

Thermal Stress in a Layered Plate

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Abstract

In this report, Group M4 members try to build a FEM solver for the thermal stress problem. Thermal stress occurs when the environment temperature changes for adhered materials with different thermal expansion coefficients. The FEM approximation formulae are derived based on principle of minimum potential energy (PMPE). First-order and second-order elements are applied. Results obtained from meshes different types of elements different degrees of fineness are compared. The maximum Mises stress occurs at the outer corner of a square layered plate. The maximum Mises stress drops about 18% after the outer corner being rounded off.

Introduction

This project tends to simulate the thermal stresses in a layered plate. The plate consists of a coating and a substrate. The coating is deposited onto the substrate at a temperature of 800 °C. The coating and the substrate are both stress-free at this temperature. The temperature is then lowered to 20 °C, and the thermal stress are examined. The material properties of the coating and the substrate are provided in Table 1:

Property	Coating	Substrate
Dimension [m]	0.04*0.04*0.005	0.04*0.04*0.02
Young's modulus [GPa]	70	130
Poisson's ratio	0.17	0.28
Density [kg/m ³]	1000	1000
Thermal expansion coefficient [K ⁻¹]	5e ⁻⁷	3e ⁻⁶

Table 1. Material properties.

Theoretical Analysis

The potential energy is:

$$\Pi = U - W = \frac{1}{2} \int_{\Omega} \sigma_{ij} \varepsilon_{ij}^{el} d\Omega - \int_{\Omega} b_i u_i d\Omega - \int_{\partial\Omega} T_i u_i dA \quad (1)$$

from which the governing equation can be derived as:

$$\sigma_{ij,j} + b_i = 0 \quad (2)$$

where b_i is the body force, T_i is the surface traction, σ_{ij} is the Cauchy stress tensor, ε_{ij}^{el} is the elastic strain tensor:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}^{el} \quad (3)$$

$$\varepsilon_{ij}^{el} = \varepsilon_{ij} - \varepsilon_{ij}^{th} \quad (4)$$

where C_{ijkl} is the linear elastic tensor, ε_{ij} is the linear strain tensor, and ε_{ij}^{th} is the thermal strain tensor:

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu [\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}] \quad (5)$$

$$\varepsilon_{ij} = \frac{1}{2} [u_{i,j} + u_{j,i}] \quad (6)$$

$$\varepsilon_{ij}^{th} = \alpha (T - T_{ref}) \delta_{ij} \quad (7)$$

Finite Element Approximation

Substituting Eq. (3), and Eq. (4) into Eq. (1), the potential energy becomes:

$$\Pi = \frac{1}{2} \int_{\Omega} \varepsilon_{ij} C_{ijkl} \varepsilon_{kl} d\Omega - \int_{\Omega} \varepsilon_{ij} C_{ijkl} \varepsilon_{kl}^{th} d\Omega - \int_{\Omega} b_i u_i d\Omega - \int_{\partial\Omega} T_i u_i dA + \frac{1}{2} \int_{\Omega} \varepsilon_{ij}^{th} C_{ijkl} \varepsilon_{kl}^{th} d\Omega \quad (8)$$

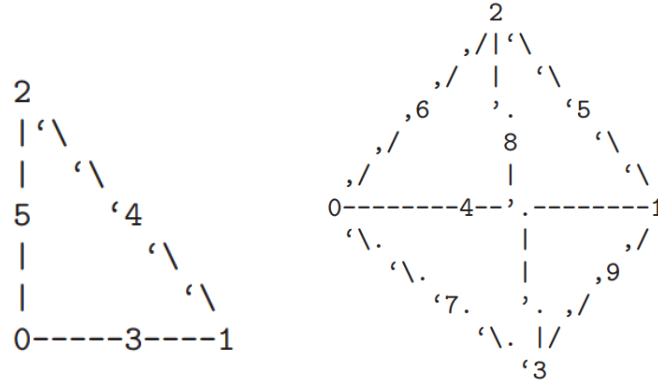


Figure 1. Triangle and tetrahedron elements (apply to both 1st & 2nd order elements) in gmsh
As shown in Figure 1, the first-order iso-parametric tetrahedron (4 nodes) is:

$$u^e(g, h, r) = (1 - g - h - r)u_1 + gu_2 + hu_3 + ru_4 \quad (9)$$

and the second-order iso-parametric tetrahedron (10 nodes) is:

$$\begin{aligned} u^e(g, h, r) = & (2(1 - g - h - r) - 1)(1 - g - h - r)u_1 + (2g - 1)gu_2 \\ & + (2h - 1)hu_3 + (2r - 1)ru_4 + 4(1 - g - h - r)gu_5 + 4ghu_6 \\ & + 4(1 - g - h - r)hu_7 + 4(1 - g - h - r)ru_8 + 4hru_9 + 4gru_{10} \end{aligned} \quad (10)$$

Notice that the 10-node sequence is a bit different in gmsh (the serial number of the last two elements are exchanged).

Suppose each element has n nodes, then we may express the nodal displacement into a 3n*1 vector:

$$\mathbf{u}^N = [\cdots u_i v_i w_i \cdots]^T \quad (11)$$

and the displacement field inside an element is:

$$\mathbf{u}^e(g, h, r) = \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} \cdots N_i & 0 & 0 & \cdots \\ \cdots 0 & N_i & 0 & \cdots \\ \cdots 0 & 0 & N_i & \cdots \end{bmatrix} \mathbf{u}^N = \mathbf{N} \mathbf{u}^N \quad (12)$$

where N_i is the shape functions for node i as defined in Eq. (9) and Eq. (10), and \mathbf{N} is a 3*3n matrix; therefore, \mathbf{u} is 3*1. The strain field is the derivative of the displacement field:

$$\boldsymbol{\varepsilon}^e = \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{bmatrix} = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial z \\ \partial/\partial y & \partial/\partial x & 0 \\ 0 & \partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & \partial/\partial x \end{bmatrix} \begin{bmatrix} u^e \\ v^e \\ w^e \end{bmatrix} = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial z \\ \partial/\partial y & \partial/\partial x & 0 \\ 0 & \partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & \partial/\partial x \end{bmatrix} \begin{bmatrix} \cdots N_i & 0 & 0 & \cdots \\ \cdots 0 & N_i & 0 & \cdots \\ \cdots 0 & 0 & N_i & \cdots \end{bmatrix} \mathbf{u}^N = \mathbf{B}^e \mathbf{u}^N \quad (13)$$

However, as \mathbf{u}^e is a function of iso-geometric variables, Eq. (13) cannot be directly applied. The relationship between the derivatives of global coordinates and iso-geometric coordinates is:

$$[\partial_g] = \begin{bmatrix} \partial/\partial g \\ \partial/\partial h \\ \partial/\partial r \end{bmatrix} = \begin{bmatrix} \partial x/\partial g & \partial y/\partial g & \partial z/\partial g \\ \partial x/\partial h & \partial y/\partial h & \partial z/\partial h \\ \partial x/\partial r & \partial y/\partial r & \partial z/\partial r \end{bmatrix} \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{bmatrix} = J(g, h, r) [\partial_x] \quad (14)$$

$$[\partial_x] = J^{-1} [\partial_g] \quad (15)$$

where J is the Jacobian matrix. Define a shape function $1 \times n$ matrix \mathbf{N} :

$$\mathbf{N} = [\dots \ N_i \ \dots] \quad (16)$$

then $[\partial_g] \mathbf{N}$ is a $3 \times n$ matrix:

$$[\partial_g] \mathbf{N} = \begin{bmatrix} \dots & \partial N_i / \partial g & \dots \\ \dots & \partial N_i / \partial h & \dots \\ \dots & \partial N_i / \partial r & \dots \end{bmatrix} \quad (17)$$

The Jacobian matrix can be obtained from:

$$J = \begin{bmatrix} \partial x/\partial g & \partial y/\partial g & \partial z/\partial g \\ \partial x/\partial h & \partial y/\partial h & \partial z/\partial h \\ \partial x/\partial r & \partial y/\partial r & \partial z/\partial r \end{bmatrix} = \begin{bmatrix} \dots & \partial N_i / \partial g & \dots \\ \dots & \partial N_i / \partial h & \dots \\ \dots & \partial N_i / \partial r & \dots \end{bmatrix} \begin{bmatrix} \vdots & \vdots & \vdots \\ x_i & y_i & z_i \\ \vdots & \vdots & \vdots \end{bmatrix} = [\partial_g] \mathbf{N} \mathbf{x} \quad (18)$$

Now $[\partial_x] \mathbf{N}$ can be calculated from $[\partial_g] \mathbf{N}$ and it contains every non-zero element in \mathbf{B}^e matrix. The potential energy of each element is:

$$\begin{aligned} \tilde{H}^e = & \frac{1}{2} [\mathbf{u}^N]^T \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \mathbf{B}^e \det J d\Omega \mathbf{u}^N - [\mathbf{u}^N]^T \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \boldsymbol{\epsilon}^{e,th} \det J d\Omega \\ & - [\mathbf{u}^N]^T \int_{\Omega^e} \mathbf{N}^T \mathbf{b} \det J d\Omega - [\mathbf{u}^N]^T \int_{\partial\Omega^e} \mathbf{N}^T \mathbf{T} \det J dA + \frac{1}{2} \int_{\Omega^e} [\boldsymbol{\epsilon}^{e,th}]^T \mathbf{C} \boldsymbol{\epsilon}^{e,th} \det J d\Omega \end{aligned} \quad (19)$$

where $\boldsymbol{\epsilon}^{e,th}$ is the thermal strain of each element which can be derived from Eq. (7) following $\boldsymbol{\epsilon}^e$ defined in Eq. (13):

$$\boldsymbol{\epsilon}^{e,th} = \alpha (T - T_{ref}) [1 \ 1 \ 1 \ 0 \ 0 \ 0]^T \quad (20)$$

and \mathbf{C} is the elastic constant matrix, which for an isotropic solid can be expressed as:

$$\mathbf{C} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \quad (21)$$

The minimum potential energy occurs at $\partial \tilde{H}^e / \partial u_i^N = 0$, yielding $\mathbf{K}^e \mathbf{u}^N = \mathbf{f}^e$, where:

$$\mathbf{K}^e = \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \mathbf{B}^e \det J d\Omega \quad (22)$$

$$\mathbf{f}^e = \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \boldsymbol{\epsilon}^{e,th} \det J d\Omega + \int_{\Omega^e} \mathbf{N}^T \mathbf{b} \det J d\Omega + \int_{\partial\Omega^e} \mathbf{N}^T \mathbf{T} \det J dA \quad (23)$$

Simulation Set Up

As the plate is symmetric, only a quarter of it will be analyzed, as shown in Figure 2:

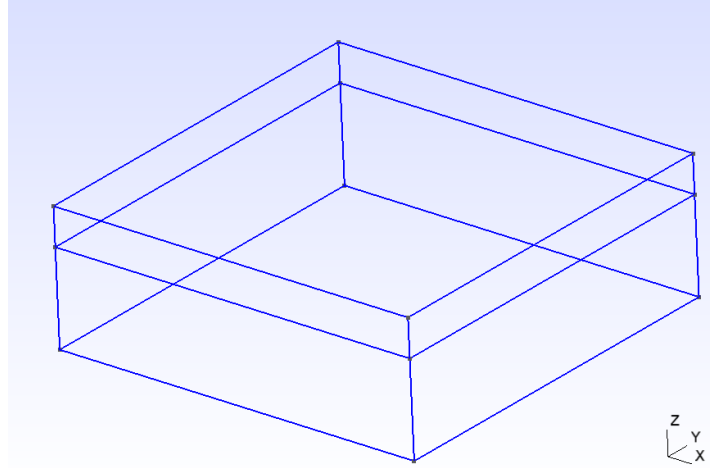


Figure 2. Model set up.

The mesh is built by Gmsh. Meshes with first- and second-order tetrahedron elements and various degrees of fineness are generated. The fineness is controlled by Gmsh Element Size Factor. The quantities of elements are the same for meshes with first- and second-order elements with the same Size Factor.

Boundary Conditions

In the case above, the body force can be neglected; assume the plate is traction free. Set $u_1 = 0$ at $x = 0$ and $u_2 = 0$ at $y = 0$. Set the vertical displacement at the lower inner corner of substrate as zero.

Results and Comparison

Conclusion

We successfully developed a set of FEM scripts that can handle thermal stress problems. The relative error between displacements obtained by this script and COMSOL simulation is