A simple boundary element method for problems of potential in non-homogeneous media

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SUMMARY

A simple boundary element method for solving potential problems in non-homogeneous media is presented. A physical parameter (e.g. heat conductivity, permeability, permittivity, resistivity, magnetic permeability) has a spatial distribution that varies with one or more co-ordinates. For certain classes of material variations the non-homogeneous problem can be transformed to known homogeneous problems such as those governed by the Laplace, Helmholtz and modified Helmholtz equations. A three-dimensional Galerkin boundary element method implementation is presented for these cases. However, the present development is not restricted to Galerkin schemes and can be readily extended to other boundary integral methods such as standard collocation. A few test examples are given to verify the proposed formulation. The paper is supplemented by an Appendix, which presents an ABAQUS user-subroutine for graded finite elements. The results from the finite element simulations are used for comparison with the present boundary element solutions. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: boundary element method; Galerkin; functionally graded materials; non-homogeneous materials; Green's function; three-dimensional analysis

1. INTRODUCTION

The governing differential equation for a potential function ϕ defined on a region Ω bounded by a surface Σ, with an outward normal $\mathbf{n}$, can be written as

$$\nabla \cdot (k(x, y, z)\nabla \phi) = 0 \tag{1}$$

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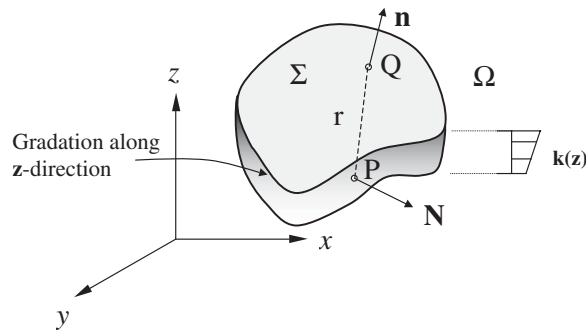
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Figure 1. Definition of the boundary value problem with boundary Σ and domain Ω. The source point is P (normal $\mathbf{N}$) and the field point is Q (normal $\mathbf{n}$).

Table I. Problems governed by Equation (1).

| Problems | Scalar function ϕ | $k(x, y, z)$ | Boundary condition | |
			Dirichlet	Neumann
Heat transfer	Temperature T	Thermal conductivity (k)	$T = \overline{T}$	Heat flow $q = -k\partial T/\partial n$
Ground water flow	Hydraulic head H	Permeability (k)	$H = \overline{H}$	Velocity flow $q = -k\partial H/\partial n$
Electrostatic	Field potential V	Permittivity (ε)	$V = \overline{V}$	Electric flow $q = -\varepsilon\partial V/\partial n$
Electric conduction	Electropotential E	Resistivity (k)	$E = \overline{E}$	Electric current $q = -k\partial E/\partial n$
Magnetostatic	Magnetic potential M	Magnetic permeability (μ)	$M = \overline{M}$	Magnetic flux density $B = -\mu\partial M/\partial n$

where $k(x, y, z)$ is a position-dependent material function. The general problem under consideration is presented in Figure 1. Equation (1) is the field equation for a wide range of problems in physics and engineering such as heat transfer, fluid flow motion, flow in porous media, electrostatics and magnetostatics. Table I presents a list of $k(x, y, z)$ used in different applications [1].

The boundary conditions of the problem can be of the following types:

$$\phi = \overline{\phi} \quad \text{on } \Sigma_1 \text{ (Dirichlet type)} \tag{2}$$

$$q = -k(x, y, z)\frac{\partial \overline{\phi}}{\partial n} = \overline{q} \quad \text{on } \Sigma_2 \text{ (Neumann type)} \tag{3}$$

with $\Sigma = \Sigma_1 + \Sigma_2$ for a well-posed problem. The boundary value problem is a Neumann problem if the flux is known on the whole boundary, and the problem is a Dirichlet problem if the potential is known on the whole boundary. Mixed boundary conditions are also frequently

encountered: flux is prescribed over some portion of the boundary and potential is prescribed over the complementary portion of the boundary.

For non-homogeneous media, $k(x, y, z)$ can assume any function of x, y and z. With recent development and research of functionally graded materials (FGMs), problems in non-homogeneous media have generated new interest. In FGMs, the composition and the volume fraction of the FGM constituents vary gradually, giving a non-uniform microstructure with continuously graded macroproperties such as thermal conductivity, elasticity, hardness, etc. In most engineering applications the spatial variation of $k(x, y, z)$ is in one co-ordinate.

There is a class of material variations, which can transform the problem equation to a Laplace or standard/modified Helmholtz equation. *The present work demonstrates that by simple change in the treatment of the boundary conditions of existing homogeneous Laplace and standard/modified Helmholtz codes, the solutions for non-homogeneous media with quadratic, exponential and trigonometric material variations can be obtained.* Numerical implementation for specific cases using these variations of $k(x, y, z)$ in one or more co-ordinates are presented. Heat transfer problems have been chosen for the numerical examples, although the numerical implementation can be used for any potential problem (See Table I).

Another contribution of this work is the development of a user-subroutine to implement graded finite elements in the finite element method (FEM) software ABAQUS. It is used for comparison purposes with the present BEM solutions.

2. RELATED WORK

The boundary element method (BEM) is an efficient solution method because only the boundary discretization is necessary for numerical implementation. It is accurate due to the fact that the Green's function, which is admissible to the governing equation, is used as the weighting function. In the context of BEM, problems in non-homogeneous media has been previously studied by Cheng [2, 3], Ang *et al.* [4], Shaw [5] and recently by Gray *et al.* [6] and Dumont *et al.* [7]. The majority of these works have emphasized on obtaining the Green's function. Cheng [2] presented a direct Green's function approach for Darcy's flow with spatially variable permeability. The formulation required that the Green's function be found for each given permeability variation. He also presented the Green's function for a class of permeability variations whose square root of hydraulic conductivity satisfies the Laplace and the Helmholtz equations in 1–3 dimensions. Shaw [8] presented a two-dimensional fundamental solution involving axisymmetric material variation and also showed the inter-relationship between the fundamental solutions for different heterogeneous potential, wave and advective–diffusion problems. Lafe and Cheng [9] used a pertubation boundary element for steady-state ground water flow for heterogeneous aquifers where the governing equation is decomposed into a Laplace equation and a sequence of Poisson's equations with known right-hand sides. Harrouni *et al.* [10, 11] used a global interpolation-based dual reciprocity boundary element method (DRBEM) for Darcy's flow in heterogeneous media where the governing equation is transformed into a Poisson-type equation with modified boundary conditions. In this technique, the domain integral that arises from the non-homogeneous part of the governing equation is interpolated by a set of complete basis functions and converted to a series of boundary integrals. Divo and Kassab [12, 13] introduced a technique for heat conduction in heterogeneous media based on a fundamental solution that is a locally radially symmetric response to a non-symmetric forcing function.

Multiple techniques have been used to deal with the numerical implementation, namely the *iterative scheme* involving domain integrals and iterations, the *domain scheme* and the *direct Green's function scheme* [2]. The domain technique requires use of domain integrals or radial basis functions [10, 14]. The iterative and the domain scheme decrease the inherent efficiency of the BEM as the boundary-only nature of the method is lost. Another simple technique is the multi-zone approach [15], where the conductivity is assumed to be constant over several zones. This approach is inefficient because in order to capture the continuous variation of the material property, a large number of sub-regions or zones are necessary.

Cheng [2] presented some forms of $k(x, y, z)$ for permeability in the context of Darcy's flow, for which closed-form expressions of the Green's function were obtained by using a variable transformation following Georghitza [16], which allows Equation (1) to be rewritten as Laplace or Helmholtz equation. In his BEM implementations, the kernels are based on the Green's function G of the heterogeneous media, where G is the free-space Green's function defined as

$$\nabla \cdot (k(x, y, z)\nabla G) = -\delta(Q - P) \tag{4}$$

where P is the source point, Q is the field point, and the gradient ∇ is taken with respect to the field point Q ($\nabla \equiv \nabla_Q$).

3. GOVERNING EQUATIONS CONSIDERING VARIABLE CONDUCTIVITY

By defining a variable

$$v(x, y, z) = \sqrt{k(x, y, z)}\phi(x, y, z) \tag{5}$$

Equation (1) can be rewritten as

$$\nabla^2 v + \left(\frac{\nabla k \cdot \nabla k}{4k^2} - \frac{\nabla^2 k}{2k}\right) v = 0 \tag{6}$$

or,

$$\nabla^2 v + k'(x, y, z)v = 0 \tag{7}$$

where

$$k' = \frac{\nabla k \cdot \nabla k}{4k^2} - \frac{\nabla^2 k}{2k} \tag{8}$$

From Equation (7), three different cases can be generated. If $k'(x, y, z) = 0$, then Equation (7) becomes the standard Laplace equation, i.e.

$$\nabla^2 v = 0 \tag{9}$$

If $k'(x, y, z) = -\beta^2$, then Equation (7) converts to the modified Helmholtz equation, i.e.

$$\nabla^2 v - \beta^2 v = 0 \tag{10}$$

while if $k'(x, y, z) = \beta^2$, then Equation (7) transforms to the standard Helmholtz equation, i.e.

$$\nabla^2 v + \beta^2 v = 0 \tag{11}$$

From the three cases of $k'(x, y, z)$ we can generate a family of variations of $k(x, y, z)$. Here we focus on variations which depend only on one Cartesian co-ordinate, namely z. From an engineering point of view (for applications such as FGMs), material variation in one co-ordinate is of practical importance as described in References [17, 18].

3.1. Reduction to the Laplace equation

In this case $k'(x, y, z) = 0$ and, according to Equation (6), $k(x, y, z)$ can be determined by

$$\frac{\nabla k \cdot \nabla k}{4k^2} - \frac{\nabla^2 k}{2k} = 0 \tag{12}$$

If k varies only with z, then Equation (12) becomes

$$\frac{((\mathrm{d}/\mathrm{d}z)k(z))^2}{4(k(z))^2} - \frac{(\mathrm{d}^2/\mathrm{d}z^2)k(z)}{2k(z)} = 0 \tag{13}$$

Solving Equation (13), one obtains

$$k(z) = (c_1 + c_2 z)^2 \tag{14}$$

where c_1 and c_2 are arbitrary constants. In a more general form Equation (14) can be written as

$$k(z) = k_0(c_1 + c_2 z)^2 \tag{15}$$

where k_0 is a reference value for k. From Equations (13) and (14), we can infer that for quadratic variation of $k(z)$, Equation (1) can be transformed to a Laplace equation. This variation can be extended to more dimensions.

3.2. Reduction to the modified Helmholtz equation

In this case $k'(x, y, z) = -\beta^2$ and, according to Equation (6), $k(x, y, z)$ can be determined by

$$\frac{\nabla k \cdot \nabla k}{4k^2} - \frac{\nabla^2 k}{2k} = -\beta^2 \tag{16}$$

For k varying only with z, Equation (16) becomes

$$\frac{((\mathrm{d}/\mathrm{d}z)k(z))^2}{4(k(z))^2} - \frac{(\mathrm{d}^2/\mathrm{d}z^2)k(z)}{2k(z)} = -\beta^2 \tag{17}$$

Solving Equation (17), one obtains

$$k(z) = k_0(a_1 \mathrm{e}^{\beta z} + a_2 \mathrm{e}^{-\beta z})^2 \tag{18}$$

where a_1 and a_2 are arbitrary constants. Equation (18) can be rewritten in terms of only hyperbolic functions as

$$k(z) = k_0(b_1 \cosh \beta z + b_2 \sinh \beta z)^2 \tag{19}$$

where b_1 and b_2 are arbitrary constants. Alternatively Equation (18) can be expressed in terms of a combination of exponential and hyperbolic functions such as

$$k(z) = k_0(b_1 \mathrm{e}^{\beta z} + b_2 \sinh \beta z)^2 \tag{20}$$

or

$$k(z) = k_0(b_1 \cosh \beta z + b_2 \mathrm{e}^{-\beta z})^2 \tag{21}$$

From Equations (18) to (21) it is apparent that for a family of variations involving hyperbolic and exponential functions, Equation (1) can be transformed into the modified Helmholtz equation Equation (10).

3.3. Reduction to the standard Helmholtz equation

In this case $k'(x, y, z) = \beta^2$ and, according to Equation (6), $k(x, y, z)$ can be determined by

$$\frac{\nabla k \cdot \nabla k}{4k^2} - \frac{\nabla^2 k}{2k} = \beta^2 \tag{22}$$

Again, for k varying only with z, we set up the following differential equation:

$$\frac{((\mathrm{d}/\mathrm{d}z)k(z))^2}{4(k(z))^2} - \frac{(\mathrm{d}^2/\mathrm{d}z^2)k(z)}{2k(z)} = \beta^2 \tag{23}$$

Solving Equation (23), one obtains

$$k(z) = k_0(a_1 \cos \beta z + a_2 \sin \beta z)^2 \tag{24}$$

where a_1 and a_2 are arbitrary constants. For a family of variations involving trigonometric sine and cosine functions, Equation (1) can be transformed into the Helmholtz equation Equation (11).

3.4. Remarks

The appeal of the transform is its generality and the fact that for all of variations of $k(x, y, z)$, the Green's function can be obtained. Table II presents a list of variations of $k(x, y, z)$ with corresponding differential equations and the closed-form Green's function.

It may be mentioned that, in the present paper, we do not use these Green's functions for the boundary element method implementation. We rather use the simpler Green's function of the modified problem (Laplace equation or standard/modified Helmholtz equation).

3.5. Boundary conditions

In order to solve the boundary value problem based on the modified variable v, the boundary conditions of the original problem have to be incorporated in the modified boundary value problem. Thus for the modified problem, the Dirichlet and the Neumann boundary conditions given by Equations (2) and (3), respectively, change as follows:

$$v = \sqrt{k}\,\overline{\phi} \quad \text{on } \Sigma_1 \tag{25}$$

$$\frac{\partial v}{\partial n} = \frac{1}{2k} \frac{\partial k}{\partial n} v - \frac{\overline{q}}{\sqrt{k}} \quad \text{on } \Sigma_2 \tag{26}$$

Note that the Dirichlet boundary condition of the original problem is affected by the factor $\sqrt{k}$. Moreover, the Neumann boundary condition of the original problem changes to a mixed

Table II. Table of Green's function for various forms of $k(z)$ given by Equation (1).

Variation $k(z)$	Differential equation	Modified prob.	Green's function (2D)	Green's function (3D)
Parabolic:				
$(c_1 + c_2 z)^2$	$(c_1 + c_2 z)\nabla^2\phi + 2c_2\phi_z = 0$	$\nabla^2 v = 0$	$-\dfrac{1}{2\pi}\dfrac{(c_1 + c_2 z')^{-1}}{(c_1 + c_2 z)}\ln r$	$\dfrac{1}{4\pi r}\dfrac{(c_1 + c_2 z')^{-1}}{(c_1 + c_2 z)}$
Exponential:				
$(a_1 e^{\beta z} + a_2 e^{-\beta z})^2$	$(a_1 e^{\beta z} + a_2 e^{-\beta z})^2\nabla^2\phi$ $+2\beta\phi_z(a_1^2 e^{2\beta z} - a_2^2 e^{-2\beta z}) = 0$	$\nabla^2 v - \beta^2 v = 0$	$\dfrac{1}{2\pi}\dfrac{(a_1 e^{\beta z'} + a_2 e^{-\beta z'})^{-1}}{(a_1 e^{\beta z} + a_2 e^{-\beta z})}K_0(\beta r)$	$\dfrac{e^{-\beta r}}{4\pi r}$ $\dfrac{(a_1 e^{\beta z'} + a_2 e^{-\beta z'})^{-1}}{(a_1 e^{\beta z} + a_2 e^{-\beta z})}$
Trigonometric:				
$(a_1\cos\beta z + a_2\sin\beta z)^2$	$(a_1\cos\beta z + a_2\sin\beta z)^2\nabla^2\phi$ $+2\beta\phi_z\left[\dfrac{1}{2}(a_2^2 - a_1^2)\right.$ $\left.\sin 2\beta z + a_1 a_2\cos 2\beta z\right] = 0$	$\nabla^2 v + \beta^2 v = 0$	$\dfrac{1}{2}\dfrac{(a_1\cos\beta z' + a_2\sin\beta z')^{-1}}{(a_1\cos\beta z + a_2\sin\beta z)}Y_0(\beta r)$	$\dfrac{\cos(\beta r)}{4\pi r}$ $\dfrac{(a_1\cos\beta z' + a_2\sin\beta z')^{-1}}{(a_1\cos\beta z + a_2\sin\beta z)}$

boundary condition or Robin boundary condition. This later modification is the only major change on the boundary value problem.

Another common boundary condition of the original problem is a prescribed relationship between the potential and the flux (e.g. convective heat transfer problems). The boundary condition of this type is

$$q = \lambda_1 \phi + \lambda_2 \text{ (Robin type)} \tag{27}$$

The corresponding boundary condition for the modified problem would be also a Robin boundary condition similar to Equation (26), i.e.

$$\frac{\partial v}{\partial n} = \left(\frac{1}{2k} \frac{\partial k}{\partial n} - \lambda_1 \right) v - \frac{\lambda_2}{\sqrt{k}} \tag{28}$$

4. GREEN'S FUNCTION VERSUS REDUCTION TO PARENT EQUATION: A COMPARISON OF APPROACHES

The Green's function approach is not attractive because each different material variation requires a different fundamental solution, and thus the kernels for the BEM implementation are different from the standard kernels usually employed for homogeneous problems. As a result each time a new computer code has to be developed. Moreover, if the treatment of singularity involves analytical integration, then the treatment becomes more involved [19]. The differential equation for the non-homogeneous medium is not self-adjoint. Consequently the Green's function for such cases are not symmetric also. On the contrary, the Green's functions for the modified problem (both Laplace equation and standard/modified Helmholtz equation) are symmetric. The symmetric property is of utmost importance if one wants to develop the symmetric Galerkin formulation of the problem.

To demonstrate the difference between the two approaches, the case of the exponential variation is considered and explained below.

We emphasize that with the modified problem, the class of functions of $k(x, y, z)$ can be addressed with the same code. Let the exponential variation $k(x, y, z)$ be defined as

$$k(x, y, z) = k(z) = k_0 e^{2\beta z} \tag{29}$$

Below we investigate the 'Green's function' approach and the 'reduction to the parent equation' approach to solve the problems with the material gradation given by Equation (29).

4.1. Green's function approach for three-dimensional (3D) problems

The Green's function for the exponential case is

$$G(P, Q) = \frac{e^{\beta(-r+R_z)}}{4\pi r} \tag{30}$$

where

$$R_z = z_Q - z_P \quad \text{and} \quad r = \|\mathbf{R}\| = \|\mathbf{Q} - \mathbf{P}\| \tag{31}$$

The boundary integral equation (BIE) for surface temperature $\phi(P)$ on the boundary Σ (see Figure 1) is therefore

$$\phi(P) + \int_{\Sigma} \phi(Q) \left(\frac{\partial}{\partial n} G(P, Q) - 2\beta n_z G(P, Q) \right) dQ = \int_{\Sigma} G(P, Q) \frac{\partial}{\partial n} \phi(Q) dQ \qquad (32)$$

that differs in form from the usual integral statements by the presence of the additional term multiplying $\phi(Q)$, i.e. $[-2\beta n_z G(P, Q)]$, which are due to the material gradation.

The kernel functions for the exponential case are

$$G(P, Q) = -\frac{1}{4\pi} \frac{e^{\beta(-r + z_Q - z_P)}}{r}$$

$$F(P, Q) = \frac{\partial}{\partial n} G(P, Q) - 2\beta n_z G(P, Q) \qquad (33)$$

$$= -\frac{e^{\beta(-r + R_z)}}{4\pi} \left(\frac{\mathbf{n} \cdot \mathbf{R}}{r^3} + \beta \frac{\mathbf{n} \cdot \mathbf{R}}{r^2} + \beta \frac{n_z}{r} \right)$$

4.2. Reduction to the modified Helmholtz equation

For the modified problem, the Green's function for the exponential case is

$$G(P, Q) = \frac{e^{-\beta r}}{4\pi r} \qquad (34)$$

The expression of $G(P, Q)$ is simpler than that of the Green's function approach (cf. Equation (30)). Moreover, Equation (34) is symmetric with respect to both P and Q. A discussion on symmetric properties is presented in the next section.

The governing BIE corresponding to Equation (10) is

$$\phi(P) + \int_{\Sigma} \phi(Q) \left(\frac{\partial}{\partial n} G(P, Q) \right) dQ = \int_{\Sigma} G(P, Q) \frac{\partial}{\partial n} \phi(Q) dQ \qquad (35)$$

The kernel functions for the exponential case in the reduction to parent equation technique are given by Equation (34) and

$$F(P, Q) = \frac{\partial}{\partial n} G(P, Q)$$

$$= -\frac{e^{-\beta r}}{4\pi} \left(\frac{\mathbf{n} \cdot \mathbf{R}}{r^3} + \beta \frac{\mathbf{n} \cdot \mathbf{R}}{r^2} \right) \qquad (36)$$

The kernels in Equation (33) have one more term than the kernels in Equation (36). But the significant difference is the exponential term in front of the kernels. In the Green's function approach, in order to take care of the singularity using the direct limit approach [20, 21], the power of the exponential plays an important role. The complexity of handling such exponential terms magnifies even more when applied to the hypersingular boundary integral equation.
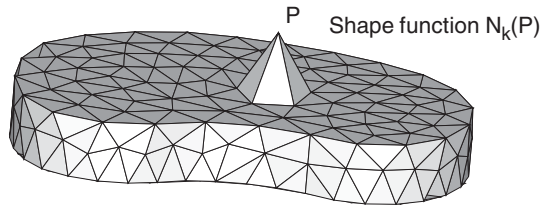
Figure 2. The local support of the Galerkin formulation at point P.

A direct treatment of singularity of the hypersingular double integrals using a hybrid analytical numerical approach has been presented by Sutradhar *et al.* [19] for exponential variation of the thermal conductivity. The treatment is based on the direct approach [21]. The direct limit approach is shown to be suitable for dealing with complicated Green's functions, which appear in applications such as those involving FGMs.

5. NUMERICAL IMPLEMENTATION

The numerical methods employed in the current work use standard Galerkin techniques. A discussion of these techniques in the context of the BEM is presented below.

5.1. Galerkin boundary integral equation

Define the collocation BIE as

$$\mathscr{B}(P) \equiv \phi(P) + \int_{\Sigma} \left(\frac{\partial}{\partial n} G(P, Q) \right) \phi(Q) \, \mathrm{d}Q - \int_{\Sigma} G(P, Q) \frac{\partial \phi}{\partial n}(Q) \, \mathrm{d}Q \tag{37}$$

and thus for an exact solution $\mathscr{B}(P) \equiv 0$.

In a Galerkin approximation, the error in the approximate solution is orthogonalized against the shape functions, i.e. the shape functions are the weighting functions and $\mathscr{B}(P) = 0$ is enforced in the 'weak sense', i.e.

$$\int_{\Sigma} N_k(P)\mathscr{B}(P) \, \mathrm{d}P = 0 \tag{38}$$

As a result the Galerkin technique possesses the important property of the *local support* as illustrated by Figure 2. This technique is especially suitable to treat corners [22]. After replacing the boundary and the boundary functions by their interpolated approximations, a set of linear algebraic equations emerges

$$[\mathbf{H}]\{\phi\} = [\mathbf{G}] \left\{ \frac{\partial \phi}{\partial n} \right\} \tag{39}$$

The matrix $\mathbf{G}$ is symmetric because its coefficients only depend on the distance (r) between the source points (P) and the fields points (Q), but matrix $\mathbf{H}$ is not because it depends on the normal vectors of the field points (Q). For Dirichlet problems, the Galerkin method gives rise to symmetric system of equations. In the context of non-homogeneous media a symmetric

Galerkin boundary element method (SGBEM) has been recently presented by Sutradhar *et al.* [19]. Details of the symmetry property and numerical implementation can be found in References [23–25].

5.2. Simple Kernel functions

- *Generalized quadratic variation of k*: For the quadratic variation of k, the problem is solved by the standard Laplace equation. The kernels corresponding to Equation (37) for the Laplace equation are

$$G(P, Q) = \frac{1}{4\pi r} \tag{40}$$

$$F(P, Q) = \frac{\partial}{\partial n} G(P, Q) = -\frac{1}{4\pi} \frac{\mathbf{n} \cdot \mathbf{R}}{r^3} \tag{41}$$

- *Generalized exponential variation of k*: For this variation, the transformed problem is the modified Helmholtz equation. The kernel functions are

$$G(P, Q) = \frac{\mathrm{e}^{-\beta r}}{4\pi r} \tag{42}$$

$$F(P, Q) = \frac{\partial}{\partial n} G(P, Q)$$

$$= -\frac{\mathrm{e}^{-\beta r}}{4\pi} \left(\frac{\mathbf{n} \cdot \mathbf{R}}{r^3} + \beta \frac{\mathbf{n} \cdot \mathbf{R}}{r^2} \right) \tag{43}$$

- *Trigonometric variation of k*: For the trigonometric variation the problem is transformed into standard Helmholtz equation. The kernel functions are

$$G(P, Q) = \frac{\cos \beta r}{4\pi r} \tag{44}$$

$$F(P, Q) = \frac{\partial}{\partial n} G(P, Q) = -\frac{1}{4\pi} \left(\cos(\beta r) \frac{\mathbf{n} \cdot \mathbf{R}}{r^3} + \beta \sin(\beta r) \frac{\mathbf{n} \cdot \mathbf{R}}{r^2} \right) \tag{45}$$

5.3. Treatment of boundary conditions

As explained in Section 3.5, in order to solve the non-homogeneous problem using codes for homogeneous materials (Laplace, Helmholtz and modified Helmholtz), the main modification in the implementation is to incorporate the boundary conditions for the modified problem. In this section, the necessary modifications are described.

Let us assume three nodes, of which nodes 1 and 3 have prescribed Neumann boundary condition and node 2 has prescribed Dirichlet boundary condition, i.e.

$$\overline{q_1}, \ \overline{\phi_2}, \ \overline{q_3} \text{ known quantities}$$

$$\phi_1, \ q_2, \ \phi_3 \text{ unknown quantities}$$

In the modified boundary value problem the variables are v and $\partial v/\partial n$. The system of algebraic equations emerges as

$$
\begin{bmatrix}
H_{11} & H_{12} & H_{13} \\
H_{21} & H_{22} & H_{23} \\
H_{31} & H_{32} & H_{33}
\end{bmatrix}
\begin{Bmatrix}
v_1 \\
v_2 \\
v_3
\end{Bmatrix}
=
\begin{bmatrix}
G_{11} & G_{12} & G_{13} \\
G_{21} & G_{22} & G_{23} \\
G_{31} & G_{32} & G_{33}
\end{bmatrix}
\begin{Bmatrix}
\dfrac{\partial v_1}{\partial n} \\[2mm]
\dfrac{\partial v_2}{\partial n} \\[2mm]
\dfrac{\partial v_3}{\partial n}
\end{Bmatrix}
\tag{46}
$$

By rearranging the equations so that the unknowns are passed to the left-hand side, we can rewrite the linear system

$$
\begin{bmatrix}
H_{11} & -G_{12} & H_{13} \\
H_{21} & -G_{22} & H_{23} \\
H_{31} & -G_{32} & H_{33}
\end{bmatrix}
\begin{Bmatrix}
v_1 \\[1mm]
\dfrac{\partial v_2}{\partial n} \\[2mm]
v_3
\end{Bmatrix}
=
\begin{bmatrix}
G_{11} & -H_{12} & G_{13} \\
G_{21} & -H_{22} & G_{23} \\
G_{31} & -H_{32} & G_{33}
\end{bmatrix}
\begin{Bmatrix}
\dfrac{\partial v_1}{\partial n} \\[2mm]
v_2 \\[1mm]
\dfrac{\partial v_3}{\partial n}
\end{Bmatrix}
\tag{47}
$$

Using Equations (25) and (26) we obtain, the final form of the set of equations

$$
\begin{bmatrix}
\left(H_{11} - \dfrac{G_{11}}{2k}\dfrac{\partial k}{\partial n}\right) & -G_{12} & \left(H_{13} - \dfrac{G_{13}}{2k}\dfrac{\partial k}{\partial n}\right) \\[3mm]
\left(H_{21} - \dfrac{G_{21}}{2k}\dfrac{\partial k}{\partial n}\right) & -G_{22} & \left(H_{23} - \dfrac{G_{23}}{2k}\dfrac{\partial k}{\partial n}\right) \\[3mm]
\left(H_{31} - \dfrac{G_{31}}{2k}\dfrac{\partial k}{\partial n}\right) & -G_{32} & \left(H_{33} - \dfrac{G_{33}}{2k}\dfrac{\partial k}{\partial n}\right)
\end{bmatrix}
\begin{Bmatrix}
v_1 \\[1mm]
\dfrac{\partial v_2}{\partial n} \\[2mm]
v_3
\end{Bmatrix}
=
\begin{bmatrix}
G_{11} & -H_{12} & G_{13} \\
G_{21} & -H_{22} & G_{23} \\
G_{31} & -H_{32} & G_{33}
\end{bmatrix}
\begin{Bmatrix}
-\dfrac{\overline{q_1}}{\sqrt{k}} \\[2mm]
\overline{\phi_2}\sqrt{k} \\[2mm]
-\dfrac{\overline{q_3}}{\sqrt{k}}
\end{Bmatrix}
\tag{48}
$$

We solve these equations for v_1, $\partial v_2/\partial n$, and v_3; and finally, by using Equations (25) and (26), we obtain

$$
\phi_1 = v_1/\sqrt{k}
$$

$$
q_2 = -\sqrt{k}\left\{\frac{\partial v_2}{\partial n} - \frac{1}{2k}\frac{\partial k}{\partial n}v_2\right\}
\tag{49}
$$

$$
\phi_3 = v_3/\sqrt{k}
$$

The extension of the current algorithm to handle multi-zone problems is doable but warrants careful housekeeping of the variables. A useful discussion on multi-zone and interface problems can be found in the paper by Gray and Paulino [26].

5.4. Boundary elements

The surface of the solution domain is divided into a number of connected elements. Over each element, the variation of the geometry and the variables (potential and flux) is approximated by

Weight function N_k

Neumann Corner
(Unknown is
potential at corner,
flux is known on
both sides)

Dirichlet Corner
(Unknowns are
fluxes on each
side, potential is
known)

Mixed Corner
(Unknown is
flux on left side,
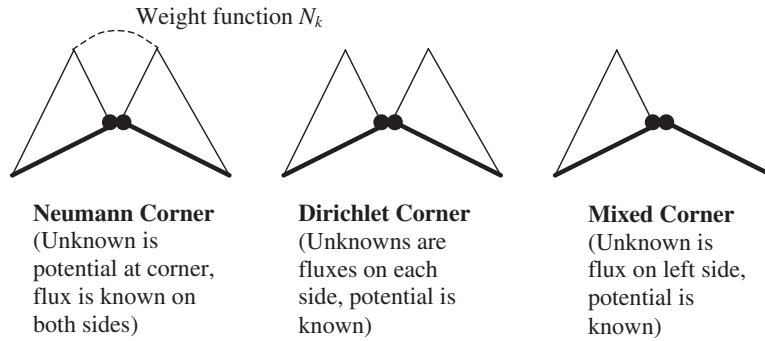potential is
known)

Figure 3. Corner treatment in the Galerkin BEM.

simple functions. Six-noded isoparametric quadratic triangular elements are used. The geometry of an element can be defined by the co-ordinates of its six nodes using appropriate quadratic shape functions as follows:

$$x_i(\xi, \eta) = \sum_{j=1}^{6} N_j(\xi, \eta)(x_i)_j \tag{50}$$

In an isoparametric approximation, the same shape functions are used for the solution variables (both potential and flux), as follows:

$$\phi_i(\xi, \eta) = \sum_{j=1}^{6} N_j(\xi, \eta)(\phi_i)_j$$
$$q_i(\xi, \eta) = \sum_{j=1}^{6} N_j(\xi, \eta)(q_i)_j \tag{51}$$

The shape functions can be explicitly written in terms of intrinsic co-ordinates ξ and η as

$$N_1(\eta, \xi) = (\xi + \sqrt{3}\eta - \sqrt{3})(\xi + \sqrt{3}\eta)/6, \quad N_4(\eta, \xi) = (\xi + \sqrt{3}\eta - \sqrt{3})(\xi - \sqrt{3}\eta - \sqrt{3})/3$$

$$N_2(\eta, \xi) = (\xi - \sqrt{3}\eta - \sqrt{3})(\xi - \sqrt{3}\eta)/6, \quad N_5(\eta, \xi) = -2\xi(\xi - \sqrt{3}\eta - \sqrt{3})/3$$

$$N_3(\eta, \xi) = \xi(2\xi - \sqrt{3})/3, \quad N_6(\eta, \xi) = -2\xi(\xi + \sqrt{3}\eta - \sqrt{3})/3 \tag{52}$$

The intrinsic co-ordinate space is the equilateral triangle with $-1 \leqslant \eta \leqslant 1$, $0 \leqslant \xi \leqslant \sqrt{3}(1 - |\eta|)$.

5.5. Corners

The treatment of corners in Galerkin BEM is simple and elegant due to the flexibility in choosing the weight function for the Galerkin approximation. Corners are represented by double nodes, and on each side two different weight functions are used. These weight functions are half of the usual weight. Figure 3 illustrates the corner treatment. For a Neumann corner (flux specified on both sides of the corner, potential is the unknown), the weight functions are added into one. In all other cases (Dirichlet corner and mixed corner) the weight functions remain separate.

6. ABAQUS USER SUBROUTINE

In general, conventional FEM softwares (including ABAQUS [27]) use homogeneous elements with constant material properties at the element level. In the present work, in order to incorporate the functional variation of the material at the finite element level, a user subroutine UMATHT was developed for ABAQUS [27]. By means of this subroutine, any functional variation can be included within an element by sampling the material property at each Gauss point. In general, graded elements approximate the material gradient better than conventional homogeneous elements and provide a smoother transition at element boundaries. Further investigations on graded elements can be found in the papers by Santare and Lambros [28] and Kim and Paulino [29] for 2D problems, and in the paper by Walters *et al.* [30] for 3D problems. The user subroutine UMATHT is included in Appendix A.

7. NUMERICAL EXAMPLES

In this section, several test cases are reported, demonstrating the implementation of the above techniques. To verify the numerical implementation, the following four examples are presented:

(1) cube with material gradation along the z-axis,
(2) cube with a 3D material gradation,
(3) inclined cylindrical cavity in a parallelepiped,
(4) rotor problem.

The first example is a cube with constant temperatures in two sides and insulated in all the other sides. The material property varies only in the z direction. This problem has analytical solution. For this problem all the three kinds of material variation i.e. quadratic, exponential and trigonometric, are prescribed. This problem is used to verify the present formulation [31]. The second example has a complicated 3D quadratic spatial material variation inside a cube with mixed boundary conditions. The third problem has a complicated geometry, an inclined cylindrical cavity in a parallelepiped. This problem is solved as a Dirichlet problem with known prescribed field. The last example is a rotor problem, which is of engineering significance in the field of functionally graded materials.

7.1. Cube with material gradation with z-axis

A unit cube ($L = 1$) with prescribed constant temperature on two sides is considered. The problem of interest and corresponding BEM mesh is shown in Figure 4. The top surface of the cube at $[z = 1]$ is maintained at a temperature of $T = 100$ while the bottom at $[z = 0]$ is zero. The remaining four faces are insulated (zero normal flux). Three different classes of variations are considered. The profiles of the thermal conductivity $k(z)$ of the three cases are illustrated in Figure 4.

- *Quadratic variation of k*: The quadratic variation of the thermal conductivity $k(x, y, z)$ is defined as

$$k(x, y, z) = k(z) = k_0(a_1 + \beta z)^2 = 5(1 + 2z)^2 \tag{53}$$
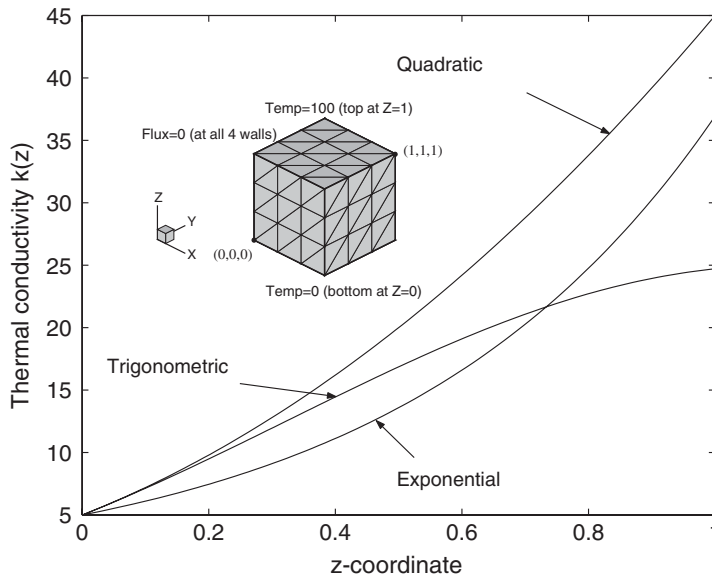
Figure 4. Thermal conductivity variation along the z direction. The quadratic variation is $k(z) = 5(1 + 2z)^2$, the trigonometric is $k(z) = 5[\cos(z) + 2\sin(z)]^2$, and the exponential variation is $k(z) = 5e^{2z}$. The insert shows the geometry, mesh and the boundary conditions of the unit cube. The BEM mesh consists of 294 nodes and 108 quadratic triangular elements.

in which β is the non-homogeneity parameter and a_1 is a constant. The analytical solution for temperature is

$$\phi(z) = 100\frac{(a_1 + \beta L)z}{(a_1 + \beta z)L} = \frac{300z}{1 + 2z} \tag{54}$$

- *Exponential variation of k*: Let the exponential variation $k(x, y, z)$ be defined as

$$k(x, y, z) = k(z) = k_0 e^{2\beta z} = 5e^{2z} \tag{55}$$

The analytical solution for temperature for this type of material variation is

$$\phi(z) = 100\frac{1 - e^{-2\beta z}}{1 - e^{-2\beta L}} \tag{56}$$

- *Trigonometric variation of k*: Let the trigonometric variation of the thermal conductivity $k(x, y, z)$ be defined as

$$k(z) = k_0(a_1 \cos \beta z + a_2 \sin \beta z)^2 = 5[\cos(z) + 2\sin(z)]^2 \tag{57}$$

The analytical solution for temperature is

$$\phi(z) = 100\frac{[a_1 \cot(\beta L) + a_2]\sin(\beta z)}{[a_1 \cos(\beta z) + a_2 \sin(\beta z)]} \tag{58}$$
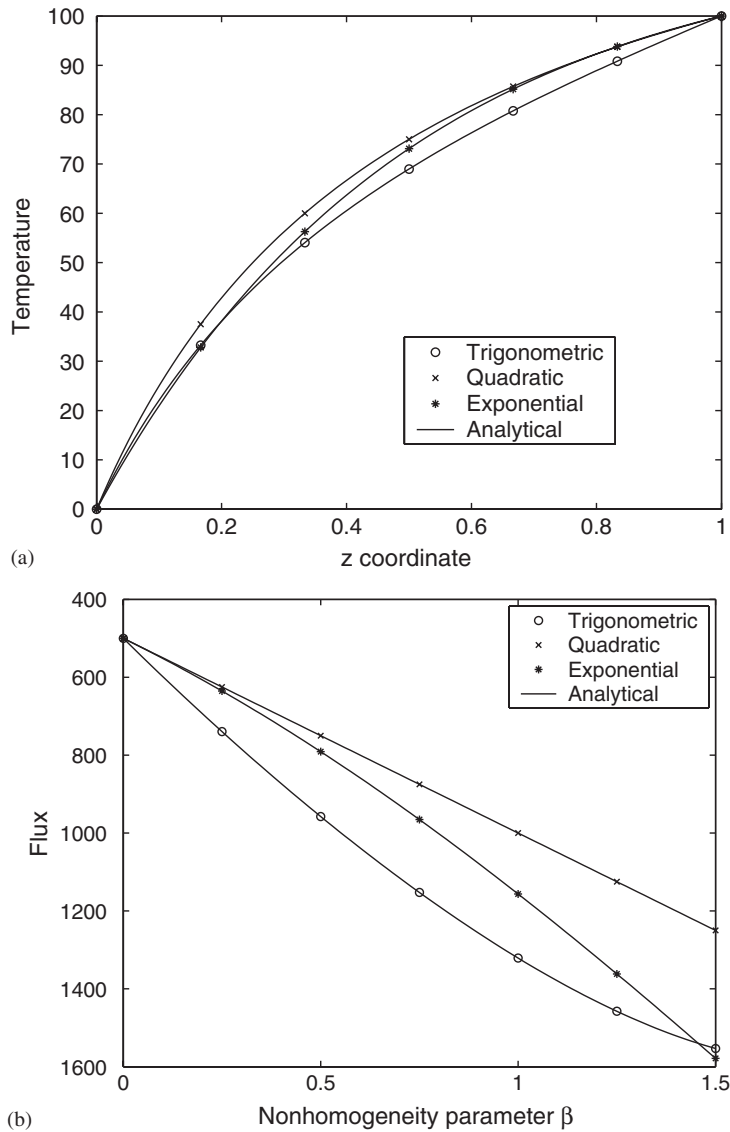
Figure 5. (a) Temperature profile in the z direction for different material variations; (b) variation of flux at $z = 1$ surface with different values of non-homogeneity parameter β.

- *Results*: The temperature profile along the z-axis is plotted for the three variations and compared with the analytical solutions in Figure 5(a). The variation of flux at the $z = 1$ surface with different values of the non-homogeneity parameter β (keeping a_1 and a_2 as constants) is plotted and compared with the analytical solution in Figure 5(b). The numerical and analytical results are in excellent agreement.
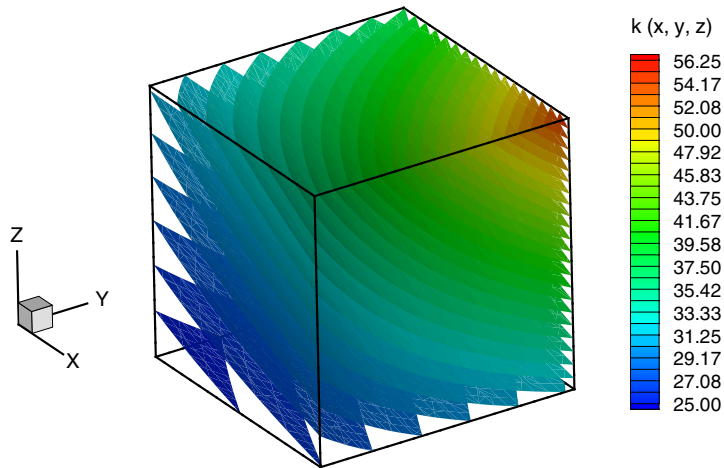
Figure 6. Representation of iso-surfaces for the three-dimensional variation of thermal conductivity $k(x, y, z)$.

7.2. Cube with a 3D material gradation

The three-dimensional thermal conductivity variation is

$$k(x, y, z) = (5 + 0.2x + 0.4y + 0.6z + 0.1xy + 0.2yz + 0.3zx + 0.7xyz)^2 \tag{59}$$

Figure 6 illustrates the iso-surfaces of the 3D variation of the thermal conductivity. It can be shown that Equation (59), in which $\sqrt{k(x, y, z)}$ is a linear combination of $1, x, y, z, xy, yz, zx,$ xyz (i.e. the most general linear function of x, y or z alone) satisfies Equation (12) and thereby allows Equation (1) to be reduced to a Laplace equation governing $v(x, y, z)$, by change of variables using Equation (5). The following function is an admissible solution for this variation

$$\phi(x, y, z) = \frac{xyz}{(5 + 0.2x + 0.4y + 0.6z + 0.1xy + 0.2yz + 0.3zx + 0.7xyz)} \tag{60}$$

The mixed boundary conditions at the six faces of the cube are prescribed as

$$\phi(0, y, z) = 0$$

$$\overline{q}(1, y, z) = -k(1, y, z) \frac{\partial \phi(x, y, z)}{\partial x} = -0.2zy(25 + 2y + 3z + zy)$$

$$\phi(x, 0, z) = 0$$

$$\overline{q}(x, 1, z) = -k(x, 1, z) \frac{\partial \phi(x, y, z)}{\partial y} = -0.1xz(50 + 2x + 6z + 3xz) \tag{61}$$

$$\phi(x, y, 0) = 0$$

$$\overline{q}(x, y, 1) = -k(x, y, 1) \frac{\partial \phi(x, y, z)}{\partial z} = -0.1xy(50 + 2x + 4y + xy)$$

(a)

(b)
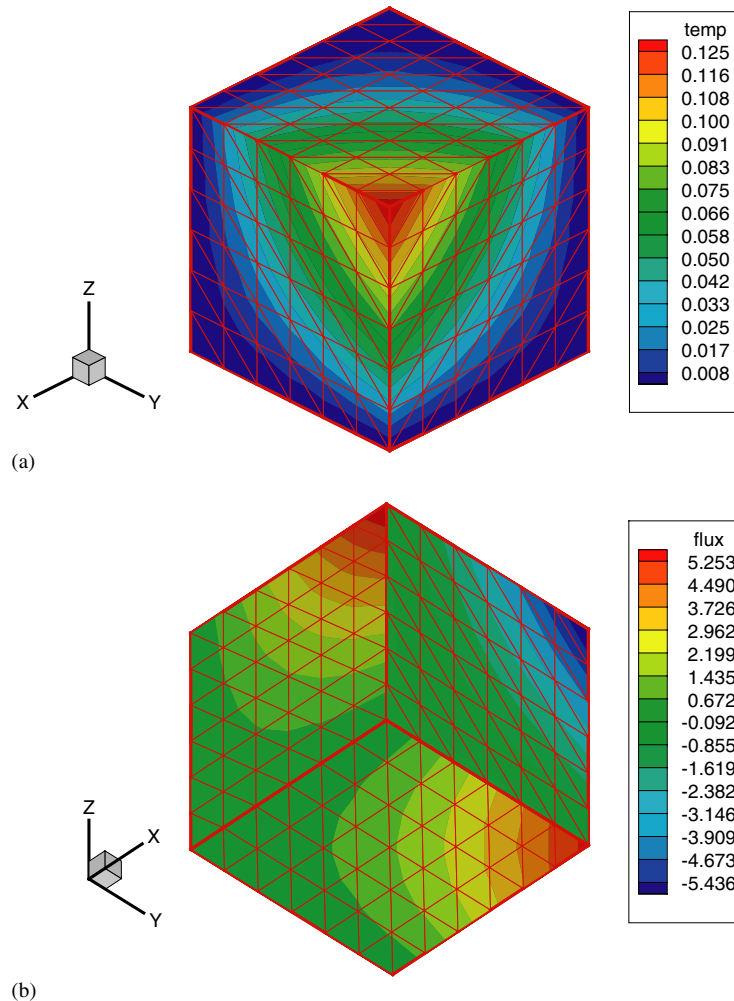
Figure 7. (a) Contour plot of temperature for the cube with 3D material variation; and (b) contour plot of flux for the cube with 3D material variation.

The cube is discretized with 294 nodes and 108 quadratic triangular elements. The results for the temperature and the flux are recovered exactly up to three decimals. Contour plots of the temperature and the flux are shown in Figure 7.

7.3. Cylindrical cavity in a parallelepiped

Figure 8 shows the geometry of the parallelepiped with a cylindrical cavity. The inspiration for this problem comes from a paper by Ingber and Martinez [32]; however, the boundary conditions here are different from their paper. The thermal conductivity varies as a trigonometrical function in one co-ordinate (see Figure 9(a)) according to

$$k(z) = 0.5[5\cos(2z) + 7.78704\sin(2z)]^2 \tag{62}$$

XY view   *YZ view*
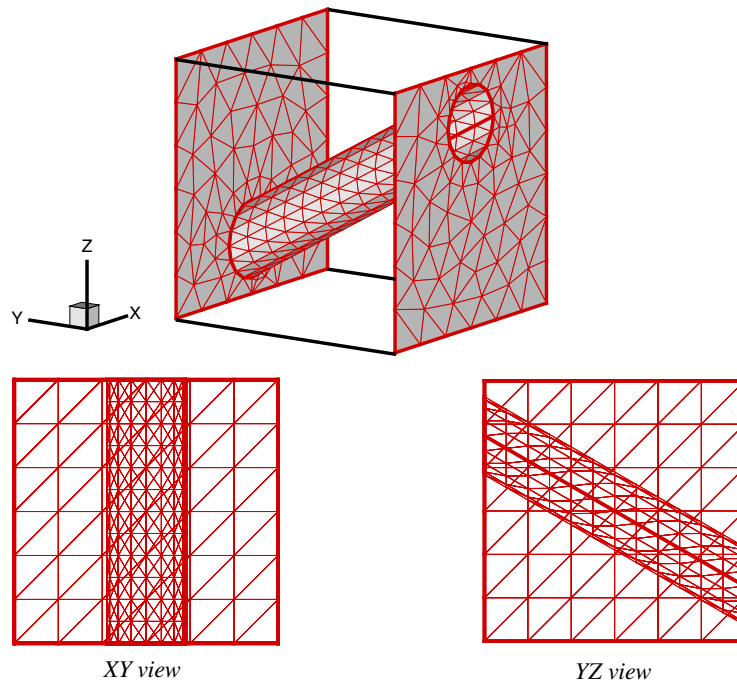
Figure 8. The mesh and the geometry of the parallelepiped. For the sake of clarity meshes in four faces of the parallelepiped have been omitted in the figure in the top. The *XY* and *YZ* views are provided which shows the mesh in those faces.

This problem is set as a Dirichlet problem where the temperature in the surface of the body is specified as

$$u(x, y, z) = \frac{4xy \sin(2z)}{[a_1 \cos(2z) + a_2 \sin(2z)]}$$

$$= \frac{4xy \sin(2z)}{[5 \cos(2z) + 7.78704 \sin(2z)]} \tag{63}$$

The analytical solution for flux is therefore

$$q(x, y, z) = -4k_0[a_1 \cos(2z) + a_2 \sin(2z)]y \sin(2z)\mathbf{n}_1$$

$$- 4k_0[a_1 \cos(2z) + a_2 \sin(2z)]x \sin(2z)\mathbf{n}_2 - 8k_0 xy a_1 \mathbf{n}_3 \tag{64}$$

The parallelepiped including the cavity is discretized using 942 T6 elements and 2121 nodes. Flux along z in $y = 0$ plane at the intersection of $x = 1$ and $y = 0$ planes is compared with the analytical results as shown in Figure 9(b), which shows that the numerical and analytical solutions are in excellent agreement. The contour plot in Figure 10 illustrates the complex nature of the flux distribution of the problem.
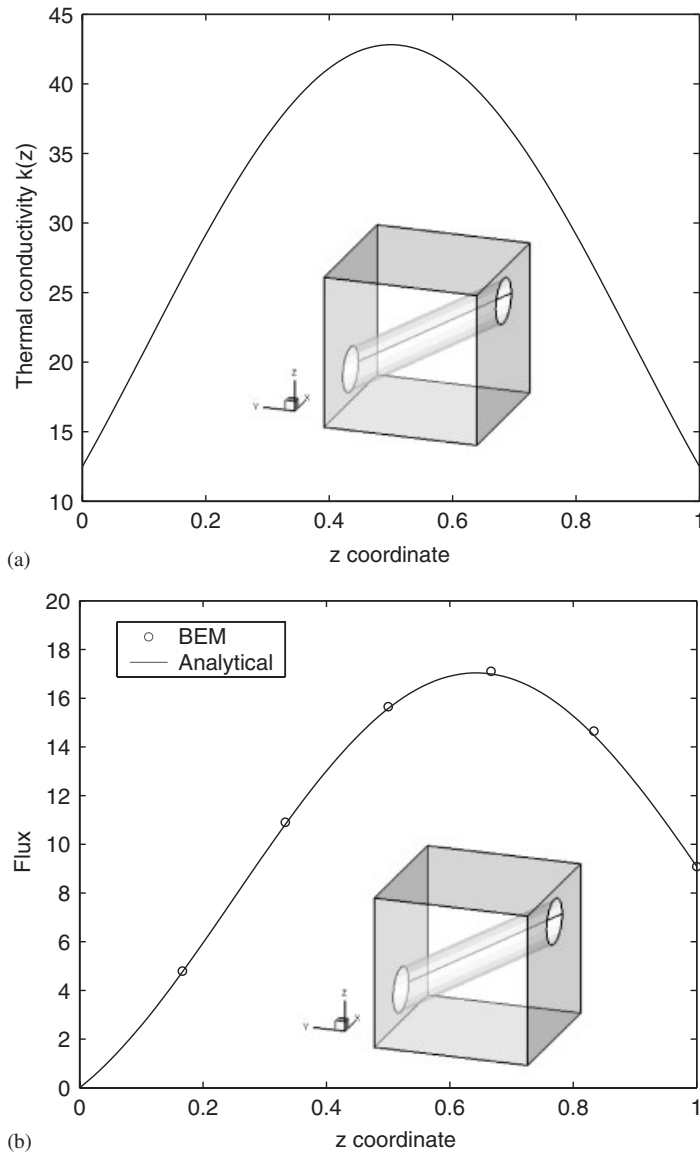
Figure 9. (a) Thermal conductivity for the parallelepiped with cylindrical cavity; and (b) flux along z in $y = 0$ plane at edge $[x = 1, \ y = 0]$ of the parallelepiped.

7.4. FGM Rotor problem

The last numerical example is an FGM rotor with eight mounting holes having an eight-fold symmetry. Owing to the symmetry, only one-eighth of the rotor is analysed. The top view of the rotor, the analysis region, and the geometry of the region are illustrated in Figure 11. The
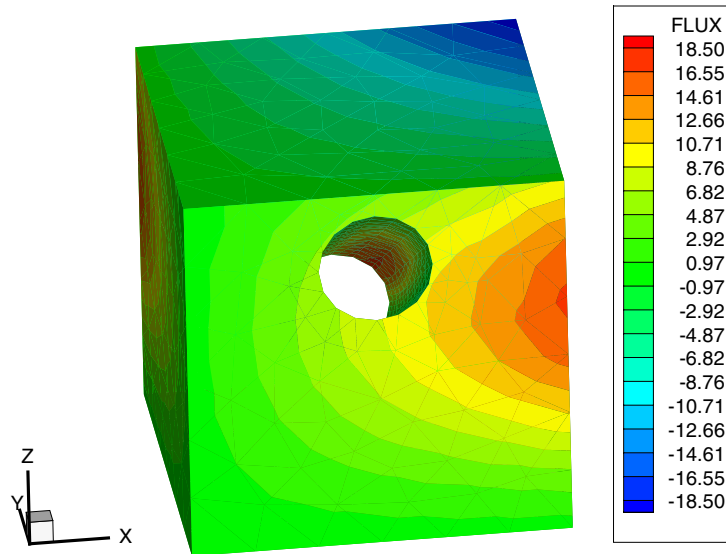
Figure 10. Contour plot of flux for cylindrical cavity in parallelepiped.
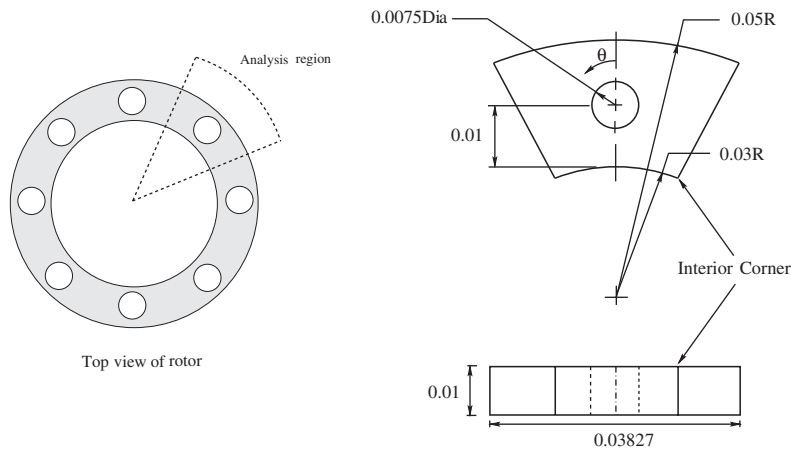
Figure 11. Geometry of the functionally graded rotor with 8-fold symmetry.

grading direction for the rotor is parallel to its line of symmetry, which is taken as the z-axis. The thermal conductivity for the rotor varies according to the following expression:

$$\text{Quadratic} \quad k(z) = 20(1 + 420.7z)^2 \tag{65}$$

The profile of the thermal conductivity $k(z)$ of the variation is illustrated in Figure 12. The temperature is specified along the inner radius as $T_{\text{inner}} = 20 + 1.25 \times 10^6 (z - 0.01)^2$ and
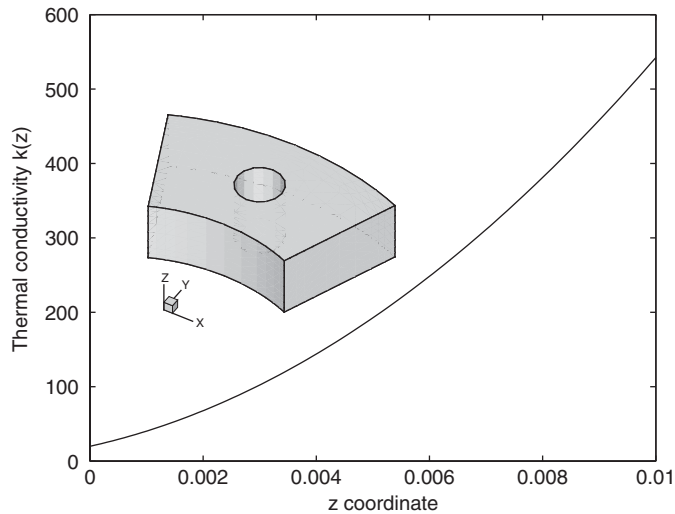
Figure 12. Profile of thermal conductivity in z direction. The quadratic variation of the conductivity is $k(z) = 20(1 + 420.7z)^2$.
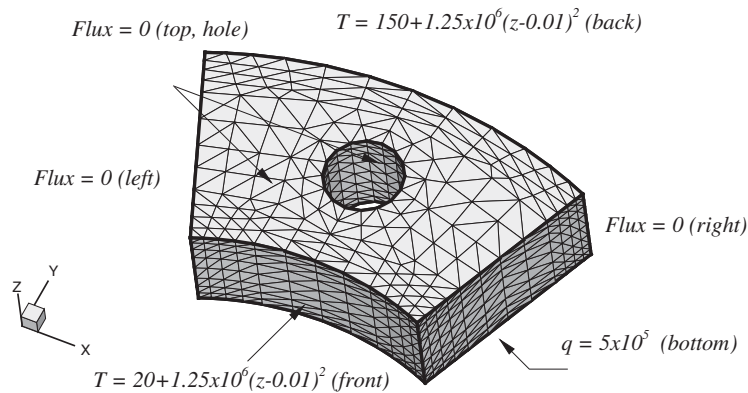
Figure 13. Thermal boundary conditions and the BEM mesh with 1584 elements and 3492 nodes.

outer radius as $T_{\text{outer}} = 150 + 1.25 \times 10^6 (z - 0.01)^2$. A uniform heat flux of 5×10^5 is added on the bottom surface where $z = 0$, and all other surfaces are insulated. The BEM mesh employs 1584 elements and 3492 nodes. A schematic for the thermal boundary conditions and the BEM mesh employed is shown in Figure 13. This problem has been solved previously using the 'Green's function' approach by means of a Galerkin BEM (non-symmetric) by Gray *et al.* [6], who considered exponential conductivity variation. Here the solution of the problem is verified using the commercially available software ABAQUS by means of the user-defined subroutine UMATHT (see Appendix A). The FEM mesh consists of 7600 20-noded brick
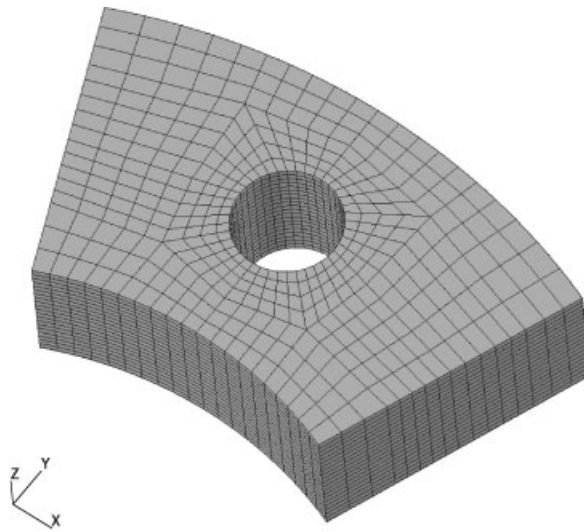
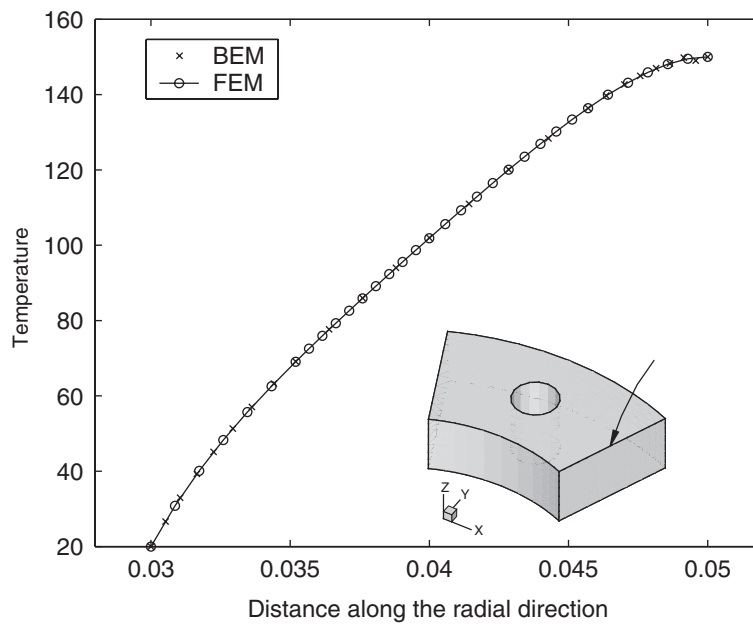Figure 14. The FEM mesh with 7600 elements and 35 514 nodes.

Figure 15. Temperature distribution along the right top edge (indicated by the arrow).

elements (quadratic) and 35 514 nodes. The FEM mesh is shown in Figure 14, which is intended simply to provide a reference solution against which the BEM results can be compared to. The temperature along the radial direction at the edge is plotted and compared with the FEM results
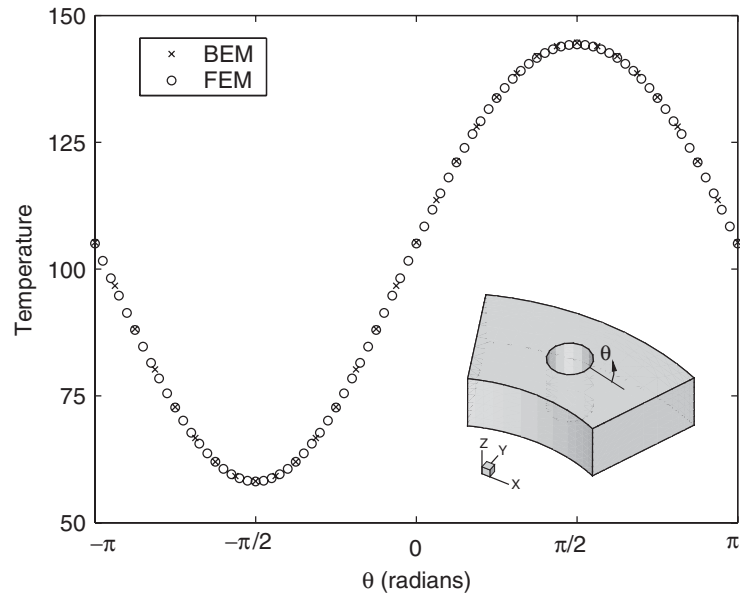
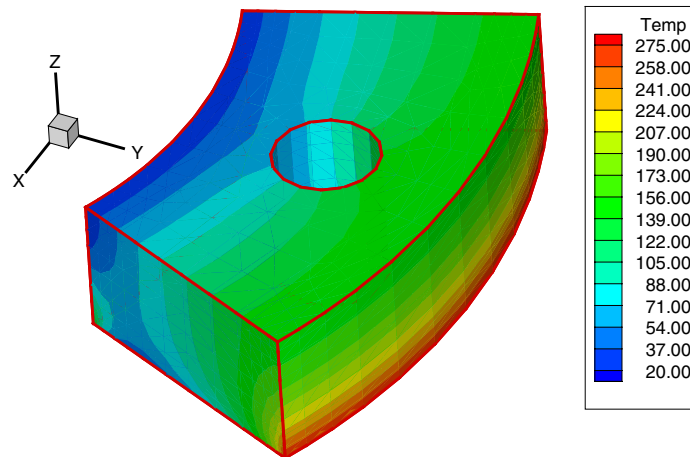Figure 16. Temperature distribution along the circular contour on the top face.

Figure 17. BEM contour plot of the temperature of the rotor.

in Figure 15. Figure 16 shows the comparison of the BEM and FEM results for the temperature around the hole. A contour plot of the temperature distribution is shown in Figure 17. The radial heat flux at the right interior corner is plotted along the interior corner in Figure 18. All the results of the BEM and FEM solution are in very good agreement.
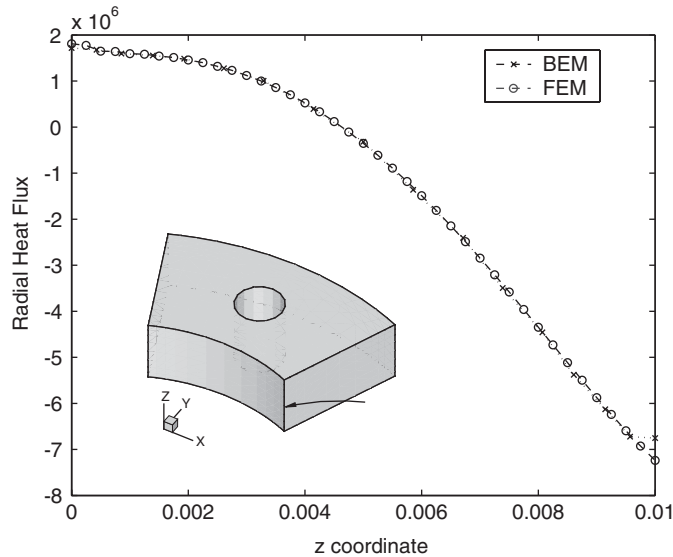
Figure 18. Radial heat flux along the interior edge (indicated by the arrow).

8. CONCLUSIONS

This paper presents a novel simple boundary element technique to address problems of potential flow for non-homogeneous media. It is shown that for quadratic material variation, the non-homogeneous problem can be transformed to a Laplace problem; for exponential variation, the problem can be transformed to a modified Helmholtz equation; and for trigonometric variation, the problem can be transformed to a standard Helmholtz equation. By simple modification of the boundary conditions, standard codes for homogeneous material problems are used. A number of examples are presented to verify the methodology. In this paper, the implementation is carried out using the Galerkin BEM (non-symmetric), but the idea and development are applicable to collocation or other boundary element methods such as meshless or symmetric Galerkin BEM. The Galerkin approximation allows standard continuous C^0 elements to be used for evaluation of hypersingular integrals, which is extremely useful for treatment of corners and fracture problems. Future work involves extension to transient heat conduction and crack problems.

APPENDIX A

The ABAQUS user subroutine UMATHT for graded elements with variable conductivity is presented here. It is written in Fortran language.

```
c        ABAQUS User subroutine umatht
c    This user subroutine implements graded elements with variable
c    conductivity in ABAQUS. It can incorporate any functional
c    variation of heat conductivity and specific heat.
```

```
c   Ref: A. Sutradhar and G. H. Paulino, 'A simple boundary element
c        method for potential problems in nonhomogeneous media'.
c        International Journal for Numerical Methods in Engineering
c
    subroutine umatht(u,dudt,dudg,flux,dfdt,dfdg,statev,temp,
   $   dtemp,dtemdx,time,dtime,predef,dpred,cmname,ntgrd,nstatv,
   $   props,nprops,coords,pnewdt,noel,npt,layer,kspt,kstep,kinc)
c
    include 'aba_param.inc'
    character*80 cmname
    dimension dudg(ntgrd),flux(ntgrd),dfdt(ntgrd),
   $   dfdg(ntgrd,ntgrd),statev(nstatv),dtemdx(ntgrd),time(2),
   $   predef(1),dpred(1),props(nprops),coords(3)
c              read in properties
c   exponential
c   beta=1.5
c   cond=5.0*exp(2.0*beta*coords(3))
c   trigonometric
c   cond=5.0*(cos(coords(3))+4.68392*sin(coords(3)))**2.d0
c   quadratic
    cond=20*(1+420.7*coords(3))**2.0
    specht=0.0
c              input specific heat
    dudt=specht
    deltu=dudt*dtemp
    u=u+deltu
c              input flux=-[k]*{dtemdx}
    do i=1, ntgrd
      flux(i)=-cond*dtemdx(i)
    end do
c              input isotropic conductivity
    do i=1, ntgrd
      dfdg(i,i)=-cond
    end do
    return
    end
```

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