Linear Systems and Mixed Finite Elements in Hydrogeology

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Outline

- ▷ Mixed and Mixed-Hybrid finite element approximations.
  - ⇒ model flow problem in porous media.
  - ⇒ variational formulations and the resulting linear systems.
- ▷ Effect of the mesh geometry on both approximations.
  - ⇒ flat elements and condition numbers.
  - ⇒ symbolic and numerical computing (stability analysis).
- ▷ Behavior of both methods on heterogenous media.
  - ⇒ condition number estimates of the algebraic linear systems.
  - ⇒ numerical error estimates of the computed velocity.
  - ⇒ choice of linear system solvers and preconditioning .
- ▷ Some numerical experiments to validate the theoretical results.

Model flow problem in porous media

The governing transient equations for the pressure head p and Darcy's velocity u are given by:

$$\begin{aligned} s\,\frac{\partial p}{\partial t} + \nabla . u = f & \quad \text{in} \quad \Omega \times (0,T), \\ u = -\mathcal{K}\,\nabla p & \quad \text{in} \quad \Omega \times (0,T), \\ p = p^0 & \quad \text{in} \quad \Omega, \\ p = p^D & \quad \text{on} \quad \Gamma^D \times (0,T), \\ u.\nu = q^N & \quad \text{on} \quad \Gamma^N \times (0,T). \end{aligned} \tag{1}$$

where,

f : sink/source term;

$\mathcal{K}$: tensor of hydraulic conductivity;

s : storage coefficient;

ν : outward unit normal vector.

Mixed and Mixed-Hybrid finite element methods

- The mass is conserved locally (over each element K)

$$\int_{\partial K} u.\nu = \int_K \nabla.u = \sum_{\partial K} flux.$$

- The pressure head and its gradient are approximated simultaneously with the same order of convergence

- They can easily handle full tensors of permeability

- The hybridization technique aims to enforce the continuity of the fluxes across the interelement boundaries

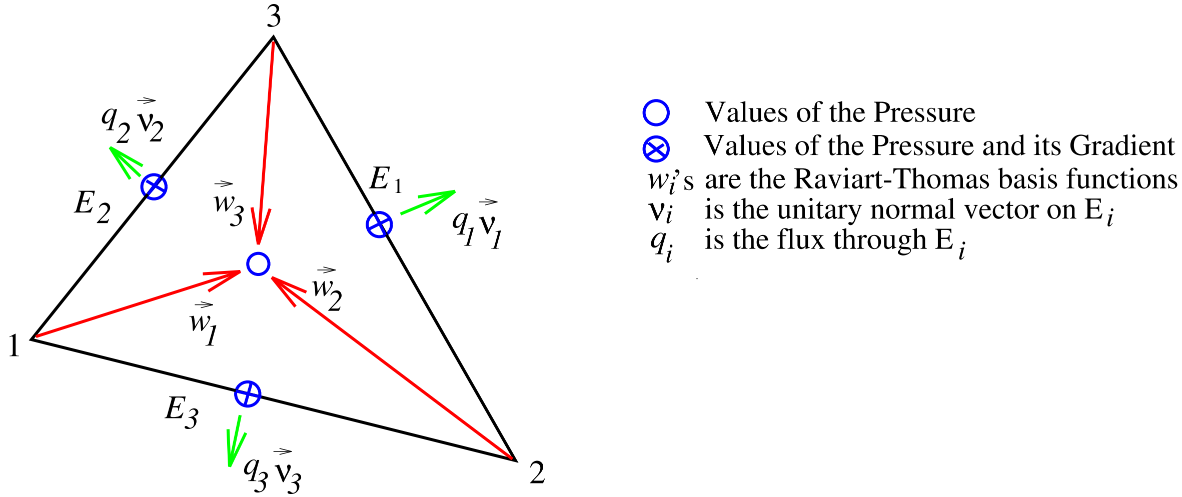
$$\int_E u.\nu_{K_1} = \int_E u.\nu_{K_2}, \quad E = \partial K_1 \cap \partial K_2.$$

Lowest order Raviart-Thomas space

The basis functions of the 3-dimensional space $RT^0(K)$ are defined as

$$w_{K,E_i} = \frac{1}{2|K|} \begin{pmatrix} x - x_i \\ y - y_i \end{pmatrix} \quad i = 1, \ldots, 3, \qquad (2)$$

where $|K|$ denotes the measure of the triangular element K.



Nodal points and basis functions on triangular elements.

- p_K: the mean of the pressure in K.
- $tp_{K,E}$: the mean of the pressure on E.

Mixed and Mixed-Hybrid formulations

The MFE formulation reads as :

Find $(u_h, p_h) \in RT^0_{q^N,N}(\mathcal{T}_h) \times \mathcal{M}^0(\mathcal{T}_h)$, such that

$$\left\{\begin{array}{lll} \displaystyle\int_\Omega (\mathcal{K}^{-1} u_h).\chi_h \, dx + \int_{\partial\Omega} p^D \, \nu.\chi_h \, d\ell & = \displaystyle\int_\Omega p_h \nabla.\chi_h \, dx & \forall\, \chi_h \in RT^0_{0,N}, \\ \displaystyle\int_\Omega s \frac{\partial p_h}{\partial t} \varphi_h \, dx + \int_\Omega \nabla.u_h \, \varphi_h \, dx & = \displaystyle\int_\Omega f \, \varphi_h \, dx & \forall\, \varphi_h \in \mathcal{M}^0. \end{array}\right. \tag{3}$$

The MHFE formulation reads as :

Find $(u_h, p_h, tp_h) \in RT^0(\mathcal{T}_h) \times \mathcal{M}^0(\mathcal{T}_h) \times \mathcal{N}^0_{p^D,D}(\mathcal{E}_h)$ such that

$$\left\{\begin{array}{ll} \displaystyle\int_\Omega (\mathcal{K}^{-1} u_h).\chi_h \, dx + \sum_{K\in\mathcal{T}_h} \int_{\partial K} tp_h \, \nu_K.\chi_h \, d\ell = \sum_{K\in\mathcal{T}_h} \int_K p_h \nabla.\chi_h \, dx & \forall\, \chi_h \in RT^0, \\ \displaystyle\int_\Omega s \frac{\partial p_h}{\partial t} \varphi_h \, dx + \int_\Omega \nabla.u_h \, \varphi_h \, dx = \int_\Omega f \, \varphi_h \, dx & \forall\, \varphi_h \in \mathcal{M}^0, \\ \displaystyle\sum_{K\in\mathcal{T}_h} \int_{\partial K} u_h.\nu_K \, \lambda_h \, d\ell = \int_{\partial\Omega} q^N \, \lambda_h \, d\ell & \forall\, \lambda_h \in \mathcal{N}^0_{0,D}. \end{array}\right. \tag{4}$$

Discetization of Darcy's law

By using $w_{K,E}$ as test functions in (3), we get

$$B_K Q_K = p_K e - T_{P_K} \qquad K \in \mathcal{T}_h, \tag{5}$$

where,

B_K : is a 3×3 symmetric positive definite matrix (elementary matrix)

$$(B_K)_{E,E'} = \int_K w_{K,E}^T \mathcal{K}_K^{-1} w_{K,E'} \, dx.$$

p_K : the pressure average over K.

e : vector of dimension 3 with unitary entries.

T_{P_K} : vector of pressure averages on ∂K.

Q_K : the fluxes across ∂K.

Discetization of Darcy's law

By inverting B_K, it is possible to eliminate the flux unknown. Thus, we obtain :

$$R^T P - M\,Tp + V = 0 \tag{6}$$

These matrices are defined as follows :

R^T is a sparse matrix of dimension $N_{\mathcal{E}} \times N_{\mathcal{T}}$

$$R = \left[R_{K,E}\right]_{N_{\mathcal{T}},N_{\mathcal{E}}},\ R_{K,E} = \alpha_{K,E} = \sum_{E' \subset \partial K} (B_K^{-1})_{E,E'}$$

M : is a $N_{\mathcal{E}} \times N_{\mathcal{E}}$ sparse matrix

$$M = \left[M_{E,E'}\right]_{\mathcal{N}_{\mathcal{E}},\mathcal{N}_{\mathcal{E}}},\ M_{E,E'} = \sum_{\partial K \supset E,E'} (B_K^{-1})_{E,E'}$$

Discretization of the mass conservation equation

Integrating (4) leads to :

$$s_K |K| \frac{\partial p_K}{\partial t} + \sum_{E \subset K} q_{K,E} = f_K \qquad K \in \mathcal{T}_h, \tag{7}$$

In matrix form, (7) is rewritten :

$$S \frac{dP}{dt} + D\,P - R\,T_P = F, \tag{8}$$

where

$S = \left[S_{K,K}\right]_{N_Q,N_Q}$ diagonal matrix:

$$S_{K,K} = |K|\, s_K$$

$D = \left[D_{K,K}\right]_{N_Q,N_Q}$ diagonal matrix:

$$D_{K,K} = \alpha_K = \sum_{E \subset \partial K} \alpha_{K,E}\,;$$

The linear systems derived from the MFE

The MHFE formulation gives rise a linear system of unknowns P and T_P

$$\underbrace{\begin{pmatrix} S & 0 \\ 0 & 0 \end{pmatrix}}_{\mathcal{L}} \begin{pmatrix} \frac{dP}{dt} \\ \frac{dT_P}{dt} \end{pmatrix} + \underbrace{\begin{pmatrix} D & -R \\ -R^T & M \end{pmatrix}}_{\mathcal{J}} \begin{pmatrix} P \\ T_P \end{pmatrix} = \begin{pmatrix} F \\ V \end{pmatrix}. \qquad (9)$$

By discretizing (9) by Backward Euler scheme, the problem is reduced to solve

$$(M - \Delta t\, N)\, T_P^n = R^T G^{-1} (S\, P^{n-1} + \Delta t F^n) + V^n.$$

where $G = (S + \Delta t D)$, $N = R^T G^{-1} R$.
$\mathcal{A} = (M - \Delta t\, N)$ can be seen as a Schur complement in S.P.D matrix.

The linear systems derived from the MFE

The MFE formulation gives rise a linear system of unknowns P and Q

$$\underbrace{\begin{pmatrix} S & 0 \\ 0 & 0 \end{pmatrix}}_{\mathcal{L}} \begin{pmatrix} \frac{dP}{dt} \\ \frac{dQ}{dt} \end{pmatrix} - \underbrace{\begin{pmatrix} 0 & -\widetilde{R} \\ -\widetilde{R}^T & \widetilde{M} \end{pmatrix}}_{\widetilde{\mathcal{J}}} \begin{pmatrix} P \\ Q \end{pmatrix} = \begin{pmatrix} \widetilde{F} \\ \widetilde{V} \end{pmatrix}. \tag{10}$$

By discretizing (10) by Backward Euler scheme, the problem is reduced to solve

$$(\widetilde{M} + \Delta t\, \widetilde{N})Q^n = \widetilde{R}^T (P^{n-1} + \Delta t\, S^{-1}\, \widetilde{F}^n) + \widetilde{V}^n.$$

where $\widetilde{N} = \widetilde{R}^T S^{-1} \widetilde{R}$.
$\widetilde{\mathcal{A}} = (\widetilde{M} + \Delta t\, \widetilde{N})$ can be seen as a Schur complement in S.P.D matrix.

Effect of the spatial discretization

Effect of the spatial discretization

Inverting method of the elementary matrix B_K

This matrix is defined by

$$(B_K)_{E,E'} = \int_K w_{K,E}^T \, \mathcal{K}_K^{-1} \, w_{K,E'} \, dx.$$

▷ The mixed hybrid formulation necessitates inverting B_K.

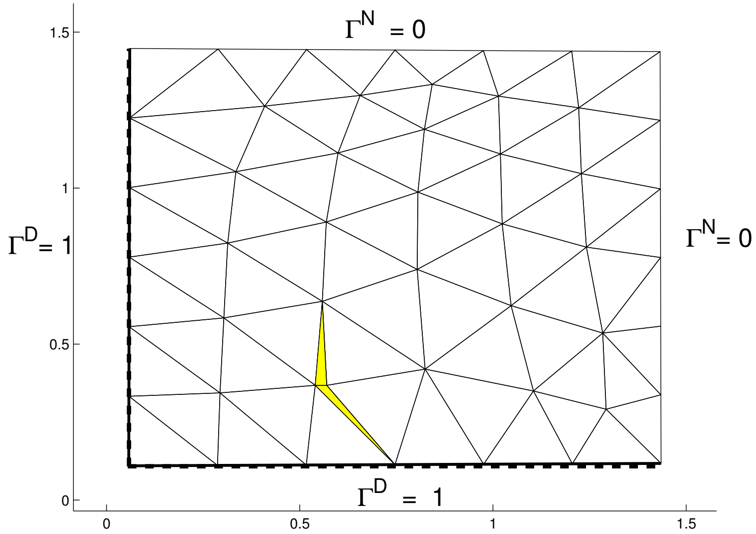
▷ The stability of the numerical code is crucial due to possible ill-conditioned matrices

▷ Two codes are used to invert B_K

1. Cramer's method (generated automatically by Maple)
2. LDL^T Factorization ($B_K^{-1} = L^{-T} D^{-1} L^{-1}$)

Effect of the spatial discretization

Numerical test:



$T = 3,\ \Delta t = 1,\ s = 1,\ \mathcal{K} = I_{2\times 2},\ f = 0.$

The quality of a triangular element K is evaluated by

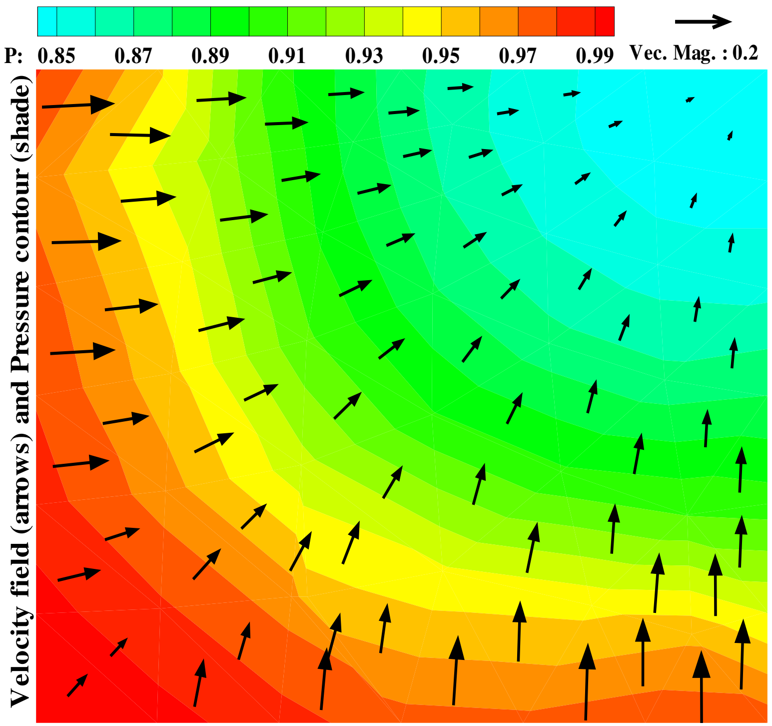
$$\mathcal{Q}(K) = 2\sqrt{3}\,\frac{\rho_K}{h_K}, \qquad (\mathcal{Q}(K) = 1 \text{ if } K \text{ equilateral triangle})$$

ρ_K: is the element diameter (the length of its longest edge).
h_K: is the in-radius.

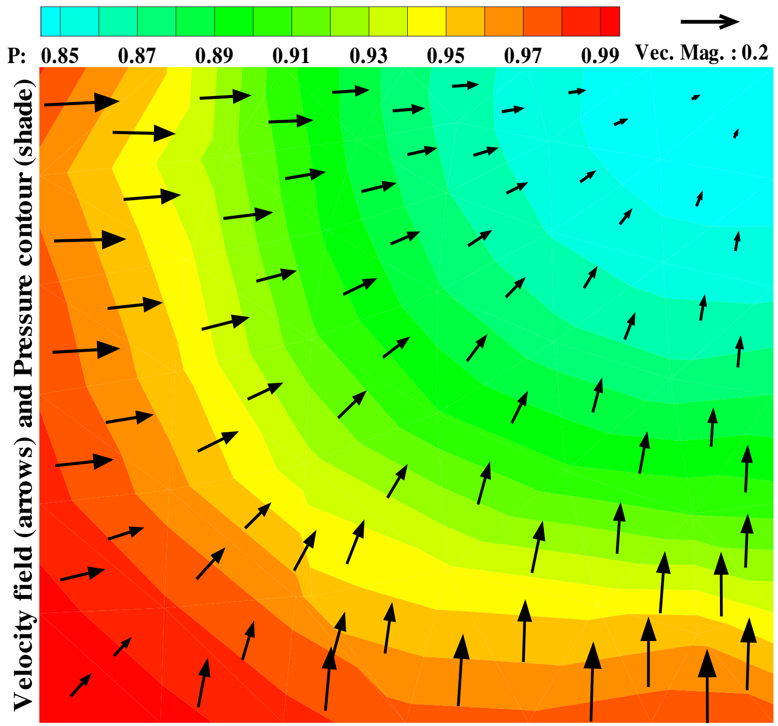
Effect of the spatial discretization

Comparison between 2 computations obtained by using the 2 codes in the MHFE algorithm

well-shaped, $\mathcal{Q}(K) \approx 0.2$



(a) Cramer - Method, Mesh quality $\approx$ 0.2



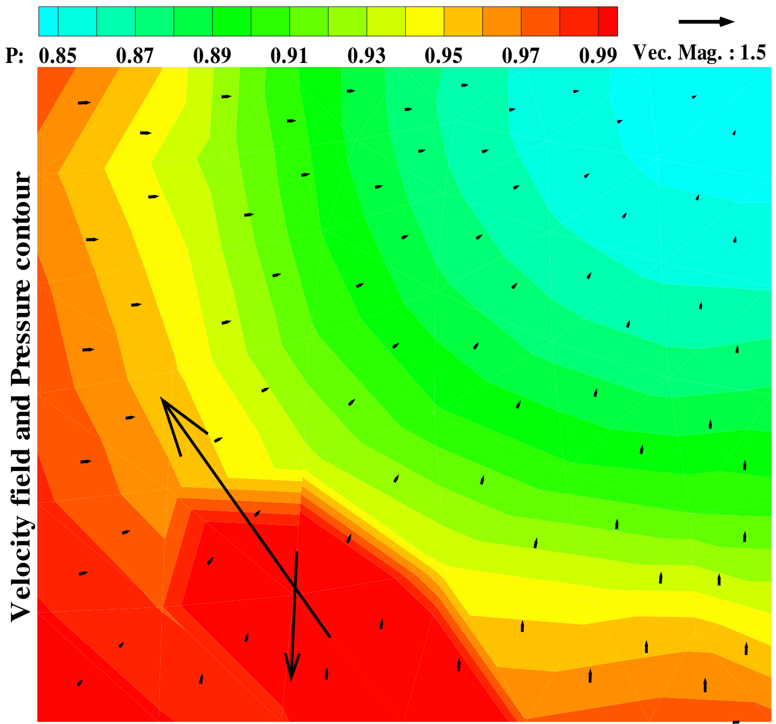
(b) LDL - Method, Mesh quality $\approx$ 0.2

Velocity field and pressure contour

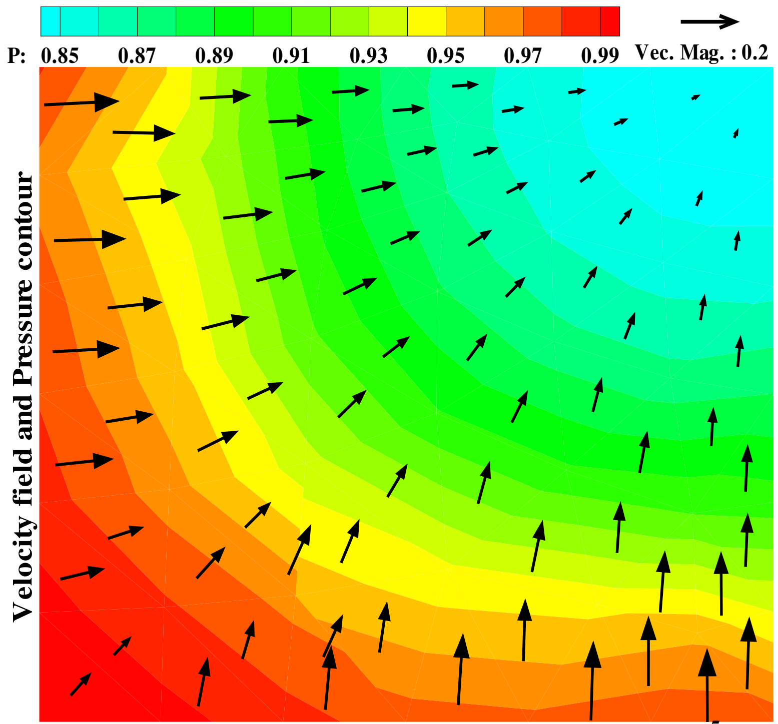
Effect of the spatial discretization

Comparison between 2 computations obtained by using the 2 codes in the MHFE algorithm

ill-shaped, $\mathcal{Q}(K) \approx 10^{-5}$



(a) Cramer - Method , Mesh quality $\approx 10^{-5}$



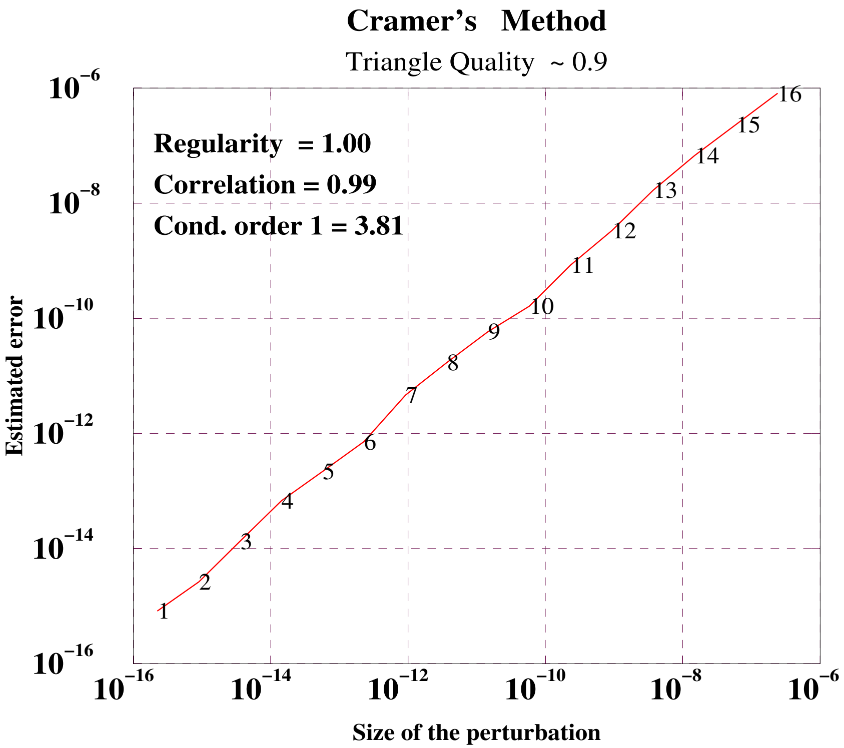
(b) LDL - Method, Mesh quality $\approx 10^{-5}$

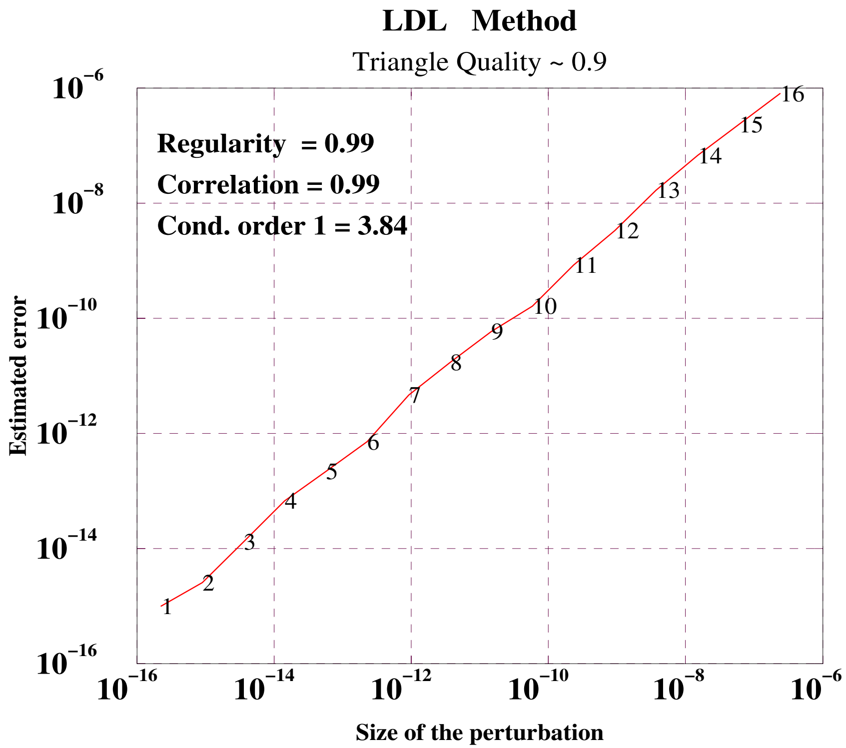
Velocity field and pressure contour

Effect of the spatial discretization

Stability analysis by Aquarels

well-shaped, $\mathcal{Q}(K) \approx 0.9$



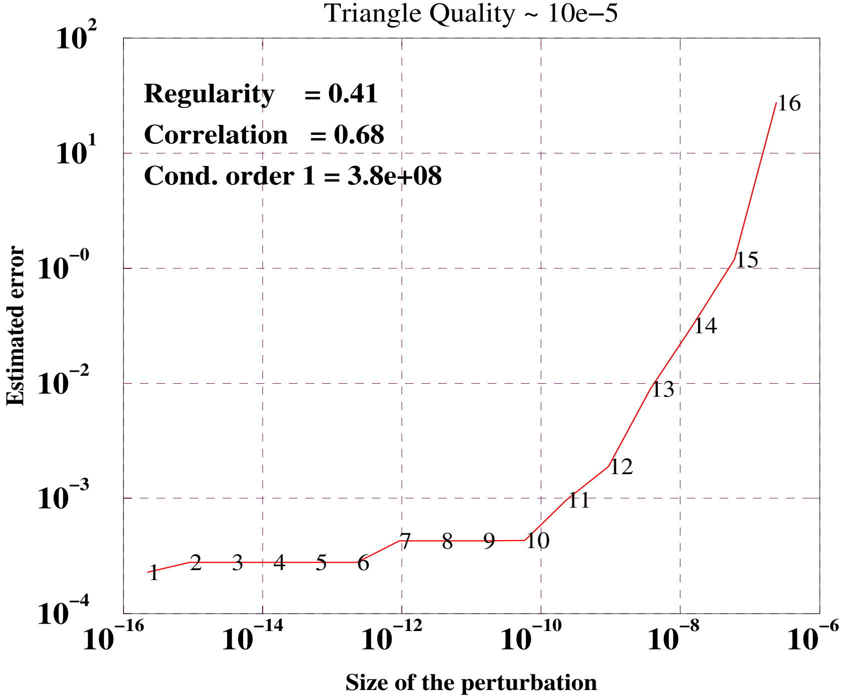


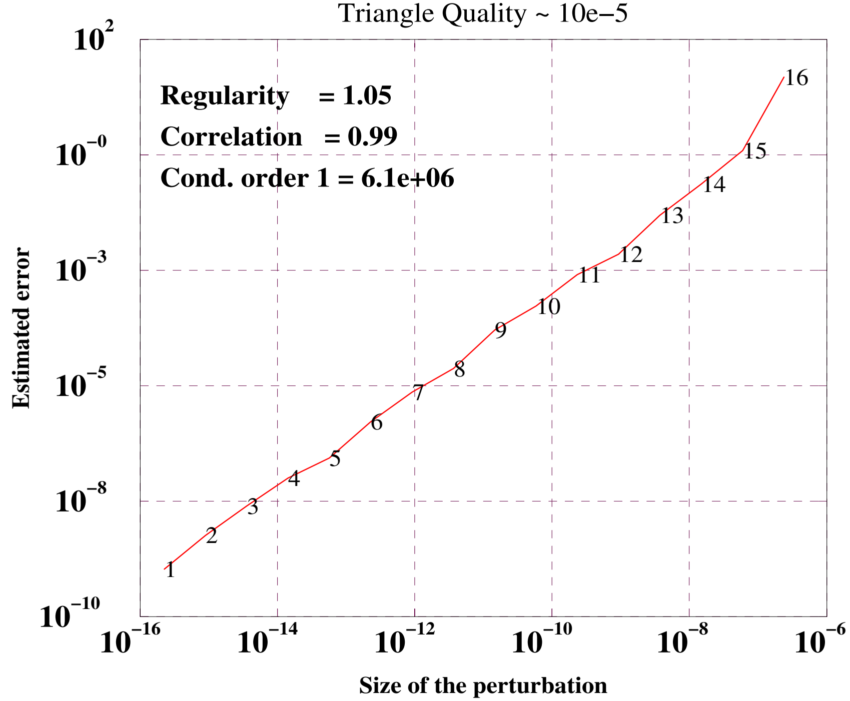
Absolute error $\|B_K^{-1} - \widetilde{B}_K^{-1}\|_2$		Relative error	
Cramer	*LDL*	Cramer	*LDL*
1.7×10^{-15}	4.4×10^{-16}	5.9×10^{-16}	1.5×10^{-16}

Effect of the spatial discretization

Stability analysis by Aquarels

ill-shaped, $\mathcal{Q}(K) \approx 10^{-5}$



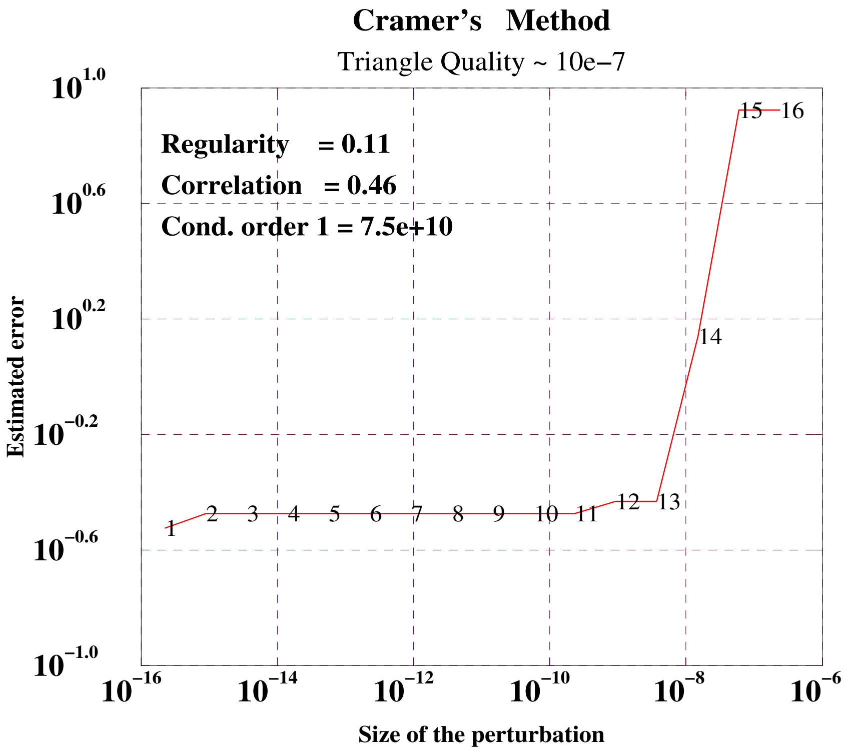


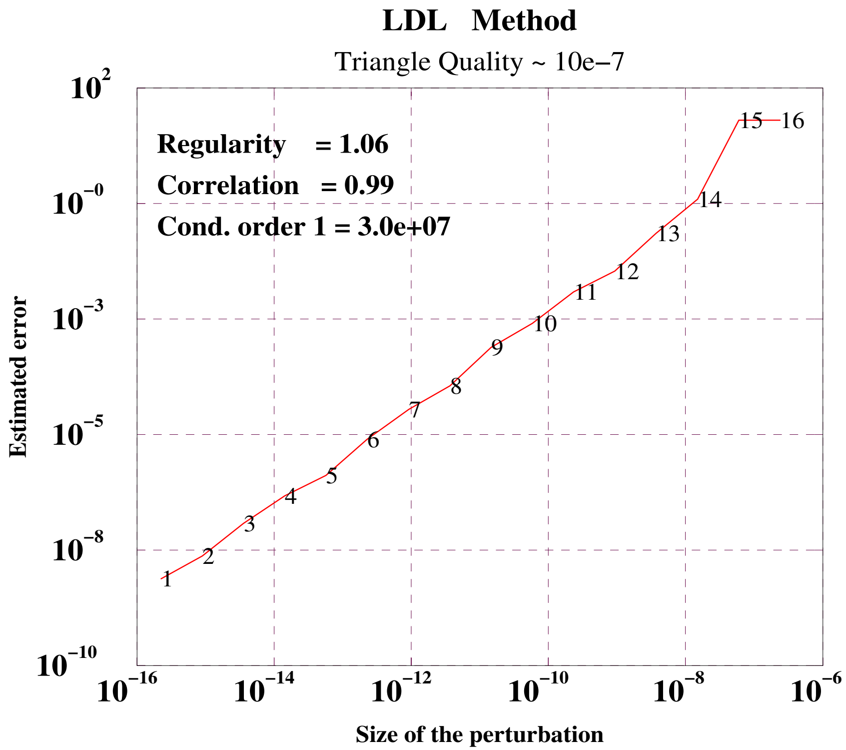
Absolute error		Relative error	
Cramer	*LDL*	Cramer	*LDL*
$1.6 \times 10^{+03}$	4.7×10^{-03}	1.1×10^{-04}	3.3×10^{-10}

Effect of the spatial discretization

Stability analysis by Aquarels

very ill-shaped, $\mathcal{Q}(K) \approx 10^{-7}$



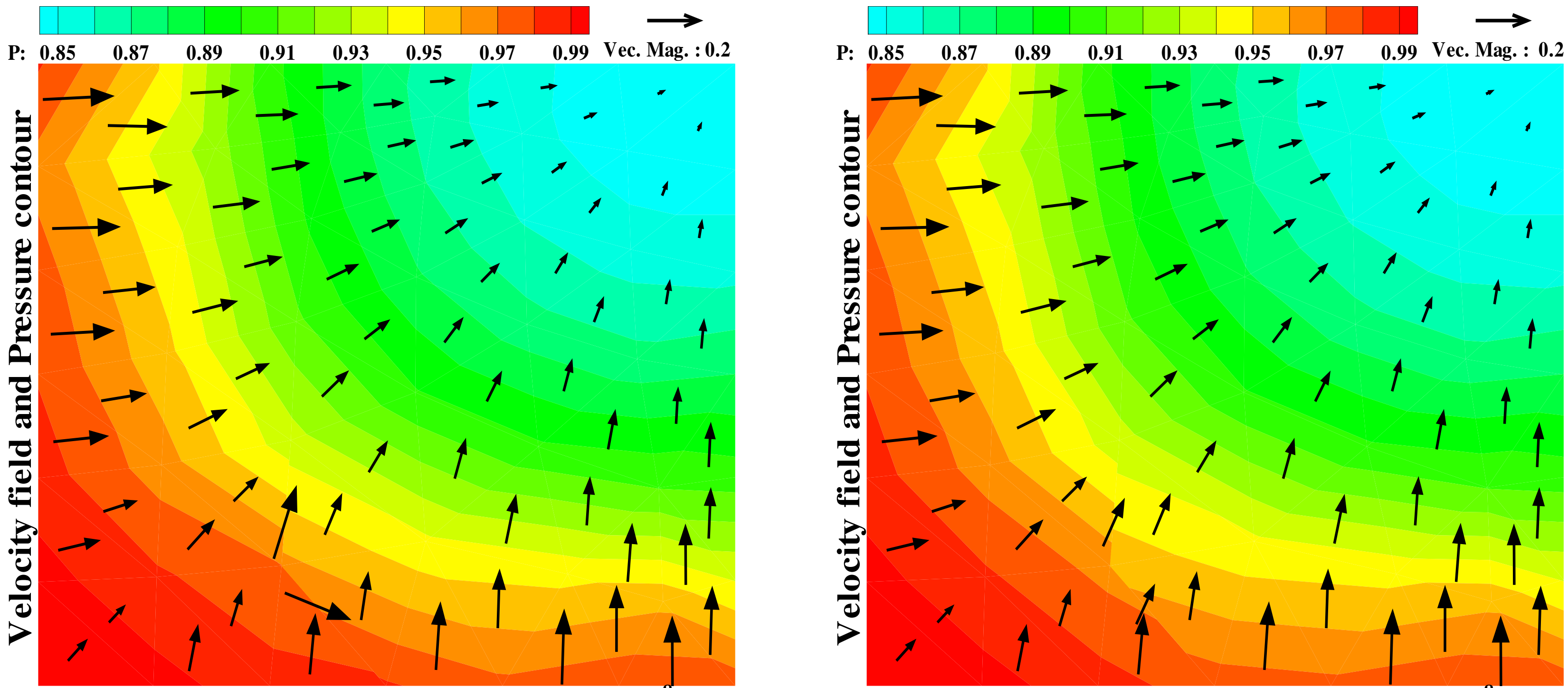


Absolute error		Relative error	
Cramer	*LDL*	Cramer	*LDL*
$3.5 \times 10^{+07}$	2.7×10^{-02}	1.6×10^{-01}	1.2×10^{-10}

Effect of the spatial discretization

Comparison between MHFE et MFE methods

$\mathcal{Q}(K) \approx 10^{-8}$, Condition number $\approx 10^{15}$



(a) MHFE- Method, Mesh quality $\approx 10^{-8}$

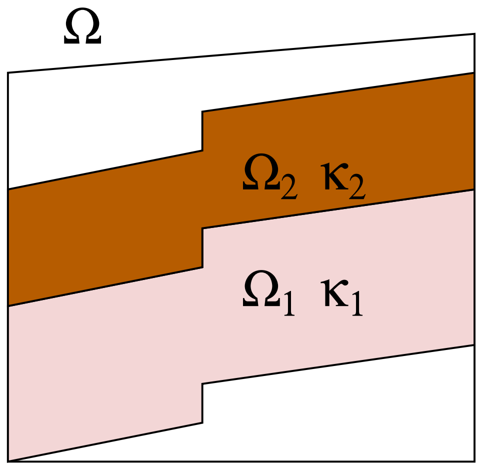
(b) MFE - Method, Mesh quality $\approx 10^{-8}$

Velocity field and pressure contour

Behavior of MFE and MHFE methods on heterogeneous media

MFE and MHFE methods in heterogeneous media

Suppose that the heterogeneous domain Ω is composed of two sub-domains Ω_i, according to their conductivities $\mathcal{K}_i = \kappa_i \, I_{2\times 2}$



Decomposition of the domain according to the permeability values.

with very high contrast of permeability: $\dfrac{\kappa_2}{\kappa_1} \gg 1$

Lemma 1.
Let A (resp. B) be a non-singular (resp. singular) matrix, then the condition number $\mathcal{X}(A)$ of A is bounded by the following inequality

$$\mathcal{X}(A) = \|A\|.\|A^{-1}\| \geq \frac{\|A\|}{\|A-B\|}$$

Proof:
Since B is a singular matrix, there exists a nonzero vector x such that $Bx = 0$, then we can write

$$\begin{aligned} \|Ax\| &= \|(A-B)x\| \leq \|A-B\|\|x\|, \\ \|x\| &= \|A^{-1}Ax\| \leq \|A^{-1}\|\|Ax\|. \end{aligned}$$

Hence, the lemma is a direct consequence of these inequalities.

Let $\mathcal{J}_{\kappa_1,\kappa_2}$(resp. $\mathcal{J}_{\kappa_1}$) denote the matrix $\mathcal{J}$ over $\Omega = \Omega_1 \cup \Omega_2$ (resp.$\Omega = \Omega_1$)

$$\mathcal{J} = \begin{pmatrix} D & -R \\ -R^T & M \end{pmatrix}$$

Proposition 1. $\mathcal{X}(\mathcal{J}_{\kappa_1,\kappa_2}) = \mathcal{O}(\frac{\kappa_2}{\kappa_1})$.

Proof: We have

$$\mathcal{J}_{\kappa_1,\kappa_2} = \begin{cases} \mathcal{J}_{\kappa_1} & \text{in } \Omega_1, \\ \mathcal{J}_{\kappa_2} & \text{in } \Omega_2, \\ \mathcal{J}_{\kappa_1,\kappa_2} & \text{on } \Omega_1 \cap \Omega_2. \end{cases}, \text{ define } \overline{\mathcal{J}}_{\kappa_1,\kappa_2} = \begin{cases} 0 & \text{in } \Omega_1, \\ \mathcal{J}_{\kappa_2} - \mathcal{J}_{\kappa_1} & \text{in } \Omega_2, \\ \mathcal{J}_{\kappa_1,\kappa_2} - \mathcal{J}_{\kappa_1} & \text{on } \Omega_1 \cap \Omega_2. \end{cases}$$

$\overline{\mathcal{J}}_{\kappa_1,\kappa_2}$ is singular with $\mathcal{J}_{\kappa_1,\kappa_2} - \overline{\mathcal{J}}_{\kappa_1,\kappa_2} = \mathcal{J}_{\kappa_1}$

Hence $\mathcal{X}(\mathcal{J}_{\kappa_1,\kappa_2}) \geq \frac{\|\mathcal{J}_{\kappa_1,\kappa_2}\|}{\|\mathcal{J}_{\kappa_1}\|} = \mathcal{O}(\frac{\kappa_2}{\kappa_1})$,

Condition number estimates

By applying **Lemma.1**, the following estimations of the condition numbers can be shown:

MHFE Schur complement matrix (unknowns Tp)

1. $\mathcal{X}(\mathcal{A}_{\kappa_1,\kappa_2}) = \mathcal{O}(\frac{\kappa_2}{\kappa_1})$

MFE Schur complement matrix (unknowns Q)

2. $\mathcal{X}(\tilde{A}_{\kappa_1,\kappa_2}) = \mathcal{O}\left(\max\left\{\kappa_1\,\Delta t\,\|S^{-1}\|,\ \frac{\kappa_2}{\kappa_1}\left(\frac{1+\kappa_1\,\Delta t\,\|S^{-1}\|}{1+\kappa_2\,\Delta t\,\|S^{-1}\|}\right)\right\}\right)$

MFE matrix without eliminating the fluxes (unknowns Q and P)

3. $\mathcal{X}(\mathcal{L} - \Delta t\,\tilde{\mathcal{J}}_{\kappa_1,\kappa_2}) = \mathcal{O}\left(\max\left\{\frac{\kappa_2}{\Delta t}\|S\|, \frac{\kappa_2}{\kappa_1}\right\}\right)$

Accumulation of numerical errors by the MHFEM

After computing the pressure and its traces, the fluxes are computed locally by solving a block diagonal system

$$B\,Q = (P - T_P). \tag{11}$$

B is a block diagonal matrix of condition number $\mathcal{X}(B) = \mathcal{O}(\frac{\kappa_2}{\kappa_1})$. Thus, the fluxes Q are computed with conditioning order $\mathcal{O}\left((\frac{\kappa_2}{\kappa_1})^2\right)$.

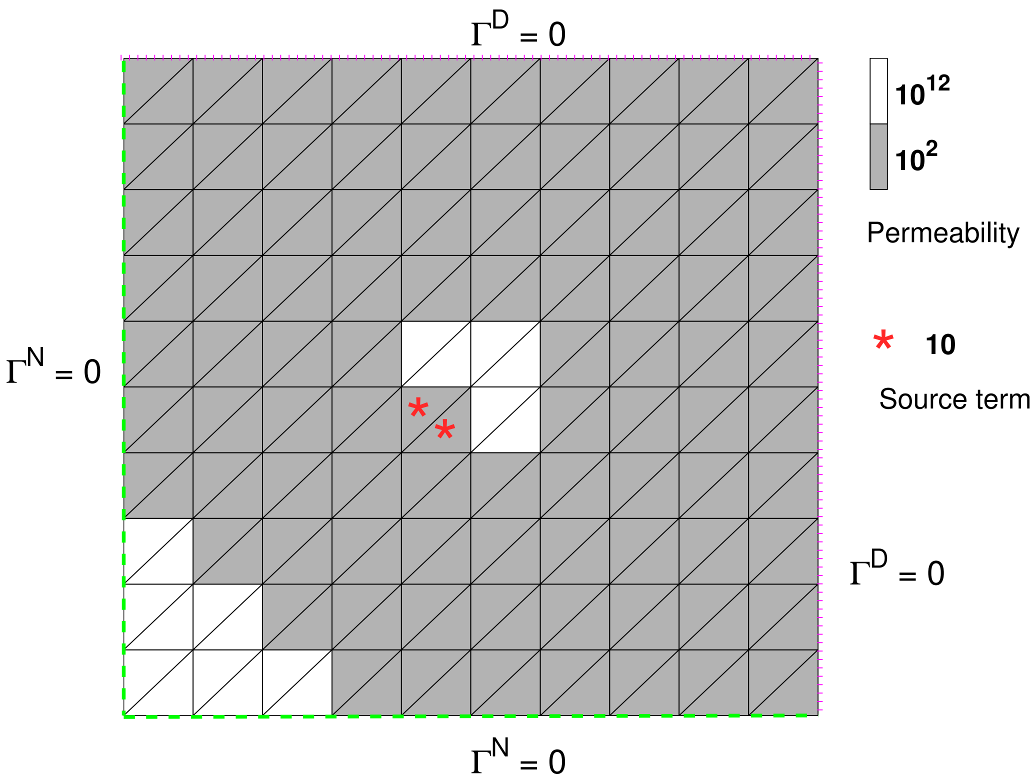
In the stationary case, the absolute roundoff error of the local mass balance can be written as

$$\left[\sum_{E\subset\partial K} q_{K,E} - f_K\right] = \kappa_K \sum_{E\subset\partial K} \epsilon_{K,E}. \tag{12}$$

where $\epsilon_{K,E}$ denotes the numerical error produced from the computation of P and T_P.

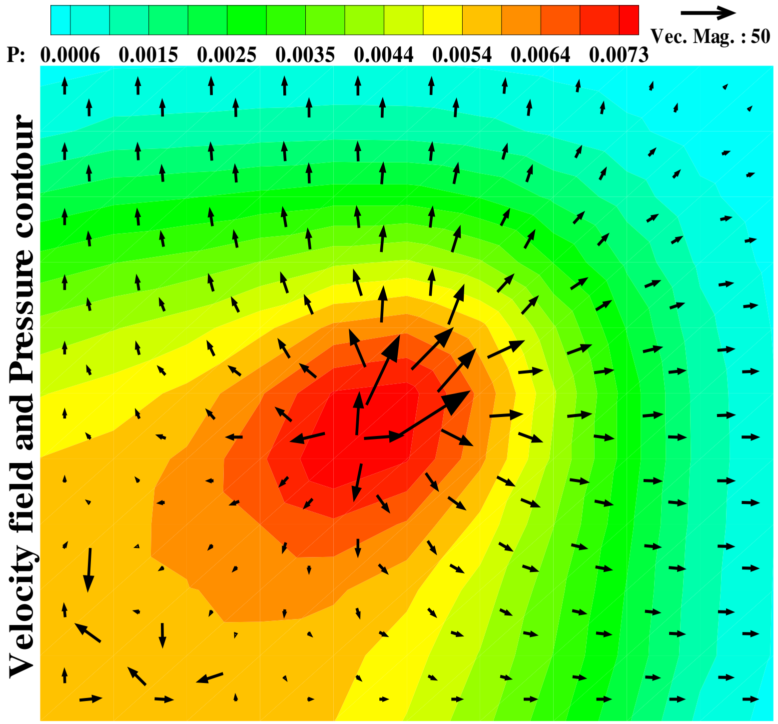
Experiment 1: stationary problem

Consider a stationary problem over a unit square with the following initial and boundary conditions.

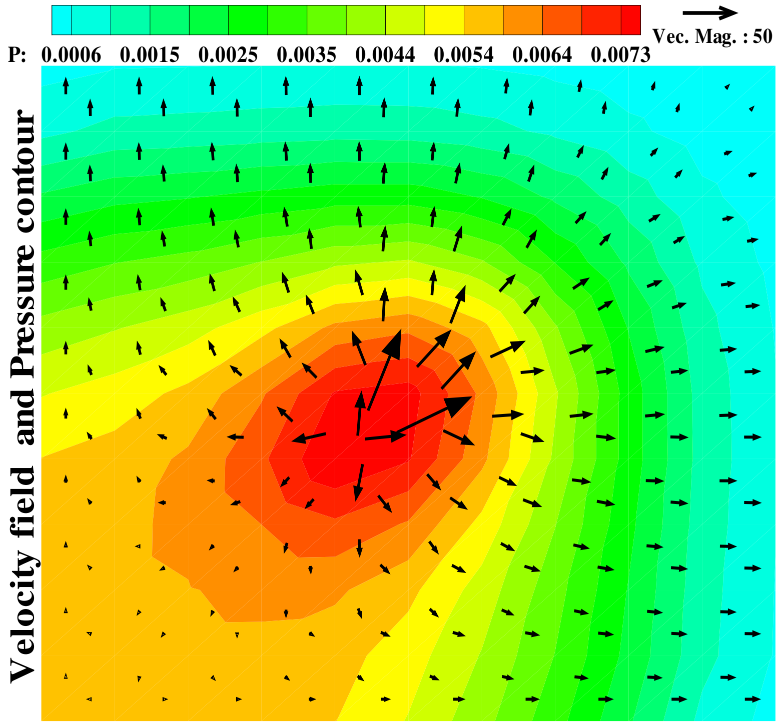


Triangulation of the unit square.

Experiment 1: stationary problem



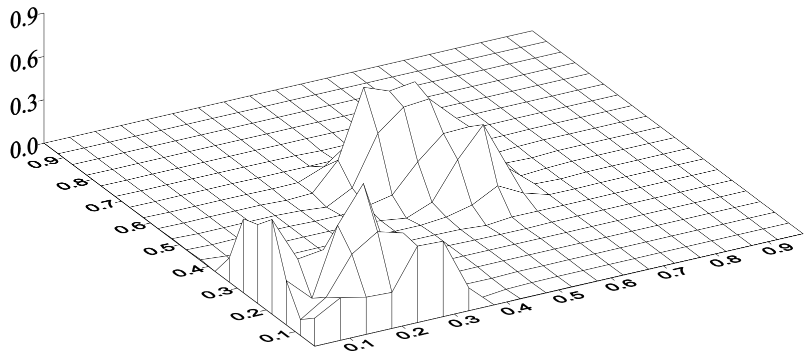
a) Results computed by MHFE method



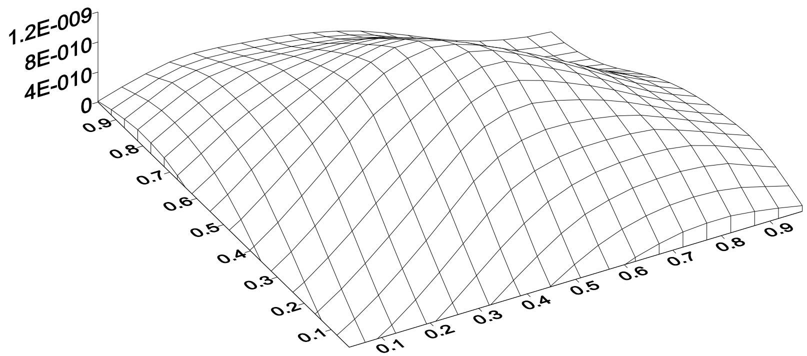
b) Results computed by MFE method

Results obtained by the MHFE and MFE methods

Experiment 1: stationary problem

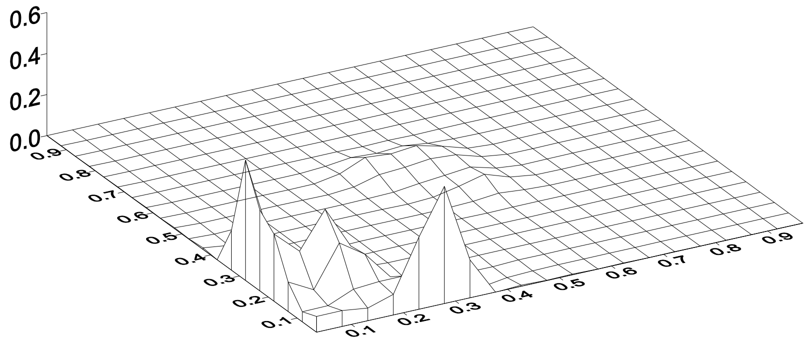


a) Absolute error , MHFE method

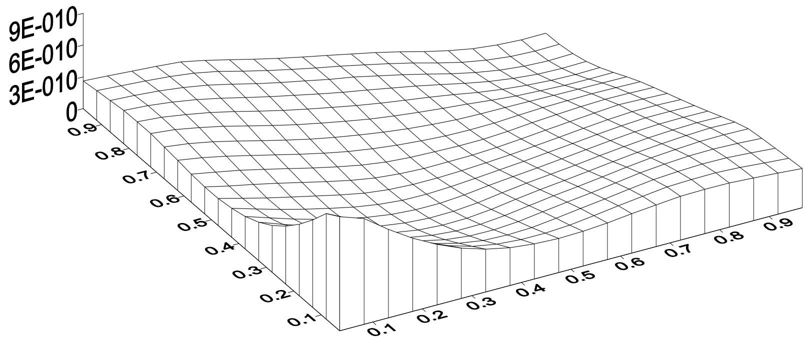


b) Absolute error, MFE method

Absolute errors of the mass balance over the domain



a) Relative error, MHFE method

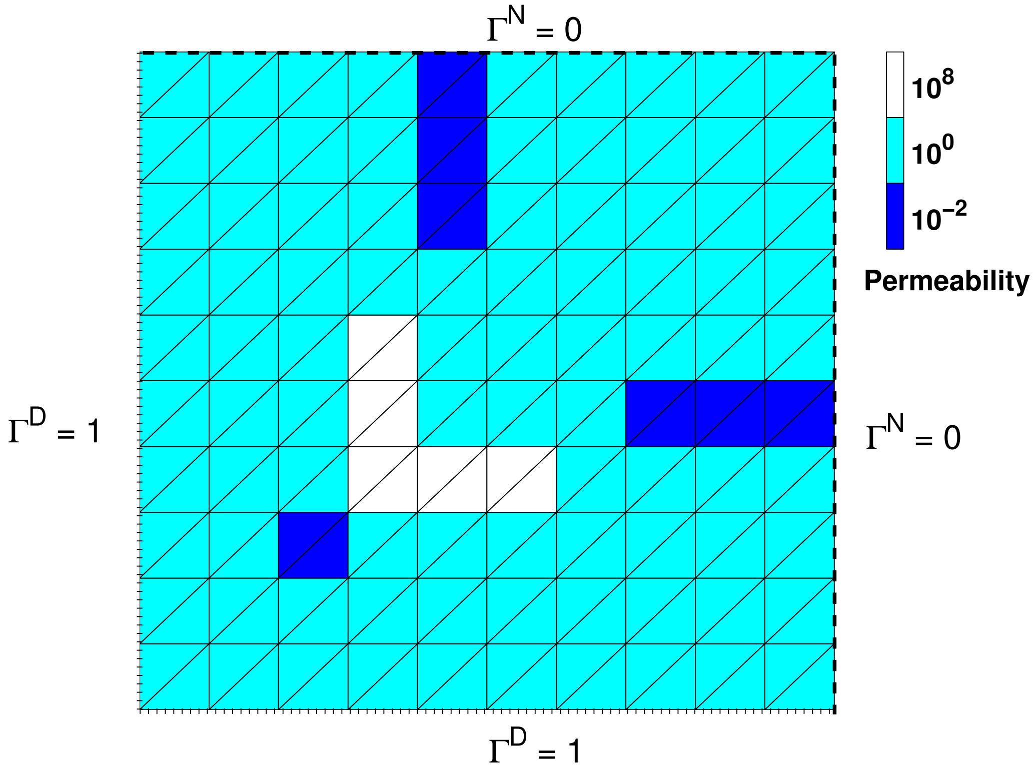


b) Relative error, MFE method

Relative errors of the mass balance over the domain

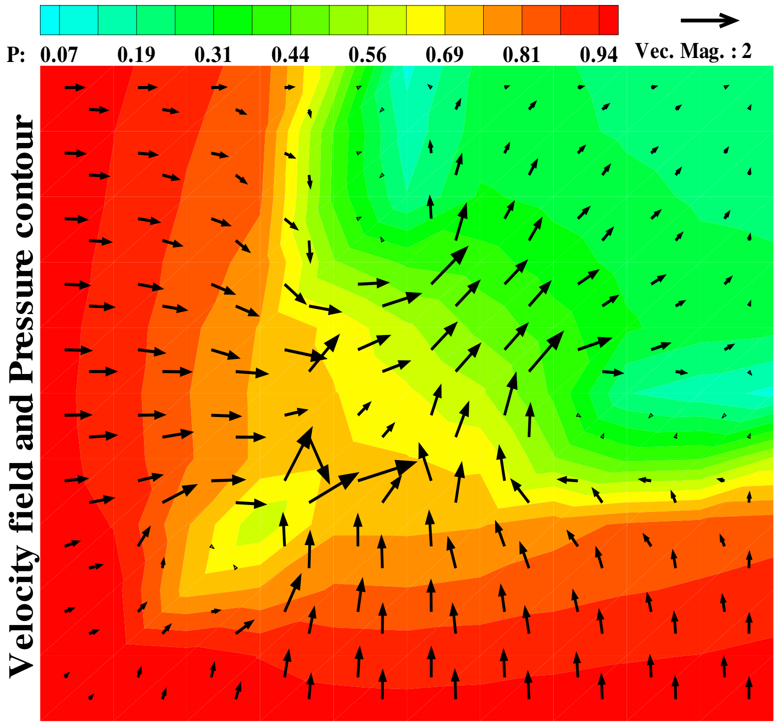
Experiment 2: transient problem

Consider a time-dependent problem over a unit square with the following initial and boundary conditions. $T =]0, 1]$, $\Delta t = \frac{1}{10}$, $s = 1$, $f = 0$.

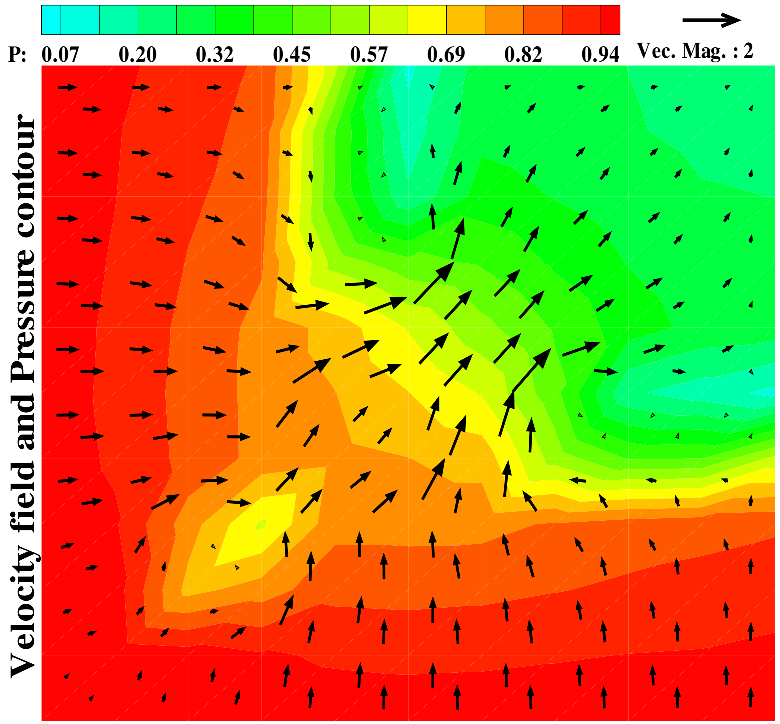


Permeability distribution and boundary conditions

Experiment 2: transient problem



a) Results computed by MHFE method



b) Results computed by MFE method

Results obtained by the MHFE and MFE methods

Eisenstat preconditioning is used with the CG algorithm to solve the S.P.D systems.

The symmetric indefinite systems are solved by using Symmlq solver without any preconditioning.

Computing times

$\Omega = \Omega_1 \cup \Omega_2$, $\Delta t = 1/10$, $s_i = 1$ $i = 1, 2$, PCG solver.

	MHFE method			MFE method		
κ_2/κ_1	CPU	Cond. Num.	# Iter.	CPU	Cond. Num.	# Iter
10^2	2.2	10.2×10^2	22–21	1.8	4.3×10^2	33–31
10^4	2.3	10.9×10^4	24–23	2.1	4.2×10^4	42–40
10^6	2.4	10.7×10^6	26–25	2.4	4.5×10^6	55–54

$\Delta t = 1/10$, $\kappa_i = 1$ $i = 1, 2$, PCG solver.

	MHFE method			MFE method		
s	CPU	Cond. Num.	# Iter.	CPU	Cond. Num.	# Iter.
10^{-2}	2.2	50.9	20–19	2.4	65.1×10^1	30–29
10^{-4}	2.2	55.1	20–19	3.2	68.3×10^3	51–50
10^{-6}	2.2	55.1	20–19	3.9	68.3×10^5	84–83

Conclusion

- ▷ The MHFE and MFE methods lead to symmetric, positive definite linear systems for parabolic problems.

- ▷ In heterogenous media, the condition numbers of both systems grow up according to the ratio between the highest and the lowest values of permeability parameters between adjacent subdomains.

- ▷ The MHFE formulation sometimes leads to senseless values in the velocity field, especially when large jumps in the hydraulic conductivity take place.

- ▷ Small values of the storage coefficient could blow up the conditioning of the MFE linear system. Thus, the symmetric indefinite linear system has to be solved.