A Simulation of Unsteady Heat Conduction Problems for Anisotropic Quadratically Graded Materials

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Abstract—**Numerical solutions for unsteady heat conduction problems governed by a Laplacian type equation with quadratically varying coefficients for anisotropic inhomogeneous media are sought using a mixed Laplace transform and boundary element method. Several examples for anisotropic quadratically graded media are considered. The results demonstrate ease of implementation and accuracy of the method.**

Index Terms—**anisotropic functionally graded materials, unsteady heat conduction, simulation, boundary element method**

I. INTRODUCTION

We will consider unsteady heat conduction problems governed by a Laplace type equation with variable coefficients of the form

$$\frac{\partial}{\partial x_i}\left[\kappa_{ij}(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial x_j}\right]=\psi(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial t}\quad i,j=1,2 \tag{1}$$

where $[\kappa_{ij}]$ is the conductivity, which is a symmetric matrix with positive determinant, T is the temperature, ψ is the rate of the temperature change, $\mathbf{x}$ is the spatial variable, and t is the time variable. In equation (1), summation convention holds for repeated indices so that explicitly equation (1) takes the form

$$\frac{\partial}{\partial x_1}\left(\kappa_{11}\frac{\partial T}{\partial x_1}\right)+\frac{\partial}{\partial x_1}\left(\kappa_{12}\frac{\partial T}{\partial x_2}\right)+\frac{\partial}{\partial x_2}\left(\kappa_{12}\frac{\partial T}{\partial x_1}\right)+\frac{\partial}{\partial x_2}\left(\kappa_{22}\frac{\partial T}{\partial x_2}\right)=\psi\frac{\partial T}{\partial t}$$

Equation (1) is usually used to model antiplane strain in elastostatics and plane thermostatic problems (see for examples [1]–[4]).

In recent years, there has been a growing interest in functionally graded materials (FGMs), and various studies have been conducted on them for different purposes. FGMs are materials that exhibit varying properties based on a mathematical function, and as such, equation (1) is pertinent to their study. These materials are usually engineered to meet specific practical requirements, and this underscores the importance of solving equation (1), as it can help in the development of FGMs that meet desired performance standards (as demonstrated, for example, in references [9], [10]).

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A number of studies on the heat conduction equation had been done for finding its numerical solutions. The studies can be classified according to the anisotropy of the media and the variability of coefficients (inhomogeneity of the media). For examples, [1]–[3] considered a *constant coefficients* (homogeneous media) anisotropic equation, [4] solved an anisotropic equation with *variable coefficients* (inhomogeneous media). Some other studies on problems of inhomogeneous anisotropic media for several types of governing equations had been done (see for examples, [5], [6], [7], [8]).

This paper is intended to extend the recently published works in [11] for steady anisotropic Laplace type equation with spatially variable coefficients of the form

$$\frac{\partial}{\partial x_i}\left[\kappa_{ij}(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial x_j}\right]=0$$

to unsteady anisotropic Laplace type equation with spatially variable coefficients of the form (1).

II. THE INITIAL-BOUNDARY VALUE PROBLEM

The goal is to find solutions and their derivatives to equation (1) for time $t\geq 0$ and inside a region Ω in R^2 with a continuous boundary $\partial\Omega$. On $\partial\Omega_1$ the dependent variable $T(\mathbf{x},t)$ $(\mathbf{x}=(x_1,x_2))$ is specified and on $\partial\Omega_2$

$$F(\mathbf{x},t)=\kappa_{ij}(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial x_i}n_j \tag{2}$$

is specified where $\partial\Omega=\partial\Omega_1\cup\partial\Omega_2$ and $\mathbf{n}=(n_1,n_2)$ denotes the outward pointing normal to $\partial\Omega$. The initial condition is taken to be

$$T(\mathbf{x},0)=0 \tag{3}$$

III. THE INTEGRAL EQUATION

The coefficients κ_{ij},ψ are required to take the form

$$\kappa_{ij}(\mathbf{x}) = \overline{\kappa}_{ij}g(\mathbf{x}) \tag{4}$$

$$\psi(\mathbf{x}) = \overline{\psi}g(\mathbf{x}) \tag{5}$$

where the $\overline{\kappa}_{ij},\overline{\psi}$ are constants. Further we assume that the coefficients $\kappa_{ij}(\mathbf{x})$ and $\psi(\mathbf{x})$ are graded quadratically according to the gradation function

$$g(\mathbf{x})=(c_0+c_ix_i)^2 \tag{6}$$

where c_0 and c_i are constants. Therefore (6) satisfies

$$\overline{\kappa}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j}=0 \tag{7}$$

Use of (4)-(5) in (1) yields

$$\overline{\kappa}_{ij}\frac{\partial}{\partial x_i}\left(g\frac{\partial T}{\partial x_j}\right)=\overline{\psi}g\frac{\partial T}{\partial t} \quad (8)$$

Let

$$T(\mathbf{x},t)=g^{-1/2}(\mathbf{x})\,\sigma(\mathbf{x},t) \quad (9)$$

therefore substitution of (4) and (9) into (2) gives

$$F(\mathbf{x},t)=-F_g(\mathbf{x})\,\sigma(\mathbf{x},t)+g^{1/2}(\mathbf{x})\,F_\sigma(\mathbf{x},t) \quad (10)$$

where

$$F_g(\mathbf{x})=\overline{\kappa}_{ij}\frac{\partial g^{1/2}}{\partial x_j}n_i \qquad F_\sigma(\mathbf{x})=\overline{\kappa}_{ij}\frac{\partial \sigma}{\partial x_j}n_i$$

Also, (8) may be written in the form

$$\overline{\kappa}_{ij}\frac{\partial}{\partial x_i}\left[g\frac{\partial\left(g^{-1/2}\sigma\right)}{\partial x_j}\right]=\overline{\psi}g\frac{\partial\left(g^{-1/2}\sigma\right)}{\partial t}$$

which can be simplified

$$\overline{\kappa}_{ij}\frac{\partial}{\partial x_i}\left(g^{1/2}\frac{\partial\sigma}{\partial x_j}+g\sigma\frac{\partial g^{-1/2}}{\partial x_j}\right)=\overline{\psi}g^{1/2}\frac{\partial\sigma}{\partial t}$$

Use of the identity

$$\frac{\partial g^{-1/2}}{\partial x_i}=-g^{-1}\frac{\partial g^{1/2}}{\partial x_i}$$

implies

$$\overline{\kappa}_{ij}\frac{\partial}{\partial x_i}\left(g^{1/2}\frac{\partial\sigma}{\partial x_j}-\sigma\frac{\partial g^{1/2}}{\partial x_j}\right)=\overline{\psi}g^{1/2}\frac{\partial\sigma}{\partial t}$$

Rearranging and neglecting the zero terms yield

$$g^{1/2}\overline{\kappa}_{ij}\frac{\partial^2\sigma}{\partial x_i\partial x_j}-\sigma\overline{\kappa}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j}=\overline{\psi}g^{1/2}\frac{\partial\sigma}{\partial t}$$

Equation (7) then implies

$$\overline{\kappa}_{ij}\frac{\partial^2\sigma}{\partial x_i\partial x_j}=\overline{\psi}\frac{\partial\sigma}{\partial t} \quad (11)$$

Taking the Laplace transform of (9), (10), (11) and applying the initial condition (3) we obtain

$$\sigma^*(\mathbf{x},s)=g^{1/2}(\mathbf{x})\,T^*(\mathbf{x},s) \quad (12)$$

$$F_{\sigma^*}(\mathbf{x},s)=\left[F^*(\mathbf{x},s)+F_g(\mathbf{x})\,\sigma^*(\mathbf{x},s)\right]g^{-1/2}(\mathbf{x}) \quad (13)$$

$$\overline{\kappa}_{ij}\frac{\partial^2\sigma^*}{\partial x_i\partial x_j}-s\overline{\psi}\sigma^*=0 \quad (14)$$

where s is the variable of the Laplace-transformed domain.

A boundary integral equation for the solution of (14) is given in the form

$$\eta(\mathbf{x}_0)\,\sigma^*(\mathbf{x}_0,s)=\int_{\partial\Omega}\left[\Gamma(\mathbf{x},\mathbf{x}_0)\,\sigma^*(\mathbf{x},s)\right.$$
$$\left.-\Phi(\mathbf{x},\mathbf{x}_0)\,F_{\sigma^*}(\mathbf{x},s)\right]dS(\mathbf{x}) \quad (15)$$

where $\mathbf{x}_0=(a,b)$, $\eta=0$ if $(a,b)\notin\Omega\cup\partial\Omega$, $\eta=1$ if $(a,b)\in\Omega$, $\eta=\frac{1}{2}$ if $(a,b)\in\partial\Omega$ and $\partial\Omega$ has a continuously turning tangent at (a,b). The so called fundamental solution Φ in (15) satisfies

$$\overline{\kappa}_{ij}\frac{\partial^2\Phi}{\partial x_i\partial x_j}-s\overline{\psi}\Phi=\delta(\mathbf{x}-\mathbf{x}_0)$$

and the Γ is given by

$$\Gamma(\mathbf{x},\mathbf{x}_0)=\overline{\kappa}_{ij}\frac{\partial\Phi(\mathbf{x},\mathbf{x}_0)}{\partial x_j}n_i$$

where δ is the Dirac delta function. For two-dimensional problems Φ and Γ are given by

$$\Phi(\mathbf{x},\mathbf{x}_0)=\begin{cases}\frac{K}{2\pi}\ln R & \text{if } s\overline{\psi}=0\\ \frac{\imath K}{4}H_0^{(2)}(\omega R) & \text{if } s\overline{\psi}<0\\ \frac{-K}{2\pi}K_0(\omega R) & \text{if } s\overline{\psi}>0\end{cases}$$

$$\Gamma(\mathbf{x},\mathbf{x}_0)=\begin{cases}\frac{K}{2\pi}\frac{1}{R}\overline{\kappa}_{ij}\frac{\partial R}{\partial x_j}n_i & \text{if } s\overline{\psi}=0\\ \frac{-\imath K\omega}{4}H_1^{(2)}(\omega R)\,\overline{\kappa}_{ij}\frac{\partial R}{\partial x_j}n_i & \text{if } s\overline{\psi}<0\\ \frac{K\omega}{2\pi}K_1(\omega R)\,\overline{\kappa}_{ij}\frac{\partial R}{\partial x_j}n_i & \text{if } s\overline{\psi}>0\end{cases} \quad (16)$$

where

$$\begin{aligned}K&=\ddot{\tau}/D\\ \omega&=\sqrt{|s\overline{\psi}|/D}\\ D&=\left[\overline{\kappa}_{11}+2\overline{\kappa}_{12}\dot{\tau}+\overline{\kappa}_{22}\left(\dot{\tau}^2+\ddot{\tau}^2\right)\right]/2\\ R&=\sqrt{(\dot{x}_1-\dot{a})^2+(\dot{x}_2-\dot{b})^2}\\ \dot{x}_1&=x_1+\dot{\tau}x_2\\ \dot{a}&=a+\dot{\tau}b\\ \dot{x}_2&=\ddot{\tau}x_2\\ \dot{b}&=\ddot{\tau}b\end{aligned}$$

where $\dot{\tau}$ and $\ddot{\tau}$ are respectively the real and the positive imaginary parts of the complex root τ of the quadratic

$$\overline{\kappa}_{11}+2\overline{\kappa}_{12}\tau+\overline{\kappa}_{22}\tau^2=0$$

and $H_0^{(2)}$, $H_1^{(2)}$ denote the Hankel function of second kind and order zero and order one respectively. K_0, K_1 denote the modified Bessel function of order zero and order one respectively, $\imath=\sqrt{-1}$. Use of (12) and (13) in (15) yields

$$\eta g^{1/2}T^* = \int_{\partial\Omega}\left[\left(g^{1/2}\Gamma-F_g\Phi\right)T^*\right.$$
$$\left.-\left(g^{-1/2}\Phi\right)F^*\right]dS \quad (17)$$

This equation provides a boundary integral equation for determining T^* and its derivatives at all points of Ω.

After solving the boundary integral equation in the Laplace transform variable using a standard boundary element method, the solutions and their derivatives in the Laplace transform variable are obtained. The Stehfest formula is then used for a numerical Laplace transform inversion to find the solutions and their derivatives in the original time variable. The obtained solutions and their derivatives are for the original variable t, which were previously transformed to the Laplace transform variable s. The Stehfest formula is

$$\begin{aligned}T(\mathbf{x},t)&\simeq\frac{\ln 2}{t}\sum_{m=1}^{N}V_mT^*(\mathbf{x},s_m)\\ \frac{\partial T(\mathbf{x},t)}{\partial x_1}&\simeq\frac{\ln 2}{t}\sum_{m=1}^{N}V_m\frac{\partial T^*(\mathbf{x},s_m)}{\partial x_1}\\ \frac{\partial T(\mathbf{x},t)}{\partial x_2}&\simeq\frac{\ln 2}{t}\sum_{m=1}^{N}V_m\frac{\partial T^*(\mathbf{x},s_m)}{\partial x_2}\end{aligned} \quad (18)$$

TABLE I
VALUES OF V_m OF THE STEHFEST FORMULA

V_m	$N=6$	$N=8$	$N=10$	$N=12$
V_1	1	$-1/3$	$1/12$	$-1/60$
V_2	-49	$145/3$	$-385/12$	$961/60$
V_3	366	-906	1279	-1247
V_4	-858	$16394/3$	$-46871/3$	$82663/3$
V_5	810	$-43130/3$	$505465/6$	$-1579685/6$
V_6	-270	18730	-236957.5	1324138.7
V_7		$-35840/3$	$1127735/3$	$-58375583/15$
V_8		$8960/3$	$-1020215/3$	$21159859/3$
V_9			164062.5	-8005336.5
V_{10}			-32812.5	5552830.5
V_{11}				-2155507.2
V_{12}				359251.2

where

$$\begin{aligned} s_m &= \frac{\ln 2}{t} m \\ V_m &= (-1)^{\frac{N}{2}+m} \times \\ & \sum_{k=\left[\frac{m+1}{2}\right]}^{\min\left(m,\frac{N}{2}\right)} \frac{k^{N/2}\,(2k)!}{\left(\frac{N}{2}-k\right)!k!\,(k-1)!\,(m-k)!\,(2k-m)!} \end{aligned}$$

A simple script is developed to calculate the values of the coefficients $V_m, m = 1, 2, \ldots, N$ for any even number N. Table (I) shows the values of V_m for several values of N.

IV. NUMERICAL EXAMPLES

To verify the analysis developed in previous sections, various problems are considered, some of which have analytical solutions and others which do not. These problems belong to a system that is governed by equation (1) with specific initial and boundary conditions, and the coefficients $\kappa_{ij}(\mathbf{x})$ and $\psi(\mathbf{x})$ in equation (1) are of the form (4) and (5), respectively, with $g(\mathbf{x})$ being a quadratic function of the form [6]. The coefficients $\kappa_{ij}(\mathbf{x})$ and $\psi(\mathbf{x})$ represent diffusivity or conductivity and the change rate of the unknown $T(\mathbf{x}, t)$, respectively. Numerical solutions are obtained using the standard boundary element method (BEM) with constant elements, and a unit square is taken as the geometrical domain for all problems. The numerical solutions are obtained for the time interval $0 \leq t \leq 5$. A FORTRAN script is developed to compute the solutions, and the elapsed CPU time is calculated using a specific FORTRAN command. The Stehfest formula is used with different values of N ($N = 6, 8, 10, 12$) to obtain the results. It is found that $N = 10$ gives the most stable and optimized results, while increasing N from 10 to 12 yields worse results due to round-off errors, as noted by Hassanzadeh and Pooladi-Darvish [12]. Therefore, $N = 10$ is used in (18) for the Stehfest formula.

For all problems the inhomogeneity function is taken to be

$$g^{1/2}(\mathbf{x}) = 1 - 0.15x_1 - 0.3x_2$$

and the constant anisotropy coefficient $\overline{\kappa}_{ij}$

$$\overline{\kappa}_{ij} = \begin{bmatrix} 1 & 0.1 \\ 0.1 & 0.85 \end{bmatrix}$$

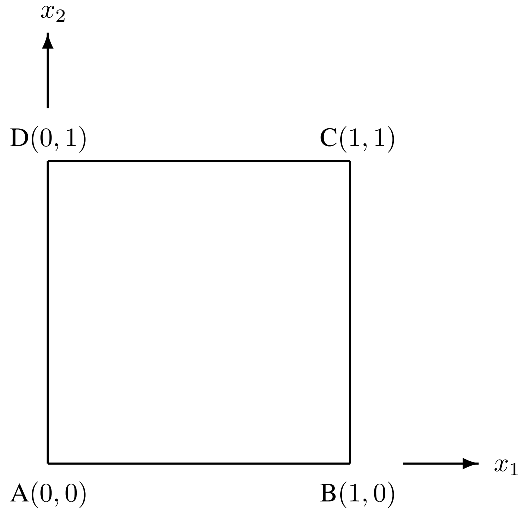

Fig. 1. The domain Ω

A. *Examples with analytical solutions*

1) Problem 1:: The analytical solutions are assumed to take a separable variables form

$$T(\mathbf{x}, t) = g^{-1/2}(\mathbf{x})\, h(\mathbf{x})\, f(t)$$

where $h(\mathbf{x}), f(t)$ are continuous functions. The boundary conditions are assumed to be (see Figure 1)

F is given on side AB
F is given on side BC
T is given on side CD
F is given on side AD

Case 1:: We take

$$\begin{aligned} h(\mathbf{x}) &= 0.5 - 0.15x_1 - 0.35x_2 \\ f(t) &= 1 - \exp(-1.75t) \end{aligned}$$

Thus for $h(\mathbf{x})$ to satisfy (14)

$$\overline{\psi} = 0$$

Case 2:: For the analytical solution we take

$$\begin{aligned} h(\mathbf{x}) &= \sin(0.5 - 0.15x_1 - 0.35x_2) \\ f(t) &= t/5 \end{aligned}$$

So that in order for $h(\mathbf{x})$ to satisfy (14)

$$\overline{\psi} = -0.137125/s$$

Case 3:: We take

$$\begin{aligned} h(\mathbf{x}) &= \exp(-0.5 + 0.15x_1 + 0.35x_2) \\ f(t) &= 0.16t(5 - t) \end{aligned}$$

Therefore (14) gives

$$\overline{\psi} = 0.137125/s$$

As shown in Figures 2, 3 and 4 for all cases the errors mainly occur in the fourth decimal place. Figures 5 and

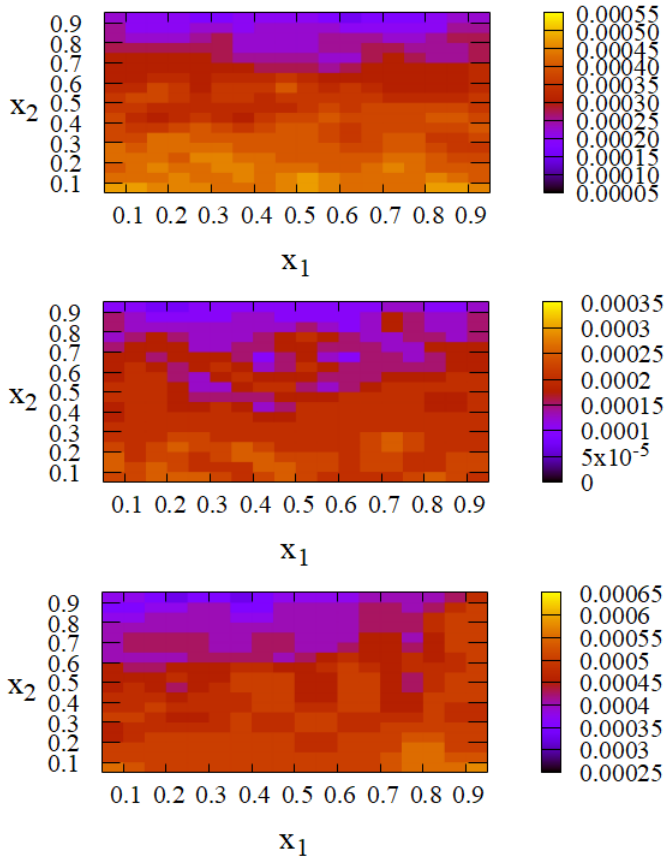

Fig. 2. The errors of interior solution T for the Case 1 (first row), Case 2 (second row), Case 3 (third row) of Problem 1

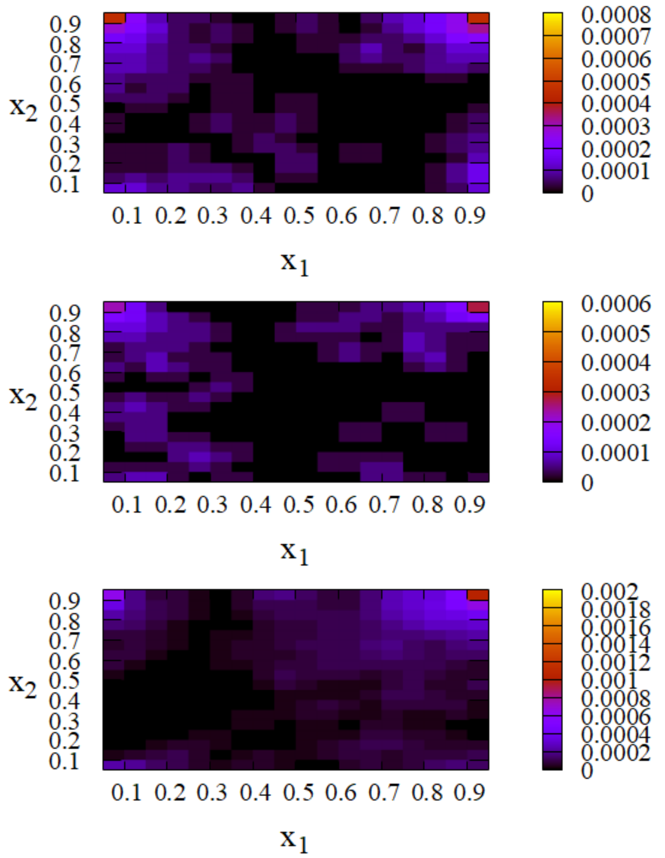

Fig. 3. The errors of interior solution $\partial T/\partial x_1$ at $t = 2.5$ for the Case 1 (first row), Case 2 (second row), Case 3 (third row) of Problem 1

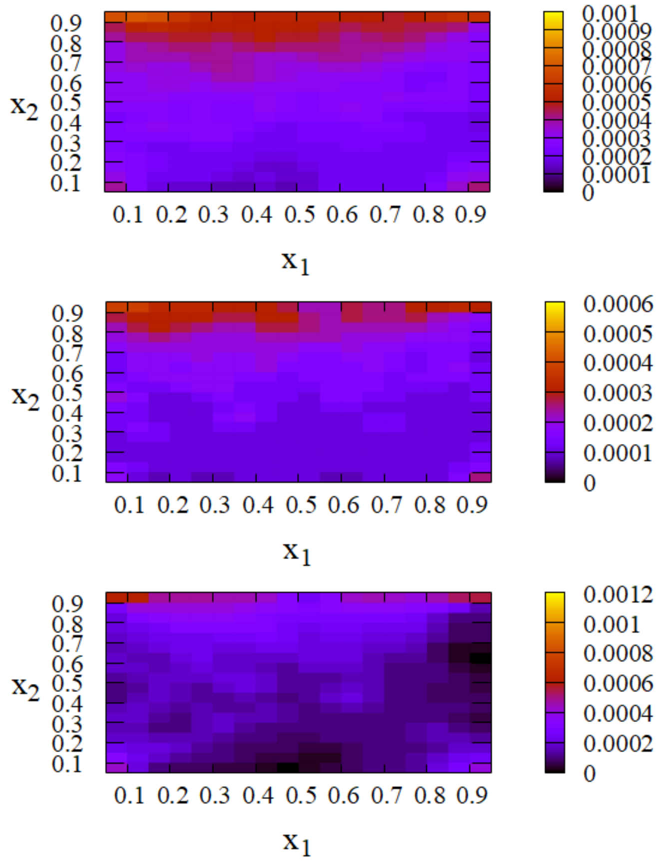

Fig. 4. The errors of interior solution $\partial T/\partial x_2$ at $t = 2.5$ for the Case 1 (first row), Case 2 (second row), Case 3 (third row) of Problem 1

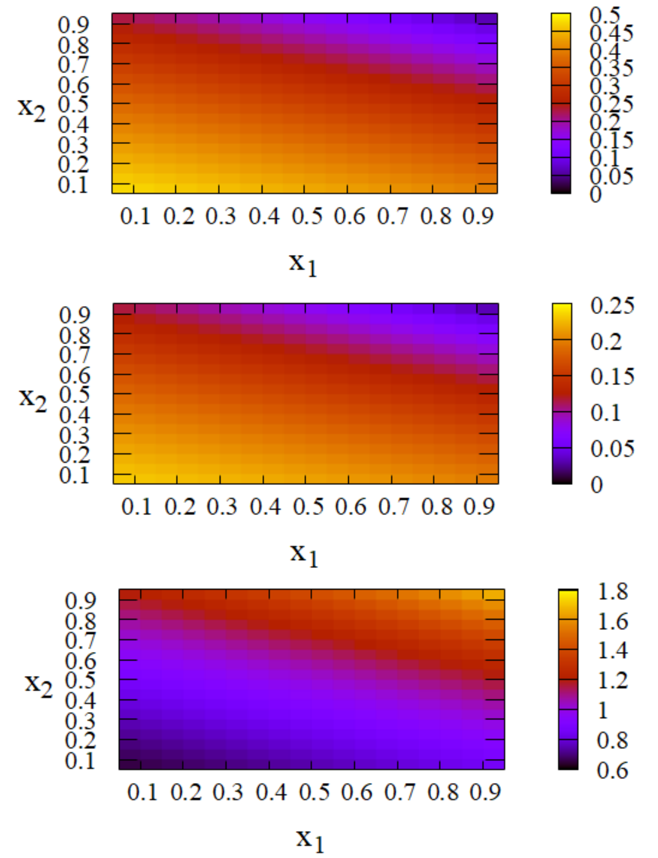

Fig. 5. The scattering T solutions at $t = 2.5$ for the Case 1 (first row), Case 2 (second row), Case 3 (third row) of Problem 1

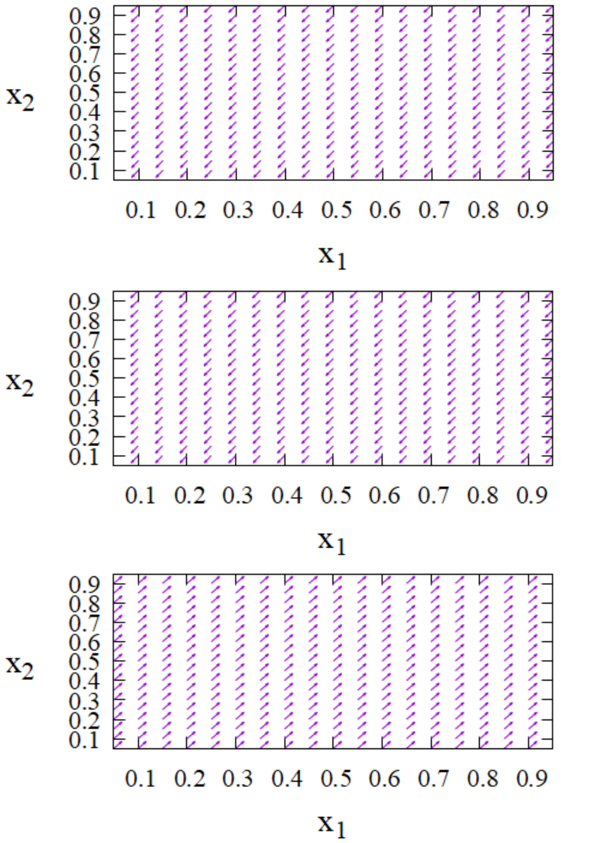

Fig. 6. The flow vector $(\partial T/\partial x_1, \partial T/\partial x_2)$ solutions at $t = 2.5$ for the Case 1 (first row), Case 2 (second row), Case 3 (third row) of Problem 1

6 indicate the consistency between the scattering and the flow solutions. Figure 7 shows that the variation of the T solution follows the way the associated function $f(t)$ changes. Specifically for the Case 1 of associated function $f(t) = 1 - \exp(-1.75t)$ the T solution will converge to 1.

For the computation of the numerical solutions the CPU elapses 401.703125 seconds for the Case 1, 6810.40625 seconds for the Case 2, and 3303.90625 seconds for the Case 3. The longer computation time for the Cases 2 and 3 is produced by the iterative calculation of the polynomial approximation of the Hankel and Bessel functions in the fundamental solutions (16).

B. Examples without analytical solutions

The aim is to show the effect of inhomogeneity and anisotropy of the considered material on the solution T.

1) Problem 2:: The material is supposed to be either inhomogeneous or homogeneous and either anisotropic or isotropic. If the material is homogeneous then

$$g(\mathbf{x}) = 1$$

and if it is isotropic then

$$\overline{\kappa}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

So that there are four cases regarding the material, namely anisotropic inhomogeneous, anisotropic homogeneous, isotropic inhomogeneous and isotropic homogeneous material. We set $\overline{\psi} = 1$ and the boundary conditions are (see Figure 1)

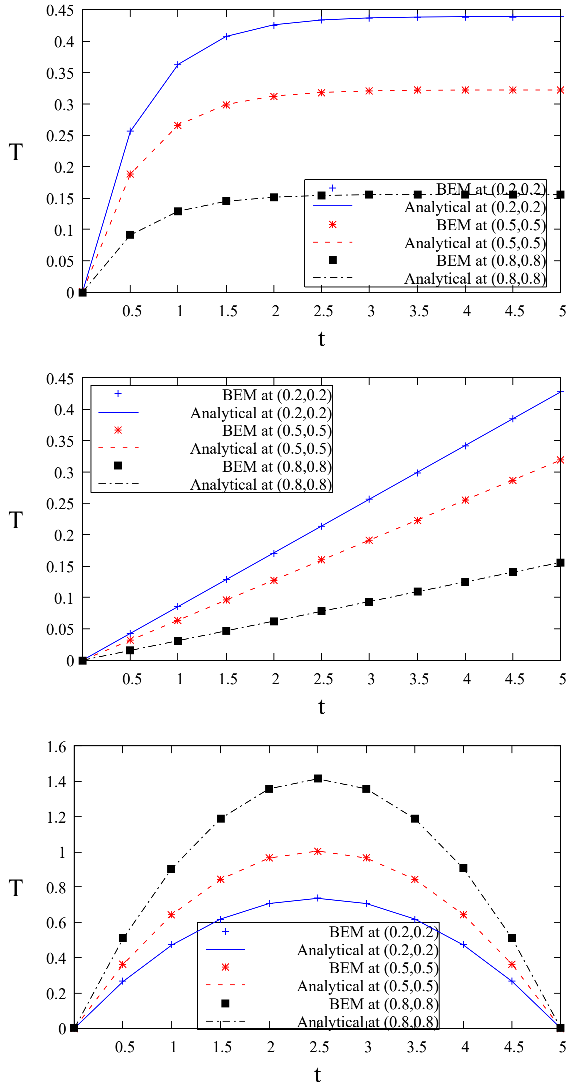

Fig. 7. Solutions T at some interior points (x_1, x_2) for the Case 1 (top), Case 2 (center) and Case 3 (bottom) of Problem 1

$$\begin{aligned} F &= f(t) \text{ on side AB} \\ F &= 0 \text{ on side BC} \\ T &= 0 \text{ on side CD} \\ F &= 0 \text{ on side AD} \end{aligned}$$

Four cases of the function $f(t)$ will be considered, namely

$$\begin{aligned} &\text{Case 1: } f(t) = 1 \\ &\text{Case 2: } f(t) = 1 - \exp(-1.75t) \\ &\text{Case 3: } f(t) = t/5 \\ &\text{Case 4: } f(t) = 0.16t(5 - t) \end{aligned}$$

In fact, for the case of isotropic and homogeneous material the system is geometrically symmetric about the axis $x_1 = 0.5$. And this is verified by the results in Figures 8 and 9. In addition, Figure 8 also shows the effect of anisotropy and inhomogeneity on the asymmetry of the solution T. And Figure 9 indicates that the solution T tends to follow the variation of the function $f(t)$ associated for the boundary condition on the side AB.

Figure 10 shows again the effect of anisotropy and inhomogeneity on the solution T and the tendency of the solution T to agree the variation of the corresponding function $f(t)$. In particular, for bigger t the boundary conditions on the

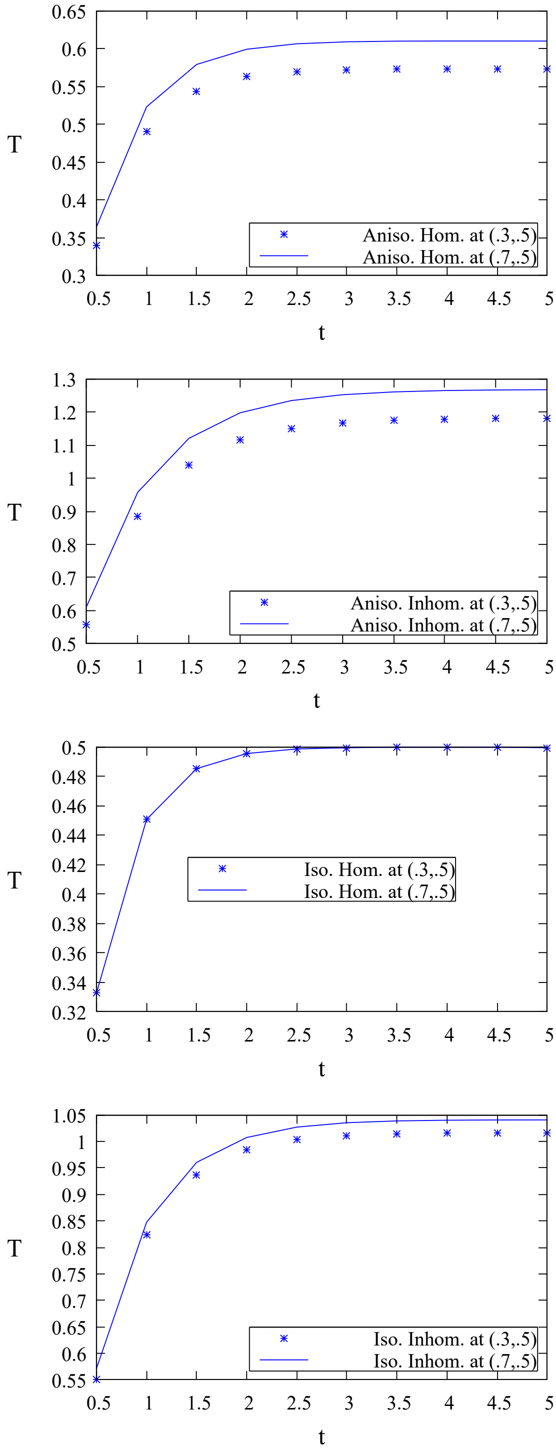

Fig. 8. Symmetry of solution T when $f(t) = 1$ for Problem 2

side AB with $f(t) = f_1(t) = 1$ and $f(t) = f_2(t) = 1 - \exp(-1.75t)$ are identical. This is verified by the results in Figure 10, the two plots for the cases when $f(t) = f_1(t) = 1$ and $f(t) = f_2(t) = 1 - \exp(-1.75t)$ will coincide as t goes to infinity.

After all, the results suggest it is important to put the anisotropy and inhomogeneity into account in any practical application.

V. Conclusion

The Laplace transform and standard boundary element method have been used together to solve unsteady heat

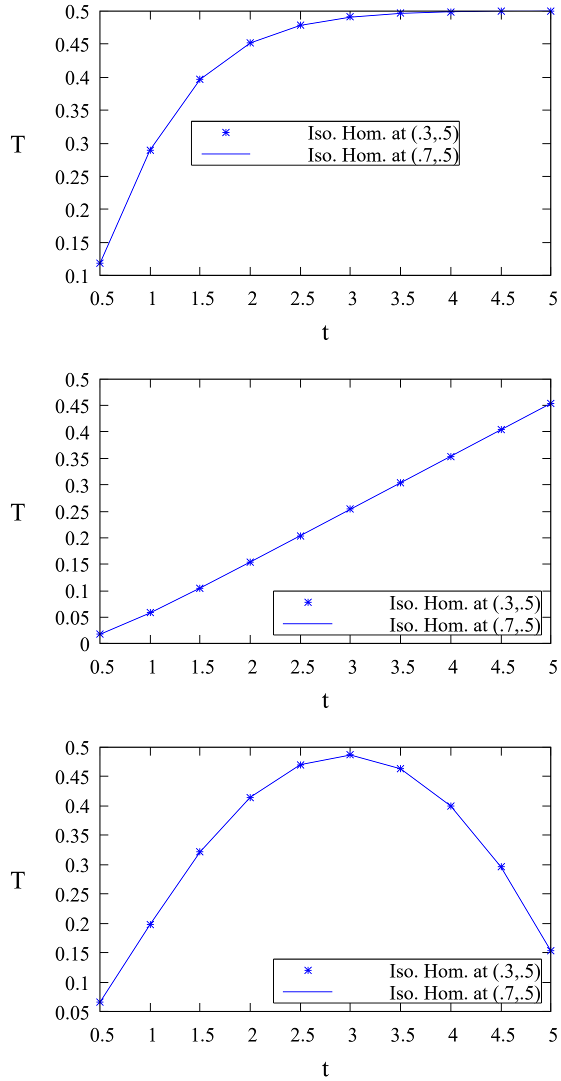

Fig. 9. Symmetry of solution T when $f(t) = 1 - \exp(-1.75t)$ (top), $f(t) = t/5$ (center) and $f(t) = 0.16t(5-t)$ (bottom) for Problem 2

conduction problems for anisotropic functionally graded materials described by the Laplace type equation (1). This numerical method used to solve the problems is quite accurate and very easy to be implemented. It involves a time variable-free fundamental solution which provides greater accuracy compared to other methods with singular time points in their fundamental solution.

The study was applied to the category of quadratically graded materials. The coefficients of diffusivity or conductivity, represented by $\kappa_{ij}(\mathbf{x})$ and the change rate of the unknown $T(\mathbf{x}, t)$, represented by $\psi(\mathbf{x})$, depend solely on the spatial variable $\mathbf{x}$ and the same inhomogeneity or gradation function $g(\mathbf{x})$. The research could be extended in the future to include cases where the coefficients depend on different gradation functions varying with the time variable t.

Before the boundary integral equation (17) can be used, the boundary conditions of $T(\mathbf{x}, t)$ or $F(\mathbf{x}, t)$ in the original system must be Laplace transformed. Therefore, at the beginning of a problem, an approximation of boundary conditions is required. To obtain accurate results, it is essential to use a precise technique for numerical Laplace transform inversion. Based on the results for problems in Section (IV-A), the

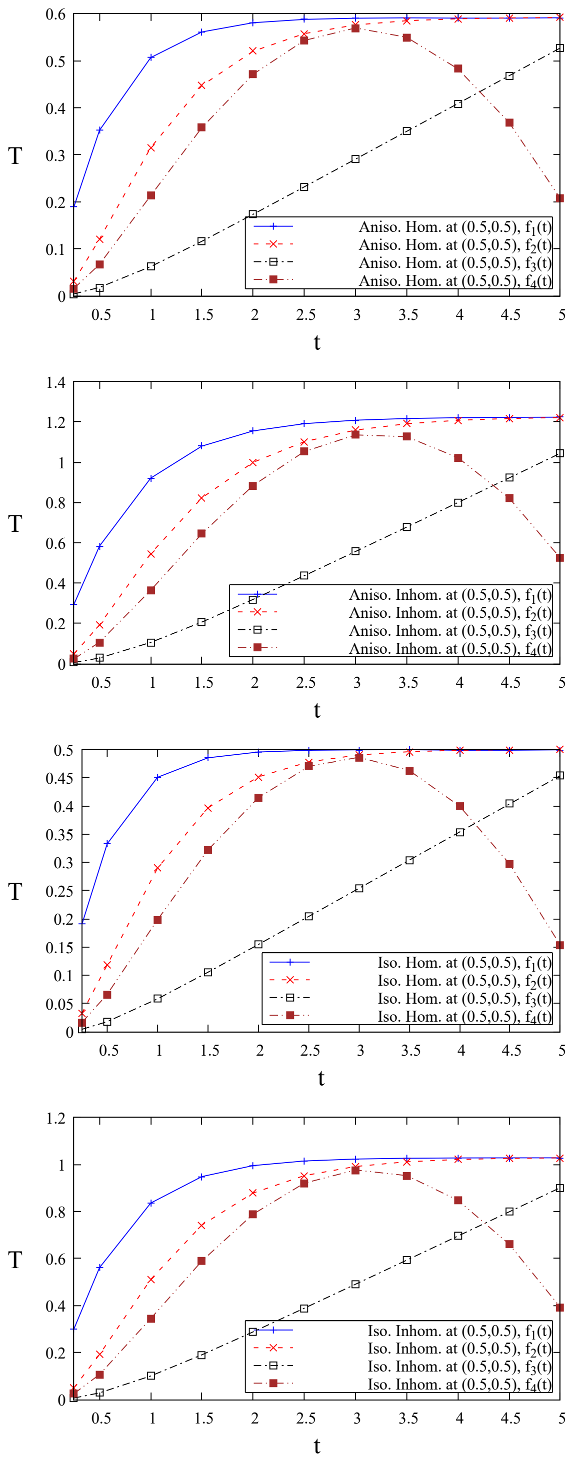

Fig. 10. Solutions T at $(x_1, x_2) = (0.5, 0.5)$ for Problem 2

Stehfest formula (18) was found to be quite accurate.

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