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Latest advances in fully coupled thermal structural calculations using finite element method (FEM) with new energy conservation equation

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Contents

1, Contemporary and new energy conservation equation derivation

First principle of thermodynamics:

$$\frac{D}{Dt}\int_{\Omega}\left(\frac{1}{2}\rho\mathbf{v}\bullet\mathbf{v}+e_c\right)dv=\int_{\partial\Omega}\left(\mathbf{t}\bullet\mathbf{v}+q_n\right)ds+\int_{\Omega}\left(\mathbf{b}\bullet\mathbf{v}+r\right)dv$$

Internal energy material derivative formulation:

$$\frac{D}{Dt}\int_{\Omega}e_c dv=\int_{\Omega}\left(\boldsymbol{\sigma}:\mathbf{d}-\nabla\bullet\mathbf{q}+r\right)dv$$

The energy conservation equation has to work properly in the following three different cases:

1, All thermal contributions are equal to zero

2, All mechanical contributions are equal to zero

3, Neither thermal nor mechanical terms are equal to zero

Case1: All thermal contributions are equal to zero

First principle of thermodynamics:

$$\frac{D}{Dt}\int_{\Omega}\left(\frac{1}{2}\rho\mathbf{v}\bullet\mathbf{v}+e_c\right)dv=\int_{\partial\Omega}\mathbf{t}\bullet\mathbf{v}ds+\int_{\Omega}\mathbf{b}\bullet\mathbf{v}dv$$

Internal energy material derivative formulation:

$$\frac{D}{Dt}\int_{\Omega}e_c dv=\int_{\Omega}\boldsymbol{\sigma}:\mathbf{d}dv$$

$$\boldsymbol{\sigma}\bullet\mathbf{n}=\mathbf{t}$$

After back substitution we have:

Mechanical energy conservation equation:

$$\frac{D}{Dt}\int_{\Omega}\frac{1}{2}\rho\mathbf{v}^2dv+\int_{\Omega}\boldsymbol{\sigma}:\mathbf{d}dv=\int_{\partial\Omega}\mathbf{t}\bullet\mathbf{v}dv+\int_{\Omega}\mathbf{b}\bullet\mathbf{v}dv$$

The result is correct!

Case 2: All mechanical energy contributions are equal to zero

First principle of thermodynamics:

$$\frac{D}{Dt}\int_{\Omega} e_c\,dv = \int_{\partial\Omega} q_n\,ds + \int_{\Omega} r\,dv$$

Internal energy material derivative formulation:

$$\frac{D}{Dt}\int_{\Omega} e_c\,dv = \int_{\Omega} (-\nabla\bullet\mathbf{q} + r)\,dv$$

$$\mathbf{q} = -\mathbf{K}\bullet\nabla T$$

$$\mathbf{q}\bullet\mathbf{n} = -q_n$$

After back substitution we arrive at the following equation:

$$\int_{\Omega} (-\nabla\bullet\mathbf{q} + r)\,dv = \int_{\Omega} (-\nabla\bullet\mathbf{q} + r)\,dv$$

$$0 = 0$$

The result is incorrect !!!!!

Gauss' theorem:

$$\int_{\partial\Omega} \mathbf{a}\bullet\mathbf{n}\,ds = \int_{\Omega} (\nabla\bullet\mathbf{a})\,dv$$

Case 3: Neither mechanical nor thermal terms are equal to zero

After back substitution for the internal energy material derivative formulation we arrive at the mechanical energy conservation equation:

Mechanical energy conservation equation:

$$\frac{D}{Dt}\int_{\Omega}\frac{1}{2}\rho\mathbf{v}^2 dv+\int_{\Omega}\boldsymbol{\sigma}:\mathbf{d}dv=\int_{\partial\Omega}\mathbf{t}\bullet\mathbf{v}dv+\int_{\Omega}\mathbf{b}\bullet\mathbf{v}dv$$

First principle of thermodynamics is equivalent with the mechanical energy conservation equation and is independent of all thermal energy contributions

The result is incorrect !!!!!

The new energy conservation equation derivation

$$\dot{w} = \dot{w}_m + \dot{w}_q = 0$$

$$\dot{w}_m = \mathbf{v} \bullet \left(\mathbf{b} + \nabla \bullet \boldsymbol{\sigma} - \rho \dot{\mathbf{v}} \right) = \mathbf{b} \bullet \mathbf{v} + \nabla \bullet (\boldsymbol{\sigma} \bullet \mathbf{v}) - \boldsymbol{\sigma} : (\nabla \mathbf{v}) - \rho \dot{\mathbf{v}} \bullet \mathbf{v} = 0$$

$$\dot{w}_q = (-\nabla \bullet \mathbf{q}) + r - \rho c \dot{T} = 0$$

$$\mathbf{q} = -\mathbf{K} \bullet (\nabla T) \qquad \nabla \bullet (a\mathbf{a}) = a \nabla \bullet \mathbf{a} + \mathbf{a} \bullet \nabla a$$

The first principle of thermodynamics of a body without temperature gradient:

$$\int_{\Omega} \left(\rho \mathbf{v} \bullet \dot{\mathbf{v}} + \boldsymbol{\sigma} : \mathbf{d} + \rho c \dot{T} \right) dv = \int_{\partial\Omega} (\mathbf{t} \bullet \mathbf{v} + q_n) ds + \int_{\Omega} (\mathbf{b} \bullet \mathbf{v} + r) dv$$

$$\frac{D}{Dt} \int_{\Omega} e_c dv = \int_{\Omega} \left(\boldsymbol{\sigma} : \mathbf{d} + \rho c \dot{T} \right) dv$$

The first principle of thermodynamics of a body with temperature gradient:

$$\sum_{i=1}^{NNode} \delta T_i \mathbf{f}_i \bullet \mathbf{v}_i + \sum_{i=1}^{NNode} \delta T_i Q_i + \int_{\Omega} \delta T \mathbf{b} \bullet \mathbf{v} dv + \int_{\partial\Omega} \delta T \mathbf{t} \bullet \mathbf{v} ds + \int_{\partial\Omega} \delta T q_n ds + \int_{\Omega} \delta T r dv =$$

$$= \int_{\Omega} \delta T \rho c \dot{T} dv - \int_{\Omega} (\nabla \delta T) \bullet \mathbf{q} dv + \int_{\Omega} \delta T \rho \dot{\mathbf{v}} \bullet \mathbf{v} dv + \int_{\Omega} \delta T (\boldsymbol{\sigma} : \mathbf{d}) dv + \int_{\Omega} (\nabla \delta T) \bullet (\boldsymbol{\sigma} \bullet \mathbf{v}) dv$$

The physical meaning of the new terms coming from the usage of the mathematical identity

Force equilibrium in CM:

$$\mathbf{b}+\nabla\bullet\boldsymbol{\sigma}-\rho\dot{\mathbf{v}}=\mathbf{0}$$
$$\boldsymbol{\sigma}\bullet\mathbf{n}=\mathbf{t}$$

Force equilibrium in FEM:

$$\delta w_m=\delta\mathbf{r}\bullet\left(\mathbf{b}+\nabla\bullet\boldsymbol{\sigma}-\rho\dot{\mathbf{v}}\right)=$$
$$=\mathbf{b}\bullet\delta\mathbf{r}+\nabla\bullet(\boldsymbol{\sigma}\bullet\delta\mathbf{r})-\boldsymbol{\sigma}:(\nabla\delta\mathbf{r})-\rho\dot{\mathbf{v}}\bullet\delta\mathbf{r}=0$$
$$\boldsymbol{\sigma}\bullet\mathbf{n}=\mathbf{t}$$

After integration over the volume of the body:

$$\int_\Omega\mathbf{b}dv+\int_{\partial\Omega}\boldsymbol{\sigma}^T\bullet\mathbf{n}da-\int_\Omega\rho\dot{\mathbf{v}}dv=\mathbf{0}$$

$$\int_\Omega\mathbf{b}\bullet\delta\mathbf{r}dv+\int_{\partial\Omega}\delta\mathbf{r}\bullet\mathbf{t}da-\int_\Omega\boldsymbol{\sigma}:(\nabla\delta\mathbf{r})dv-\int_\Omega\rho\dot{\mathbf{v}}\bullet\delta\mathbf{r}dv=0$$

Force equilibrium of a rigid body

$$\int_{\partial\Omega}\mathbf{a}\bullet\mathbf{n}ds=\int_\Omega(\nabla\bullet\mathbf{a})dv$$

$$\int_{\partial\Omega}\mathbf{A}^{\mathrm{T}}\bullet\mathbf{n}ds=\int_\Omega(\nabla\bullet\mathbf{A})dv$$

Force equilibrium of a deformable body

$$\nabla\bullet(\mathbf{A}^T\bullet\mathbf{a})=(\nabla\bullet\mathbf{A})\bullet\mathbf{a}+\mathbf{A}:(\nabla\mathbf{a})$$

The physical meaning of the new terms coming from the usage of the mathematical identity 2

Heat equation in CM:

$$\dot{w}_q = (-\nabla \bullet \mathbf{q}) + r - \rho c \dot{T} = 0$$
$$\mathbf{q} = -\mathbf{K} \bullet (\nabla T)$$
$$\mathbf{q} \bullet \mathbf{n} = -q_n$$

Heat equation in FEM:

$$\delta T \dot{w}_q = \delta T \left[(-\nabla \bullet \mathbf{q}) + r - \rho c \dot{T} \right] =$$
$$= (\nabla \delta T) \bullet \mathbf{q} - \nabla (\delta T \mathbf{q}) + \delta T r - \delta T \rho c \dot{T} = 0$$
$$\mathbf{q} \bullet \mathbf{n} = -q_n$$

After integration over the volume of the body:

$$\int_{\partial\Omega} q_n da + \int_{\Omega} r dv - \int_{\Omega} \rho c \dot{T} dv$$

$$\int_{\partial\Omega} \delta T q_n da + \int_{\Omega} \delta T r dv + \int_{\Omega} (\nabla \delta T) \bullet \mathbf{q} dv - \int_{\Omega} \delta T \rho c \dot{T} dv = 0$$

Body without a temperature gradient

Body with nonzero temperature gradient

$$\nabla \bullet (a\mathbf{a}) = a \nabla \bullet \mathbf{a} + \mathbf{a} \bullet \nabla a$$

$$\int_{\partial\Omega} \mathbf{a} \bullet \mathbf{n} ds = \int_{\Omega} (\nabla \bullet \mathbf{a}) dv$$

2, Material model

Modified NoIHKH model for large strain / large deformation cyclic plasticity of metals:

Yield surface: $f = \sigma_{eq} - \sigma_y - R \le 0$

$$\sigma_{eq} = \sqrt{\frac{3}{2}\left(\hat{\boldsymbol{\Sigma}} - \hat{\mathbf{X}}\right) : \left(\hat{\boldsymbol{\Sigma}} - \hat{\mathbf{X}}\right)}$$

$$\hat{\boldsymbol{\sigma}} = \mathbf{R}^T \bullet \boldsymbol{\sigma} \bullet \mathbf{R} \qquad \hat{\mathbf{X}} = \mathbf{R}^T \bullet \mathbf{X} \bullet \mathbf{R}$$

NoIH rule for isotropic hardening:

$$R = Q\left(1 - e^{\left(-b\varepsilon^p\right)}\right)$$

NoKH rule for kinematic hardening for large strain formulation:

$$\dot{\hat{\mathbf{X}}} = \mathbb{C}_{cycl} : \hat{\mathbf{d}}^p - \gamma\left(\varepsilon^p\right)\hat{\mathbf{X}}\dot{\varepsilon}^p$$

Green – Naghdi objective rate

$$\mathbf{R} \bullet \frac{\partial \hat{\mathbf{X}}}{\partial t} \bullet \mathbf{R}^T = \dot{\mathbf{X}} - \boldsymbol{\Omega} \bullet \mathbf{X} - \mathbf{X} \bullet \boldsymbol{\Omega}^T = \mathbb{C}_{cycl} : \mathbf{d}^p - \gamma\left(\varepsilon^p\right)\mathbf{X}\dot{\varepsilon}^p$$

$$tr\left(\hat{\mathbf{X}}\right) = 0$$

$$\gamma\left(\varepsilon^p\right) = \gamma_\infty - \left(\gamma_\infty - \gamma_0\right)e^{\left(-\omega\varepsilon^p\right)}$$

$$\hat{\mathbf{d}}^p = \mathbf{R}^T \bullet \mathbf{d}^p \bullet \mathbf{R} = \lambda \frac{\partial f}{\partial \hat{\boldsymbol{\sigma}}}$$

Rotating tensor formulation

Jaumann objective rate:

$$\boldsymbol{\sigma}^{\nabla J} = \frac{D(\boldsymbol{\sigma})}{Dt} - \mathbf{W}.\boldsymbol{\sigma} - \boldsymbol{\sigma}.\mathbf{W}^{T}$$

Green – Naghdi objective rate:

$$\boldsymbol{\sigma}^{\nabla G} = \frac{D(\boldsymbol{\sigma})}{Dt} - \boldsymbol{\Omega}.\boldsymbol{\sigma} - \boldsymbol{\sigma}.\boldsymbol{\Omega}^{\mathrm{T}}$$

$$\boldsymbol{\Omega}(t) = \dot{\mathbf{R}}(t).\mathbf{R}^{\mathrm{T}}(t)$$

Equivalence condition:

$$\dot{\mathbf{R}}(t) = \mathbf{W}.\mathbf{R}(t)$$

IC: $\mathbf{R}(t = t_0) = \mathbf{R}_0$

Exact solution:

$$\mathbf{R}(t) = \exp[(t - t_0)\mathbf{W}].\mathbf{R}_0$$

Rotating tensor at midpoint and endpoint configuration

$$\mathbf{R}^{n+\frac{1}{2}} = \exp\left[\frac{\Delta t}{2}\mathbf{W}^{n+\frac{1}{2}}\right]\bullet\mathbf{R}^{n}$$

$$\mathbf{R}^{n+1} = \exp\left[\Delta t\mathbf{W}^{n+\frac{1}{2}}\right]\bullet\mathbf{R}^{n}$$

Rodrigues formula:

Let $\mathbf{X}$ be a skew-symmetric tensor ($\mathbf{X} = -\mathbf{X}^T$). Then

$$\mathbf{Q} = \exp[\mathbf{X}]$$

is a proper orthogonal tensor (a rotation) and the exponential map has the following representation known as Rodrigues' formula:

$$\exp[\mathbf{X}] = \mathbf{I} + \frac{\sin(\|\mathbf{x}\|)}{\|\mathbf{x}\|}\mathbf{X} + \frac{1}{2}\left[\frac{\sin\left(\frac{\|\mathbf{x}\|}{2}\right)}{\frac{\|\mathbf{x}\|}{2}}\right]^2\mathbf{X}^2$$

where

$\mathbf{x}$ is the axial vector of $\mathbf{X}$. If $\|\mathbf{x}\| \neq n\pi$ for any odd n, then we have the additional equivalent representation:

3, Numerical implementation

1, Fully coupled thermal-structural problem using large strain / large deflection formulation with updated Lagrange method.

2, Eight node 3D solid element with linear shape function in element matrices formulation

3, Full numerical integration in element matrices calculation

4, Proper linearization = no simplifications in gradient, element matrix, etc. formulation

4, Numerical example

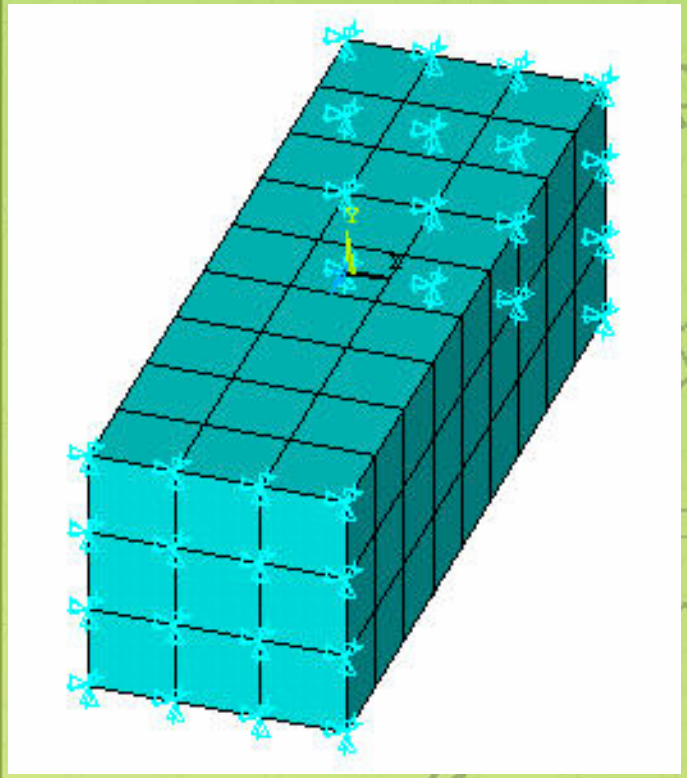

Fig. 1 Numerical model

Table 1: Material properties

$c = 15.0\,\mathrm{J}/(\mathrm{kg}\cdot\mathrm{K})$	$\mu = 0.3$
$k_{xx}, k_{yy}, k_{zz} = 50.0W/(m\cdot K)$	$\mu_{cycl} = 0.3$
$\alpha_x, \alpha_y, \alpha_z = 0.000012\,K^{-1}$	$\sigma_y = 250000.0\,Pa$
$h = 0.5W/(m^2\cdot K)$	$Q = 100000.0\,Pa$
$T_{bulk} = 0.0\,K$	$b = 3.0$
$\rho = 7800.0kg/m^3$	$\gamma_\infty = 20.0$
$E = 2100000.0\,Pa$	$\gamma_0 = 10.0$
$E_{cycl} = 550000.0\,Pa$	$\omega = 10.0$

Initial conditions: The bar is initially at the state of rest.

Initial temperature of the bar is zero.

5, Numerical results

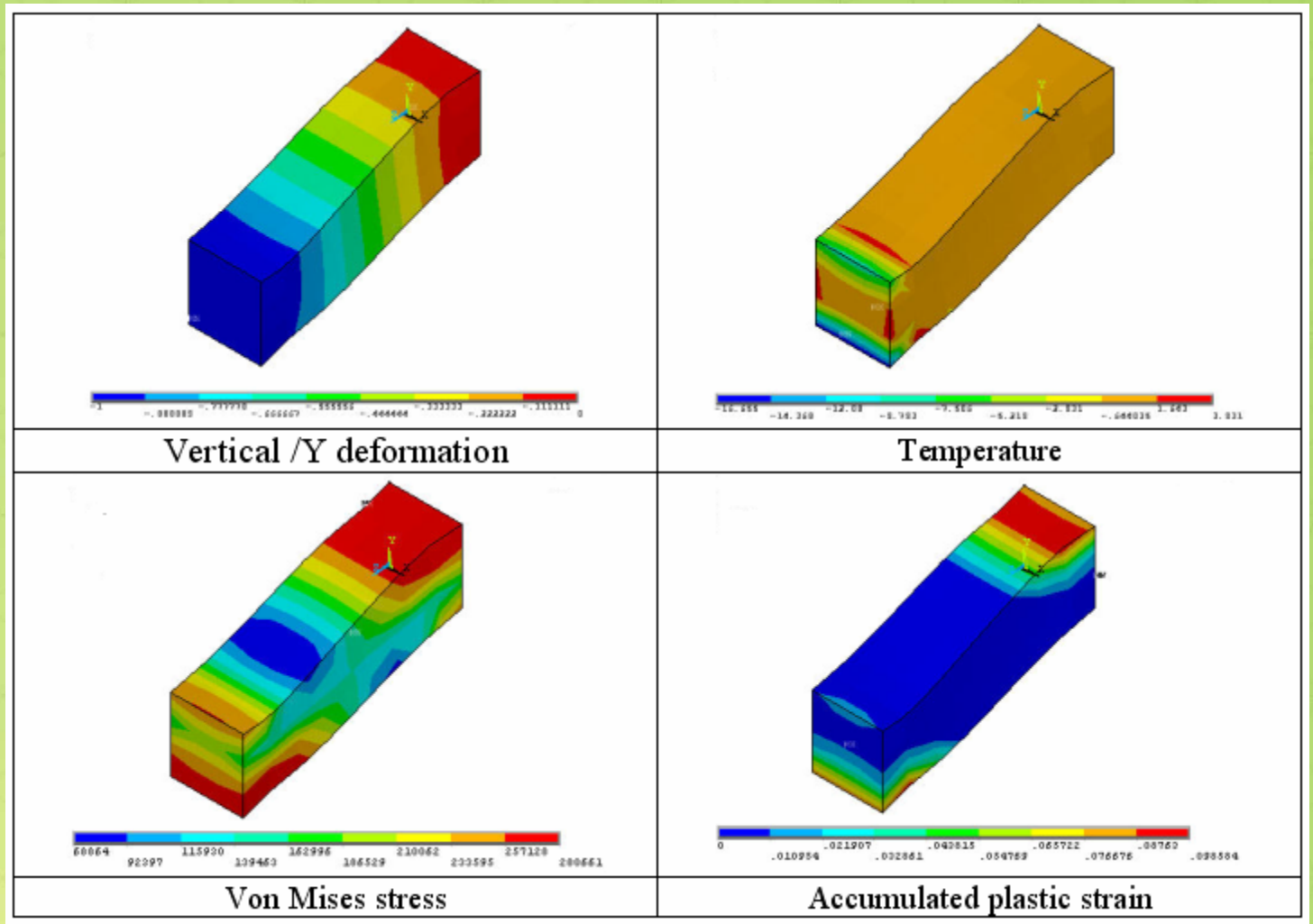

Fig. 2 Some results corresponding to the maximum downward deformation of the bar

Static elastic-plastic analysis

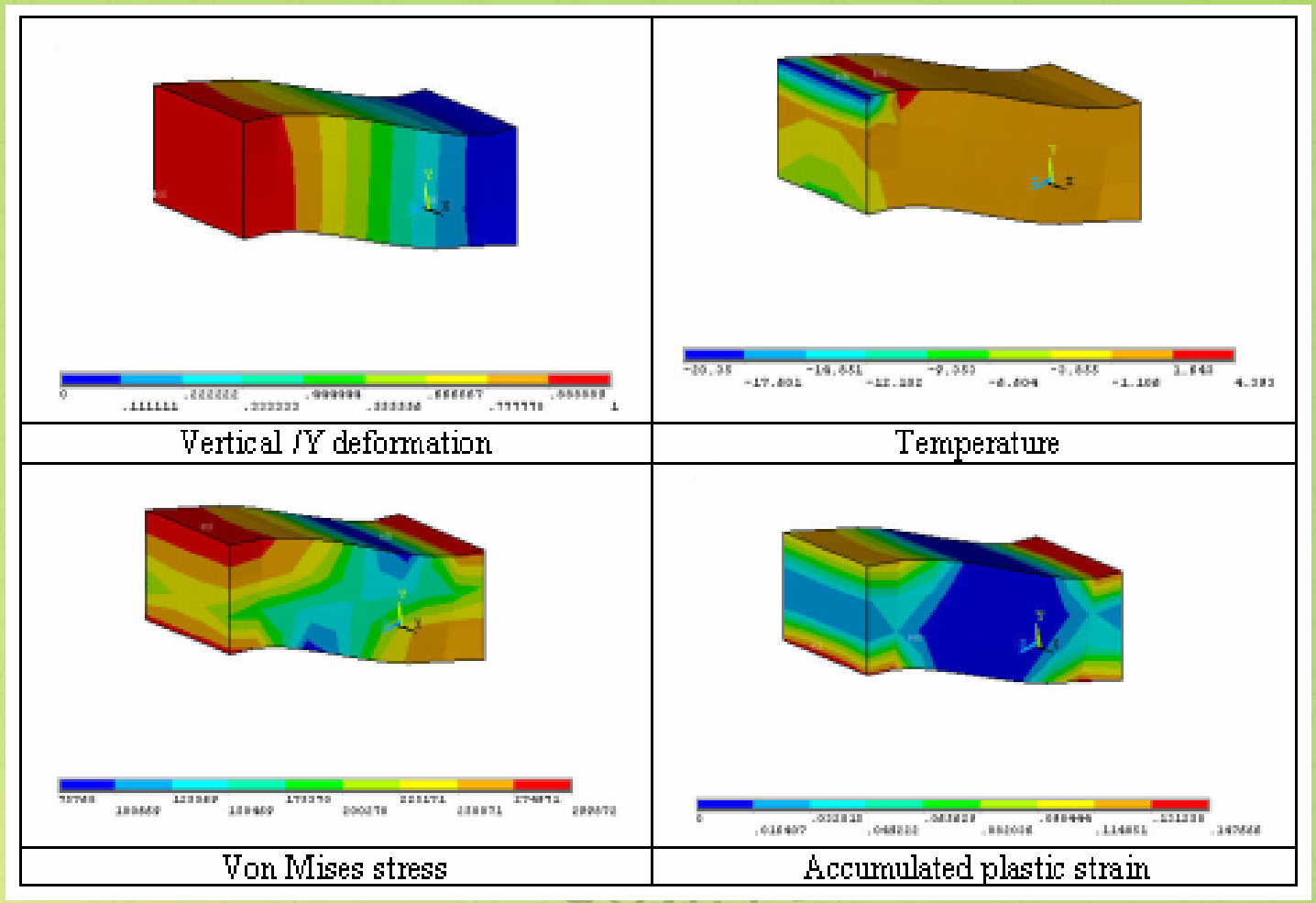

Fig. 3 Some results corresponding to the maximum upward deformation of the bar

6, Conclusions

1, The derived energy conservation equation is complete with respect to the thermal and mechanical energy contributions and the author believes that it represents a more accurate solution of fully coupled thermal structural problems, mainly in fast / ultra fast thermoelasticity / thermoplasticity. However this assertion still needs to be proved experimentally.

2, Since on a 32 bit personal computer (PC) there was a need to decrease some material values to prevent the global stiffness matrix from being nearly singular, in order to use real material properties, these analyses will need a 64 bit PC.

Thank you for your attention!