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Temperatures field calculation in an anisotropic solid through finite elements method, tridimensional case

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Abstract

This calculation is part of numeric thermo-mechanical strains simulation in anisotropic solids. The objective is to apply Fourier's law for anisotropic materials in tridimensional case. The study domain is a cube with unit dimension, representing some crystalline systems having one internal heat source equal to 10^9 Kw/m^3 and convective borders with a convection coefficient equal to 20 w/m^2.K. Domain and heat transfer equation are discretized by finite elements method, obtained equations set is resolved via Crout's method. Each crystalline system is identified by its heat conductivity tensor. Obtained results agree well with thermal transfer theory and clearly illustrate crystalline structure symmetry. This calculation can predict eventual thermal strains in a solid anisotropic.

Keywords: Temperature, anisotropic, discretization, finite element, simulation;

1. Introduction

The work consists on enlarging temperature fields calculation in anisotropic solids, already completed for the two-dimensional case [1]. This paper aims to implement a program for numerical temperature field calculation in an anisotropic solid into tridimensional case. To achieve this, we have chosen a cubic domain submitted to a volumical heat source effect and convective heat exchange in the borders. Via Galerkin's discretization method, we obtain an elementary-four order linear equations system, and then we assemble all element effects to obtain the global system which will be resolved via LU decomposition technique of Crout's method.

2. Fourier's law for an anisotropic solid

In anisotropic solids, heating flow vector projections according to space coordinates are temperature gradients function under same coordinates [2]:

$$\begin{cases} q_x = -k_{xx}\dfrac{\partial\theta}{\partial x} - k_{xy}\dfrac{\partial\theta}{\partial y} - k_{xz}\dfrac{\partial\theta}{\partial z} \\ q_y = -k_{yx}\dfrac{\partial\theta}{\partial x} - k_{yy}\dfrac{\partial\theta}{\partial y} - k_{yz}\dfrac{\partial\theta}{\partial z} \\ q_z = -k_{zx}\dfrac{\partial\theta}{\partial x} - k_{zy}\dfrac{\partial\theta}{\partial y} - k_{zz}\dfrac{\partial\theta}{\partial z} \end{cases} \quad (1)$$

Where

q_x, q_y, q_z: Heat flow thru x,y,z axis (w/m^2).
k_{ij} : Thermal conductivity tensor (w/m K).
θ: *Temperature* (K).

In a condensed form, the energy balance equation into an anisotropic solid is written as [3], [4]:

$$\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial \theta}{\partial x_j}\right)+w=\rho c_p\frac{\partial \theta}{\partial t} \quad i,j=x,y,z \qquad (2)$$

Where

w: Internal heat source in domain D (w/m^3).

ρ: Density (kg/m^3).

c_p: Specific-massic heat capacity (J/kg K).

t: Time (s).

3. Heat conductivity tensors [k_i] for different solids

For each system and taking into account symmetry in crystalline systems, thermal conductivity tensors became [7]:

Monoclinic system:

$$[k_{ij}]=\begin{bmatrix} k_{11} & k_{12} & 0 \\ k_{21} & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix}$$

Cubic system:

$$[k_{ij}]=\begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{11} & 0 \\ 0 & 0 & k_{11} \end{bmatrix}$$

Orthorhombic system:

$$[k_{ij}]=\begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix}$$

Trigonal system:

$$[k_{ij}]=\begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{11} & 0 \\ 0 & 0 & k_{33} \end{bmatrix}$$

Triclinic system:

$$[k_{ij}]=\begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}$$

4. Finite elements method application to calculate temperatures

4.1 Domain discretization

To manage automatic mesh of studied domain on fig.1, we proceed with a first clipping on elementary cubes noted (e) of eight nodes (i,j,k,l,m,r,p,q) as shown on fig.2. Then, we discretized every cube (e) on five tetrahedron noted (ee), each of four node (i,j,k,l) fig.3.

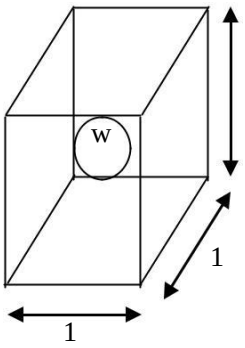

Figure 1. Study domain

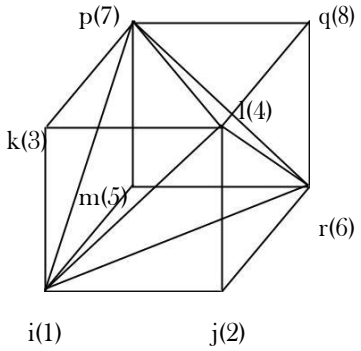

Figure 2. Elementary cube (e)

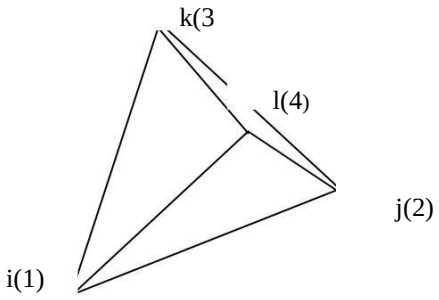

Figure 3. Elementary tetrahedron (ee)

4.2 Equation discretization

For stationary case, equation (2) became:

$$\frac{\partial}{\partial x}\left[k_{11}\frac{\partial \theta}{\partial x}+k_{12}\frac{\partial \theta}{\partial y}+k_{13}\frac{\partial \theta}{\partial z}\right]+$$

$$\frac{\partial}{\partial y}\left[k_{21}\frac{\partial \theta}{\partial x}+k_{22}\frac{\partial \theta}{\partial y}+k_{23}\frac{\partial \theta}{\partial z}\right]+$$

$$\frac{\partial}{\partial z}\left[k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right]+w=0 \qquad (3)$$

The equation (3) is discretized by Galerkin's method, [5], [6].

$$\int_v (\Phi_k)\left[\mathcal{L}\left(\sum_{j=1}^{n} C_j\Phi_j\right)-f\right]dV=0 \qquad (4)$$

$$k=1,\dots n$$

Where

Φ_i: State variable.

$\mathcal{L}U=f$: Problem's state equation.

$U=\sum_{j=1}^{n} C_j\Phi_j$: Approached problem solution.

C_i: Constants to be calculated.

4.3 Interpolating function choice

We choose the following interpolating function [4]

$$N^{ee}(x,y,z)=\alpha_1+\alpha_2 x+\alpha_3 y+\alpha_4 z \qquad (5)$$

$\alpha_1, \alpha_2, \alpha_3, \alpha_4$: Constants to be determined.

Interpolating function in a four nodes tetrahedron component is :

$$\theta^{ee}(x,y,z)=N_1(x,y,z)\theta_1+N_2(x,y,z)\theta_2+$$

$$N_3(x,y,z)\theta_3+N_4(x,y,z)\theta_4 \qquad (6)$$

Where: θ_1, θ_2, θ_3 and θ_4 are temperatures at i, j, k and l nodes.

We apply Galerkin's method described in (4), then:

$$\int_{D^e}\begin{bmatrix}\frac{\partial}{\partial x}\left(k_{11}\frac{\partial\theta}{\partial x}+k_{12}\frac{\partial\theta}{\partial y}+k_{13}\frac{\partial\theta}{\partial z}\right)+\\ \frac{\partial}{\partial y}\left(k_{21}\frac{\partial\theta}{\partial x}+k_{22}\frac{\partial\theta}{\partial y}+k_{23}\frac{\partial\theta}{\partial z}\right)+\\ \frac{\partial}{\partial z}\left(k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right)+w\end{bmatrix}N_i dD^e=0$$

$$i=1,2,3,4 \qquad (7)$$

Using Green's theorem we integer the first term of (7) we obtain:

$$\int_{\Sigma^e}\begin{bmatrix}\left(k_{11}\frac{\partial\theta}{\partial x}+k_{12}\frac{\partial\theta}{\partial y}+k_{13}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{21}\frac{\partial\theta}{\partial x}+k_{22}\frac{\partial\theta}{\partial y}+k_{23}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right)\end{bmatrix}N_i d\Sigma^e-$$

$$\int_{D^e}\begin{bmatrix}\left(k_{11}\frac{\partial\theta}{\partial x}+k_{12}\frac{\partial\theta}{\partial y}+k_{13}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{21}\frac{\partial\theta}{\partial x}+k_{22}\frac{\partial\theta}{\partial y}+k_{23}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right)\end{bmatrix}\left[\frac{\partial N_i}{\partial x}+\frac{\partial N_i}{\partial y}+\frac{\partial N_i}{\partial z}\right]dD^e=0 \qquad (8)$$

Let

$$I_{\Sigma^e}=\int_{\Sigma^e}\begin{bmatrix}\left(k_{11}\frac{\partial\theta}{\partial x}+k_{12}\frac{\partial\theta}{\partial y}+k_{13}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{21}\frac{\partial\theta}{\partial x}+k_{22}\frac{\partial\theta}{\partial y}+k_{23}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right)\end{bmatrix}N_i d\Sigma^e \qquad (9)$$

and

$$I_{D^e}=\int_{D^e}\begin{bmatrix}\left(k_{11}\frac{\partial\theta}{\partial x}+k_{12}\frac{\partial\theta}{\partial y}+k_{13}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{21}\frac{\partial\theta}{\partial x}+k_{22}\frac{\partial\theta}{\partial y}+k_{23}\frac{\partial\theta}{\partial z}\right)+\\ \left(k_{31}\frac{\partial\theta}{\partial x}+k_{32}\frac{\partial\theta}{\partial y}+k_{33}\frac{\partial\theta}{\partial z}\right)\end{bmatrix}\left[\frac{\partial N_i}{\partial x}+\frac{\partial N_i}{\partial y}+\frac{\partial N_i}{\partial z}\right]dD^e \qquad (10)$$

The term I_{Σ^e} exists only for elements with segments situated on frontiers exchanging heat with external medium, with a convection coefficient h. This term is estimated as follows:

$\int_{\sum^e} h\,\theta N_i d\sum^e =$

$$\int_{\sum^e} h\,(N_1 N_i \theta_1 + N_2 N_i \theta_2 + N_3 N_i \theta_3) d\sum^e \qquad (11)$$

i=1, 2, 3, 4

where $\sum^e$ is the four surface areas sum of a tetrahedron.
Second term equation integral is given by

$$\int_{D^e} w.N_i dD^e = w \int_{D^e} N_i dD^e \quad i = 1,2,3,4 \qquad (12)$$

Once every calculation made, discretization from (3) for one tetrahedron element (ee) of i, j, k and l nodes, may be written in a matrix form:

a) $$[K]^e\{\theta\}^e = \{W\}^e \qquad (13)$$

when no face exchanges heat with external medium,

b) $$\{[K]^e + [K_h]^e\}\{\theta\}^e = \{W\}^e \qquad (14)$$

when one, two or three surfaces are within solid boundary.

$[K]^e$, $[K_h]^e$: Square matrix of four order.
$\{W\}^e$, $\{\theta\}^e$: Column vectors of four order.

5. Suitable mesh choice

Once mathematical formula finished, which describes solid thermal behavior given by Fourier's law, and following model discretization finite elements method; we proceeded to numerical calculation concerning several solid types. To achieve these calculations, we performed a program in FORTRAN language. We choose a cubical solid with unit dimension, which experienced temperature variations through volume heat source of 10^3 Kw/m^3. Before temperature field distribution is described, we made a preliminary estimation to choose finite element mesh. First, we started with an uniform grid of six (6) order along three axis. While temperatures are calculated by increasing mesh order, we noted temperature field variation which decreases more and more, we consider that it will be appropriate to further increase the mesh to a grid of nine (9) order, that we maintained for any subsequent solid type calculations.

6. Temperature field calculation results for different solids

To illustrate calculation results, we have chosen as numerical value for conductivity tensors

Monoclinic system:

$$[k_{ij}] = \begin{bmatrix} 100 & 120 & 0 \\ 120 & 200 & 0 \\ 0 & 0 & 300 \end{bmatrix}$$

Cubic system:

$$[k_{ij}] = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 100 \end{bmatrix}$$

Orthorhombic system

$$[k_{ij}] = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 200 & 0 \\ 0 & 0 & 300 \end{bmatrix}$$

Trigonal system:

$$[k_{ij}] = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 200 \end{bmatrix}$$

Triclinic system:

$$[k_{ij}] = \begin{bmatrix} 100 & 120 & 150 \\ 120 & 200 & 190 \\ 150 & 190 & 300 \end{bmatrix}$$

7. Discussion

Temperature distribution in the (x, y, z) coordinates is shown in Fig.4 to 8 with Tecplot software, representing solids: monoclinic, cubic, orthorhombic, trigonal and triclinic, respectively.

For all presented cases, we find that maximum calculated temperature is at field centre, it is equal to 1200°K, 1160°K, 1120°K, 1140°K and 1250°K for monoclinic, cubic, orthorhombic, trigonal and triclinic solid cases, respectively.

All figures present symmetries to median and diagonal planes as per thermal conductivity tensor symmetry and imposed boundary conditions.

The results that seems qualitatively identical in bi-dimensional case for cubic/trigonal and monoclinic/triclinic solids, on the fact that $k_{11}= k_{22}$ and $k_{12}= 0$; however, in the three-dimensional case, they are clearly different because $k_{33} \neq k_{11}$ and $k_{33} \neq k_{22}$, and also k_{12}, k_{13} and k_{23} are different from 0.

In fig.5, temperature distribution is obviously different from the two previous cases because $k_{11} = k_{22}= k_{33}$, also k_{12}, k_{13} and k_{23} are non-zero; the difference between the results shown in fig.4 and fig.8 is well visible because k_{13} and k_{23} are non-zero, which was expected in results discussion of the bi-dimensional case.

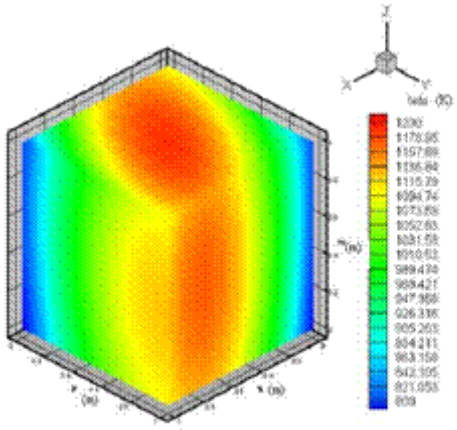

Figure 4. Monoclinic solid

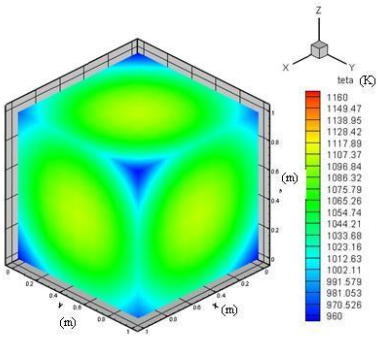

Figure 5. Cubic solid

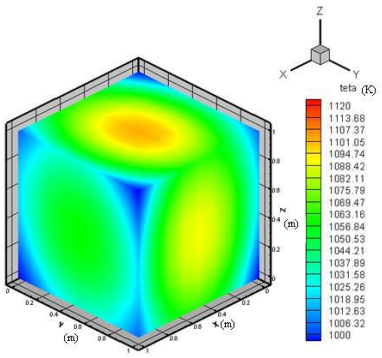

Figure 6. Orthorombic solid

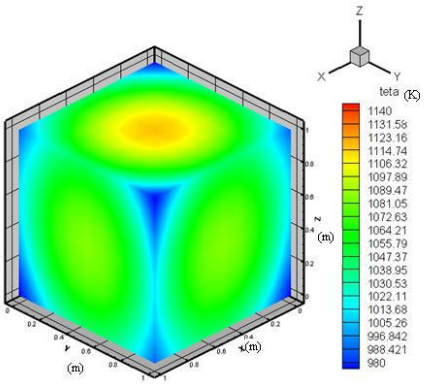

Figure 7. Trigonal solid

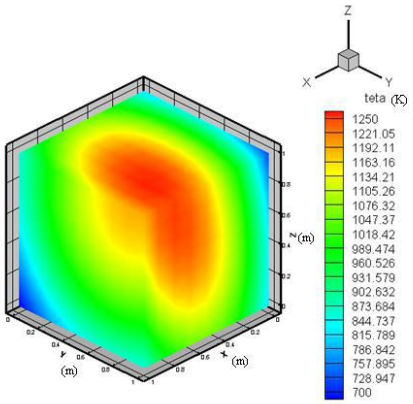

Figure 8. Triclinic solid

8. Conclusion

Elaborated program enabled us to identify Fourier's law implementation to calculate temperature distribution within anisotropic solids in tridimensional case.

Results agreed with heat conduction theory and crystalline systems symmetry. These results can contribute to calculate thermal elastic strains of anisotropic solids in tridimensional case which will be used as data for subsequent thermo-mechanical strain calculations in anisotropic solids.

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