
Modelling and Simulation of complex GeoTechnical Problems

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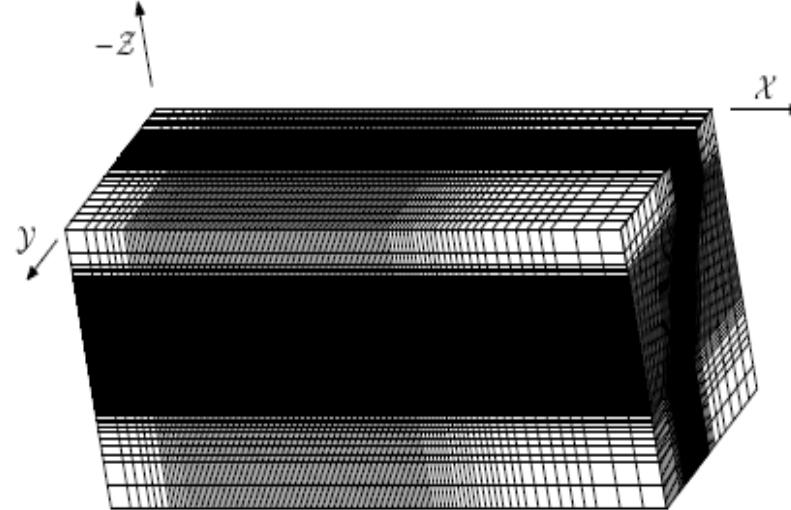
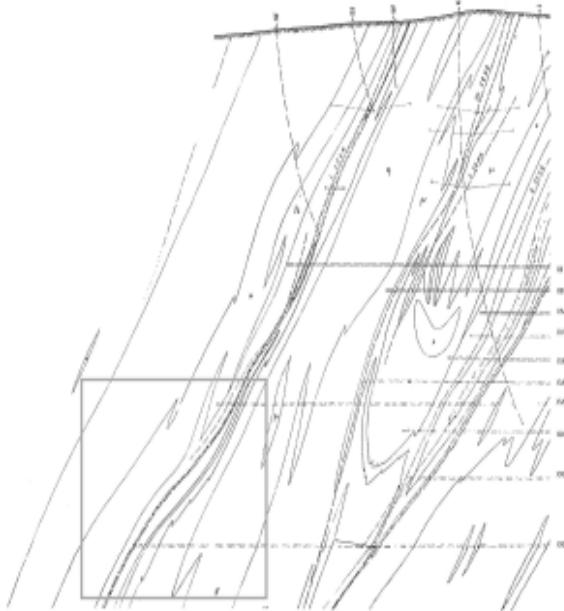
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Outline

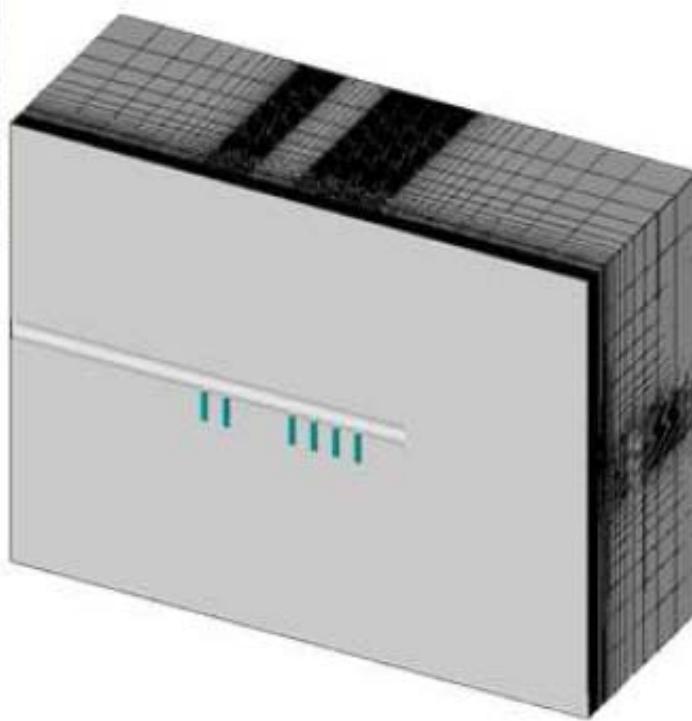
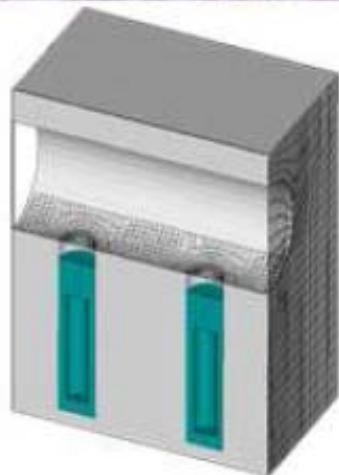
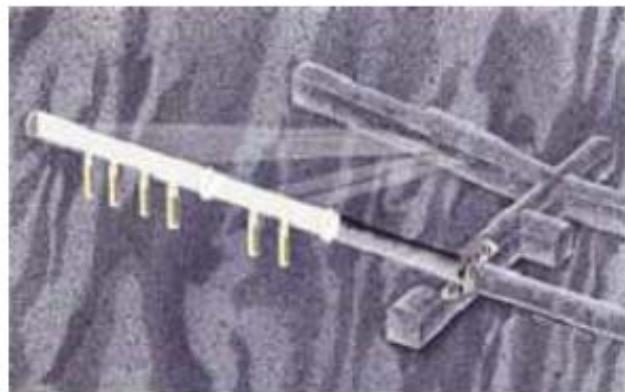
- Project “Modelling and Simulation of complex Technical Problems”
 - numerical methods
 - computer implementation
 - engineering applications
- GeoTechnical Problems
- Krylov space method problems
- Parallel preconditioners
- Results

Problem – GEAM Uranium mine



- Renewed interest
- Mining sequence, general in situ stress, large-scale
- Previous computations: Multiscale, 4+1 million DOF's

Äspö – underground deposition of the spent nuclear fuel (T-M-H) Decovalex 2011

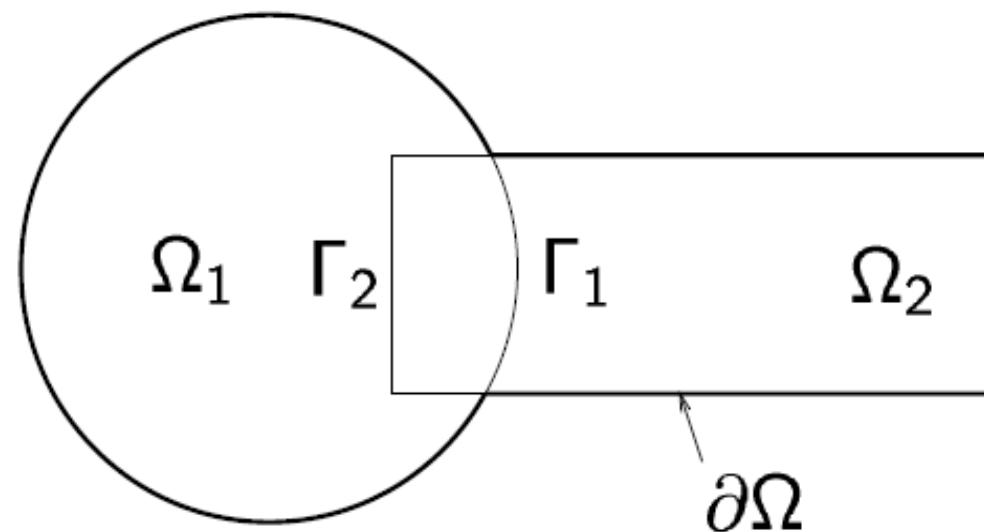


- thermo
- elastic.
- 2.5
- + 7.5
- MDOF
- time-
step.
meth.

Development of numerical methods based on Schwarz overlapping domain decomposition



- H.A. Schwarz, 1869
- P.L. Lions 1988, hundreds (?) papers
- SNA 2005

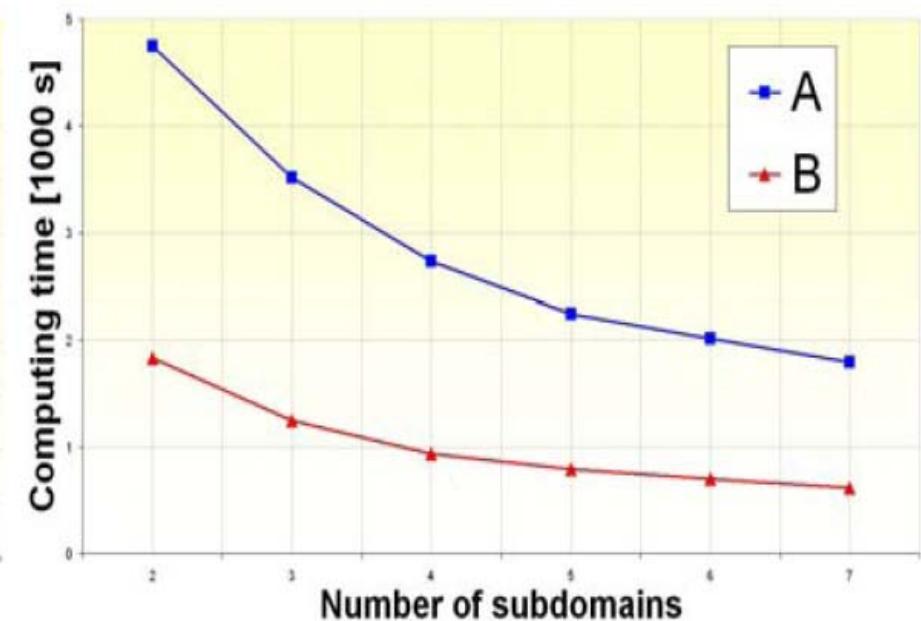
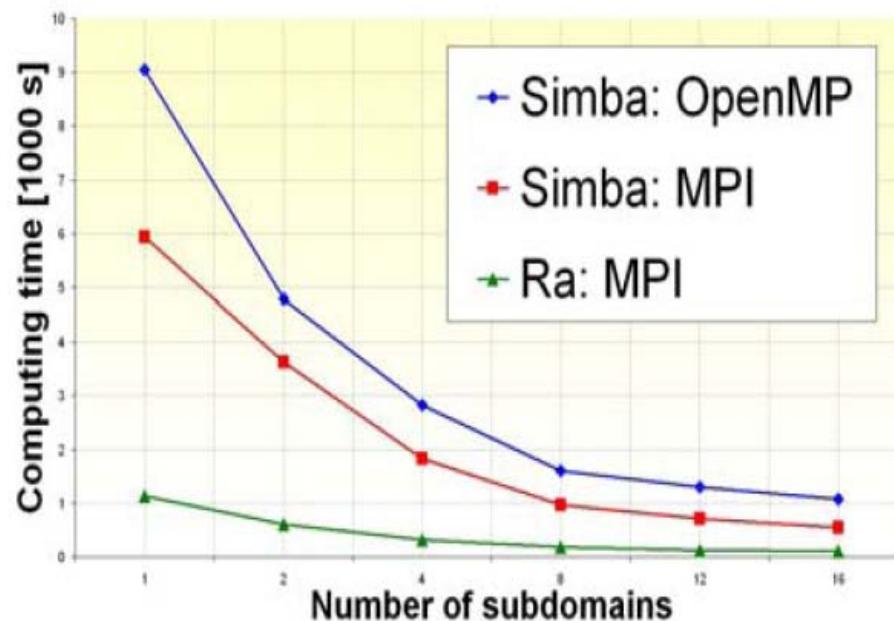


Our implementation (SNA 2004)

- a **black box method** working with
 - Decomposition of the stiffness matrix based on a domain decomposition
 - Coarse approximation created algebraically by **aggregation**
 - **Inexact solution** of subproblems
 - Hybrid **nonsymmetric variant** of two-level preconditioning
 - modification (stabilization) of the outer CG method (**GPCG**)
- parallel implementation with **MPI and OpenMP**
- code optimization
- **difference** between the solution of stationary and evolution problems

Schwarz methods – Äspö problem

one-level $A^{-1} \sim \sum_k R_k^T A_k^{-1} R_k$ or two-level $A^{-1} \sim \sum_k R_k^T A_k^{-1} R_k + R_0^T A_0^{-1} R_0$



New: stationary saturated Darcy flow

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

$$\mathbf{v} = -K_H \nabla p \text{ in } \Omega,$$

$$Lp - \mathbf{v} \cdot \mathbf{n} = g \text{ on } \Gamma = \partial\Omega$$

\mathbf{v} is the Darcy velocity, \mathbf{G} is the source/sink term, \mathbf{K} is the hydraulic conductivity tensor, \mathbf{p} is the pressure (total head), \mathbf{L} , \mathbf{g} are given functions on

$$\partial\Omega = \Gamma_* \cup \Gamma_0, L \neq 0 \text{ on } \Gamma_*, L = 0 \text{ on } \Gamma_0$$

Mixed variational formulation

find $v \in V \subset H(\text{div}, \Omega)$, $p \in L_2(\Omega)$

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

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

- This variational formulation is a basis for the **mixed finite element method**
- 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.

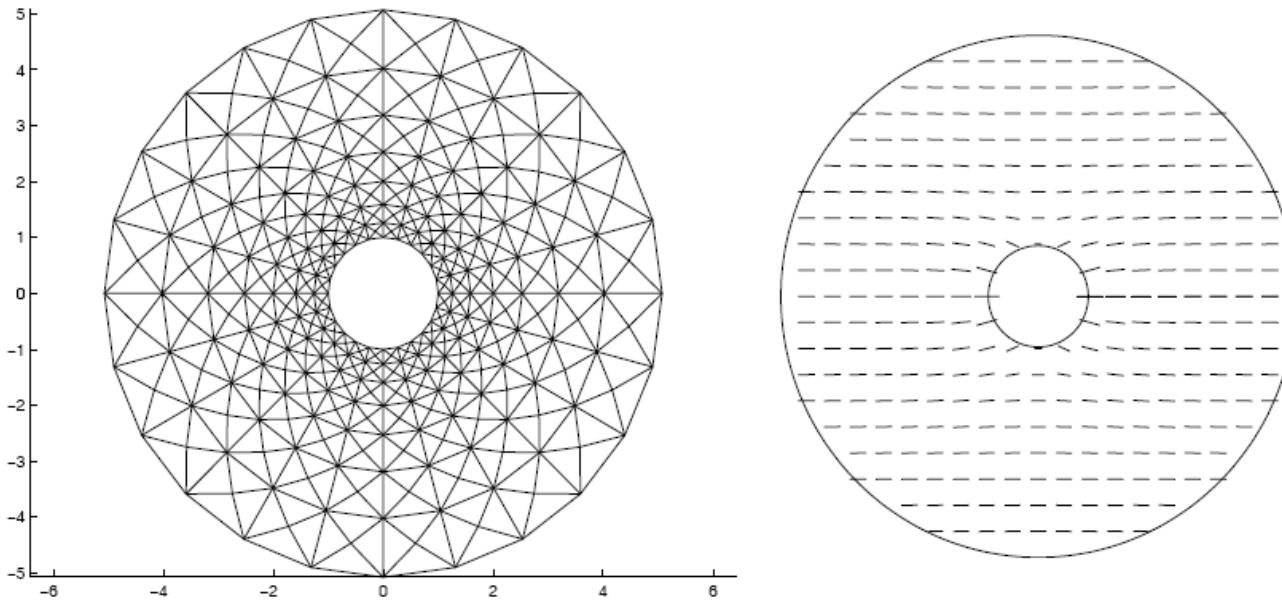
Mixed FEM => Saddle point system

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

$$M_H + \eta^{-1} B^T B \iff K_H^{-1} - \text{grad div}$$

- Use of the Schwarz method for the first block
- Assembling subdomain contributions to Block11
- Homogeneous Dirichlet BC on inner boundaries
- Inexact solvers

Model Darcy flow problem



$\operatorname{div}(v(x)) = 0$ 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} .

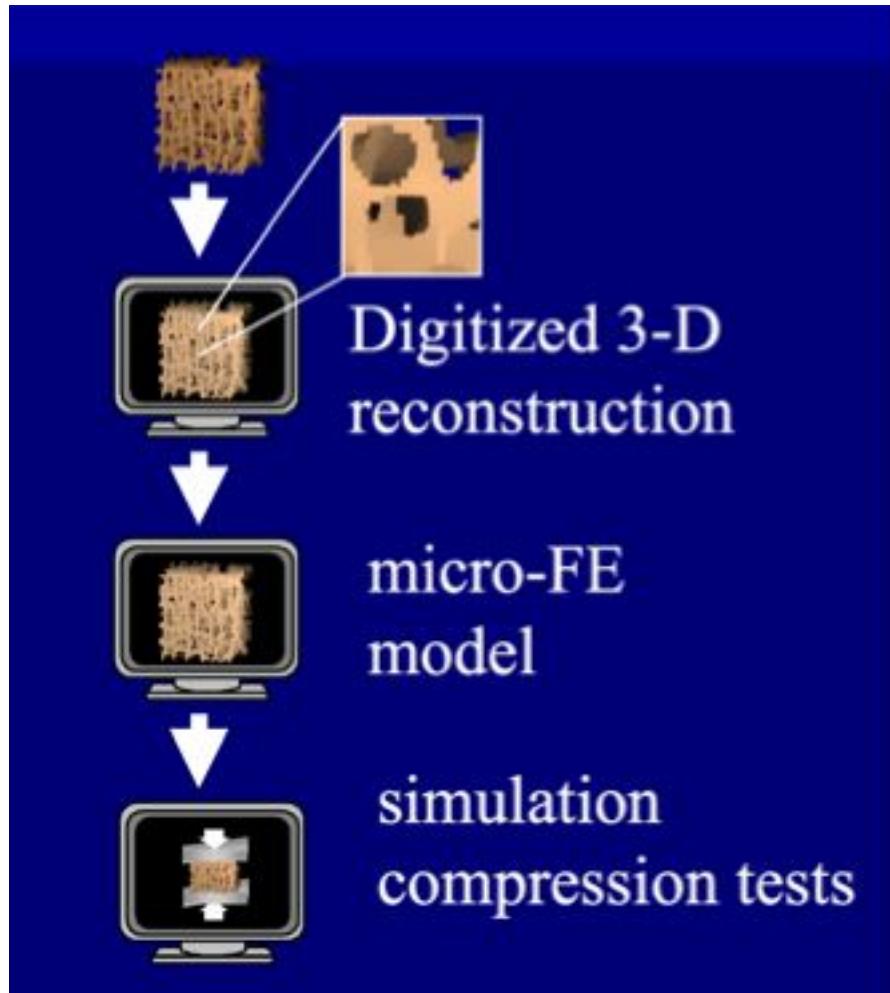
Numerical results

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} .

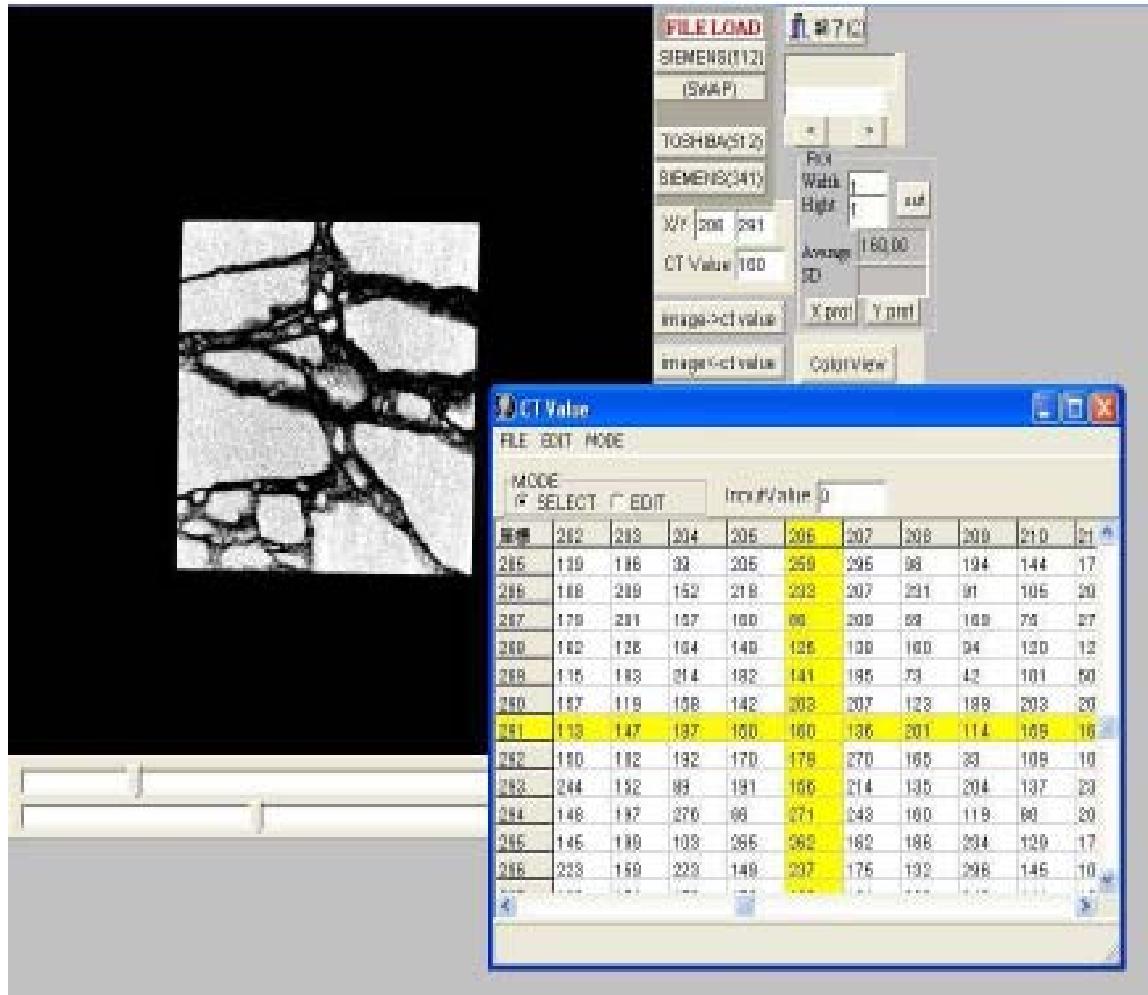
- Hypothesis: for $\eta=1$, one-level Schwarz is sufficient

Microstructure modelling – micro FEM



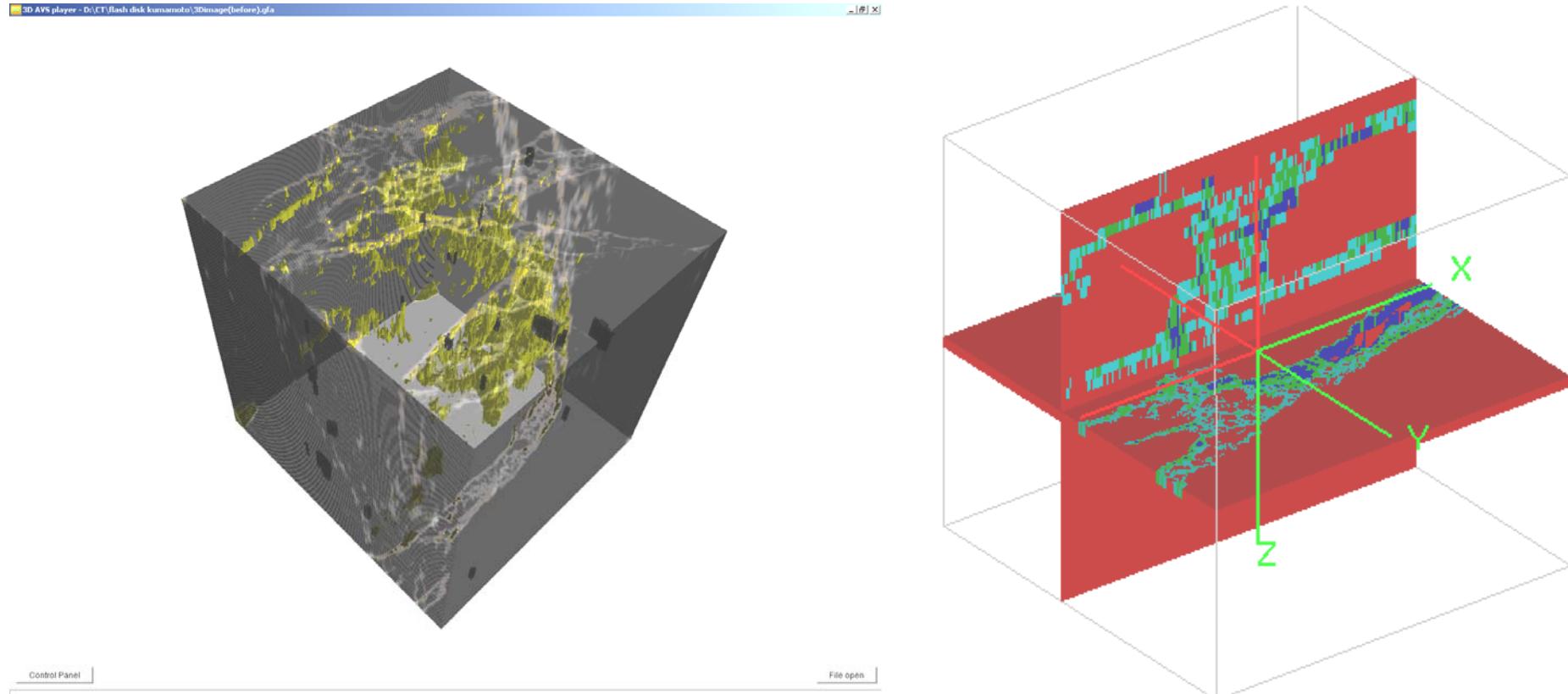
- CT scan (Kumamoto U.) >investigation of fracture, wetting, permeability changes etc.
- micro FEM analysis > upscaling, developing constitutive relations for poroelasticity, clearing up the H-M coupling effects etc.

Coal geocomposites – voxel FEM analysis



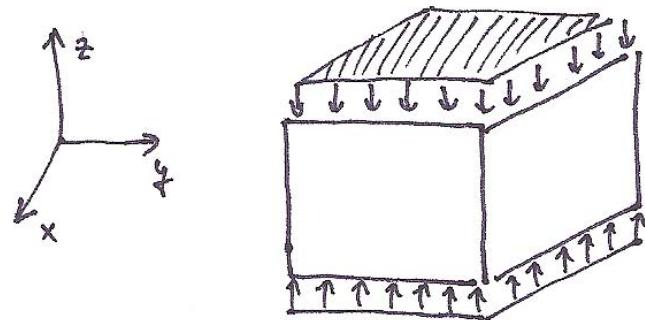
- 75×75×75mm
- CT
- voxel grid 0.3 × 0.3 × 2.0 mm
- 6.5 MDOF's
- CT values > material prop.
- Num. pasting >larger REV's

Visualization of the microstructure



- Toshiba CT vs. FEM grid visualization. Data smoothing.

Upscaling



$$\begin{aligned} \bar{\epsilon}_x &= \bar{\epsilon}_{y\perp} = \bar{\epsilon}_{x\perp} = \bar{\epsilon}_{xy} = \bar{\epsilon}_{yz} \\ &= \bar{\epsilon}_{zx} = 0 \end{aligned}$$

$$\bar{\epsilon}_z \text{ ; } \bar{\epsilon}_y, \bar{\epsilon}_x$$

$$\begin{bmatrix} \bar{\epsilon}_x \\ \bar{\epsilon}_y \\ \bar{\epsilon}_z \\ \bar{\epsilon}_{xy} \\ \bar{\epsilon}_{yz} \\ \bar{\epsilon}_{zx} \end{bmatrix} = \begin{bmatrix} 1 & -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} \\ -\frac{1}{\sqrt{m}} & 1 & -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} \\ -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} & 1 & -\frac{1}{\sqrt{m}} \\ -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} & -\frac{1}{\sqrt{m}} & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

- simplest and more general anisotropic upscaling
- upscaling strength parameters
- different loadings

Singular systems

given u^0

$$w = Au^0$$

$$r^0 = b - w$$

$$v^0 = g^0 = Gr^0$$

for $i = 0, 1, \dots$ **until** $\|r^i\| \leq \varepsilon \|b\|$ **do**

$$w = Av^i$$

$$\alpha = \langle r^i, g^i \rangle / \langle w, v^i \rangle$$

$$u^{i+1} = u^i + \alpha v^i$$

$$r^{i+1} = r^i - \alpha w$$

$$g^{i+1} = Gr^{i+1}$$

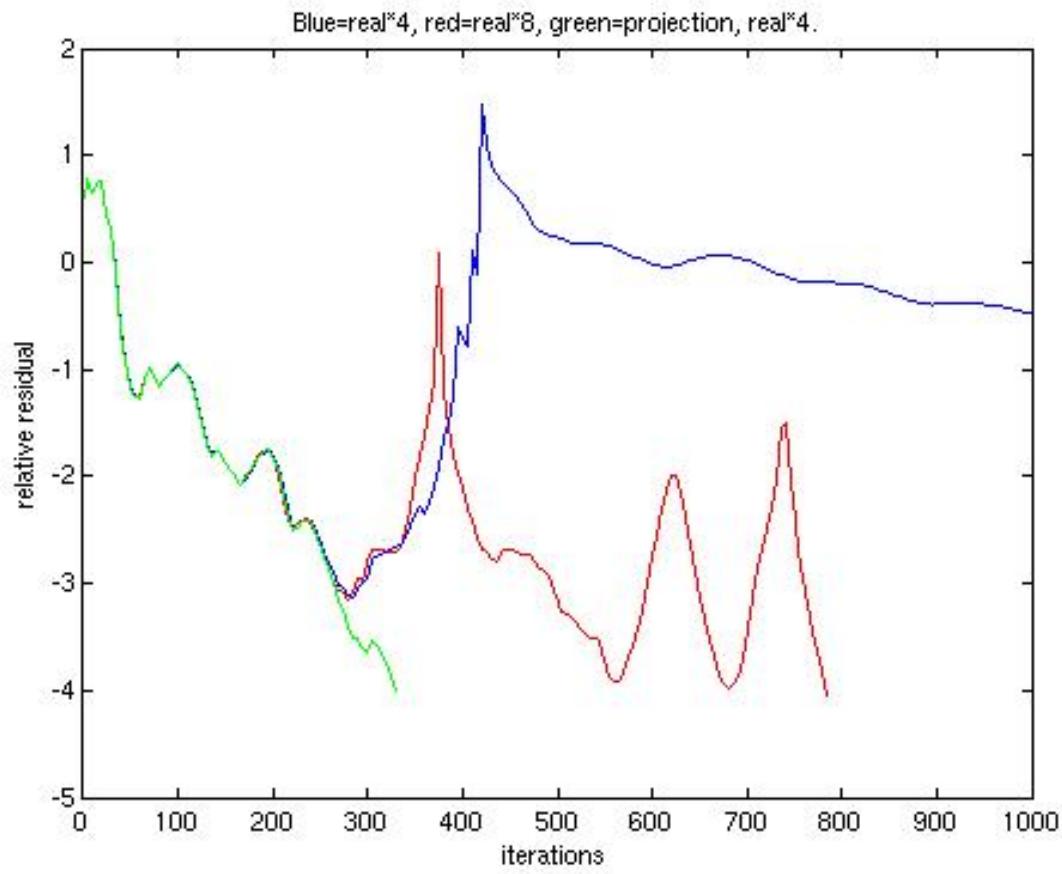
$$\beta = \langle r^{i+1}, g^{i+1} \rangle / \langle r^i, g^i \rangle$$

$$v^{i+1} = g^{i+1} + \beta v^i$$

end for

- $Au=b$
- singular & consistent \Rightarrow CG
- $R^n = N_0 + R_0$
- $P: R^n \rightarrow R_0$
- $PAPu = Pb$
- $A \leftarrow PAP$
- $b \leftarrow Pb$
- $G \leftarrow PGP$
- $R \leftarrow PR$

Convergence of PCG in singular case



- Model problem
58x58x38
layered structure
- **Blue:** real*4 for
matrix and
vectors
- **Red:** real*8,
matrix created in
real*4
- **Green:** use of
projections r*4

Singular systems – another issues

- Alternative approach – use of augmented system
(Axelsson etc., Marek 60 - Pilsen)
- More clear information about the spectrum
- Stopping criteria

Publications

- R. Blaheta, P. Byczanski, O. Jakl, R. Kohut, A. Kolcun, K. Krečmer, J. Starý,, Future Generation Computer Systems - special issue "Numerical Modelling in Geomechanics and Geodynamics". 22 (2006) 449-459
- Blaheta, Radim ; Kohut, Roman ; Neytcheva, M. ; Starý, Jiří.. Mathematics and Computers in Simulation, 76(2007), 1-3, pp. 18-27.
- R. Blaheta, P. Byczanski, R. Kohut, J. Starý, Modelling THM Processes in Rocks with the Aid of Parallel Computing, GeoProc 2008, Lille, France (accepted)
- R. Blaheta, P. Byczanski, R. Kohut, J. Starý, Parallel Computing Methods for Modelling THM Processes in Rocks, IACMAG 2008, Goa (accepted)



Thank you for your attention !
