Solving augmented systems in the potential fluid flow problem

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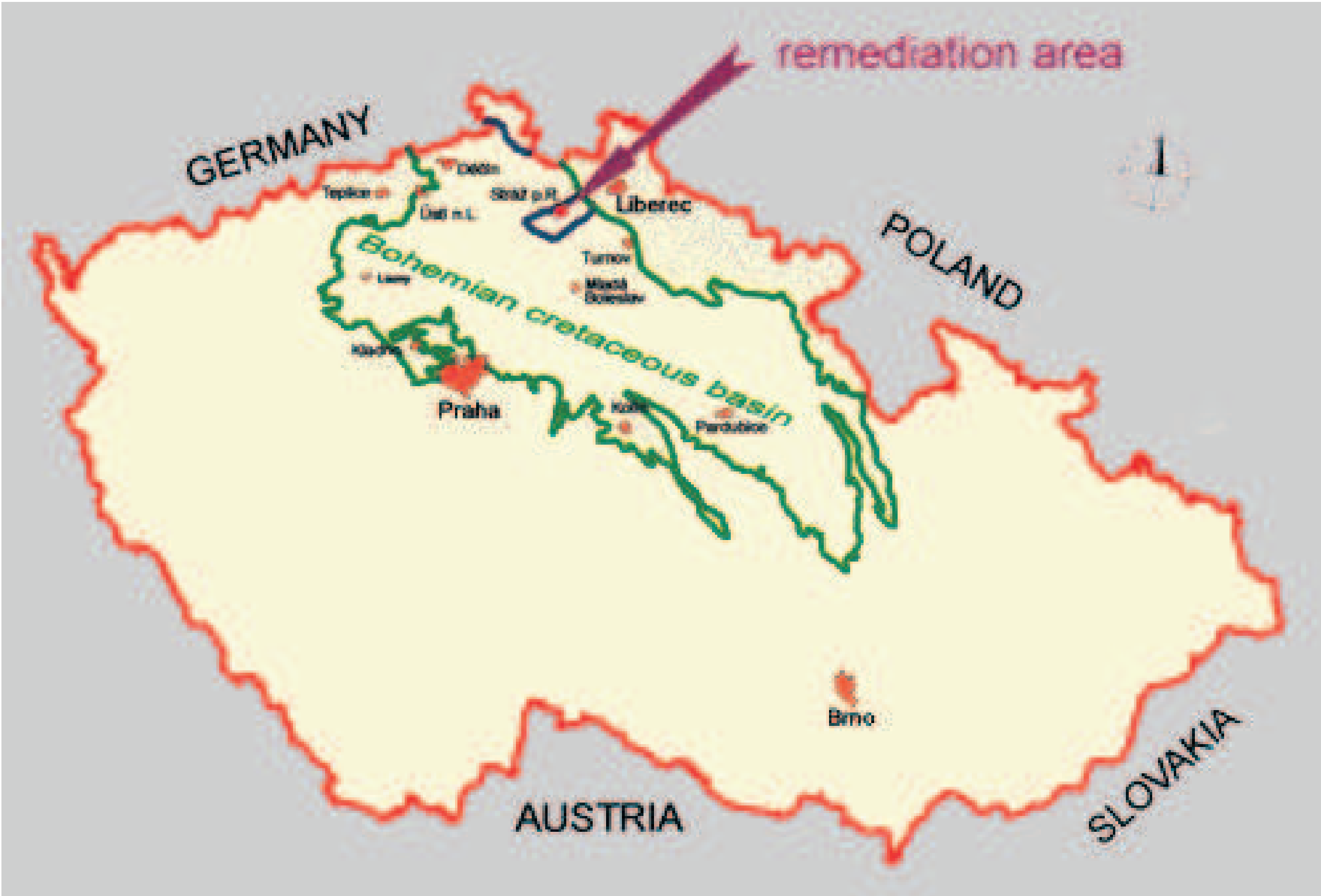
Outline

1. Application
2. Continuous formulation and discretization
3. The system matrix
   - Structural properties
   - Spectral properties
4. Solution Approaches
   - Iterative indefinite solver MINRES
   - Schur complement approach
   - Null Space Approach
   - Direct LDL^T solver
5. Conclusions

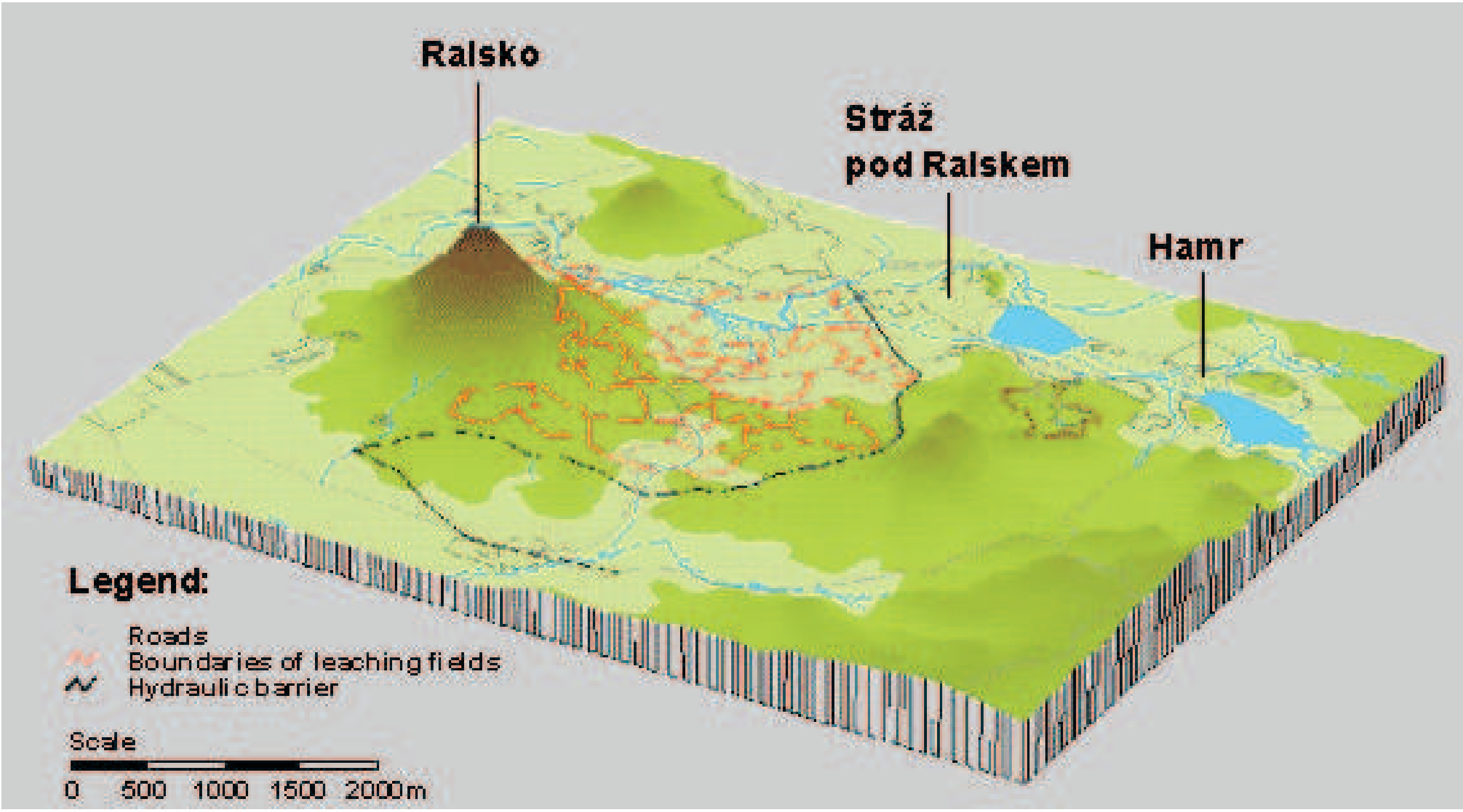
1. Application / I.

region under consideration



1. Application / II.

detailed 3D view



1. Application / III.

Specific 3D Applications

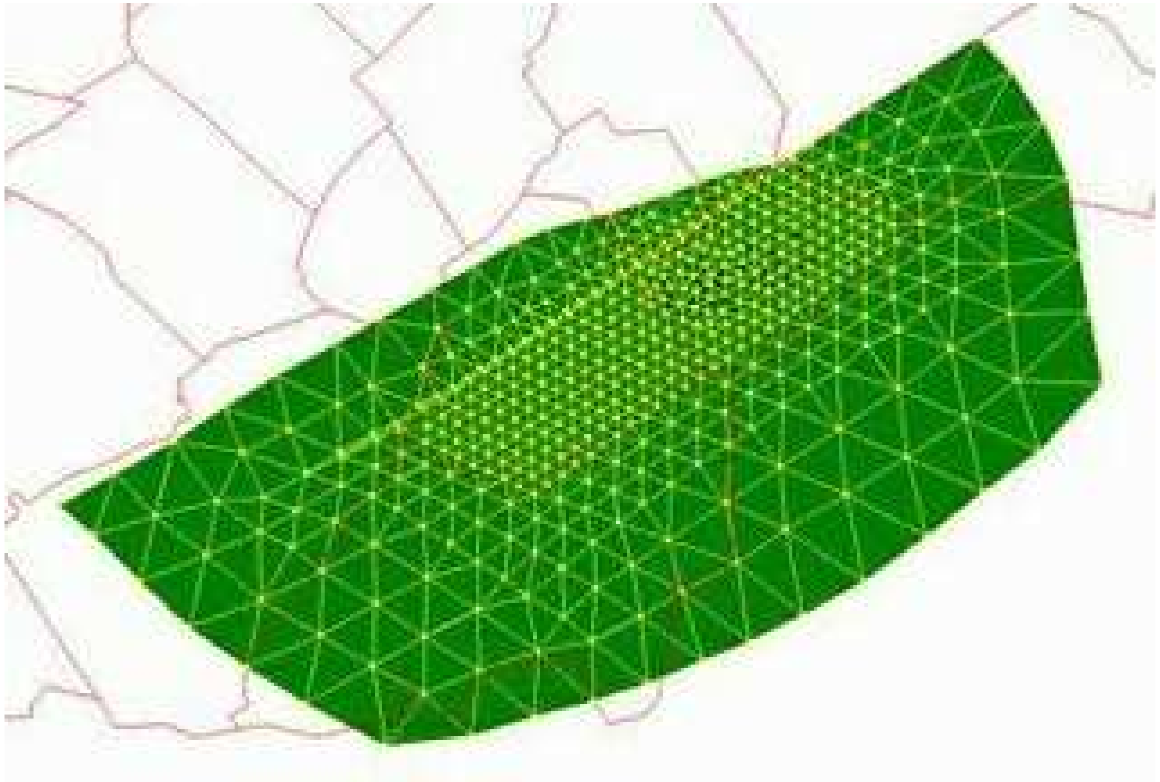
- Transport of contaminants in porous media
  - ⁕ Finite volumes, splitting convection and diffusion at each time step
- Flow in fractured and anisotropic rocks
  - ⁕ Combining two grids: network of fractures and FEM discretization of porous substrate
- Calibration of flow/transport models

(Vohralík, 2004)

1. Application / IV.

Examples

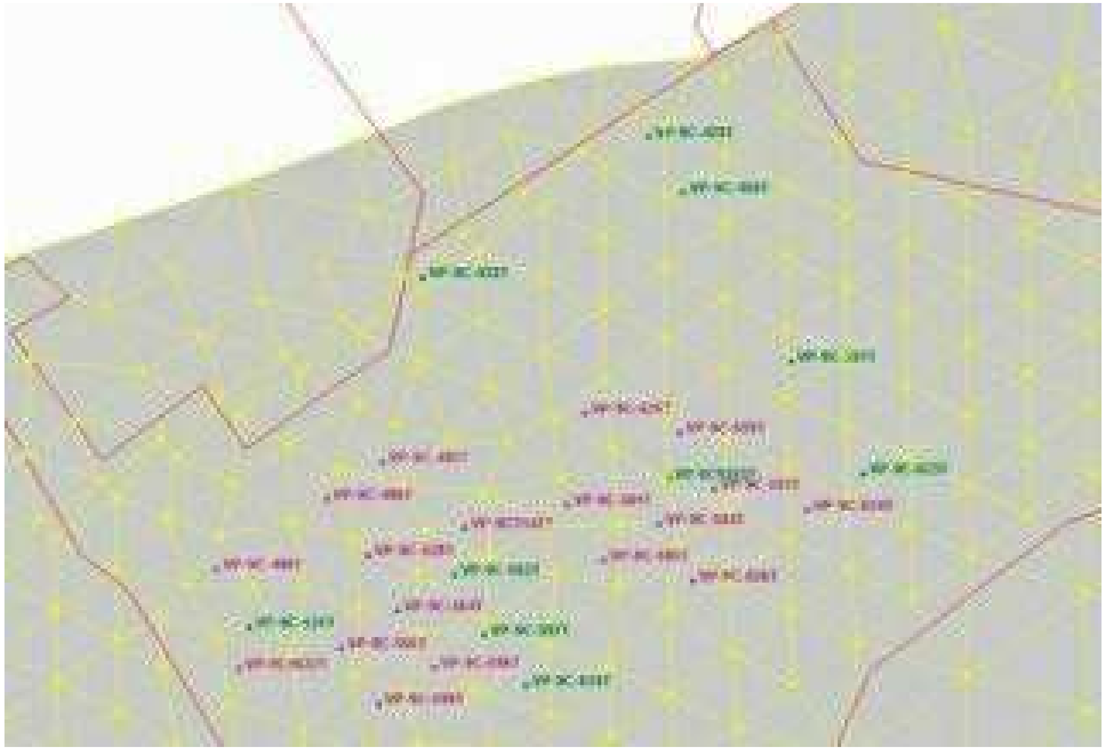
- Contaminant transport with dual porosities for remediation (grid)



1. Application / V.

Examples

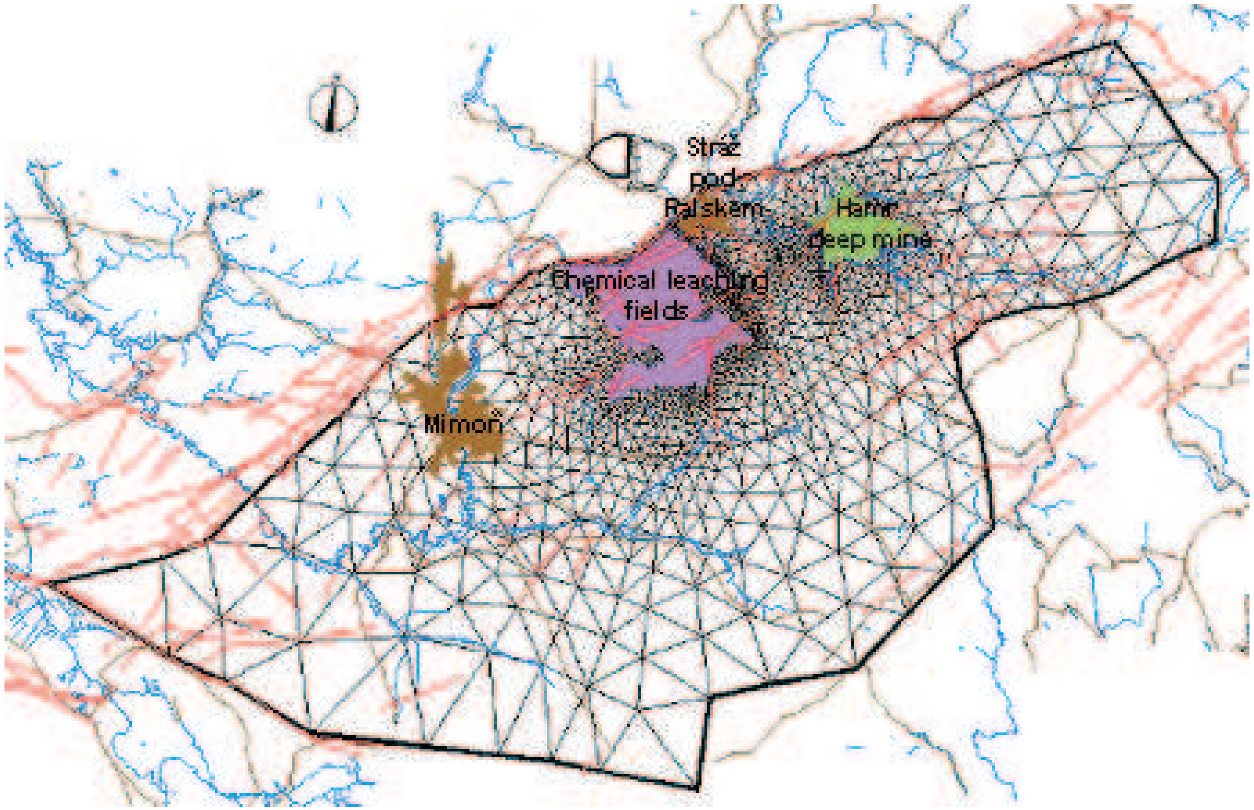
- Contaminant transport with dual porosity for remediation (drilled holes)



1. Application / VI.

Examples

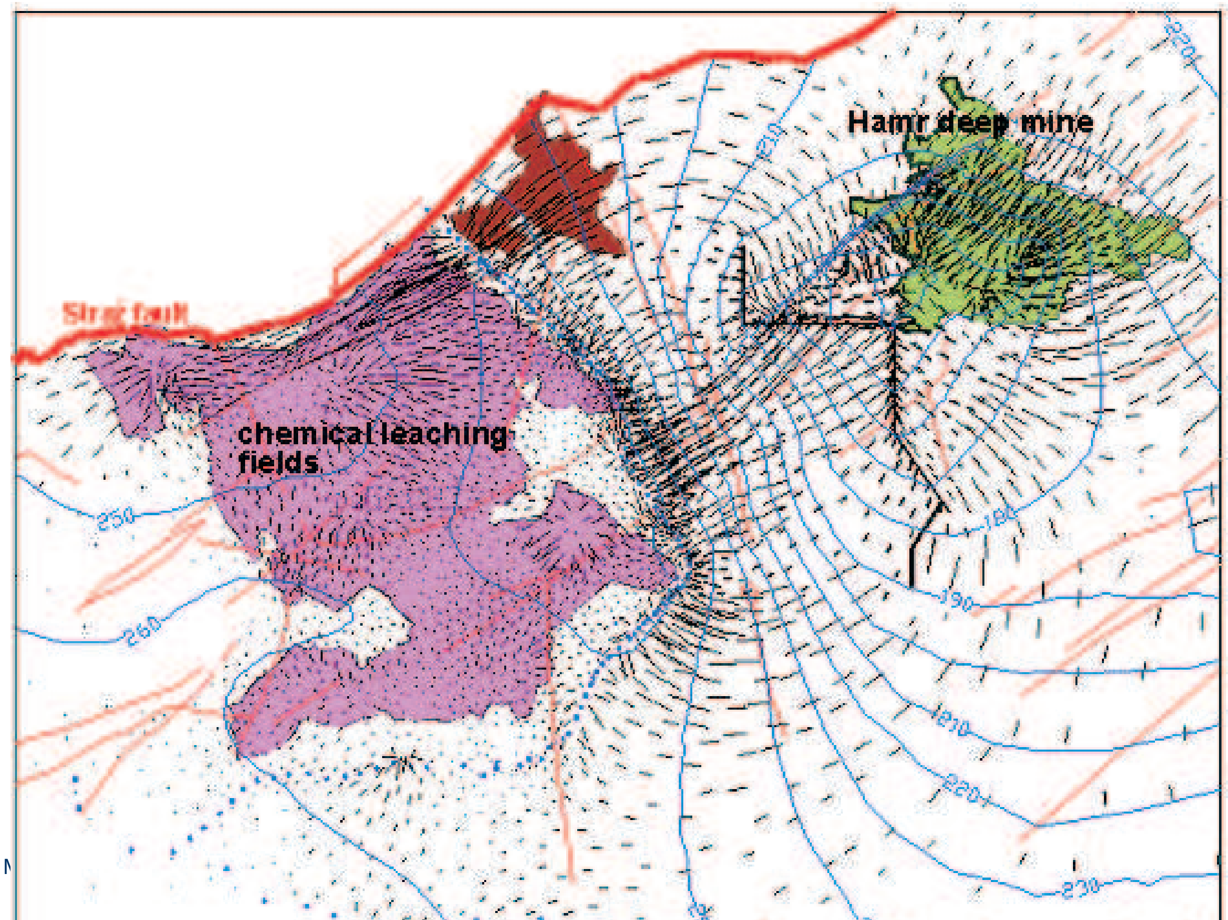
- Mine flooding (grid)



1. Application / VII.

Examples

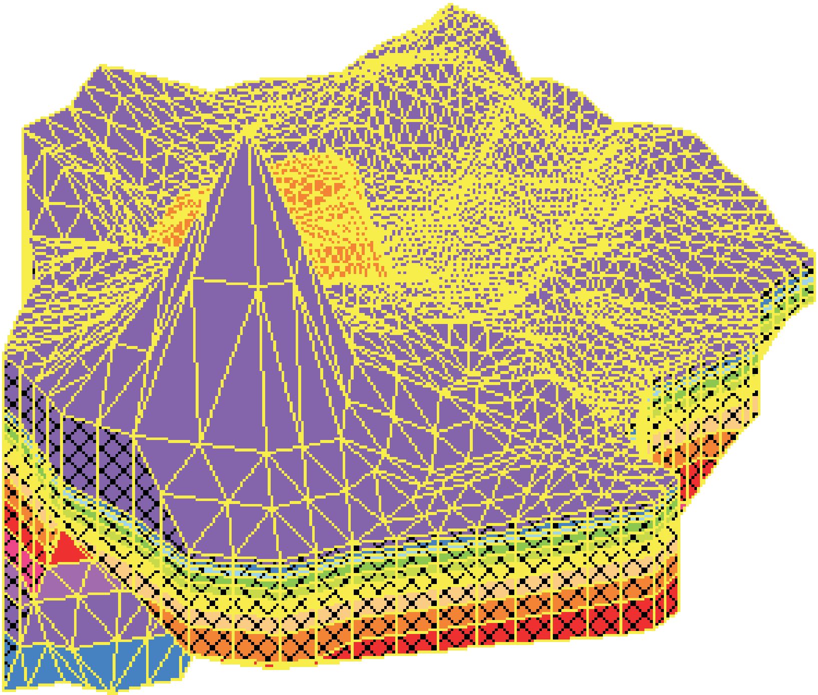
- Mine flooding (grid with velocities)



1. Application / VIII.

Examples

- Mine flooding (3D grid)



1. Application / IX.

Animations

Mine flooding (animation of **pressure development**)

Mine flooding (animation of **contamination development**)

General model of contaminant transport

$$\frac{\partial \beta(c)}{\partial t} \; \nabla.(\mathbf{S}\nabla c) + \mu \nabla.(c\mathbf{v}) + F(c) = q$$

- degenerate parabolic equation: for convection - reaction - diffusion
- c: concentration of contaminant
- $\mathbf{S}$: diffusion - dispersion tensor
- $\mathbf{v}$: velocity of the convection
- μ: scalar parameter
- F: changes due to chemical reactions
- q: sources

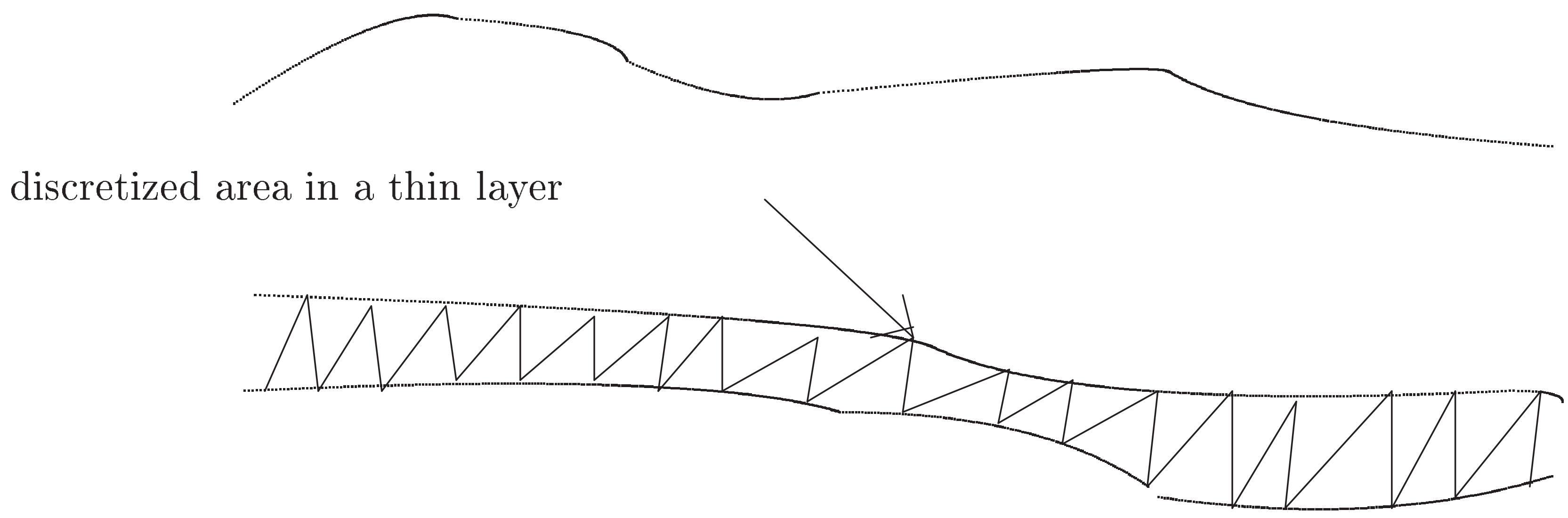
2. Continuous formulation and discretization: II.

Our restrictions

- We restrict ourselves to the flow problem only: computing velocity $\mathbf{v}$ for the model from the Darcy's law
- Application-based discretization
  - ⁎ in 2D projection determined by physically drilled holes
  - ⁎ possible different vertical positions of points of measurements
- Only partially interested in **asymptotic complexity:**
  - ⁎ **size of constants** in efficiency evaluations is crucial
- **Physical conditioning** (in the flow tensor) is important

2. Continuous formulation and discretization: III.

The modelled domain is flat and layered



2. Continuous formulation and discretization: IV.

Equations for the velocity vector
(Stationary potential fluid flow problem)

The Continuity Equation

$$\nabla \cdot \mathbf{u} \;=\; q,$$

Darcy's Law

$$\mathbf{u} \;=\; -\mathbf{A}\;\nabla p$$

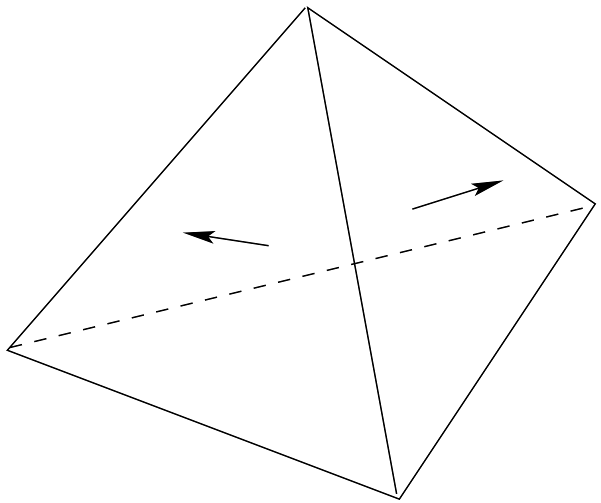
The Boundary Conditions

$$p = p_D \quad \text{on } \partial\Omega_D$$

$$-\mathbf{n}.(\mathbf{A}\nabla p) = \mathbf{n}.\mathbf{u} = u_N \quad \text{on } \partial\Omega_N$$

FEM Approximation

- Lowest-order Raviart-Thomas-Nédelec elements:
  - ∗ extension of 2D elements (Raviart, Thomas, 1977) into 3D elements (Nédelec, 1980)
  - ∗ pressure $\mathbf{p}$ is elementwise constant
  - ∗ velocity $\mathbf{u}$ is elementwise linear



2. Continuous formulation and discretization: VI.

Hybridization / Problem stretching

- enables natural condensation of unknowns to those coresponding to non-Dirichlet faces (Fraejis de Veubeke, 1965)
- larger, but more transparent system matrix
- other ways of condensation of unknowns (Maryška, Rozložník, T., 1998)
- simple aposteriori updates in the matrix

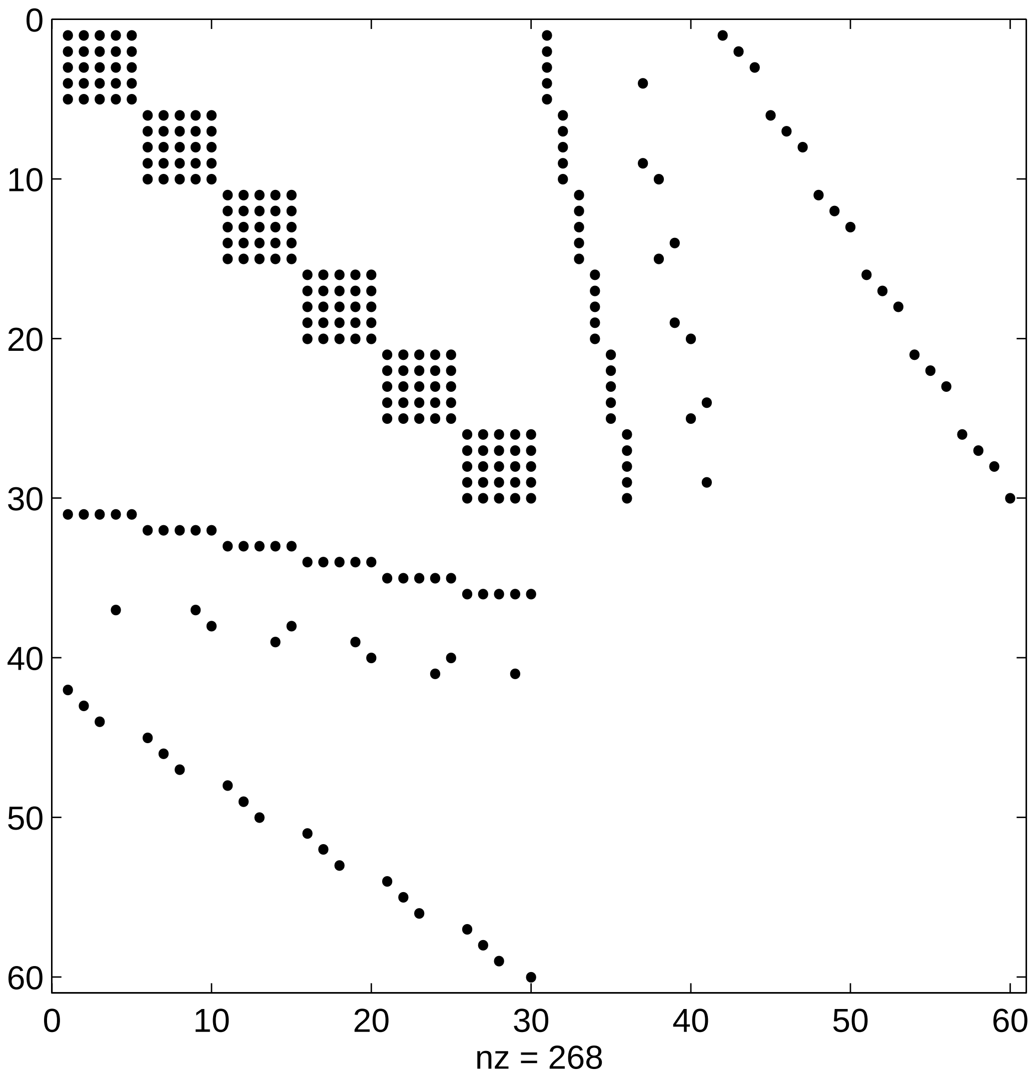
3. System matrix: I.

Matrix Structural Properties

$$\mathcal{A} = \begin{pmatrix} A & B & C \\ B^T & & \\ C^T & & \end{pmatrix}$$

- $(B|C_1|C_2)$ is an incomplete incidence matrix of a graph (some columns are missing)
- At least one Dirichlet condition $\Longrightarrow$ matrix regularity

3. System matrix: II.



3. System matrix: III.

Matrix Spectral Properties

$$\sigma(A) \subset [\frac{c_1}{h}, \frac{c_2}{h}]$$

from the properties of the discretization

$$sv(B\ C) \subset [c_3 h, c_4]$$

using the Courant-Fischer theorem and properties of paths in weighted graphs (see Maryška, Rozložník, T., 1995, 1996)

3. System matrix: IV.

Using Rusten and Winter, 1992:

$$\sigma(\mathcal{A}) \subset [-\frac{c_4^2}{c_1}h, -\frac{c_3^2}{c_2}h^3] \cup [\frac{c_1}{h}, \frac{c_2}{h}]$$

Conditioning of A: O(h^{-4})

$\Downarrow$

Scaling is necessary

3. System matrix: V.

Scaling I.

$$\begin{pmatrix} h^{\frac{1}{2}} I & \\ & I \end{pmatrix} \begin{pmatrix} A & (B\ C) \\ (B\ C)^T & \end{pmatrix} \begin{pmatrix} h^{\frac{1}{2}} I & \\ & I \end{pmatrix}$$

$$= \begin{pmatrix} hA & h^{\frac{1}{2}}(B\ C) \\ h^{\frac{1}{2}}(B\ C)^T & \end{pmatrix}$$

$$\Downarrow$$

$$[-\frac{c_4^2}{c_1}h, -\frac{c_3^2}{c_2}h^3] \cup [c_1, c_2]$$

3. System matrix: VI.

Scaling II.

$$\begin{pmatrix} h^{\frac{1}{2}} I & \\ & h^{-\frac{1}{2}} I \end{pmatrix} \begin{pmatrix} A & (B\ C) \\ (B\ C)^T & \end{pmatrix} \begin{pmatrix} h^{\frac{1}{2}} I & \\ & h^{-\frac{1}{2}} I \end{pmatrix}$$

$$= \begin{pmatrix} hA & (B\ C) \\ (B\ C)^T & \end{pmatrix}$$

$$\Downarrow$$

$$[\frac{1}{2}(c_1 - \sqrt{c_1^2 + 4c_4^2}), -\frac{c_3^2}{c_2} h^2] \cup [c_1, \frac{1}{2}(c_2 + \sqrt{c_2^2 + 4c_4^2})]$$

4. Solution approaches: MINRES: I.

$A)$ Indefinite Iterative Solver MINRES

Asymptotic convergence factor (optimal polynomial known only for specific sequences of inclusion sets)

$$\lim_{n\to+\infty}\left(\frac{\|r_n\|}{\|r_0\|}\right)^{1/n} \leq \lim_{n\to+\infty}\left[\min_{P\in\Pi_n}\max_{\lambda\in\mathcal{G}}|P(\lambda)|\right]^{\frac{1}{n}}$$

Unscaled problem (Maryška, Rozložník, T., 1995, using technique of Wathen, Fischer, Silvester, 1995):

$\Downarrow$

1

4. Solution approaches: MINRES: II.

a) considering size of constants:

$$\mathcal{G} : [-\frac{c_4^2}{c_1}h, -\frac{c_3^2}{c_2}h^3] \cup [\frac{c_1}{h}, \frac{c_2}{h}] \to [-c_4, -\frac{c_3^2}{c_2}h^3] \cup [\frac{c_1}{h}, c_4]$$

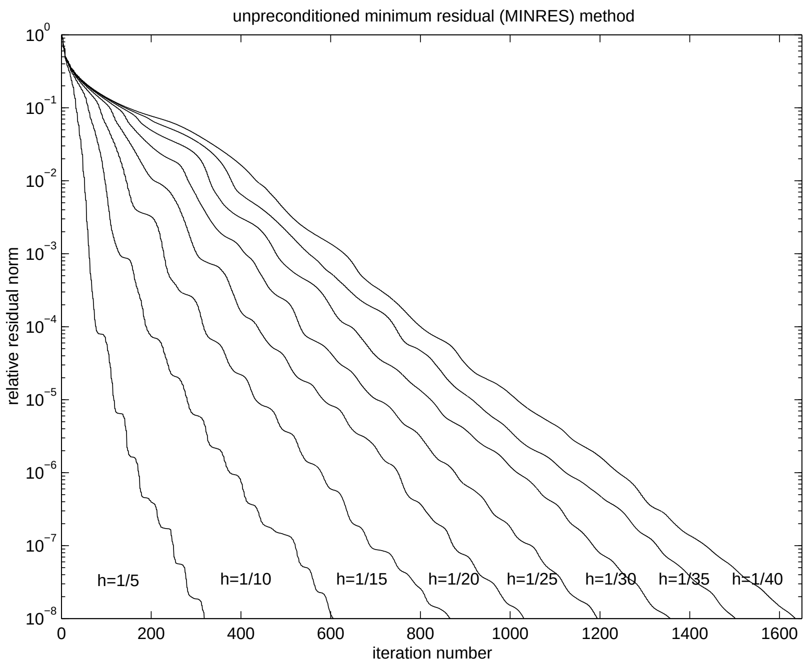
b) or scaled matrix problem:

$$\Downarrow$$

$$\lim_{n\to+\infty} \left(\frac{\|r_n\|}{\|r_0\|}\right)^{\frac{1}{n}} \leq 1 - c_6 h$$

4. Solution approaches: MINRES: III.

Unpreconditioned MINRES applied to the whole indefinite system



both in theory and in practice:

$$\lim_{n\to\infty} \left(\frac{\|r_n^{MINRES}\|}{\|r_0\|} \right)^{\frac{1}{n}} \leq 1 - c_1 h$$

4. Solution approaches: MINRES: IV.

- preconditioning helps a lot in terms of number of iterations
- it still keeps the same behaviour of the curves: the same asymptotic complexity
- the implementation is easily parallelizable
- the implementation is often preferred when only a small precision needed, cf. Maryška, Rozložník, T., 1999

4. Solution approaches: Schur complement: I.

$B)$ **Schur Complement Approach**

the matrix

$$\mathcal{A} = \begin{pmatrix} A & B & C_1 & C_2 \\ B^T & & & \\ C^T & & & \\ C_2^T & & & \end{pmatrix}$$

C_1: internal faces
C_2: Neumann boundary conditions

$$|C_1|/|C_2| \approx volume/surface \text{ ratio}$$

4. Solution approaches: Schur complement: II.

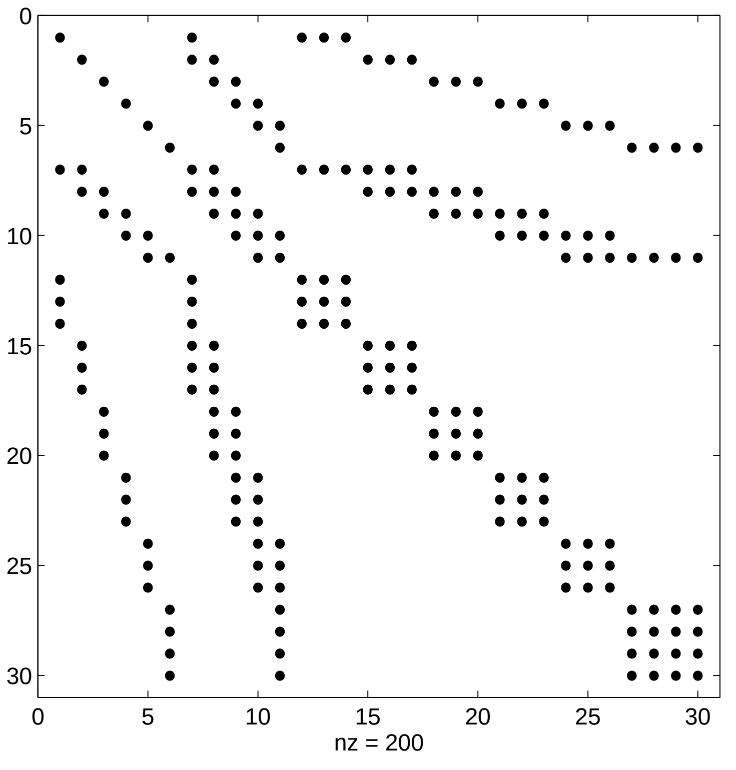
- First Schur complement

$$-\mathcal{A}/A = (B\ C_1\ C_2)^T A^{-1} (B\ C_1\ C_2)$$

  ⁎ can be formed cheaply (A is block diagonal - Brezzi, Fortin, 1991)

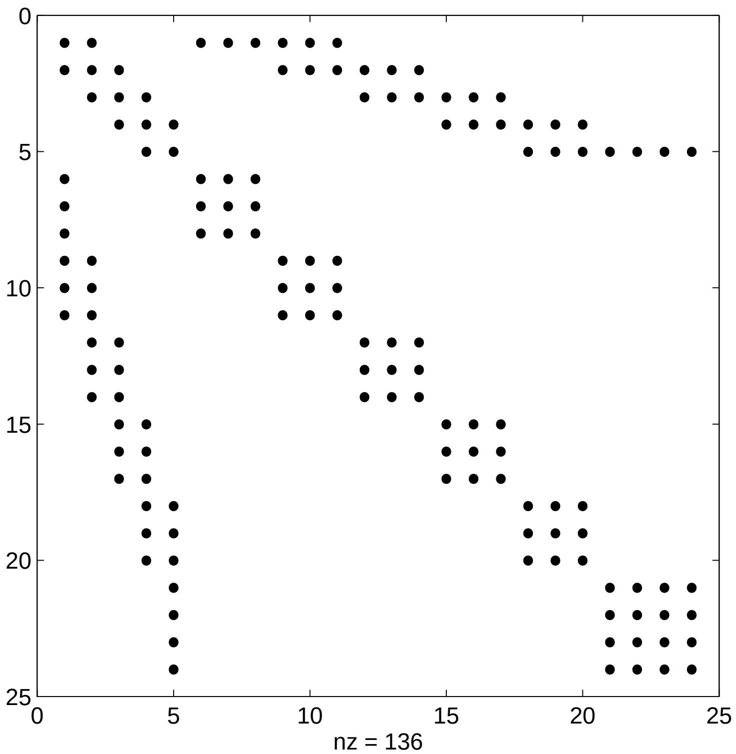
- Further Schur complements: $-\mathcal{A}/A$ induced by B and C_2
  ⁎ can be formed with no fill-in (Maryška, Rozložník, T., 1999)

4. Solution approaches: Schur complement: III.



Structural pattern of the (first) Schur complement matrix $\mathcal{A}/A$

4. Solution approaches: Schur complement: IV.



Structural pattern of the (second) Schur complement matrix $-\mathcal{A}/A)/A_{11}$

4. Solution approaches: Schur complement: V.

Schur Complement Spectral Properties

Estimate for the scaled matrix

$$\sigma(-\mathcal{A}/A) \subset [\frac{c_3^2}{c_2} h^2, \frac{c_4^2}{c_1}]$$

Residual norm for smoothed CG/CR method

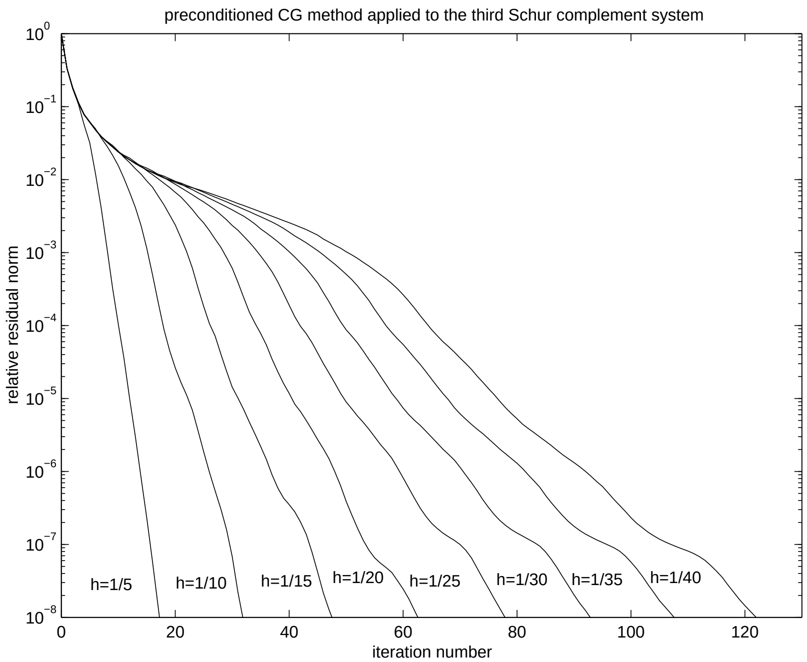
$$\frac{\|r_n\|}{\|r_0\|} \leq 2 \left(\frac{1 - \frac{c_3}{c_4}\sqrt{\frac{c_1}{c_2}}h}{1 + \frac{c_3}{c_4}\sqrt{\frac{c_1}{c_2}}h} \right)^n$$

$$\Downarrow$$

$$\lim_{n \to +\infty} \left(\frac{\|r_n\|}{\|r_0\|} \right)^{\frac{1}{n}} \leq 1 - c_9 h$$

4. Solution approaches: Schur complement: VI.

Successive Schur Complements: preconditioned and smoothed CG applied to third Schur complement



both in theory and in practice:

$$\lim_{n\to\infty}\left(\frac{\|r_n^{CR}\|}{\|r_0\|}\right)^{\frac{1}{n}} \leq 1 - c_2 h$$

4. Solution approaches: Schur complement: VII.

- preconditioning helps a lot in terms of number of iterations
- keeps the same behaviour of the curves: the same asymptotic complexity
- modelling of thin layers may use domain information in order to increase solver efficiency

$C)$ **Null-space approach**

Motivation

- useful when iteratively changing material properties (solving inverse problems)
- sequences of time-dependent and nonlinear problems
- must be as efficient as possible

Two basic strategies

- use **divergence-free finite elements**: the null-space approach embedded in formulation
- **algebraic** null-space basis construction

4. Solution approaches: Null-space approach: II.

divergence-free finite elements

- needed vector potentials of functions in an appropriate Sobolev space
- Raviart-Thomas-Nédelec elements as 3D curls of these potentials
- finding a linearly independent set of the potentials can be based on Nédelec edge elements
  - ⁕ taking curls of all edge elements, eliminating the kernel later (Hiptmair, Hoppe, 1999)
  - ⁕ finding a basis based on a spanning tree graph of the discretization (Cai, Parashkevov, Russell, Ye, 2002; Scheichl, 2003)
  - ⁕ not clear how to generalize the procedure to unstructured meshes

4. Solution approaches: Null-space approach: III.

Algebraic null-space based approaches

- Find a null-space basis Z

$$(B\ C_1\ C_2)^T Z = 0$$

- Solve the projected system

$$Z^T A Z u_2 = Z^T (q_1 - A u_1)$$

Possible methods

1. (**fundamental; spanning tree-based**) cycle null-space basis based on incidence vectors of cycles in the mesh
2. **orthogonal** null space basis
   based on QR decomposition of $(B\ C_1\ C_2)$
3. **partial** null space basis (formed only for a part of offdiagonal blocks of the matrix, namely for the matrix $(C_1\ C_2)$)

4. Solution approaches: Null-space approach: IV.

C.1 Fundamental cycle null-space basis

- find a (shortest path) spanning tree
- form cycles using non-tree edges

$$sv(Z) \subset [1, \frac{c_{10}}{h^2}]$$

- notice the problem of long cycles!

$$\sigma(Z^T \mathbf{A} Z) \subset [c_1, \frac{c_2 c_{10}^2}{h^4}]$$

(Arioli, Maryška, Rozložník, T., 2001)

4. Solution approaches: Null-space approach: V.

Relative residual norm

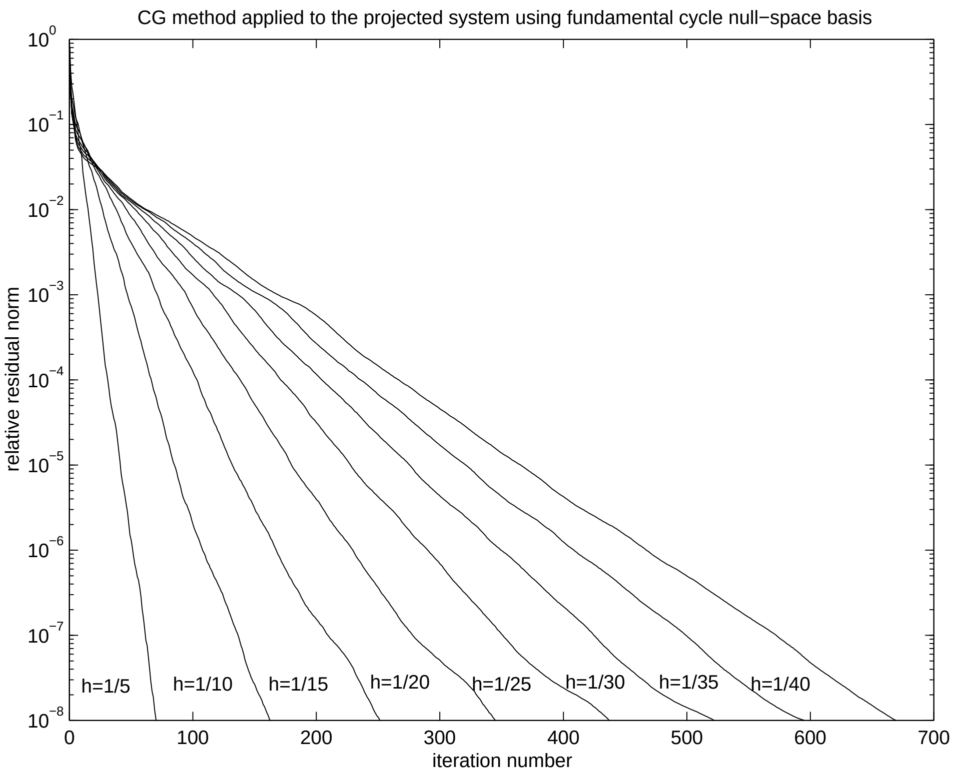
$$\frac{\|r_n\|}{\|r_0\|} \leq 2 \left(\frac{1 - \frac{1}{c_{10}} \sqrt{\frac{c_1}{c_2}} h^2}{1 + \frac{1}{c_{10}} \sqrt{\frac{c_1}{c_2}} h^2} \right)^n$$

$$\Downarrow$$

$$\lim_{n \to +\infty} \left(\frac{\|r_n\|}{\|r_0\|} \right)^{\frac{1}{n}} \leq 1 - c_{11} h^2$$

4. Solution approaches: Null-space approach: VI.

Fundamental Cycle Null-Space Approach: unpreconditioned and smoothed CG applied to the projected system



$$\lim_{n\to\infty}\left(\frac{\|r_n^{CR}\|}{\|r_0\|}\right)^{\frac{1}{n}} \leq 1 - c_3 h^2$$

4. Solution approaches: Null-space approach: VII.

- in practice better than in theory
- explicit assembly of the projected system is feasible, but: difficult to precondition

C.2 Orthogonal null-space basis

- based on sparse QR of $(B\ C_1\ C_2)$ (in our case, MA49 from HSL)
- projected system independent of h
- subsequent table: comparison of fundamental cycle approach (FC) versus orthogonal null-space basis approach (QR)

4. Solution approaches: Null-space approach: IX.

h	memory requirements		iteration counts	
	QR	FC	QR	FC
	$NNZ(QR)$	$NNZ(Z1)$	QR/SN	UN
1/5	28360 (3e-2)	3360 (7e-3)	22/20 (0.17/0.44)	71 (0.08)
1/10	410466 (0.97)	47120 (0.07)	22/21 (1.87/4.23)	163 (1.57)
1/15	1979203 (9.73)	226780 (0.30)	22/21 (8.48/17.1)	252 (19.9)
1/20	7120947 (59.6)	697840 (0.93)	22/21 (25.0/48.6)	346 (75.9)
1/25	18105131 (237)	1675800 (2.21)	22/21 (57.2/107)	438 (222)
1/30	40837823 (980)	3436160 (4.60)	21/21 (110/214)	523 (510)
1/35	—	6314420 (8.64)	—	596 (1009)
1/40	—	10706080 (14.8)	—	670 (1900)

4. Solution approaches: Null-space approach: X.

C.3 Null-space basis for the block $(C_1 \ C_2)$

$$(C_1 \ C_2)^T Z = 0$$

(Arioli, Maryška, Rozložník, T., 2001)

$$\begin{pmatrix} Z^T \mathbf{A} Z & Z^T B \\ B^T Z & \end{pmatrix} \begin{pmatrix} u_2 \\ p \end{pmatrix} = \begin{pmatrix} Z^T (q_1 - \mathbf{A} u_1) \\ q_2 - B^T u_1 \end{pmatrix}$$

Singular values of $Z^T B$

$$sv(Z^T B) \subset [c_{12} h, c_{13}]$$

4. Solution approaches: Null-space approach: XI.

Inclusion set

$$[\frac{1}{2}(c_1 - \sqrt{c_1^2 + 4c_{13}^2}, -\frac{c_{12}^2}{c_2}h^2] \cup [c_1, \frac{1}{2}(c_2 + \sqrt{c_2^2 + 4c_{13}^2})]$$

Asymptotic convergence factor

$$\lim_{n \to +\infty} \left(\frac{\|r_n\|}{\|r_0\|} \right)^{\frac{1}{n}} \leq 1 - c_{14}h$$

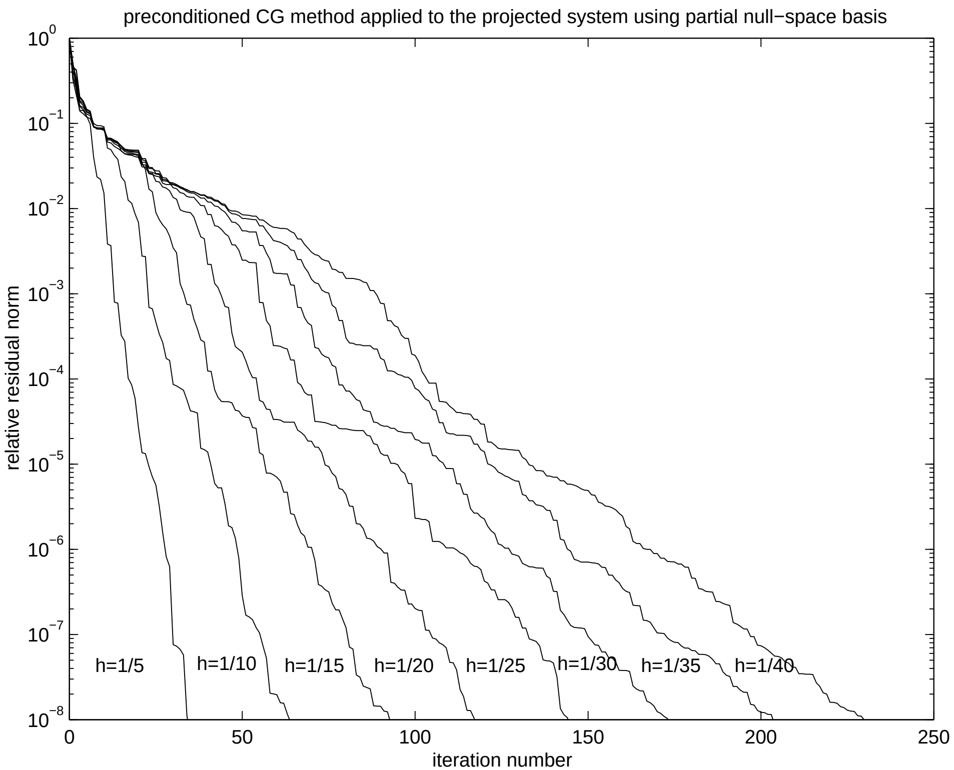
Some results with the partial null-space approach follow

4. Solution approaches: Null-space approach: XII.

h	NNZ	implicit	sparse QR	
		IP/IQ	$NNZ(QR)$	QR/SN
1/5	14375	62/35 (0.05/0.03)	20834 (0.02)	18/14 (0.09/0.09)
1/10	123000	103/64 (0.68/0.48)	356267 (0.35)	19/16 (1.11/0.89)
1/15	424125	144/93 (5.17/3.79)	1840670 (3.14)	21/15 (6.09/4.63)
1/20	1016000	186/118 (20.2/14.2)	6322468 (17.97)	21/15 (18.3/14.94)
1/25	1996875	225/145 (50.8/37.4)	16661544 (86.6)	23/15 (47.0/27.8)
1/30	3465000	260/174 (111/84.2)	40669978 (584)	22/15 (96.7/85.5)
1/35	5518625	295/204 (224/173)	—	—
1/40	8256000	331/230 (383/295)	—	—

4. Solution approaches: Null-space approach: XIII.

Partial null-space approach: preconditioned and smoothed CG applied to the projected system



both in theory and in practice:

$$\lim_{n\to\infty}\left(\frac{\|r_n^{CR}\|}{\|r_0\|}\right)^{\frac{1}{n}} \le 1 - c_3 h$$

$D)$ **Direct indefinite LDL^T decomposition**

- symmetric quasidefinite matrices are strongly factorizable (Vanderbei, 1995)

$$\begin{pmatrix} A & B \\ B^T & -D \end{pmatrix}$$

A is SPD, D is SPD

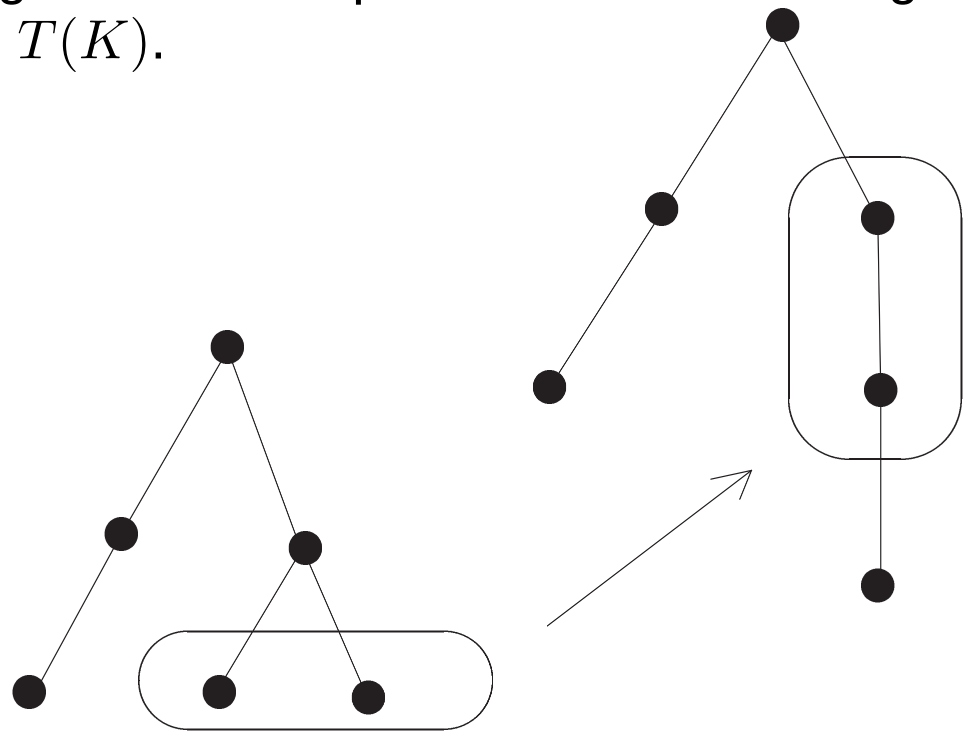
- Our matrix has zero block instead of D: Is there a LDL^T decomposition?

4. Solution approaches: Direct solver: II.

$$
\begin{array}{cc}
 & \begin{array}{cc} \boldsymbol{R} & \boldsymbol{C} \end{array} \\
\begin{array}{c} \boldsymbol{R} \\ \boldsymbol{C} \end{array} &
\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}
\end{array}
$$

Supporting assertions

- **Fact:** Matrix K is factorizable only if leafs of the elimination tree $T(K)$ belong to $\mathcal{R}$.
- **Problem:** Some leafs of $T(K)$ are from $\mathcal{C}$.
- **Cure:** Change the current permutation of K using a traversal through postordered $T(K)$.

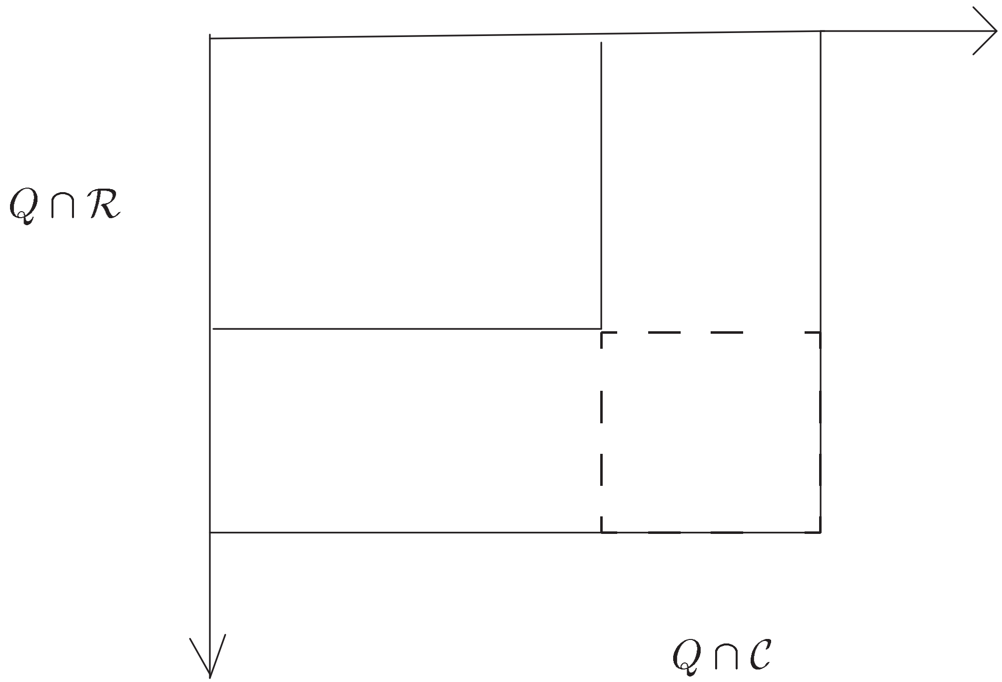


4. Solution approaches: Direct solver: IV.

- **Fact:** Matrix K is factorizable only if each of its leading principal submatrices have the number of indices from $\mathcal{R}$ greater or equal to the number of indices from $\mathcal{C}$.
- **Problem:** The assertion is not satisfied.
- **Cure:** Again, change the current permutation of K using a traversal through postordered $T(K)$.

4. Solution approaches: Direct solver: V.

$$Q = \{1, \ldots, i\}$$



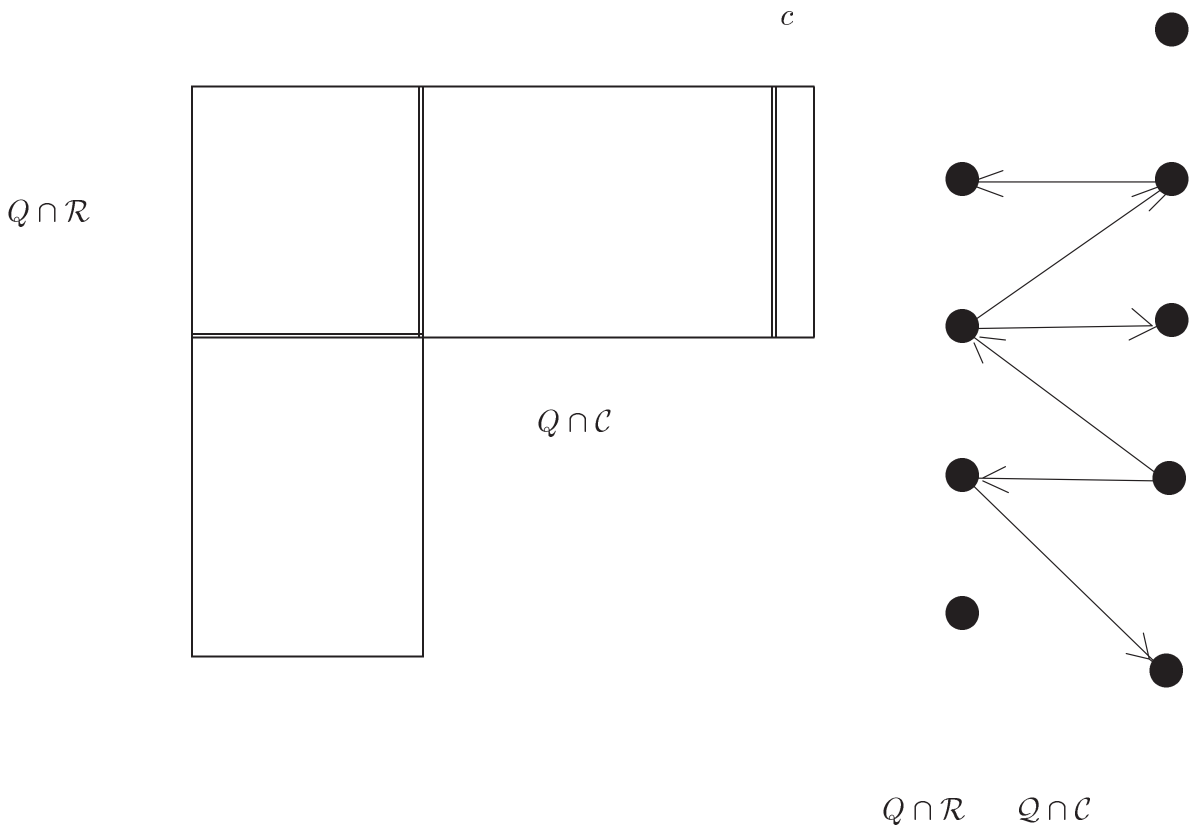
$$|Q \cap \mathcal{R}| \leq |\mathcal{Q} \cap \mathcal{C}|$$

4. Solution approaches: Direct solver: VI.

- **Fact:** Our matrix K is factorizable if and only if there are no paths of odd lengths in search trees rooted in nodes from $\mathcal{C}$ in the bipartite graph of the outdiagonal block of the principal leading submatrices.
- **Problem:** The assertion is not satisfied.
- **Cure:** Change the current permutation of K constructing the set of search trees.

(T., 2002)

4. Solution approaches: Direct solver: VII.



4. Solution approaches: Direct solver: VIII.

Global Algorithmic Strategy

- MMD ordering.
- Delaying nodes coresponding to **leaves** of the elimination tree from $\mathcal{C}$.
- Delaying nodes from $\mathcal{C}$ which **do not satisfy criterion which balances nodes** from $\mathcal{R}$ and $\mathcal{C}$ in the current offdiagonal graph.
- Delaying nodes based on **search trees construction**.

$$\Downarrow$$

Supernodal LDL^T solver

4. Solution approaches: Direct solver: IX.

Fill-in Comparison

MAT	$n+m$	n	nnz	$SCHUR$	$SQSD$
S3P	477	270	1539	3151	2957
LI5	868	480	2208	5098	4686
LI6	3707	2100	9575	40269	34498
M3P	3744	2160	12312	46504	44002
DRT2	12992	7515	42935	296818	231312
DORT	22967	13360	76199	641828	551215

5. Conclusions

Conclusions

- FEM hybridization is an important tool also from algebraic point of view
- No-fill construction of the third Schur complement makes it attractive for modelling of thin layers.
- Null-space approach (its partial variant) is a reasonable alternative for solving nonlinear and time-dependent problems.
- All the basic approaches have asymptotic convergence rate $1 - O(h)$ after appropriate scaling.