Abstract: The analysis of stability and safety of underground repositories of the spent nuclear fuel requires the use of mathematical modelling of coupled T-H-M phenomena. The realization of reliable numerical simulations is a difficult task from many points of view including the aspect of high computational requirements concentrated mainly in the necessity of a repeated solution of large linear systems.

In our contribution, we address this aspect and describe numerical methods based on the use of efficient iterative solvers, which exploit the conjugate gradient (CG) method, its generalization and the space decomposition preconditioners. The efficiency of these solvers will be illustrated by the solution of elasticity and thermo-elasticity problems arising from the finite element analysis of selected benchmarks with computations performed on a PC cluster. The introduced ideas could be useful also for the solution of more complicated coupled problems.

1. INTRODUCTION

The solution of many geotechnical problems requires the use of mathematical modelling for understanding of natural and induced phenomena in the geological environment. This is the case of thermal, hydrological, mechanical (T-H-M) and other phenomena induced by mining, building of underground constructions, deep geological deposition of the spent nuclear fuel and other geotechnical activities. In some cases, the T-H-M phenomena can be investigated separately, neglecting their interactions. In other cases, more accurate coupled analysis is required. Such coupled analysis was shown to be important for the investigation of deep geological repositories of the nuclear waste, see Stephansson (1996, 2001).

The mathematical modelling of the T-H-M phenomena uses initial – boundary value problems for differential or variational equations involving the physical principles. We shall assume that these problems are discretized by the finite element or similar methods. What we want to point out is that the numerical solution can be computationally very expensive due to

- solution of problems in large 3D domains,
- requirements for an accurate analysis in some parts of the computational domains,
- possibly large time-scale of the investigated phenomena,
- complexity of the material behaviour and requirements of the coupled analysis.

The large computational demands indicate that a special care must be given to searching for accurate, robust and efficient numerical methods, which are capable to exploit the power of high-performance (parallel) computers.

In this paper, we shall touch the development of such numerical methods intended for the solution of the coupled evolution problems as e.g. thermo-elasticity, which is described in Section 2. Here we also discuss the discretization of the evolution problems. As the computational demands are concentrated mainly in the solution of the arising linear systems, we shall focus on the application of suitable, efficient and parallelizable iterative solvers for these linear systems. Section 3 deals with some general techniques enhancing the efficiency of the iterative solution of discrete evolution problems. Section 4 is devoted to a short discussion of the numerical results. In Section 5, we shall describe solvers, which exploit the domain decomposition and parallel computations. Here we also mention another division techniques as displacement decomposition or composite grid methods.

The performance of the introduced numerical methods will be illustrated by solving a simple 2D model extracted from the DECOVALEX project and large-scale real-life 3D model arising from a computation of stress changes induced by uranium ore mining. In a near future, we would like to test the introduced methods also by solving 3D thermo-elasticity problems relevant to the assessment of underground repositories of the spent nuclear fuel.
2. THERMO-ELASTICITY

In this section, we describe problems of thermoelasticity and focus on their robust numerical solution. The considered problems are important for the investigation of nuclear waste repositories, as is illustrated by the simple model problem shown in Figure 1.

This problem represents a 2D cut through a repository tunnel located at the depth of 500 m. The nuclear waste, which is the source of the heat, is disposed in a borehole below the tunnel. We are interested in the temperature and stress changes in the near field. This model problem, which arose by simplification of the BMT3 benchmark formulated in the DECOVALEX project, see Jing et al. (1994), will be used for an illustration of the behaviour of some of the numerical methods presented later. For this, we shall use the discretization by linear triangular finite elements, see Figure 2.

![Figure 1. The model problem BMT3.](image)

The thermo-elasticity problem is to find the temperature \( \tau \) and displacement \( u \),

\[
\tau : \Omega \times (0,T) \rightarrow R, \quad u : \Omega \times (0,T) \rightarrow R^d (d = 2,3),
\]

which fulfil the following equations

\[
\begin{align*}
\kappa \rho \frac{\partial \tau}{\partial t} - \sum_j \frac{\partial}{\partial x_j} \left( k_{ij} \frac{\partial \tau}{\partial x_i} \right) &= q \quad \text{in} \ \Omega \times (0,T), \\
- \sum_j \frac{\partial \sigma_{ij}}{\partial x_j} &= f_i \quad \text{in} \ \Omega \times (0,T),
\end{align*}
\]

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

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

together with the initial and boundary conditions.

Above, \( \Omega \subset R^d \) represents the considered domain, \( (0,T) \) is the time interval, \( q \) is the density of the heat source, \( f \) is the density of the volume forces, \( \kappa \) is the specific heat, \( \rho \) is the density of material, \( k_{ij} \) are coefficients of the heat conductivity, \( c_{ijkl} \) are the elastic moduli and \( \alpha_{ij} \) are the coefficients of the heat expansion.

![Figure 2. The FE mesh and time step sizes determined by the adaptive algorithm.](image)

The initial-boundary value problem of thermoelasticity can be discretized by the finite elements in space and the finite differences in time. Using the linear finite elements and the simplest time discretization, we come to the computation of vectors \( \tau^j, u^j \) of nodal temperatures and displacements at the time levels \( t_j, j = 1,\ldots,N \), with the time steps \( \Delta t_j = t_j - t_{j-1} \). This leads to the following algorithm:

\[
\text{find} \quad \tau^0 : M_h \tau^0 = \tau_0, \quad u^0 : A_h u^0 = b^0 = b_h(\tau^0),
\]

for \( j = 1,\ldots,N : \)

\[
\begin{align*}
\text{find} \quad \tau^j : \quad &B_h^{(j)} \tau^j = [M_h + \theta \Delta t_j K_h] \tau^j = c^j, \\
\text{find} \quad u^j : \quad &A_h u^j = b^j.
\end{align*}
\]

Above, \( M_h \) is the capacitance matrix, \( K_h \) is the conductivity matrix, \( A_h \) is the stiffness matrix, \( \theta \in (0,1) \) is a parameter,

\[
c^j = [M_h - (1-\theta)\Delta t_j K_h] \tau^{j-1} + \theta q_h^{j-1} + (1-\theta) q_h^{j-1},
\]

\[
b^j = b_h(\tau^j) \quad \text{and} \quad \tau_0 \quad \text{is from the initial condition.}
\]
Note that \( q_h \) represents the heat sources and \( b_h \) represents volume and surface forces including the thermal expansion term.

We aim at the development of fully robust, stable methods and therefore we restrict our attention to implicit methods with \( \theta \in \{ \frac{1}{2}, 1 \} \). Particularly, we shall consider two cases with \( \theta = \frac{1}{2} \) and \( \theta = 1 \), which correspond to the Crank–Nicolson (CN) and backward Euler (BE) method, respectively. More details can be found e.g. in Quarteroni & Valli (1994). Finally, we chose the BE method for its higher stability (the CN scheme can show some local oscillations for large time steps).

The use of the BE method allows also to use adaptive time stepping scheme based on a local comparison of the BE and CN steps. To make this comparison computationally cheap, we shall use only the residual corresponding to the substitution of the BE time step \( \tau^j \) into the CN equation,

\[
\left( M_h + 0.5 \Delta t_j K_h \right) \tau^j = \left( M_h - 0.5 \Delta t_j K_h \right) \tau^{j-1} - 0.5 q_h^j - 0.5 q_h^{j-1}. 
\]

Then the CN step can be approximated by the value \( \tau_{CN}^j = \tau^j - r^j \) and the time steps can be controlled with the aid of the ratio \( \eta = \| r^j \| / \| \tau^j \| \) according to the following algorithm (\( k \) counts time step adaptation cycles):

\[ \text{for } k=1,2,... \text{ until stop do } \]

- compute \( \tau^{j,k}, r^{j,k} \) and evaluate \( \eta_k \),
- if \( \eta_k < \epsilon_{\text{min}} \) then \( \Delta t_j \leftarrow 2 \star \Delta t_j \),
- if \( \eta_k > \epsilon_{\text{max}} \) then \( \Delta t_j \leftarrow \Delta t_j / 2 \),
- if \( \eta_k \in (\epsilon_{\text{min}}, \epsilon_{\text{max}}) \) and \( \eta_k < \epsilon_{\text{min}} \) then \( \Delta t_{j+1} = \Delta t_j / 2 \), \( \tau^{j,k} = \tau^{j,k-1} \), stop,
- if \( \eta_k > \epsilon_{\text{max}} \) and \( \eta_{k-1} < \epsilon_{\text{min}} \) then \( \Delta t_{j+1} = \Delta t_j / 2 \), \( \tau^{j,k} = \tau^{j,k-1} \), stop,

\[ \text{end} \]

As a change in the step-size induces the change of the matrix \( B^{(j)}_h \), it may be advantageous to do the step-size adaptation only in each \( k \)-th time step. In Figure 2 (right), we can see the step size adaptation in each time step (solid line) and each 10\(^{10} \) time step (dashed line) for parameters \( \epsilon_{\text{min}}, \epsilon_{\text{max}} \) equal to \( 10^{-3}, 10^{-2} \), respectively.

### 3. THE USE OF ITERATIVE SOLVERS

The computational requirements of the time stepping algorithm are concentrated in the solution of linear systems with the matrices \( B^{(j)}_h \) and \( A_h \).

For large-scale and accurate models, the dimension of these matrices will be very large. Therefore, it will be advantageous to solve them iteratively.

Then we have to answer the following questions

- which iterative method is suitable to use,
- what is the right accuracy of the iterations,
- what are suitable initial guesses for the solution of systems arising in the time steps.

As the matrices \( B^{(j)}_h \) and \( A_h \) are symmetric and positive definite in our case, it seems that a good choice of the solution technique is the conjugate gradient (CG) method with a suitable preconditioning. This question will be further discussed in the next section.

The accuracy of solving the systems with matrices \( B^{(j)}_h \) should be in correspondence with the accuracy of the time stepping scheme. We performed numerical tests with the adaptively controlled time stepping schemes \( \epsilon_{\text{min}}, \epsilon_{\text{max}} \) equal to \( 10^{-3}, 10^{-2} \) or \( 10^{-4}, 10^{-3} \). These tests show that the accuracy of computed results is not deteriorated when we use a lower accuracy \( \epsilon = 0.01 \) for stopping the iterations,

\[ \| c^j - B^{(j)}_h \tau^j \| \leq \epsilon \| c^j \|. \]

Surprisingly, even \( \epsilon = 0.1 \) works still well with the less accurate adaptive scheme. The adaptive scheme only somewhat increased the number of time steps in this case. But with the more accurate adaptive scheme such low accuracy of iterations caused infinite cycling.

The efficiency of the iterative solution can be also increased by using a suitable initial guesses. There are several possibilities:

(i) using the previous time step (PS) values \( \tau^{j-1}, u^{j-1} \) as initial guesses for \( \tau^{j+1}, u^{j+1} \),
(ii) using the initial guesses given by the linear extrapolation (LE), i.e. for $\Delta t_j = \Delta t_{j-1}$, we get $\tau^{j+1} = 2\tau^j - \tau^{j-1}$, $u^{j+1} = 2u^j - u^{j-1}$, 
(iii) improvement of the initial guesses by exploiting the conjugate directions (CD) from application of the CG method to the solution of the systems in some previous time step.

In the CD technique, we assume that $B_h^{j(k)} = B_h$ does not change in a selected sequence of time steps $j = j_0, \ldots, j_1$. Then the conjugate directions $\{v_i\}, i = 1, \ldots, m$ from solving the system in the step $j_0$ can be used for improving the initial guesses in the subsequent steps where we take

$$\tau^{j,0} = \tau_{ini} + \sum_{i=1}^m \eta_i v_i, \quad \eta_i = \frac{\langle r_{ini}, v_i \rangle}{\langle Av_i, v_i \rangle}.$$

Here $\langle, \rangle$ denotes the inner product and $\langle Av_i, v_i \rangle$ are known from the previous application of the CG method. Then computation of $\tau^{j,0}$ requires only computation of the residual $r_{ini} = c^j - B_h \tau_{ini}$ and $m$ inner products $\langle r_{ini}, v_i \rangle$. The same technique is applicable also for solving elasticity systems.

Let us focus again on the systems $B_h \tau = c^j$. The slow change of the right hand sides (RHS) $c^j$ with changing $j$ motivates introduction of another technique, which consists in the gradual construction of an orthonormal basis for the representation or approximation of the next RHS vectors. This technique requires the solution of the system with the matrix $B_h$ only in the case that the existing basis is not sufficient for the representation of the next RHS. In this case, the base is extended.

To be more specific, let us consider the $j$-th time step. Let $\{e_k\}$, $k \in K_j$, be the existing basis and let $\theta_k$ be (approximate) solutions of the systems $B_h \theta_k = e_k$. Then $c^j$ can be represented as

$$c^j = \sum_{k \in K_j} \lambda_k e_k + \nu e_\perp,$$

where $e_\perp$ is orthogonal to all $e_k, k \in K_j, \|e_\perp\| = 1$, $\lambda_k = \langle c^j, e_k \rangle$.

If $|\nu| \leq \varepsilon \|c^j\|$ then we take the solution $\tau^j$ as

$$\tau^j = \sum_{k \in K_j} \lambda_k \theta_k,$$

otherwise we solve the system $B_h \theta_\perp = e_\perp$ and take

$$\tau^j = \sum_{k \in K_j} \lambda_k \theta_k + \nu \theta_\perp.$$

If some of $\lambda_k$ is small (typically $\lambda_k \leq \varepsilon/10$), then the new pair $e_j = e_\perp, \theta_j = \theta_\perp$ can replace $e_k, \lambda_k$. Otherwise the new pair extends the existing base. Due to the rounding errors, $e_j$ should be reorthogonalized to the previous basis vectors $e_k$.

Note that this technique, which can be denoted as the combination of the previous solutions (CPS), does not need the symmetry of $B_h$ and is applicable also to the elasticity systems.

The efficiency of the described ideas is illustrated by the solution of the benchmark problem BMT3. The results are summarized in Table 1. The systems are reformulated in unknown increments of temperatures and displacements.

<table>
<thead>
<tr>
<th>Initial $\tau$: $\Delta t_j = 0.25$</th>
<th>$u$: $\Delta t_j = 0.25$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>gues:</strong></td>
<td></td>
</tr>
<tr>
<td>$\varepsilon = 10^{-2}$</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>$\varepsilon = 10^{-2}$</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td><strong>Zero</strong></td>
<td></td>
</tr>
<tr>
<td>2420</td>
<td>3632</td>
</tr>
<tr>
<td>3632</td>
<td>8362</td>
</tr>
<tr>
<td>8362</td>
<td>11159</td>
</tr>
<tr>
<td><strong>PS</strong></td>
<td></td>
</tr>
<tr>
<td>590</td>
<td>1457</td>
</tr>
<tr>
<td>1457</td>
<td>810</td>
</tr>
<tr>
<td>810</td>
<td>4526</td>
</tr>
<tr>
<td><strong>PS + CD</strong></td>
<td></td>
</tr>
<tr>
<td>399</td>
<td>899.10</td>
</tr>
<tr>
<td>899.10</td>
<td>210.22</td>
</tr>
<tr>
<td>210.22</td>
<td>1126.30</td>
</tr>
<tr>
<td><strong>LE</strong></td>
<td></td>
</tr>
<tr>
<td>689</td>
<td>697</td>
</tr>
<tr>
<td>697</td>
<td>501</td>
</tr>
<tr>
<td>501</td>
<td>840</td>
</tr>
<tr>
<td><strong>LE + CD</strong></td>
<td></td>
</tr>
<tr>
<td>423.8</td>
<td>459.10</td>
</tr>
<tr>
<td>459.10</td>
<td>207.22</td>
</tr>
<tr>
<td>207.22</td>
<td>311.30</td>
</tr>
<tr>
<td><strong>CPS</strong></td>
<td></td>
</tr>
<tr>
<td>101.18</td>
<td>181.21</td>
</tr>
<tr>
<td>181.21</td>
<td>199.9</td>
</tr>
<tr>
<td>199.9</td>
<td>351.12</td>
</tr>
</tbody>
</table>

In the above table, $\varepsilon$ denotes the relative accuracy of the iterative solution or the parameter in the CPS technique. The LE helps in the case of smooth results, which are not the case in column 2 due to a low accuracy $\varepsilon$. To emphasize the effect of the initial guess, we present here the results for constant $\Delta t_j = 0.25$ but the described ideas are useful also for some adaptive schemes.
4. BMT3 RESULTS

We use the BMT3 benchmark for an illustration of the efficiency of the described ideas concerning the acceleration of the iterative solution. As concerns the computed results, the temperature field is in a good agreement with the results reported by Jing et al (1994), see also Fig.3. The comparison of computed stresses and displacement is more complicated, because the original BMT3 assumed fractured rocks, which require to use homogenized properties. There is also a bigger variance in the corresponding results presented in Jing et al (1994).

The BMT3 problem was solved by means of a simple code implemented in MATLAB. In near future, the described ideas will be also implemented and tested within a scientific FEM system GEM (Institute of Geonics AS CR). This system aims at the solution of large 3D problems, for which the iterative solvers are crucial. In the next section, we try to give an idea about the expected efficiency of a large 3D modelling with parallel computations.

5. SPACE DECOMPOSITION SOLVERS AND LARGE 3D MODELLING

In Section 3, we discussed an acceleration of iterative solvers, now we shall touch the question of the choice of a suitable iterative methods and show that efficient methods can be found in the class of space decomposition - subspace correction methods, see Blaheta et. al. (2003). Remember that we are interested in the solution of linear systems with symmetric positive definite matrices $B_k$ and $A_k$ for finding the unknown temperature and displacement increments, respectively.

The well-known domain decomposition (DD) methods, see e.g. Chan & Mathew (1994), use data partition induced by a decomposition of the computational domain. This decomposition can be used for two purposes: Firstly for parallel implementation of vector updates, inner products and matrix-vector multiplication, i.e. for parallel implementation of the CG method. Secondly, for a construction of efficient preconditioners.

The preconditioner $C$ is an approximation of the FEM matrix $A$, which can be used for computations of pseudoresiduals $g=C^{-1}r$ and search directions, which are closer to errors $e=A^{-1}r$. Of course, the operation $C^{-1}r$ should be sufficiently computationally cheap. The basic preconditioner induced by a domain decomposition is the block diagonal one and its efficiency can be increased by extending the blocks or correspondingly extending the subdomains into overlapping ones, see Figure 4 (right). But even more important is to enable a global exchange of information by adding a small (coarse) but global subproblem. This defines so-called two-level preconditioner. The global subproblem can be created by discretization of the solved problem on a coarser grid or e.g. by the use of a simpler construction with aggregation of unknowns, see Blaheta et. al. (2003a, 2003b). The subproblems can be solved exactly by a direct method or approximately by inner iterations with accuracy $\varepsilon_0$. The latter approach can be more efficient and correctly used within a generalized CG method, see Blaheta (2002).
elasticity problem represents the computation of stresses induced by mining at the uranium ore deposit Rožná (DR) in the Czech Republic, for more details see Blaheta et al. (2002a, 2002b).

Figure 5. The FE mesh for the benchmark DR, about 4 million DOF.

The computations were done in parallel on a cheap Beowulf cluster consisting of 8 PCs with the processors AMD Athlon 1.4 GHz, 768 MB RAM. The PCs are interconnected by Fast Ethernet LAN. The results in Table 2 correspond to computations on 3 and 8 PC’s from the cluster.

Table 2. Solving the problem DR on a PC cluster.

<table>
<thead>
<tr>
<th>method</th>
<th># proc’s</th>
<th># iter’s</th>
<th>time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG-DD-one-level</td>
<td>3</td>
<td>102</td>
<td>283</td>
</tr>
<tr>
<td>CG-DD-two-level</td>
<td>3</td>
<td>56</td>
<td>242</td>
</tr>
<tr>
<td>CG-DD-one-level</td>
<td>8</td>
<td>128</td>
<td>161</td>
</tr>
<tr>
<td>CG-DD-two-level</td>
<td>8</td>
<td>72</td>
<td>111</td>
</tr>
</tbody>
</table>

Note that similar methods can be applied also to the solution of systems arising from the time-dependent heat conduction – convection problems. There are also other space decomposition methods. Let us mention the displacement decomposition technique for solving the elasticity problems and composite grid technique, for solving problems, which need a local resolution. More details can be found in Blaheta (2002) and Blaheta et al. (2002b).

6. FINAL REMARKS

The aim of this paper was to show numerical techniques suitable for efficient modelling of large-scale coupled problems, which are typical for the assessment of repositories of the spent nuclear fuel. The use of iterative solvers and parallel computing is the essential part of these methods.

Note that the efficiency of the considered numerical methods is important not only for solving large-scale and complicated coupled problems but also for performing a further analysis of the obtained results for the assessment of sensitivity to changes of input parameters, influence of uncertainty in the model data, etc.

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