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Parallel Computing Methods for Modelling THM Processes in Rocks

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ABSTRACT: The paper concerns numerical modelling of complicated GeoTechnical problems as mine stability, performance of underground radioactive waste repositories or microstructure modelling of geocomposites. The modelling uses finite elements and parallel computing based on overlapping domain decomposition. Important implementation issues for this approach are discussed: inexact solution of subproblems, creation of a global approximation of the problem by aggregation, stabilization of the outer CG type method and programming with the aid of MPI or OpenMP. The domain decomposition technique is also applied to the solution of saddle point systems arising from the use of mixed finite element method (FEM).

1 Introduction

The paper is organized as follows. First, it provides three examples of geotechnical rock engineering problems which require mathematical modelling by usage of efficient numerical methods and powerful parallel computers. These examples give a motivation and exploit numerical methods, which are described in the next section. Finally, numerical results, which illustrate parallel solution of a model thermo-elasticity problem, are described.

The presented paper deals mainly with modelling of thermal and mechanical processes in rocks, which are important for the assessment of many geotechnical projects including deep underground deposition of the spent nuclear fuel. The hydogeological aspect is only shortly mentioned and will be described more deeply elsewhere. Our interest is focused on the finite element analysis of the processes. The application of parallel computing is easy for assembling the finite element matrices or other element-by-element computations and the crucial task is the development of parallel solution methods for arising linear algebraic systems. Here, the use of parallelizable iterative solution methods with parallelizable preconditioning is crucial.

The considered iterative solution approach is based on overlapping domain decomposition and Schwarz-type preconditioning methods, see (Toselli and Widlund, 2005). For elliptic problems, well represented by linear elasticity or stationary heat conduction, we use Schwarz-type methods using both subproblems defined on subdomains and additionally a subproblem representing a coarse discretization of the whole problem. We show that such preconditioning can be efficiently implemented with inexact solution of the subproblems and with coarse discretization, which is constructed algebraically by aggregation. Then the solution method is of a black-box type and can be successfully applied to the solution of many geotechnical problems, see (Blaheta et al., 2006; 2007a).

The evolution heat transfer problems can be solved by time stepping algorithms. In this case, we show that for time steps appearing from standard adaptive time stepping schemes, the Schwarz-type methods are very efficient even without any additional coarse discretization (Blaheta et al., 2007a).

The newest results have been obtained for the systems arising from solving Darcy flow problems by mixed finite elements, which guarantee local conservativeness and good approximation of velocities (Chen et al., 2006). Then the finite element matrices are not further positive definite and application of the Schwarz method is not direct, see (Toselli and Widlund, 2005). From several ways how to overcome this situation, we shall show one technique based on grad-div-Schwarz preconditioner, see (Blaheta, 2006b; Blaheta et al., 2008).

2 Complex GeoTechnical problems

This section provides three examples of geotechnical problems which motivate the use of efficient numerical methods and powerful parallel computers.

2.1 Stability of mine openings

An extensive finite element analysis of stability of mining openings at the uranium mine GEAM Dolní Rožínka was performed in the years 1996-2002, see Fig. 1. The final conclusions of this analysis advocate the use of a new mining technology (underhand stoping) and safety of mining in greater depths 950-1100 meters under the surface. At present, the GEAM mine prolonged its production life and new plans assume mining at depths up to 1200 meters. Therefore a new very large modelling will be performed in a near future.

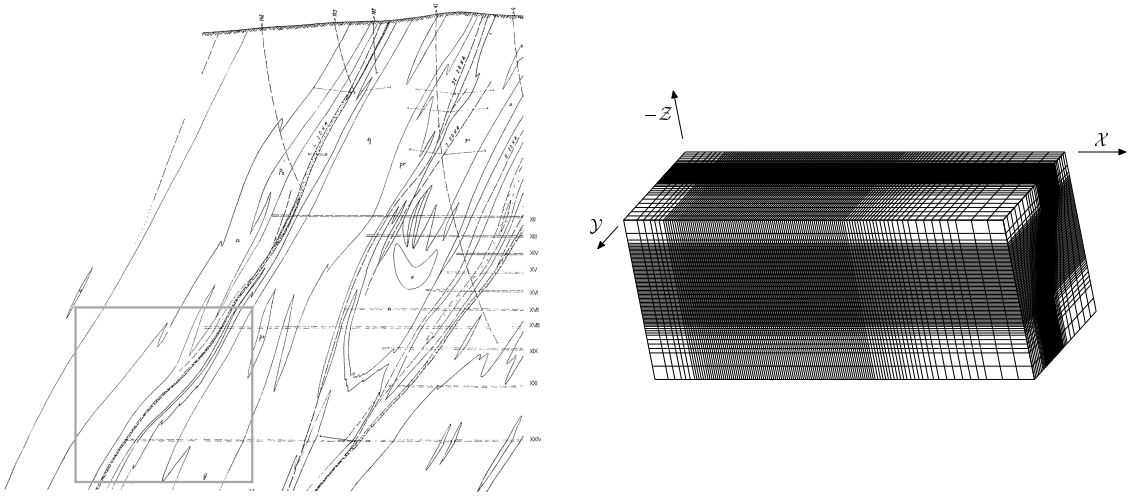

Figure 1. Cross section through Rožná deposit with modelled area left-down and the computational grid.

More details concerning the past finite element modelling for GEAM can be found in (Blaheta et al., 2006). Let us summarize the main features taken into account for the construction of the numerical model:

- the uranium ore is located in several meters thick veins coupled in zones of thickness from 4 to 20 meters, see Fig. 1,
- our domain of interest has dimensions 1430×550×600 metres,
- according to the initial stress measurement by the hydrofracturing method, the mechanical loading is given by horizontally anisotropic initial stress and weight of rocks.

The performed finite element analysis

- uses a basic global discretization with linear triangular finite elements and the grid of 124×137×76 nodes,
- assumes linear elastic behaviour of all materials (ore, surrounding rocks, crushed goaf material) and results in elastic model with almost 4 million DOFs,
- meets with a big difference between the scale of the whole domain (hundreds of meters) and dimensions of veins and mine openings (metres, decimetres). It requires highly refined mesh and/or some multiscale approach. We used the composite grid method, see (Blaheta et al., 2006),
- simulates the loading by a general anisotropic initial stress by using pure force boundary condition. If different weights of rocks are considered, then analysis leads to a singular slightly inconsistent linear algebraic system and seeking for its generalized solution.

The numerical solution is performed with the aid of an in-house FEM software called GEM, which implements the following numerical methods including a black-box two-level Schwarz preconditioning (Blaheta et al., 2006):

- iterative solution of the large scale linear system by the CG method,
- use of parallel computation of the iterations with the aid of data partition corresponding to a domain decomposition (DD), see Fig. 5,
- preconditioning of the CG method by Schwarz type overlapping DD method with subproblems corresponding to subdomains solved approximately by incomplete factorization,
- improved Schwarz preconditioning by adding a global coarse problem in an additive or multiplicative way. The coarse problem is created algebraically by aggregation,
- approximate solution of the coarse problem by inner CG iterations preconditioned by incomplete factorization,

- stabilization of the outer CG by explicit orthogonalization of the search directions, see (Blaheta, 2002). It enables to use inner CG iterations as well as nonsymmetric multiplicative combinations of overlapping Schwarz preconditioner with the coarse problem solution,
- stabilization of the iterative solution of singular system by deflation (Blaheta 2006a).

2.2 Underground deposition of spent nuclear fuel

Whereas the modelling of previous section concerns only the mechanical behaviour of rocks, the assessment of nuclear waste repository includes mechanical behaviour, thermal loading and groundwater flow with transport of species, especially of radionuclides. Thus the mathematical analysis considers thermo-hydro-mechanical processes (T-H-M) plus chemistry (C). The chemistry becomes important due to very long time periods for which the repository should operate as a barrier between the radioactive waste and the environment. In many cases, the T-H-M-C processes should be considered as coupled, see e.g. (Stephansson et al., 2004).

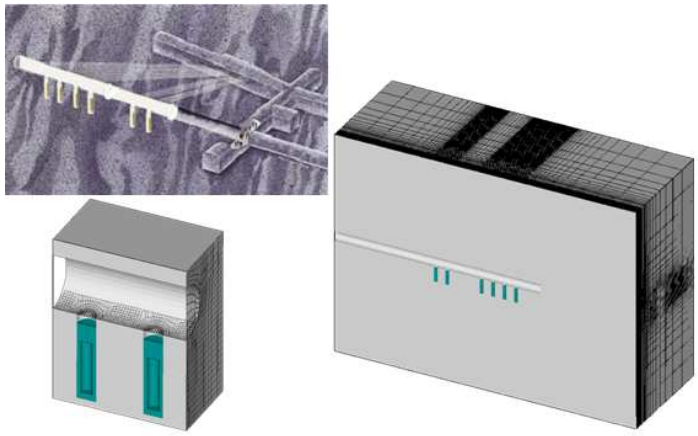

Figure 2. Äspö prototype repository: the considered domain and detail with two deposition holes. Discretization uses a regular grid.

A simple example of problems arising from mathematical simulation of performance of underground nuclear waste repositories is modelling of thermoelastic aspects of the prototype repository experiment in the underground hard rock laboratory in Äspö in Sweden, see Fig. 2 and also (Cleall et al., 2006), (Blaheta et al., 2005; 2007) for more details and material parameters. The basic features of this modelling are the following:

- 3D domain of interest has dimensions 200×100×200 metres, this domain contains tunnel with six deposition holes equipped with canisters (heaters),
- the mechanical loading is given by the weight of rocks and the overburden,
- thermoelastic behaviour is considered in the period of 50 years after installation of canisters.

The finite element analysis uses

- the discretization with linear triangular finite elements and with a regular grid containing 391×63×105=2 586 465 nodes. It means that more than 2.5 million DOFs is used for heat conduction and more than 7.75 million DOFs for elasticity,
- the FE grid which again reflects a big difference between the scale of the whole domain (hundreds of meters) and dimensions of canisters, deposition holes and pillars (metres, centimetres). It requires highly refined mesh or multiscale approach.

The problem is again solved by the in-house GEM software, which implements the following numerical methods, cf. (Blaheta et al., 2005; 2007a):

- time discretization by a backward Euler method, which guarantees full stability without any oscillations of the solution,
- time step determination by adaptive scheme based on a comparison of the first and second order approximation in time, see (Blaheta et al., 2004),
- iterative solution of large scale linear systems by CG method and parallel computation of the iterations with the aid of data partition corresponding to domain decomposition,

- preconditioning of the CG method by Schwarz type DD method, the subdomain subproblems are solved approximately by incomplete factorization,
- improved preconditioning of elasticity part by adding a coarse problem created algebraically by aggregations. It is important, that in the heat evolution part, this addition is not necessary, see (Blaheta et al., 2007a).

2.3 Microstructure modelling

The H-M processes in geomaterials depend heavily on the microstructure. The CT scan can be used for investigation of fracture, wetting, permeability changes etc,, see e.g. (Otani and Obara, 2004). The consequent FE analysis of the microstructure can be used for computation of homogenized material parameters, developing constitutive relations for poroelasticity, clearing up the coupling effects etc.

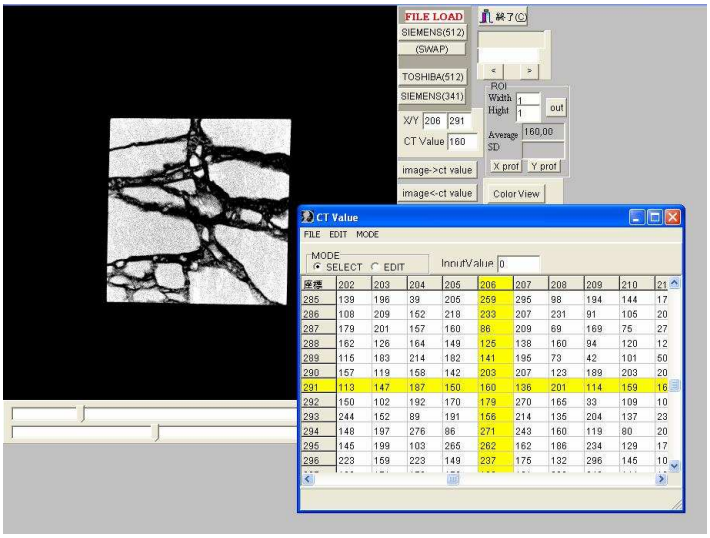

Figure 3. A coal geocomposite consisting of coal and polyurethane resin.
2D cut and CT values in a selected voxel and its neighbours.

A specific application of microstructure FEM (μFEM) is an analysis of properties of coal geocomposites, see Fig. 3. This analysis allows to compute homogenized characteristics as well as to investigate optimal properties of polyurethane resin filled into the geomaterial (coal) matrix. Specific features of this problem are:

- an analysis of 3D cubes with edge 75mm discretized by an uniform voxel grid with 251×251×38=2 394 038 nodes and more than 7 million DOFs in the case of elasticity,
- the use of uniform grid with assuming homogeneous material in voxels. Material properties of voxels are assigned according to X-ray CT scan.

More details can be found in (Blaheta and Krečmer, 2007) and in a future paper.

3 Numerical methods

This section briefly characterizes the numerical methods used for implementation of the finite element method on parallel computers and solution of problems from the previous section. Our approach is characterized by iterative solution with conjugate gradient (CG) type method, domain decomposition, Schwarz type preconditioning with inexact solution of subproblems and stabilization of outer iterations. Basic references are (Toselli and Widlund, 2005), (Blaheta, 2002), (Blaheta et al., 2006; 2007).

3.1 Parallel CG solution of FEM systems

Solution of boundary value problems of elasticity, heat conduction etc. by the finite element method leads to the linear systems

$$Au = b \tag{1}$$

where A and b are typically the stiffness matrix and load vector, which are constructed in an element by element way. Thus the assembling procedure is very easily parallelizable. Similar type systems can be found in time stepping and Newton type algorithms.
Therefore, we shall concentrate only on the parallel solution of the linear system (1). It can be solved by both direct and iterative solvers. We prefer the latter one due to several reasons: better efficiency for very large sparse systems, simpler implementation, better parallelizability as well as possible incomplete solution, which can save the effort e.g. when solving subproblems (see later) or in some THM coupling via staggered schemes or in inexact Newton like algorithms etc.
The system (1) can be solved iteratively by the standard preconditioned conjugate gradient (CG) method or its generalized variant (GPCG), see Fig. 4 and e.g. (Blaheta, 2002). In GPCG, the new search direction is explicitly orthogonalized to a selected number $z_i = \min\{m, i\}$ of previous search directions as the standard implicit CG orthogonality is disturbed not only due to use of computer arithmetic but also due to use preconditioner including nonsymmetry or inner iterations.

given u^0
$w = Au^0$
$r^0 = b - w$
$v^0 = g^0 = Gr^0$
for $i = 0, 1, \ldots$ **until** $\|r^i\| \le \varepsilon\|b\|$ **do**
  $w = Av^i$
  $\alpha = \langle r^i, g^i\rangle / \langle w, v^i\rangle$
  $u^{i+1} = u^i + \alpha v^i$
  $r^{i+1} = r^i - \alpha w$
  $g^{i+1} = Gr^{i+1}$
  $\beta = \langle r^{i+1}, g^{i+1}\rangle / \langle r^i, g^i\rangle$
  $v^{i+1} = g^{i+1} + \beta\, v^i$
end for

given u^0
$w = Au^0$
$r^0 = b - w$
$v^0 = g^0 = Gr^0$
for $i = 0, 1, \ldots$ **until** $\|r^i\| \le \varepsilon\|b\|$ **do**
  $w = Av^i$
  $\alpha_i = \langle r^i, v^i\rangle / \langle w, v^i\rangle$
  $u^{i+1} = u^i + \alpha_i v^i$
  $r^{i+1} = r^i - \alpha_i w$
  $g^{i+1} = Gr^{i+1}$
  $v^{i+1} = g^{i+1} + \sum_{k=1}^{z_{i+1}} \beta_{i+1}^{(k)} v^{i+1-k}$
end for

Figure 4. Preconditioned conjugate gradient method (left) and its generalized variant (right).

Each iteration of CG or GPCG consists of matrix by vector multiplication, inner products, scalar by vector multiplication and additions of vectors and preconditioning (computing of pseudoresidual $g = Gr$). We can imagine first the simplest diagonal preconditioning with $g = D^{-1}r$, where D is the diagonal part of A.
In the case of vectors decomposed into blocks and the corresponding decomposition of the matrix, each of the above mentioned operations (and therefore also the whole iteration) is easily parallelizable. The decomposition of the vectors can be defined through a nonoverlapping decomposition of the computational domain, see Fig. 5.

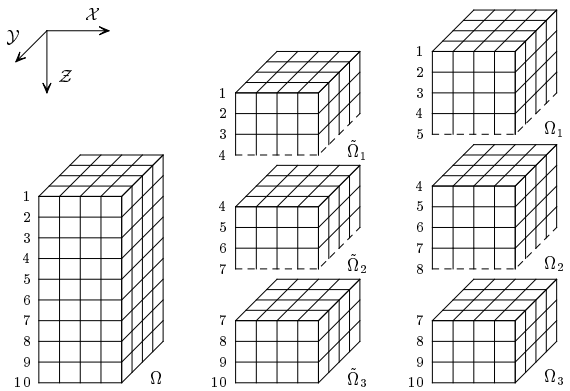

Figure 5. Domain decomposition: nonoverlapping and overlapping.

3.2 Parallel Schwarz type preconditioning

A remaining problem is necessity of accelerating the convergence via preconditioning, which is parallelizable and more efficient than the simplest diagonal one described above. A first idea can be to use a block diagonal Jacobi preconditioner corresponding to the same partition of vectors and matrix as used for parallelization of the basic operations. But the efficiency of this preconditioner is still not sufficient (it approximates the diagonal preconditioner with increasing number of subdomains). Therefore, a further efficiency enhancement was suggested, which takes into account bigger blocks (subproblems) corresponding to an overlapping domain decomposition $\Omega = \bigcup_k \Omega_k$, see Fig. 5. It gives Schwarz type preconditioner in the form

$$G = \sum_k R_k^T A_k^{-1} R_k \ , \tag{2}$$

where A_k are finite element matrices that correspond to FE spaces of functions in the domains Ω_k fulfilling homogeneous Dirichlet type boundary conditions on the inner boundaries and main boundary conditions of the whole problem on the outer boundaries. R_k denote restrictions to algebraic counterparts of these subspaces.

The operations with inverses $w = A_k^{-1} v$ are implemented approximately as $w = U_k^{-1} L_k^{-1} v$, where $L_k U_k$ is an incomplete factorization of A_k. We use MIC(0) incomplete factorization combined with displacement decomposition in the case of elasticity, see (Blaheta, 1994) for more details.

3.3 Two-level Schwarz type preconditioning with aggregations

The efficiency of the (one-level) Schwarz preconditioner (2) is enough for solving linear systems arising from time stepping solution of problems like evolutionary heat conduction, see (Blaheta et al., 2007a). For stationary problems, it should be further improved by using the two-level Schwarz method with an additional subproblem A_0 corresponding to a discretization of the solved problem with the aid of a coarser finite element division. The global subproblem A_0 can be also constructed algebraically by aggregation, which means that $A_0 = R_0 A R_0^T$ where R_0 is a rectangular $n_0 \times n$ restriction matrix with just one unity in each column, for more details see (Blaheta et al. , 2006) and the references therein. Note that n is the dimension of the square matrix A and $n_0 << n$. The coarse subproblem can be added additively, which gives

$$G = G_A = \sum_k R_k^T A_k^{-1} R_k + R_0^T A_0^{-1} R_0 \tag{3}$$

or multiplicatively. The simplest multiplicative version means that $g = Gr = G_M r$ is computed in two steps

$$\begin{aligned} g &\leftarrow \sum_k R_k^T A_k^{-1} R_k \, r, \\ g &\leftarrow g + R_0^T A_0^{-1} R_0 (r - Ag). \end{aligned} \tag{4}$$

This preconditioner is not symmetric, but can be symmetrized, of course at the expense of an additional step with solving global or local subproblems and at the cost of additional multiplication with A. It motivates the use of cheaper nonsymmetric variant. It is also called hybrid as it combines multiplicative approach with additive one in the step dealing with local subproblems, see (Toselli and Widlund, 2005). The use of nonsymmetric multiplicative variant requires stabilization by using the already described GPCG method.

The global subproblem $w = A_0^{-1} v$ can be again solved approximately. The experience shows that the use of inner CG iterations with the displacement decomposition-incomplete factorization preconditioning discussed above and relative residual criterion with the accuracy about $\varepsilon_0 = 10^{-1}$ is a good choice.

3.4 Stabilization of outer iterations in the case of singular systems

The application of loading by a general anisotropic initial stress or computation of upscaled homogenized modules leads to the solution of singular systems. Sometime we seek for a generalized solution of a slightly inconsistent linear system, i.e.

$$\text{solution of } Au = b \text{ is replaced by seeking for } u: \quad \|b - Au\| = \min . \tag{5}$$

For seeking standard or generalized solution of the described singular systems, we can use the PCG or GPCG methods after a slight modification of the described preconditioners. It is sufficient to equip them with a preliminary step, which project the residual into the (theoretical) range of A, i.e.

$$r \leftarrow r - \sum \gamma_i w_i, \quad \gamma_i : (r - \sum \gamma_i w_i)^T w_i = 0 . \tag{6}$$

Here, w_i create basis of the (theoretical) null space of A (e.g. w_i are rigid body displacements in the case of elasticity). Note that by "theoretical", we understand that the effects of the finite computer arithmetic are neglected.

3.5 Parallel Schwarz type mixed FEM for Darcy flow

Here we only mention one possible approach. First of all, the use of mixed FEM with lowest order Thomas-Raviart elements (Chan et al., 2006), (Toselli and Widlund, 2005) leads to the system

$$A_H = \begin{bmatrix} M_H & B^T \\ B & 0 \end{bmatrix}, \qquad A_H \approx \begin{bmatrix} M_H + \eta^{-1} B^T B & 0 \\ 0 & \eta I \end{bmatrix} \tag{7}$$

with indefinite matrix A_H. This system can be iteratively solved e.g. by the MINRES method instead of CG, see (Paige and Saunders 1975). It is not straightforward to apply Schwarz preconditioners to this system, see (Toselli and Widlund, 2005). One successful approach is described in (Blaheta, 2006b; Blaheta et al., 2008). It consists of use of block diagonal preconditioning from (7-right) and application of Schwarz technique just to the first block $M_H + \eta^{-1} B^T B$.

4 Some numerical results

Let us consider the Äspö prototype repository thermo-elasticity problem described in Section 2.2. 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 ten selected time levels.

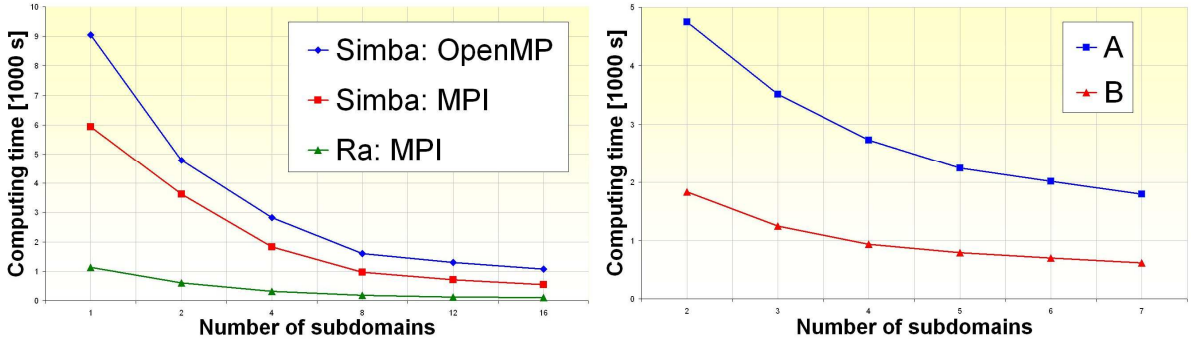

Figure 6. Äspö model problem: Computing times for the whole heat evolution in 47 time steps (left) and for one elasticity problem with one-level (A) and two-level (B) Schwarz preconditioning (right).

Fig. 6 shows decrease of computing times with increasing number of subdomains (processors). Fig. 6 – left considers the parallel solution of the arising linear systems in the whole time evolution for 50 years. The PCG here uses one-level Schwarz preconditioner (2) and the approximate solution of subproblems as described in Section 3. The computations performed on parallel computers in the UPPMAX centre. The first one is Simba with 48 UltraSPARC-III/900 CPU's, the second newer and more powerful one is cluster Ra with 280 AMD Opteron processors, see UPPMAX web page for more details. Two parallel codes are developed and compared. They differ in using OpenMP and MPI parallel programming paradigma.
The parallel speed up is good for the computations on up to 16 processors. Later, the size of subdomains constructed by parallel horizontal cutting (see Fig. 5) 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 provides simpler code development but MPI code proved to be 35-60% faster.

Fig. 6 - right shows the results from solving elasticity part of Äspö model problem with both one level (2) and two-level (3) Schwarz method. The coarse subproblem is then created with aggressive 6×6×6 aggregations, i.e. $n_0 = n/216$. Computing times correspond to an older Beowulf cluster with AMD Athlon 1.4 GHz processors.

5 Conclusions

The paper firstly shows that all thermal, deformation and flow processes in rocks can be efficiently modelled by the FEM with parallel solvers based on overlapping domain decomposition and Schwarz-type preconditioning. In the case of elasticity or heat conduction, we use standard Schwarz method enhanced by specific implementation details concerning inexact solution of subproblems, the use of subproblem constructed by aggregation, stabilization of the outer iterative method etc. For flow processes discretized by mixed FEM, we describe a new technique.
The importance of efficient solvers is further strengthened by solving nonlinear and coupled problems and by attempts to evaluate influence of uncertainty in model definition.

6 Acknowledgements

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