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SOLUTION OF TRANSIENT PROBLEMS OF THERMOELASTICITY*

Roman Kohut

Abstract

The paper deals with a finite element solution of transient thermoelasticity problems. For each time step the system of linear algebraic equations is solved using the conjugate gradient method preconditioned by incomplete factorization of the matrix derived from the original matrix. The time step is chosen adaptively. The results of numerical tests are presented. A procedure for the solution of large practical problems is proposed.

1. Introduction

The design and construction of a deep geological repository for spent nuclear fuel require the use of mathematical modelling for understanding natural and induced phenomena in the geological environment. This geotechnical activity induces thermal, hydrological, mechanical (T–H–M) and other phenomena. In this paper we will study thermo-mechanical (T–M) processes only. This is not a fully coupled problem, we consider strains and stresses induced by heat loading, but the mechanical and heat parameters don't depend on temperature. We assume the material is isotropic.

2. Thermoelasticity

The thermoelasticity problem is concerned with finding the temperature $\tau = \tau(x,t)$ and the displacement $u = u(x,T)$,

$$\tau : \Omega \times (0,T) \to R, \quad u : \Omega \times (0,T) \ \to R^3,$$

that fulfill the following equations

$$\kappa\rho\frac{\partial\tau}{\partial t} = k\sum_i \frac{\partial^2\tau}{\partial {x_i}^2} + Q(t) \qquad in \quad \Omega\times(0,T)\,, \tag{1}$$

$$-\sum_j \frac{\partial\sigma_{ij}}{\partial x_j} = f_i \quad (i=1,\dots,d) \quad in \quad \Omega\times(0,T)\,, \tag{2}$$

$$\sigma_{ij} = \sum_{kl} c_{ijkl}\left[\varepsilon_{kl}(u) - \alpha_{kl}(\tau-\tau_0)\right] \quad in \quad \Omega\times(0,T)\,, \tag{3}$$

$$\varepsilon_{kl}(u) = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) \quad in \quad \Omega\times(0,T), \tag{4}$$

together with the boundary conditions

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$$\tau(x,t) = \hat{\tau}(x,t), \quad \text{on } \Gamma_0 \times (0,T)\,, \tag{5}$$

$$-k\sum_i \frac{\partial \tau}{\partial x_i} n_i = q \quad \text{on } \Gamma_1 \times (0,T)\,, \tag{6}$$

$$-k\sum_i \frac{\partial \tau}{\partial x_i} n_i = H(\tau - \hat{\tau}_0) \quad \text{on } \Gamma_2 \times (0,T)\,, \tag{7}$$

$$u_n = \sum_i u_i n_i = 0, \quad \text{on } \tilde{\Gamma}_0 \times (0,T)\,, \tag{8}$$

$$\sigma_t = 0 \quad \text{on } \tilde{\Gamma}_0 \times (0,T)\,, \tag{9}$$

$$\sum_j \sigma_{ij}\, n_j = g_i \quad (i = 1,\ldots,3) \quad \text{on } \tilde{\Gamma}_1 \times (0,T)\,, \tag{10}$$

where $\partial\Omega = \Gamma = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2$ for equation (1) and $\partial\Omega = \Gamma = \tilde{\Gamma}_0 \cup \tilde{\Gamma}_1$ for equations (2)–(4), and the initial conditions

$$\tau(x,0) = \tau_0(x) \quad \text{in } \Omega. \tag{11}$$

The boundary conditions represent the temperature (5), heat flow (6), heat transfer (7), displacement (8), stresses(9), surface loading(10).

Note that the T–M coupling in the problem (1) – (11) is done by adding heat deformations to the generalized Hooke's law (3). Thus stresses do not influence temperature fields and we can compute them only in predefined time points as post-processing to the solution of the equation (1).

Thus the problem (1)–(11) can be divided in two parts. Firstly, the temperature distribution is computed. Secondly, the corresponding displacements, strains and stresses are determined. The stress determinantion at given time points represents a post-processing for the heat conduction problem, when the determined temperature field modifies the right-hand side for the elasticity problem. After the displacement is computed, stresses are determined according to the relation (3).

The finite element method (FEM) is based on a weak formulation of the heat conduction problem, which can be written after application of Green's theorem as follows:

find $\tau = \tau(x,t)$, $(x,t) \in \Omega \times (0,T)$, $\tau(.,t) \in V_D$ such that the following equations hold:

$$(\kappa\rho\,\dot{\tau}, v)_0 + a(t,\tau,v) = b(t,v) \quad \forall v \in V_0,\ t \in (0,T), \tag{12}$$

$$(\tau(x,0), v)_0 = (\tau_0, v)_0 \quad \forall v \in V_0. \tag{13}$$

In these equations

$$V_0 = \left\{ v \in H^1(\Omega) : v = 0 \quad \text{on} \quad \Gamma_0 \right\},$$

$$V_D = \left\{ v \in H^1(\Omega) : v = \hat{\tau} \quad \text{on} \quad \Gamma_0 \right\},$$

where $(\ ,\ )_0$ is the scalar product in the space of square-integrable functions $L_2(\Omega)$, $H^1(\Omega) \subset L_2(\Omega)$ is the Sobolev space of functions having first weak derivatives in the the space $L_2(\Omega)$. For a, b there holds

$$a(t,\tau,v) = \int_\Omega \sum_{ij} k_{ij} \frac{\partial \tau}{\partial x_j} \frac{\partial v}{\partial x_i} dx + \int_{\Gamma_2} H\tau v ds\,, \tag{14}$$

$$b(t,v) = \int_\Omega Q(t) v dx - \int_{\Gamma_1} qv ds + \int_{\Gamma_2} H\hat{\tau}_0 v ds\,. \tag{15}$$

The direct application of the finite element method means to transfer the above mentioned variational formulation to the finite element space. We'll consider the space $V_{0,h} = \text{span}\,\{\varphi_i\} \subset V_0$, where φ_i is a standard FEM basis, and span presents linear combination of these base functions.

3. Time discretization

We find $\tau = \tau(x,t), (x,t) \in \Omega \times (0,T), \tau(\cdot,t) \in V_D$ such, that (12), (13) hold. We transfer the problem to the FEM formulation. Consider the space $V_{0,h} = \text{span}\,\{\varphi\} \subset V_0$. We find

$$\tau_h(x,t) = \hat{\tau}(x,t) + \sum_i \underline{\tau_i}(t)\varphi_i(x), \tag{16}$$

where $\hat{\tau}(x,t)$ acquires the prescribed values on Γ_0. In our case we use the function $\hat{\tau}(x,t) = \tau_0(x)$, which represents the initial condition for the non-stationary problem. Substituting (16) into the equation (12), for the determination of the coefficient vector $\underline{\tau} = [\underline{\tau_i}]$ we receive the system of linear differential equations

$$\begin{aligned} M_h \dot{\underline{\tau}}(t) + A_h(t)\underline{\tau}(t) &= \underline{b}_h(t) \quad \forall t \in (0,T), \\ \frac{1}{\kappa\rho} M_h \underline{\tau}(0) &= 0, \end{aligned} \tag{17}$$

where

$$\begin{aligned} M_h &= [(\kappa\rho\varphi_i, \varphi_j)_0]\,, \\ A_h(t) &= [a(t, \varphi_i, \varphi_j)]\,, \\ \underline{b}_h(t) &= [b(t,\varphi_i) - a(t,\hat{\tau},\varphi_i)]. \end{aligned} \tag{18}$$

Remark: If we express the solution in the form (16), the original problem is transformed to the problem (17) with the homogeneous boundary conditions and with the zero initial condition. Thus we determine the increment of the temperature τ with respect to the initial condition τ_0. The initial condition in (17) can be replaced with the condition $\underline{\tau}(0) = 0$.

We divide the interval $\langle 0,T\rangle, 0=t_0<t_1<\ldots<t_p=T, \Delta_i=t_i-t_{i-1}$. We find values $\underline{\tau}_i^j=\underline{\tau}_i(t_j)$. Using the time discretization we obtain

$$\begin{aligned} M_h\frac{1}{\Delta_j}(\underline{\tau}^j-\underline{\tau}^{j-1})+\theta A_h(t_j)\underline{\tau}^j+(1-\theta)A_h(t_{j-1})\underline{\tau}^{j-1} &= \varphi^j, \\ \underline{\tau}^0 &= 0, \end{aligned} \tag{19}$$

where $\theta\in\langle 0,1\rangle, \varphi^j=\theta\underline{b}_h(t_j)+(1-\theta)\underline{b}_h(t_{j-1})$. In each time step we have to solve the system

$$[M_h+\Delta_j\theta A_h(t_j)]\underline{\tau}^j=[M_h-(1-\theta)\Delta_j A_h(t_{j-1})]\underline{\tau}^{j-1}+\Delta_j\varphi_j. \tag{20}$$

For $\theta=0$ we obtain the so-called explicit Euler scheme, for $\theta=1$ we obtain the backward Euler (BE) scheme, $\theta=0.5$ gives the Crank-Nicholson(CN) scheme.

In our case we will use the BE scheme, which is more stable. Because the matrix A_h is not time dependent, we can write $A_h(t_j)=A_h$. Then the system (20) is replaced by

$$[M_h+\Delta_j A_h]\underline{\tau}^j=M_h\underline{\tau}^{j-1}+\Delta_j\varphi_j, \tag{21}$$

where $\Delta_j\varphi_j=\Delta_j\underline{b}_h(t_j)$. If we substitute

$$\underline{\tau}^j=\underline{\tau}^{j-1}+\Delta\underline{\tau}^j$$

into (21), we obtain the system of equations for the increment of temperature

$$[M_h+\Delta_j A_h]\Delta\underline{\tau}^j=\Delta_j(\varphi_j-A_h\underline{\tau}^{j-1}). \tag{22}$$

Remark: We denote the system matrix in (22) by $B_h^{(j)}$, $B_h^{(j)}=M_h+\Delta_j A_h$.

Using the constant time-step, the system (22) must be solved hundreds times which consumes, especially in 3D, huge time. Therefore it is necessary to optimize the computation.([1])

The first step is the adaptive choice of time-step. The use of the BE method allows to use the adaptive time stepping scheme based on a local comparison of the BE and CN steps. We solve the system (20) in the incremental form only for $\theta=1$. If this solution $\underline{\tau}^j=\underline{\tau}^{j-1}+\Delta\underline{\tau}^j$ is considered as the initial approximation for the solution of system (20) for $\theta=0.5$ (CN scheme), then the first iteration of the Richardson's method presents an approximation of the solution of the system (20) for $\theta=0.5$. Thus $\underline{\tau}_{CN}^j\cong\underline{\tau}^j-r^j$, where

$$r^j=(M_h+0.5\Delta_j A_h)\underline{\tau}^j-(M_h-0.5\Delta_j A_h)\underline{\tau}^{j-1}-0.5\underline{b}_h(t_j)-0.5\underline{b}_h(t_{j-1}). \tag{23}$$

The time steps can be controlled with the aid of the ratio $\eta=\frac{\|r^j\|}{\|\underline{\tau}^j\|}$ according to the following algorithm ($k=1,2,\ldots$ denotes the adaptive changes, $\underline{\tau}^{j,k}$ corresponding solutions of system (20)):

for $k = 1, 2, \ldots$ **until** *stop* **do**
solve system (20) $\rightarrow \underline{\tau}^{j,k}$, **compute** $r^{j,k}$ a η_k
if $\eta_k < \varepsilon_{\min}$ **then** $2\Delta_j \rightarrow \Delta_j$
if $\eta_k > \varepsilon_{\max}$ **then** $\Delta_j/2 \rightarrow \Delta_j$
if $\eta_k \in < \varepsilon_{\min}, \varepsilon_{\max} >$ **or** $\eta_k < \varepsilon_{\min}$ & $\eta_{k-1} > \varepsilon_{\max}$ **then**
$\Delta_{j+1} = \Delta_j, \underline{\tau}^j = \underline{\tau}^{j,k}, stop$
if $\eta_k > \varepsilon_{\max}$ & $\eta_{k-1} < \varepsilon_{\min}$ **then**
$\Delta_{j+1} = \Delta_j/2, \quad \underline{\tau}^j = \underline{\tau}^{j,k-1}, stop$
end

Because the matrix in (22) changes in every time step, it may be advantageous to adapt the step-size only in each k-th time step. For parameters $\varepsilon_{\min}, \varepsilon_{\max}$ we usually take values $10^{-3}, 10^{-2}$.

In each time step we solve system (22). The efficiency of the iterative solution can be also increased by using a suitable initial approximation. There are several possibilities:
1. using the previous time step value $\Delta\underline{\tau}^j$ as initial approximation for $\Delta\underline{\tau}^{j+1}$.
2. using the initial approximation given by the linear extrapolation, i.e. for $\Delta_j = \Delta_{j-1}$ we get $\Delta\underline{\tau}^{j+1} = 2\Delta\underline{\tau}^j - \Delta\underline{\tau}^{j-1}$.
3. the improvement of the initial approximations by exploiting the conjugate directions $\{\nu_i\}$, $i = 1, \ldots, m$ from the application of the CG method to the solution of the system in some previous time step. Here we assume that $B_h^{(j)} = B_h$ does not change in a selected sequence of time steps $j_0, \ldots, j_1$. Then

$$\underline{\tau}^{j,0} = \underline{\tau}_{ini} + \sum_{i=1}^{m} \mu_i \nu_i, \quad \mu_i = \frac{(r_{ini}, \nu_i)}{(A\nu_i, \nu_i)}.$$

The inner products $(A\nu_i, \nu_i)$ are known from the previous application of the CG method, we must only compute the residual $r_{ini} = c^j - B_h \underline{\tau}_{ini}$ and m inner products (r_{ini}, ν_i).

4. Numerical tests

The numerical tests were realized on the BMT3 benchmark problem setting up in framework of DECOVALEX project([2]). In this test case, the repository tunnel is located at the depth of $500m$ and the nuclear waste, which is a source of heat, is disposed in a borehole below this tunnel (see Figure 1). The heat source simulating the waste canister is assumed to decay exponentially with time according to the following relation

$$Q(t) = Q_0 exp(-\beta t).$$

The test problem is defined as a 3D problem with the grid dimension $45 \times 51 \times 46$, whose nodes present 316710 unknowns. The tests were done on the workstation IBM RS/6000 43P - 260.

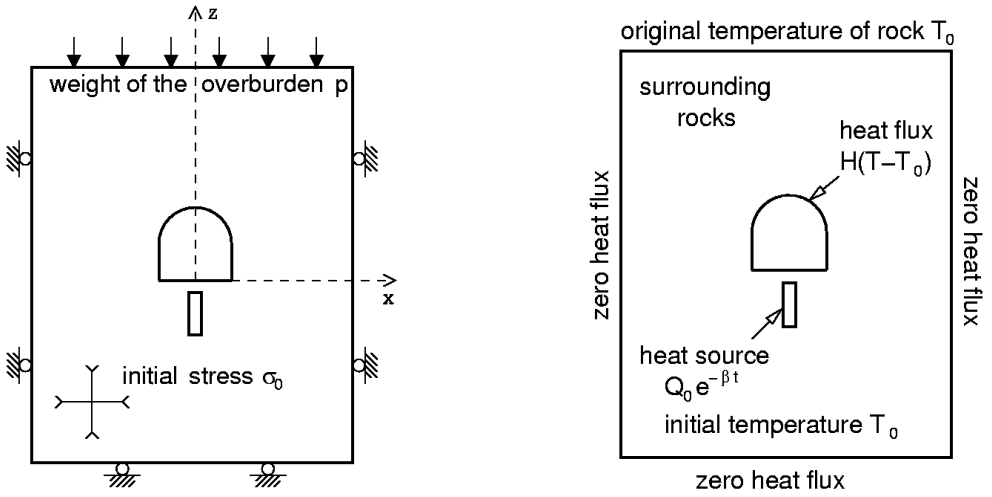

Fig. 1: *The model problem BMT3.*

a) Preconditioning

We solve the system of the equation (22) using the preconditioned CG method in each time step. The system matrix is composed from two matrices, the matrix M_h which is not an M-matrix, and the matrix $\Delta_j A_h$. For small values of Δ_j the matrix $M_h + \Delta_j A_h$ is not an M-matrix, so we cannot use the incomplete factorization for preconditioning. But it is possible to apply the incomplete factorization of matrix $M_h^L + \Delta_j A_h$, where M_h^L is the lumped matrix to the matrix M_h, which means that its diagonal has diagonal elements equal to the sum of the elements on the corresponding row. For small values of Δ_j giving approximately the same order of elements in matrices M_h and $\Delta_j A_h$ the tests show that it is better to use the matrix $0.5M_h^L$ instead of the matrix M_h^L. Table 1 shows the number of iterations for various types of preconditioning and for various values of the time step Δ_j. The number of iterations represents the sum of CG iterations for ten time steps; the system is solved with the accuracy 10^{-6}.

Note that in our test problem the elements of both matrices are approximately of the same order for $\Delta t = 0.001$. We can also see that the condition number decreases with the decrease of Δt.

Δt	$M_h + \Delta t A_h$	$M_h^L + \Delta t A_h$	$0.5M_h^L + \Delta t A_h$	$diag(M_h + \Delta t A_h)$
1.0	318	318	323	1593
0.1	145	145	154	822
0.01	87	94	83	405
0.001	72	76	55	189
0.0001	nonconv.	64	49	122

Tab. 1: *The number of iterations for various types of preconditioning.*

b) Initial approximation
The adaptive time stepping evokes that the temperature increments in successive time increments differ only little. Because the temperature increments reach the value of several degrees in our problems, the use of the temperature increment from the previous time step as the initial approximation seems to be better than the use of the zero initial approximation. For the total time 10 years (63 time steps) and the accuracy 10^{-6} for the solution of linear systems we needed 1127 iterations for the zero initial approximation, and 966 iterations if the solution from the previous time increment had been used.

c) The influence of the accuracy of the solution of the system
The accuracy $0.01 - 0.0001$ for the solution of the system (22) gives practically the same solution vector, the solution vector for the accuracy 0.1 differs a little, the difference is 0.5% (in l_∞ norm).

d) The frequency of the adaptive modification
We tested the adaptive changing of the time step after 2 or 5 time steps. The difference between the corresponding solution vectors is about 0.2%.

e) The criteria for adaptive changing of time steps
We used the criteria presented in Section 2 and tested 3 various intervals $\langle \varepsilon_{\min}, \varepsilon_{\max} \rangle$, namely $\langle 0.01, 0.001 \rangle$, $\langle 0.001, 0.0001 \rangle$, and $\langle 0.0001, 0.00001 \rangle$. The difference among the solution vectors is less than 2%.

f) CPU time and the numbers of iterations
We denote the various approaches to the solution by 3 characters abc, where

a=1 => accuracy for the solution of linear system is $\varepsilon = 0.0001$
a=2 => accuracy for the solution of linear system is $\varepsilon = 0.001$
a=3 => accuracy for the solution of linear system is $\varepsilon = 0.01$
a=4 => accuracy for the solution of linear system is $\varepsilon = 0.1$

b=1 => the adaptive changing of the time step after 5 iterations
b=2 => the adaptive changing of the time step after 2 iterations

c=1 => the interval for the adaptive changing is $\langle 0.01, 0.001 \rangle$
c=2 => the interval for the adaptive changing is $\langle 0.001, 0.0001 \rangle$
c=3 => the interval for the adaptive changing is $\langle 0.0001, 0.00001 \rangle$

We solved the problem for the global time 100 years. The results are presented in Table 2. The first column presents the type of the computation, the second the number of the time steps, the third the global number of CG iterations, the fourth the global CPU time, the last column presents the length of the time step in the last time step.

1	2	3	4	5
111	43	956	498s	13.11
211	43	722	458s	13.11
311	43	472	414s	13.11
411	54	291	436s	6.55
121	37	924	463s	13.11
221	37	702	425s	13.11
321	37	465	382s	13.11
421	57	301	452s	3.28
112	121	1714	1046s	3.28
212	121	1187	953s	3.28
312	121	765	879s	3.28
412	195	346	1202s	1.64
122	102	1597	936s	3.28
222	102	1135	855s	3.28
322	106	757	812s	3.28
422	170	341	1075s	1.64
113	320	2720	2310s	1.64
213	321	1855	2167s	1.64
313	370	1092	2291s	0.82
413	825	528	4683s	0.41
123	307	2676	2252s	1.63
223	307	1821	2102s	1.63
323	357	1088	2241s	0.82
423	786	507	4520s	0.41

Tab. 2: *The number of iterations and CPU times for various types of computing.*

5. Conclusion

In the paper, the solution of the thermoelasticity problem is described. The numerical tests were done using the sequential code. At present we work on a new version of code for parallel computations.

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