Thermal Stress in a Layered Plate

Group M4: Matthew Minjiang Zhu, Yong Ye, Travis Jeremiah Zook

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:

$$\Pi = U - W = \frac{1}{2}\int_{\Omega} \sigma_{ij}\varepsilon_{ij}^{el}\,\mathrm{d}\Omega - \int_{\Omega} b_i u_i \,\mathrm{d}\Omega - \int_{\partial\Omega} T_i u_i \,\mathrm{d}A \tag{1}$$

from which the governing equation can be derived as:

$$\sigma_{ij,j} + b_i = 0 \tag{2}$$

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:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}^{el} \tag{3}$$

$$\varepsilon_{ij}^{el} = \varepsilon_{ij} - \varepsilon_{ij}^{th} \tag{4}$$

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

$$\varepsilon_{ij}^{th} = \alpha(T - T_{ref})\delta_{ij} \tag{5}$$

Finite Element Approximation

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

$$\Pi = \frac{1}{2}\int_{\Omega} \varepsilon_{ij}C_{ijkl}\varepsilon_{kl}\,\mathrm{d}\Omega - \int_{\Omega} \varepsilon_{ij}C_{ijkl}\varepsilon_{kl}^{th}\,\mathrm{d}\Omega - \int_{\Omega} b_i u_i \,\mathrm{d}\Omega - \int_{\partial\Omega} T_i u_i \,\mathrm{d}A + \frac{1}{2}\int_{\Omega} \varepsilon_{ij}^{th}C_{ijkl}\varepsilon_{kl}^{th}\,\mathrm{d}\Omega \tag{6}$$

```
2
|`\
|  `\
5    `4
|      `\
|        `\
0-----3----1
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```
           2
         ,/|`\
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0--------4--'.--------1
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       `7.   '. ,/
          `\. |/
             `3
```

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:

$$u^e(g,h,r) = (1-g-h-r)u_1 + gu_2 + hu_3 + ru_4 \tag{7}$$

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

$$\begin{aligned} u^e(g,h,r) = {} & (2(1-g-h-r)-1)\,(1-g-h-r)u_1 + (2g-1)gu_2 \\ & + (2h-1)hu_3 + (2r-1)ru_4 + 4(1-g-h-r)gu_5 + 4ghu_6 \\ & + 4(1-g-h-r)hu_7 + 4(1-g-h-r)ru_8 + 4hru_9 + 4gru_{10} \end{aligned} \tag{8}$$

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:

$$\mathbf{u}^N = [\cdots \;\; u_i \;\; v_i \;\; w_i \;\; \cdots]^T \tag{9}$$

and the displacement field inside an element is:

$$\mathbf{u}^e(g,h,r) = \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} \cdots & N_i & 0 & 0 & \cdots \\ \cdots & 0 & N_i & 0 & \cdots \\ \cdots & 0 & 0 & N_i & \cdots \end{bmatrix} \mathbf{u}^N = \mathbf{N}\mathbf{u}^N \tag{10}$$

where N_i is the shape functions for node i as defined in Eq. (7) and Eq. (8), and $\mathbf{N}$ is a 3*3n matrix; therefore, $\mathbf{u}$ is 3*1. The strain field is the derivative of the displacement field:

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

(11)

However, as $\mathbf{u}^e$ is a function of iso-geometric variables, Eq. (11) cannot be directly applied. The relationship between the derivatives of global coordinates and iso-geometric coordinates is:

$$[\partial_g] = \begin{bmatrix} \partial/\partial g \\ \partial/\partial h \\ \partial/\partial r \end{bmatrix} = \begin{bmatrix} \partial x/\partial g & \partial y/\partial g & \partial z/\partial g \\ \partial x/\partial h & \partial y/\partial h & \partial z/\partial h \\ \partial x/\partial r & \partial y/\partial r & \partial z/\partial r \end{bmatrix} \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{bmatrix} = J(g,h,r)\,[\partial_x] \tag{12}$$

$$[\partial_x] = J^{-1}[\partial_g] \tag{13}$$

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

$$\boldsymbol{N} = [\cdots \quad N_i \quad \cdots] \tag{14}$$

then $[\partial_g]\boldsymbol{N}$ is a 3*n matrix:

$$[\partial_g]\boldsymbol{N} = \begin{bmatrix} \cdots & \partial N_i/\partial g & \cdots \\ \cdots & \partial N_i/\partial h & \cdots \\ \cdots & \partial N_i/\partial r & \cdots \end{bmatrix} \tag{15}$$

The Jacobian matrix can be obtained from:

$$J = \begin{bmatrix} \partial x/\partial g & \partial y/\partial g & \partial z/\partial g \\ \partial x/\partial h & \partial y/\partial h & \partial z/\partial h \\ \partial x/\partial r & \partial y/\partial r & \partial z/\partial r \end{bmatrix} = \begin{bmatrix} \cdots & \partial N_i/\partial g & \cdots \\ \cdots & \partial N_i/\partial h & \cdots \\ \cdots & \partial N_i/\partial r & \cdots \end{bmatrix} \begin{bmatrix} \vdots & \vdots & \vdots \\ x_i & y_i & z_i \\ \vdots & \vdots & \vdots \end{bmatrix} = [\partial_g]\boldsymbol{N}\boldsymbol{x} \tag{16}$$

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

$$\begin{aligned} \widetilde{\Pi}^e = & \frac{1}{2}[\mathbf{u}^N]^T \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C}\mathbf{B}^e \det J \, \mathrm{d}\Omega \, \mathbf{u}^N - [\mathbf{u}^N]^T \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \boldsymbol{\varepsilon}^{e,th} \det J \, \mathrm{d}\Omega \\ & - [\mathbf{u}^N]^T \int_{\Omega^e} \mathbf{N}^T \mathbf{b} \det J \, \mathrm{d}\Omega - [\mathbf{u}^N]^T \int_{\partial\Omega^e} \mathbf{N}^T \mathbf{T} \det J \, \mathrm{d}A + \frac{1}{2} \int_{\Omega^e} [\boldsymbol{\varepsilon}^{e,th}]^T \mathbf{C} \boldsymbol{\varepsilon}^{e,th} \det J \, \mathrm{d}\Omega \end{aligned} \tag{17}$$

where $\boldsymbol{\varepsilon}^{e,th}$ is the thermal strain of each element which can be derived from Eq. (5) following $\boldsymbol{\varepsilon}^e$ defined in Eq. (11):

$$\boldsymbol{\varepsilon}^{e,th} = \alpha(T - T_{ref})[1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0]^T \tag{18}$$

and $\mathbf{C}$ is the elastic constant matrix, which can be found from lecture slides. The minimum potential energy occurs at $\partial\widetilde{\Pi}^e / \partial u_i^N = 0$, yielding $\mathbf{K}^e \mathbf{u}^N = \mathbf{f}^e$, where:

$$\mathbf{K}^e = \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C}\mathbf{B}^e \det J \, \mathrm{d}\Omega \tag{19}$$

$$\mathbf{f}^e = \int_{\Omega^e} [\mathbf{B}^e]^T \mathbf{C} \boldsymbol{\varepsilon}^{e,th} \det J \, \mathrm{d}\Omega + \int_{\Omega^e} \mathbf{N}^T \mathbf{b} \det J \, \mathrm{d}\Omega + \int_{\partial\Omega^e} \mathbf{N}^T \mathbf{T} \det J \, \mathrm{d}A \tag{20}$$

Simulation Set Up

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

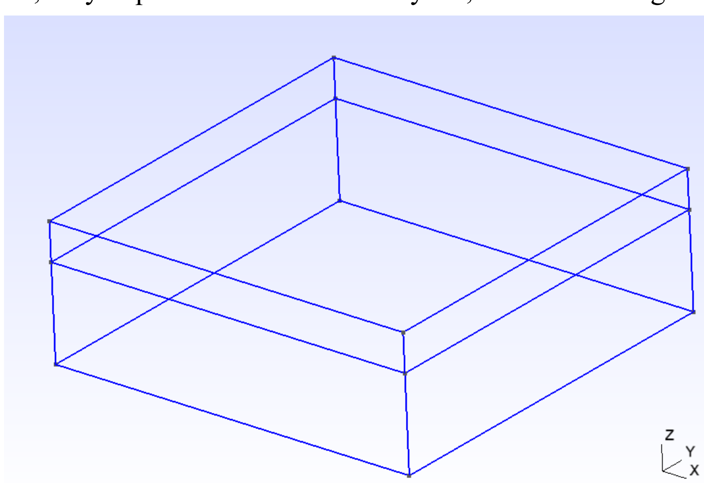

Figure 2. Model set up (Gmsh).

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 (ESF). The quantities of elements are the same for meshes with first- and second-order elements with the same Size Factor.

Boundary Conditions and Loading 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

For ESF = 100%, the nodal displacement field plots like:

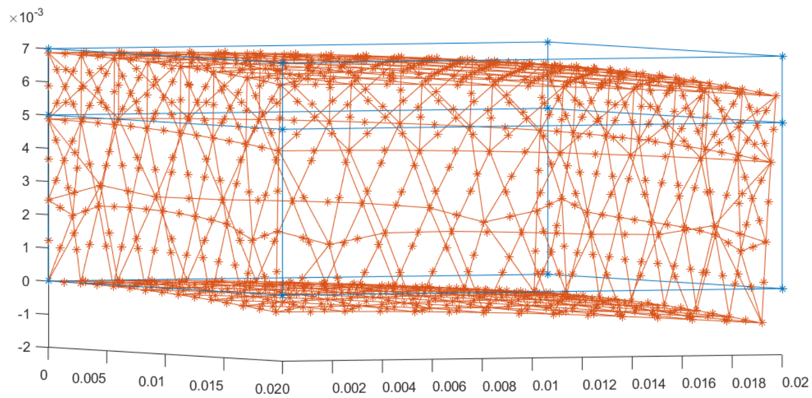

Figure 3. Nodal displacement (ESF = 100%, second-order tetrahedral elements)

The blue frame shows the original position. The displacement is magnified by 10 times. This is close to COMSOL results:

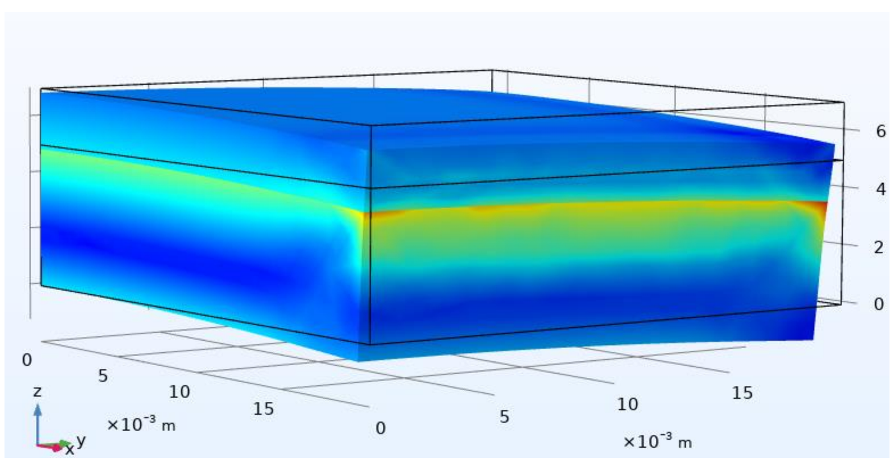

Figure 4. COMSOL result (Similar fineness of mesh)

Von Mises stress is also plotted for the same simulation case, as shown in

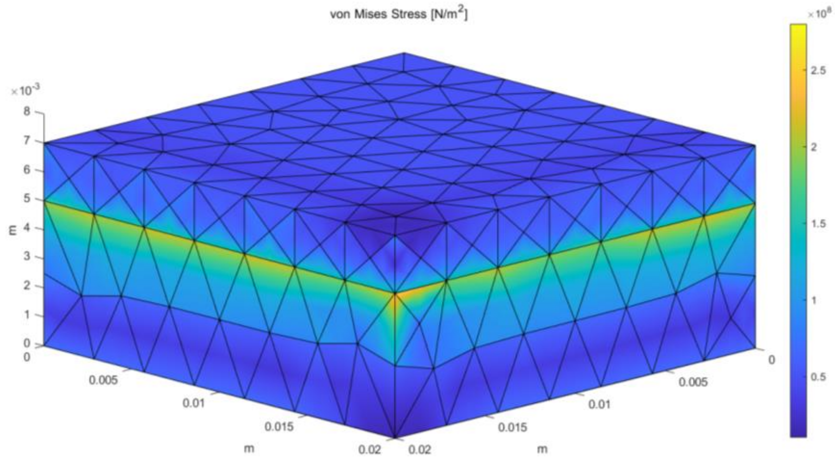

Figure 5. Von Mises stress (ESF = 100%, second-order tetrahedral elements)

which is also close to COMSOL simulation result:

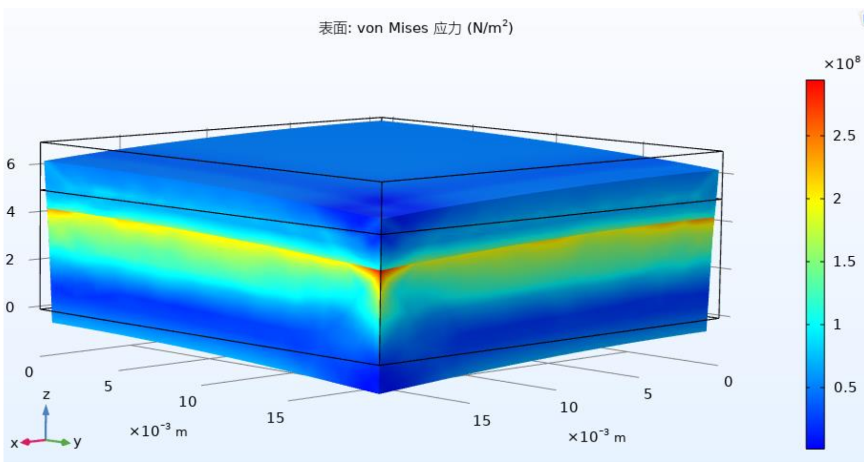

Figure 6. Von Mises stress by COMSOL (Similar fineness of mesh, second-order tetrahedral elements)

Discussion

As shown in Figure 3 to Figure 6, the greatest von Mises stress appears at the outer corner of the substrate, whose thermal expansion coefficient is higher. This should be a type of stress concentration. The adhered material could tear apart at this corner, and stress concentration will appear at the newly developed fissure 'front'. Even if the material is strongly adhered, the long-standing stress will continuously damage the material and magnify any imperfection inside the material. The potential strategies to avoid thermal include:

1. Use materials with close thermal expansion coefficients.
2. Avoid sharp corners.
3. Slowly cooling; heat treatment.

Convergence

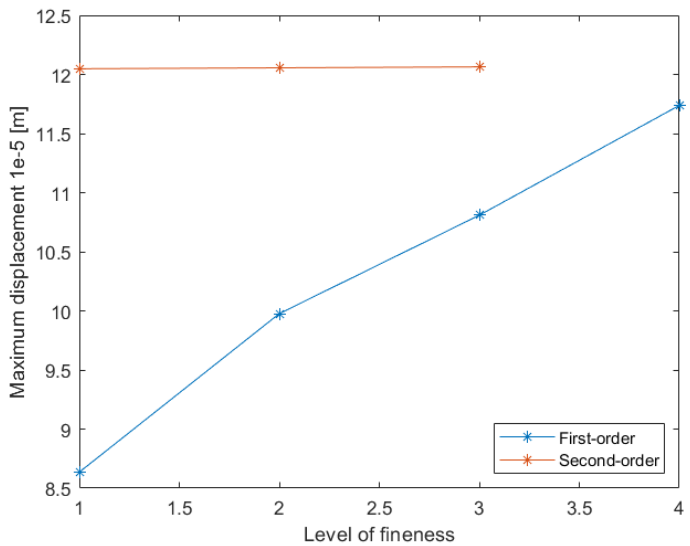

Figure 7. Convergence comparison

Convergence of FEM solutions is plotted in Figure 7. In Figure 7, level of fineness = 1 refers to ESF = 100%; level of fineness = 2 refers to ESF = 75%, and so on. ESF is proportional to the edge length of elements. The COMSOL solution for a mesh with ESF ≈100% is 12.055e-4, which is very close to the second-order solutions, thus we can assume the solutions are roughly correct. We see clearly that the first-order solutions deviate a lot in coarse meshes, and they gradually approach the second-order solutions. The second-order solutions seem almost unchanged, although it is actually slowly increasing. Notice that when Level of fineness = 4, which corresponds to ESF = 25%, the mesh is too fine for a personal computer to handle for the second-order case. However, if we assume the convergence is fulfilled, the second-order solutions are still much more accurate than first-order solutions under close level of computation cost.

Multiple-loading Conditions

As required, if set the reference temperature (the initial temperature) as 3000°C, though not physical, the von Mises stress is shown in Figure 8:

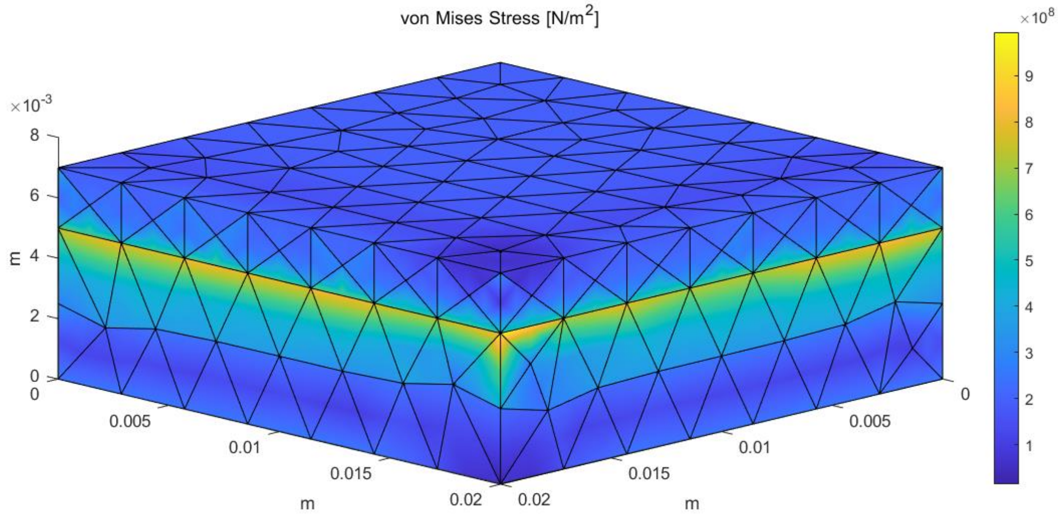

Figure 8. Von Mises stress (T_ref = 8000℃)

As MATLAB scales the colorbar by itself and the solver is linear, the color seems nothing different with that obtained when T_ref = 800℃. Nevertheless, the greatest von Mises stress is now around 1 GPa. The stress can even go higher if the thermal expansion coefficients of two material differs more.

Improved System

If we round off the sharp outer corner, the von Mises stress will drop from 0.29GPa to 0.24 GPa (about 18%), as shown in Figure 9:

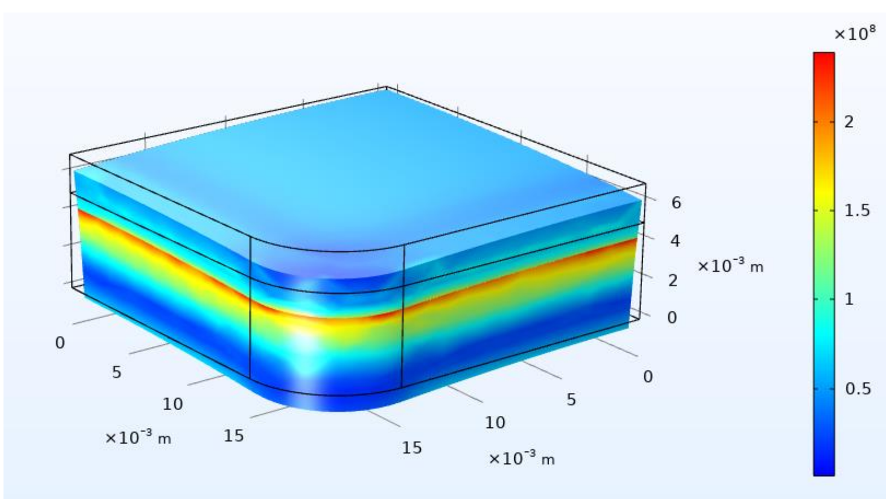

Figure 9. Von Mises stress of a layered plate with rounded outer corner

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 0.06% for second-order elements and 28% for first-order elements in coarse mesh. The potential hazard of thermal stress is discussed. The convergence is observed and discussed. The design of structure is improved such that the von Mises stress is reduced by around 18%.