Numerical methods for hydro-mechanics in standard and disturbed continua

Radim Blaheta
joint work with
O. Axelsson, M. Béreš, S. Domesová, D. Horák, J. Kružík and T. Luber

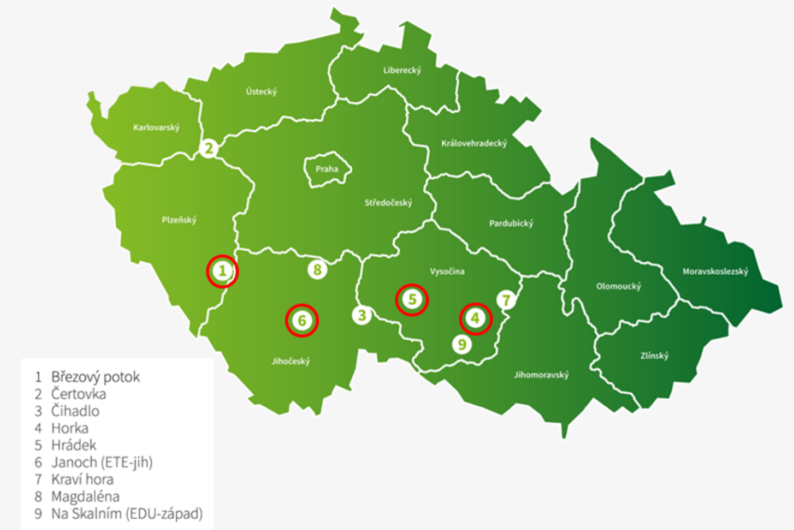
PANM Hejnice, June 21-26, 2020

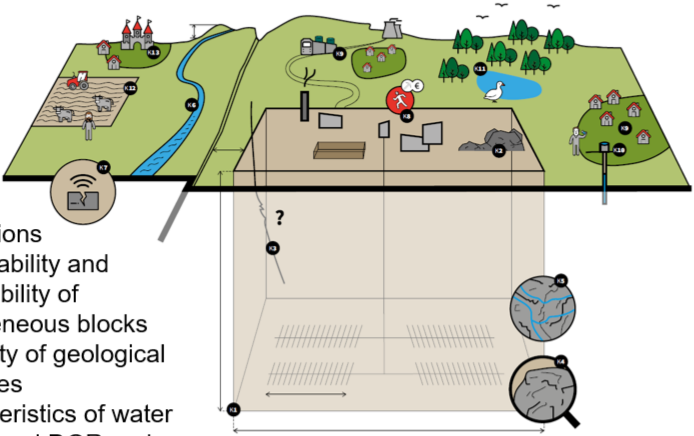
(version June 23, 2020)

Outline

Motivation

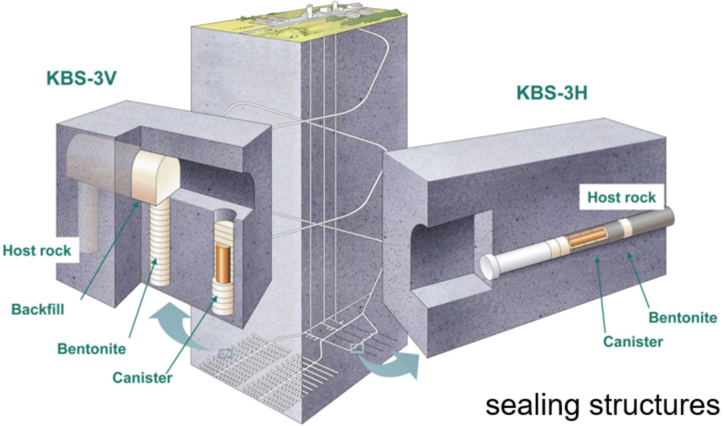
Localities CR



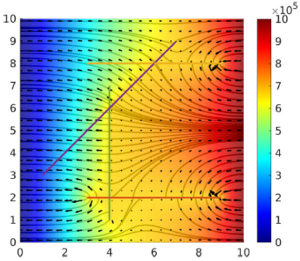


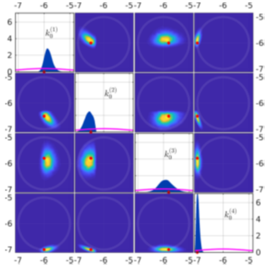
1. Dimensions
2. Describability and predictability of homogeneous blocks
3. Variability of geological properties
4. Characteristics of water flow around DGR and transport
5. etc.

Nuclear waste deposition - barriers



sealing structures





- Flow in porous media with fractures
- Fractures as domains of reduced dimension
- Mechanics – elasticity + contact on fractures
- Iterative coupling of flow + mechanics
- Bayesian inversion

- R. Blaheta · M. Béreš · S. Domesová · D. Horák: Bayesian inversion for steady flow in fractured porous media with contact on fractures and hydro-mechanical coupling. Computational Geosciences 2020, on-line

  https://doi.org/10.1007/s10596-020-09935-8

CouFrac 2018, Wuhan

Poroelasticity - hydro-mechanics
linear models / linear couplings

Darcy flow

One-field formulation p - pressure in fluid

$$c_{pp}\frac{\partial}{\partial t}p = \mathrm{div}(\kappa\nabla p) + f_p \quad in\ \Omega \times T.$$

Two-field formulation $(p,\ v)$ - pressure & velocity

$$\begin{array}{lll} \kappa^{-1}v & +\nabla p & = 0, \\ \mathrm{div}(v) & +c_{pp}\frac{\partial}{\partial t}p & = f_p, \end{array} \quad in\ \ \Omega \times T.$$

κ represents hydraulic conductivity, c_{pp} storativity , f_p is a source term.

Boundary-initial conditions

$$p = \hat{p}\ \ on\ \Gamma_p, \quad v \cdot n = -\kappa\nabla p \cdot n = \hat{v}\ \ on\ \Gamma_v, \tag{1}$$

$$p(x, 0) = p_0(x). \tag{2}$$

Poro-elasticity

Two-field formulation (u, p) - displacement and pore fluid pressure

$$
\begin{aligned}
-\mathrm{div}(C : \varepsilon(u)) \qquad & +\nabla(\alpha p) && = f_u, \\
\alpha \tfrac{\partial}{\partial t}\mathrm{div}(u) \qquad & + c_{pp}\tfrac{\partial}{\partial t} p - \mathrm{div}(\kappa \nabla p) && = f_p,
\end{aligned}
$$

three-field fomulation

$$
\begin{array}{cccc}
-\mathrm{div}(C : \varepsilon(u)) & & +\nabla(\alpha p) & = f_u, \\
 & \kappa^{-1} v & +\nabla p & = 0, \\
\alpha \tfrac{\partial}{\partial t}\mathrm{div}(u) & +\mathrm{div}(v) & +c_{pp}\tfrac{\partial}{\partial t} p & = f_p.
\end{array}
$$

The Terzaghi-Biot model, linear couplings: (1) effective stress

$$\sigma = \sigma_{eff} - \alpha p I$$

(2) change of bulk volumes $\Rightarrow$ change of pore (fluid) volumes, flow induced by deformation

$$\triangle V / V = \frac{\partial}{\partial t}\varepsilon_v = \frac{\partial}{\partial t}\mathrm{div}(u)$$

$$\frac{\triangle V_p}{V} = \frac{\triangle V - \triangle V_s}{V} = \frac{\triangle V}{V}\left(1 - \frac{\triangle V_s}{\triangle V}\right) = \frac{\triangle V}{V}\left(1 - \frac{\triangle\sigma / K_s}{\triangle\sigma / K_b}\right) = \alpha \frac{\triangle V}{V}$$

Variational formulation of two-field poro-elasticity

For a.e. $t \in T = \langle 0,\ t_{max} \rangle$ find $(u(t,\cdot),\ p(t,\cdot)) \in \boldsymbol{U}_D \times W_D$ such that $\frac{\partial}{\partial t} p \in L^2(\Omega)$ and

$$\begin{aligned} & & a_u(u,\ w) + (\nabla(\alpha p),\ w) &= F_u(w) \quad \forall w \in \boldsymbol{U}_0, \\ (c_{pp}\tfrac{\partial}{\partial t} p, q) + & & \left(\tfrac{\partial}{\partial t}\left(\alpha div(u)\right),\ q\right) + a_p(p,\ q) &= F_p(q) \quad \forall q \in W_0. \end{aligned}$$

where $(\cdot,\cdot)$ denotes the inner product in $L_2(\Omega)$,

$$a_u(u, w) = \int_\Omega C\varepsilon(u) : \varepsilon(w)\, dx, \quad a_p(p, q) = \int_\Omega \kappa \nabla p \cdot \nabla q\, dx$$

$u, w \in \boldsymbol{U} = [H^1(\Omega)]^d, \quad p, q \in W = H^1(\Omega).$ Moreover,

$$\begin{aligned} \boldsymbol{U}_{tD} &= \{u \in \boldsymbol{U},\ u = \hat{u}(t) \ \ on\ \Gamma_u\}, \quad \boldsymbol{U}_0 = \{u \in \boldsymbol{U},\ u = 0 \ \ on\ \Gamma_u\}, \\ W_D &= \{p \in W, p = \hat{p}(t) \ \ on\ \Gamma_p\}, \quad W_0 = \{p \in W,\ p) = 0 \ \ on\ \Gamma_p\}. \end{aligned}$$

For existence and uniqueness see

- Zenisek, A.: The existence and uniqueness theorem in Biot's consolidation theory. Apl. Mat. 3(29), 194–211 (1984) - with $c_{pp} = 0$
- Showalter, R.E.: Diffusion in poro-elastic media. J. Math. Anal. Appl. 1(251), 310–340 (2000)

Step 0

$$(u^0,\, w) = (u_0,\, w)\ \ \forall w \in \boldsymbol{U}_0, \quad (p^0,\, q) = (p_0,\, q)\ \ \forall q \in V_0.$$

Step $k > 0$

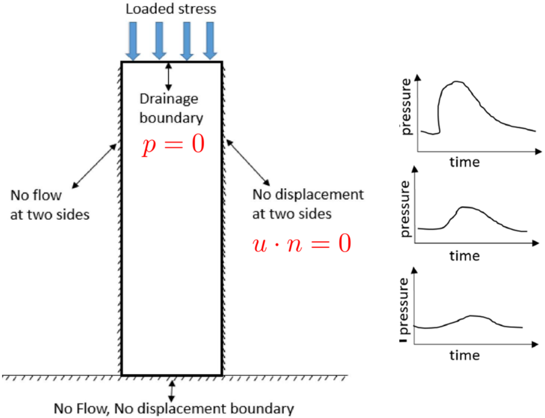
$$a_u(u^k,\, w) + b_1(w, p) = F_u^k(w)\ \ \forall w \in \boldsymbol{U}_0,$$
$$b(u^k, q) - c(p^k, q) = F_p^k(q)\ \ \forall q \in W_0,$$

Next time step

$$c(p^k, q) = (c_{pp}p^k, q) + \tau_k a_p(p^k,\, q)$$

Nonsymmetry $b_1 \neq b$

$$(\nabla(\alpha p),\, w) = \int_{\partial\Omega} \alpha p w \cdot n\, dx - \int_{\Omega} \alpha p\, div(w)\, dx = \int_{\partial\Omega} \alpha p w \cdot n\, dx + b(w, p)$$
$$= \int_{\partial\Omega \setminus \Gamma_{pu}} \alpha p w \cdot n\, dx + b(w, p) = b_1(w, p), \quad p = 0 \ \ or \ \ u \cdot n = 0 \ on \ \Gamma_{pu}$$



- P.M. Delgado V. M. Krushnarao Kotteda, V. Kumar, Hybrid Fixed-Point Fixed-Stress Splitting Method for Linear Poroelasticity. Geosciences 2019
- Cheng An, P. Zhou, B. Yan, Y. Wang, J. Killough, Adaptive Time Stepping with the Modified Local Error Method for Coupled Flow-Geomechanics Modeling. Conference SPE-186030-MS, 2017

Full discretization

FE spaces $\boldsymbol{U}^h$, $\boldsymbol{U}_0^h$ and V^h, V_0^h, algebraic spaces $X = R^n$ and $Y = R^m$,

$u \in X \leftrightarrow u_{fem} \in U_h$ and $p \in Y \leftrightarrow p_{fem} \in W_h$.

$a_u \leftrightarrow A_u$, $a_p \leftrightarrow A_p$, $\int_\Omega u \cdot w \leftrightarrow M_u$, $(\cdot,\cdot)_{2,0} \leftrightarrow M_p$, $\int_\Omega \nabla(\alpha q) \cdot w \leftrightarrow B_1^T$,

$\int_\Omega \alpha div(w) q \leftrightarrow B_2$

Time stepping algorithm in discrete form

- Step 0
- For $k = 1, 2, \ldots$
  - Step $k > 0$: find $(u^k, p^k) \in X \times Y$ such that

$$\begin{bmatrix} A_u & B_1^T \\ B_2 & -C \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix} = \begin{bmatrix} v \\ p \end{bmatrix},$$

where $C = c_{pp} M_p + \tau_k A_p$

- Next time step

Analysis of the saddle point problem I

Problem formulation with two bilinear forms: Find $(u,p) \in U_0 \times W_0$

$$(P1) \quad \begin{aligned} a(u,v) + b(v,p) &= f(v) \qquad \forall v \in U_0 \\ b(u,q) - c(p,q) &= g(q) \qquad \forall q \in W_0 \end{aligned}$$

Problem formulation with one bilinear form: Find $(u,p) \in U_0 \times W_0$

$$(P2) \quad \mathbb{A}((u,p),(v,q)) = F(v,q) \qquad \forall (v,q) \in U \times P$$

$$\begin{aligned} \mathbb{A}((u,p),(v,q)) &= a(u,v) + b(v,p) - b(u,q) + c(p,q) \\ F(v,q) &= f(v) - g(q) \end{aligned}$$

Theorem: The problems (P1) and (P2) are equivalent and have a unique solution.

$$\begin{gathered} \mathbb{A}((u,p),(v,0)) = a(u,v) + b(v,p) = f(v) \\ \mathbb{A}((u,p),(0,q)) = b(u,q) - c(p,q) = g(q) \\ \mathbb{A}((u,p),(v,0)+(0,q)) = F(v,q) \end{gathered}$$

+ Lax-Milgramm lemma for problem (P2)

- According to the previous Theorem there is a unique solution, but the stability depends on c,

$$\gamma_u \|u\|_{2,1} + \gamma_p \|p\|_{2,1} \leq \frac{1}{\gamma_u} \|f\|_{2,0} + \frac{1}{\gamma_p} \|g\|_{2,0} \,,$$

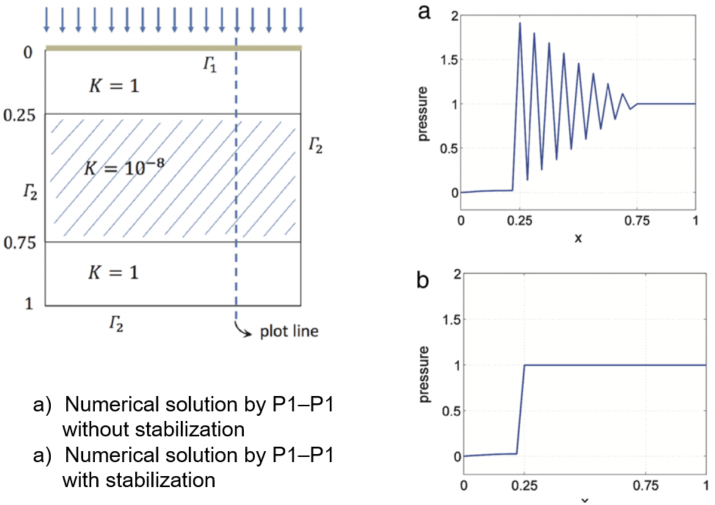
  see [Boffi, Brezzi, Fortin], γ_u and γ_p are elipticity constants.

- Inf-sup - ex. $\beta > 0$

$$??? \quad \sup_{w \in U} \frac{(div(w), p)}{\|w\|_{2,1}} \geq \beta \|p\|_{2,1} \,,$$

- Note that
    - C becomes close to zero if c_{pp} and $\tau_k \kappa$ are small.
    - For P1/P1 finite element pairs instability was observed if $C \sim 0$.
    - Robustness w.r.t. discretization and problem parameters.
    - Recent results for 2 and 3 field poroelasticity

Spurious oscillations in computed pressure



a) Numerical solution by P1–P1 without stabilization

a) Numerical solution by P1–P1 with stabilization

C. Rodrigo et al. / Comput. Methods Appl. Mech. Engrg. 298 (2016) 183–204

PDE system for 3-field poroelasticity

Physical structure - putting elasticty and flow together

$$
\begin{array}{llll}
-\mathrm{div}\, C : \varepsilon(u) & & +c_{up} \nabla p & = f_m, \\
& K^{-1} v & +\nabla p & = 0, \\
-c_{pu} \frac{\partial}{\partial t} \mathrm{div}(u) & -\mathrm{div}(v) & -c_{pp} \frac{\partial}{\partial t} p & = -f_s
\end{array}
$$

Analytical structure

$$
\begin{array}{llll}
-\mathrm{div}\, C : \varepsilon(u) & & +c_{up} \nabla p & = f_m, \\
& K^{-1} v & +\nabla p & = 0, \\
-c_{pu} \frac{\partial}{\partial t} \mathrm{div}(u) & -\mathrm{div}(v) & -c_{pp} \frac{\partial}{\partial t} p & = -f_s
\end{array}
$$

In time steps $k = 1, 2, \dots$ find

$u^k \in U_D \subset H^1(\Omega),\ v^k \in V_{bc} \subset H(div,\, \Omega),\ p^k \in Q = L_2(\Omega)$

$$
\begin{array}{cccc}
a_u(u^k, \eta) & & -(\mathrm{div}(\eta),\, p^k) & = f^k(\eta) \\
 & m(v^k, w) & -(\mathrm{div}(w),\, p^k) & = G^k(w), \\
-\frac{1}{\tau}(\mathrm{div}(u^k),\, q) & -(\mathrm{div}(v^k),\, q) & -\frac{1}{\tau}(c_{pp} p, q) & = -f_s^k(q) + \dots
\end{array}
$$

$$\forall \eta \in U_0,\ \forall w \in V_0,\ \forall q \in Q$$

Here we found the already defined bilinear forms of elasticity a_u , mass matrix of velocities m, etc.

$$m(v,\, w) = \int_\Omega k^{-1} v \cdot w \, d\Omega, \quad b_u(u,\, p) = (\mathrm{div}(u),\, p),$$

$$b_v(v,\, p) = (\mathrm{div}(v),\, p), \quad c(p,\, q) = (c_{pp} p, q)$$

Possible nonsymmetry b_u and b_{u1}. Another nonsymmetry due to τ can be removed by scaling with $\mathrm{diag}(1, \tau,\, \tau)$.

Consider the arrangement $((u,v),\, p) \in \mathbb{V} \times W$,

$\mathbb{V}_{bc} = U_D \times V_{bc}$, $\mathbb{V}_0 = U_0 \times V_0$

$\|((u,v)\|^2_{\mathbb{V}} = \|u\|^2_{H^1(\Omega)} + \|v\|^2_{H(div,\Omega)}$, $\|q\|_W = \|q\|_{2,0}$

Define the bilinear forms

$\mathbb{A}((u,v),(\eta,w)) = a(u,\eta) + \tau m(v,w)$

$\mathbb{B}((u,v),q) = b_u(u,q) + \tau b_v(v,q)$

Variational formulation - find $(u,v) \in \mathbb{V}_{bc},\ p \in W_D$

$$
\begin{array}{cccc}
\mathbb{A}((u,v),\,(\eta,w)) & +\mathbb{B}((\eta,w),\,p) & = & f^k(\eta) + G^k(w), \\
\mathbb{B}((u,v),\,q) & -\frac{c_{pp}}{\tau}(p,q) & = & -F_s^k(p) + \ldots
\end{array}
$$

$$\forall\,(\eta,\,w) \in \mathbb{V}_0,\ q \in W$$

$$\mathbb{Z} = \{(\eta, w) : \ \mathbb{B}((\eta, w), q) = 0 \ \forall q \in W\}$$

$$(div(u),\ q) = -\tau(div(v),\ q) \ \forall q \in W$$

Coerciveness on $\mathbb{Z}$

$$\mathbb{A}((u, v), (\eta, w)) = a(u, u) + \tau m(v, v) \geq \gamma_u \|u\|^2_{H^1(\Omega)} + \tau\gamma_v \|v\|^2_{L_2(\Omega)}$$

$$\geq \gamma \left(\|u\|^2_{H^1(\Omega)} + \|div(u)\|^2_{L_2(\Omega)} + \|v\|^2_{L_2(\Omega)}\right)$$

$$= \gamma \left(\|u\|^2_{H^1(\Omega)} + \|v\|^2_{H(div,\Omega)}\right) = \gamma \|((u, v)\|^2_{\mathbb{V}}$$

LBB

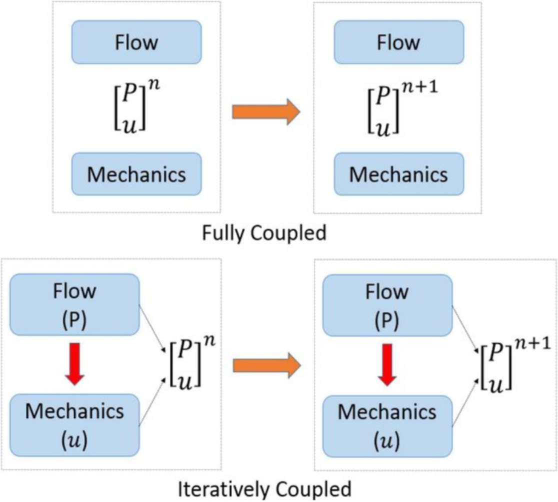
$$\sup_{(\eta,w)\in\mathbb{V}} \frac{|\mathbb{B}((\eta,w),p)|}{\|(\eta,v)\|_{\mathbb{V}}} \geq \sup_{(0,w)\in\mathbb{V}} \frac{|\mathbb{B}((0,w),p)|}{\|(0,v)\|_{\mathbb{V}}} \geq \beta \|p\|_W$$

Locking and nonconforming FEM for poroelasticity

- Discretization with P1/P1 and P1/RT0/P0 may cause locking effect in poroelasticity, pressure oscillations for a two- and three-field Biot's model, not parameter robustness
- recent papers
  - X. Hua, C. Rodrigo, FJ. Gaspar, LT. Zikatanov, JCAM 310 (2017) 143–154, Crouzeix–Raviart (CR) FEM for elasticity
  - C. Rodrigo, X. Hu, P. Ohm, JH. Adler, FJ. Gaspar, L. Zikatanov, New stabilized discretizations for poroelasticity and the Stokes' equations, arXiv:1706.05169 [math.NA] 2017 (P1 elements enriched by bubbles)
  - C. Rodrigo, X., FJ. Gaspar, X. Hu, L. Zikatanov, Stability and monotonicity for some discretizations of the Biot's consolidation model. Comput. Methods Appl. Mech. Engrg. 298 (2016) 183–204

Iterative coupling

Iterative coupling for linear/linear HM



P.M. Delgado V. M. Krushnarao Kotteda, V. Kumar, Hybrid Fixed-Point Fixed-Stress Splitting Method for Linear Poroelasticity. Geosciences 2019

- Step 0
- For $k = 1, 2, \ldots$
  - Step $k > 0$: find $(u^k, p^k) \in X \times Y$ such that

$$\begin{bmatrix} A_u & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix} = \begin{bmatrix} v \\ p \end{bmatrix},$$

where $C = c_{pp} M_p + \tau_k A_p$

- full coupling, monolithic scheme
- iterative coupling
- staggered scheme (one pass, one iteration)
- loose coupling (one process is updated after several time steps)

Gauss-Seidel for semidiscretization

$$
\begin{aligned}
a_u(u^k,\ w) + b_1(w, p^k) &= F_u^k(w) \ \ \forall w \in \boldsymbol{U}_0, \\
b(u^k, q) - c(p^k, q) &= F_p^k(q) \ \forall q \in W_0,
\end{aligned}
$$

can be solved iteratively, e.g. using the inital guess

$$
u^{k,0} = u^{k-1}, \ \ p^{k,0} = p^{k-1}
$$

and e.g. iterations for $i = 0, 1, \dots$

$$
\begin{aligned}
a_u(u^{k,i+1},\ w) + b_1(w, p^{k,i+1}) &= F_u^k(w) \ \ \forall w \in \boldsymbol{U}_0, \\
b(u^{k,i}, q) - c(p^{k,i+1}, q) &= F_p^k(q) \ \forall q \in W_0,
\end{aligned}
$$

$$\mathcal{A}z = \begin{bmatrix} A_u & B_1^T \\ B_2 & -C \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix} = \begin{bmatrix} f_u^k \\ f_p^k \end{bmatrix} = \mathcal{F}^k.$$

Note that if A_u is regular and $C + B_2 A_u^{-1} B_1^T$ is regular, then $\mathcal{A}$ is regular (block elimination, factorization).

$$z^{k,i+1} = z^{k,i} + \omega \begin{bmatrix} A_u & B_1^T \\ & -C \end{bmatrix}^{-1} \left(\mathcal{F}^k - \mathcal{A} z^{k,i} \right),$$

For $C \sim 0$ or $C = 0$ it is possible to use the iterations

$$z^{k,i+1} = z^{k,i} + \begin{bmatrix} A_u & B_1^T \\ & -(\omega^{-1} P + C) \end{bmatrix}^{-1} \left(\mathcal{F}^k - \mathcal{A} z^{k,i} \right).$$

Here $\omega > 0$ and $\omega^{-1} P \sim B_2 A_u^{-1} B_1^T$ of the Schur complement component.

If $u^\star, p^\star$ is the exact solution, $e_u^i = u^i - u^\star$ and $e_p^i = p^i - p^\star$ are the components of the error, then

$$e_u^{i+1} = -A_u^{-1} B_1^T e_p^i$$

$$e_p^{i+1} = (\omega^{-1} P + C)^{-1} \left(\omega^{-1} P + C - (C + B_2 A_u^{-1} B_1^T) \right) e_p^i.$$

If $B_1 = B_2 = B$, A_u is SPD, C is SPSD and $P = I$ then the Uzawa method can be reducted to Richardson method the equation for p,

$$e_p^{i+1} = (I - \omega B A_u^{-1} B^T) e_p^i, \quad \text{convergence for } \omega < \frac{2}{\lambda_{max}(B A_u^{-1} B^T)}.$$

$$\mathcal{A}_{u-p} = \begin{bmatrix} A_u & B_1^T \\ B_2 & -C \end{bmatrix} = \begin{bmatrix} I & \\ B_2 A_u^{-1} & I \end{bmatrix} \begin{bmatrix} A_u & \\ & -S_A \end{bmatrix} \begin{bmatrix} I & A_u^{-1} B_1^T \\ & I \end{bmatrix}.$$

Note that for 2-field poroelasticity we prefer this factorization with the Schur complement $S = S_A = C + B_2 A_u^{-1} B_1^T$ as

- (1) C can be close to zero and S_A provides a stabilization of C,
- (2) there is a good approximation to $B_2 A_u^{-1} B_1^T$, $B_2 A_u^{-1} B_1^T \sim M_p$.

$$\mathcal{P}_T = \begin{bmatrix} A_u & \\ & -S_A \end{bmatrix} \begin{bmatrix} I & A_u^{-1} B_1^T \\ & I \end{bmatrix} = \begin{bmatrix} A_u & B_1^T \\ & -S_A \end{bmatrix},$$

$$\mathcal{P}_D = \begin{bmatrix} A_u & \\ & -S_A \end{bmatrix}.$$

Theorem [Elman, Silvestr, Wathen, Finite Elements and Fast Iterative Solvers]:

$$C \leq C + BA_u^{-1}B^T \leq C + \tfrac{1}{c}M_p$$

$$\beta M_p \leq BA_u^{-1}B^T \leq \frac{1}{c}M_p$$

Proof.

$$\langle Bw, q\rangle^2 = (\alpha div(w),\ q)^2$$
$$\leq \tfrac{\alpha}{\lambda} a_u(w,\ w)(q, q) = \tfrac{1}{c}\langle A_u w,\ w\rangle \langle M_p q,\ q\rangle$$

Taking $w = A_u^{-1}B^T q$, we get

$$\left\langle BA_u^{-1}B^T q, q\right\rangle^2 \leq \frac{1}{c}\left\langle B_1^T q,\ A_u^{-1}B_1^T q\right\rangle \langle A_p q,\ q\rangle .$$

If the (Stokes type) inf-sup condition is valid,

$$\sup_w \tfrac{(\alpha div(w),\, q)}{a_u(w,\, w)^{1/2}} = \sup_w \tfrac{\langle Bw, q\rangle}{\langle A_u w, w\rangle^{1/2}} \geq \tfrac{\left\langle BA_u^{-1}B^T q, q\right\rangle}{\left\langle B^T q, A_u^{-1}B^T q\right\rangle^{1/2}}$$
$$= \left\langle BA_u^{-1}B^T q, q\right\rangle^{1/2} \geq \beta \langle M_p q,\ q\rangle^{1/2}$$

Analysis of diagonal preconditioner

Let

$$\mathcal{M} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \ \mathcal{P} = \begin{bmatrix} \tilde{A}_{11} & \\ & -A_{22} \end{bmatrix}$$

with A_{11}, $-A_{22}, \tilde{A}_{11}$ being SPD,

Lemma 1: Let $\tilde{A}_{11} = S = A_{11} - A_{21}A_{22}^{-1}A_{12}$, then

$$\sigma(\mathcal{P}^{-1}\mathcal{M}) \subset \left\langle \frac{-1-\sqrt{5}}{2}, -1 \right\rangle \cup \left\langle \frac{-1+\sqrt{5}}{2}, 1 \right\rangle$$

Lemma 2: Let there be $\xi_0, \xi_1 > 0$ such that $\xi_0 S \leq \tilde{A}_{11} \leq \xi_1 S$, then

$$\sigma(\mathcal{P}^{-1}\mathcal{M}) \subset \left\langle -\frac{1}{2} - \frac{1}{2}\sqrt{1+\frac{4}{\xi_0}}, \ -1 \right\rangle \cup \left\langle -\frac{1}{2} + \frac{1}{2}\sqrt{1+\frac{4}{\xi_1}}, \ \frac{1}{\xi_0} \right\rangle$$

RB: Report IGAS 2012, 2015. Note in the case $A_{22} = 0$, there is result from M. F. Murphy, G. H. Golub, and A. J. Wathen, SIAM J. Sci. Comput., 21 (2000)

Block triangular preconditioners

$$\mathcal{A}_{u-p}\mathcal{P}_t^{-1} = \begin{bmatrix} I & \\ B_2 A_u^{-1} & I \end{bmatrix} = I + X,$$

$$X = \begin{bmatrix} 0 & \\ B_2 A_u^{-1} & 0 \end{bmatrix}, \quad X^2 = 0.$$

- Right preconditioned system $\mathcal{A}_{u-p}\mathcal{P}_t^{-1}$ has minimal polynomial $p(\lambda) = (\lambda - 1)^2$,
- For the left preconditioning, $\mathcal{P}_t^{-1}\mathcal{A}_{u-p} = \mathcal{P}_t^{-1}\left(\mathcal{A}_{u-p}\mathcal{P}_t^{-1}\right)\mathcal{P}_t$, therefore $p\left(\mathcal{P}_t^{-1}\mathcal{A}_{u-p}\right) = \mathcal{P}_t^{-1}p\left(\mathcal{A}_{u-p}\mathcal{P}_t^{-1}\right)\mathcal{P}_t = 0$, i.e. left preconditioned system has also minimal polynomial of order 2.
- Inexact solution of the block subproblems?
- Spectral analysis [Axelsson], analysis through field of values [Rodrigo et al.]

Discrete 3-field poroelasticity system

The space discretization provides DAE

$$\mathcal{A}_1 \frac{\partial}{\partial t}\mathcal{U} + \mathcal{A}_0\mathcal{U} = \mathcal{F}$$

with the matrices $\mathcal{A}_1$and $\mathcal{A}_0$ and blocks $A \leftrightarrow a$, $M \leftrightarrow m$, $B_u \leftrightarrow b_u$, $B_v \leftrightarrow b_v$, $C \leftrightarrow c$,

$$\mathcal{A}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ B_u & 0 & -C \end{bmatrix}, \quad \mathcal{A}_0 = \begin{bmatrix} A & 0 & B_u^T \\ 0 & M & B^T \\ 0 & B & 0 \end{bmatrix}, \quad \mathcal{U} = \begin{bmatrix} u \\ v \\ p \end{bmatrix}$$

Backward Euler provides in k+1th step the system

$$(\mathcal{A}_1 + \tau\mathcal{A}_0)\mathcal{U}^{k+1} = \mathcal{F}(t_{k+1}) + \mathcal{A}_1\mathcal{U}^k$$

with the Euler matrix $\mathcal{A}_E$,

$$\mathcal{A}_\tau = \begin{bmatrix} A & 0 & B_u^T \\ 0 & M & B^T \\ \frac{1}{\tau}B_u & B & -\frac{1}{\tau}C \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1/\tau & \\ & & 1/\tau \end{bmatrix} \begin{bmatrix} A & 0 & B_u^T \\ 0 & \tau M & \tau B^T \\ B_u & \tau B & -C \end{bmatrix}$$

There are several block type preconditioners for the symmetrized Euler matrix

$$\mathcal{A}_E = \mathcal{A}_\tau^{sym} = \begin{bmatrix} A & 0 & B_u^T \\ 0 & \tau M & \tau B^T \\ B_u & \tau B & -C \end{bmatrix}.$$

Restricting to block diagonal, SPD ones, we can consider

$$\mathcal{P} = \begin{bmatrix} A & 0 & \\ 0 & \tau M & \\ & & S_{AM} \end{bmatrix} \quad or \quad \mathcal{P} = \begin{bmatrix} S_{11} & S_{12} & \\ S_{21} & S_{22} & \\ & & C \end{bmatrix} \quad or \quad \mathcal{P} = \begin{bmatrix} \color{red}{S_{11}} & \color{blue}{S_{12}} & \\ & \color{red}{S_{22}} & \\ & & \color{red}{C} \end{bmatrix}$$

$$\mathcal{P} = \begin{bmatrix} A + B_u^T C^{-1} B_u & \color{blue}{\tau B_u^T C^{-1} B} & \\ & \tau M + \tau^2 B^T C^{-1} B & \\ & & C \end{bmatrix}$$

O. Axelsson, RB, P. Byczanski, Computing and Visualization in Science. Vol. 15, No. 4 (2012), pp. 191-207

Diagonalization

- There is spectral equivalence[1]

$$(1-\gamma)\begin{bmatrix} S_{11} & \\ & S_{22} \end{bmatrix} \leq \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \leq (1+\gamma)\begin{bmatrix} S_{11} & \\ & S_{22} \end{bmatrix},$$

where $0 \leq \gamma < 1$ such that

$$|\langle S_{12}v,\, u\rangle| \leq \gamma\sqrt{\langle S_{11}u,\, u\rangle}\sqrt{\langle S_{22}v,\, v\rangle}\ \ \forall u, v,$$

$$\gamma^2 \leq (1+c_{pp}c_{el})^{-1}, \ \text{ where } \ c_{el}\,\|\mathrm{div}(u_h)\|^2_{L_2} \leq \langle Au,\, u\rangle$$

For isotropic elasticity with Lamè constants λ and μ, $c_{el} \geq \lambda$.

- Robustness w.r.t. k and h
- Typical values[2] of storativity and $\lambda = \frac{E\nu}{(1-2\nu)(1+\nu)}$,
  $c_{pp} \sim 10^{-6} - 10^{-4}$, $c_{el} \sim 10^6 - 10^9 \Rightarrow \gamma \leq (\ll)1/2$

(1) O. Axelsson, RB, T. Luber, LSSC 2015, LNCS 9374, Springer, 2015, pp. 3-14,

(2) Data Collection Handbook to Support Modelling Impacts of Radioactive Material in Soil and Building Structures, Argonne Nat. Lab. 2015

Fixed strain iterations

The Gauss-Seidel method,

$$z^{k,i+1} = z^{k,i} + \begin{bmatrix} A_u & B_1^T \\ & -C \end{bmatrix}^{-1} \left(\mathcal{F}^k - \mathcal{A}z^{k,i}\right),$$

uses triangular preconditioner which requires to solve the system with C or in the variational form

$$-c(p^{k,i+1}, q) = -(c_{pp}p^{k,i+1}, q) - \tau_k a_p(p^{k,i+1},\, q) = R_p^k(q) \;\; \forall q \in W_0.$$

Such equation correspond to PDE

$$\underbrace{\alpha \frac{\partial}{\partial t}\mathrm{div}(u)}_{=0} + c_{pp}\frac{\partial}{\partial t}p - \mathrm{div}(\kappa \nabla p) = r_p.$$

With respect to $\alpha \frac{\partial}{\partial t}\mathrm{div}(u) = 0$, the procedure is called fixed strain iterations.

Fixed stress iterations

We already know, that better preconditioning should use the Schur complement S_A, or its sparse approximation, instead of C alone. Such sparse approximation of S_A can be also derived as follows:

The volume deformation is in a relation with volumetric stress,

$$\frac{\partial}{\partial t}\sigma_{vol} = K_b \frac{\partial}{\partial t}\mathrm{div}(u) - \alpha \frac{\partial}{\partial t} p,$$

where K_b is the bulk modulus of the porous material, which can be expressed through Lame moduli as $K_b = \lambda + \frac{2}{3}\mu$.

The assumption $\frac{\partial}{\partial t}\sigma_{vol} = 0$, fixed stress, then provides $K \frac{\partial}{\partial t}\mathrm{div}(u) = \frac{\alpha}{K}\frac{\partial}{\partial t} p$ and

$$\left(c_{pp} + \frac{\alpha^2}{K}\right)\frac{\partial}{\partial t} p - \mathrm{div}(\kappa \nabla p) = r_p.$$

Variationally, $p^{k,i+1}$ is computed from

$$-c(p^{k,i+1},q) = -(\left(c_{pp} + \frac{\alpha^2}{K}\right) p^{k,i+1}, q) - \tau_k a_p(p^{k,i+1},\ q) = R_p^k(q)\ \forall q \in W_0.$$

Consequently, the triangular preconditioner uses modified $\widetilde{C}$ which is a sparse matrix approximation to S_A.

The additional term is algebraically $\frac{\alpha^2}{K} M_p$ and it can be used for modification of the original discretized system, which gets the form

$$\mathcal{A}z = \begin{bmatrix} A_u & B_1^T \\ B_2 & -C - \frac{\alpha^2}{K} M_p \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix} = \begin{bmatrix} f_u^k \\ f_p^k \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & -\frac{\alpha^2}{K} M_p \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix}.$$

The Gauss-Seidel method then get the form

$$\begin{bmatrix} A_u & B_1^T \\ & -\widetilde{C} \end{bmatrix} z^{k,i+1} = \begin{bmatrix} f_u^k \\ f_p^k \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ B_2 & -\frac{\alpha^2}{K} M_p \end{bmatrix} z^{k,i}.$$

HO time discretizarion

Backward Euler time discretization - time step systems:

$$\mathcal{A}_E \mathcal{U}^{k+1} = \mathcal{F}^{k+1} + \frac{1}{\tau}\mathcal{A}_1 \mathcal{U}^k$$

$$\mathcal{A}_E = \frac{1}{\tau}\mathcal{A}_1 + \mathcal{A} = \begin{bmatrix} M & B^T \\ B & -\frac{1}{\tau}C \end{bmatrix}$$

Radau IIA time discretization uses time step with two substeps

$$\begin{bmatrix} \frac{1}{\tau}\mathcal{A}_1 + \frac{5}{12}\mathcal{A} & -\frac{1}{12}\mathcal{A} \\ \frac{3}{4}\mathcal{A} & \frac{1}{\tau}\mathcal{A}_1 + \frac{1}{4}\mathcal{A} \end{bmatrix} \begin{bmatrix} \mathcal{U}^{k+1/3} \\ \mathcal{U}^{k+1} \end{bmatrix} = RHS$$

Block diagonal and triangular preconditioners with Euler type blocks on the diagonal are introduced and analyzed in Axelsson, Blaheta and Luber[1].

[1] O. Axelsson, RB and T. Luber, I. Lirkov et al. (Eds.): LSSC 2015, LNCS 9374, pp. 3–14, Springer 2015.

Nonlinear Hydromechanics

Hydro-mechanics with nonlinearities

- linear models - linear couplings (poroelasticity)
- non-linear models - linear couplings (Richards model, multiphase model)
- linear models - non-linear couplings
- non-linear models - non-linear couplings

Examples of nonlinearities can be different

1. nonlinear elasticity with variable bulk modulus
2. plasticity
3. unsaturated Richards model
4. two-phase flow
5. Kozeny-Carman
6. cubic law

Time stepping algorithm in discrete form

- Step 0
- For $k = 1, 2, \ldots$
  - Step $k > 0$: find $(u^k, p^k) \in X \times Y$ which solve the nonlinear system

$$\begin{bmatrix} A_u(u^k, p^k) & B^T \\ B & -C(u^k, p^k) \end{bmatrix} \begin{bmatrix} u^k \\ p^k \end{bmatrix} = \begin{bmatrix} f^k \\ g^k \end{bmatrix},$$

$$\mathcal{G}(z^k)z^k = \mathcal{F}^k, \;\; z^k = \begin{bmatrix} u^k \\ p^k \end{bmatrix},$$

where $C(u^k, p^k) = c_{pp}M_p + \tau_k A_p(u^k, p^k)$

end time stepping

Time stepping algorithm with nonlinear iterations

- Step 0
- For $k = 1, 2, \ldots$
  - Step $k > 0$: find $(u^k,\, p^k) \in X \times Y$ by iterations:
    take $u^{k,0}$ and $p^{k,0}$
    iterate for $l = 0, 1, 2, \ldots$

$$z^{k,l+1} = z^{k,l} + \mathcal{D}(z^k)^{-1}\left(\mathcal{F}^k - G(z^k)\right),\ \ \mathcal{D} = D\mathcal{G}.$$

end time stepping

Nonlinear couplings, Biot-Kozeny model

We shall consider the model with conductivity depending on volumetric deformation, $\kappa = \kappa(\nabla \cdot u)$,

$$a_p(p, q) = (\kappa(\nabla \cdot u)\nabla p,\, \nabla q)_{2,0}.$$

The function κ is assumed to be continuously differentiable, $\kappa_{min} \leq \kappa \leq \kappa_{max}$ more properties of κ will be specified later.

Particularly, κ can be determined by **Kozeny-Carman formula,**

$$\kappa = \kappa_0 \frac{(1-\phi_0)^2}{\phi_0^3} \frac{\phi^3}{(1-\phi)^2},$$

where ϕ_0 is the initial porosity giving the conductivity κ_0, $\phi = \phi_0 + \alpha \nabla \cdot u$.

- Josef Kozeny 1927, Prof. at U of Agricultural Sciences in Vienna, since 1929 at TU Vienna.
- Philipe Carman, 1937 (modified equation), 1956. Prof. at University College London, UCL Department of Chemical Engineering.

Picard method for Biot-Kozeny model

$$
\begin{aligned}
a_u(u^k,\, w) + b_1(w, p^k) &= F_u^k(w) \;\; \forall w \in \boldsymbol{U}_0,\\
b(u^k, q) - c(u^k; p^k, q) &= F_p^k(q) \;\; \forall q \in W_0
\end{aligned}
\tag{3}
$$

with nonlinearity involved in

$$
c(u^k; p^k, q) = ((c_{pp} + m)p^k, q) + \tau_k(\kappa(\nabla \cdot u^k)\nabla p^k,\, \nabla q),
$$

where $m = \frac{\alpha^2}{K_b}$ is the fixed stress stabilization term.

Picard method with iterations $l = 1, 2, \ldots$

$$
\begin{aligned}
a_u(u^{k,l},\, w) + b_1(w, p^{k,l}) &= F_u^k(w) \;\; \forall w,\\
b(u^{k,l}, q) - ((c_{pp} + m)p^{k,l}, q) - \tau_k(\kappa(\nabla \cdot u^{k,l-1})\nabla p^{k,l},\, \nabla q) &= F_p^k(q) \;\; \forall q.
\end{aligned}
$$

Theorem

Let $\xi = \tau_k \frac{c_2^2}{\kappa_{min}\lambda} < 1$ *then for* $l \to \infty$,

$$c_{Fu} \left\| e_u^{k,l} \right\|_{2,1} \leq \left\| e_u^{k,l} \right\|_{a_u} \to 0$$

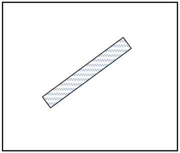
and

$$c_{Fp} \left\| e_p^{k,l} \right\|_{2,1} \leq \left\| \nabla e_p^{k,l} \right\|_{2,0} \leq \frac{c_2^2}{\kappa_{min}\lambda} \left\| e_u^{k,l-1} \right\|_{a_u} \to 0,$$

where c_{Fu} *and* c_{Fp} *are constants from the corresponding Korn and Friedrichs identities, The linear convergence of both* $u^{k,l} \to u^k$ *and* $p^{k,l} \to p^k$ *in the Sobolev* H^1*-norms is proven.*

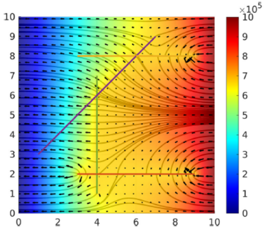
Disturbed continua

Models for disturbed zones / fractures



We can consider Biot-Kozeny as a simple possibility to model Faults / Fractures:

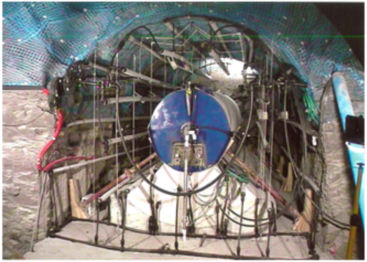
- Mechanically F/F behaves as a week material. It can be modified to material which becomes stiffer when F/F is closing,
- Hydraulic conductivity is decreasing with closing the F/F (volumetric change), the flow in F/F communicate with the flow in the porous matrix,
- Couplings are given by fluid pressure contributing to the total stress, change of conductivity with pore space change and fluid movement due to opening or closing of pores inside F/F.

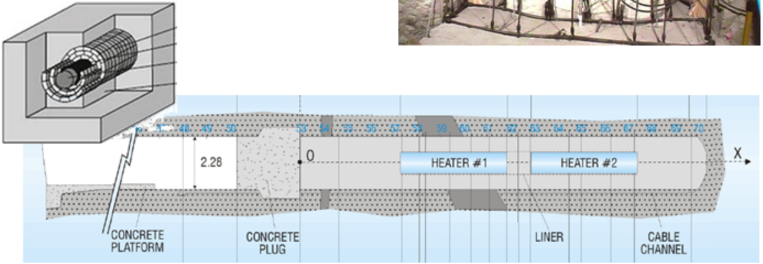


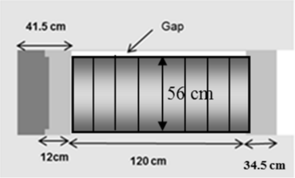
In the model from [Comp. Geosciences 2020] we consider the steady regime which is still described by two-way coupling as mechanics influence the conductivity (not the case of poroelasticity). This model assumes that:

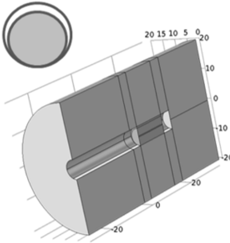
- Mechanically F/F behaves without its own response to outer load, mutual penetration of F/F walls is avoided by Signorini type conditions,
- Hydraulic conductivity is connected with aperture (cubic law) and decreasing with closing the F/F (decreasing aperture), the flow in F/F communicate with the flow in the porous matrix,
- The coupling is due to fluid pressure on F/F walls and change of conductivity with the change of aperture.

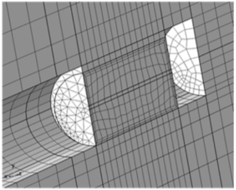
Applications




2.28
0
HEATER #1
HEATER #2
X
CONCRETE PLATFORM
CONCRETE PLUG
LINER
CABLE CHANNEL







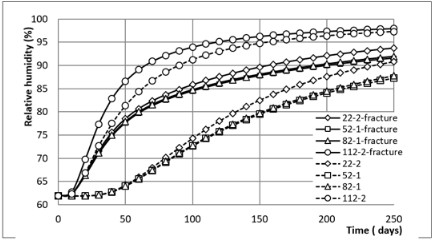


Fig. 4.2: Development of relative humidity in four sensor positions (see Fig. 1.3). The simulations with (suffix fracture) and without (no suffix) of the inter-block fractures in the model.

Conclusions

Important applications in geomechanics (nuclear waste, geothermal energy, energy accummulation), biomechanics etc.

Interesting mathematics

- coupled processes,
- saddle point structure, stable discretization
- three levels of iterative methods - (1) nonlinear, (2) linear systems, (3) solution of individual block systems,
- robustness w.r.t. discretization, convergence of iterative solvers

Faults / fractures in granite type rocks - TACR ENDORSE, H2020 EURAD

Thank you for your attention !