Modelling of THM processes in rocks [Geonics 2007]

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Abstrakt

Článek se zabývá matematickým modelováním teplotních (T), hydraulických (H) a mechanických (M) procesů v horninách, které jsou významné pro posouzení různých geotechnických projektů, specielně podzemních úložišť jaderného odpadu. V článku je naznačena problematika analýzy oddělených i sdružených THM problémů a diskutována možnost použití paralelních výpočtů metodou rozdělení oblasti Schwarzova typu. Efektivita tohoto přístupu je demonstrována na analýze T-M procesů v případě prototypového úložiště jaderných odpadů, které odpovídá švédské koncepci geologického úložiště KBS3 a je realizováno v podzemní laboratoři Äspö ve Švédsku.

Introduction

This paper is devoted to modelling thermal (T), hydraulic (H) and mechanical (M) processes in rocks. These physical processes seem to be the most important ones for many engineering applications ranging from the classical mining, tunnelling and underground constructions to new geotechnologies of waste disposal or geothermal energy utilization.

In the first plan, the T, H, M processes are investigated separately with the aid of mathematical modelling methods. The mathematical models themselves are not unique, but for each physical phenomenon, it is possible to develop a hierarchy of models including more and more specific features. For example,

- the simplest thermal model is stationary linear heat conduction, which can be developed to include anisotropy, nonlinearity, time evolution, heat convection, etc.
- the simplest hydraulic model is linear Darcy flow in saturated porous media, more sophisticated models allow nonsaturation, nonlinearities, multicomponent flow, etc.
- the simplest mechanical model is linear elasticity, more complex models include different reaction of rocks under different load, irreversible deformations caused by rock damage, etc.

In all cases, we restrict our attention to modelling processes in rocks under the concept of continuous medium. Then T, H, M models are formulated as boundary value problems and solved numerically. Among several possible numerical methods we consider the finite element method for all the considered physical processes.

The second plan of refining the modelling consists in taking in the account the couplings of the physical processes. In this case, we speak about THM processes. The

modelling of coupled THM processes is important for some applications among which belongs investigation of the safety and performance of repositories for the spent nuclear fuel. In this respect, much work has been done within the DECOVALEX project, see e.g. Stephansson (2001), Hudson et al (2001) and (2005).

The computational demands of the separated and coupled THM modelling can be very high so that implementation of complex models in large 3D domains may require use of advanced numerical methods and parallel computer facilities. In this paper, we briefly discuss the parallel solution methods of Schwarz type, more details can be found in Blaheta (2006), Blaheta et al (2006a, 2006b). We also provide an example, which serves us as a benchmark for testing the parallel solution methods, an Äspö prototype repository T-M model.

Separated T, H, M processes

The basic T, H, M models are as follows:

(T) find the temperature $\tau : \Omega \times (0,T) \to R,$ which fulfils the following equations

$$c_s \rho \frac{\partial \tau}{\partial t} - \sum_{ij} \frac{\partial}{\partial x_i}\left(k_{ij} \frac{\partial \tau}{\partial x_j} \right) = Q \quad \text{in } \Omega \times (0,T),$$

where c_s is the specific heat, ρ is the density of material, k_{ij} are coefficients of the heat conductivity, Q is the density of the heat source, in isotropic case, $k_{ij} = k$,

(H) find the hydraulic potential $\phi : \Omega \to R,$ which fulfils the following equations

$$-\sum_{ij} \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial \phi}{\partial x_j} \right) = 0 \quad \text{in } \Omega,$$

where K_{ij} are components of the hydraulic conductivity tensor,

(M) find the displacement $u : \Omega \to R^d \ (d = 2,3),$ which fulfils the equations

$$-\sum_{j} \frac{\partial \sigma_{ij}}{\partial x_j} = f_i \quad \text{in } \Omega,$$

$$\sigma_{ij} = \sum_{kl} c_{ijkl} \varepsilon_{kl}(u), \quad \varepsilon_{kl}(u) = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad \text{in } \Omega,$$

where f is the density of the volume (gravitational) forces, c_{ijkl} are the elastic moduli.

All T, H, M models require proper definition of the domain of interest and boundary conditions on its boundary $\partial\Omega$. For evolution problems, we need also to define the initial conditions.

As concerns the finite element (FE) solution of the basic T, H, M models, the most standard is the case of elasticity. It represents an elliptic boundary value problem, which can be solved by introducing proper FE spaces of displacement, which are continuous and piecewise polynomial on elements (triangles, tetrahedral etc.) of a given FE division of the domain of interest. The algebraic formulation leads to the solution of linear system

(**M**) $Au = b$

with the stiffness matrix A, which is sparse, mostly positive definite and typically large and ill conditioned, see e.g. Blaheta et al (2006b, 2007) for more details.

The evolution heat conduction is an example of a parabolic problem. It can be discretized by the FE method under a time stepping scheme. For the basic Euler or Crank-Nicolson schemes, we have to solve the systems

(**T**) $\left(M + \Theta \Delta t B\right)\tau = c,$

in each time step. Here Δt is the time step size, $\Theta \in \{0,1,1/2\}$ is a parameter. The system matrix is now a combination of the capacity M and conductivity B matrices. It is again sparse, positive definite and typically large, see e.g. Blaheta et al (2007).

The basic Darcy flow is again an elliptic problem, but the use of the standard FE method gives an approximate solution, which is not locally conservative. It can be a substantial drawback for modelling unsaturated flow, transport of pollutants etc. A remedy is in the use of the mixed FE method, which provides an approximation for both the piesometric head and fluxes. Algebraically, it leads to a larger system

(**H**) $Z\phi = d,$

where Z is indefinite, but has a natural 2×2 structure, see e.g. Blaheta (2006).

For all algebraic systems (**M**), (**T**), (**H**), it is possible to construct efficient parallel solvers by the overlapping domain decomposition technique. This construction is discussed in a next section.

Coupled THM processes

In some geotechnical applications, it is important to consider also the coupling of different T, H, M processes. Generally, the T, H, M processes are coupled the following mechanisms (YX: X→Y):

- HT thermal changes of viscosity, density, etc.
- MT thermal volume expansion,
- MH pore pressure,
- TH heat convection,
- TM conversion of mechanical energy,
- HM change of porosity and apertures.

T	TH	TM
HT	H	HM
MT	MH	M

T	
MT	M

H	HM
MH	M

Obr. 1. THM procesy: Úplné spojení (vlevo), termo-pružnost (uprostřed), konsolidace (vpravo)
Fig. 1. THM processes: Full coupling (left), thermo-elasticity (center), consolidation (right)

Depending on the considered situation, some of the coupling mechanisms can be neglected. In the field of assessment of safety and performance of underground nuclear waste repositories, an extensive research on importance of modelling coupled THM processes has been done within the DECOVALEX project, see e.g. Hudson et al (2002, 2005). One of the conclusions discussed here is the change of importance of different

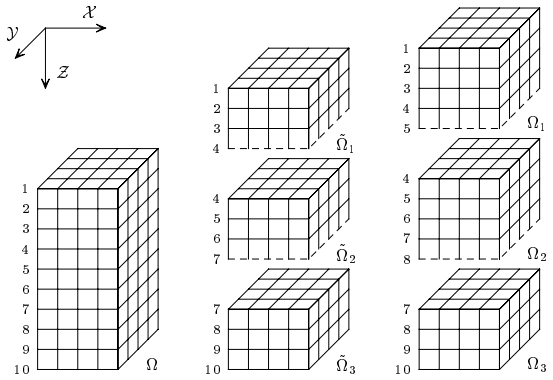
processes and couplings in different stages of the repository life: excavation, operation, post-closure.

Practically, we usually select only some subset of the full coupling scheme. Two such subsets are shown in Fig. 1, thermo-elasticity and consolidation. The first case is one side coupled, which allows a decomposition of the coupled problem – it is possible to solve the thermal problem first and then to add the thermal expansion term into elasticity equation. This decomposition can be also used for the numerical solution.

The second case, consolidation, is two-side coupled, which makes the problem and its solution more difficult. Nevertheless, a lot of results can be found in both theory and numerical analysis of this problem. From the algebraic point of view, the FE system corresponding to the coupled problem can be used by a direct or iterative solver or block relaxation type iterations, which decompose the processes.

FE analysis and parallel computations

The computational demands of FE analysis of T, H, M processes may require the use of high performance parallel computer systems (clusters, symmetric multiprocessors - SMP) and appropriate numerical methods.



Obr. 2. Rozklad oblasti: bez překrytí a s překrytím
Fig. 2. Domain decomposition: non-overlapping and overlapping

The FE method generally requires the following numerical procedures:

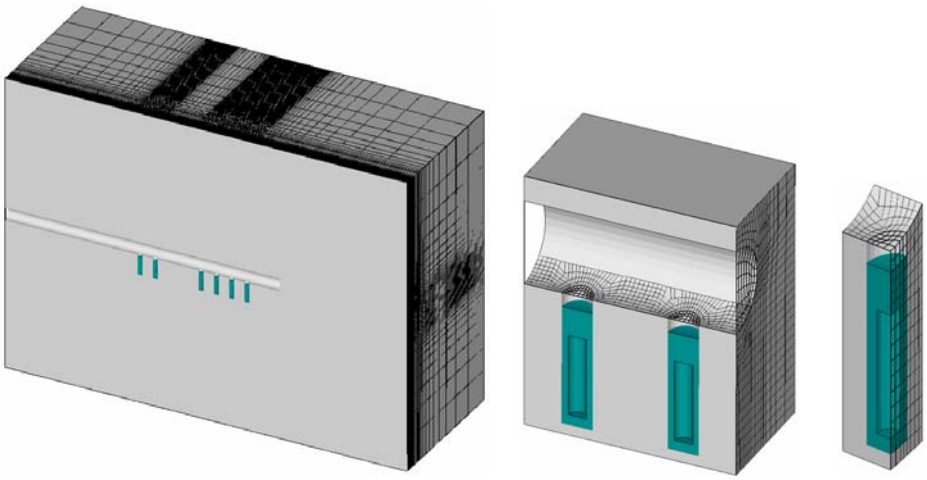
(1) assembling of matrices and vectors,
(2) solving linear systems,
(3) computation of output data.

The procedures (1) and (3) involve local (element by element) computations and therefore are easily parallelizable. The solution of linear system can be approximated by means of iterative methods, which again involve easily parallelizable components (matrix-vector multiplication, scalar products and vector updates). It is e.g. the conjugate gradient (CG) method for (**M**) and (**T**) systems or the MINRES method for (**H**) system. But the efficiency of these methods should be enhanced by a suitable preconditioning.

The domain decomposition (DD) is a common approach for decomposition and parallelization of the basic matrix and vector operations as well as for construction of preconditioners. We investigated construction of preconditioners based on overlapping DD, see Fig.2. For (**M**) such Schwarz type preconditioner constructed from local

approximate solvers on subdomains requires to add a coarser problem, possibly constructed algebraically, see e.g. Blaheta et al (2006). For (**T**) systems Schwarz preconditioner is efficient even without a coarse problem, see e.g. Blaheta et al (2007). For (**H**) system the construction of Schwarz preconditioner is not unique and less straightforward. A promising approach is described in Blaheta (2006).

For illustration, we shall solve a benchmark problem – solution of a 3D Äspö model see Figure 3 and Blaheta et al (2005). The thermo-elasticity problem is discretized by linear tetrahedral FE with 15 088 320 tetrahedra, 2 586 465 DOF for heat transfer and 7 759 395 DOF for elasticity computations. The TM problem is solved by the in-house GEM-FEM software on a SunFire 15000 SMP computer installed at Uppsala University in 2001. The efficiency of parallel computations using MPI and OpenMP programming paradigma can be seen in Fig. 4.



Obr. 3. Konečněprvková síť pro Äspö model
Fig. 3. Finite element mesh for the Äspö model

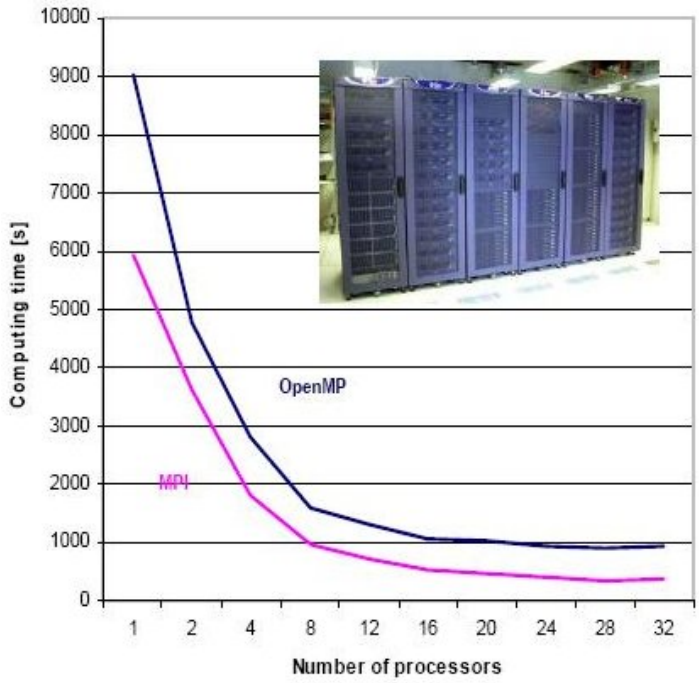
Conclusions

The paper outlines numerical parallel solution methods applicable to modelling of both separated and coupled THM processes in rocks. More details can be found in references Blaheta (2006) and Blaheta et al (2006a, 2006b, 2007).

The THM processes can be further coupled with transport of chemical species and modelling chemical reactions, see Hudson (2005).

The selection of the proper model, formulation of the boundary value problem and obtaining the input data involve degrees of uncertainty. The whole output should be therefore calibrated and validated. The uncertainty in input data and its influence to the outputs create a specific subproblem of a particular importance as the geological continuous media are very heterogeneous and therefore it is necessary to work with averaged effective input data strongly influenced by uncertainty. The analysis of such uncertainty is possible by several concepts of input-output mapping, from deterministic, through interval (worst scenario), fuzzy to stochastic concepts. This uncertainty analysis further strengthens the need of high performance computing methods.

Acknowledgement The work is supported by the Academy of Sciences of the Czech Rep. projects AV0Z30860518 and 1ET400300415 and Uppsala Univ. UPPMAX project p2004009.



Obr. 4. Výpočetní čas vs. počet procesorů pro úlohu vývoje tepla v období 100 let
Fig. 4. Comuting time vs. number of processors for the heat evolution in period 100 years.

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