Parallel Computing of Thermoelasticity Problems

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Introduction

Problem: solution of the TE problem which is not fully coupled

We can divide the problem into two parts:

- the temperature distribution - determined by solving the nonstationary heat equation
- the linear elasticity problem - solved at given time levels

The numerical solution of the original problem leads to the repeated solution of large systems of linear equations. Therefore, our aim is to find efficient and parallelizable iterative solution methods.

For the solution of each linear system, we use the CG method with Schwarz-type preconditioners. If the Schwarz method is used for elliptic problems, the efficiency of the preconditioners decreases with the increasing number of subproblems. To avoid this, it is necessary to involve a coarse space correction. We use the algebraic coarse space created by aggregation.

In case of the parabolic problem, the corresponding system matrix depends on the time stepsize Δt. For suitable small Δt, the one-level additive Schwarz method is efficient enough.

Thermoelasticity

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

$$\tau\colon\ \Omega \times (0,T) \to R, \qquad u\colon\ \Omega \times (0,T) \to R^3$$

that fulfill the following equations

$$\begin{aligned}
\kappa\rho\frac{\partial \tau}{\partial t} &= k\sum_i \frac{\partial^2 \tau}{\partial {x_i}^2} + Q(t) && \text{in} \quad \Omega \times (0,T)\,, \\
-\sum_j \frac{\partial \sigma_{ij}}{\partial x_j} &= f_i \quad (i = 1,\ldots,d) && \text{in} \quad \Omega \times (0,T)\,, \\
\sigma_{ij} &= \sum_{kl} c_{ijkl}\left[\varepsilon_{kl}(u) - \alpha_{kl}(\tau - \tau_0)\right] && \text{in} \quad \Omega \times (0,T)\,, \\
\varepsilon_{kl}(u) &= \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) && \text{in} \quad \Omega \times (0,T)
\end{aligned}$$

together with the corresponding boundary and initial conditions.

Initial and boundary conditions

$$\begin{aligned}
\tau(x,t) &= \hat{\tau}(x,t) && \text{on} \quad \Gamma_0 \times (0,T)\,, \\
-k \sum_i \frac{\partial \tau}{\partial x_i} n_i &= q && \text{on} \quad \Gamma_1 \times (0,T)\,, \\
-k \sum_i \frac{\partial \tau}{\partial x_i} n_i &= H(\tau - \hat{\tau}_{out}) && \text{on} \quad \Gamma_2 \times (0,T)\,, \quad \text{where} \quad \Gamma = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2\,,
\end{aligned}$$

$$\begin{aligned}
u_n &= \sum_i u_i n_i \;=\; 0 && \text{on} \quad \tilde{\Gamma}_0 \times (0,T)\,, \\
\sigma_t &= 0 && \text{on} \quad \tilde{\Gamma}_0 \times (0,T)\,, \\
\sum_j \sigma_{ij} n_j &= g_i \quad (i = 1, \ldots, d) && \text{on} \quad \tilde{\Gamma}_1 \times (0,T)\,, \quad \text{where} \quad \Gamma = \tilde{\Gamma}_0 \cup \tilde{\Gamma}_1\,,
\end{aligned}$$

$$\tau(x,0) = \tau_0(x) \quad \text{in} \quad \Omega \qquad \text{are the initial conditions}\,.$$

The boundary conditions represent the temperature, heat flow, heat transfer, displacement, stresses, surface loading.

Linear equations

Using the variational formulation, space discretization by the finite element method and time discretization by the backward Euler method, we get:

- The system of equations for the heat,

$$(M + \Delta t B)\tau = q\,,$$

  which must be solved in each time step. This system depends on the time stepsize Δt. To optimize the computation, we use adaptive choice of time stepsize based on a local comparison of the backward Euler and Crank-Nicholson steps.

- The linear system for the elasticity at given time levels,

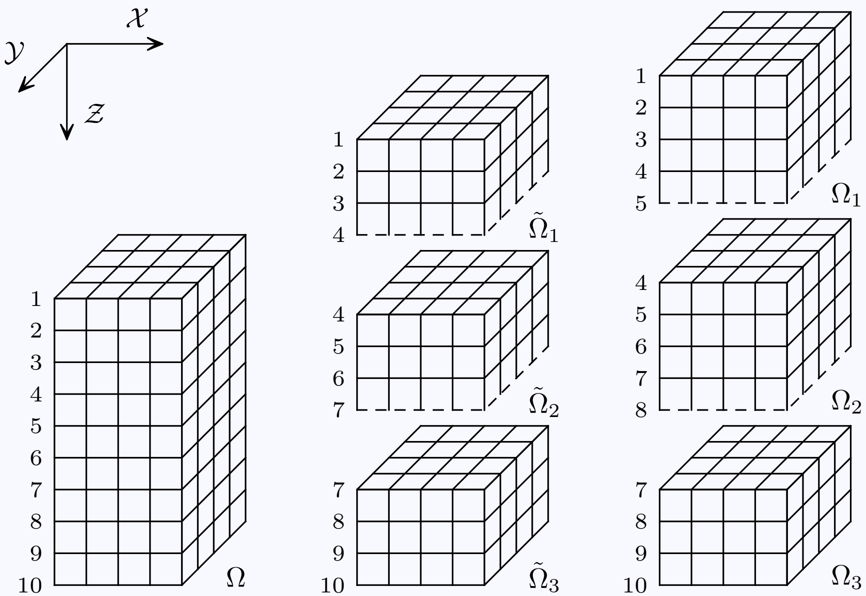
$$Au = f\,.$$

Solution of linear equations

For the solution of both linear systems, we use the preconditioned CG method. The domain is decomposed into m subdomains Ω_k. In our case, the domain is divided only in $\mathcal{Z}$ direction.

The preconditioning is given by the one-level additive Schwarz method,

$$g = Gr = \sum_{k=1}^{m} I_k A_k^{-1} R_k r \,.$$



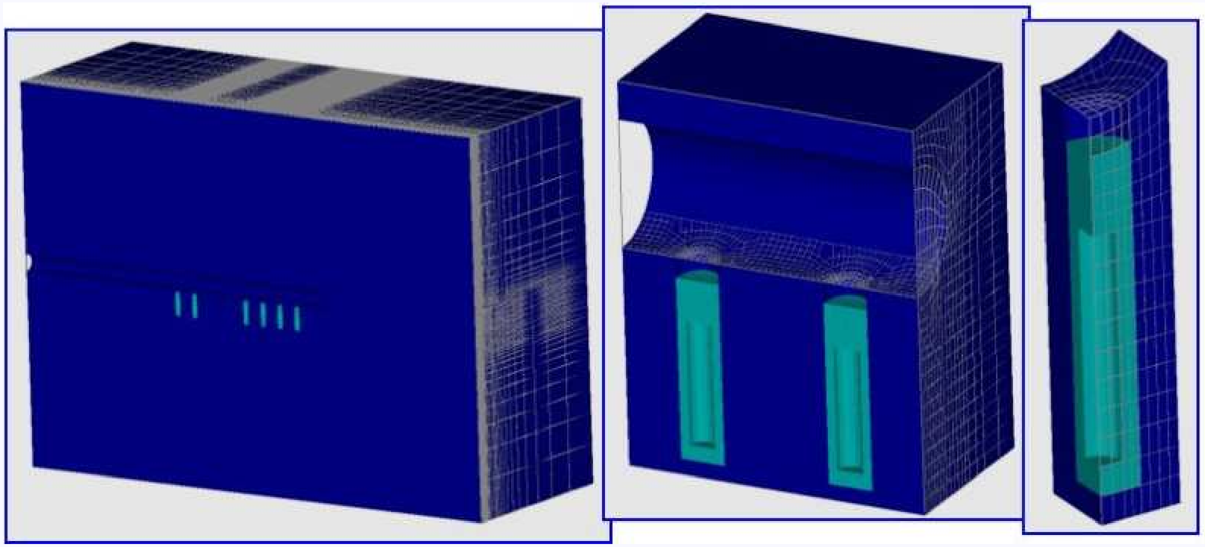
If the Schwarz method is used for elliptic problems, the efficiency of G decreases with the increasing number of subproblems and it is necessary to apply the coarse mesh solution in G (to set the two-level Schwarz method).

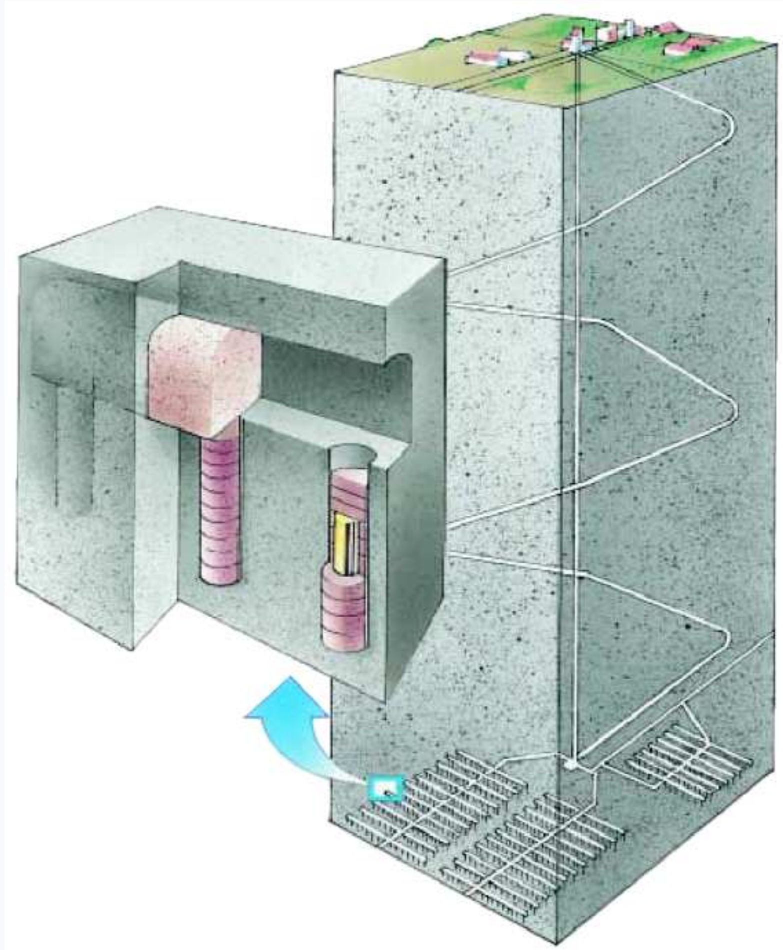
For the parabolic problems under the assumption that $\Delta t/H^2$ is reasonably bounded, the method remains numerically scalable even if the coarse mesh space is eliminated. Here, Δt is in order of the time stepsize and H is the diameter of the largest subdomain.

Model of the prototype repository in Äspö

The studied domain 200×200×100 m, located 450 m bellow surface, surrounds 65 m long tunnel with two sections including 4 and 2 deposition holes (1.75 m diameter, 8 m deep).

The FE mesh has 391×63×105 nodes, the considered time interval is 100 years.





For the heat - 2 586 465 DOF (radioactive waste as the heat source, heat conduction in rock, buffer and backfill).

For the elasticity - 7 759 395 DOF (initial stress loading, tunnel excavation, heat load from the nuclear waste).

Experiments with preconditioners

We tested the usage of the one-level additive Schwarz method. The efficiency of the two-level method in dependence on Δt was tested for 4 processors. The local and coarse (60×10×17 nodes) problems are solved inexactly by using an incomplete factorization. The system was solved up to the relative residual accuracy 10^{-6}.

#P	Δt									
	0.0001	0.001	0.01	0.1	1.0	5.0	10.0	100.0	1000.0	
1	11	11	16	26	38	46	60	109	193	
2	12	12	16	26	38	49	64	118	222	
4	12	12	16	26	38	49	64	125	238	
4	*18*	*17*	*17*	*27*	*41*	*50*	*53*	*83*	*142*	Aggr.
8	14	16	20	26	39	50	68	146	281	
12	14	16	20	25	42	54	78	183	328	
16	14	16	20	26	42	56	84	212	395	

The two-level preconditioner is efficient if Δt is 10 years and more.

Solution of the full nonstationary problem

The described solution methods were implemented in Fortran and parallelized by OpenMP and MPI paradigms:

- OpenMP allows a simple and scalable directive-based shared-memory parallel programming. It reduces the time by exploiting loop-level parallelism, by executing iterations of the loops across multiple processors.
- MPI applies the universal concept of concurrent processes communicating through message passing and portable on a wide range of parallel architectures including distributed-memory systems.

Now, we shall consider the whole sequence of time steps. In this, the system

$$(M + \Delta t B)\tau = q$$

is solved up to the relative residual accuracy 10^{-6} and with the initial guess taken from the previous time step. The adaptive choice of Δt is done and the total number of time steps is 47.

Symmetric multiprocessor Ngorongoro

Sun Fire 15000 installed at UPPMAX, Uppsala. The theoretical top performance is 86 GFlops/s.

SMP consists of 48 UltraSPARC III/900, 48 GB of shared memory, 8 MB of L2 cache, 12× 18 GB drives + Fibrenetix RAID controller with 3.4 TB disk storage. The used Sun Fireplane system interconnect has the peak data bandwith of 9.6 GB/s.

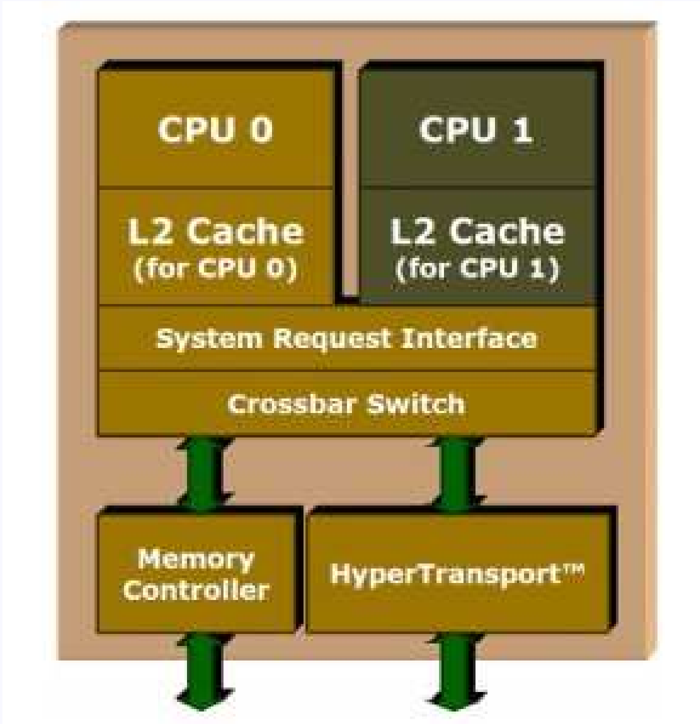
The machine has 4 parts: Simba (has 36 CPU's, 36 GB of memory), Mbogo, Tembo, Duma (each has 4 CPU's, 4 GB of memory).

The operating system is Solaris 5.9. Software includes Sun Grid Engine and MPI (Sun).

Opteron cluster Ra

The cluster, giving the total peak performance of 1.34 TFlops/s, consists of 99 nodes with 280 CPU cores, 688 GB of distributed memory and 16 TB of disk space. It is configured as:

- Front-end: Sun Fire V20z server;
- Back-end:
  - 64 nodes Sun Fire V20z server (9.6 GFlops/s): 2 AMD Opteron 250 procesors, 1 MB of L2 cache per core, 4 GB of shared memory, 150 GB of local disk space;
  - 32 nodes Sun Fire V40z server (19.2 GFlops/s): 4 AMD Opteron 850 procesors, 1 MB of L2 cache per core, 12 GB of shared memory, 300 GB of local disk space;
  - 3 nodes Sun Fire V40z server (35.2 GFlops/s): 4 AMD Opteron 875 dual core procesors, 1 MB of L2 cache per core, 16 GB of shared memory, 300 GB of local disk space;



Opteron cluster Ra - II

- Interconnection:
  - a fast low-latency InfiniBand fabric, the main switch is TopSpin 270 with 96 ports, each running at 4X speed or 10Gbit/s;
  - Gigabit Ethernet through a HP switch.
- Shared disk system: 12 TB storage capacity.

The operating system is Scientific Linux, which is a Red Hat Enterprise Linux recompiled from source. Installed software includes Sun Grid Engine for distributed resource managementa family of Portland Group compilers 5.2 and 6.0 and MPI implementations MPICH and SCALI for message-passing communication of parallel processes.

Numerical tests

# P	Simba - OpenMP			Simba - MPI			Ra - MPI		
	# It	T [s]	S	# It	T [s]	S	# It	T [s]	S
1	1341	6292		1344	5931		1344	1144	
2	1421	4101	1.63	1424	3169	1.87	1421	643	1.78
4	1425	2082	3.44	1428	1577	3.76	1426	314	3.64
8	1514	1120	6.34	1514	833	7.12			
12	1578	872	8.48	1581	596	9.95			
16	1614	751	10.09	1618	483	12.28			

Both solvers show very good scalability up to 16 processors. However, a comparison of the computing times on Simba confirms a higher performance of the MPI solver, which is faster than the OpenMP one. The difference is up to 36 % and shows necessity of the further optimization of the OpenMP code.

The computing times on Ra are approximately 5× shorter than on Simba.

Conclusion

The work outlines applications of parallel computing in geotechnics. The experiments with the solution of the nonstationary heat transfer part of the model KBS confirm a good efficiency of the used parallel solvers based on the CG method and domain decomposition technique. Especially in the case of the resulting MPI code, the solver shows to be very efficient for the solution of such kind of large practical problems.

Thank you for your attention

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