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Sensitivity analysis for viscoelastic bodies in object-oriented finite element environment†

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In this paper the constitutive model of thermoviscoelastic model is presented. To obtain the parameter sensitivity equations the direct differentiation method is applied. The paper also deals with the finite element for equilibrium and sensitivity analysis problems. Consistent tangent operator for the model is derived. To integrate the creep evolution equation the backward-Euler scheme is efficiently applied. The thermoviscoelastic model with parameter sensitivity analysis is implemented in object-oriented finite element system. Many advantages of the object-oriented approach in FE programming are described in the paper. Two numerical examples are solved. Very good agreement between the FE and analytical results is observed.

Keywords: viscoelasticity, transient heat transfer, sensitivity analysis, object-oriented approach

1. Introduction

Constitutive modelling of materials exhibiting thermo-viscoelastic behaviour, together with object-oriented applications of the finite element method to solve corresponding initial-boundary value problems, can now be considered as a classical subject with some three decade history.

The sensitivity formulation is a crucial ingredient in working out effective, numerical procedures for solving practical problems of structural optimization, parameter identification, optimal control, structural reliability, etc.

For better transparency of the formulation, we confine ourselves to mechanically and thermally isotropic materials characterized by only two distinct sets of relaxation behaviour: one associated with the shear modulus and the other, with the bulk modulus. No difficulties arise if more complex behaviour is considered.

2. Thermo-viscoelastic material model

The standard model is taken as the constitutive equation defining the class of linear viscoelastic materials on hand,

$$\sigma_{ij}(\tau) = \int_0^\tau C_{ijkl}(\xi - \xi')\, \frac{\mathrm{d}}{\mathrm{d}\tau'} \left[\varepsilon_{kl}(\tau') - \varepsilon_{kl}^{(\theta)}(\tau') \right] \mathrm{d}\tau' \tag{1}$$

where τ is the time coordinate, ξ is a reduced time coordinate defined as

$$\xi = \xi(\tau) = \int_0^\tau \frac{\mathrm{d}\zeta}{A(\theta(\zeta))}\,. \tag{2}$$

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ξ' has a similar definition with integration extending up to the time instant τ'

$$\xi' = \xi(\tau') = \int_0^{\tau'} \frac{\mathrm{d}\zeta}{A(\theta(\zeta))} \,. \tag{3}$$

$A(\theta)$ is a given temperature dependent shift factor and $\varepsilon_{ij}^{(\theta)}$ is the thermal strain assumed as

$$\varepsilon_{ij}^{(\theta)}(\tau) = \alpha[\theta(\tau) - \theta_0]\delta_{ij} \,. \tag{4}$$

with $\alpha(\theta)$ being the instantaneous thermal expansion coefficient, θ – the absolute temperature and $\theta_0 = \theta(0)$ – the natural state temperature.

To make the presentation more compact, still we shall be explicitly considering from now on materials with only one relaxation time

$$C_{ijkl}(\tau) = C_{ijkl}^{\infty} + \widetilde{C}_{ijkl} \exp\left[-\frac{\xi(\tau)}{\varrho}\right], \tag{5}$$

with the given parameters C_{ijkl}^{∞} being the so-called equilibrium moduli, $\widetilde{C}_{ijkl}$ – the magnitudes of transient decay and ϱ – the relaxation times. Consequently, all the derivations below based on these assumptions can easily be extended to cover more general situations. At $\tau = 0$ (i.e. also $\xi = 0$) the moduli C_{ijkl} become the glassy moduli of the form

$$C_{ijkl}(0) = C_{ijkl}^{\infty} + \widetilde{C}_{ijkl} \,. \tag{6}$$

The fundamental constitutive equation can be presented in the form

$$\sigma_{ij}(\tau) = C_{ijkl}^{0} \left[\varepsilon_{kl}(\tau) - \varepsilon_{kl}^{(\theta)}(\tau)\right] - \sigma_{ij}^{(c)}(\tau),$$

where the fictitious "creep" stress (difference between the purely elastic stress $C_{ijkl}^{0}[\varepsilon_{kl}(\tau) - \varepsilon_{kl}^{(\theta)}(\tau)]$ based on the glassy moduli and the actual stress σ_{ij}) is defined as

$$\sigma_{ij}^{(c)}(\tau) = \int_0^{\tau} \widetilde{C}_{ijkl} \left[1 - \exp\left[-\frac{\xi - \xi'}{\varrho}\right]\right] \frac{\mathrm{d}}{\mathrm{d}t'} \left[\varepsilon_{kl}(\tau') - \varepsilon_{kl}^{(\theta)}(\tau')\right] \mathrm{d}\tau'. \tag{7}$$

The temperature distribution $\theta(x, \tau)$ is obtained by solving the transient heat transfer problem consisting of the field equation

$$\nabla(\lambda \nabla^T \theta) + \dot{g} = \rho c \frac{\partial \theta}{\partial \tau}, \qquad (x, \tau) \in \Omega \times [0, \bar{t}], \tag{8}$$

where the boundary conditions

$$\theta = \hat{\theta}, \qquad \lambda \frac{\partial \theta}{\partial x_i} n_i = \hat{q}, \qquad (x, \tau) \in \partial\Omega_\theta \times [0, \bar{t}], \tag{9}$$

and the initial condition

$$\theta = \theta_0, \qquad (x, \tau) \in \Omega \times \{0\}, \tag{10}$$

in which $\nabla = \{\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\}$, $\dot{g}$ is the internal heat generation, ρ is the material density, c is the material specific heat, $\partial\Omega_\theta$, and $\partial\Omega_q$ are the boundary parts with prescribed temperature $\hat{\theta}$ and heat flux $\hat{q}$, respectively and $\underline{n} = \{n_i\}$ is the unit outward-drawn vector normal to the boundary surface. We assume that the temperature distribution is not affected by the mechanical behaviour of the material while – as seen from the previous discussion – the latter does depend on the former.

Differentiating Eq. (7) with respect to time to obtain

$$\frac{\mathrm{d}\sigma_{ij}^{(c)}(\tau)}{\mathrm{d}\tau} = \frac{1}{\varrho A(\tau)} \left[\widetilde{C}_{ijkl} \widetilde{\varepsilon}_{kl}(\tau) - \sigma_{ij}^{(c)}(\tau) \right] \tag{11}$$

where

$$\widetilde{\varepsilon}_{ij} \stackrel{\text{def}}{=} \varepsilon_{ij} - \varepsilon_{ij}^{(\theta)} \tag{12}$$

Equation (11) is a useful form of the time evolution equations for the creep stress $\sigma_{ij}^{(c)}$.

The constitutive description based on Eqs. (7), (11) allows its easy incorporation in the standard time stepping finite element algorithms. The stresses $\sigma_{ij}^{(c)}$ are treated as some internal parameters whose time evolution is governed by Eq. (11).

3. Finite element formulation

Box 1. Basic solution philosophy

(a) solve the heat transfer problem (8)–(10) at that instant for $\theta(\tau)$

(b) find the thermal strain $\varepsilon_{ij}^{(\theta)}$ at τ by Eq. (4)

(c) find the reduced time coordinate ξ at τ by Eq. (2)

(d) compute the integral in Eq. (1)

According to Box 1 the first problem to be solved at the given time step is the heat transfer equation (8). The regular FEM discretization procedure applied to that equation leads to the following (possibly nonlinear [5]) system of $\widetilde{N}$ first order time differential equations,

$$\mathbf{C}\dot{\boldsymbol{\theta}} + \mathbf{K}\boldsymbol{\theta} = \mathbf{P}. \tag{13}$$

in which the $\widetilde{N} \times \widetilde{N}$ matrices $\mathbf{K}$ and $\mathbf{C}$ (both possibly dependent on θ) are known as the capacitance and conductance matrices, $\boldsymbol{\theta}$ is the $\widetilde{N}$-dimensional vector of nodal temperatures while $\mathbf{P}$ is the $\widetilde{N}$-dimensional "load" vector due to the action of the internally generated heat and externally applied surface heat flux.

The system (13) may be solved by replacing the time derivative of the vector $\boldsymbol{\theta}$ with the finite difference scheme. We may use, for instance, expressions

$$\begin{aligned} {}^{t+\alpha\Delta t}\boldsymbol{\theta} &= (1-\alpha)\, {}^{t}\boldsymbol{\theta} + \alpha\, {}^{t+\Delta t}\boldsymbol{\theta}, \qquad \alpha \in [0,1] \\ {}^{t+\alpha\Delta t}\dot{\boldsymbol{\theta}} &= \frac{1}{\Delta t}({}^{t+\Delta t}\boldsymbol{\theta} - {}^{t}\boldsymbol{\theta}), \end{aligned} \tag{14}$$

which, substituted into Eq. (13) specified at time $t + \Delta t$, give

$${}^{t+\alpha\Delta t}\widehat{\mathbf{K}}\, {}^{t+\Delta t}\boldsymbol{\theta} = {}^{t+\alpha\Delta t}\widehat{\mathbf{P}} \tag{15}$$

where

$${}^{t+\alpha\Delta t}\widehat{\mathbf{K}} = \left[\frac{1}{\Delta t}\, {}^{t+\alpha\Delta t}\mathbf{C} + \alpha\, {}^{t+\alpha\Delta t}\mathbf{K} \right], \tag{16}$$

$${}^{t+\alpha\Delta t}\widehat{\mathbf{P}} = {}^{t+\alpha\Delta t}\mathbf{P} + \left[\frac{1}{\Delta t}{}^{t+\alpha\Delta t}\mathbf{C} - (1-\alpha)\, {}^{t+\alpha\Delta t}\mathbf{K} \right] {}^{t}\boldsymbol{\theta}. \tag{17}$$

These equations may be solved for the unknown vector ${}^{t+\Delta t}\boldsymbol{\theta}$ by using any available iterative scheme in which ${}^{t}\boldsymbol{\theta}$ is assumed to be known, while the matrices ${}^{t+\alpha\Delta t}\mathbf{C}$ and ${}^{t+\alpha\Delta t}\mathbf{K}$ are approximated by using the last available temperature ${}^{t+\Delta t}\boldsymbol{\theta}$. For the linear problem in which both $\mathbf{C}$ and $\mathbf{K}$ are temperature-independent, no iterations are clearly needed.

The basic ingredients required by the solution of the mechanical part of the problem are the time integration scheme and the consistent (algorithmic) stiffness matrix. The implicit time integration of the creep evolution equation to be performed at each spatial integration point within the FEM methodology may be based on the backward-Euler scheme to compute the end-of-the-step value of $\sigma_{ij}^{(c)}$ by Eq. (11) according to

$$\frac{{}^{t+\Delta t}\boldsymbol{\sigma}^{(c)} - {}^{t}\boldsymbol{\sigma}^{(c)}}{\Delta t} = \frac{1}{\varrho\ {}^{t+\Delta t}A}\left[\widetilde{\mathbf{C}}\,{}^{t+\Delta t}\widetilde{\boldsymbol{\varepsilon}} - {}^{t+\Delta t}\boldsymbol{\sigma}^{(c)}\right] \tag{18}$$

resolved for ${}^{t+\Delta t}\boldsymbol{\sigma}^{(c)}$ to yield

$${}^{t+\Delta t}\boldsymbol{\sigma}^{(c)} = \left[\frac{1}{\Delta t} + \frac{1}{{}^{t+\Delta t}A\varrho}\right]^{-1}\left[\frac{{}^{t}\boldsymbol{\sigma}^{(c)}}{\Delta t} + \frac{\widetilde{\mathbf{C}}\,{}^{t+\Delta t}\widetilde{\boldsymbol{\varepsilon}}}{{}^{t+\Delta t}A\varrho}\right]. \tag{19}$$

The constitutive equation (7) is used as

$${}^{t+\Delta t}\boldsymbol{\sigma} = \mathbf{C}^{0}\,{}^{t+\Delta t}\widetilde{\boldsymbol{\varepsilon}} - {}^{t+\Delta t}\boldsymbol{\sigma}^{(c)}. \tag{20}$$

The tangent operator consistent with the time integration scheme has the form

$${}^{t+\Delta t}\mathbf{C}^{*} = \frac{\partial\,{}^{t+\Delta t}\boldsymbol{\sigma}}{\partial\,{}^{t+\Delta t}\widetilde{\boldsymbol{\varepsilon}}} = \mathbf{C}^{0} - \frac{\Delta t\,\widetilde{\mathbf{C}}}{\Delta t + {}^{t+\Delta t}A\varrho}. \tag{21}$$

The system of equation governing the thermo-viscoelastic problem has the form

$$\begin{bmatrix} {}^{t+\alpha\Delta t}\widehat{\mathbf{K}} & \mathbf{0} \\ \mathbf{K}_S & \mathbf{K}^{*} \end{bmatrix}\begin{bmatrix} {}^{t+\Delta t}\boldsymbol{\theta} \\ \Delta\mathbf{q} \end{bmatrix} = \begin{bmatrix} {}^{t+\alpha\Delta t}\widehat{\mathbf{P}} \\ {}^{t+\Delta t}\widehat{\mathbf{Q}} \end{bmatrix}, \tag{22}$$

where

$$\mathbf{K}^{0} = \int_{\Omega} \mathbf{B}^{T}\mathbf{C}^{0}\,\mathbf{B}\,\mathrm{d}\Omega, \tag{23}$$

$$\widetilde{\mathbf{K}} = \left[\int_{\Omega} \widetilde{D}\,\mathbf{B}^{T}\widetilde{\mathbf{C}}\,\mathbf{B}\,\mathrm{d}\Omega\right], \tag{24}$$

$$\mathbf{K}^{*} = \int_{\Omega} \mathbf{B}^{T}\mathbf{C}^{*}\,\mathbf{B}\,\mathrm{d}\Omega = \mathbf{K}^{0} - \widetilde{\mathbf{K}}, \tag{25}$$

$$\mathbf{K}_S = \int_{\Omega} \overline{\mathbf{N}}^{T}\boldsymbol{\alpha}^{T}\mathbf{C}^{*}\mathbf{B}\,\mathrm{d}\Omega, \tag{26}$$

$${}^{t+\Delta t}\mathbf{Q} = \left[\int_{\Omega}\left({}^{t}\widehat{\mathbf{f}} + \Delta\widehat{\mathbf{f}}\right)^{T}\mathbf{N}\,\mathrm{d}\Omega\right] + \left[\int_{\partial\Omega_\sigma}\left({}^{t}\widehat{\mathbf{t}} + \Delta\widehat{\mathbf{t}}\right)^{T}\mathbf{N}\,\mathrm{d}\partial\Omega_\sigma\right], \tag{27}$$

$${}^{t}\mathbf{F}^{0} = \left[\int_{\Omega} \mathbf{B}^{T}\mathbf{C}^{0}\mathbf{B}\,\mathrm{d}\Omega\right]{}^{t}\mathbf{q}, \tag{28}$$

$$\mathbf{F}^{(\theta)} = \int_{\Omega} \boldsymbol{\alpha}^{T}\theta_0\mathbf{C}^{*}\mathbf{B}\,\mathrm{d}\Omega, \tag{29}$$

$$
\begin{aligned}
{}^t\widetilde{\mathbf{F}} &= \left[\int_\Omega \widetilde{D}\,\mathbf{B}^T\widetilde{\mathbf{C}}\,\mathbf{B}\,\mathrm{d}\Omega\right] {}^t\mathbf{q} = \widetilde{\mathbf{K}}\,{}^t\mathbf{q}, &&(30)\\
\Delta\widetilde{\mathbf{F}} &= \left[\int_\Omega \widetilde{D}\,\mathbf{B}^T\widetilde{\mathbf{C}}\,\mathbf{B}\,\mathrm{d}\Omega\right] \Delta\mathbf{q} = \widetilde{\mathbf{K}}\Delta\mathbf{q}, &&(31)\\
{}^t\overline{\mathbf{F}}^{(c)} &= \left[\int_\Omega D^{(c)}\,\mathbf{B}^T\,{}^t\boldsymbol{\sigma}^{(c)}\,\mathrm{d}\Omega\right], &&(32)\\
{}^t\mathbf{F}^{(c)} &= {}^t\widetilde{\mathbf{F}} + \overline{\mathbf{F}}^{(c)}, &&(33)\\
{}^{t+\Delta t}\widehat{\mathbf{Q}} &= {}^{t+\Delta t}\mathbf{Q} - {}^t\mathbf{F}^0 + {}^t\mathbf{F}^{(c)} + \mathbf{F}^{(\theta)}, &&(34)
\end{aligned}
$$

$$
{}^{t+\Delta t}\widetilde{D} = \frac{\Delta t}{\Delta t + {}^{t+\Delta t}A\varrho}, \qquad {}^{t+\Delta t}D^{(c)} = \frac{{}^{t+\Delta t}A\varrho}{\Delta t + {}^{t+\Delta t}A\varrho}. \tag{35}
$$

The system (22) consists of two subsystems which can be solved in succession.

4. Parameter sensitivity analysis

We assume now that our interest lies in finding a computationally effective technique of evaluating the gradient of any response functional with respect to a material parameter (say, h) entering the theory – such a gradient is referred to as the first order sensitivity response. It has been shown in the literature, see [6] for instance, that the gradient of any response functional can be expressed in terms of the displacement sensitivity $\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}h}$. Thus, our objective now is to develop a system of equations to be used for the computation of $\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}h}$ – in the context of the FEM methodology the goal is clearly fulfilled once a technique is developed to determine the value of $\frac{\Delta\mathbf{q}}{\mathrm{d}h}$.

In this paper, the so-called direct differentiation (DDM) method is used. The method requires differentiation of the governing equation with respect to the parameter h – any material parameter entering the theory can be substituted for h in specific applications.

4.1. Temperature sensitivity

Using DDM we obtain from Eq. (13) the equation governing the heat transfer sensitivity problem as

$$
\frac{\partial\mathbf{K}}{\partial h}\theta + \mathbf{K}\frac{\mathrm{d}\theta}{\mathrm{d}h} + \frac{\partial\mathbf{C}}{\partial h}\dot{\theta} + \mathbf{C}\frac{\mathrm{d}\dot{\theta}}{\mathrm{d}h} = \frac{\partial\mathbf{P}}{\partial h}. \tag{36}
$$

Using the same difference scheme as used in the heat transfer problem (14), this equation may be rewritten as

$$
{}^{t+\alpha\Delta t}\widehat{\mathbf{K}}\,\frac{\mathrm{d}\,{}^{t+\Delta t}\boldsymbol{\theta}}{\mathrm{d}h} = \frac{\mathrm{d}\,{}^{t+\alpha\Delta t}\widehat{\mathbf{P}}}{\mathrm{d}h} - \frac{\mathrm{d}\,{}^{t+\alpha\Delta t}\widehat{\mathbf{K}}}{\mathrm{d}h}\,{}^{t+\Delta t}\boldsymbol{\theta}. \tag{37}
$$

4.2. Displacement and stress sensitivity

Using the above results we differentiate Eq. (22) with respect to h to obtain

$$
\begin{bmatrix} \widehat{\mathbf{K}} & \mathbf{0} \\ {}^{t+\Delta t}\mathbf{K}_S & \mathbf{K}^* \end{bmatrix}
\begin{bmatrix} \dfrac{\mathrm{d}\,{}^{t+\Delta t}\boldsymbol{\theta}}{\mathrm{d}h} \\ \dfrac{\mathrm{d}\Delta\mathbf{q}}{\mathrm{d}h} \end{bmatrix}
=
\begin{bmatrix} \dfrac{\mathrm{d}\,{}^{t+\alpha\Delta t}\widehat{\mathbf{P}}}{\mathrm{d}h} \\ \dfrac{\mathrm{d}\,{}^{t+\Delta t}\widehat{\mathbf{Q}}}{\mathrm{d}h} \end{bmatrix}
-
\begin{bmatrix} \dfrac{\mathrm{d}\,{}^{t+\alpha\Delta t}\widehat{\mathbf{K}}}{\mathrm{d}h} & \mathbf{0} \\ \dfrac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{K}_S}{\mathrm{d}h} & \dfrac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{K}^*}{\mathrm{d}h} \end{bmatrix}
\begin{bmatrix} {}^{t+\Delta t}\boldsymbol{\theta} \\ \Delta\mathbf{q} \end{bmatrix} \tag{38}
$$

where

$$
\begin{aligned}
\frac{\mathrm{d}\mathbf{K}^0}{\mathrm{d}h} &= \int_\Omega \mathbf{B}^T \frac{\mathrm{d}\,\mathbf{C}^0}{\mathrm{d}h} \mathbf{B}\,\mathrm{d}\Omega, \\
\frac{\mathrm{d}\widetilde{\mathbf{K}}}{\mathrm{d}h} &= \int_\Omega \mathbf{B}^T \left[\frac{\mathrm{d}\,\widetilde{D}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h}\widetilde{\mathbf{C}} + \widetilde{D}\frac{\mathrm{d}\,\widetilde{\mathbf{C}}}{\mathrm{d}h} \right] \mathbf{B}\,\mathrm{d}\Omega, \\
\frac{\mathrm{d}\mathbf{K}^*}{\mathrm{d}h} &= \int_\Omega \mathbf{B}^T \frac{\mathrm{d}\,\mathbf{C}^*}{\mathrm{d}h} \mathbf{B}\,\mathrm{d}\Omega, \\
\frac{\mathrm{d}\mathbf{K}_S}{\mathrm{d}h} &= \int_\Omega \overline{\mathbf{N}}^T \boldsymbol{\alpha}^T \left[\frac{\mathrm{d}\mathbf{C}^*}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h}\boldsymbol{\varepsilon}^{(\theta)} + \mathbf{C}^*\frac{\mathrm{d}\boldsymbol{\varepsilon}^{(\theta)}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h} \right] \mathbf{B}\,\mathrm{d}\Omega, \\
\frac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{F}^{(\theta)}}{\mathrm{d}h} &= \int_\Omega \boldsymbol{\alpha}^T \theta_0^{t+\Delta t} \left[\frac{\mathrm{d}\mathbf{C}^*}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h}\boldsymbol{\varepsilon}^{(\theta)} + \mathbf{C}^*\frac{\mathrm{d}\boldsymbol{\varepsilon}^{(\theta)}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h} \right] \mathbf{B}\,\mathrm{d}\Omega, \\
\frac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{F}^0}{\mathrm{d}h} &= \left[\int_\Omega \mathbf{B}^T \frac{\mathrm{d}\,\mathbf{C}^0}{\mathrm{d}h} \mathbf{B}\,\mathrm{d}\Omega \right] {}^i\mathbf{q} + \mathbf{K}^0 \frac{\mathrm{d}\,{}^t\mathbf{q}}{\mathrm{d}h}, \\
\frac{\mathrm{d}\,{}^t\widetilde{\mathbf{F}}}{\mathrm{d}h} &= \left[\int_\Omega \mathbf{B}^T \frac{\mathrm{d}}{\mathrm{d}\theta}(\widetilde{D}\mathbf{C})\frac{\mathrm{d}\theta}{\mathrm{d}h} \mathbf{B}\,\mathrm{d}\Omega \right] {}^t\mathbf{q} + \left[\int_\Omega \mathbf{B}^T \widetilde{D}\mathbf{C}\,\mathbf{B}\,\mathrm{d}\Omega \right] \frac{\mathrm{d}\,{}^t\mathbf{q}}{\mathrm{d}h} \\
&= \frac{\mathrm{d}}{\mathrm{d}h}(\widetilde{\mathbf{K}}\,{}^t\mathbf{q}) = \frac{\partial\widetilde{\mathbf{K}}}{\partial h}{}^t\mathbf{q} + \widetilde{\mathbf{K}}\frac{\mathrm{d}\,{}^t\mathbf{q}}{\mathrm{d}h}, \qquad (39) \\
\frac{\mathrm{d}\,\Delta\widetilde{\mathbf{F}}}{\mathrm{d}h} &= \left[\int_\Omega \mathbf{B}^T \frac{\mathrm{d}}{\mathrm{d}\theta}(\widetilde{D}\mathbf{C})\frac{\mathrm{d}\theta}{\mathrm{d}h} \mathbf{B}\,\mathrm{d}\Omega \right] \Delta\mathbf{q} + \left[\int_\Omega \mathbf{B}^T \widetilde{D}\mathbf{C}\,\mathbf{B}\,\mathrm{d}\Omega \right] \frac{\mathrm{d}\,\Delta\mathbf{q}}{\mathrm{d}h} \\
&= \frac{\mathrm{d}}{\mathrm{d}h}(\widetilde{\mathbf{K}}\Delta\mathbf{q}) = \frac{\partial\widetilde{\mathbf{K}}}{\partial h}\Delta\mathbf{q} + \widetilde{\mathbf{K}}\frac{\mathrm{d}\,\Delta\mathbf{q}}{\mathrm{d}h}, \\
\frac{\mathrm{d}\,{}^t\overline{\mathbf{F}}^{(c)}}{\mathrm{d}h} &= \left[\int_\Omega \frac{\mathrm{d}}{\mathrm{d}\theta}\Big(D^{(c)}\Big)\frac{\mathrm{d}\theta}{\mathrm{d}h}\mathbf{B}^T\,{}^t\boldsymbol{\sigma}^{(c)}\,\mathrm{d}\Omega \right] + \left[\int_\Omega D^{(c)}\mathbf{B}^T \frac{\mathrm{d}\,{}^t\boldsymbol{\sigma}^{(c)}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}h}\,\mathrm{d}\Omega \right], \\
\frac{\mathrm{d}\,{}^t\mathbf{F}^{(c)}}{\mathrm{d}h} &= \frac{\mathrm{d}\,{}^t\overline{\mathbf{F}}^{(c)}}{\mathrm{d}h} + \frac{\mathrm{d}\,{}^t\widetilde{\mathbf{F}}}{\mathrm{d}h}, \\
\frac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{Q}}{\mathrm{d}h} &= \mathbf{0}, \\
\frac{\mathrm{d}\,{}^{t+\Delta t}\widehat{\mathbf{Q}}}{\mathrm{d}h} &= -\frac{\mathrm{d}\,{}^t\mathbf{F}^0}{\mathrm{d}h} + \frac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{F}^{(c)}}{\mathrm{d}h} + \frac{\mathrm{d}\,{}^{t+\Delta t}\mathbf{F}^{\theta}}{\mathrm{d}h}.
\end{aligned}
$$

System (38) containing two subsystems can be calculated separately in succession.

5. Object-oriented approach

5.1. Introduction

Application of object-oriented approach in the finite element method has already a decade long history. Especially in recent years we have observed an increasing popularity of object-oriented finite element implementations which is due to their efficiency for building and analyzing of computational models for complex engineering problems. Increasing complexity of finite element programs requires the use of efficient tools for their analysis [3], design [4] and programming [2]. The traditional structural programming emphasizes particular algorithms while data structures are not treated as crucial. For example, the nodal coordinates or the stiffness matrix are stored in the same type of vector; nevertheless, they are completely different entities from the conceptual point of view. Therefore, the natural language of the problem is far away from the implementation one. Moreover, any changes require modifications throughout the whole program and make the program maintenance very expensive and time-consuming. The object-oriented approach gives the possibility of combining the variables and subroutines in the complete bodies. This advantage allows to create the model of real-world problems very efficiently. In this paper, the thermo-viscoelastic material model with sensitivity analysis has been implemented in an object-oriented VFEM++ program.

5.2. Object-oriented model

In structural programming variables and subroutines are declared separately. This is however, related to a common entity. One of the fundamental concepts of the object-oriented approach is connection of variables (so-called *attributes*) and procedures (so-called *methods*) in one data structure (so-called *class*). This approach (so-called *encapsulation*) allows to create the data structure which completely models the entity selected from a considered problem domain. Attributes allow to store the properties of the entity and the methods usually acting on these attributes and its activities are conceptually assigned to the entity. Having the class declared we can define an object which is the variable of programming language defined similarly as the simple variables.

Considering as the problem domain the finite element analysis we can easily identify the entities that can be represented by classes. For example, a single element. A set of nodes is the attribute of the element. The class element contains also several methods. For compactness, we give one example of the method which calculates the element stiffness matrix named GetStiffnessMatrix.

Another most prominent concept of object-oriented modelling is its ability to create structures of classes. The mechanism called *inheritance* allows to make a structure of classes called *hierarchy of classes*. The hierarchy is a kind of graph similar to the genealogical tree. We discuss this structure on the basis of the example of the hierarchy of the finite elements classes shown in Fig. 1. The connection between classes i.e. inheritance, means that the lower class (so-called *subclass*) inherits the attributes and method from the upper class (*superclass*). It allows efficiently to utilize common properties of classes. In the case of elements classes the common attribute is the vector q containing nodal displacements, the results of FEM analysis. Because all elements must have this vector, it is declared in the base class and thanks to inheritance all classes posses it.

Another common property of each finite element is GetStiffnessMatrix method. All elements must have it; however, the algorithm of calculation of stiffness matrix in the case of a particular finite element (Truss, Frame, Isoparametric) is different. Thanks to the mechanism called *polymorphism* the inherited method can be redefined by declaring this method in the class once again and defining its own version of the body. It allows to cope easily with differences between classes. That class structure is also called a *generalization-specialization* (*gen-spec* for compactness) because the base class declares most general behaviours of the object while the descending classes are getting more and more specific. This structure reflects the natural classification of objects in the problem domain and assumes the object-oriented model is very close to the real problem domain allowing to effectively utilize all common features of particular hierarchy members and it easily gets along with differences.

It is clear that many entities in a real world consist of parts. The *whole-part* structure allows to reflect this obvious property of real entities in the object-oriented model and gives the mechanism for assembling composite objects. The whole-part structure is realized by calling member function of both objects (master object and parts). We can easily identify objects and its parts in the finite element analysis. For example each finite element is composed of an approximation, nodes, material and element load. In Fig. 2 the element and its parts are presented.

It is an interesting advantage of combining *whole-part* and *gen-spec* being essentially important in object-oriented approach. Let us consider Approximation, the base class for approximations. This class declares a member function GetShapeFunctionValues. This function calculates the values of the shape functions at a point. Thanks to *polymorphism*, each particular, implemented approximation

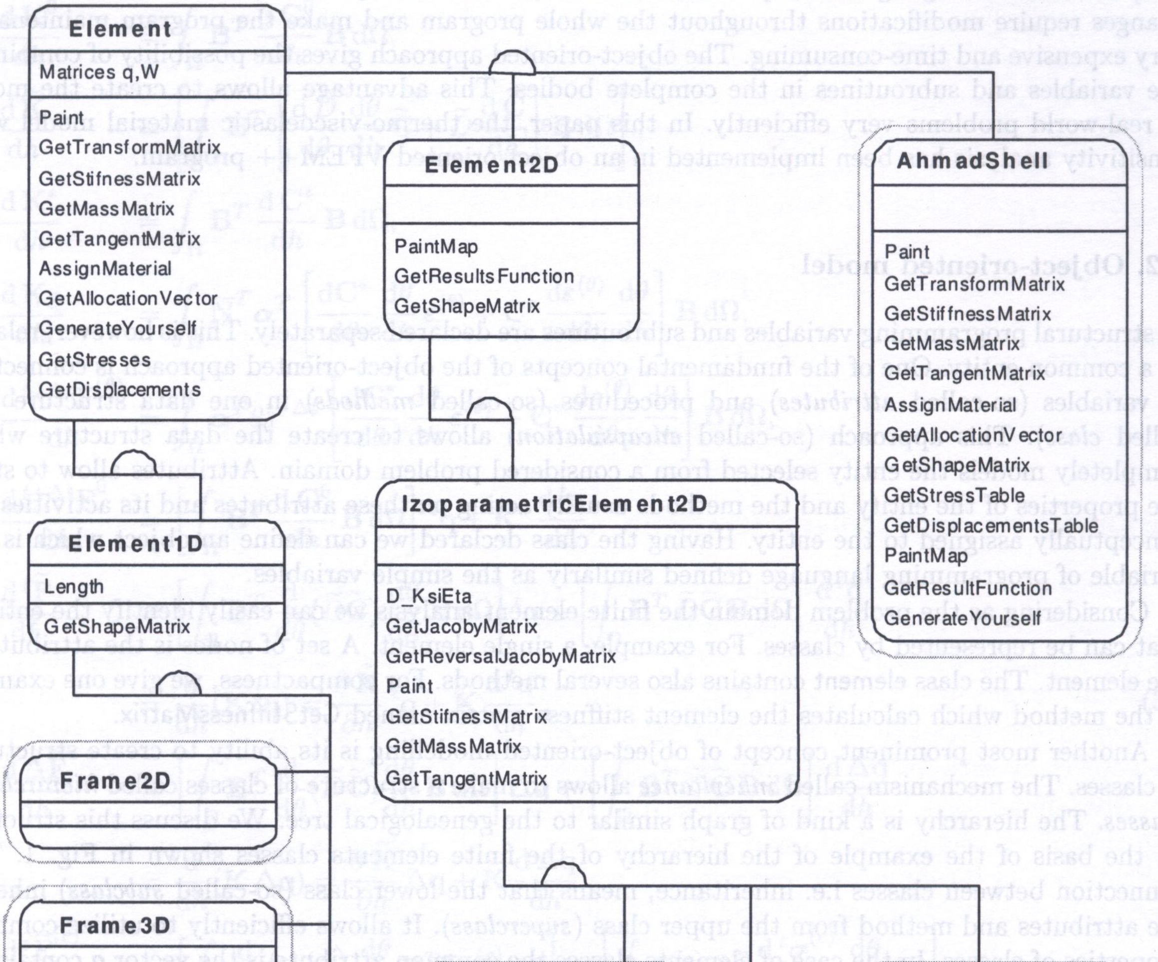

Fig. 1. Example of the finite element class hierarchy

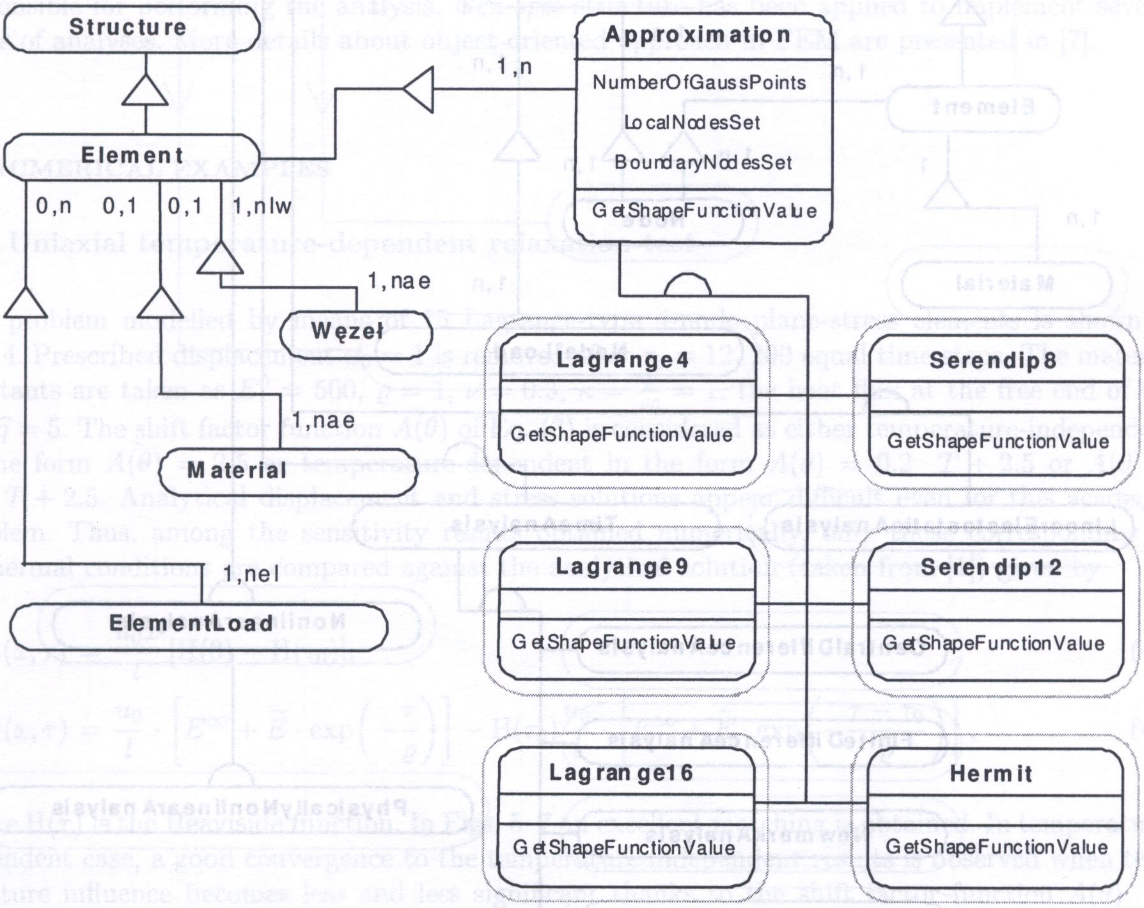

Fig. 2. Finite element object with its parts

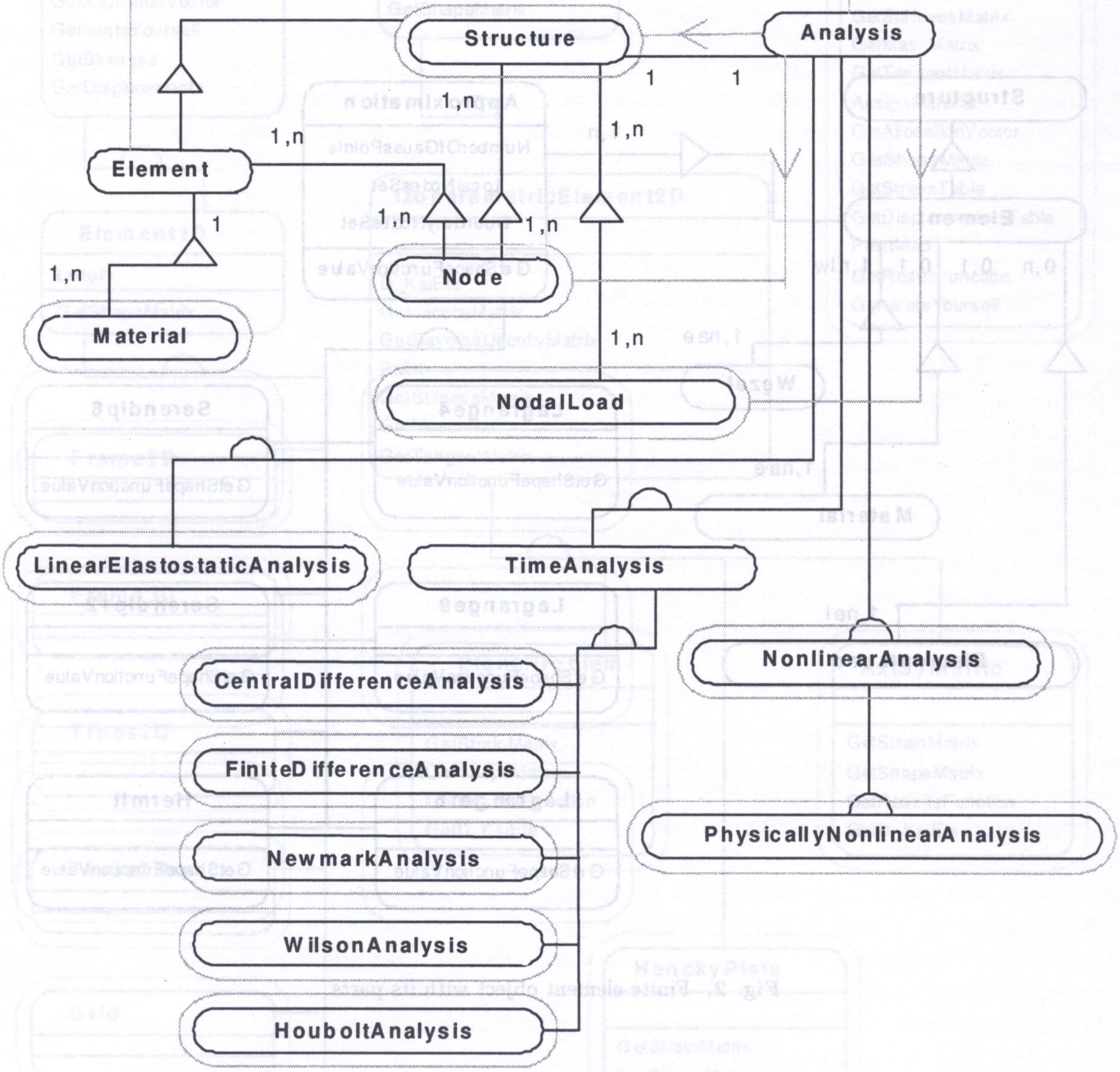

Fig. 3. Connections between main objects in VFEM++ program

derived from the base class, has its own version of this function. The object element has only a pointer to the approximation object and "doesn't have to know" what kind of approximation it actually cooperates with because all approximations must have the functions declared at the top of hierarchy of approximation. Thus a new approximation may be added to the system and no changes are necessary in the element class. In the case of implementing new finite elements we are also sure that the new element will cooperate with all already implemented approximations. Thus the structure allows to extend the system easily without many changes at many points of code.

Similar considerations apply to other parts of the object-oriented finite element system. In Fig. 3, we can see the main structures of VFEM++. Structure is the object containing all data of the structure such as nodes, elements, materials etc. These objects are, as we can see the parts of the structure (*whole-part* structure). Structure also cooperates with the Analysis objects which are responsible for performing the analysis. *Gen-spec* structure has been applied to implement several types of analyses. More details about object-oriented approach in FEM are presented in [7].

6. Numerical examples

6.1. Uniaxial temperature-dependent relaxation test

The problem modelled by means of 15 Lagrange-type 4-node plane-stress elements is shown in Fig. 4. Prescribed displacement $u_0 = 1$ is removed after $\tau_0 = 12$. 200 equal time steps. The material constants are taken as $E^0 = 500$, $\varrho = 1$, $\nu = 0.3$, $\kappa = \frac{\lambda}{\rho c} = 1$, the heat flux at the free end of the rod $\widehat{q} = 5$. The shift factor function $A(\theta)$ of Eq. (3) is considered as either temperature-independent in the form $A(\theta) = 2.5$ or temperature-dependent in the form $A(\theta) = 0.2 \cdot T + 2.5$ or $A(\theta) = 0.5 \cdot T + 2.5$. Analytical displacement and stress solutions appear difficult even for this academic problem. Thus, among the sensitivity results obtained numerically, only those corresponding to isothermal conditions are compared against the analytical solution (taken from [1]) given by

$$u(x,\tau) = \frac{u_0 x}{l}\,[\mathrm{H}(0) - \mathrm{H}(\tau_0)], \tag{40}$$

$$\sigma(x,\tau) = \frac{u_0}{l} \cdot \left[E^\infty + \widetilde{E} \cdot \exp\left(-\frac{\tau}{\varrho}\right)\right] - \mathrm{H}(\tau_0)\frac{u_0}{l} \cdot \left[E^\infty + \widetilde{E} \cdot \exp\left(-\frac{\tau - \tau_0}{\varrho}\right)\right], \tag{41}$$

where $\mathrm{H}(\tau)$ is the Heaviside function. In Figs. 5–7 an excellent matching is obtained. In temperature-dependent case, a good convergence to the temperature-independent results is observed when temperature influence becomes less and less significant thanks to the shift factor function $A(\theta)$. Increasing the shift factor function, we observe a softening of the material. Numerical stress results in Fig. 5 confirm this fact.

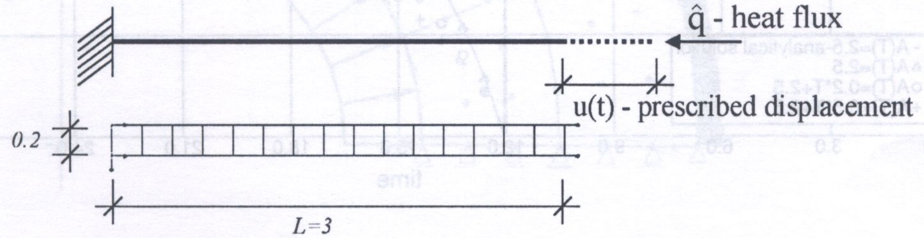

Fig. 4. Uniaxial test example with 15 Lagrange-type 4-node elements

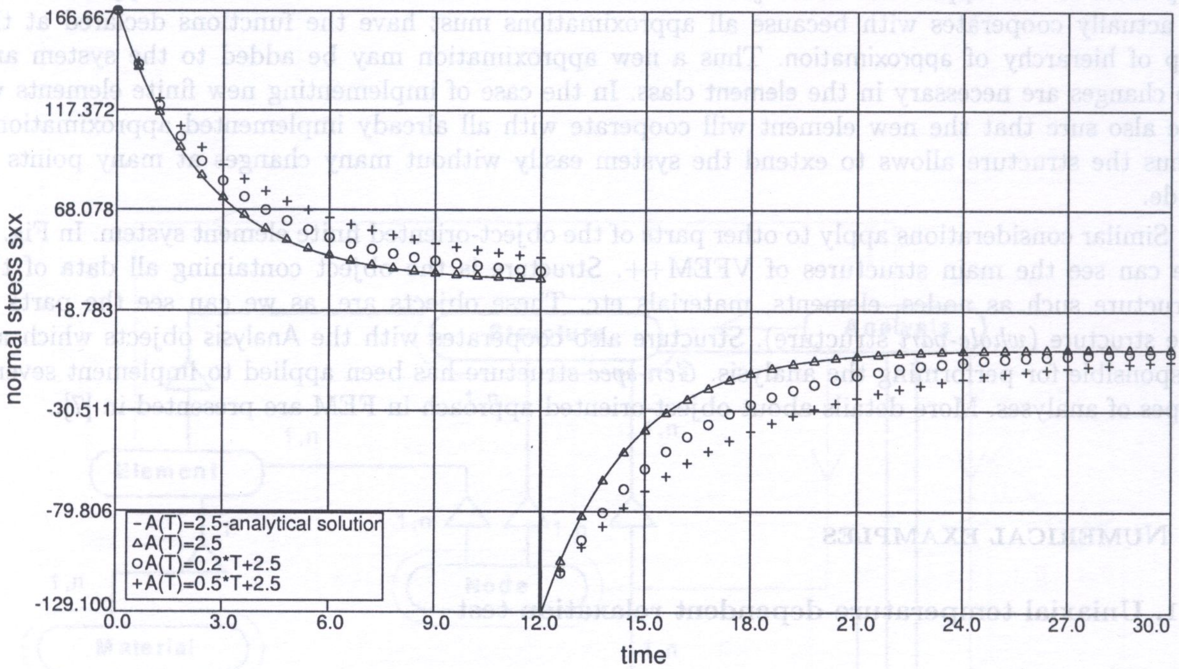

Fig. 5. Normal stress σ_x at the end of bar

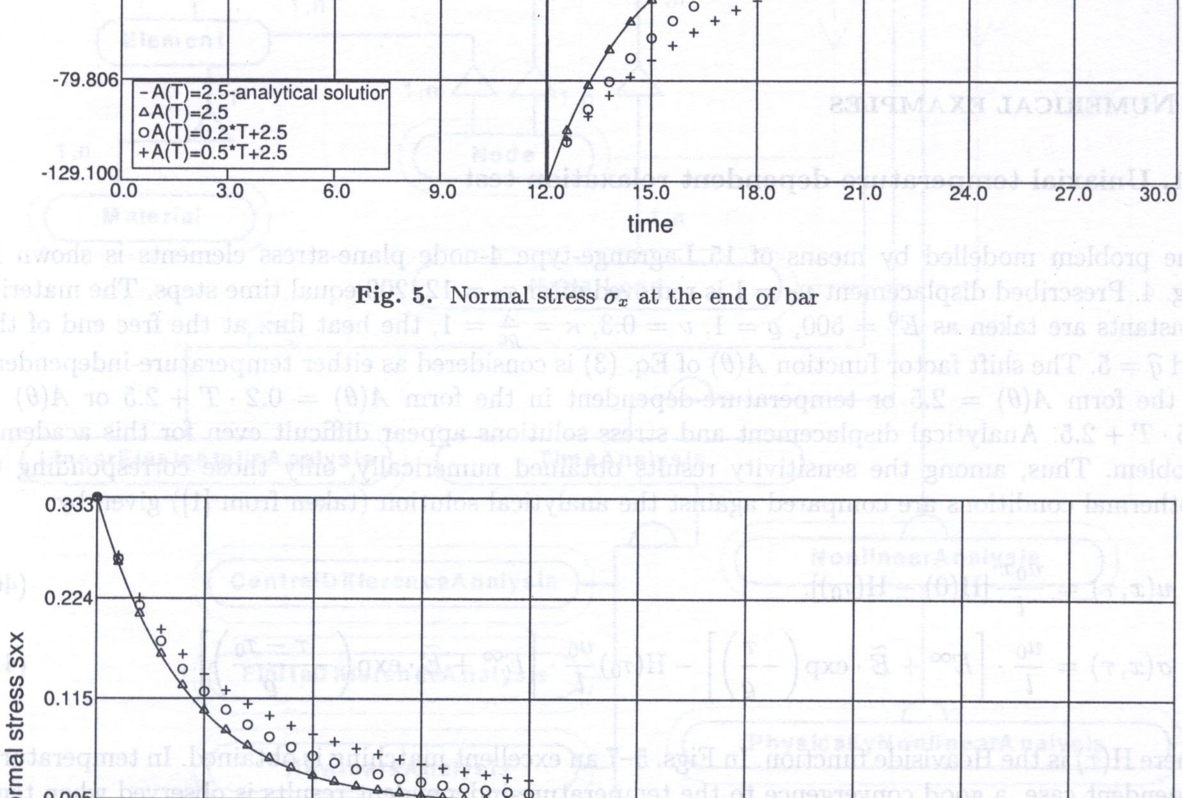

Fig. 6. Sensitivity of normal stress σ_x at the end of bar w.r.t. E^0

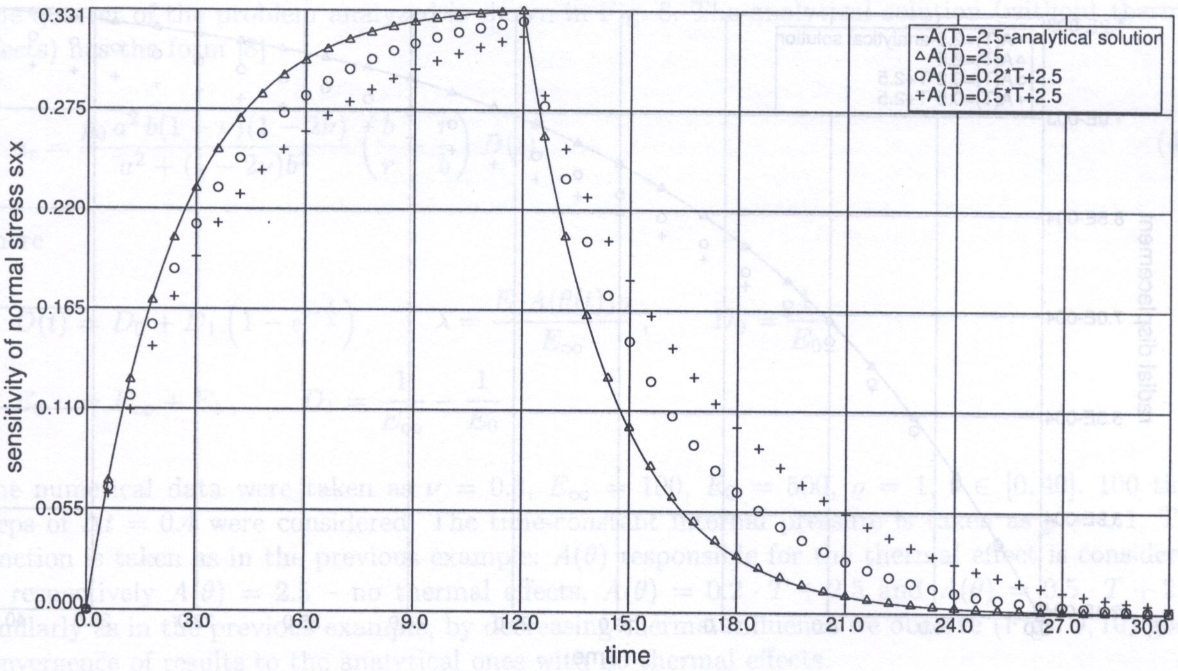

Fig. 7. Sensitivity of normal stress σ_x at the end of bar w.r.t. E^{∞}

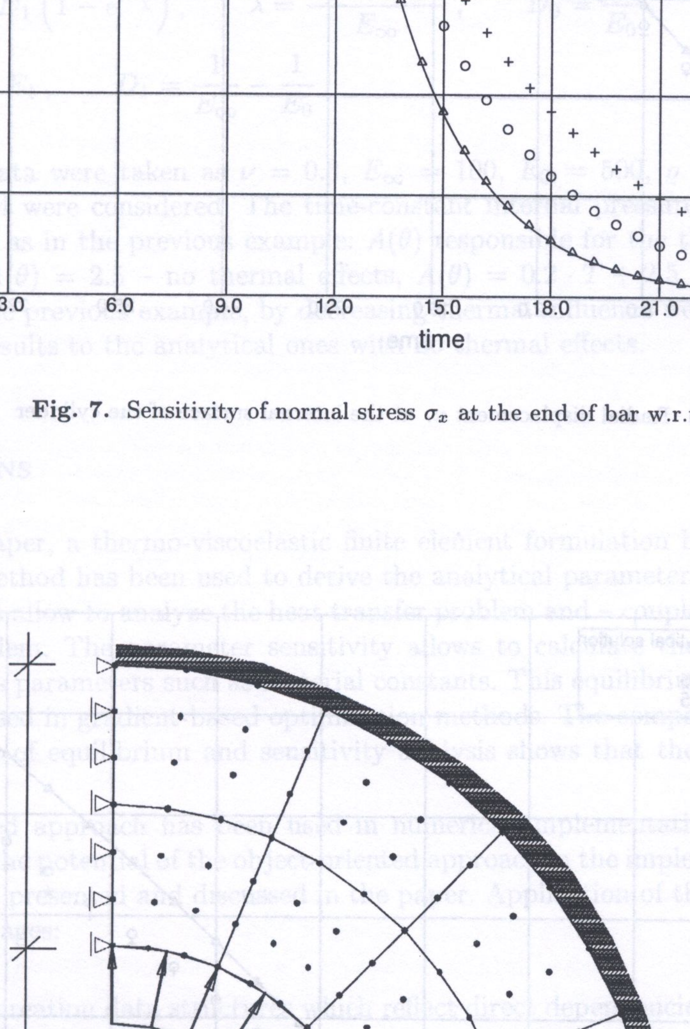

Fig. 8. Model definition

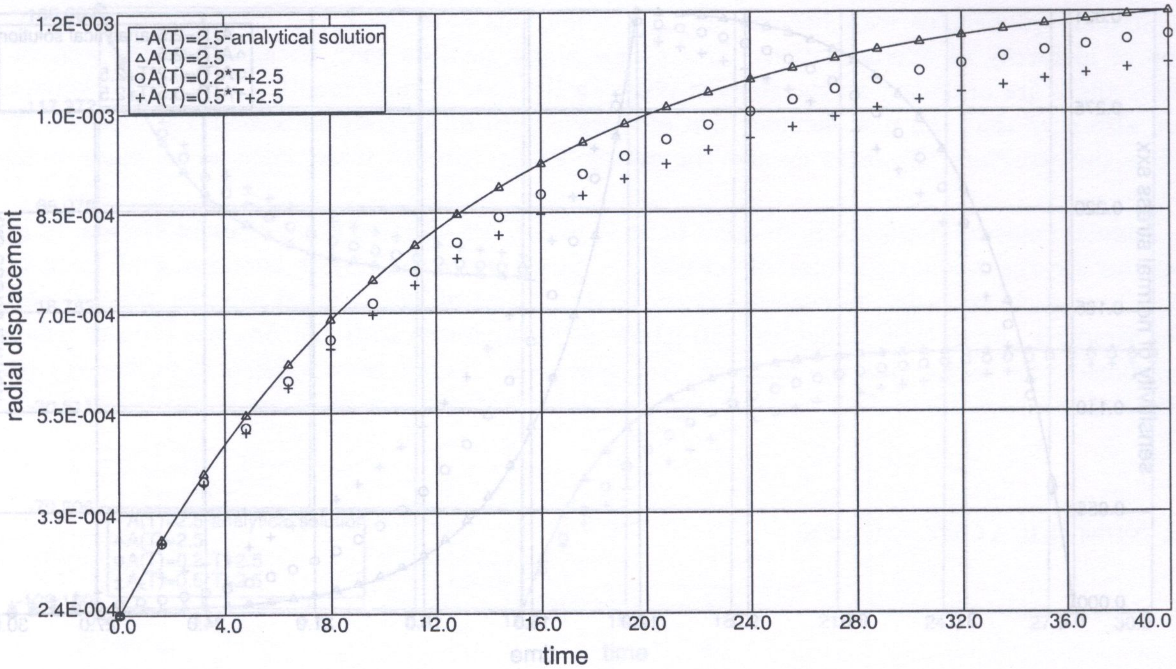

Fig. 9. Radial displacement u_r at the internal surface of the cylinder

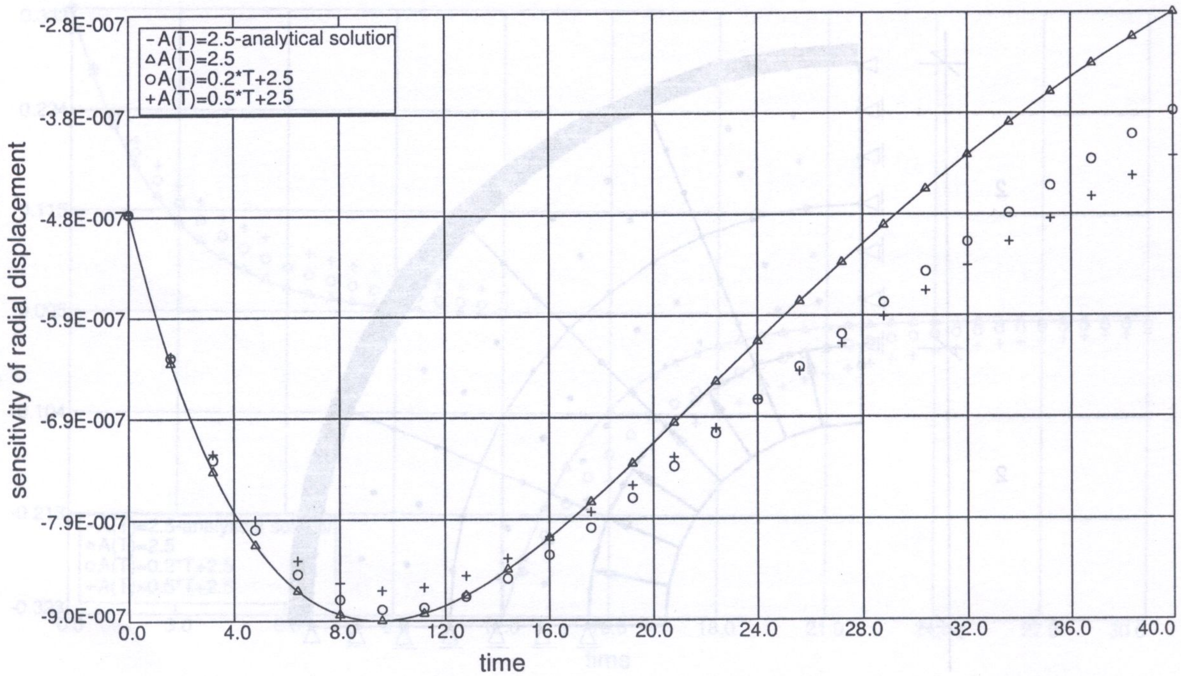

Fig. 10. Sensitivity of radial displacement u_r at the internal surface of the cylinder w.r.t. E^0

6.2. Thick walled cylinder

One quarter of the problem analyzed is shown in Fig. 8. The analytical solution (without thermal effects) has the form [8]

$$u_r = \frac{p_0\, a^2 b(1-\nu)(1-2\nu)}{a^2+(1-2\nu)b^2}\left(\frac{b}{r}-\frac{r}{b}\right)D(t), \tag{42}$$

where

$$D(t) = D_0 + D_1\left(1-e^{-\frac{t}{\lambda}}\right), \qquad \lambda = \frac{E_0 A(\theta(t))\varrho}{E_\infty}, \qquad D_0 = \frac{1}{E_0},$$

$$E_0 = E_\infty + E_1, \qquad D_1 = \frac{1}{E_\infty} - \frac{1}{E_0}.$$

The numerical data were taken as $\nu = 0.3$, $E_\infty = 100$, $E_0 = 500$, $\varrho = 1$, $t \in [0, 40]$. 100 time steps of $\Delta t = 0.4$ were considered. The time-constant internal pressure is taken as $p = 0.1$. The function is taken as in the previous example: $A(\theta)$ responsible for the thermal effect is considered as respectively $A(\theta) = 2.5$ – no thermal effects, $A(\theta) = 0.2 \cdot T + 2.5$ and $A(\theta) = 0.5 \cdot T + 2.5$. Similarly as in the previous example, by decreasing thermal influence we observe (Figs. 9, 10) good convergence of results to the analytical ones with no thermal effects.

7. Conclusions

In the present paper, a thermo-viscoelastic finite element formulation has been developed. Direct differentiation method has been used to derive the analytical parameter sensitivity equations. The derived equations allow to analyze the heat transfer problem and – coupled with it – the mechanical viscoelastic problem. The parameter sensitivity allows to calculate the first order gradient with respect to various parameters such as material constants. This equilibrium and sensitivity solutions can be directly used in gradient-based optimization methods. The comparison of the analytical and numerical results of equilibrium and sensitivity analysis shows that the two solutions are in very good agreement.

Object-oriented approach has been used in numerical implementation of the developed FEM equations. Also, the potential of the object-oriented approach in the implementation of finite element method has been presented and discussed in the paper. Application of the object-oriented methods has many advantages:

- Possibility of creation data structures which reflect direct dependencies of a real-worlds problem.
- Better modelling tools allow to cope with more complex problems the traditional structural approach does not.
- Flexibility of code allows to introduce easily some changes in the code.
- Order in structures of data enables faster searching of errors in the code.
- Object-oriented code, through the better data structures causes that the code is more reliable.

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