Modelling of Thermo-Mechanical Phenomena Arising from the Underground Disposal of the Spent Nuclear Fuel.

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Models and numerical simulations for problems

in Geophysics and Geotechnics

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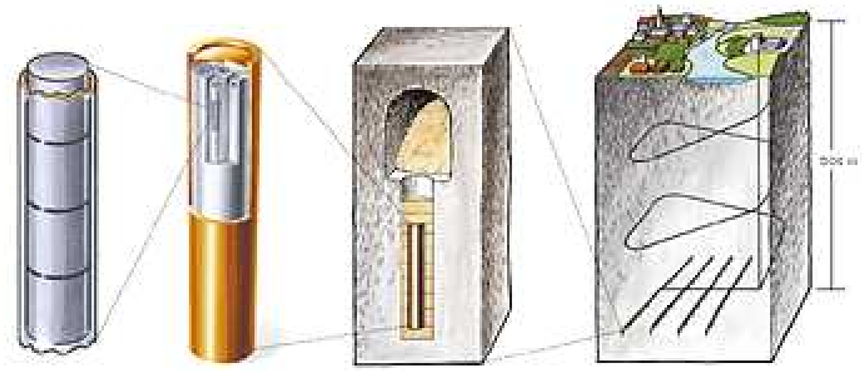
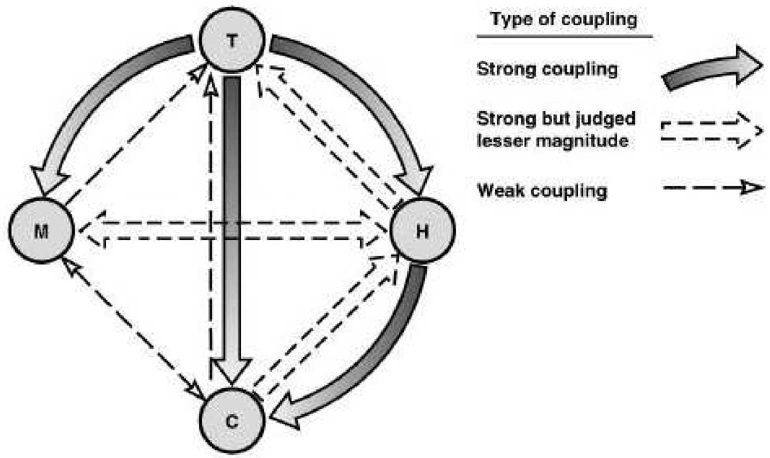
Outline of the talk

- Modelling of coupled T-H-M processes
- Model formulations of NWR problems
- Thermo-elasticity
- Radiation heat transfer
- Space and time discretization
- Solution of non-linear problems
- Iterative solution of evolution systems
- Overlapping DD
- Computed results
- Sensitivity analysis
- Concluding remarks

Assessment of NWR & T-H-M modelling



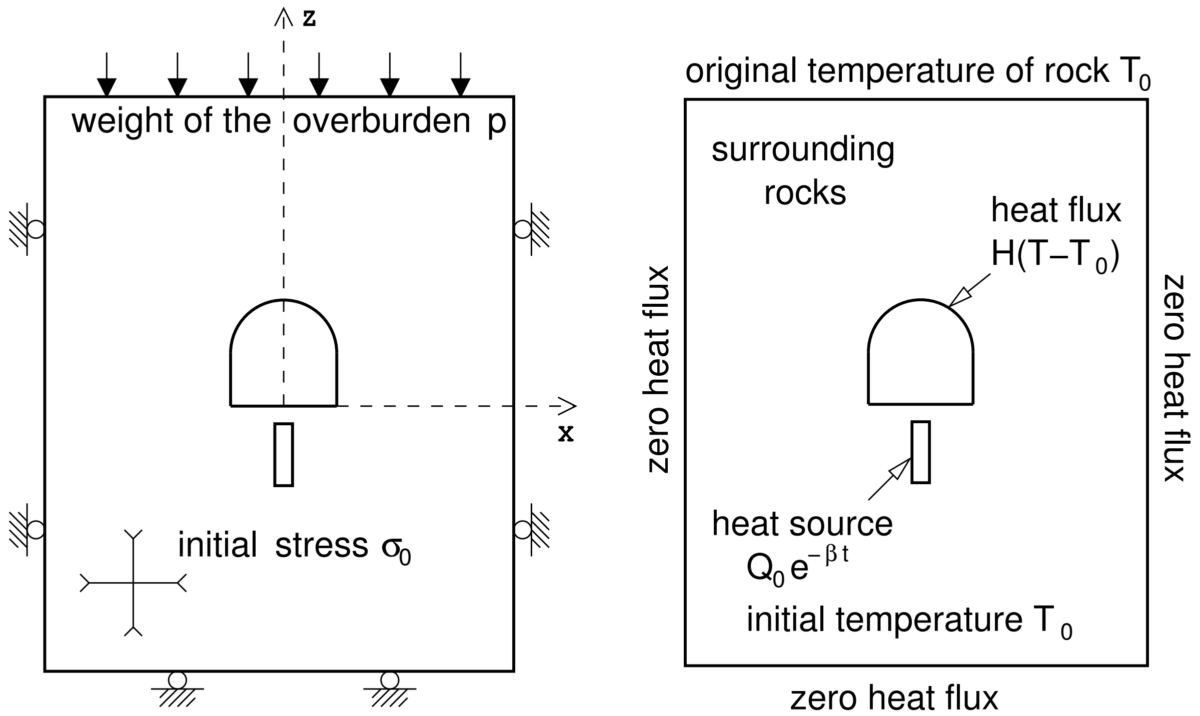


1. Need for formulation and validation of the mathematical models for the assessment of nuclear waste repositories.

2. Need for development of numerical methods and their computer implementation: parallel HPC becomes necessary due to requirements:

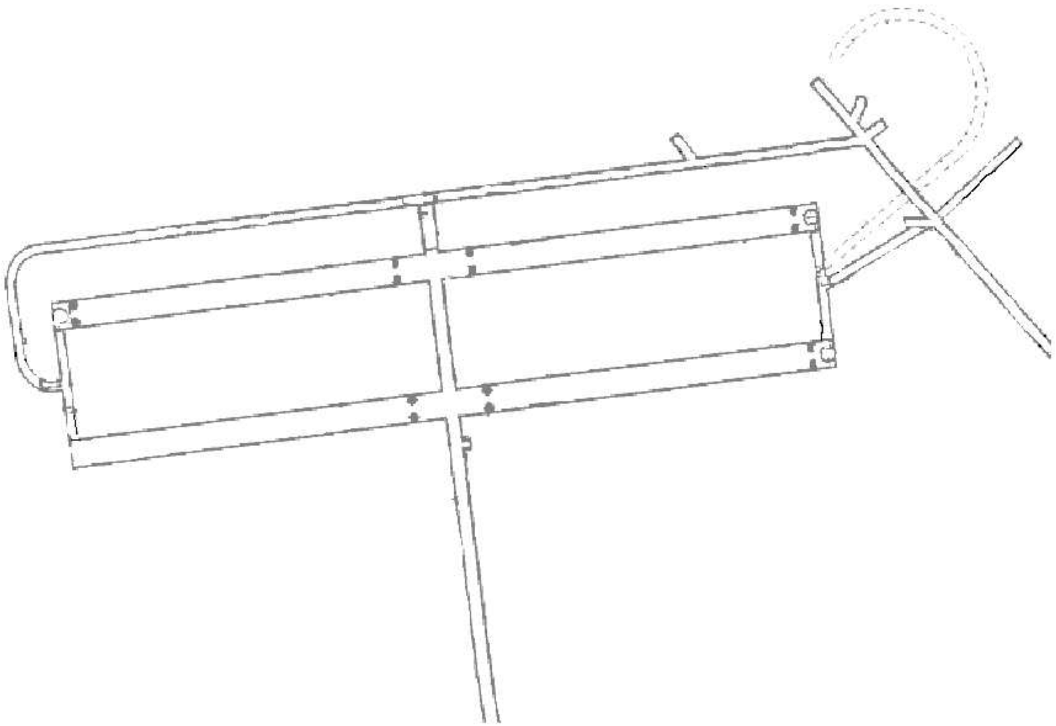
- modelling in large 3D domain, far-near field, construction steps and large time scale, multiphysics (T-H-M-C), nonlinearity, anisotropy, heterogenity and multiscale, discontinuity (rok fractures) of materials, uncertainty of material parameters, sensitivity analysis etc.

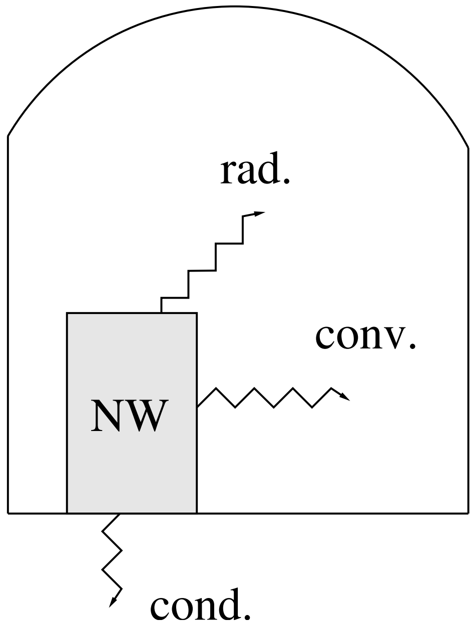
MP1 - BMT3 Decovalex benchmark



- Thermal part: radioactive waste as heat source, heat conduction in rock, heat convection to ventilation air
- Mechanical part: initial stress loading, tunnel excavation, heat load from the NW
- Groundwater flow - not considered now.

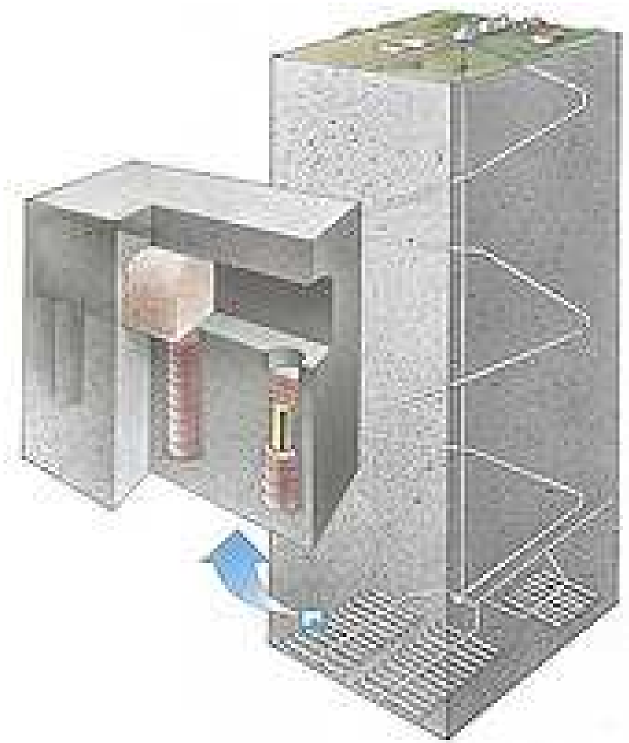
MP2 - Skalka interim repository

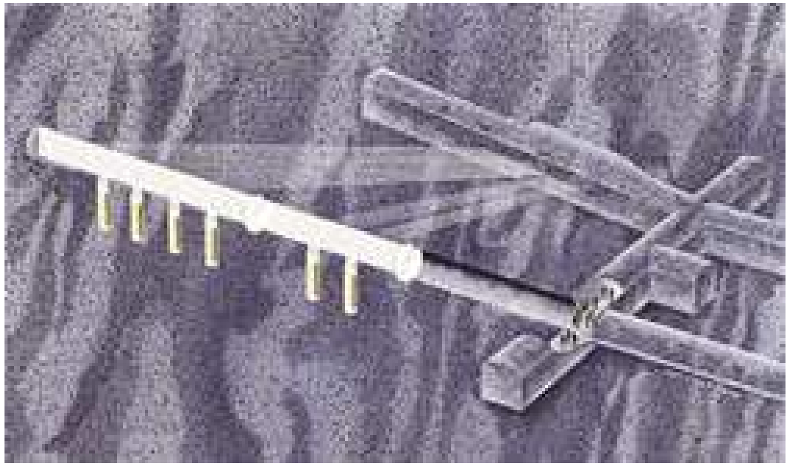




- Thermal part: radioactive waste as heat source, heat conduction in rock and lining, heat conduction to ventilation air, heat radiation
- Mechanical part: initial stress loading, tunnel excavation, heat load from the NW

MP3 - KBS-3V and Äspö prototype repository





- Thermal part: radioactive waste (heater) as heat source, heat conduction in rock, buffer and backfill (3D model)
- Mechanical part: initial stress loading, tunnel excavation, heat load from the NW (3D model)

Thermo-Elasticity

Find the temperature $\tau : \Omega \times (0,T) \rightarrow R$ and the displacement $u : \Omega \times (0,T) \rightarrow R^d \; (d = 2,3)$ such that

$$c\rho \frac{\partial \tau}{\partial t} = \sum_{ij} \frac{\partial}{\partial x_i}\left(k_{ij} \frac{\partial \tau}{\partial x_j} \right) + q \quad \textit{in } \Omega \times (0,T) \quad \textit{heat cond.}$$

$$-\sum_{j} \frac{\partial \sigma_{ij}}{\partial x_j} = f_i \quad (i = 1, \ldots, d) \quad \textit{in } \Omega \times (0,T) \quad \textit{balance}$$

$$\sigma_{ij} = \sum_{kl} c_{ijkl} \left[\varepsilon_{kl}(u) - \alpha_{kl}(\tau - \tau_R) \right] \quad \textit{in } \Omega \times (0,T) \quad \textit{const. rel.}$$

$$\varepsilon_{kl}(u) = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad \textit{in } \Omega \times (0,T) \quad \textit{small strains}$$

Initial & boundary conditions

Boundary - initial conditions

$$
\begin{aligned}
\tau(x,t) \;&=\; \hat{\tau}(x,t) \quad && \textit{on } \Gamma_0 \times (0,T) \quad && \textit{given temperature} \\
\sum_{ij} k_{ij}\,\frac{\partial \tau}{\partial x_j} n_i &= 0 && \textit{on } \Gamma_1 \times (0,T) && \textit{given heat flux} \\
-\sum_{ij} k_{ij}\,\frac{\partial \tau}{\partial x_j} n_i &= H(\tau - \hat{\tau}_0) && \textit{on } \Gamma_2 \times (0,T) && \textit{heat convection} \\
u_n \;=\; \sum_i u_i n_i \;=\; 0,\;\; \sigma_t &= 0 && \textit{on } \tilde{\Gamma}_0 \times (0,T) && \textit{symm. cond.} \\
\sum_j \sigma_{ij}\, n_j = g_i \quad & (i = 1, \ldots, d) && \textit{on } \tilde{\Gamma}_1 \times (0,T) && \textit{given pressure}
\end{aligned}
$$

the initial condition

$$\tau(x,0) \;=\; \tau_R(x) \quad \text{in } \Omega$$

Radiation heat transfer

The simplest case (two plane surfaces, the external is ideal absorber)

$$-n^T \mathcal{K} grad(\tau) = H(\tau - \tau_{out}) + \varepsilon c_{SB}(\tau^4 - \tau_{out}^4) \;\; on \; \Gamma_R,$$

where ε is relative emmisivity, c_{SB} is the Stefan-Boltzmann constant.

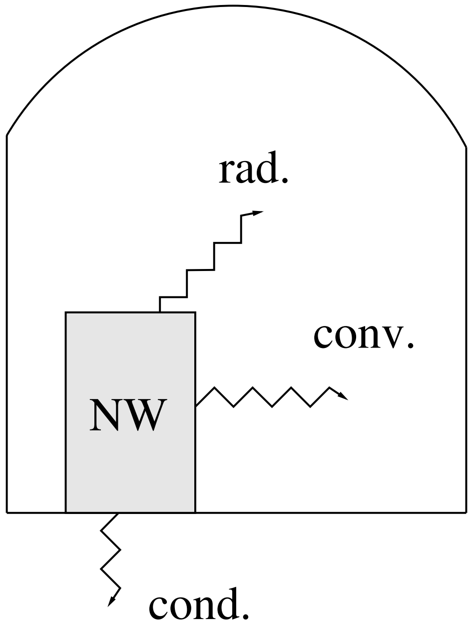
Weak formulation

$$B(\tau, v) = a_{heat}(\tau, v) + \int_{\Gamma_R} \varepsilon c_{SB} \tau^4 v \, ds$$

$$J(\tau) = \frac{1}{2} a_{heat}(\tau, \tau) + \int_{\Gamma_R} \varepsilon c_{SB} \tau^5 \, ds \; - b(\tau)$$

If $\Omega \subset R^2$ then: J is well defined in $H^1(\Omega)$, weakly semicontinuous and strongly convex in $\{\tau \in H^1(\Omega) : \; \tau \geq 0\}$. It guarantees the existence and uniqueness of the weak solution. For the linear FE, we get the convergence and for the reguar solution an estimate $\|\tau - \tau_h\| \leq C h^{1/4}$.

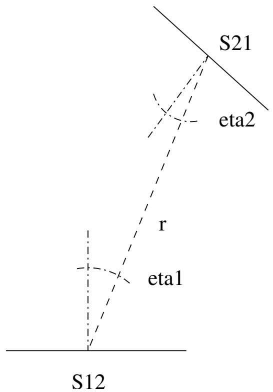
Radiation heat transfer



More general case:

- inner boundary: tunnel walls and canister surface
- parts of this inner boundary Γ_R radiate to others
- the surface absorbes ε-part and reflect the rest
- let $Z_k \subset \Gamma_R$ be zones with constant ε_k, τ_k
- let $S_{kl} \subset Z_k$ be part of Z_k visible from Z_l

- heat flux $\bar{q}_l$ emitted from Z_k to Z_l is $\bar{q}_l = |S_{lk}|\, R_{lk} q_k$, $q_k = \varepsilon c_{SB} \tau_k^4$
- $R_{lk} = \int_{S_{lk}} \int_{S_{kl}} \frac{\cos\vartheta_k \cos\vartheta_l}{r_{kl}}\, ds_k ds_l$, $R = (R_{kl})$
- $\bar{q} = E[I - SR(I-E)]^{-1}\, SRE\,\Theta(\tau)$,
  $S = (|S_{lk}|^{-1})$, $E = diag(\varepsilon_k)$, $\Theta_k = \tau_k^4$.



Space discretization

FEM:
$$\begin{aligned} \tau_h(x,t) &= \hat{\tau}(x,t) + \sum_i \tau_i(t)\phi_i(x), \\ u_h(x,t) &= \sum_i u_i(t)\tilde{\phi}_i(x)\,, \end{aligned}$$

where $\phi_i, \tilde{\phi}_i$ are basis functions. Denote $\underline{\tau} = (\tau_i)$ and $\underline{u} = (u_i)$ then:

- for elasticity $\tilde{A}_h\underline{u} = \underline{\tilde{b}}_h\,,\quad \tilde{A} = \left[\tilde{a}(\tilde{\phi}_i, \tilde{\phi}_j)\right],\ \underline{\tilde{b}} = [\tilde{b}(t, \tilde{\phi}_i)]$

- for heat conduction $$\begin{aligned} M_h\underline{\dot{\tau}}(t) + K_h(t)\underline{\tau}(t) &= \underline{b}_h(t) \quad \forall t \in (0,T)\,, \\ M_h\underline{\tau}(0) &= \underline{\tau}_0 \end{aligned}$$

  where $M_h = [(c\rho\phi_i, \phi_j)_0]\,,\ K_h(t) = [a(t, \phi_i, \phi_j)]$.

M_h is *capacity matrix*, K_h is *conductivity matrix*, $\tilde{A}_h$ is *stiffness matrix*.

Time discretization

Let $\langle 0, T\rangle$ is divided:

$0 \;=\; t_0 < t_1 < \ldots < t_j < \ldots < t_m \;=\; T\,, \quad \Delta_i = t_i - t_{i-1}$

then we seek the values $\underline{\tau}_i^j \sim \underline{\tau}_i(t_j),\; j = 1, \ldots, m$ from

$$\begin{aligned} M_h \frac{1}{\Delta_j}\left(\underline{\tau}^j - \underline{\tau}^{j-1}\right) + \theta K_h(t_j)\underline{\tau}^j + (1-\theta)K_h(t_{j-1})\underline{\tau}^{j-1} &= \varphi^j, \\ M_h\underline{\tau}^0 &= \underline{\tau}_0 \end{aligned}$$

where $\theta \in \langle 0, 1\rangle\,,\;\; \varphi^j = \theta \underline{b}_h(t_j) + (1-\theta)\, b_h(t_{j-1})\,.$

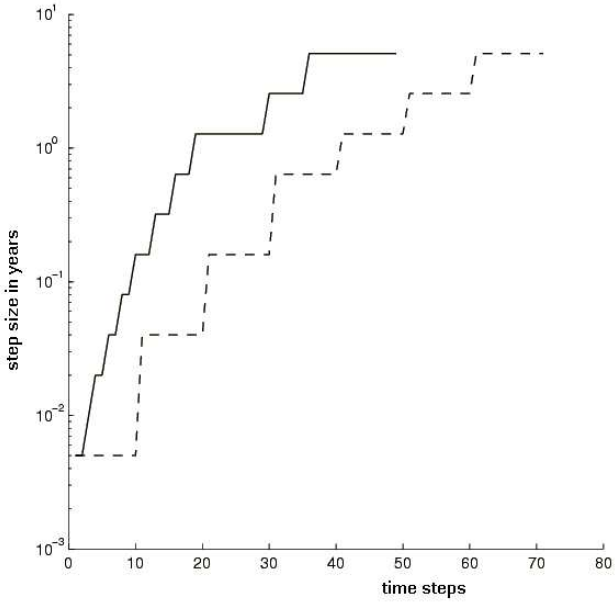
- $\theta = 0$ gives explicit Euler scheme, stable only for $\Delta t < h^2/c$
- $\theta = 1$ gives implicit Euler scheme, unconditionally stable,
- $\theta = \frac{1}{2}$ gives Crank-Nicolson scheme.

Adaptive time stepping

Time step adaptation can be based on

- variance $\rho_k(x) = |\tau_k(x) - \tau_{k-1}(x)|$
- simplified comparison of the Backward Euler and Crank Nicolson steps based on the residual (substitution BE step into the CN equation) $r^k = (M_h + 0.5\Delta t_k K_h)\tau_k - (M_h - 0.5\Delta t_k K_h)\tau_{k-1} - 0.5(c_h^k - c_h^{k-1})$.

Then according to the comparison
$\eta_* \leq \eta_k$?, $\eta_k \leq \eta^*$?
where $\eta_k = \max \rho_k(x)/\tau_k(x)$ or $\eta_k = \left\| r^k \right\| / \left\| \tau_k \right\|$,
the time step can be *shortened* and repeated
or the next step can be *prolongated*.



Solution of nonlinear systems

Damped Inexact Newton method (DIN).

Let u^0 be given,

for $i = 0, 1, \ldots$ **until** convergence **do**

$$\text{compute } v^i: \quad DF(u^i)v^i \sim b - F(u^i)$$
$$u^{i+1} = u^i + \lambda_i v^i, \quad \lambda_i \in (0, 1\rangle$$

endfor

$$\lambda_i = \max\{\lambda \in (0,1\rangle : \varphi(\lambda) \le 0\},$$
$$\varphi(\lambda) = \| b - F(u^i + \lambda v^i) \| - (1 - \alpha\lambda) \| b - F(u^i) \| \quad (Armijo)$$
$$\varphi(\lambda) = \| F(u^i + \lambda v^i) - F(u^i) - \lambda DF(u^i)v^i \| - \beta\lambda \| DF(u^i)v^i \| \ (Byczanski)$$

where α and β are parameters.

Adaptive continuation method

Find $u(t)\ :\ F(u(t)) = (1-t)b_0 + tb \quad \forall t \in \langle 0,1\rangle,\ \ u(0) = u^0,\ b^0 = F(u^0)$

Continuation steps: $(t_i, u^i) \mapsto (t_{i+1}, u^{i+1}),\ \ t_{i+1} = t_i + \tau,\ \ u^{i+1} = u^i + w$.
If τ is given, then w can be computed by the linearization:

Adaptive continuation algorithm

Given u^0 , $b^0 = F(u^0)$, $t_0 = 0$

for $i = 0, 1 \ldots$ **until** $t_i = 1$ **do**

compute z : $\qquad DF(u^i)z = (1-t_i)(b - b^0)$

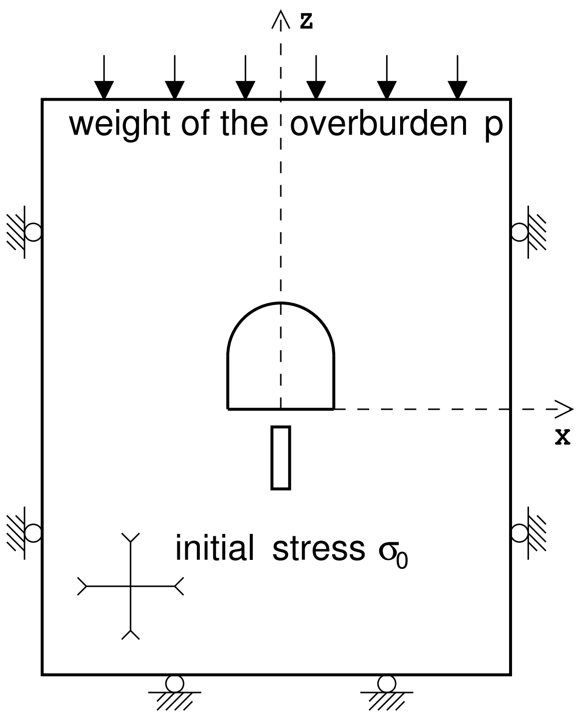
find : $\quad \kappa_i = \max\{\kappa \in (0,1\rangle : \varphi(\kappa) \le 0\}$

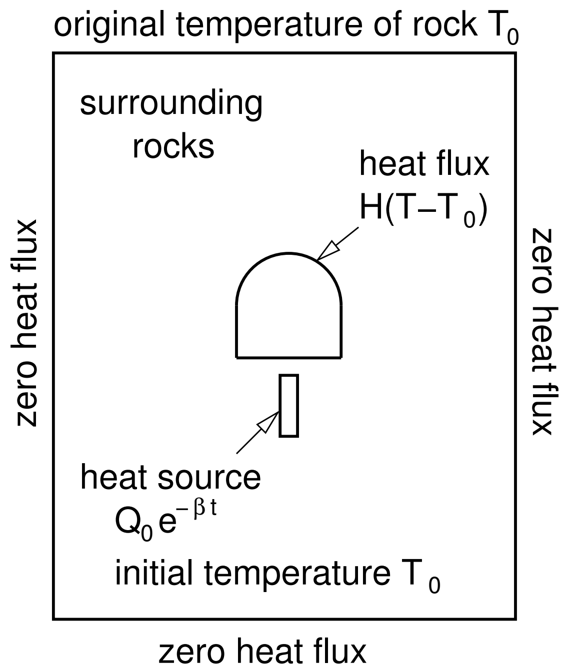
let : $\quad \tau = \kappa_i(1-t_i), \quad t_{i+1} = t_i + \tau$

$\qquad w = \kappa_i z, \quad u^{i+1} = u^i + w$

enddo, $\quad \varphi(\kappa) = \| F(u^i + \kappa z) - F(u^i) - \kappa DF(u^i)z \| - \beta\kappa \| DF(u^i)z \|$.

Iterative solution of T-M problems





FEM discretization in space, FD discretization in time: *find nodal temperatures* τ^k *and nodal displacements* u^k *in time steps* t_k

for $k = 1, \ldots, N$

find τ^k : $\quad B_k \tau^k = c^k \quad (1)$

find u^k : $\quad A u^k = b^k \quad (2)$

- in the elasticity part (2): the system with constant matrix is solved,
- in the heat part (1) with backward Euler: the system matrix $B_k = M + \Delta t_k K$ does not change if Δt_k is not changed

BMT3 model problem - Iterative solution

for $k = 1,\ldots,$ N

find τ^k : $B_k \tau^k = c^k$ (1)

find u^k : $Au^k = b^k$ (2)

solution: (1) $\varepsilon = 0.01$, (2) not always

A, $B_k = M + \Delta t_k K$ fixed

PS: $x^{k+1,0} = x^k$

PS+CD: $x^{k+1,0} = x^k + \sum \frac{\langle r_{ini}, v_i \rangle}{\langle Av_i, v_i \rangle} v_i$,

v_i conjugate directions from the solution in previous time step

LE: $x^{k+1,0} - x^k = x^k - x^{k-1}$,

CPS (generalization of LE):

storage previous $\{(rhs, sol)_j\}$,

new rhs=combination -> solution

init. guess	$\tau: \ \Delta t_j = 0.25$		$u: \ \Delta t_j = 0.25$	
$\varepsilon =$	0.01	0.001	0.01	0.001
zero	2420	3632	8362	11159
PS	590	1457	810	4526
PS + CD	399	899	210	1126
LE	689	697	501	840
LE + CD	423	459	207	311
CPS	101	181	199	351

Reduction of the number of iterations for 400 constant time steps (period 100 years).

Overlapping DD for evolution problems

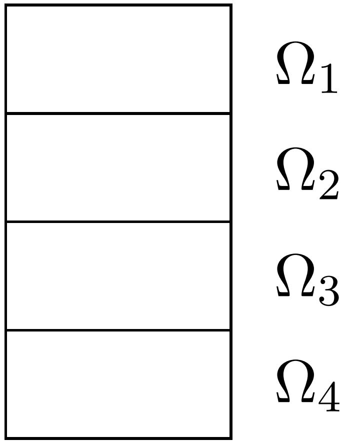
Model problem:

$\Omega = \langle 0, 2 \rangle \times \langle 0, 3 \rangle$

$\frac{\partial u}{\partial t} - \triangle u = f$

$u = 0$ on $\partial\Omega$

h=1/30, n=5100



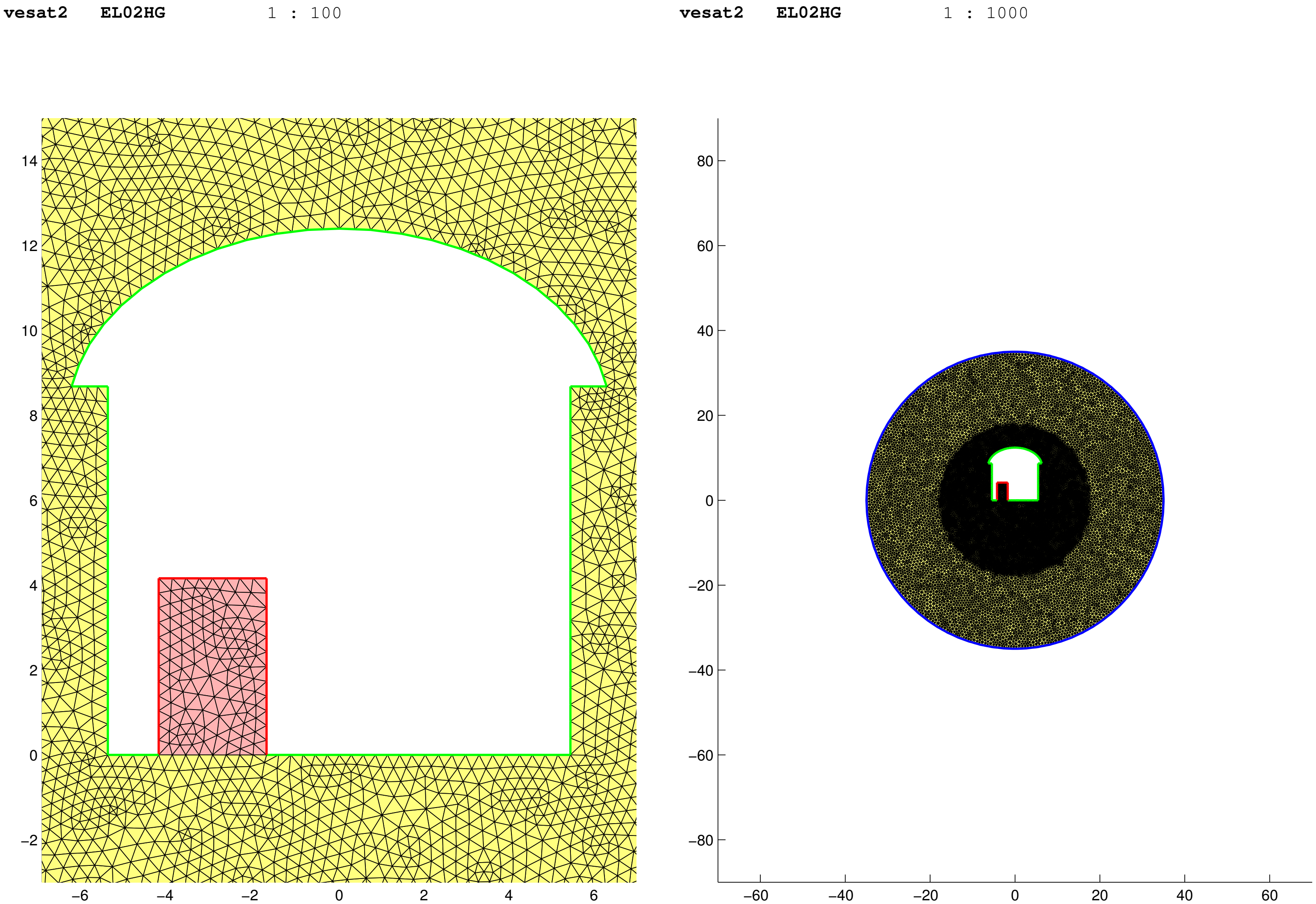
Overlap 2h, #subd's:	4			8			16		
no coarse grid	16	8	3	22	9	3	31	13	3
c-grid H=3h, AP	7	8	4	8	8	4	7	10	5
c-grid H=3h, HP	6	8	3	6	8		6	10	4
aggreg. 2h, AP	13	8	5	15	8	5	17	10	5
aggreg. 2h, HP	10	6		11	8		11	8	
interf. & aggr. 2h, AP	14	9	5	14	10	5	14	10	5
interf. & aggr. 2h, HP	8	5	3	7	5	3	8	5	3

Numbers of iterations for $\varepsilon = 10^{-3}$. AP=additive preconditioner,

HP=hybrid preconditioner + GPCG[1].

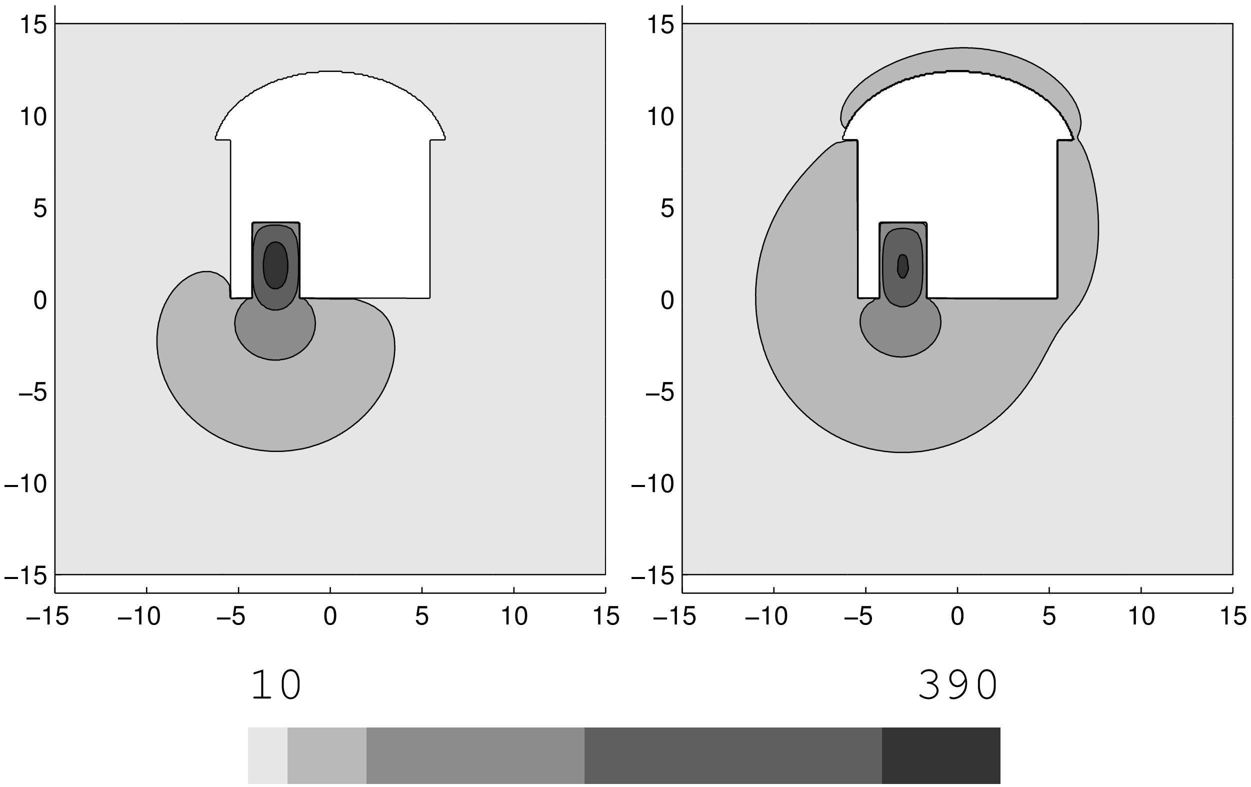
SubColumns: 1= matrix K, 2=matrix $M + \xi K$, $\xi = h$, 3=... ,$\xi = h^2$.

Skalka model problem



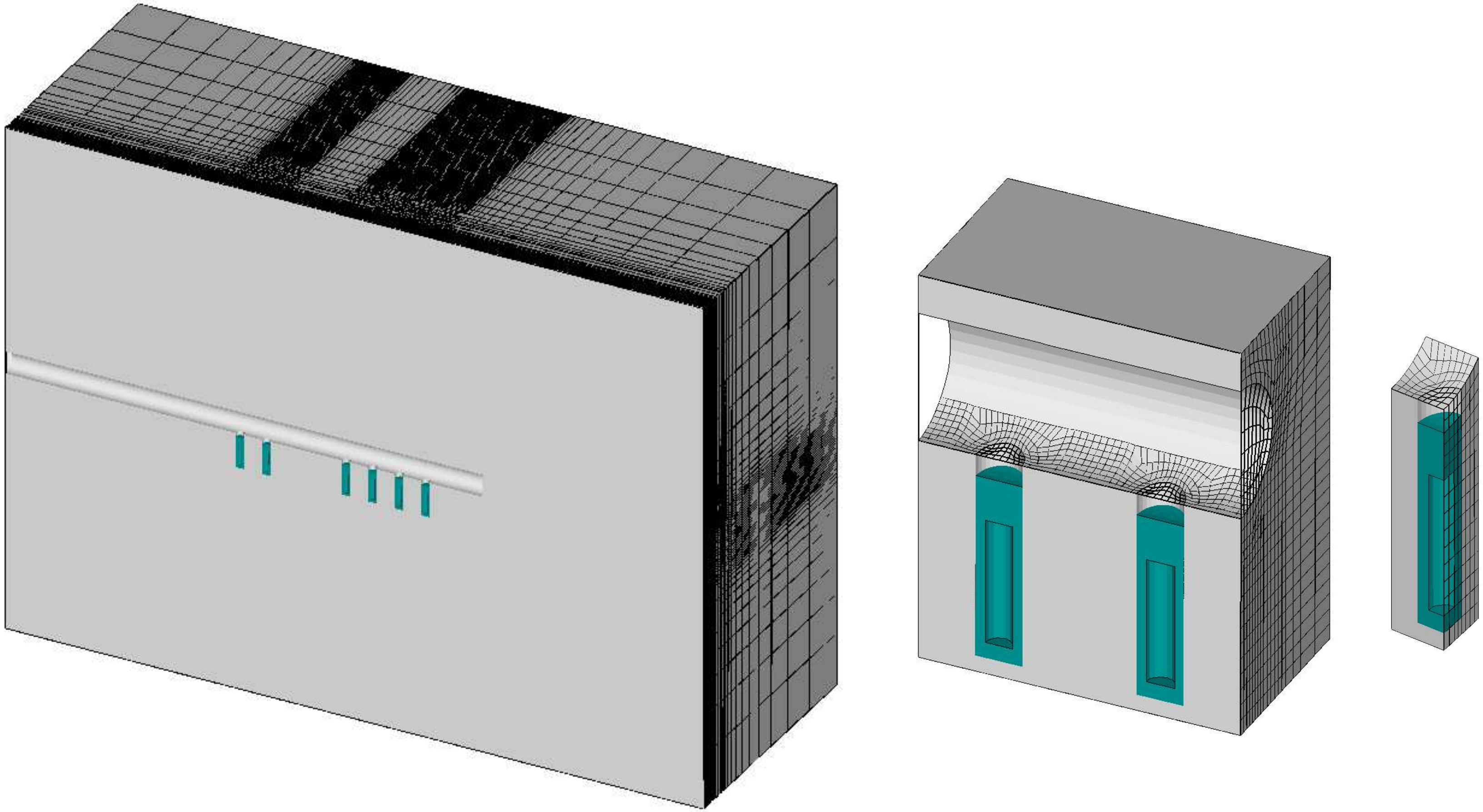
34 660 triangles, 17 584 nodes, 190 zones. 103 min. PC Pentium 2GHz

Skalka model problem - results



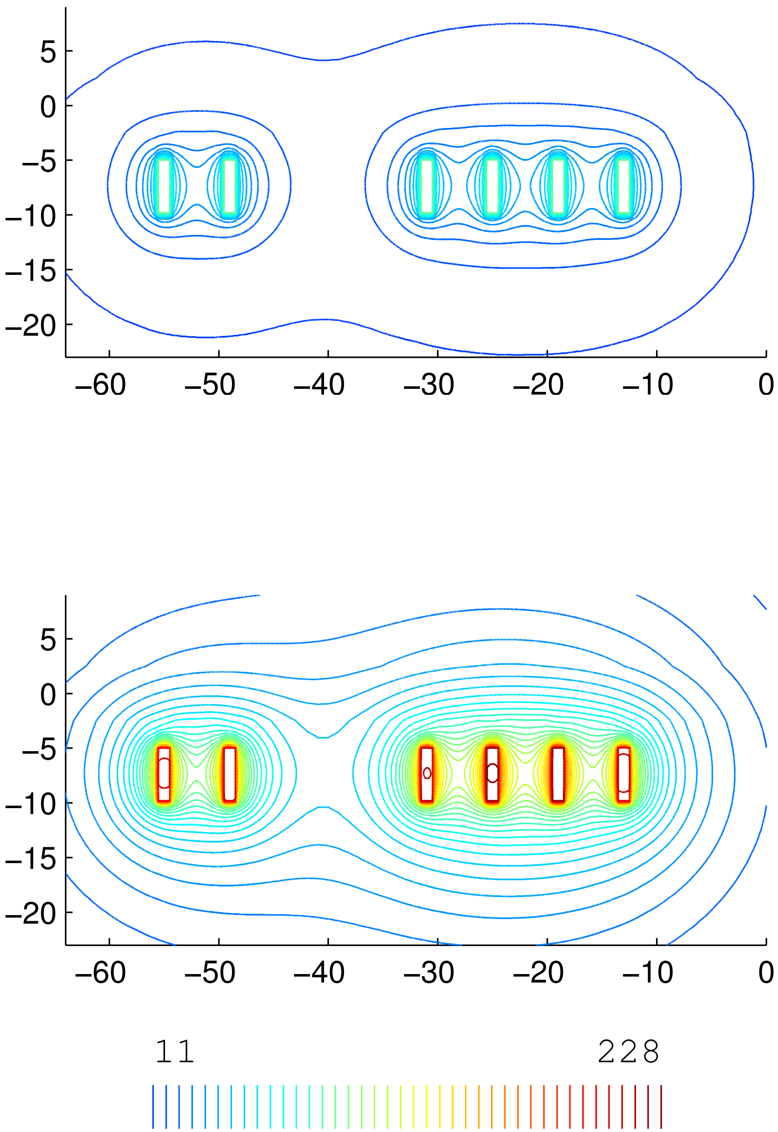
The radiation heat transfer is important, see above (under increased emmisivity of the canister).

Äspö model problem



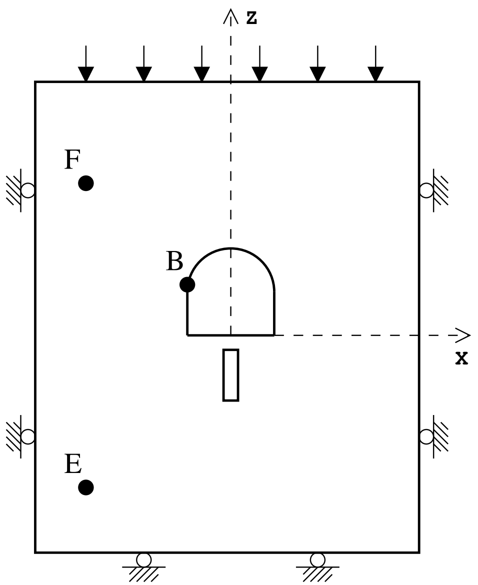
Linear tetrahedral FE (15 mil. tetrahedra), >2.5 mil. DOF for heat transfer, >7.5 mil DOF for elastic displacements, time period 50 years.

Äspö model problem - results



1 and 10 years after canister installation; equidistant temperature isolines
Computation on IBMxSeries 435, Thea cluster

Uncertainty - Sensitivity analysis



$D_pV\,(point, time) = \frac{V_{1.01p} - V_p}{0.01p}$. Results for t=10 years

	$\tau\ [deg]$			$\sigma_{vol}\ [MPa]$			$\bar{\sigma}_{shear}\ [MPa]$		
point	B	E	F	B	E	F	B	E	F
O	30	76	38	39	43	25	17	2	7
Dk	0	0.4	0.1	0.1	0.3	0	0.2	2.5	0.1
Dc	0	0.2	0.2	0.1	0.2	0.2	0.2	2.1	0.2
Dα	0	0	0	0.1	0.5	0.2	0	4.9	0.2
DE	0	0	0	0.1	0.5	0.2	0	4.9	0.2
Dν	0	0	0	0.2	0.4	0.4	0.3	3.7	0.7

Basic parameters:

k - conductivity

c - specific heat

α- thermal expansion

E - elastic modulus

ν- Poisson ratio

Semi-analytic: $A(p)u(p) = b \;\Rightarrow A(p)D_pu(p) = -D_pA(p)u(p)$

Final remarks

- We focused on some computational aspects of solving T-M problems relevant for NWR assessment (research results of grant project of GACR).
- Next development - improving efficiency and parallel computing of 3D T-M problems (also next talk by J. Stary).
- Development of GEM3 software of the Institute of Geonics (solvers, visualization etc.)
- Modelling of radiation and convection of heat in ventilation air in 3D.
- Accuracy of the discretization.
- Uncertainty in input data and evaluation of its influence.
- Coupled modeling with groundwater flow.

Thank you for your attention.