# Preconditioned iterative methods based on dual variable reduction for solving 3D potential fluid flow problem

Miroslav Tůma

Institute of Computer Science

Academy of Sciences of the Czech Republic

and Technical University in Liberec

joint work with

Mario Arioli, Jiří Maryška, Miroslav Rozložník

Supported by the project “Information Society” of the

Academy of Sciences of the Czech Republic under No. 1ET400300415

Atlanta, May 20, 2005

# Outline

1. Continuous formulation and discretization
2. The system matrix
   - Structural properties
   - Spectral properties
3. Solution Approaches: Null space approach
4. Other solution approaches (will be skipped here)
   - Iterative indefinite solver MINRES
   - Schur complement approach
   - Direct $LDL^T$ solver
5. Application
6. Conclusions

# 1. Continuous formulation and discretization: I.

## 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
- $\mu$: scalar parameter
- $F$: changes due to chemical reactions
- $q$: sources

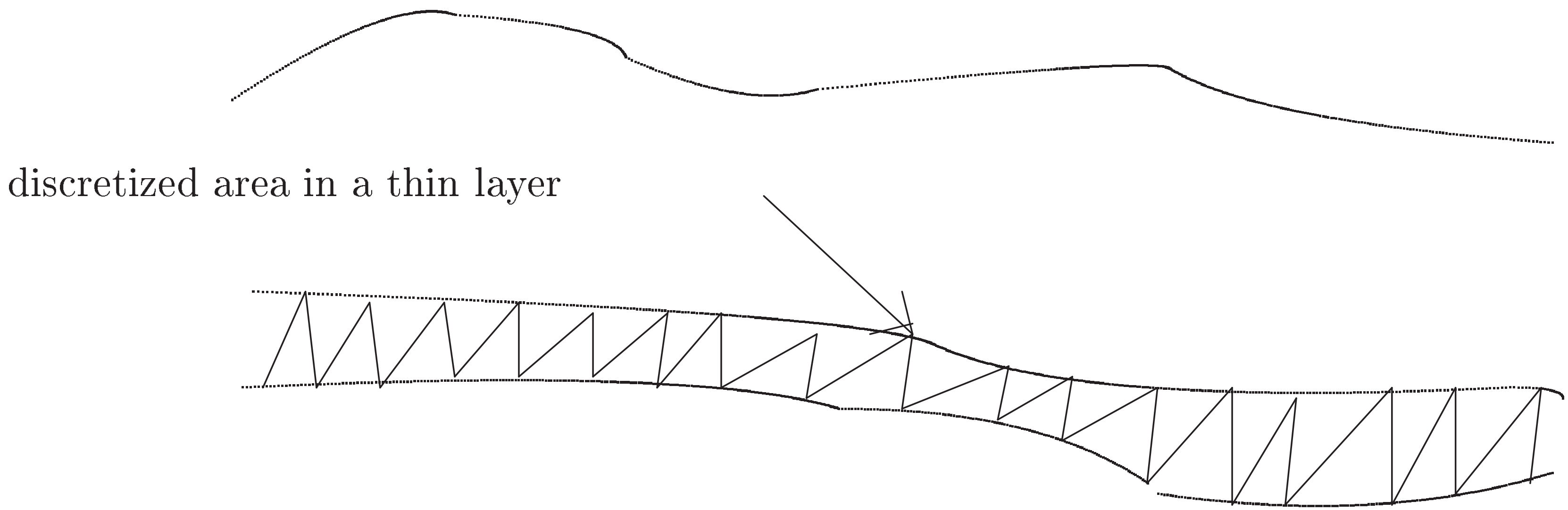
# 1. Continuous formulation and discretization: II.

## Our restrictions / specific features

- Here we restrict ourselves to the flow problem only: computing velocity $v$ for the model from the Darcy's law
- Follow-up: preconditioning sequences of linear systems: talk at Seven Springs, May 23–27, 2005
- 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

# . Continuous formulation and discretization: III.

The modelled domain is flat and layered



# 1. 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

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

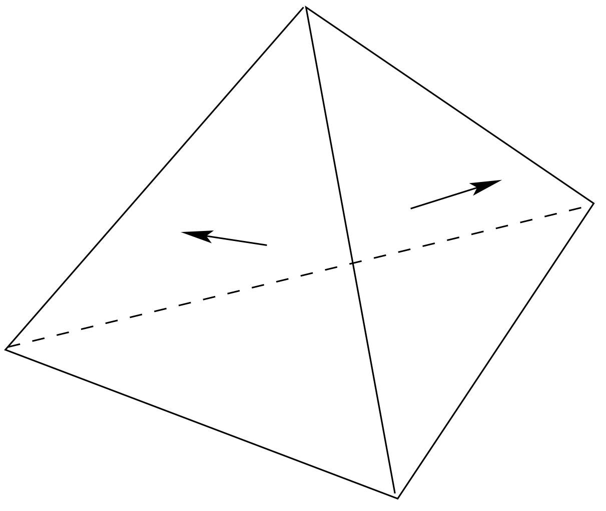
The Boundary Conditions

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

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

## 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



# 1. 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

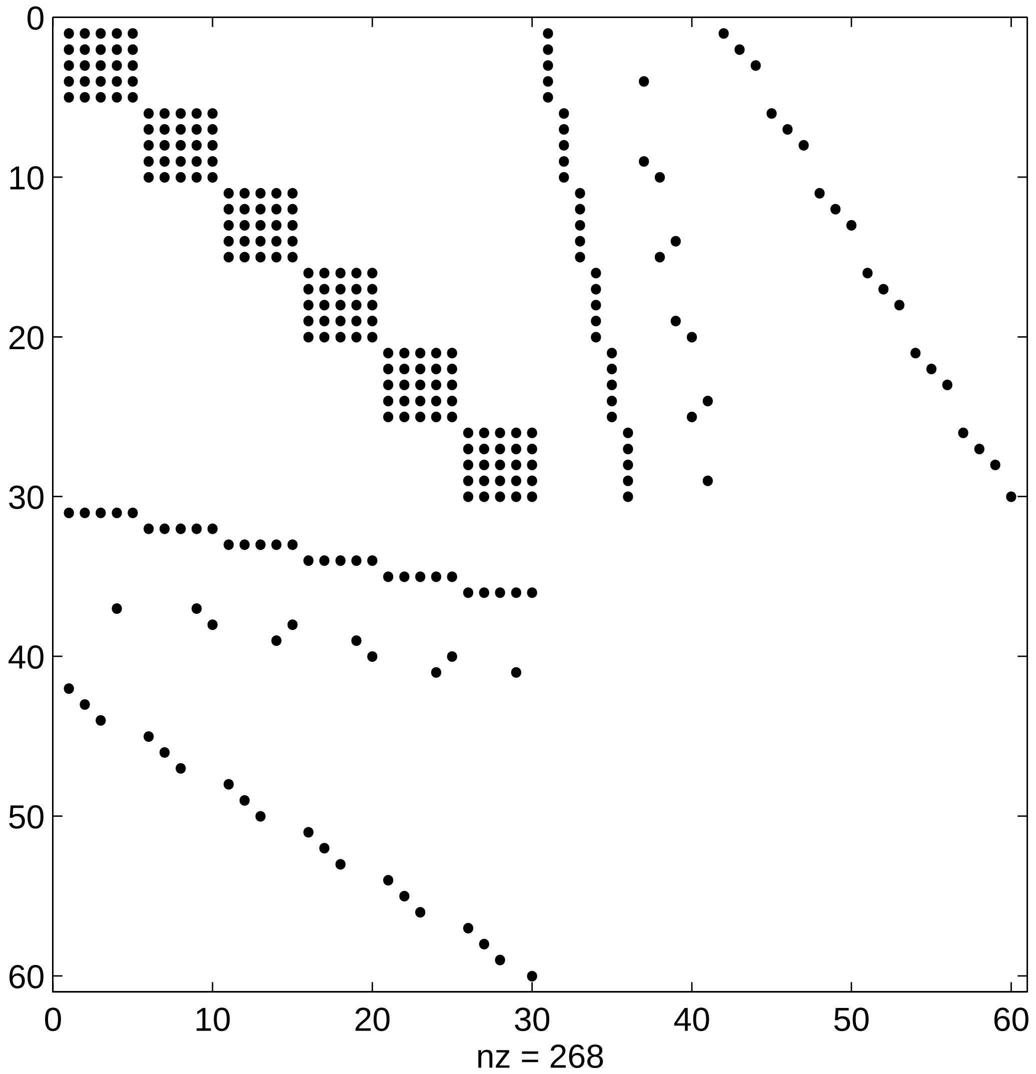
# 2. System matrix: I.

## 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

# 2. System matrix: II.



# 2. System matrix: III.

## Matrix Spectral Properties

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

from the properties of the discretization

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

Conditioning of the whole indefinite matrix after appropriate diagonal scaling of the matrix: $O(h^{-2})$

(see Maryška, Rozložník, T., 1995, 1996)

# 3. Solution approaches: Null-space approach: I.

## Motivation

Methods based on null-space basis of $(B\ C)^T$

- useful when geometry fixed and iterative changes in material properties (solving inverse problems)
- sequences of time-dependent and nonlinear problems

## Two basic strategies

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

# 3. 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

## 3. 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 $(C_1\ C_2)$)

# 3. Solution approaches: Null-space approach: IV.

## 1. Fundamental cycle null-space basis

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

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

- 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)

# 3. Solution approaches: Null-space approach: V.

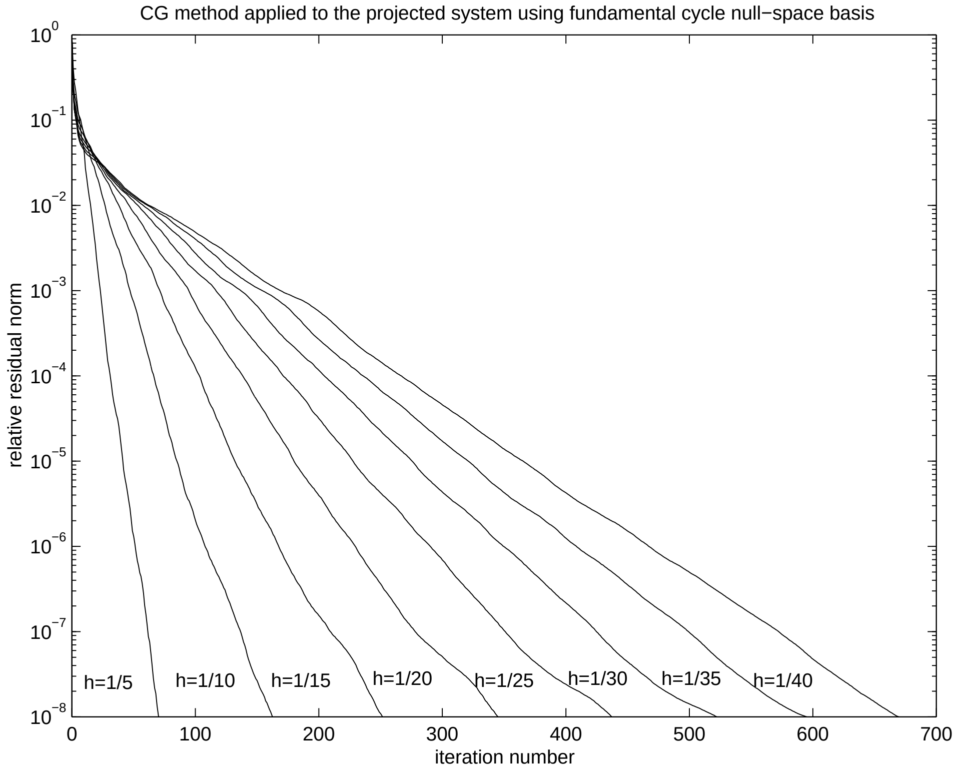
Relative residual norm

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

$$\Downarrow$$

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

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




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

# 3. Solution approaches: Null-space approach: VII.

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

## 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)

# 3. 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) |

# 3. Solution approaches: Null-space approach: X.

3. (Partial) 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 $Z^T B$

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

# 3. 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

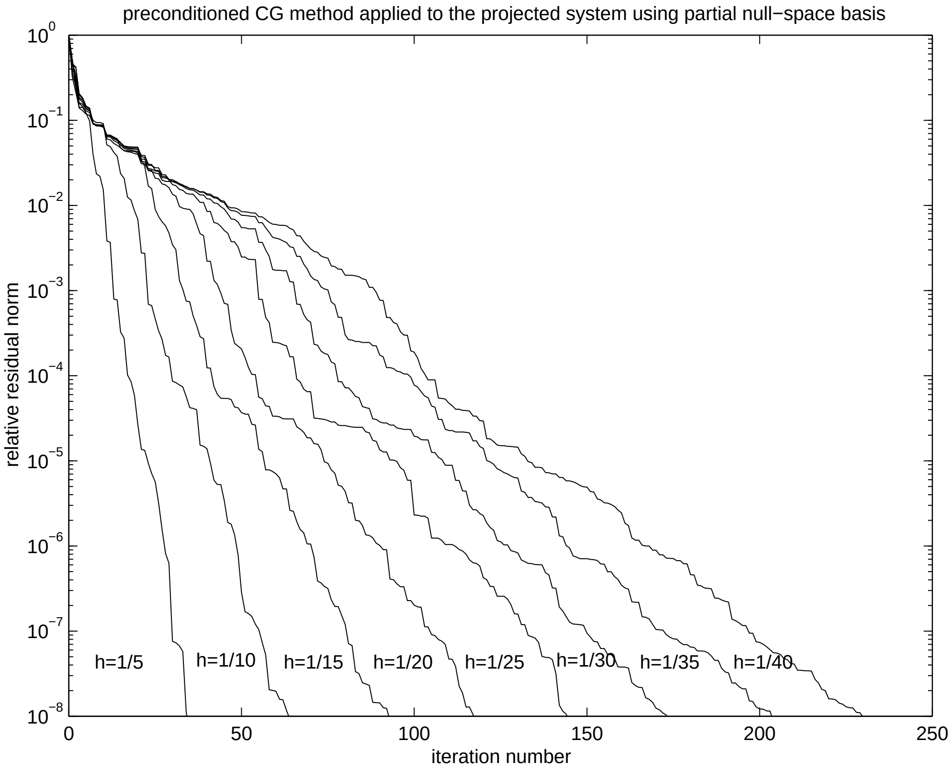
$$\lim_{n \to +\infty} \left( \frac{\|r_n\|}{\|r_0\|} \right)^{\frac{1}{n}} \leq 1 - c_{14}h$$

Some results with the partial null-space approach follow

# 3. Solution approaches: Null-space approach: XII.

| $h$ | NNZ | partial IP/IQ | sparse QR $NNZ(QR)$ | sparse 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) | — | — |

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

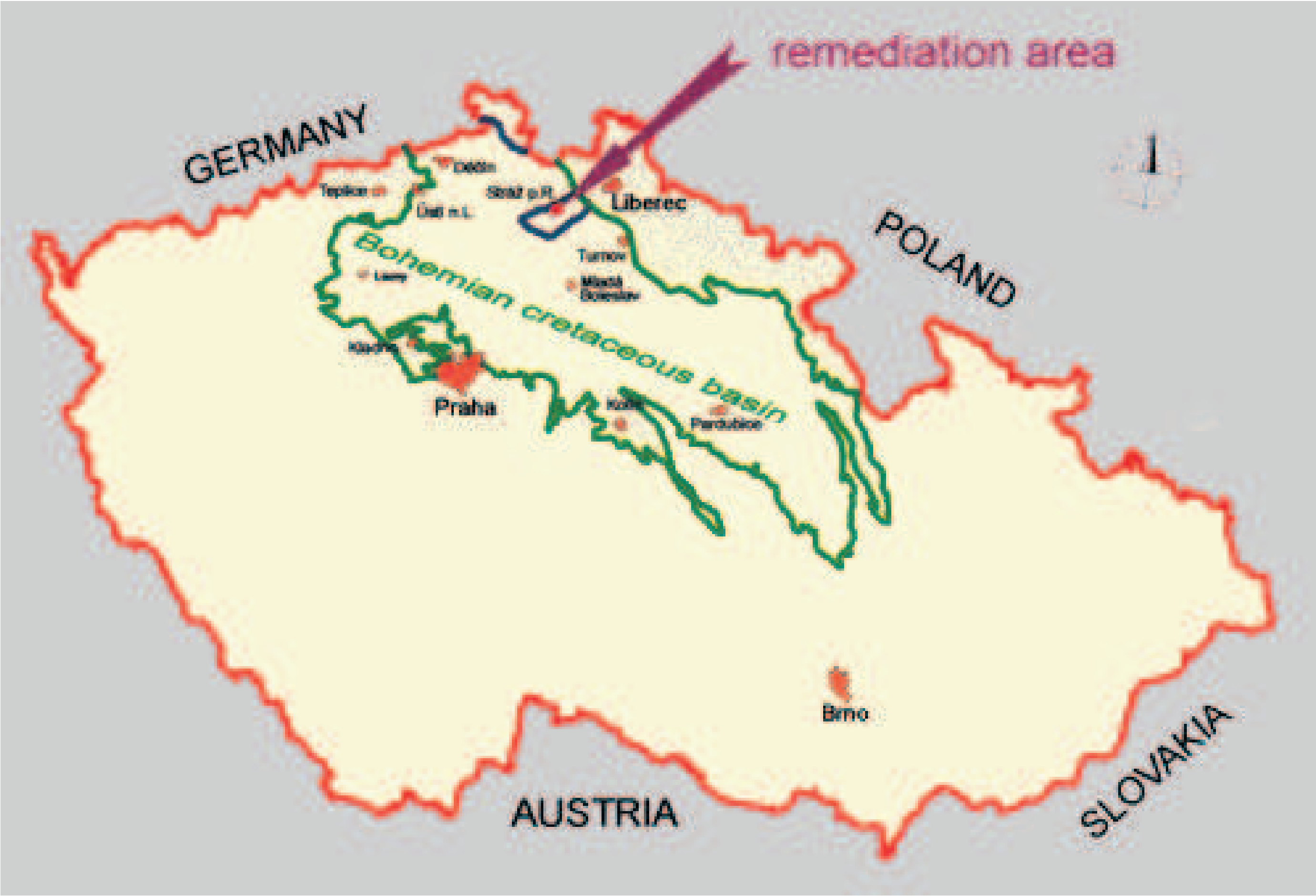



both in theory and in practice:

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

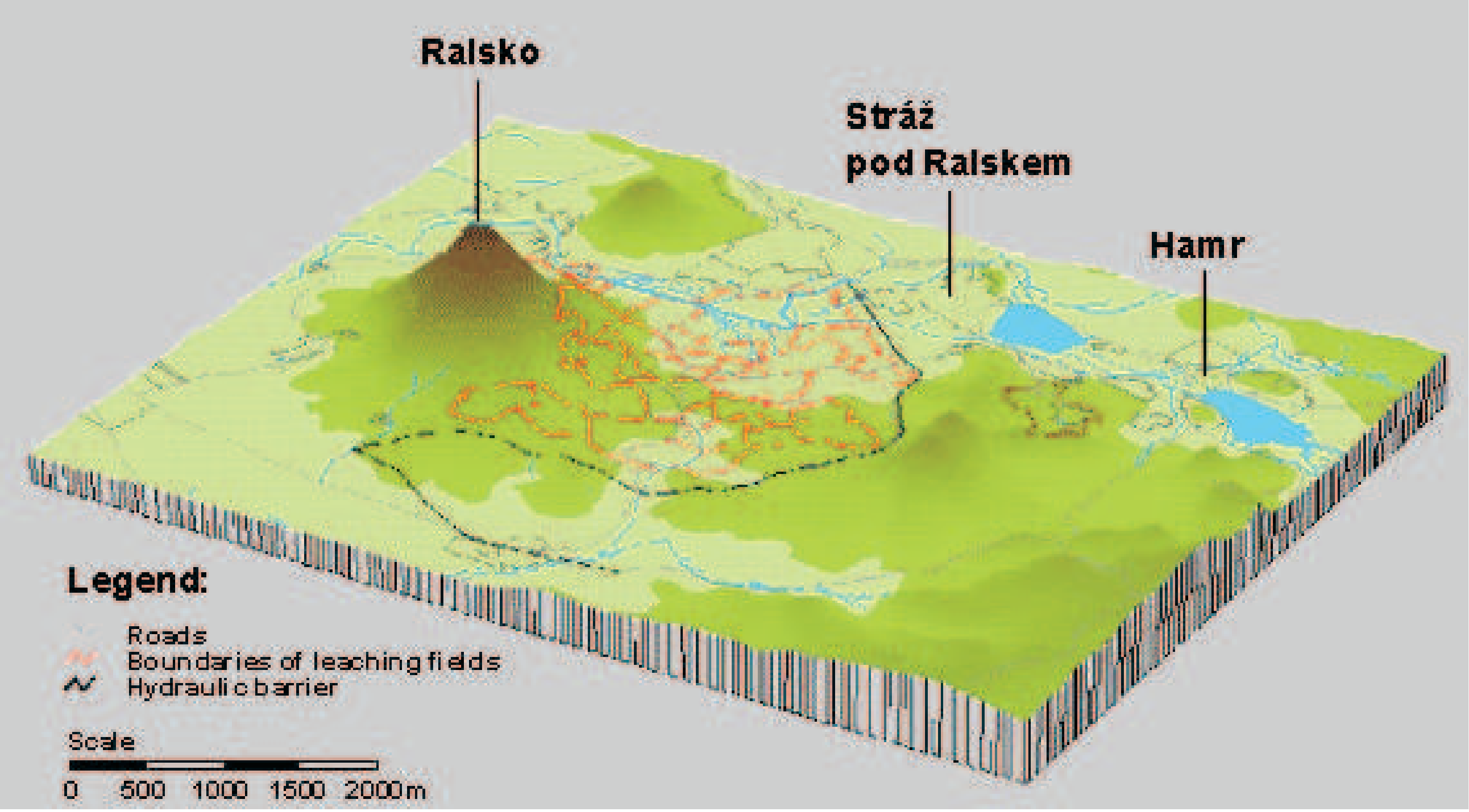
# 5. Application / I.

## Region under consideration



# 5. Application / II.

Detailed 3D view



# 5. Application / III.

## Specific 3D Applications

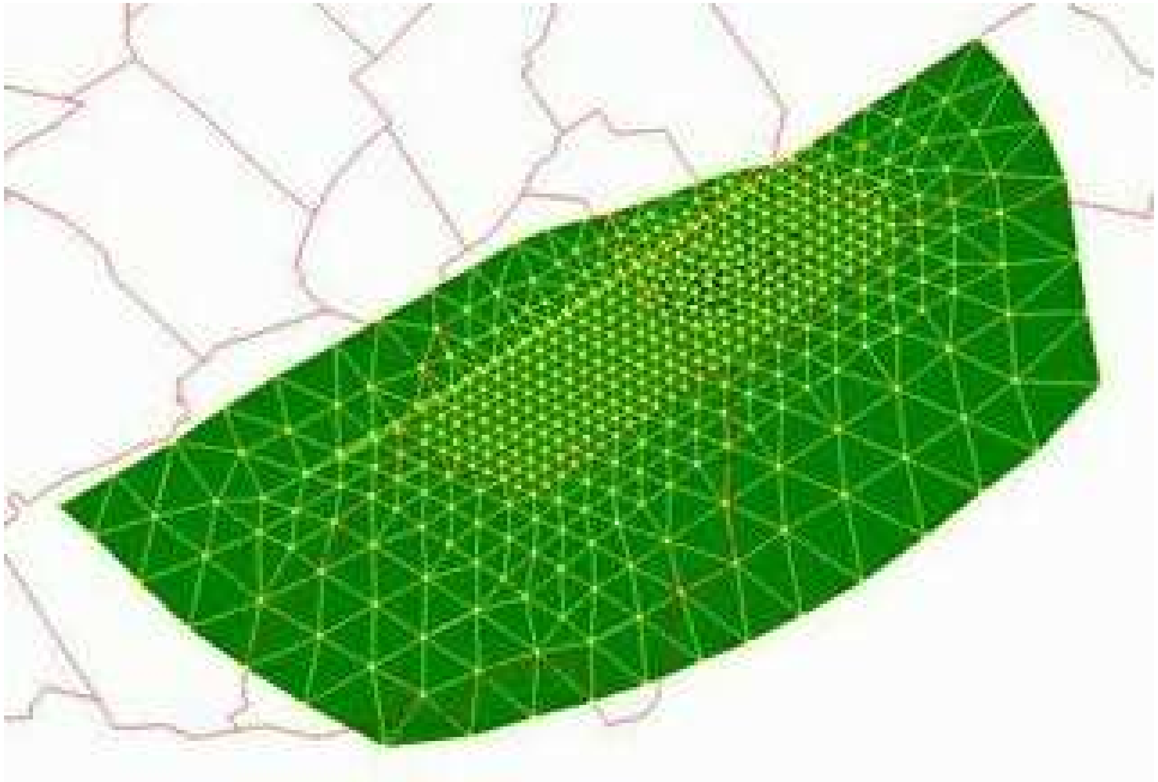
- Transport of contaminants in porous media
  - Finite volumes, splitting convection and diffusion at each time step
- Flow in fractured and anisotropic rocks
  - Combining two grids: network of fractures and FEM discretization of porous substrate
- Calibration of flow/transport models

(Vohralík, 2004)

# 5. Application / IV.

## Examples

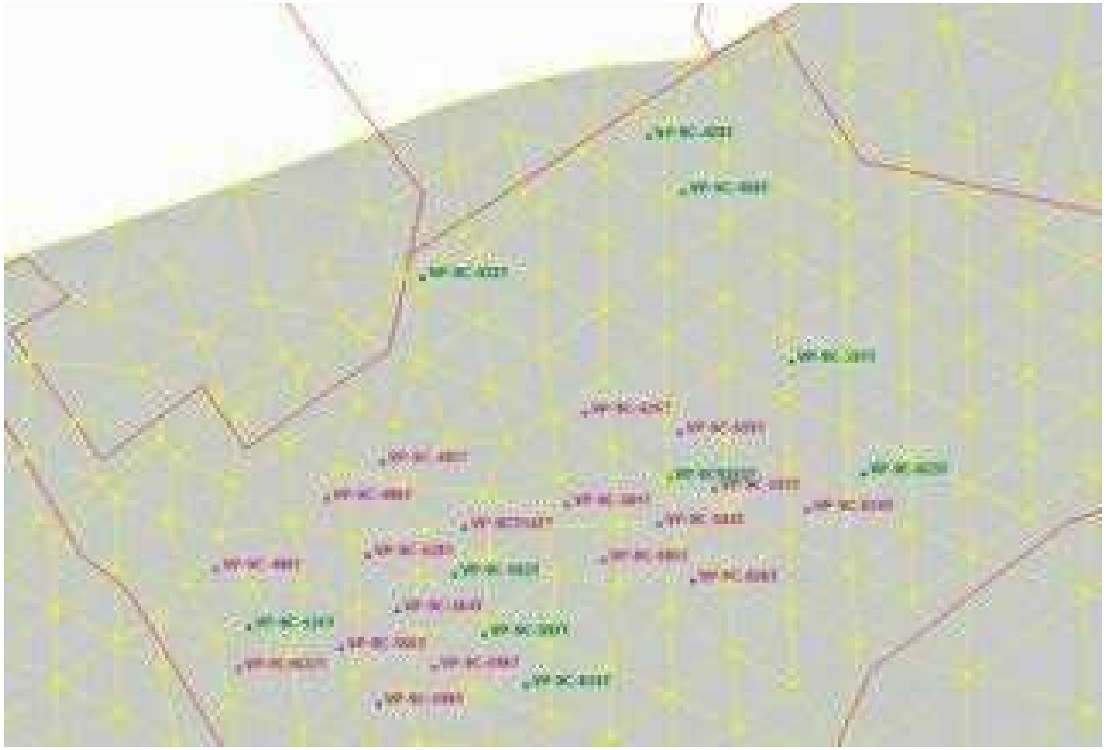
- Contaminant transport with dual porosities for remediation (grid)



# 5. Application / V.

## Examples

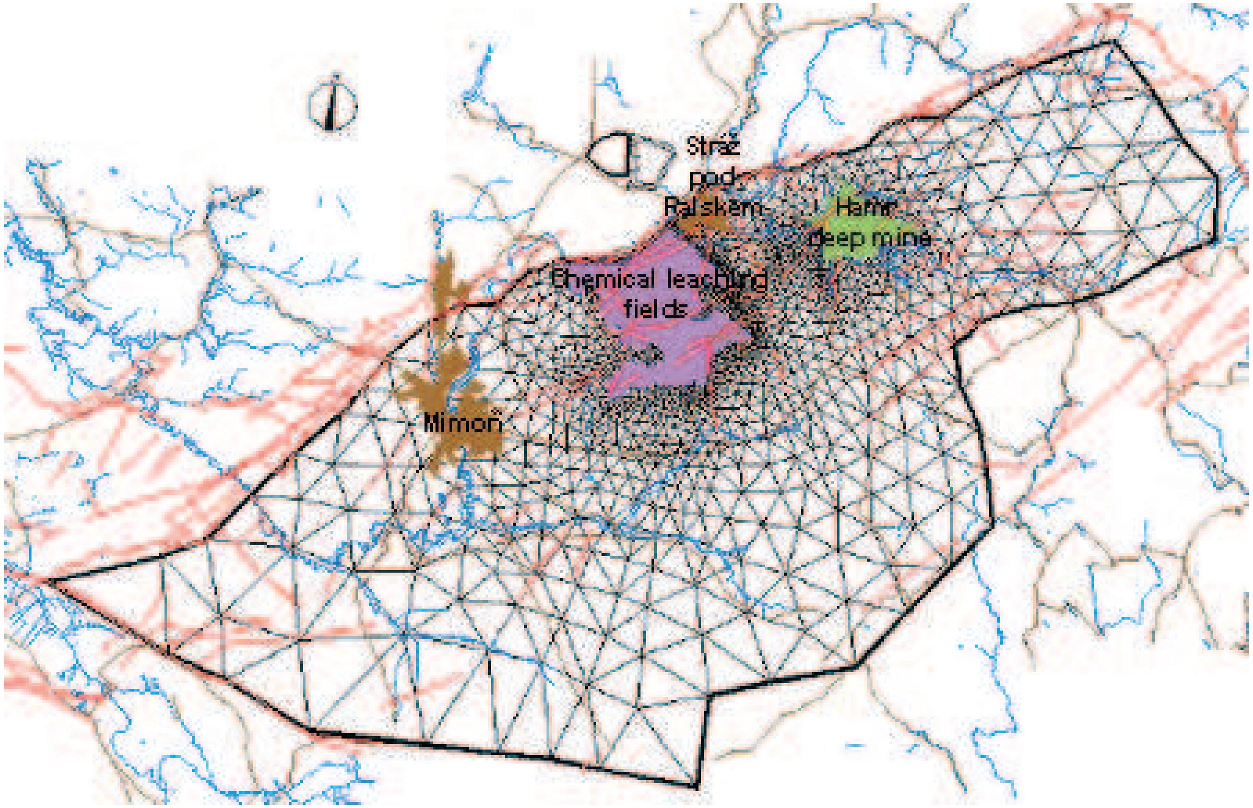
- Contaminant transport with dual porosity for remediation (drilled holes)



# 5. Application / VI.

## Examples

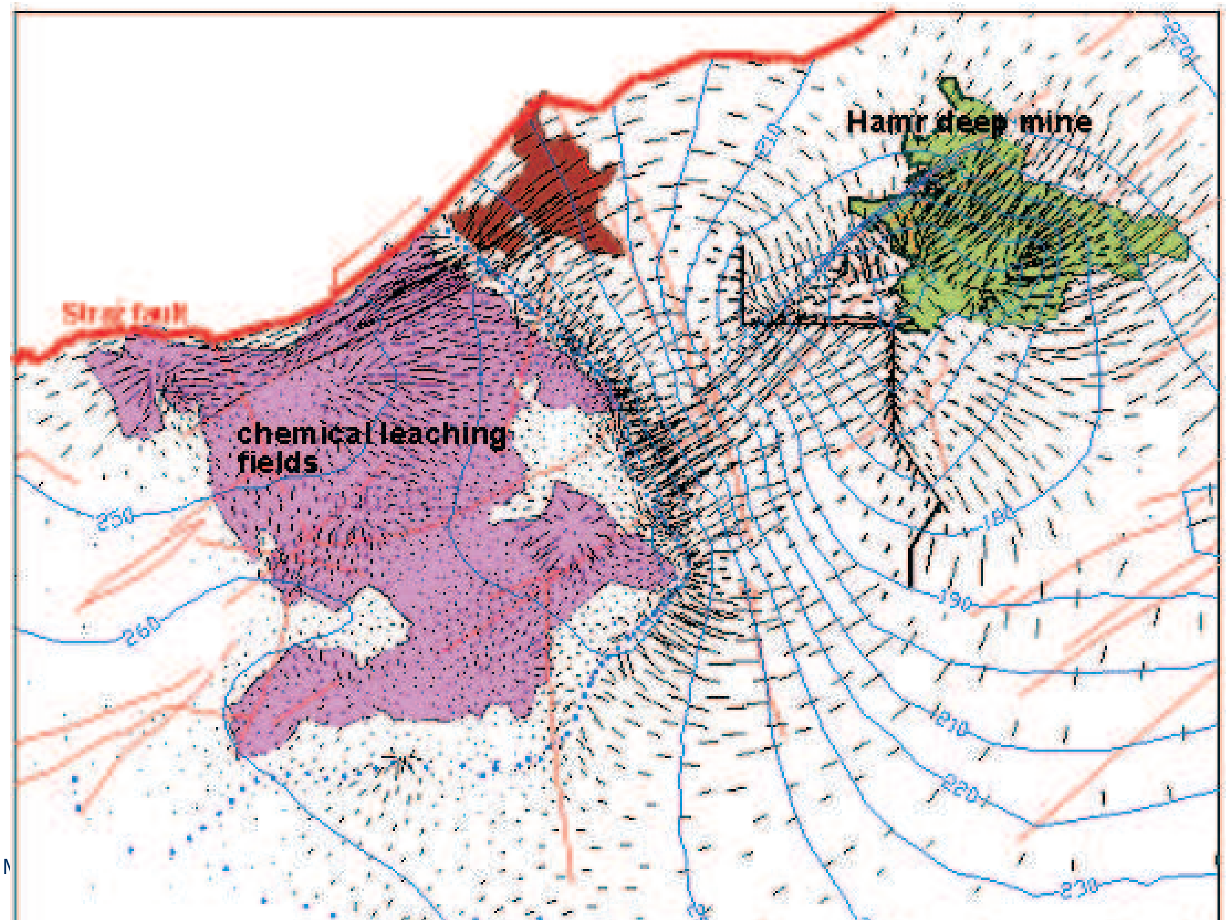
- Mine flooding (grid)



# 5. Application / VII.

Examples

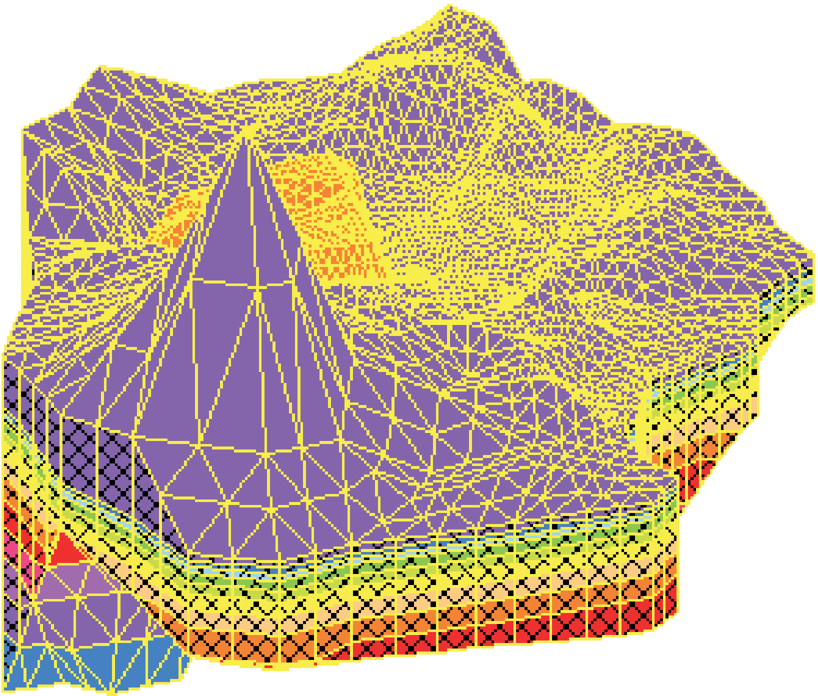
- Mine flooding (grid with velocities)



# 5. Application / VIII.

## Examples

- Mine flooding (3D grid)



# 5. Application / IX.

Animations

Mine flooding (animation of pressure development)

Mine flooding (animation of contamination development)

# 5. Conclusions

## Conclusions

- FEM hybridization is an important tool also from algebraic point of view.
- Algebraic null-space based methods useful feasible in 3D.
- Null-space approach (its partial variant) is a reasonable alternative for solving nonlinear and time-dependent problems.
- A step for cheap solving sequences of linear systems (see the talk at Seven Springs in a couple of days)