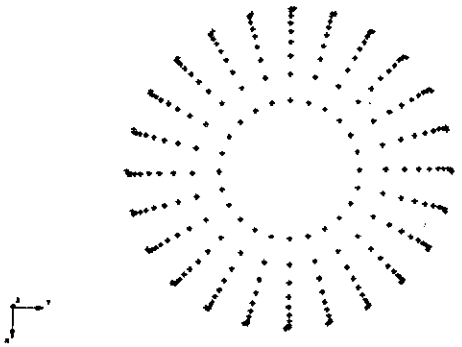
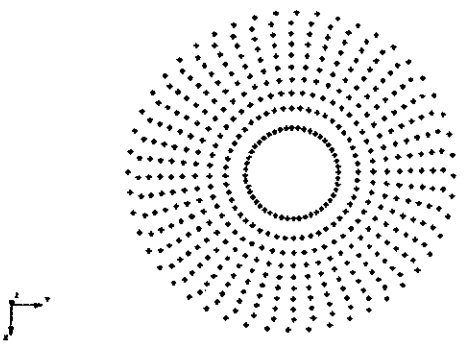


Figure 1: Branch Cut Parameters



240 Integration Points on North Hemisphere

Figure 2: Location of CVBEM integration points on northern hemisphere.



480 Test Points on North Hemisphere

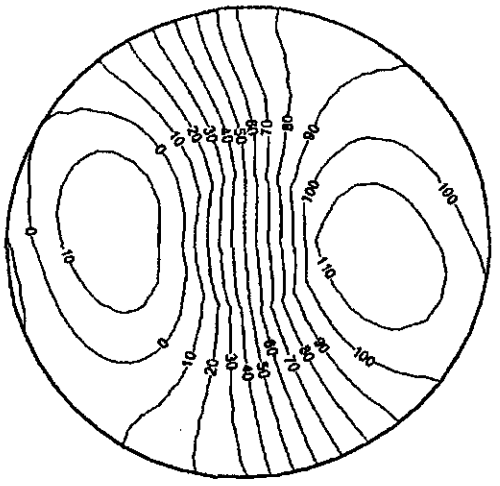
Figure 3: Location of test points on northern hemisphere.

can be solved to obtain a least squares solution so that the error, e, given by

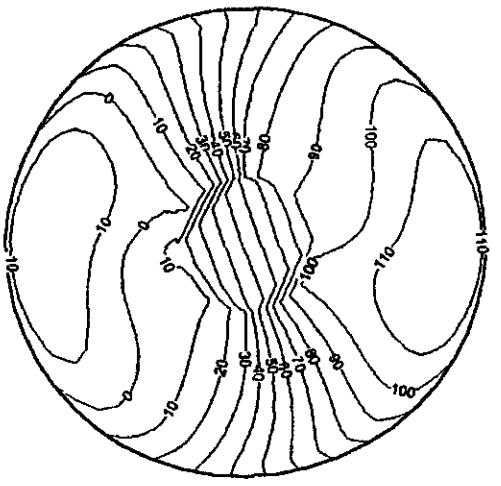
$$e = \|E - Cy\|_2 \tag{15}$$

is a minimum, i.e. the residual in matching boundary conditions is minimized.

For modeling purposes, the 3D sphere is discretized into latitudes and longitudes such that there are 240 integration points located in both the north and the south hemisphere, double counting the equator points. Another set of "test" points are also located on the sphere in order to evaluate the approximation results in between integration points. In our case, 480 test points are used in both hemispheres. Figures 2 to 3 depict these two schemes as viewed from above the north pole of the sphere. (A similar arrangement occurs in the south hemisphere.) In order to avoid coincident projections of integration points on any of the 2D planes, both of the two hemispheres are "twisted"

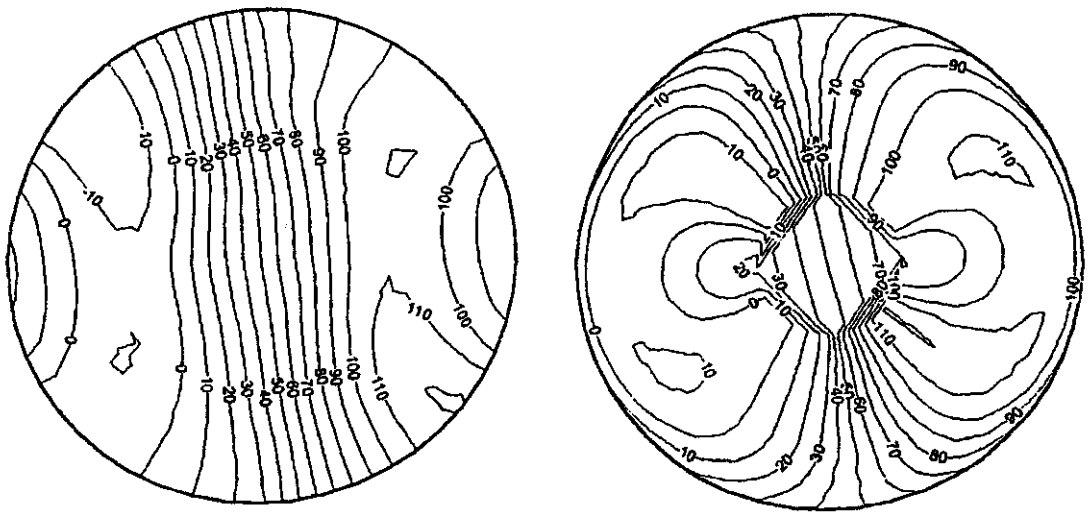


North Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
Without Rotation



South Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
Without Rotation

Figure 4: North and South hemisphere approximations without rotation.



North Hemisphere Approximation of F(x,y,z) = 100 on East Hemisphere F(x,y,z) = 0 on West Hemisphere With Rotation I

South Hemisphere Approximation of F(x,y,z) = 100 on East Hemisphere F(x,y,z) = 0 on West Hemisphere With Rotation I

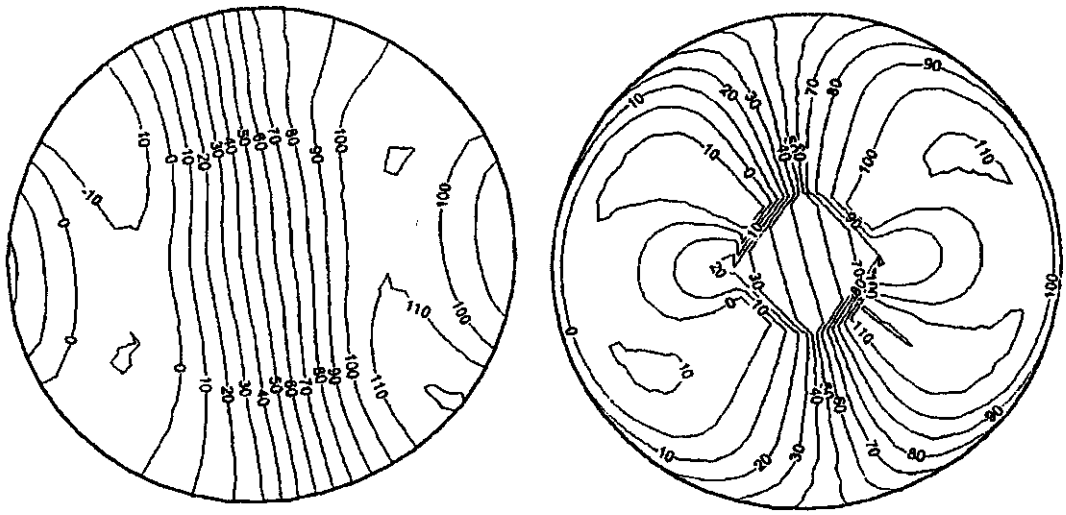
Figure 5: North and South hemisphere approximations with rotation I.

one degree, in opposite directions, so that all points are "seen" in each of the three 2D projections. Other angles could be used for this "twist". What is important is to reduce the number of coincident integration points that are lost due to the projection process. This "twist" technique is only needed if one uses the same number of nodes as the number of integration points, resulting in a collocation technique. Because the maximum approximation error must occur on the problem boundary, evaluation of the boundary fit is all that is normally needed in order to evaluate the accuracy of the approximation function.

The CVBEM basis function set can be increased by rotating the problem domain, Ω, with respect to the original three 2D CVBEM projection planes, and resolving the problem but using the error of matching the original boundary conditions (BCs) as the new BCs for the rotated problem. After solving for the rotated domain problem, the second CVBEM approximation is rotated backwards to the original orientation and then added to the original CVBEM approximation, resulting in an improved CVBEM approximation. The improved approximation can be further increased in accuracy by repeating the above steps but using different rotation settings, including rotations in each of the three axes. Indeed, one need only use a single nodal point in the first CVBEM approximation and then use several non-coincident rotations of the problem domain to improve modeling results analogous to using several nodes in a CVBEM approximation. Another approach is to assemble all of the CVBEM basis functions, generated by the rotation technique and then solve for the best approximation with respect to the entire basis function set simultaneously.

6.1 Application: Dirichlet Problem on a sphere – 100° C temperature on East Hemisphere, 0° C on West Hemisphere

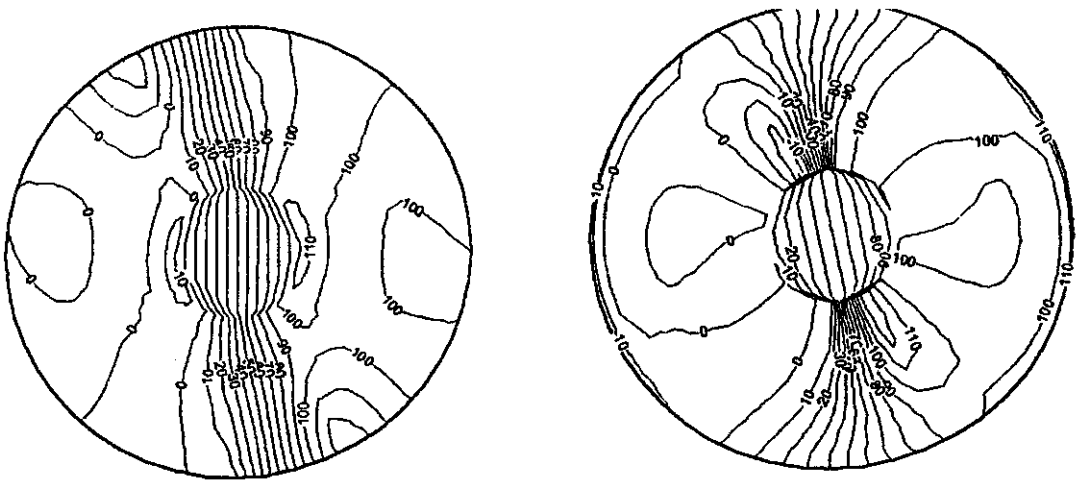
Given the sphere geometry and integration and test point setup shown in Figures 2 and 3, a Dirichlet steady-state heat transport problem is examined where a temperature of 100° C occurs on the East Hemisphere, and linearly decreases to 0° C a short distance (between integration points) into the



North Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotation I

South Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotation I

Figure 6: North and South hemisphere approximations with rotations I and II.



North Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotations I, II and III

South Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotations I, II and III

Figure 7: North and South hemisphere approximations with rotations I, II and III.

North Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotations I, II, III and IV

South Hemisphere Approximation of
F(x,y,z) = 100 on East Hemisphere
F(x,y,z) = 0 on West Hemisphere
With Rotations I, II, III and IV

Figure 8: North and South hemisphere approximations with rotations I, II, III and IV.

West Hemisphere, and is 0° C in the remainder of the West Hemisphere. Using these initial boundary conditions, a CVBEM 3D model was setup, with resulting approximation of temperature isocontours as shown in Figure 4. These isocontours are developed by use of approximations determined from equations (4) to (6). The next step was to compute the residual error in matching the BC values, at the integration points, and use this error as a new set of BC's. But first, the domain is rotated (rotation 1) 15-degrees (using the new BC values). In the rotated geometry, the 3D CVBEM model was reapplied. The resulting approximations, of the residual error in fitting the original BC's, were rotated backwards to the original position, and then summed with the original 3D CVBEM approximation results to arrive at an improved approximation. Isocontours from this second effort are shown in Figure 5. Continuing this approach, approximations of successive residual errors for a 30-degree (rotation 2) and 45-degree rotation (rotation 3) were obtained and summed (see Figures 6 and 7, respectively). Finally an approximation of residual error (remaining after all of the above three rotation enhancement efforts) using a 45-degree rotation (rotation 4), in another axis of rotation, was obtained and summed to the results shown in Figure 7 (see Figure 8). As is seen from the application results, using rotations to improve approximation accuracy is analogous to adding nodal points assuming rotations do not result in identical locations of nodal points.

7 CONCLUSIONS

In this paper, the two-dimensional (2D) CVBEM is extended to solving potential problems on a three dimensional sphere. This is achieved by applying the CVBEM to three coupled projections of the 3D problem domain, in 2D orthogonal planes, and then superimposing the resulting corresponding 2D CVBEM solutions. By rotating the problem domain and resolving the problem, but using the error in matching boundary conditions as the rotated problem boundary conditions, an improve-

ment in the results obtained is achieved. Using a sequence of such rotation solutions reduces the approximation error analogous to adding sets of nodal points to the original problem setup. The extension of the above formulations to other 3D geometries follows directly from the work presented in this paper.

REFERENCES

1. Hromadka II, T.V., 1993, *The Best Approximation Method in Computational Mechanics*, Springer-Verlag, 250 pages.
2. Hromadka II, T.V. and Whitley, R.J., 1998, *Advances in The Complex Variable Boundary Element Method*, Springer-Verlag, New York, 400 pages.
3. Hromadka II, T.V. and Guymon, G.L., 1984, A Complex Variable Boundary Element Method: Development, *International Journal for Numerical Methods in Engineering*, Vol. 20, pg. 25-37.
4. Brebbia, C.A. and Dominguez, J., 1989, *Boundary Elements: An Introductory Course*, Computational Mechanics Publications, McGraw-Hill Book Company.
5. Hromadka II, T.V., 2000, Approximating Three-Dimensional Potential Problems Using The Complex Variable Boundary Element Method (CVBEM), *Numerical Methods for Partial Differential Equations Journal*, pg. 535-560.
6. Hromadka II, T.V., Approximating Three-Dimensional Potential Problems On a Sphere Using The Complex Variable Boundary Element Method (CVBEM), *Applied Mathematical Modeling*, (2001), in-review.
7. Whitley, R.J. and Hromadka II, T.V., A General Complex Variable Boundary Element Method, *Numerical Methods for Partial Differential Equations*, (2001a), in-review.
8. Whitley, R.J. and Hromadka II, T.V., Approximating Harmonic Functions on Rn With One Function of a Single Complex Variable, *Annals of Mathematics*, (2001b), in-review.