Modelling THM Processes in Rocks with the Aid of Parallel Computing

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ABSTRACT: *In this paper, we show the use of parallel computing in the finite element analysis of thermo-hydro-mechanical problems. Our approach is based on iterative solvers, partitioning of vectors and use of Schwarz type overlapping domain decomposition preconditioners. This technique is applied to standard, time-stepping and mixed finite element analysis, respectively.*

KEY WORDS: *thermo-hydro mechanical processes in rocks, finite element analysis, domain decomposition methods, parallel computing*

1. Introduction

For many nowadays geotechnical project, it is required to analyse thermo-hydro-mechanical (T-H-M) processes in rocks. An illustrative example is the performance and safety assessment of projects for deep underground deposition of the spent nuclear fuel, for which the analysis of T-H-M processes in the host rocks is crucial, cf. (Blaheta et al. 2005, 2007), (Hudson et al. 2005).

Numerical modelling of such processes is mostly based on the finite element method and requires considerable computational effort. The use of special numerical method and parallel computing then create a basis for a possible solution of complex multiphysics and nonlinear problems, modelling of multiscale problems given by high heterogeneity of geomaterials and the size of considered domains, analysing of uncertainty, use of back analysis etc.

In this paper, we do not consider the problems in full complexity described above. Instead of this, we select here representative model problems

- elasticity as simplest mechanical problem (M),
- time dependent heat conduction as thermal problem (T),
- saturated Darcy flow as hydraulic problem (H).

Then, from the point of view of the finite element method, we consider

- standard (primal) finite element formulation for the elasticity case,
- time-stepping scheme for heat conduction,
- mixed finite element formulation for the Darcy flow.

Finally, we describe the use of overlapping domain decomposition technique for enabling parallel computations in the finite element analysis. We shall point out some differences for application to stationary and time–dependent problems and to the mixed finite element schemes. The behaviour of the methods is illustrated by solving selected model problems.

2. THM processes and their finite element analysis

First, we consider a mechanical response of a part Ω of the rock mass. The elastic deformation process is described by the following equations

$$div(\sigma(x)) + F(x) = 0 \ \text{ for all } \ x \in \Omega\,, \tag{1}$$

$$\sigma = C\varepsilon, \quad \varepsilon = \varepsilon(u) = \frac{1}{2}\left(\nabla u + (\nabla u)^T\right) \ \text{ in } \ \Omega\,, \tag{2}$$

$$u = 0 \ \text{ on } \ \Gamma_u\,, \quad \sigma\, n = f \ \text{ on } \ \Gamma_\sigma\,. \tag{3}$$

Above, $x \in \Omega \subset R^3$, $\sigma(x) \in R^{3\times 3}$ is the Cauchy stress tensor, F is the density of body forces, $C \in R^{3\times 3\times 3\times 3}$ is the elasticity tensor, ε is the small strain tensor, u is the displacement, n is the unit outward normal vector, Γ_u, Γ_σ are disjoint parts of the boundary $\partial\Omega$ of Ω, $\partial\Omega = \Gamma_u \cup \Gamma_\sigma$.

Further, we consider a thermal process governed by the equations

$$c\rho \frac{\partial \tau(x,t)}{\partial t} = div(K_T \nabla \tau(x,t)) + Q(x,t) \quad \text{for all } \ x \in \Omega, \quad t \in [0,T]\,, \tag{4}$$

$$\tau(x,t) = \tau_B(x,t) \quad \text{for all } \ x \in \Gamma_\tau, \, t \in [0,T]\,, \tag{5}$$

$$-K_T \nabla \tau(x,t) = q(x,t) \quad \text{for all } \ x \in \Gamma_q, \ \ t \in [0,T]\,, \tag{6}$$

$$\tau(x,0) = \tau_0(x) \quad \text{for all } x \in \Omega . \tag{7}$$

Above, $x \in \Omega$ is the space variable, $t \in [0,T]$ is the time variable, τ is the temperature, c is heat capacity, $K_T \in R^{3\times 3}$ is the conductivity tensor, Q represents the density of heat sources in Ω, τ_B is the prescribed temperature on Γ_τ, q is the heat flux through Γ_q, τ_0 is the initial temperature in Ω.

Finally, we consider the stationary saturated Darcy flow described as follows

$$-div(v(x)) + G(x) = 0 \quad \text{for all } x \in \Omega , \tag{8}$$

$$v = -K_H \nabla p \quad \text{in } \Omega , \tag{9}$$

$$Lp - v\,n = g \quad \text{on } \Gamma = \partial\Omega \tag{10}$$

Above, v is the Darcy velocity, G is the source/sink term, K_H is the hydraulic conductivity tensor, p is the pressure (total head), L, g are given functions on $\partial\Omega = \Gamma_* \cup \Gamma_0$, $L \neq 0$ on Γ_*, $L = 0$ on Γ_0.

3. Parallel finite element analysis

The elasticity problem (1)-(3) can be discretized by the standard finite element method, which means that we use the variational formulation in terms of the displacements in a finite element space V_h. For simplicity, we restrict here to the linear tetrahedral finite elements. Then we are ready to assembly the linear system

$$Au=b \tag{11}$$

where $A = A_M$ is a symmetric positive definite stiffness matrix, u is the vector of unknowns (nodal displacements) and b is the load vector.

The assembling itself is easily parallelizable. Thus we shall concentrate only on the parallel solution of the linear system (11). It can be solved by both direct and iterative solvers. We prefer the latter one due to several reasons: better efficiency for very large systems, simpler implementation, better parallelizability as well as possible incomplete solution, which can save the effort e.g. in some THM coupling via staggered schemes.

The system (11) can be solved iteratively by the conjugate gradient (CG) method. Then each iteration consists from matrix by vector multiplication, inner products, scalar by vector multiplication and additions of vectors. In the case of vectors

decomposed into blocks and the corresponding decomposition of the matrix, each of the mentioned operations (and therefore also the whole iteration) is easily parallelizable. Note that the decomposition of the vectors can be defined through a decomposition of the computational domain Ω.

The remaining issue is a necessity for accelerating the convergence via a suitable preconditioning, i.e. via an approximation of the inverse A^{-1}. It can be done by using the block diagonal part of A as the preconditioner or by using more efficient Schwarz type preconditioners:

$$\text{one-level } A^{-1} \sim \sum_k R_k^T A_k^{-1} R_k \text{ or two-level } A^{-1} \sim \sum_k R_k^T A_k^{-1} R_k + R_0^T A_0^{-1} R_0 . \quad (12)$$

To define the preconditioner, we first decompose the domain Ω into non-overlapping subdomains Ω_k, which are subsequently extended into overlapping subdomains Ω_k^δ. Then A_k are the finite element matrices, which correspond to the finite element subspaces $V_k = \left\{ v \in V_h : v = 0 \text{ in } \Omega \setminus \Omega_k^\delta \right\}$, R_k define restrictions to the subspaces. For solving (11), the efficiency of one-level method can be improved by two-level Schwarz method using an extended decomposition with an additional subspace $V_0 \subset V_h$ corresponding to a discretization of the solved problem with the aid of a coarser finite element division. The coarse space V_0 can be also constructed from V_h by aggregation, which means that the basis functions of V_h are divided into disjoint groups (aggregates) and sums of the basis functions in the individual groups create the basis of V_0. For more details see (Blaheta et al. 2006, 2007) and the references therein.

For the time dependent heat flow problem, we can use a finite element discretization in space and a finite difference discretization in time. If the latter is done via standard θ method, we get a time stepping scheme

for $k = 1, \ldots, n_T$:

$$\begin{aligned} &\textit{find } \underline{\tau}^{(k)} : A_T \, \underline{\tau}^{(k)} = \left[M_T + \theta \Delta t_k C_T \right] \underline{\tau}^{(k)} = c^{(k)}, \\ &c^{(k)} = \left[M_T - (1-\theta) \Delta t_k C_T \right] \underline{\tau}^{(k-1)} + \theta q_h^{(k)} + (1-\theta) q_h^{(k-1)} . \end{aligned} \quad (13)$$

Above C_T is the conductance matrix, M_T is the capacitance matrix, $\underline{\tau}^{(k)}$ is the vector of nodal temperatures, $\theta \in \langle 0, 1 \rangle$ is a parameter and $q_h^{(k)}$ is the source/sink vector in the k-th time step, Δt_k is the size of the k-th time step.

The linear system (12) can be again solved by the CG method with Schwarz type preconditioning. Unlike to the elasticity case, it is not necessary to use two-level Schwarz methods for reasonable sizes of the time steps, see (Blaheta et al. 2007).

For the Darcy flow problem, we use less standard mixed variational formulation and mixed finite element method. The advantage of this method is twofold – better approximation of fluxes and conservativeness of the discretization. We shall use the following variational formulation – find $v \in V \subset H(div,\Omega)$, $p \in L_2(\Omega)$ such that

$$\int_\Omega K_H^{-1} v \cdot w + \int_{\Gamma_*} L^{-1}(v \cdot n)(w \cdot n) \quad - \quad \int_\Omega p \cdot div(w) = -\int_{\Gamma_*} L^{-1} g (w \cdot n),$$

$$-\int_\Omega \zeta \cdot div(v) = -\int_\Omega G\zeta \quad \text{for all } w \in V_0 \subset H(div,\Omega),\ \zeta \in L_2(\Omega).$$

This variational formulation is a basis for the mixed finite element method. In our paper we consider the lowest order Thomas-Raviart finite elements, which are triangular or tetrahedral finite elements with constant pressure in the element and constant flux along the edges. Mixed formulation leads to 2×2 block system

$$A_H \begin{bmatrix} \underline{v} \\ \underline{p} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \quad A_H = \begin{bmatrix} M_H & B \\ B & 0 \end{bmatrix} \approx \begin{bmatrix} M_H + \eta^{-1} B^T B & 0 \\ 0 & \eta I \end{bmatrix} \tag{14}$$

with the matrix A_H which is symmetric, but indefinite.

This system can be solved e.g. by the MINRES method instead of CG. The parallelization of one iteration remains the same, the preconditioner is again necessary for acceleration of the convergence. The preconditioner can be defined in two steps. First A_H is approximated as shown in (14). Then the first block $M_H + \eta^{-1} B^T B$, corresponding to the differential operator $K_H^{-1} - grad\ div$, is approximated by the Schwarz method. For bigger values of η, it is again not necessary to use the two-level Schwarz method.

The methods and statements from this Section are illustrated by the solution of two model problems.

4. An example of parallel TM computations – Äspö problem

The 3D Äspö prototype repository problem aims at the solution of thermo-elasticity problem, see (Blaheta et al. 2005) for more details and material parameters. It 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 time interval is

selected to be 50 years, the adaptive time stepping begins with the step of 0.0001 year and requires totally 47 time steps. The development of stresses is monitored in selected time levels.

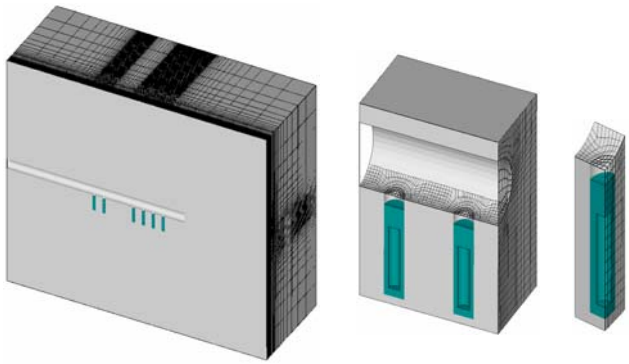

Figure 1. *Finite element mesh for the Äspö model*

#P	#D	#It	Simba - OpenMP		Simba – MPI		Ra – MPI	
			T[s]	**S**	**T[s]**	**S**	**T[s]**	**S**
1	105	1341	9044		5931		1131	
2	54	1423	4782	1.89	3624	1.64	609	1.86
4	29	1426	2818	3.21	1823	3.25	310	3.65
8	16	1514	1594	5.67	967	6.13	176	6.43
12	12	1580	1298	6.97	704	8.42	128	8.84
16	10	1617	1076	8.41	545	10.88	101	11.20
20	9	1689	1022	8.55	484	12.25	92	12.29
24	8	1709	948	9.54	407	14.57	85	13.31

Table 1. Äspö model problem – heat conduction in 50 years. #P – number of processors, #D –size of subdomains, #It – number of iterations, T[s] computing time in seconds, S – parallel speedup

The parallel solution of the arising linear systems uses CG with one level Schwarz preconditioners and approximate implementation of A^{-1} (incomplete factorization). The computations were performed on parallel computers of the UPPMAX centre. The first one is Ngorongoro-Simba with 48 UltraSPARC-III/900 CPU's, the second one is a cluster Ra with 280 AMD Opteron processor cores, see (Komminaho 2007) for more details. Two parallel codes are developed and compared. They differ in using OpenMP and MPI parallel programming paradigma.

Table 1 reports the numbers of iterations and computing times for the whole temperature evolution during 50 years. The parallel speed up is good for the computations on up to 16 processors. Later, the size of subdomains constructed by parallel cutting stagnates. For better speed up on more processors, we should solve larger problems. Code based on OpenMP and MPI are compared in the case of shared memory computer Simba. OpenMP proved to be simpler for code development but MPI proved to be 35-60% faster.

Table 2 shows the result from solving elasticity part of Äspö model problem with two-level Schwarz method with aggressive $6 \times 6 \times 6$ aggregations. Computing time are from code runs on a Beowulf cluster with AMD Athlon 1.4 GHz processors.

	without coarse grid			with aggregations		
#P	#it	CPU	CPU/it	#it	CPU	CPU/it
3	560	4747s	8.46s	208	1836s	8.77s
5	606	2733s	4.5s	201	939s	4.64s
8	651	1798s	2.76s	206	620s	2.99s

Table 2. Äspö model problem – elastic deformation.
One- and two-level Schwarz methods.

5. Mixed finite element modelling of Darcy flow

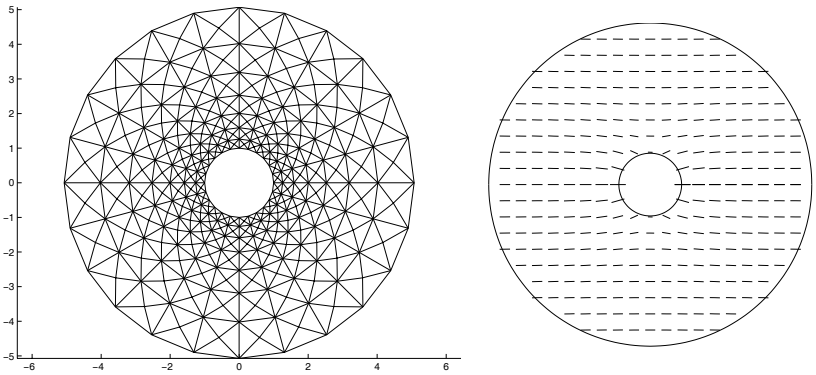

Fig. 2. *The model Darcy flow problem- mesh type (left) and velocities (right).*

We solve only a 2D model problem described as follows

$div(v(x)) = 0$ and $v = -2\nabla p$ for all $x \in \Omega$,

$7p - v \cdot n = 56$ on Γ_{inner} and $-v \cdot n = 2n_1$ on Γ_{outer} if $n = (n_1, n_2)$.

The computational domain is an annulus see Fig. 2, the discretization is done in the style of Fig. 2 with 8 832 nodes, 17 408 triangles and 26 240 sides by a code implemented in MATLAB. The purpose is to demonstrate the efficiency of the MINRES iterations with the described grad-div Schwarz preconditioner, see Table 3. The subdomains are again of an annulus shape, the overlap is given by two-element layer, subproblems are solved exactly. The parallel 3D implementation will be done in a future.

MINRES	no precond.	grad-div precond.	grad-div Schwarz preconditioner		
			2 subdom.	4 subdom.	8 subdom.
$\eta = 1$	2184	66	121	125	121
$\eta = 0.1$	2184	27	48	60	81

Table 1. *Numbers of iterations for the model Darcy flow problem, accuracy* 10^{-6}.

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