METHODES NUMERIQUES POUR DES EQUATIONS ELLIPTIQUES ET PARABOLIQUES NON LINEAIRES

Application à des problèmes d'écoulement en milieux poreux et fracturés

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Thèse présentée pour obtenir le grade de

Docteur en sciences de l'Université Paris XI Orsay en mathématiques

&

Docteur de l'Université Technique Tchèque à Prague en modélisation mathématique

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Outline

Motivation

Chapter 1, part A: A combined finite volume–nonconforming/mixed-hybrid finite element scheme for degenerate parabolic problems

Chapter 1, part B: A combined finite volume–finite element scheme for contaminant transport simulation on nonmatching grids

Chapter 2: Discrete Poincaré–Friedrichs inequalities

Chapter 3: Equivalence between lowest-order mixed finite element and multi-point finite volume methods

Chapter 4: Mixed and nonconforming finite element methods on a fracture network

Perspectives and future work

Motivation

General motivation

- development and analysis of efficient numerical methods
- simulation of flow and contaminant transport in porous and fractured media (e.g. depollution or GdR MoMaS problems)

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Underground water flow

$$\begin{aligned} \mathbf{u} &= -\mathbf{K}(\nabla p + \nabla z) \\ \nabla \cdot \mathbf{u} &= q \end{aligned}$$

p	pressure head	$\mathbf{K}$	hydraulic conductivity tensor
$\mathbf{u}$	Darcy velocity	z	elevation
		q	sources and sinks

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Difficulties

- high contrasts of parameters
- complex domains

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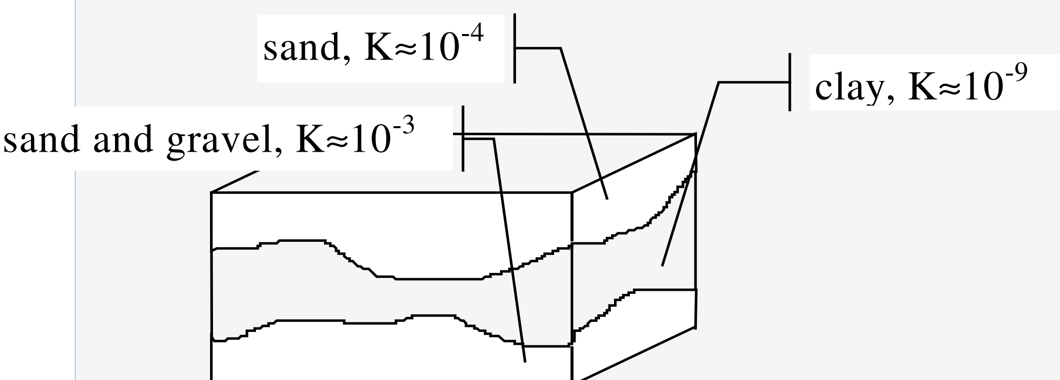
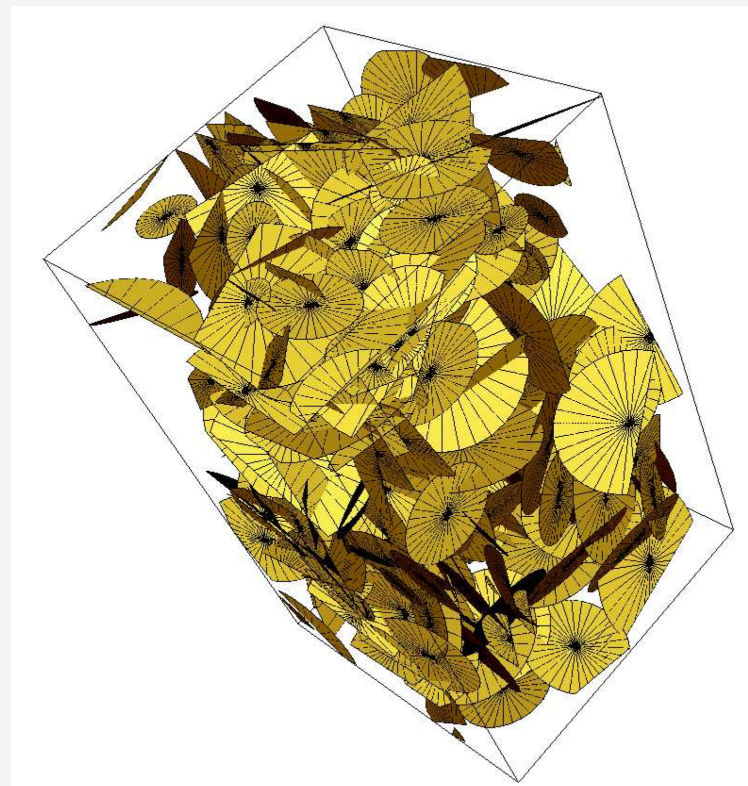


Porous media



Fracture network

Motivation

Contaminant transport

$$\frac{\partial \beta(c)}{\partial t} - \nabla \cdot (\mathbf{S} \nabla c) + \nabla \cdot (c \mathbf{v}) + F(c) = q \qquad (1)$$

c unknown concentration of a contaminant

β time evolution and equilibrium adsorption

t time

$\mathbf{S}$ diffusion–dispersion tensor

$\mathbf{v}$ velocity field

F chemical reactions

q sources and sinks

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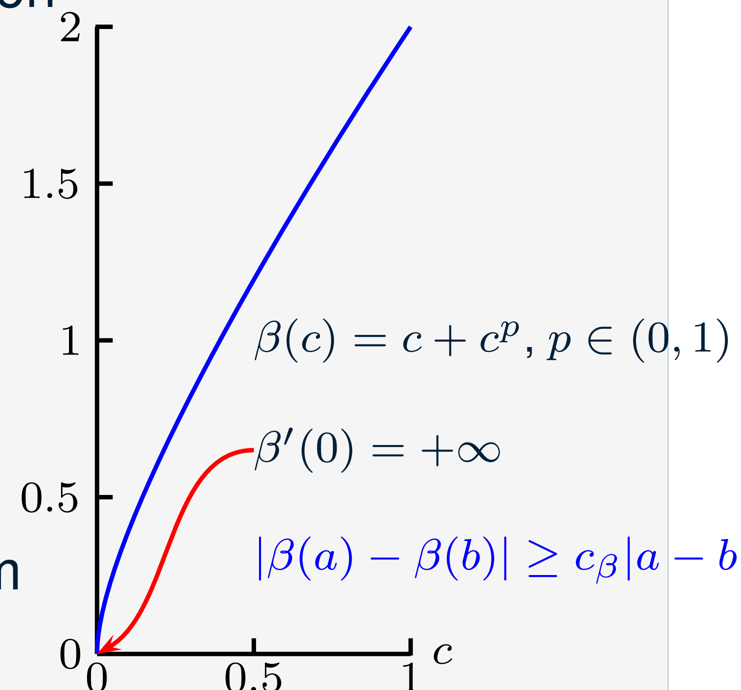

Difficulties

- nonlinear, degenerate parabolic problem
- convection dominates over diffusion
- inhomogeneous and anisotropic (nonconstant full-matrix) tensor $\mathbf{S}$
- general unstructured meshes (local refinement possible)

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Nonlinear convection–reaction–diffusion equation

Equation

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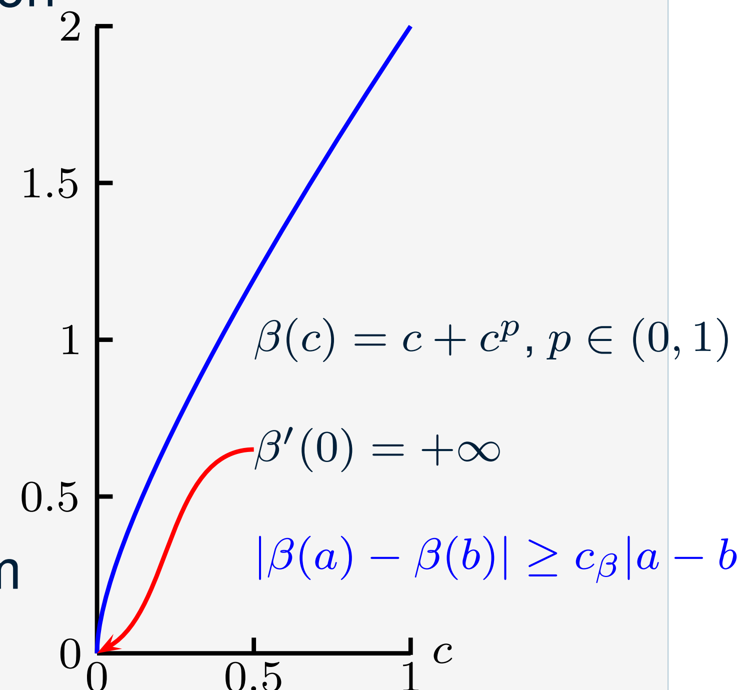

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FEMs and FVMs for degenerate parabolic problems

Finite elements for degenerate parabolic problems

- Barrett & Knabner (1997); $\frac{\partial \beta(c)}{\partial t} - \triangle c = q$, a priori error estimates
- Nochetto, Schmidt, & Verdi (1999); $\frac{\partial \beta(c)}{\partial t} - \triangle c = q$, a posteriori error estimates
- Chen & Ewing (2001); $\frac{\partial c}{\partial t} - \triangle \varphi(c) + \nabla \cdot (\theta(c)\mathbf{v}) = 0$, a priori error estimates

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Cell-centered finite volumes for degenerate parabolic problems

- Eymard, Gallouët, Hilhorst, & Naït Slimane (1998); $\frac{\partial \beta(c)}{\partial t} - \triangle c = q$, convergence
- Eymard, Gallouët, Herbin, & Michel (2002); $\frac{\partial c}{\partial t} - \triangle \varphi(c) + \nabla \cdot (\theta(c)\mathbf{v}) = 0$, convergence

FEMs and FVMs for convection–diffusion problems

Finite elements for convection–diffusion problems

- $\oplus$ no restrictions on the mesh, discretization of full diffusion tensors
- $\ominus$ oscillations in the velocity dominated case

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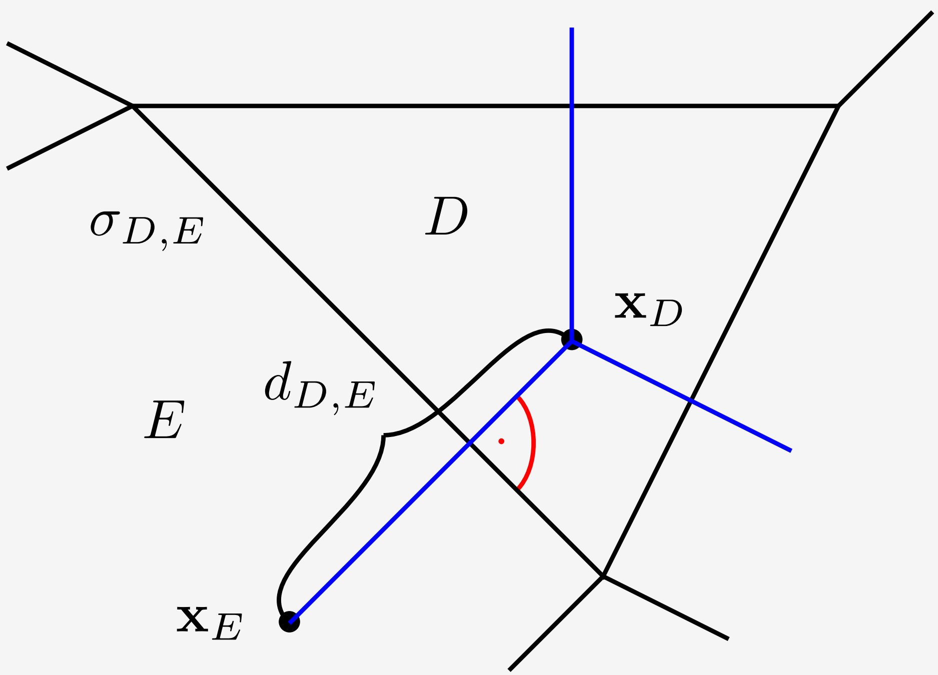
Finite volumes for convection–diffusion problems

- ⊖ restrictions on the mesh, how to discretize full diffusion tensors?



$$\int_{\sigma_{D,E}} \mathbf{S}\nabla c \cdot \mathbf{n}_D \, \mathrm{d}\gamma(\mathbf{x})$$

$$\mathbf{S} = Id \qquad \approx \frac{c_E - c_D}{d_{D,E}} |\sigma_{D,E}|$$

$$\mathbf{S} \neq Id \qquad ?$$

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Solution: combined schemes

$$-\nabla \cdot \mathbf{S}\nabla c + \nabla \cdot (c\mathbf{v}) = 0$$

finite elements   finite volumes

Combined finite volume–finite element schemes

Combined FV–FE method

- Feistauer, Felcman, Medviďová-Lukáčová, & Warnecke (1997, 1999); $\frac{\partial c}{\partial t} - \triangle c + \nabla \cdot (\theta(c)\mathbf{v}) = 0$, convergence, error estimates

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Combined FV–nonconforming FE method

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Our aims

- extend these ideas to degenerate parabolic problems
- include inhomogeneous and anisotropic diffusion tensors
- consider general meshes (namely: local refinement possible, no maximal angle condition, no orthogonality condition)
- consider also space dimension three
- combine the finite volume with the mixed-hybrid method

Continuous problem

Problem

Equation (1) in a polygonal domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, on a time interval $(0, T)$, with initial and boundary conditions

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}) \qquad \mathbf{x} \in \Omega \tag{2}$$

$$c(\mathbf{x}, t) = 0 \qquad \mathbf{x} \in \partial\Omega\,,\; t \in (0, T) \tag{3}$$

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Weak solution

Function c is a weak solution of the problem (1) – (3) if (F. Otto)

$$c \in L^2(0, T; H_0^1(\Omega))\,,\ \beta(c) \in L^\infty(0, T; L^2(\Omega))\,,$$

$$-\int_0^T \int_\Omega \beta(c)\varphi_t \,\mathrm{d}\mathbf{x}\,\mathrm{d}t - \int_\Omega \beta(c_0)\varphi(\cdot, 0)\,\mathrm{d}\mathbf{x} + \int_0^T \int_\Omega \mathbf{S}\nabla c \cdot \nabla\varphi \,\mathrm{d}\mathbf{x}\,\mathrm{d}t -$$

$$-\int_0^T \int_\Omega c\mathbf{v} \cdot \nabla\varphi \,\mathrm{d}\mathbf{x}\,\mathrm{d}t + \int_0^T \int_\Omega F(c)\varphi \,\mathrm{d}\mathbf{x}\,\mathrm{d}t = \int_0^T \int_\Omega q\varphi \,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

for all $\varphi \in L^2(0, T; H_0^1(\Omega))$ with $\varphi_t \in L^\infty(Q_T)$, $\varphi(\cdot, T) = 0\,.$

Combined FV–nonconforming/mixed-hybrid FE scheme

$$\frac{\partial \beta(c)}{\partial t} - \nabla \cdot (\mathbf{S} \nabla c) + \nabla \cdot (c\mathbf{v}) + F(c) = q$$

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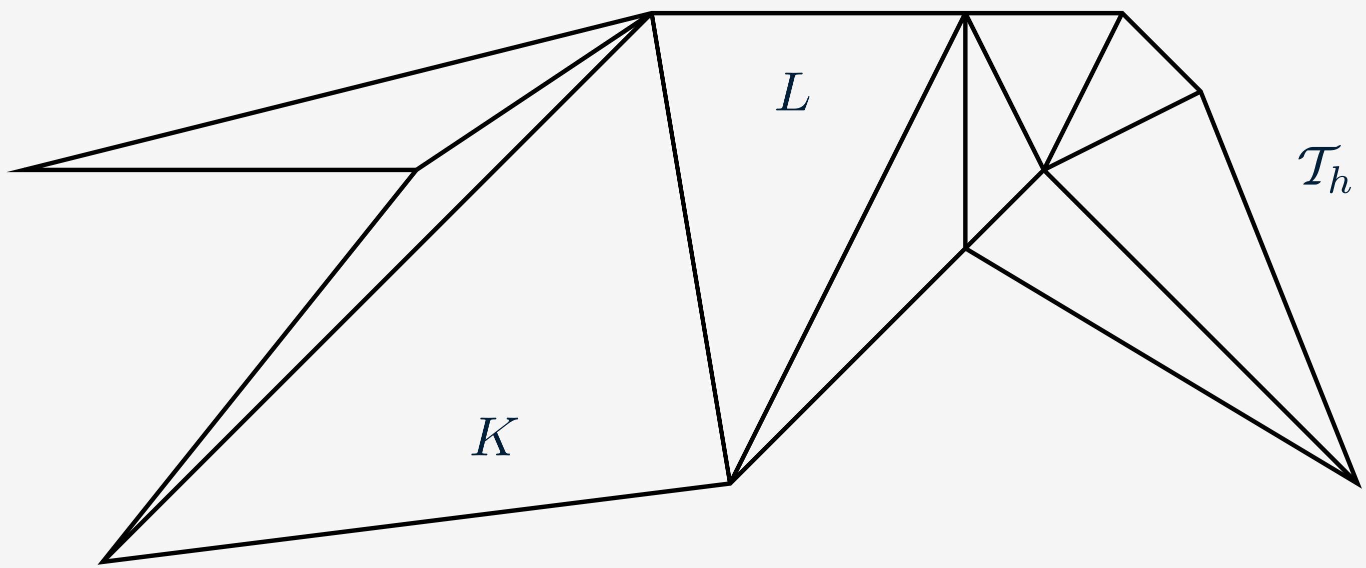

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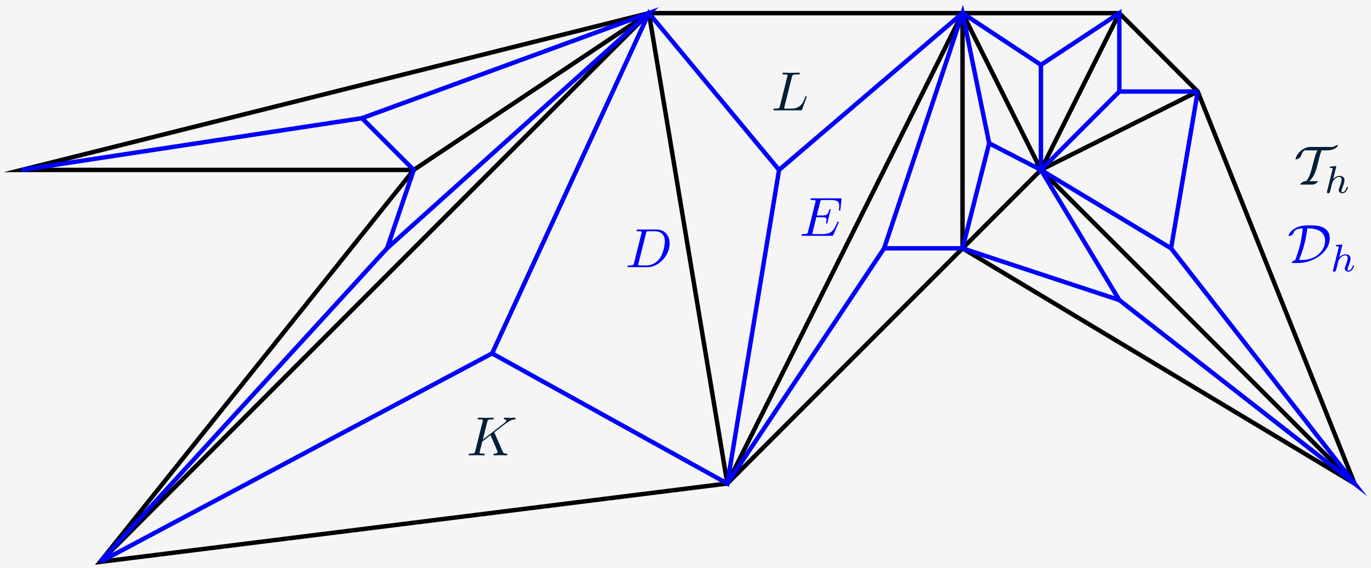

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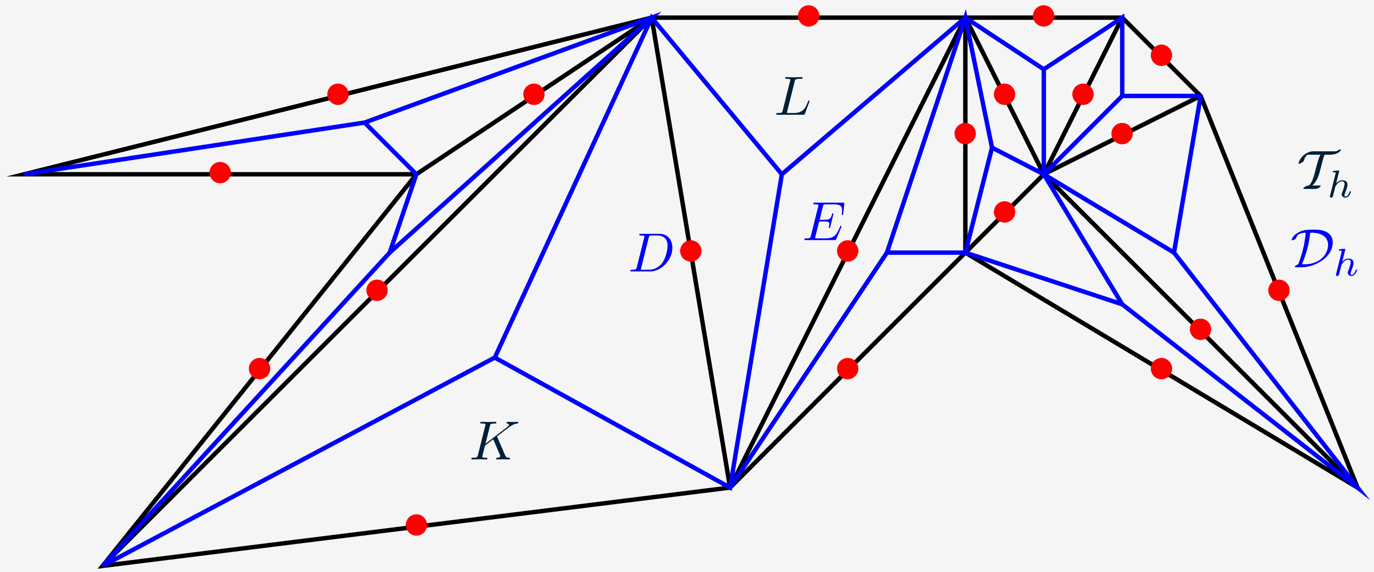

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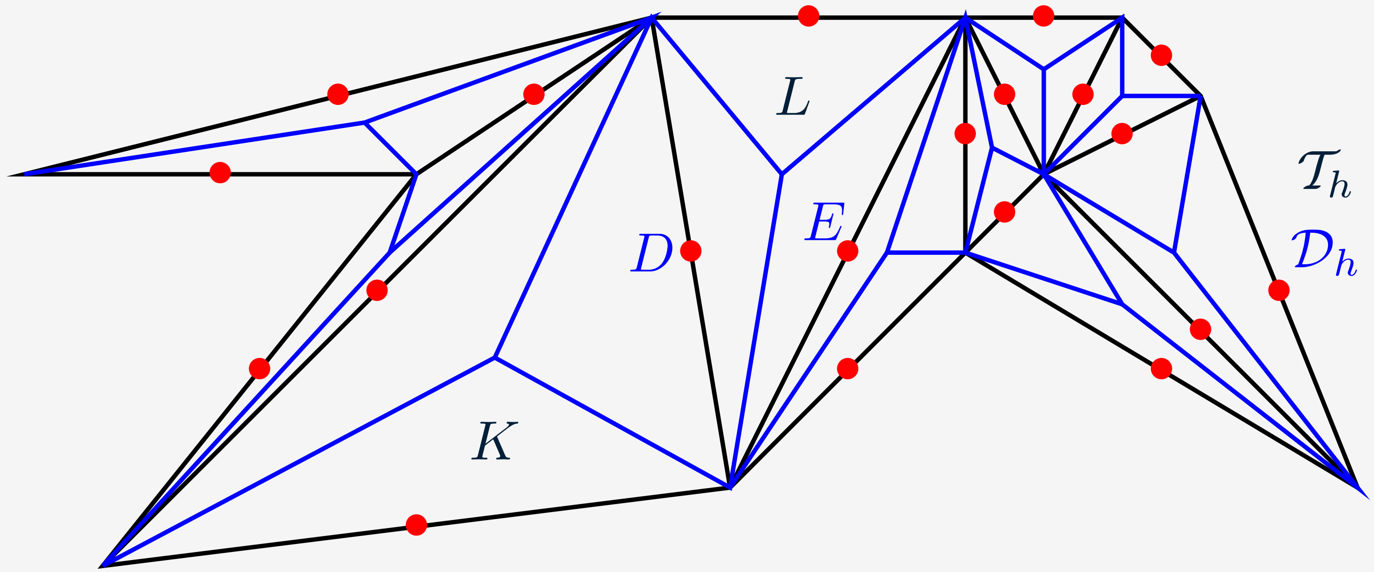

Find c_D^n, $D \in \mathcal{D}_h$, $n \in \{0, 1, \ldots, N\}$:

$$\frac{\beta(c_D^n) - \beta(c_D^{n-1})}{\triangle t_n} |D| - \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^n (c_E^n - c_D^n) +$$

$$+ \sum_{E \in \mathcal{N}(D)} \mathbf{v}_{D,E}^n \, \overline{c_{D,E}^n} + F(c_D^n) \, |D| = q_D^n \, |D|$$

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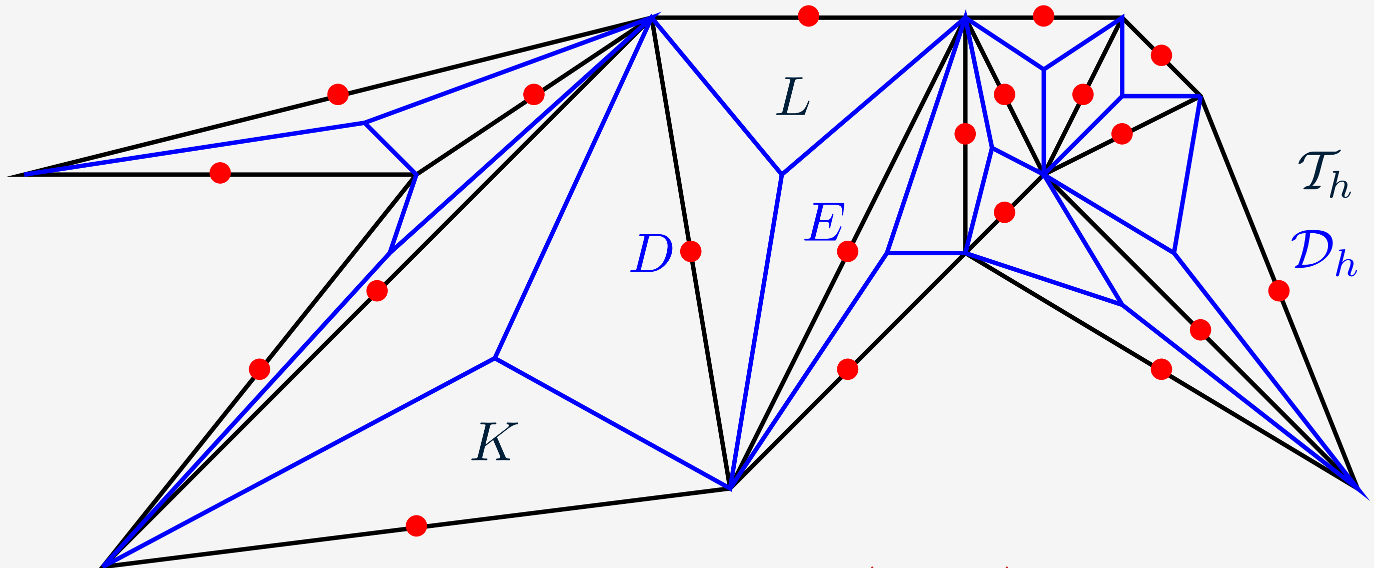

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FV: $\dfrac{|\sigma_{D,E}|}{d_{D,E}}$

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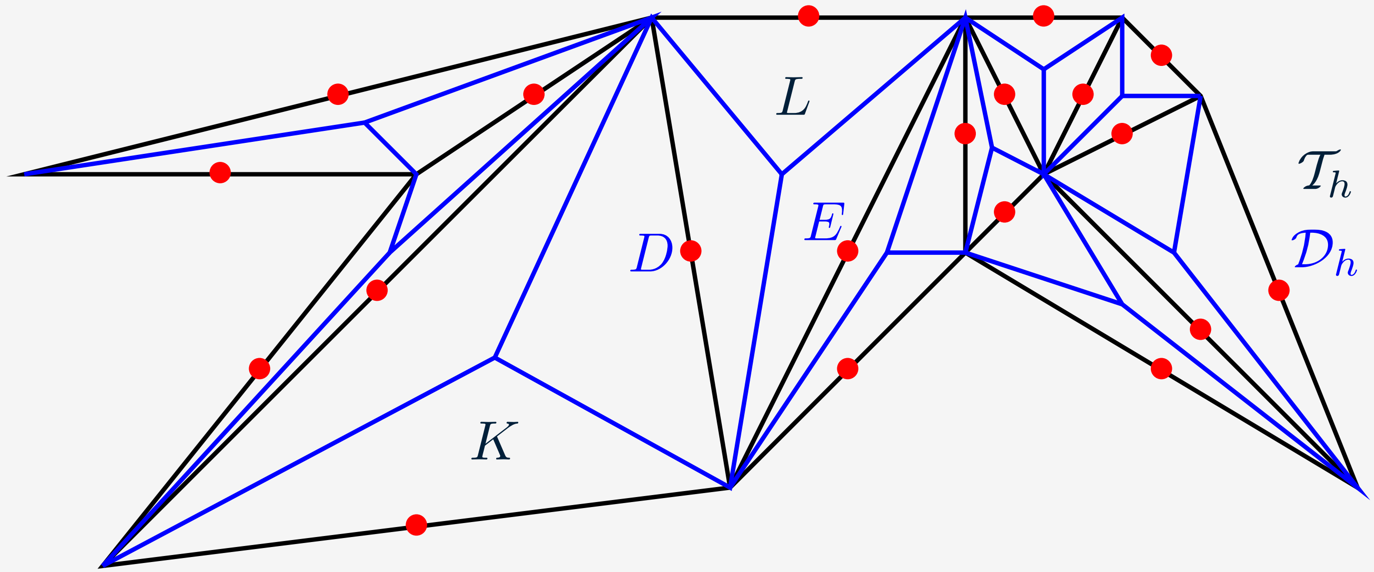

Find c_D^n, $D \in \mathcal{D}_h$, $n \in \{0, 1, \ldots, N\}$: NCFE: $-\sum_{K \in \mathcal{T}_h} (\mathbf{S}^n \nabla \varphi_E, \nabla \varphi_D)_{0,K}$

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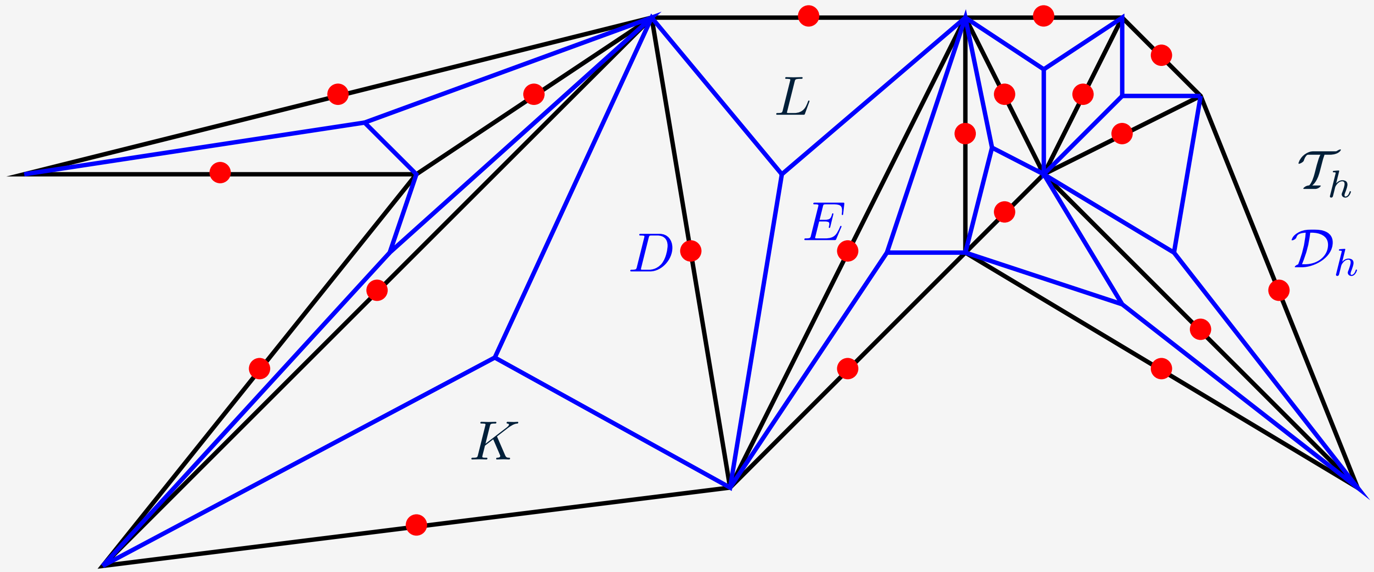

Find c_D^n, $D \in \mathcal{D}_h$, $n \in \{0, 1, \ldots, N\}$:

MHFE: Schur complement

$$\frac{\beta(c_D^n) - \beta(c_D^{n-1})}{\triangle t_n} |D| - \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^n (c_E^n - c_D^n) +$$

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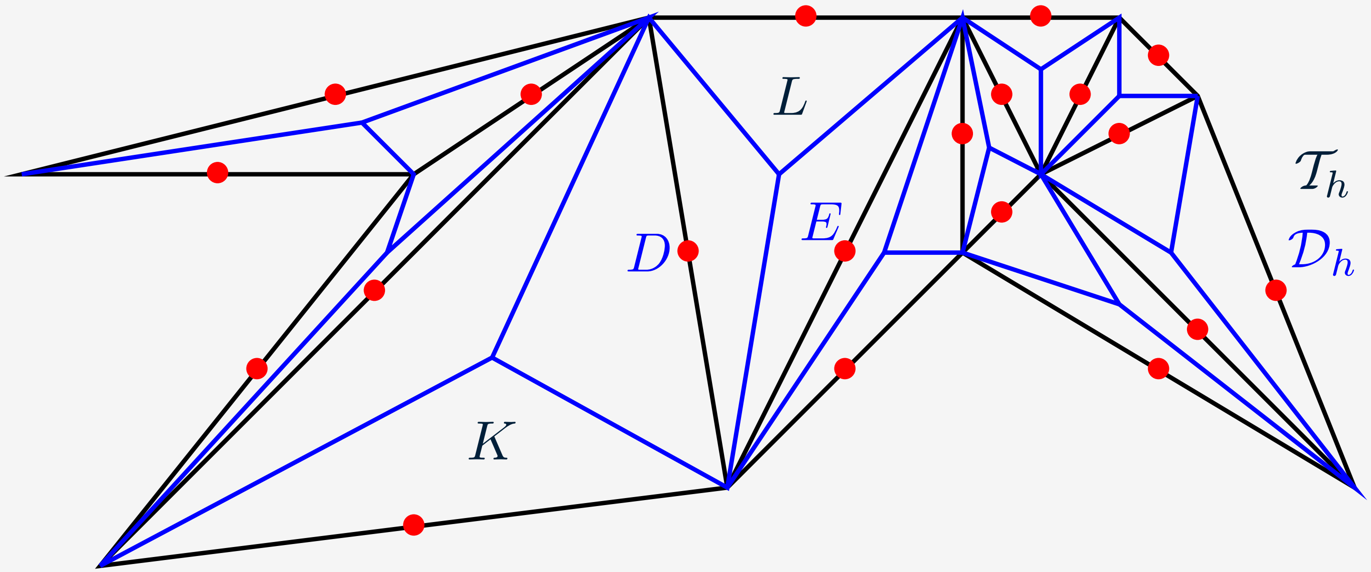

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Local Péclet upstream weighting

Flux through a side $\sigma_{D,E}$:

$$\mathbf{v}_{D,E}^n := \frac{1}{\triangle t_n} \int_{t_{n-1}}^{t_n} \int_{\sigma_{D,E}} \mathbf{v}(\mathbf{x}, t) \cdot \mathbf{n}_{D,E} \, \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}t$$

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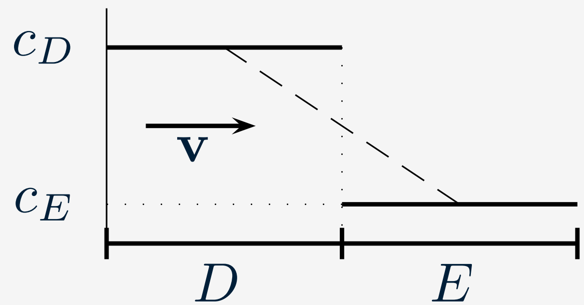
1-D:



$(1-\alpha)c_D + \alpha c_E$

$\alpha = 0$: full upstream weighting

$\alpha = 0.5$: centered weighting

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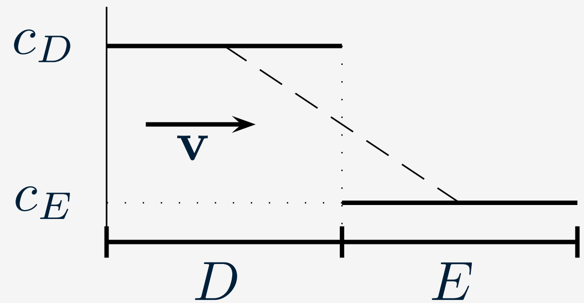

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Local Péclet upstream weighting:

$$\begin{array}{llcll} \text{if} \quad \mathbf{v}^n_{D,E} \geq 0 & \overline{c^n_{D,E}} & := & (1-\alpha^n_{D,E})c^n_D & + \quad \alpha^n_{D,E} c^n_E \\ \text{if} \quad \mathbf{v}^n_{D,E} < 0 & \overline{c^n_{D,E}} & := & (1-\alpha^n_{D,E})c^n_E & + \quad \alpha^n_{D,E} c^n_D \end{array} ,$$

$$\alpha^n_{D,E} := \frac{\max\left\{\min\left\{\mathbb{S}^n_{D,E}, \frac{1}{2}|\mathbf{v}^n_{D,E}|\right\}, 0\right\}}{|\mathbf{v}^n_{D,E}|} \quad , \quad \mathbf{v}^n_{D,E} \neq 0$$

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Discrete properties of the scheme

Existence of the discrete solution

- Brouwer topological degree

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Local conservativity

- FE/FV conservative $\rightarrow$ combined scheme conservative

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Discrete maximum principle

- under assumption $\mathbb{S}^n_{D,E} \geq 0$ for all $D \in \mathcal{D}_h^{\text{int}}$, $E \in \mathcal{N}(D)$,

$$0 \leq c_D^n \leq M$$

- satisfied e.g. when $\mathbf{S}$ is scalar and when all angles between $\mathbf{n}_{\sigma_D}$, $\sigma_D \in \mathcal{E}_K$ for all $K \in \mathcal{T}_h$ are greater or equal to $\pi/2$

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A priori estimates

A priori estimates

$$L^\infty(0,T;L^2(\Omega)) \quad c_\beta \max_{n\in\{1,2,\ldots,N\}} \sum_{D\in\mathcal{D}_h} (c_D^n)^2|D| \leq C_{\mathrm{ae}}$$

$$\max_{n\in\{1,2,\ldots,N\}} \sum_{D\in\mathcal{D}_h} [\beta(c_D^n)]^2|D| \leq C_{\mathrm{ae}}$$

$$c_{\mathbf{S}} \sum_{n=1}^{N} \triangle t_n \|c_h^n\|_{X_h}^2 \leq C_{\mathrm{ae}}$$

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$$L^2(0,T;H_0^1(\Omega)) \quad c_{\mathbf{S}} \sum_{n=1}^{N} \triangle t_n \|c_h^n\|_{X_h}^2 \leq C_{\mathrm{ae}}$$

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$$L^2(0,T;H_0^1(\Omega)) \quad c_{\mathbf{S}} \sum_{n=1}^{N} \triangle t_n \|c_h^n\|_{X_h}^2 \leq C_{\mathrm{ae}}$$

Approximate solutions piecewise constant in time, $c_{h,\triangle t}$ piecewise linear on $\mathcal{T}_h$, $\tilde{c}_{h,\triangle t}$ piecewise constant on $\mathcal{D}_h$:

$$\|c_{h,\triangle t} - \tilde{c}_{h,\triangle t}\|_{0,Q_T} \longrightarrow 0 \quad as \quad h \to 0$$

Time and space translate estimates

Lemma (Time translate estimate) *There exists a constant* $C_{\mathrm{tt}} > 0$*, such that for all* $\tau \in (0, T)$*,*

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Proofs: use of the discrete schemes and the a priori estimates.

Convergence

Theorem (Strong convergence in $L^2(Q_T)$) *Subsequences of* $\tilde{c}_{h,\triangle t}$ *and* $c_{h,\triangle t}$ *converge strongly in* $L^2(Q_T)$ *to some function* $c \in L^2(0,T;H_0^1(\Omega))$.

- Kolmogorov compactness theorem: a priori estimates and time and space translate estimates imply $\tilde{c}_{h,\triangle t}$, $c_{h,\triangle t} \stackrel{L^2(Q_T)}{\longrightarrow} c$
- space translate estimate: $c \in L^2(0,T;H_0^1(\Omega))$

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Theorem (Convergence to a weak solution) *The function c is a weak solution of the continuous problem.*

- strong convergence: passage to the limit in nonlinearities

Numerical experiments

For $\Omega = (0,1) \times (0,1)$ and $T = 1$, we consider:

$$\frac{\partial(c^{1/2})}{\partial t} - \nabla \cdot (\delta \nabla c) + \nabla \cdot (cv, 0) = 0$$

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Initial and Dirichlet boundary conditions given by the solution (traveling wave)

$$\begin{aligned} c(x,y,t) &= \left(1 - e^{\frac{v}{2\delta}(x-vt-0.2)}\right)^2 \text{ for } x \leq vt + 0.2\,, \\ c(x,y,t) &= 0 \text{ for } x \geq vt + 0.2 \end{aligned}$$

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Implementation: search for discrete unknowns corresponding to $\beta(c)$

- permits to avoid parabolic regularization
- resulting matrices are diagonal for the part where $c = 0$

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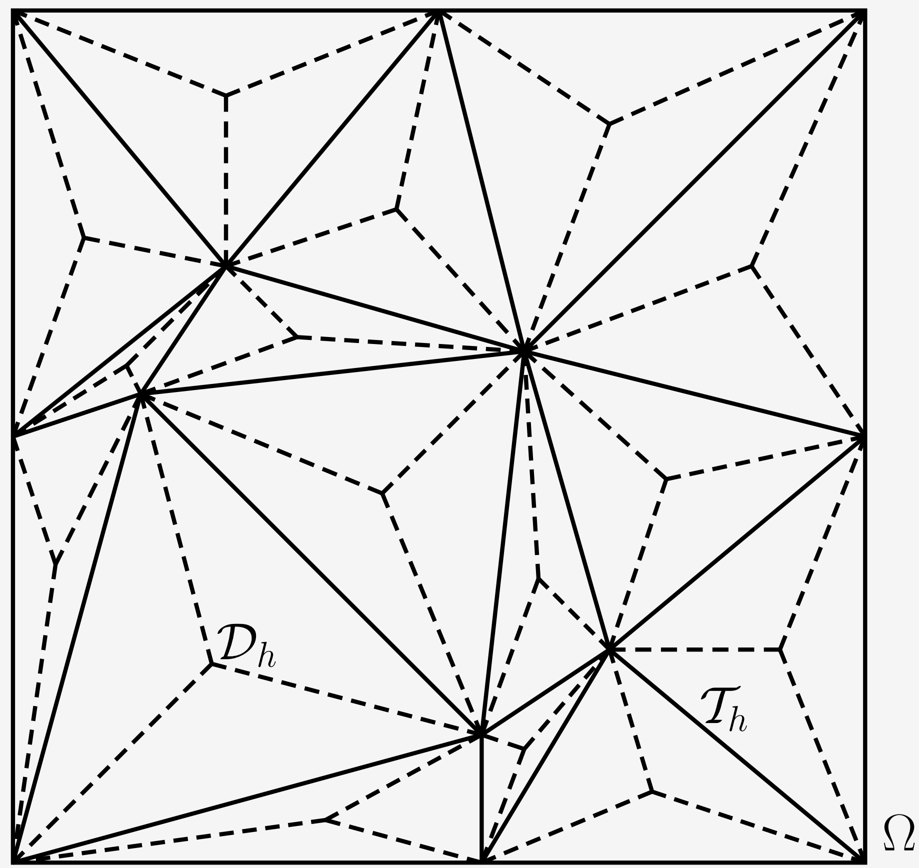
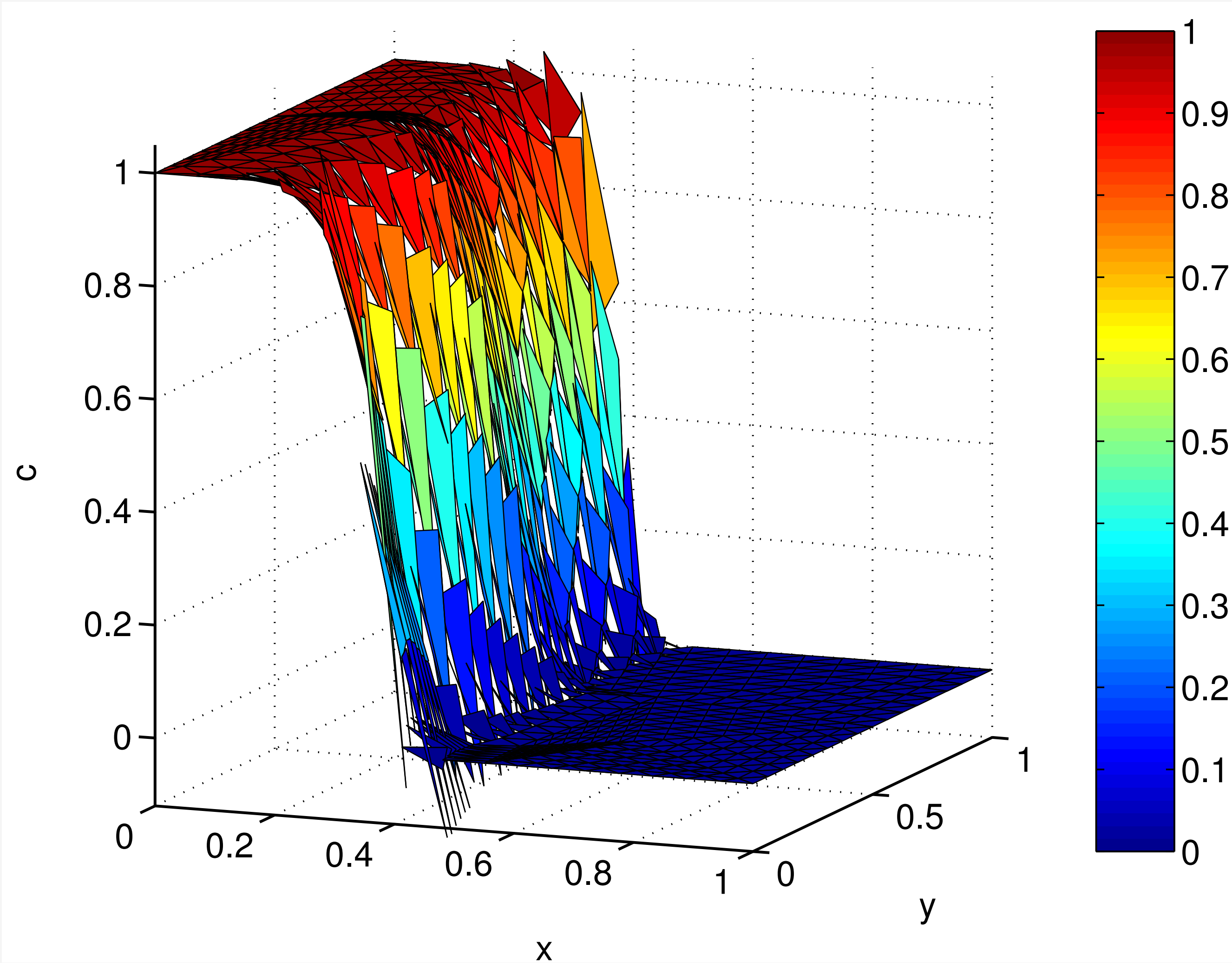
Numerical experiments



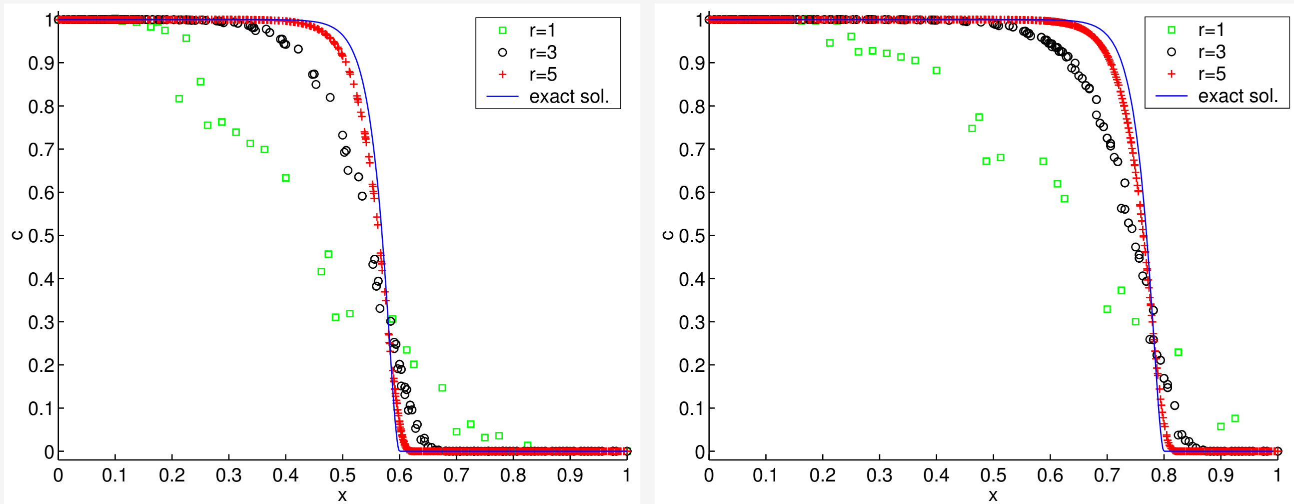
Initial triangulation

Numerical experiments

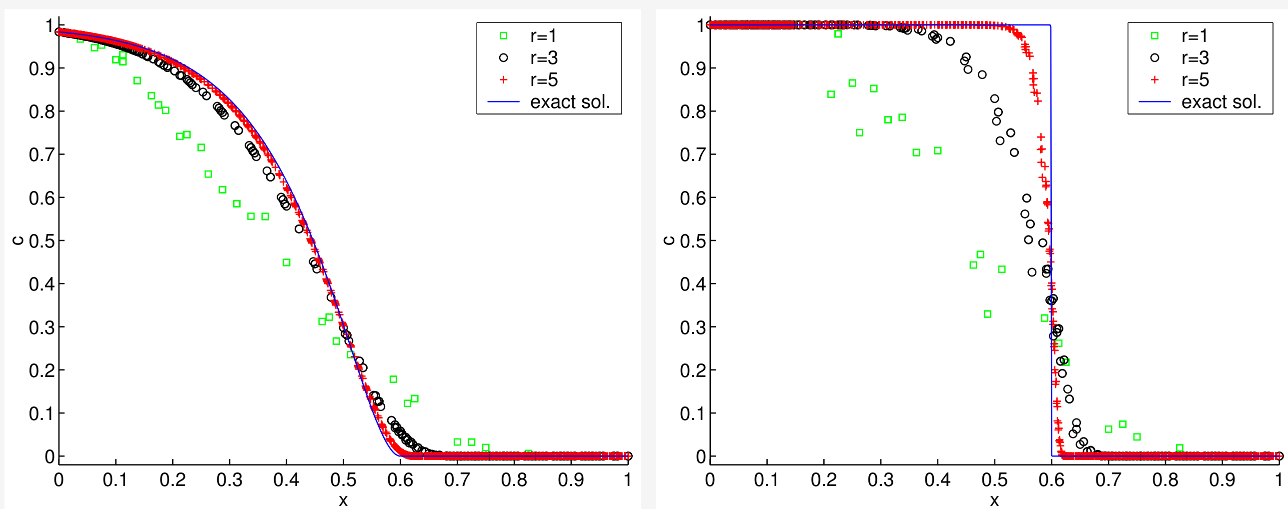


Solution for $\delta = 0.01$, $v = 0.8$, and $r = 3$ at $t = 0.25$

Numerical experiments



Solution for $\delta = 0.01$ at $t = 0.5$ (left) and at $t = 0.75$ (right)



Solution at $t = 0.5$, $\delta = 0.05$ (left) and $\delta = 0.0001$ (right)

Outline

Motivation

Chapter 1, part A: A combined finite volume–nonconforming/mixed-hybrid finite element scheme for degenerate parabolic problems

Chapter 1, part B: A combined finite volume–finite element scheme for contaminant transport simulation on nonmatching grids

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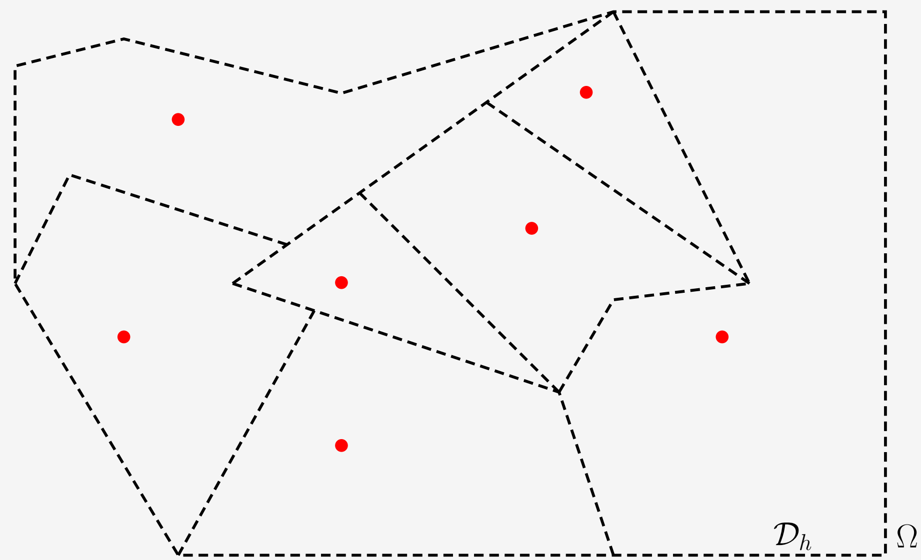
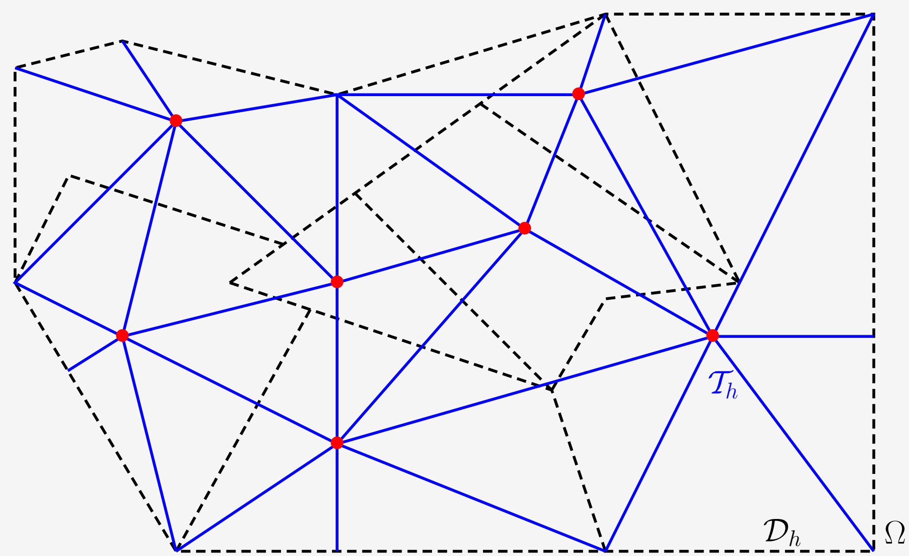
Perspectives and future work

Combined FV–FE scheme for nonmatching grids



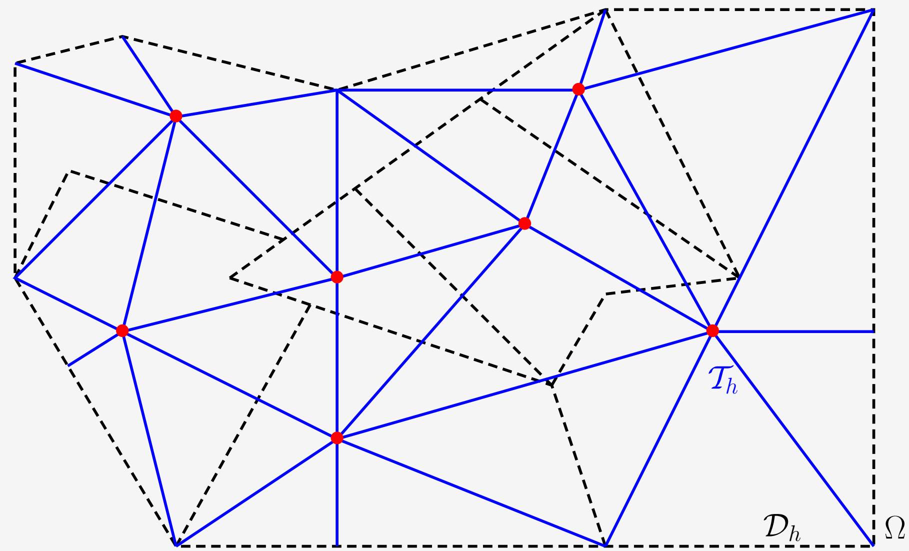
Given nonmatching grid

Combined FV–FE scheme for nonmatching grids



Nonmatching grid and dual triangular grid

Combined FV–FE scheme for nonmatching grids



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Combined FV–FE scheme

- finite elements on $\mathcal{T}_h$, finite volumes on $\mathcal{D}_h$

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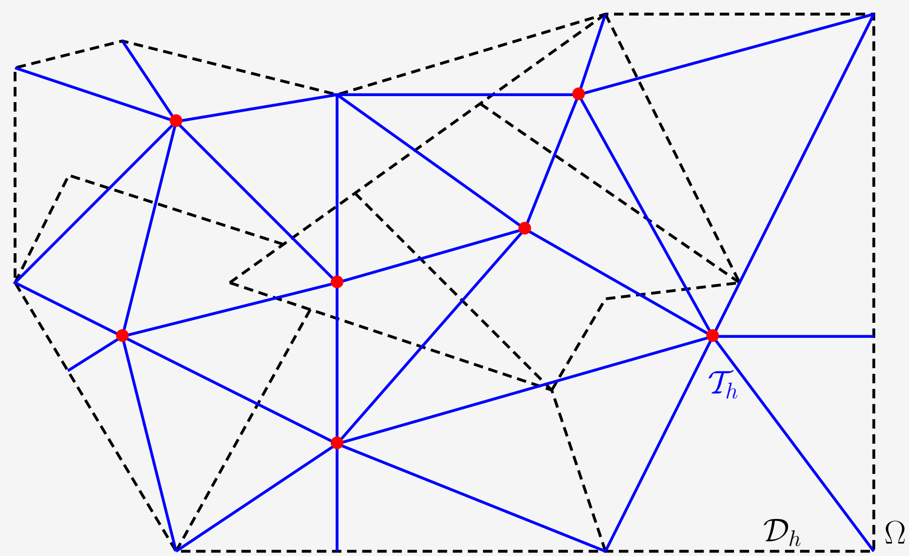

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Local conservativity

- FE/FV conservative $\rightarrow$ combined scheme conservative

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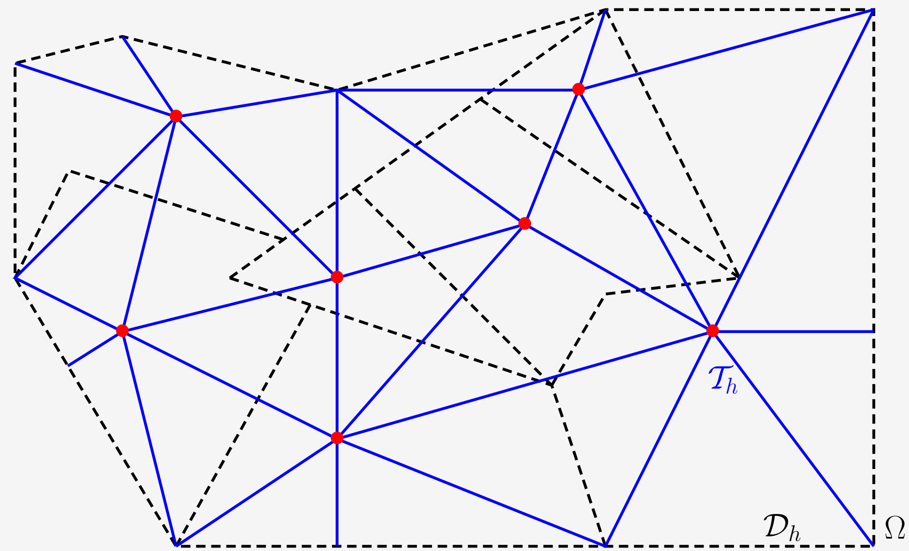

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Combined FV–FE scheme

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Discrete maximum principle

- under assumption $\mathbb{S}^n_{D,E} \geq 0$

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Implementation in the TALISMAN code

TALISMAN

- finite volume code of the society HydroExpert, Paris
- developed in cooperation with the group of D. Hilhorst, Orsay
- multi-layer approach

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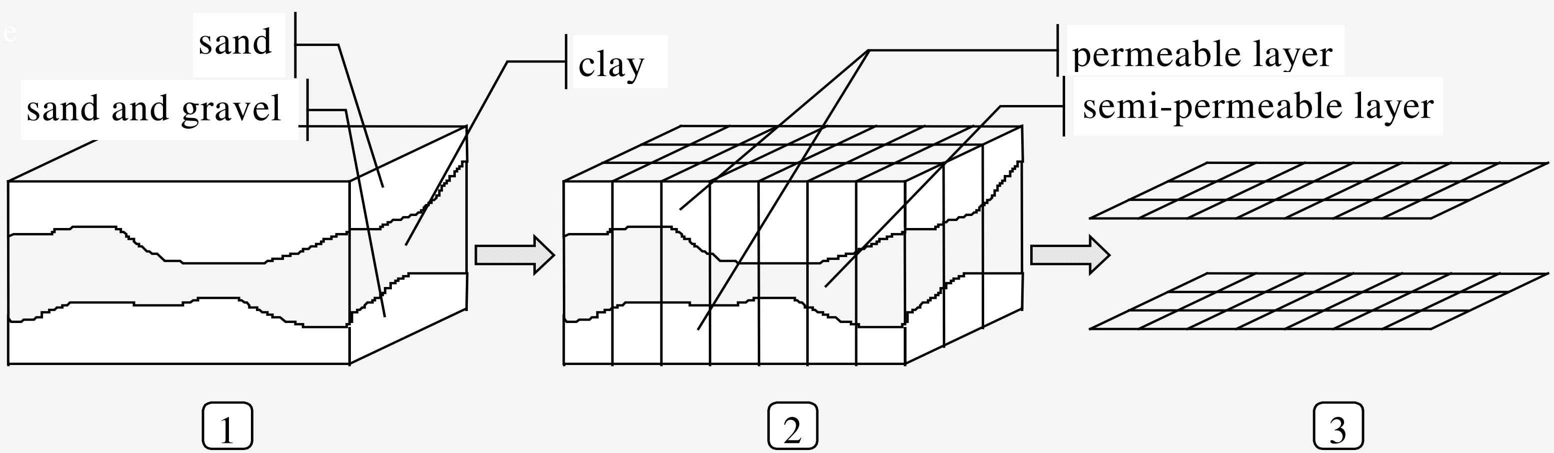

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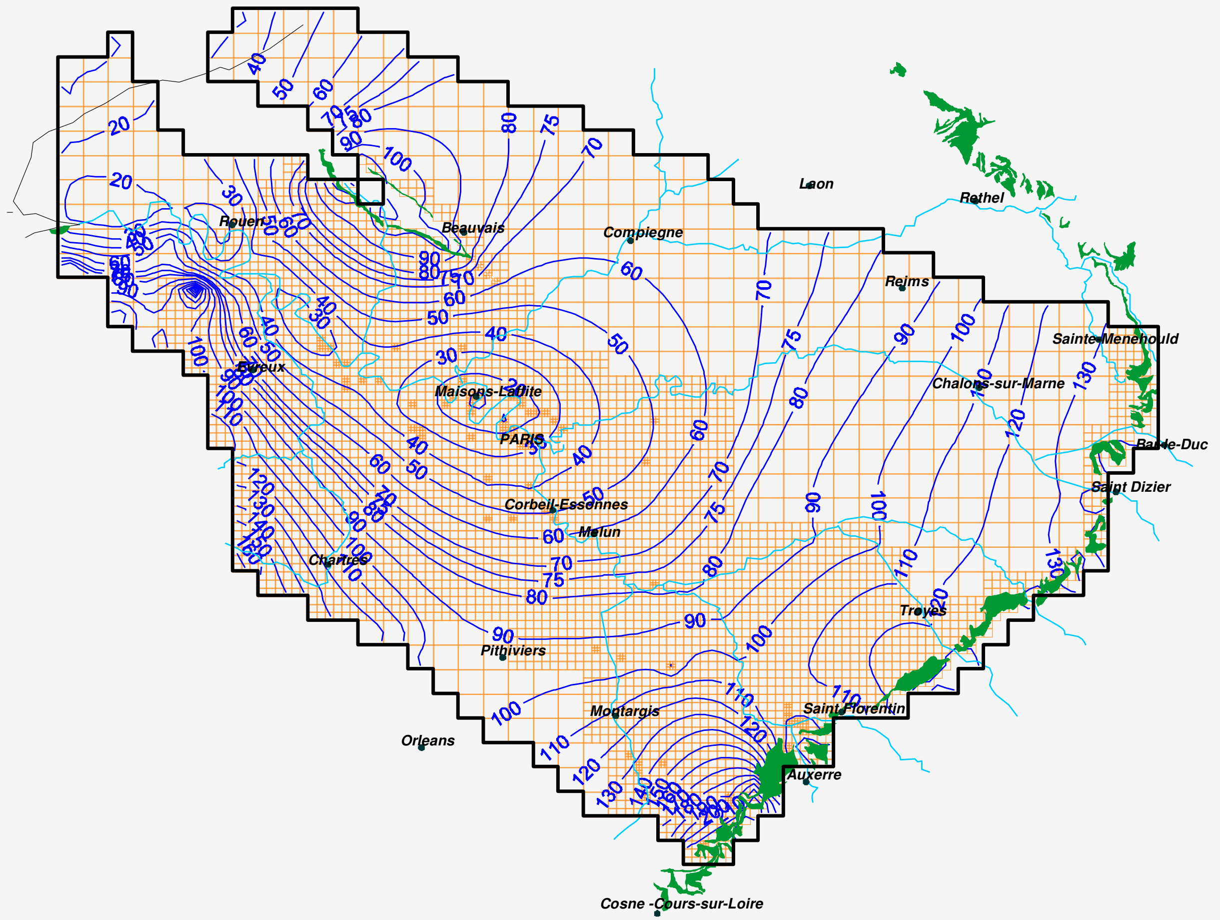
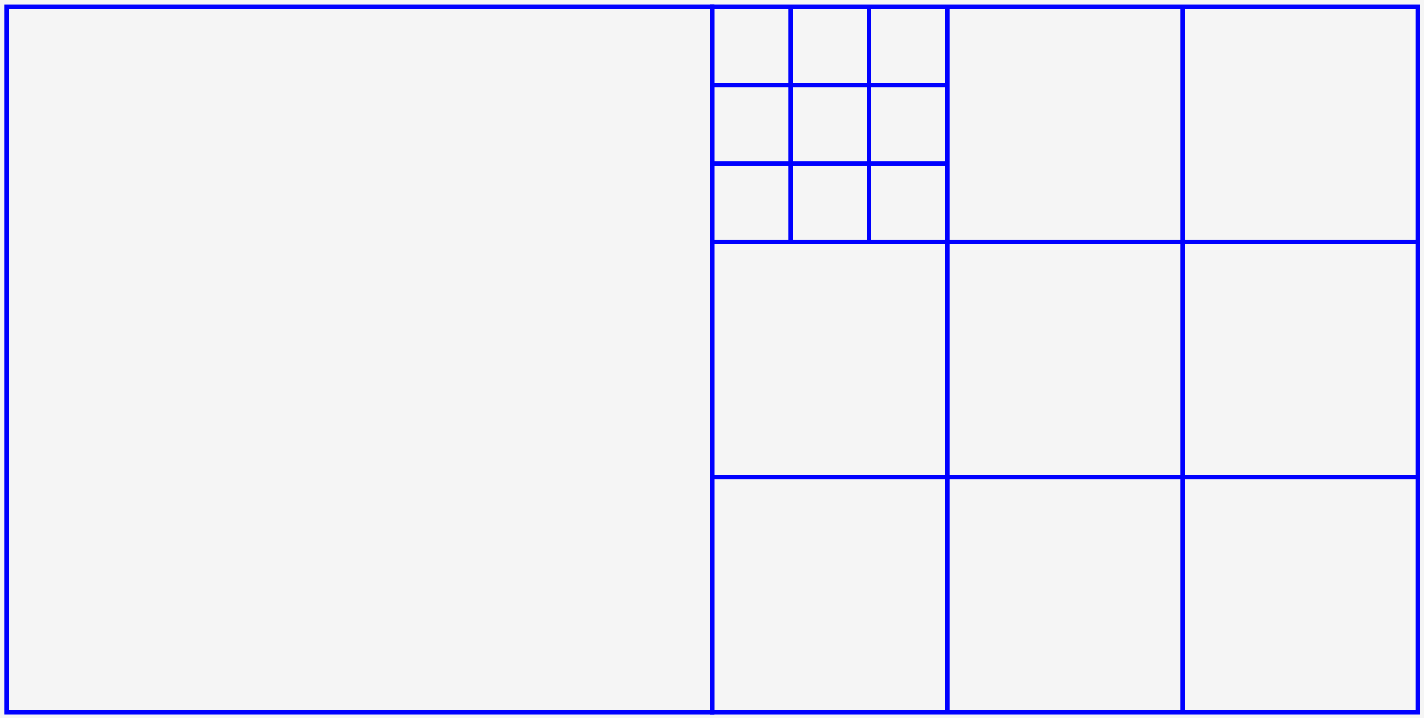


Simulation of the Ile-de-France region

Implementation in the TALISMAN code



- how to work with full diffusion tensors ?

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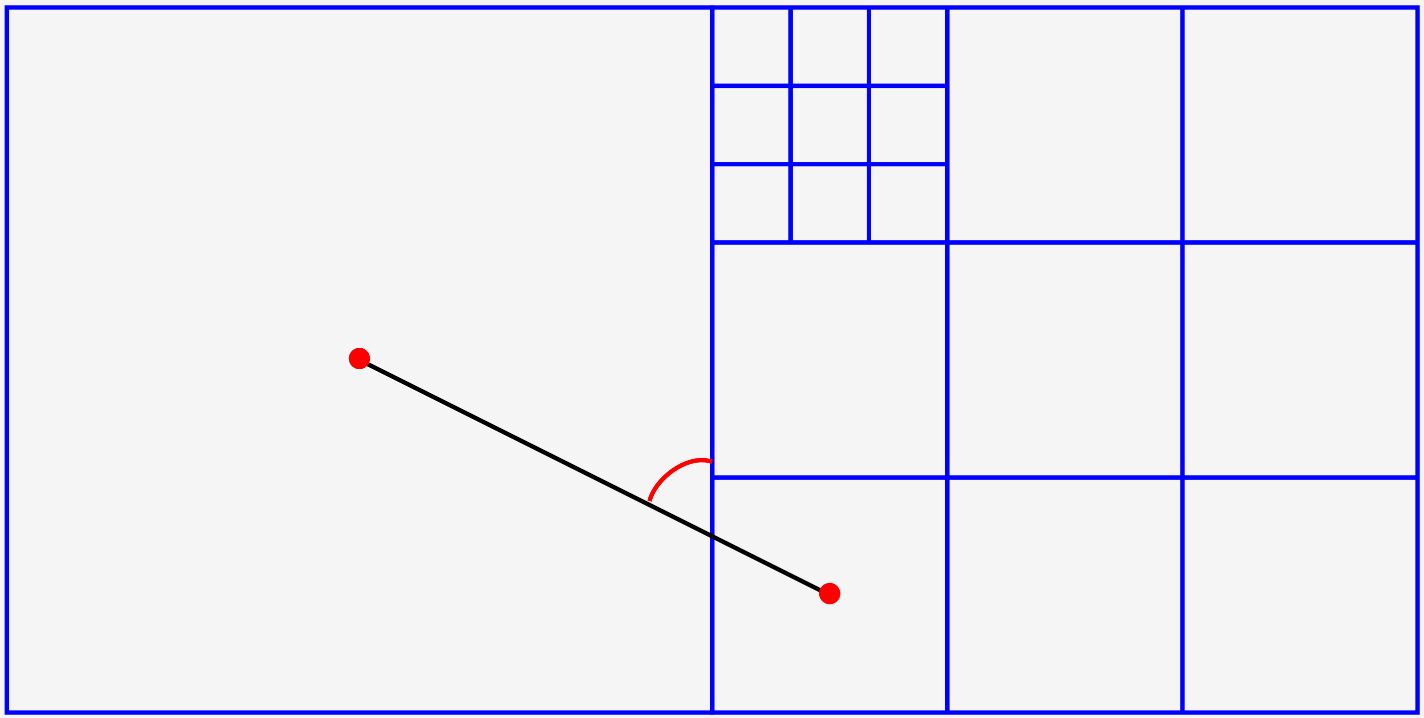
Implementation in the TALISMAN code



- how to work with full diffusion tensors ?
- nonconsistent approximation of gradients at the refinements

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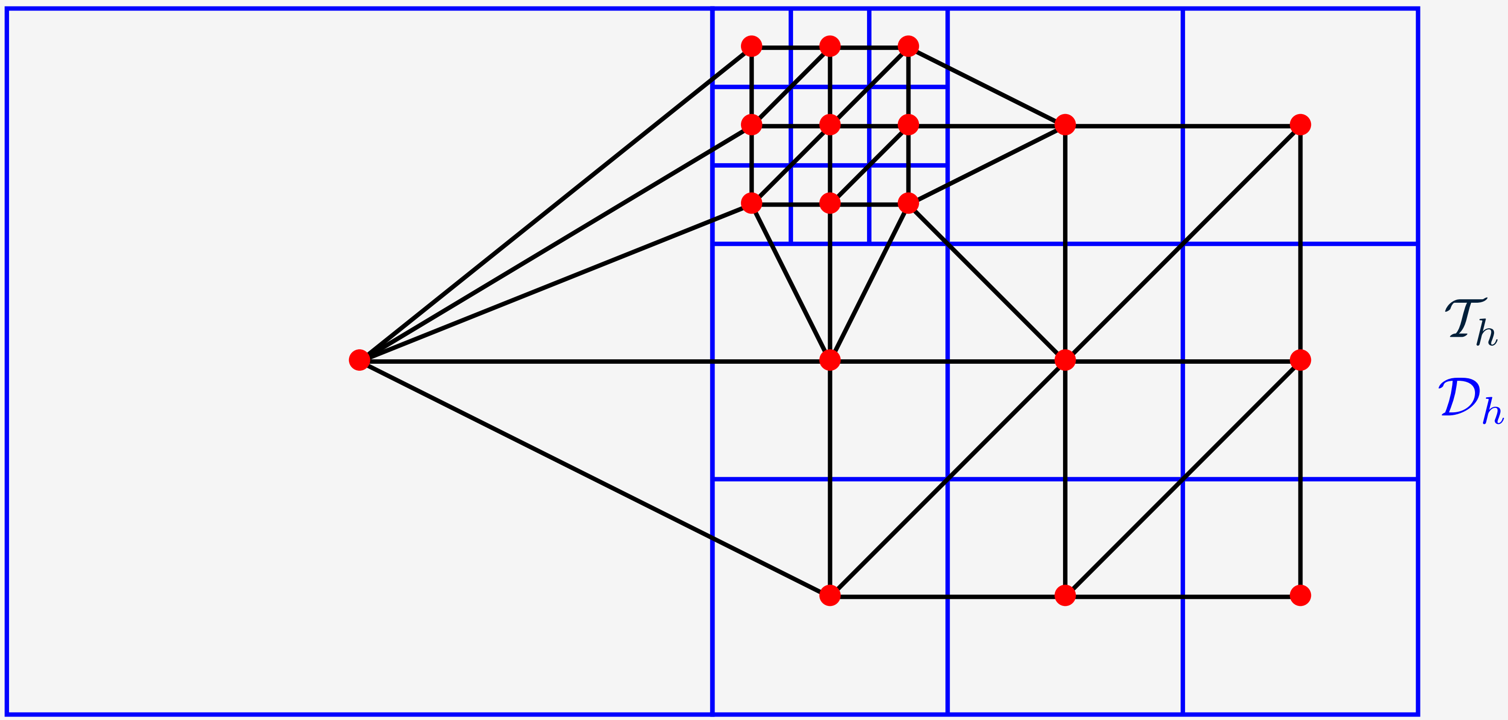

- how to work with full diffusion tensors ?
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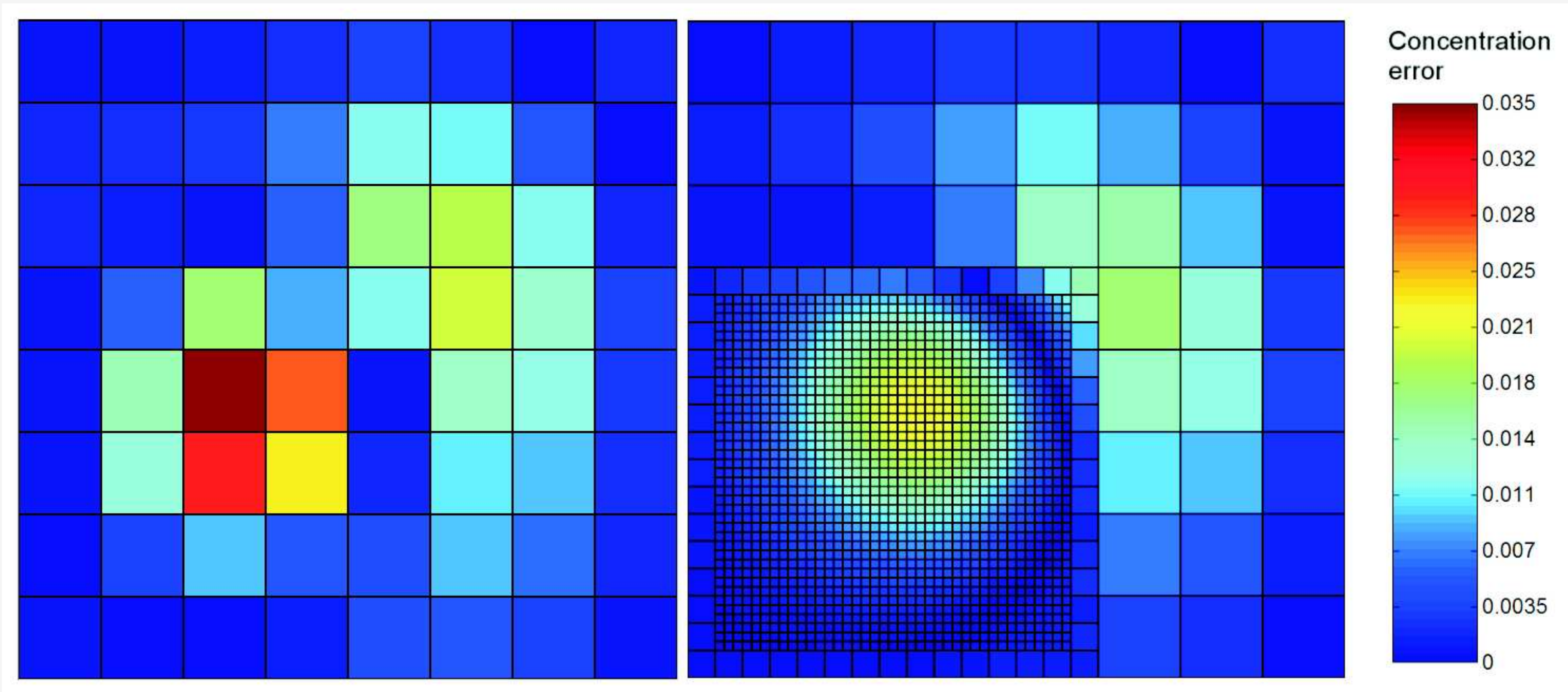
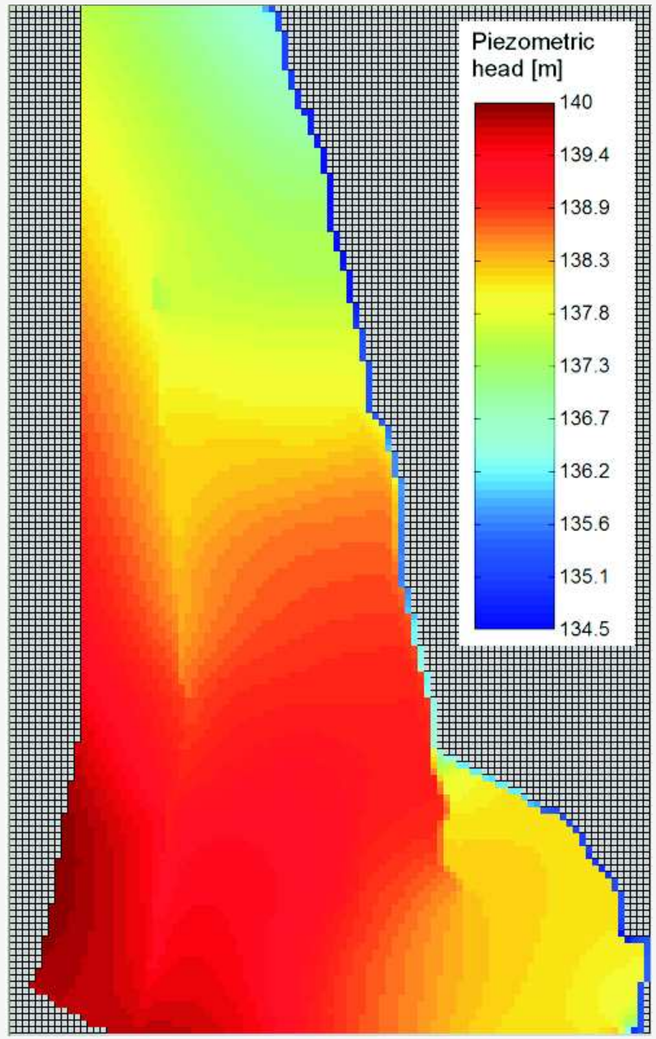
Solution: combined scheme

Model problem with known solution



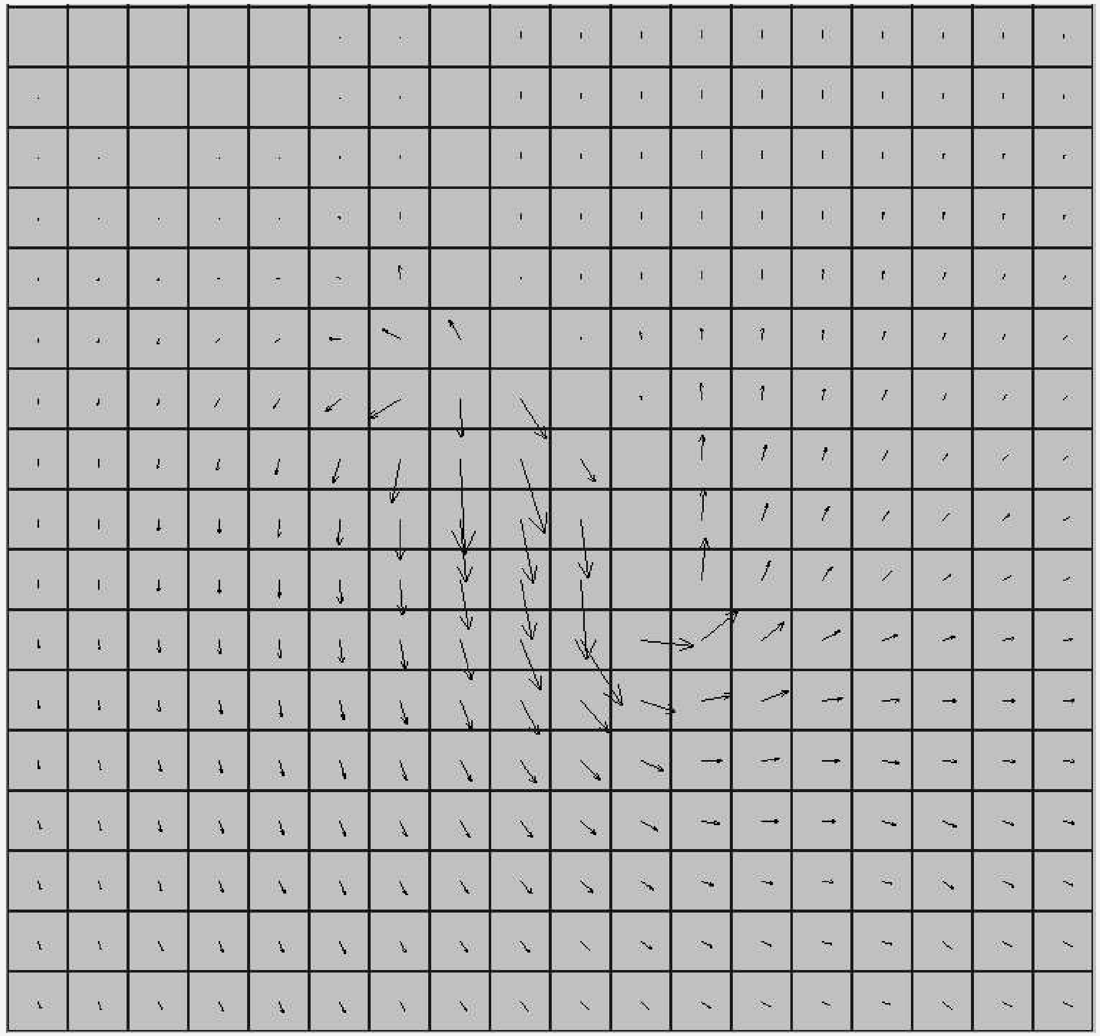
Errors on unrefined (left) and locally refined (right) grids

Contaminant transport simulation



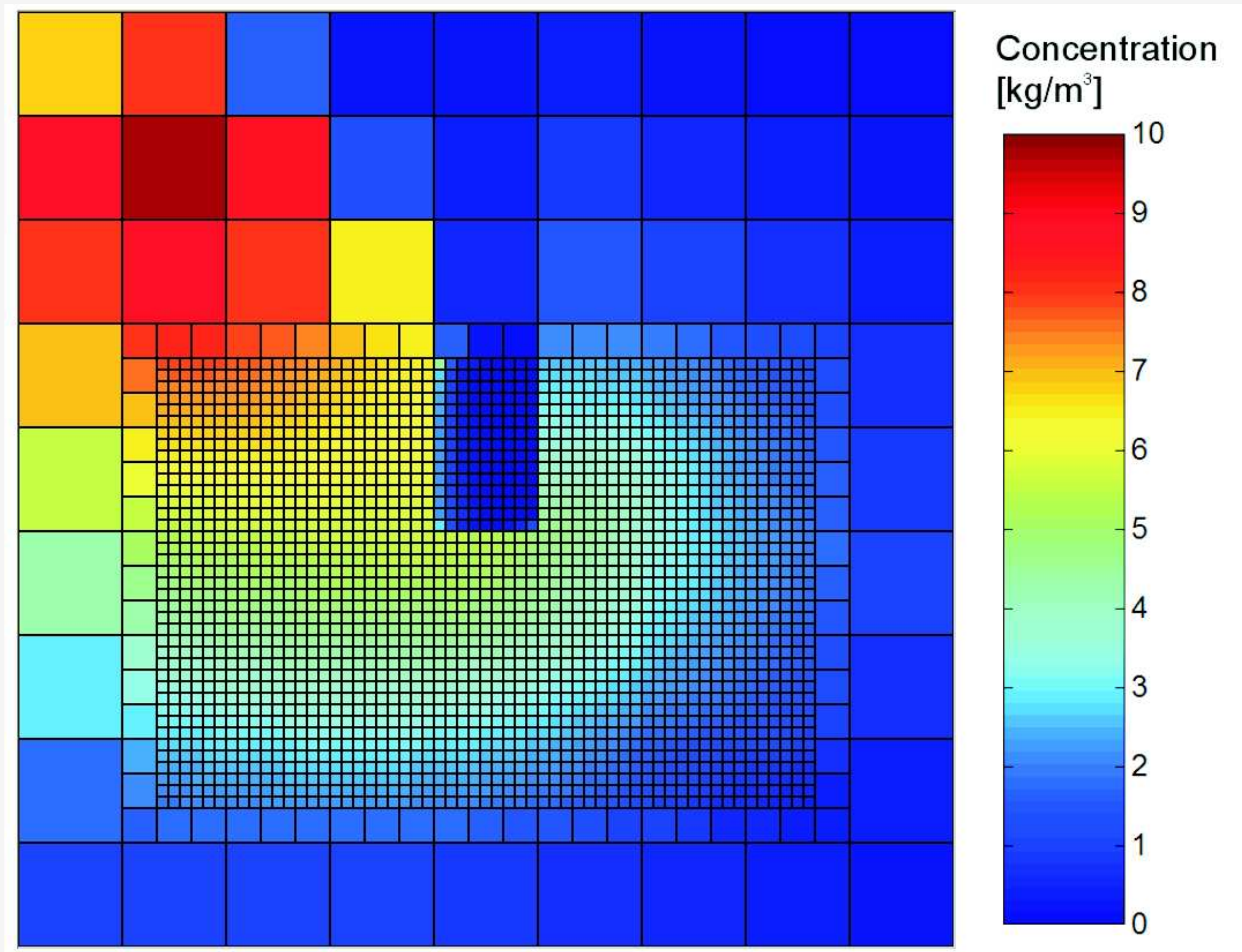
Piezometric head

Contaminant transport simulation



Darcy velocity

Contaminant transport simulation



Concentration

Conclusions and future work

Conclusions

- combined schemes integrate the advantages of the finite volume and finite element methods
  - enable robust, efficient, conservative, and stable discretization

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  - almost no regularity of data required
  - no maximal angle condition, local refinement possible
  - extensions of the “finite volume techniques” for negative transmissibilities and general meshes

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Future work

- error estimates
- complete flow – transport model

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Perspectives and future work

Discrete Poincaré–Friedrichs inequalities

Friedrichs (Poincaré) inequality

$$\int_\Omega g^2(\mathbf{x})\,\mathrm{d}\mathbf{x} \le c_F \int_\Omega |\nabla g(\mathbf{x})|^2\,\mathrm{d}\mathbf{x} \qquad \forall g \in H_0^1(\Omega)$$

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Nonconforming approximation of $H_0^1(\Omega)$

$$W_0(\mathcal{T}_h) := \Big\{ g \in \prod_{K\in\mathcal{T}_h} H^1(K)\,;\, \int_\sigma g(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{x}) = 0 \qquad \forall \sigma \in \mathcal{E}_h^{\mathrm{ext}}$$

$$\int_{\sigma_{K,L}} g|_K(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{x}) = \int_{\sigma_{K,L}} g|_L(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{x}) \qquad \forall \sigma_{K,L} \in \mathcal{E}_h^{\mathrm{int}} \Big\}$$

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Known results and opened problems

Literature overview

- Temam (1979); piecewise linear functions, inverse assumption, convex bounded domains
- Dolejší, Feistauer, & Felcman (1999); piecewise linear functions, inverse assumption, nonconvex bounded domains
- Knobloch (2001); general spaces, no inverse assumption, nonconvex bounded domains
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- value of the constant C_F ?
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- Eymard, Gallouët, & Herbin (1999); piecewise constant functions

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Proof of the discrete Friedrichs inequality

Interpolation operator $W_0(\mathcal{T}_h) \to Y_0(\mathcal{D}_h)$

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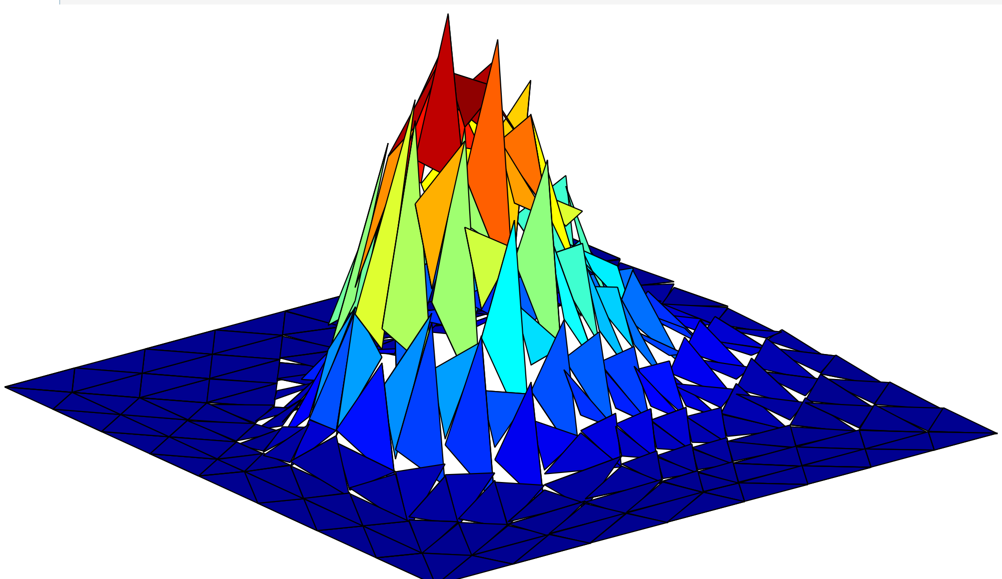
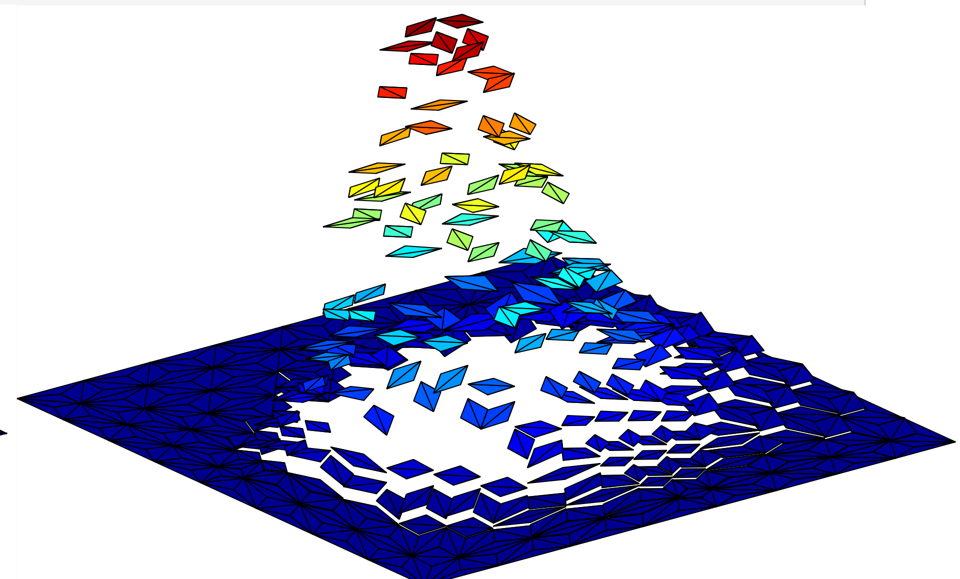


Pw linear nonconforming function



Its pw constant approximation

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Theorem (Discrete Friedrichs inequality for piecewise constant functions) *It holds that*

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Constant C_F for $d = 2$

$C_F = \dfrac{c(d)}{\kappa_{\mathcal{T}}^2}|\Omega|$, where $\kappa_{\mathcal{T}}$ is given by $\min_{K\in\mathcal{T}_h} \dfrac{|K|}{\text{diam}(K)^d} \ge \kappa_{\mathcal{T}} \quad \forall h > 0$

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Constant C_F for $d=2,3$

$C_F = C(d,\kappa_{\mathcal{T}})[\inf_{\mathbf{b}}\{\mathrm{diam}_{\mathbf{b}}(\Omega)\}]^2$, where $\mathbf{b}$ is a unit vector

- $\{\mathcal{T}_h\}_h$ satisfying the inverse assumption: $C(d,\kappa_{\mathcal{T}}) \approx 1/\kappa_{\mathcal{T}}^2\zeta_{\mathcal{T}}^d$

$$\max_{K\in\mathcal{T}_h} \frac{h}{\mathrm{diam}(K)} \le \zeta_{\mathcal{T}} \quad \forall h>0$$

- $\{\mathcal{T}_h\}_h$ only shape-regular: more complicated dependence on $\kappa_{\mathcal{T}}$

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Extensions, discrete Poincaré inequality, conclusions

Extensions

- can be extended to functions only fixed to zero on a part of the boundary
- can be extended to domains only bounded in one direction
- simplified form for Crouzeix–Raviart finite elements in two space dimensions
- optimality of C_F shown via examples

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Importance

- analysis of nonconforming methods (nonconforming FEs, discontinuous Galerkin methods)

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RT Mixed FEM for second-order elliptic problems

Second-order elliptic problem:

$$\begin{aligned} -\nabla \cdot \mathbf{S}\nabla p &= q && \text{in } \Omega\,, \\ p &= p_D && \text{on } \partial\Omega \end{aligned}$$

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Second-order elliptic problem:

$$\begin{aligned} -\nabla \cdot \mathbf{S}\nabla p &= q && \text{in } \Omega\,, \\ p &= p_D && \text{on } \partial\Omega \end{aligned} \quad \longrightarrow \quad \begin{aligned} \mathbf{u} &= -\mathbf{S}\nabla p && \text{in } \Omega\,, \\ \nabla \cdot \mathbf{u} &= q && \text{in } \Omega\,, \\ p &= p_D && \text{on } \partial\Omega \end{aligned}$$

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$$\begin{aligned} (\mathbf{S}^{-1}\mathbf{u}_h, \mathbf{v}_h)_\Omega - (\nabla\cdot\mathbf{v}_h, p_h)_\Omega = -\langle \mathbf{v}_h\cdot\mathbf{n}, p_D\rangle_{\partial\Omega} \qquad \forall\, \mathbf{v}_h \in \mathbf{V}_h\,,\\ -(\nabla\cdot\mathbf{u}_h, \phi_h)_\Omega = -(q, \phi_h)_\Omega \qquad \forall \phi_h \in \Phi_h \end{aligned}$$

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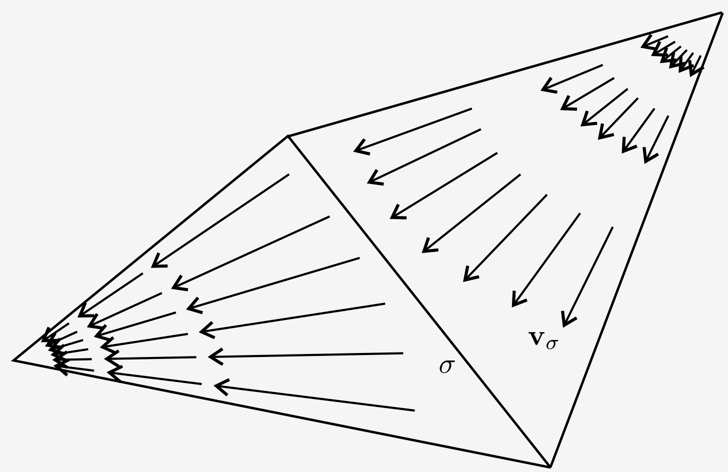

Velocity basis function $\mathbf{v}_\sigma$

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Associated matrix problem:

$$\begin{pmatrix} \mathbb{A} & \mathbb{B}^t \\ \mathbb{B} & 0 \end{pmatrix} \begin{pmatrix} U \\ P \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix}$$

Implementation and equivalences: known results

Equivalence with the nonconforming finite element method

- Lagrange multipliers, mixed-hybrid FEM $\longrightarrow \mathbb{M}\Lambda = J$
  - Arnold & Brezzi (1985)
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Equivalence with the finite volume method

- using numerical integration $\rightsquigarrow \mathbb{S}P = H$
  - Russell & Wheeler (1983); rectangles, $\mathbb{S}$ diag.
  - Agouzal, Baranger, Maitre, & Oudin (1995); triangles & rectangles, $\mathbb{S}$ diag.
  - Arbogast, Wheeler, & Yotov (1997); rectangles, $\mathbb{S}$ full

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- exact $\longrightarrow \tilde{\mathbb{S}}\tilde{P} = \tilde{H}$
  - Younès, Mose, Ackerer, & Chavent (1999); triangles

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Expressing fluxes through edges using scalar unknowns

Aim: $$\begin{pmatrix} \mathbb{A} & \mathbb{B}^t \\ \mathbb{B} & 0 \end{pmatrix} \begin{pmatrix} U \\ P \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix} \longrightarrow \mathbb{S}P = H$$

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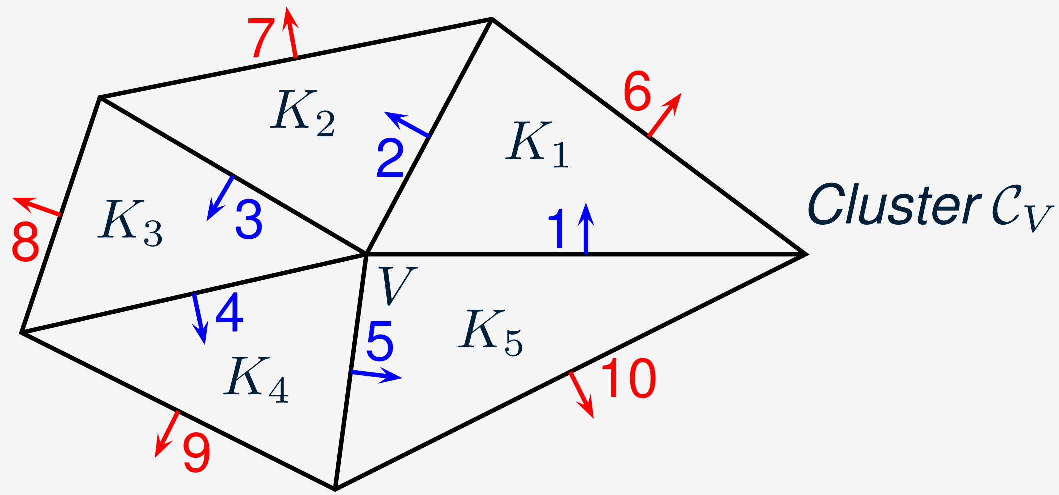

Local linear system in $\mathcal{C}_V$:

$$\begin{pmatrix} \mathbb{A}_V & \mathbb{C}_V \\ \mathbb{D}_V & \mathbb{I}_V \end{pmatrix} \begin{pmatrix} U_V^{\text{int}} \\ U_V^{\text{ext}} \end{pmatrix} = \begin{pmatrix} -\mathbb{B}_V^t P_V + F_V \\ G_V \end{pmatrix}$$

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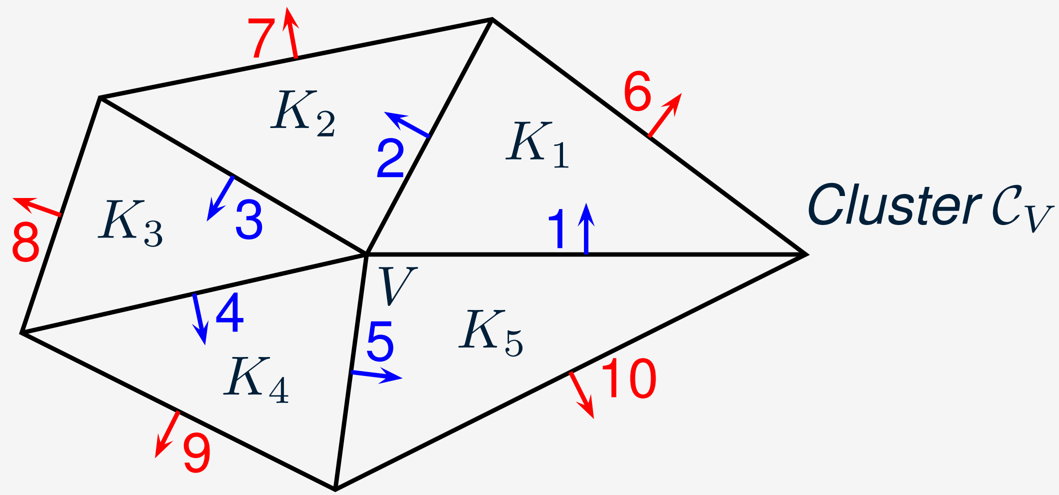

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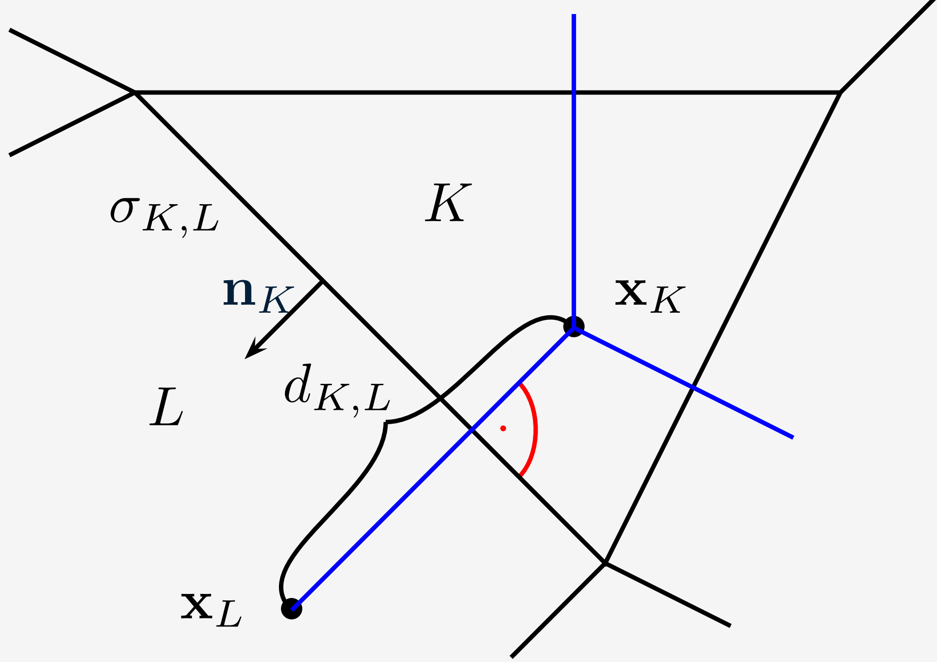
Eliminating U_V^{ext}: $(\mathbb{A}_V - \mathbb{C}_V \mathbb{D}_V) U_V^{\text{int}} = -\mathbb{B}_V^t P_V + F_V - \mathbb{C} G_V$

$(\mathbb{A}_V - \mathbb{C}_V \mathbb{D}_V) = \mathbb{M}_V$ *local condensation matrix*

Remark: the finite volume method

4-point finite volume scheme (orthogonality condition, $\mathbf{S}$ scalar):

$$-\int_{\partial K} \nabla p \cdot \mathbf{n}_K = -\sum_{L \in \mathcal{N}(K)} \int_{\sigma_{K,L}} \nabla p \cdot \mathbf{n}_K \approx -\sum_{L \in \mathcal{N}(K)} \frac{p_L - p_K}{d_{K,L}} |\sigma_{K,L}|$$



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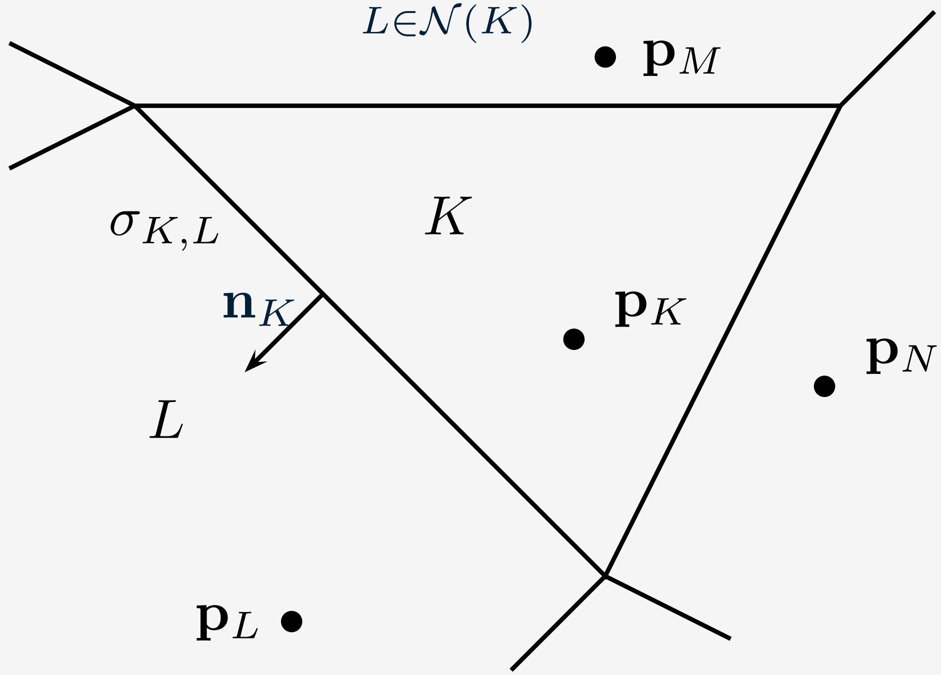
Multi-point finite volume scheme ($\mathcal{T}_h$ and S general):

$$-\int_{\partial K} \mathbf{S} \nabla p \cdot \mathbf{n}_K \approx -\sum_{L \in \mathcal{N}(K)} f(p_K, p_L, p_M, p_N, \ldots) |\sigma_{K,L}|$$



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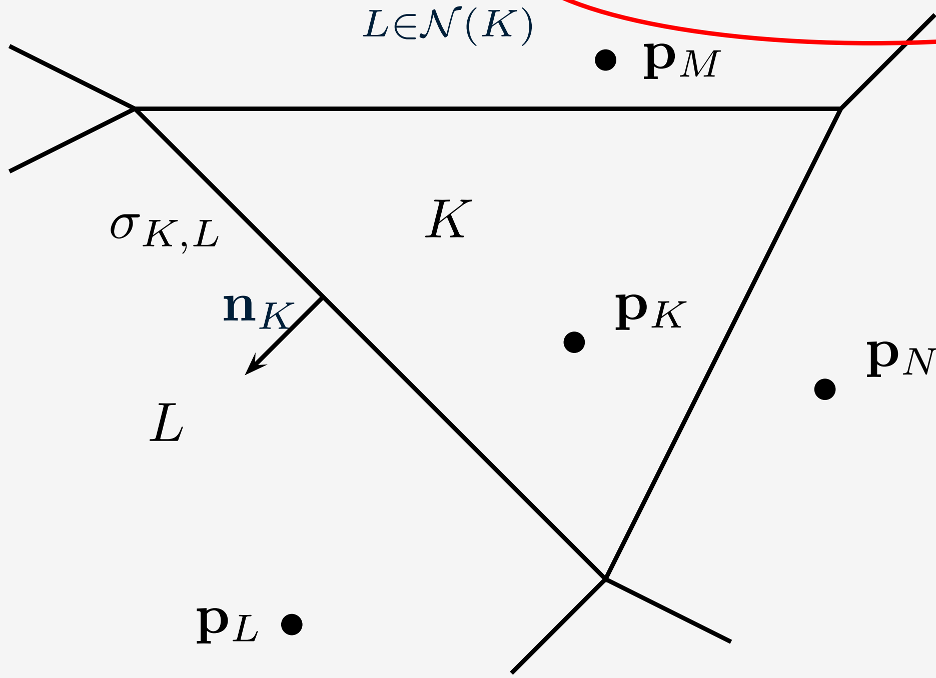

Equivalence between RT MFEM and multi-point FVM

Theorem (Equivalence between RT MFEM and multi-point FVM)
Let the matrices $\mathbb{M}_V$ be invertible for all $V \in \mathcal{V}_h$. Then the lowest-order Raviart–Thomas mixed finite element method is equivalent to a particular multi-point finite volume scheme.

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Remark (Comparison with a classical multi-point FVM)

- not only the scalar unknowns, but also the *sources* and possibly *boundary conditions* associated with the neighboring elements are used to express the flux of $\mathbf{u} = -\mathbf{S}\nabla p$ through a given side
- one has to solve a local linear problem

Properties of the global system matrix $\mathbb{S}$

Theorem (Stencil) *Let* $\mathbb{M}_V$ *be invertible for all* $V \in \mathcal{V}_h$*. Then* $\mathbb{S}_{K,L}$ *is possibly nonzero only if* K *and* L *share a common vertex.*

- The flux through a side σ is expressed only using the scalar unknowns of the elements sharing a common vertex with σ.

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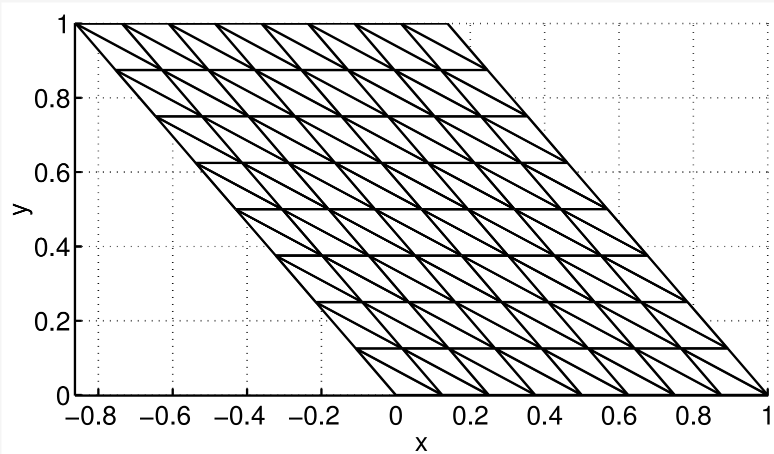
- The flux through a side σ is expressed only using the scalar unknowns of the elements sharing a common vertex with σ.

Theorem (Positive definiteness) *Let $\mathbb{M}_V$ be positive definite for all $V \in \mathcal{V}_h$. Then $\mathbb{S}$ is also positive definite.*

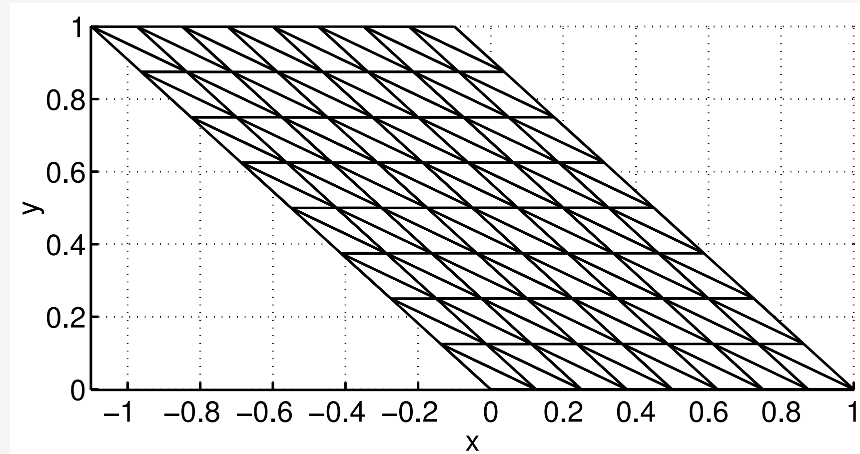
- criterion for the positive definiteness of $\mathbb{M}_V$: geometry of each triangle, tensor $\mathbf{S}$

Properties of the global system matrix $\mathbb{S}$

Example (Positive definiteness for a deformed square)



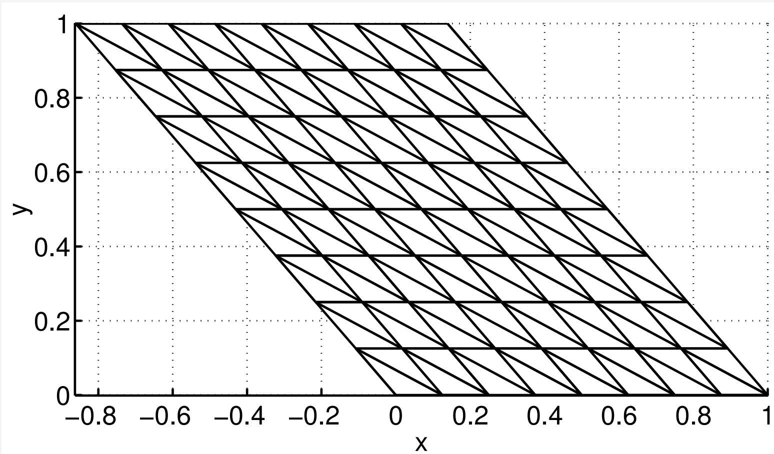
Theoretical limit



Experimental limit

Properties of the global system matrix $\mathbb{S}$

Example (Positive definiteness for a deformed square)



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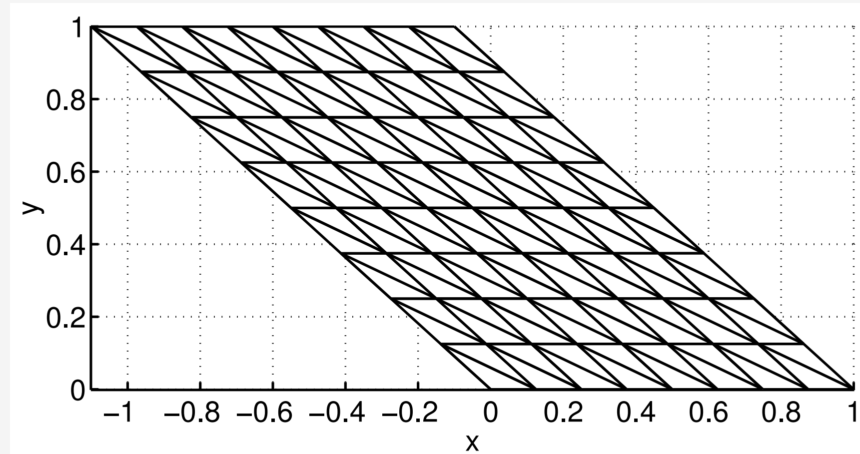
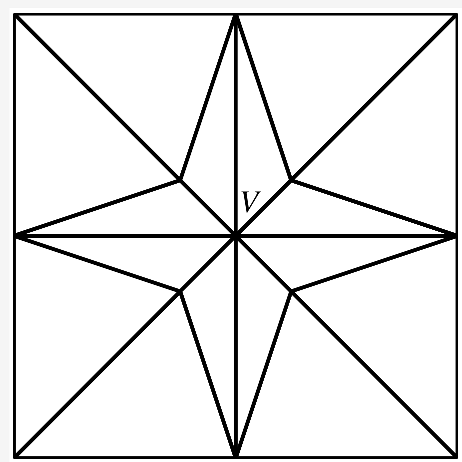


Experimental limit

Example (Singular local condensation matrix)



Properties of the global system matrix $\mathbb{S}$

Theorem (Stencil) *Let $\mathbb{M}_V$ be invertible for all $V \in \mathcal{V}_h$. Then $\mathbb{S}_{K,L}$ is possibly nonzero only if K and L share a common vertex.*

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Theorem (Positive definiteness) *Let $\mathbb{M}_V$ be positive definite for all $V \in \mathcal{V}_h$. Then $\mathbb{S}$ is also positive definite.*

- criterion for the positive definiteness of $\mathbb{M}_V$: geometry of each triangle, tensor $\mathbf{S}$

Theorem (Symmetry) *Let $\mathbb{M}_V$ be invertible and symmetric for all $V \in \mathcal{V}_h$. Then $\mathbb{S}$ is also symmetric.*

- satisfied if $\mathcal{T}_h$ consists of equilateral simplices and if $\mathbf{S}$ is pw constant and scalar

Numerical experiments: linear elliptic case

For $\Omega = (0,1) \times (0,1)$, we consider:

$$-\triangle p = q \, ,$$

$$q = -2e^x e^y \, .$$

< > − +

Numerical experiments: linear elliptic case

For $\Omega = (0,1) \times (0,1)$, we consider:

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Dirichlet BC given by the solution

$$p(x,y) = e^x e^y \, .$$

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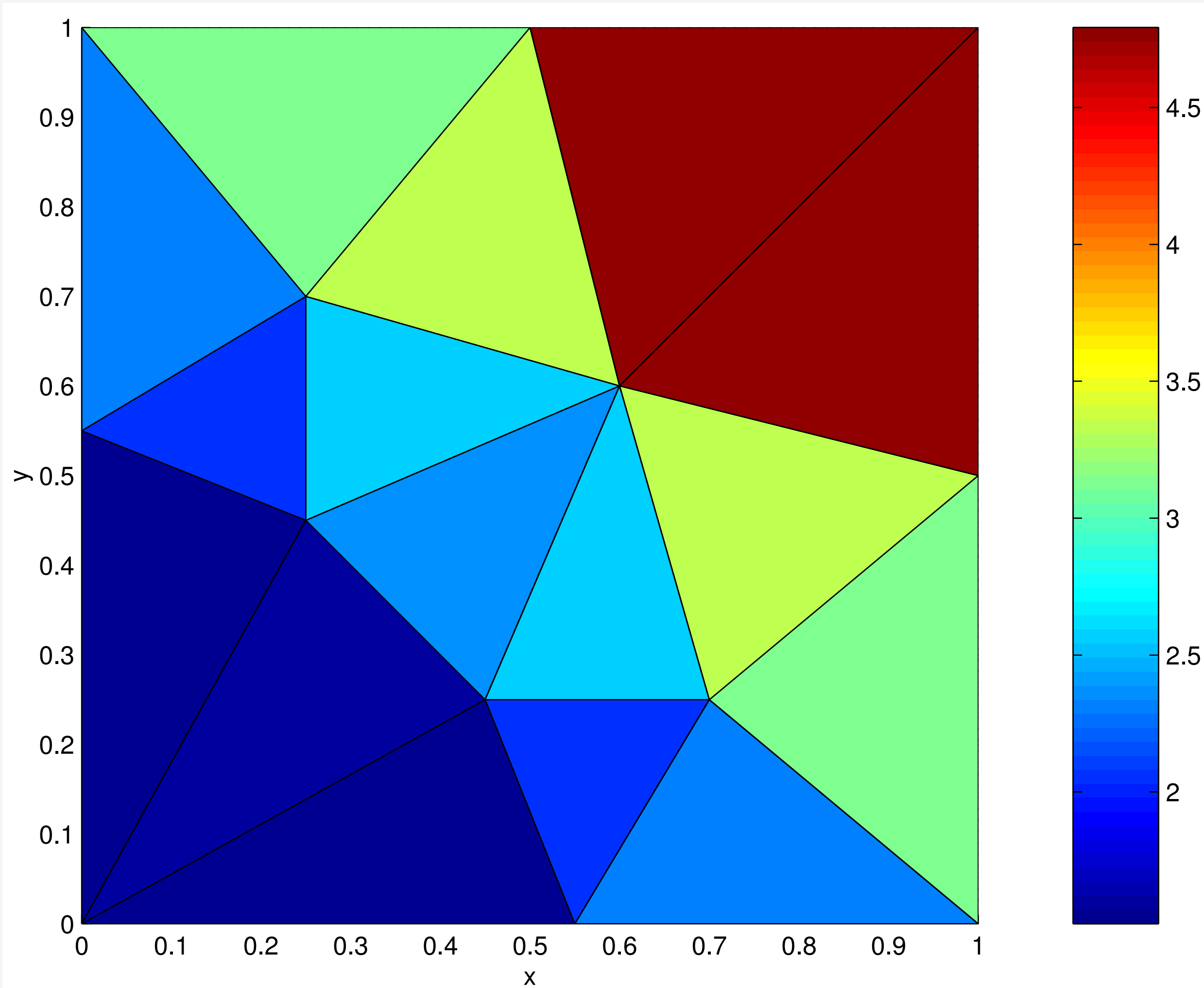
Numerical experiments: linear elliptic case



Initial triangulation and solution

Numerical experiments: linear elliptic case

Condensation

Ref.	Unkn.	Cond.	Bi-CGS	Iter.		
4	4096	2882	1.43	147.5		
5	16384	11523	12.55	295.5		
6	65536	46093	117.58	555.5		

Hybridization

Ref.	Unkn.	Cond.	Bi-CGS	Iter.	CG	Iter.
4	6080	5616	2.43	230.5	1.75	316
5	24448	22499	23.40	449.5	16.87	623
6	98048	89995	227.04	864.0	162.09	1226

Finite volumes

Ref.	Unkn.	Cond.	Bi-CGS	Iter.	CG	Iter.
4	4096	5268	1.44	211.5	1.03	297
5	16384	21089	12.96	431.5	8.30	586
6	65536	84356	139.73	893.5	92.23	1151

Application to nonlinear parabolic problems

Nonlinear parabolic convection–reaction–diffusion problem

$$\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} + F(p) = q \quad \text{in} \quad \Omega\,,$$

$$\mathbf{u} = -\mathbf{S}\nabla\varphi(p) + \psi(p)\mathbf{w} \quad \text{in} \quad \Omega\,,$$

$$p = p_0 \quad \text{in} \quad \Omega \text{ for } t = 0\,,\; p = p_D \quad \text{on} \quad \partial\Omega \times (0,T)\,.$$

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$$(\mathbf{S}^{-1}\mathbf{u}_h^n, \mathbf{v}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, \varphi(p_h^n))_\Omega - (\psi(p_h^n)\mathbf{w}, \mathbf{S}^{-1}\mathbf{v}_h)_\Omega$$

$$= -\langle \mathbf{v}_h \cdot \mathbf{n}, \varphi(p_D)\rangle_{\partial\Omega} \qquad \forall\, \mathbf{v}_h \in \mathbf{V}_h\,,$$

$$(\frac{p_h^n - p_h^{n-1}}{\triangle t_n}, \phi_h)_\Omega + (\nabla \cdot \mathbf{u}_h^n, \phi_h)_\Omega + (F(p_h^n), \phi_h)_\Omega$$

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$$= (q, \phi_h)_\Omega \qquad \forall \phi_h \in \Phi_h\,.$$

Assemblage and inversion of local condensation matrices only once; linearization and time steps—only scalar unknowns as in the FVM.

Numerical experiments: nonlinear parabolic case

For $\Omega = (0,2) \times (0,1)$ and $T = 1$, we consider:

$$\frac{\partial(p + p^{\frac{1}{2}})}{\partial t} - \nabla \cdot (\mathbf{S}\nabla p) + \nabla \cdot (p\mathbf{w}) + \frac{p^{\frac{1}{2}}}{2} = 0\,.$$

< > − +

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Case A:

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ in } \Omega\,, \quad \mathbf{w} = (3,0) \text{ in } \Omega\,.$$

Case B:

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ for } x < 1\,, \quad \mathbf{S} = \begin{pmatrix} 8 & -7 \\ -7 & 20 \end{pmatrix} \text{ for } x > 1\,,$$

$$\mathbf{w} = (3,0) \text{ for } x < 1\,, \quad \mathbf{w} = (3,12) \text{ for } x > 1\,.$$

< > − +

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$$\mathbf{w} = (3,0) \text{ for } x < 1\,, \quad \mathbf{w} = (3,12) \text{ for } x > 1\,.$$

Initial and Dirichlet BC given by the solution

$$p(x,y,t) = \frac{1}{e^3} e^x e^y e^{-t}\,.$$

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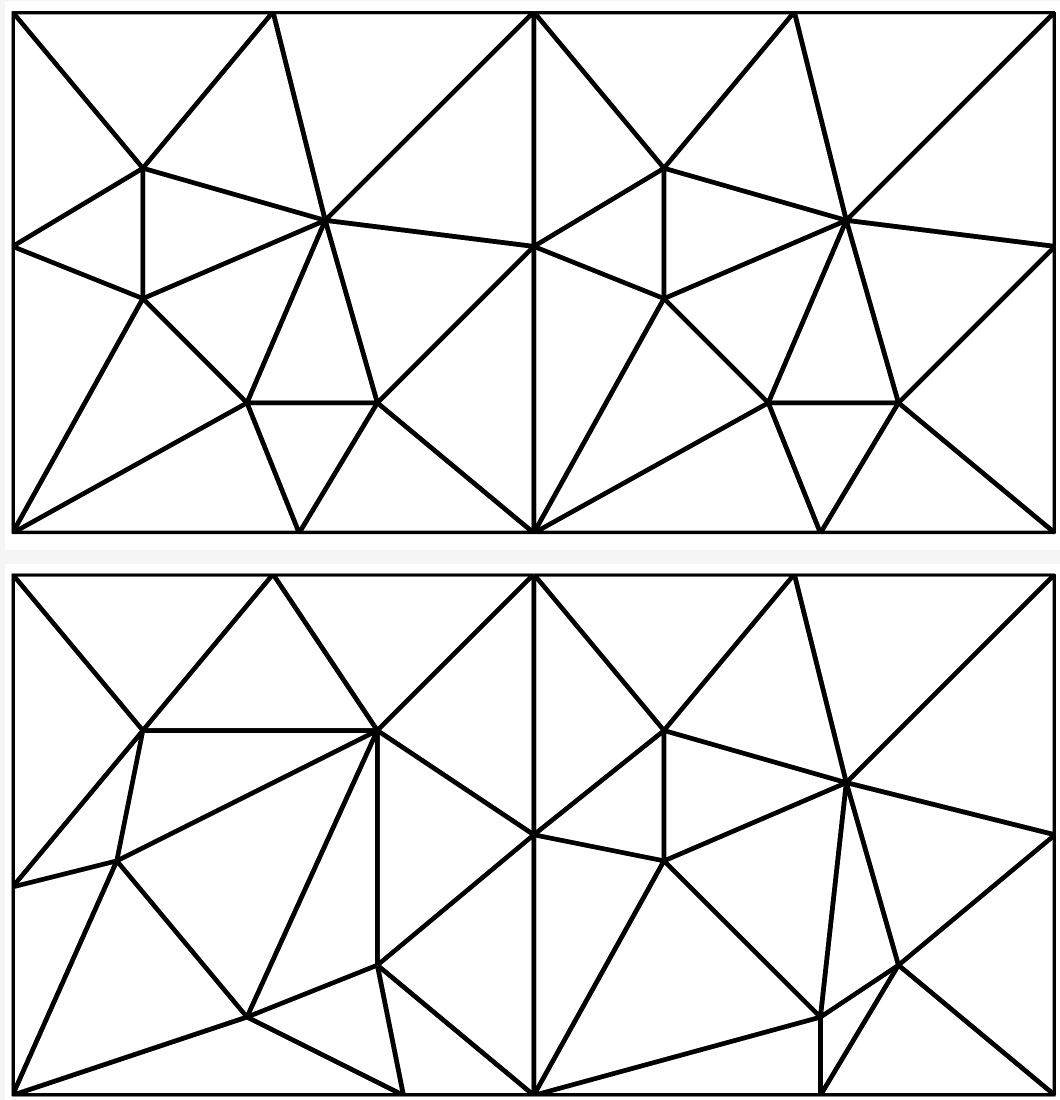
Numerical experiments: nonlinear parabolic case



Initial triangulations, case A (top), case B (bottom)

Numerical experiments: nonlinear parabolic case A

Condensation

Unkn.	St.	Cond.	Bi-CGS	Iter.	CPU	ILU	PBi-CGS	Iter.
128	14	39	0.02	27.0	0.02	0.01	0.01	2.0
512	14	116	0.07	56.5	0.02	0.01	0.01	2.5
2048	14	311	0.38	82.5	0.11	0.06	0.05	3.5
8192	14	768	2.65	139.0	0.75	0.41	0.34	5.5
32768	14	1782	17.14	191.5	4.85	2.95	1.90	7.0

Standard MFE

Unkn.	St.	Cond.	Bi-CGS	Iter.	CPU	ILU	PBi-CGS	Iter.
204	5	405	0.06	95.5	0.02	0.01	0.01	2.0
792	5	917	0.22	153.0	0.07	0.03	0.04	3.0
3120	5	1949	1.36	282.0	0.34	0.14	0.20	4.0
12384	5	4016	8.47	406.5	2.57	0.94	1.63	5.0
49344	5	8181	51.18	553.0	17.63	6.94	10.69	6.0

Numerical experiments: nonlinear parabolic case B

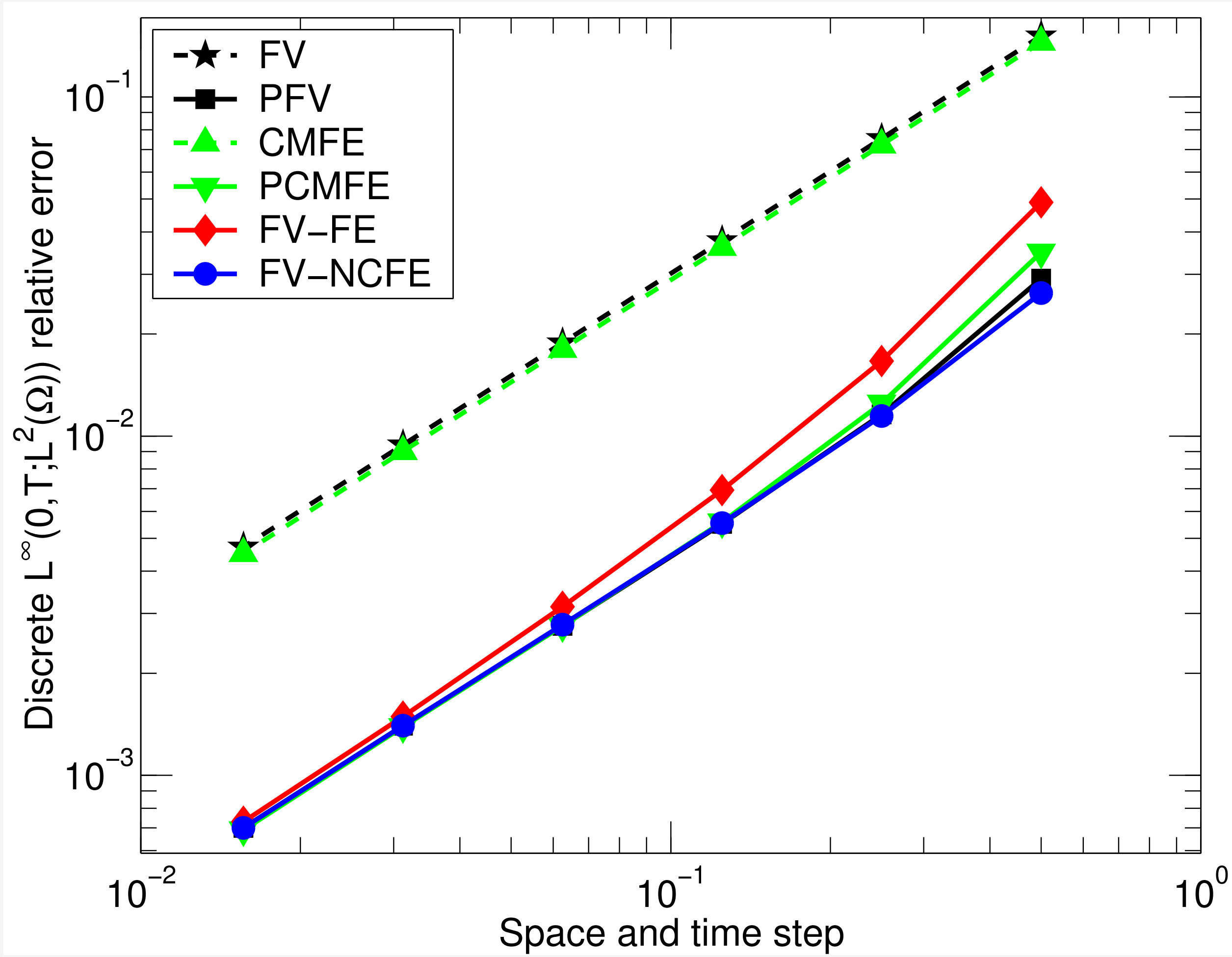
Condensation

Unkn.	St.	Cond.	Bi-CGS	Iter.	CPU	ILU	PBi-CGS	Iter.
128	14	470	0.04	70.0	0.02	0.01	0.01	2.0
512	14	1665	0.21	149.5	0.03	0.01	0.02	2.5
2048	14	4824	1.47	322.5	0.12	0.07	0.05	3.5
8192	14	12523	8.66	474.5	0.88	0.56	0.32	5.0
32768	14	31368	61.53	787.5	7.47	5.46	2.01	5.5

Standard MFE

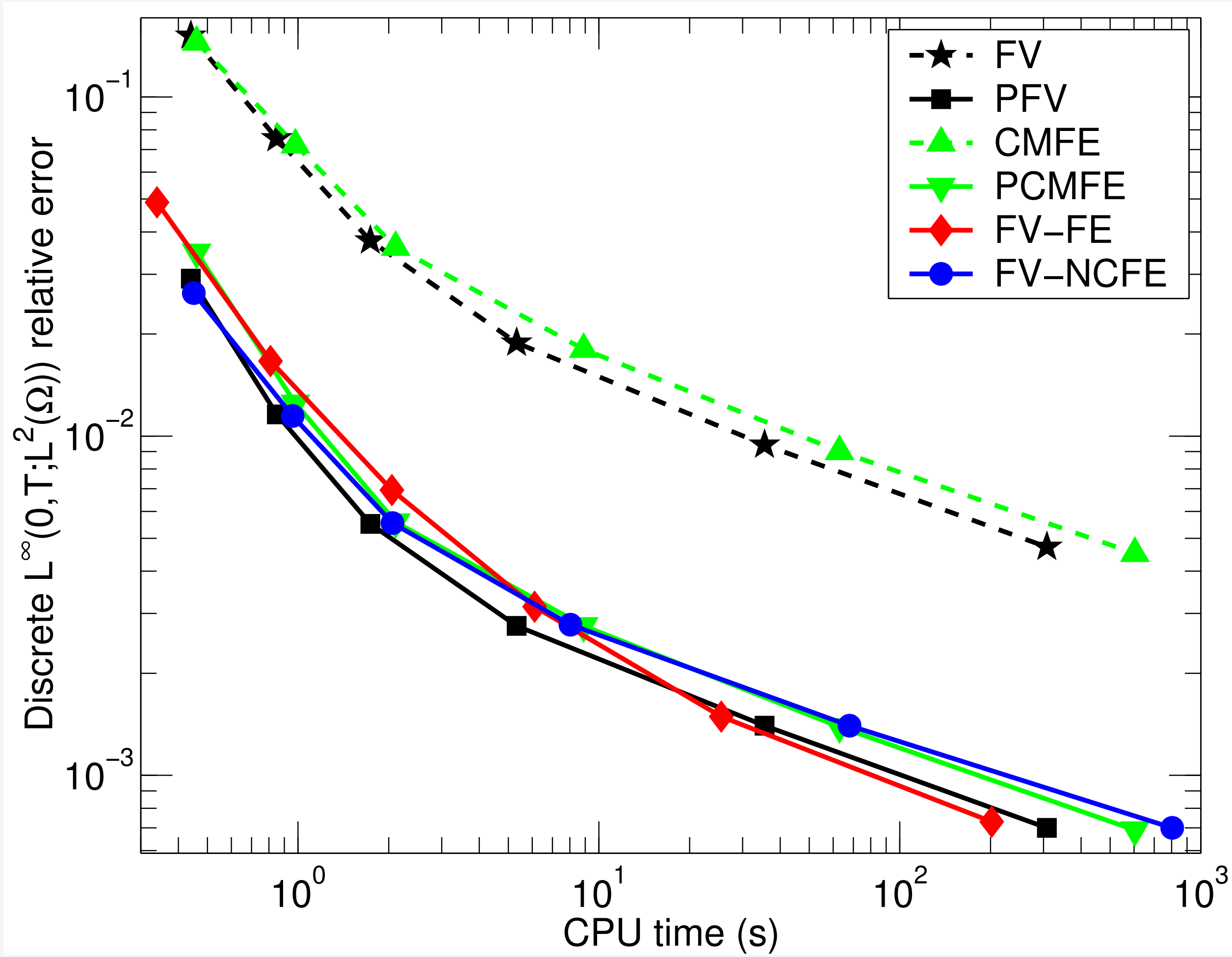
Unkn.	St.	Cond.	Bi-CGS	Iter.	CPU	ILU	PBi-CGS	Iter.
204	5	13849	0.23	412.5	0.02	0.01	0.01	2.0
792	5	39935	1.38	1105.5	0.04	0.02	0.02	2.5
3120	5	131073	12.12	2419.5	0.41	0.18	0.23	3.0
12384	5	250923	103.42	5390.5	3.06	1.32	1.74	3.5
49344	5	586375	617.26	7145.5	29.88	14.96	14.92	4.0

Comparison of different schemes, case A



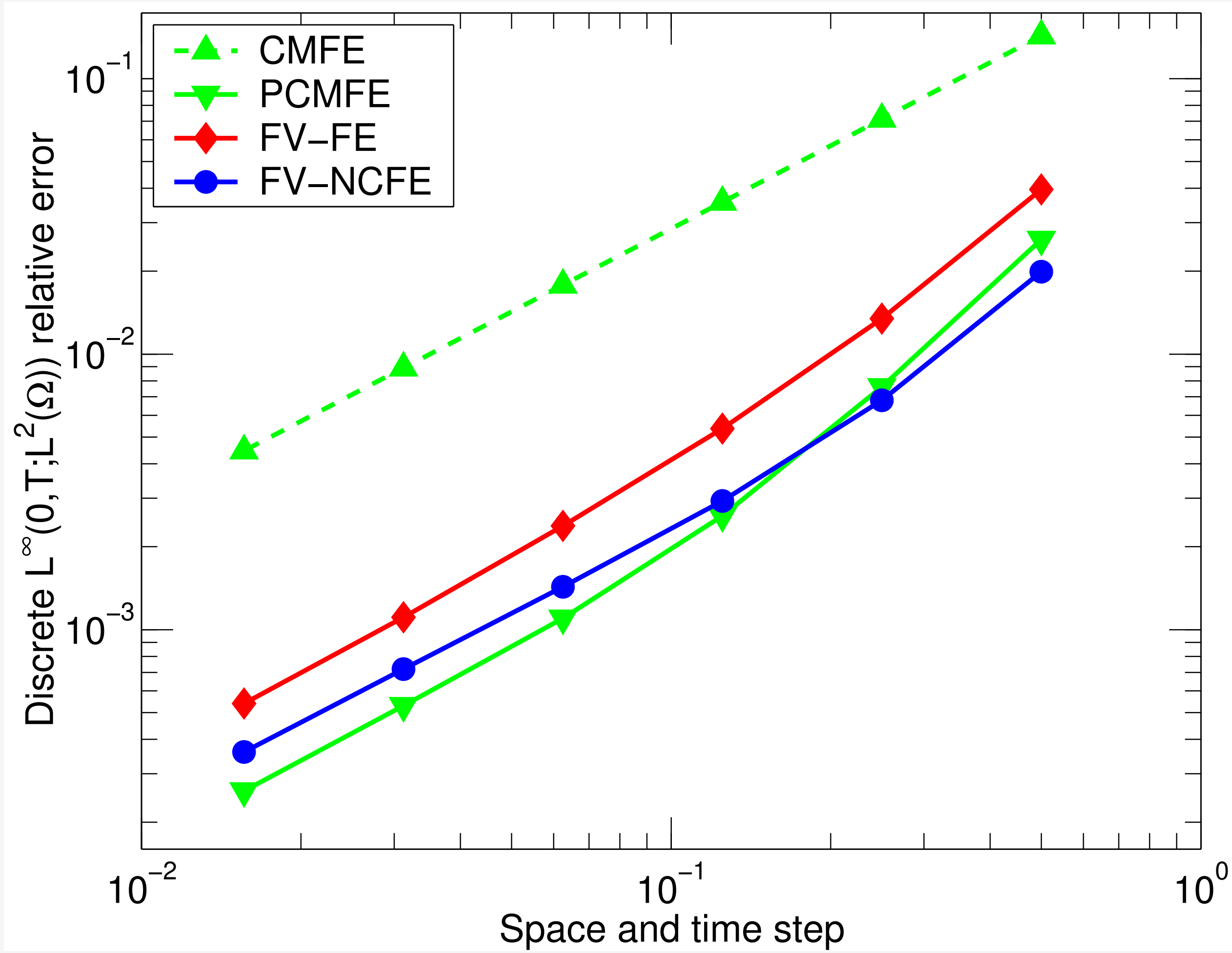
Precision comparison of different schemes, case A

Comparison of different schemes, case A



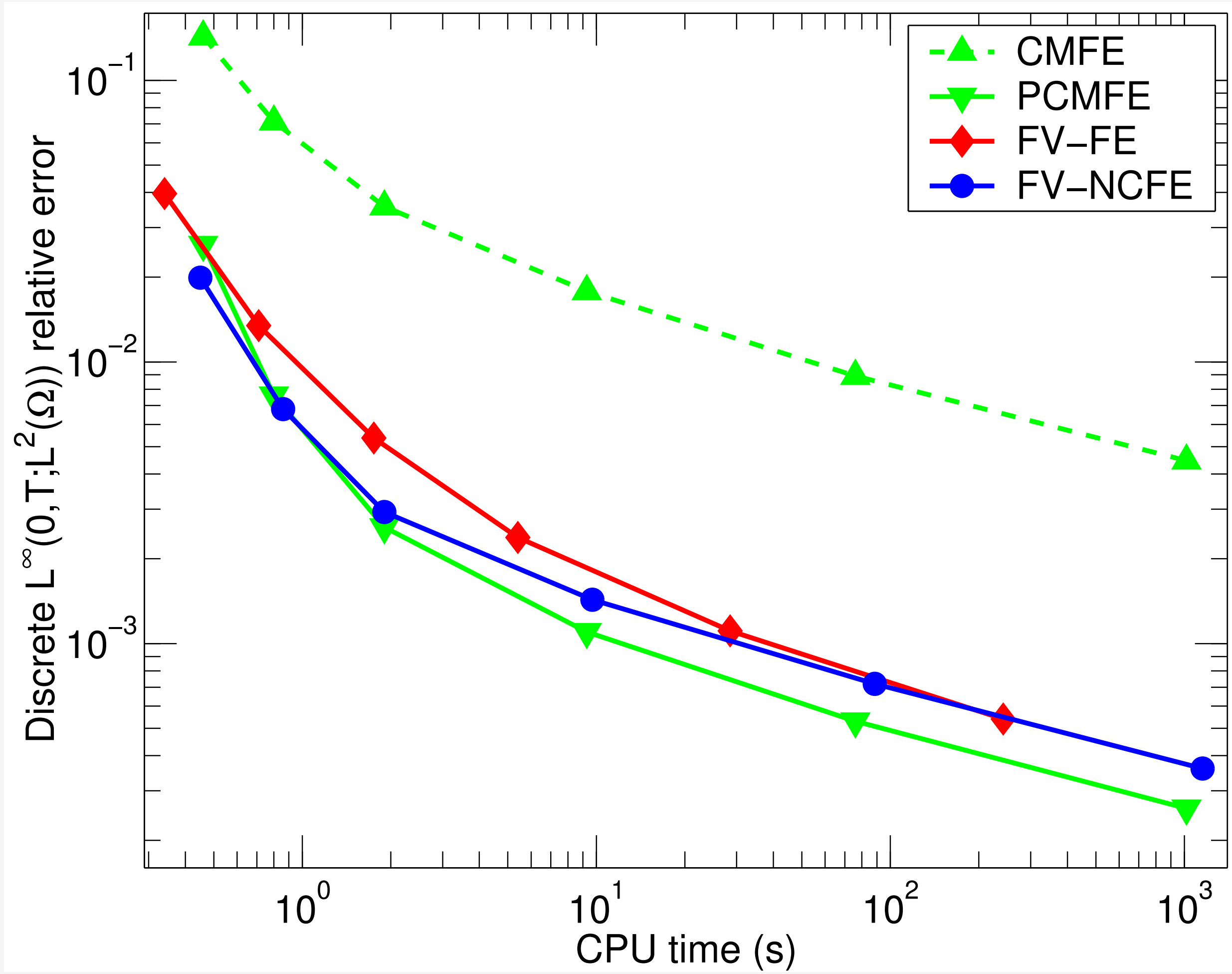
Efficiency comparison of different schemes, case A

Comparison of different schemes, case B



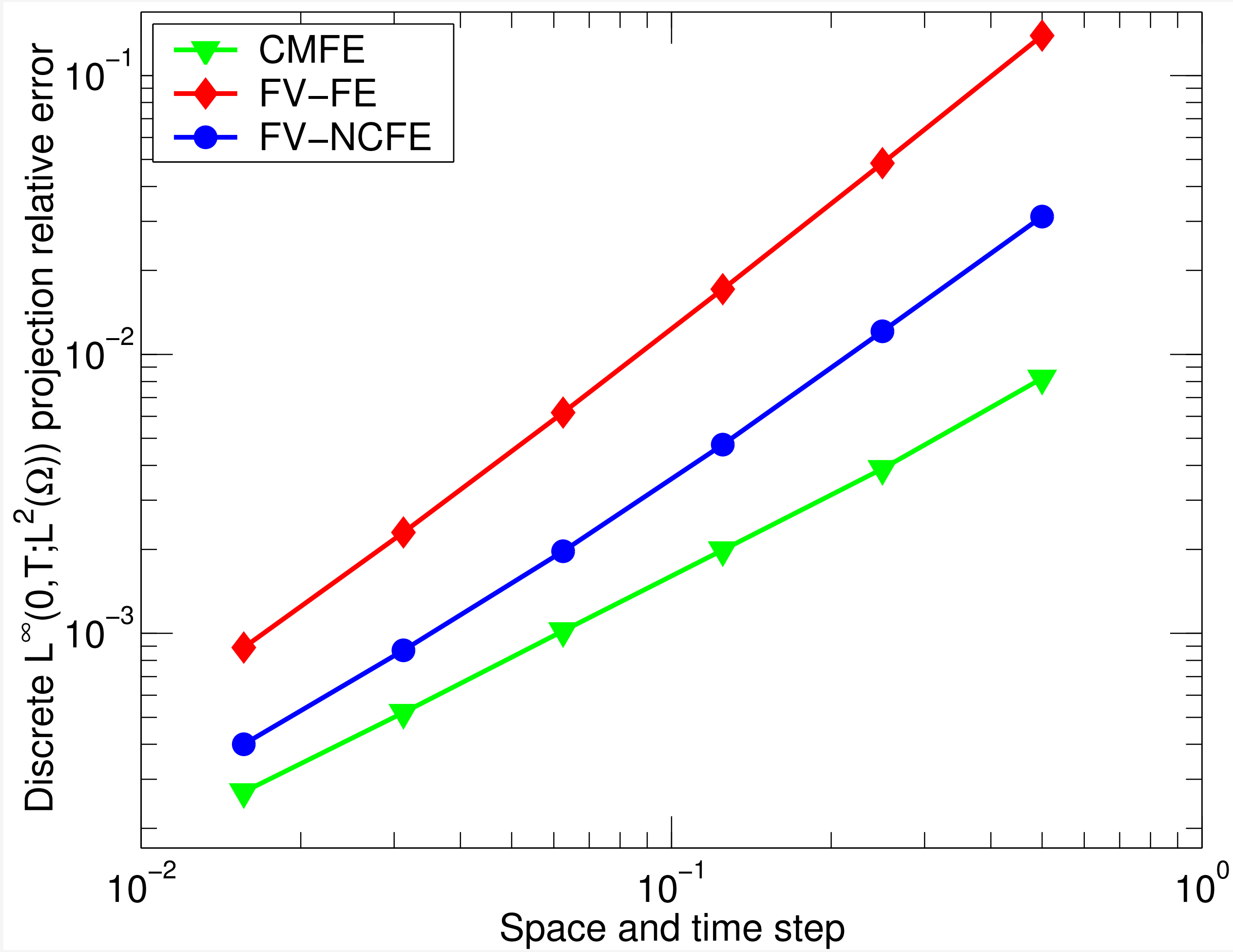
Precision comparison of different schemes, case B

Comparison of different schemes, case B



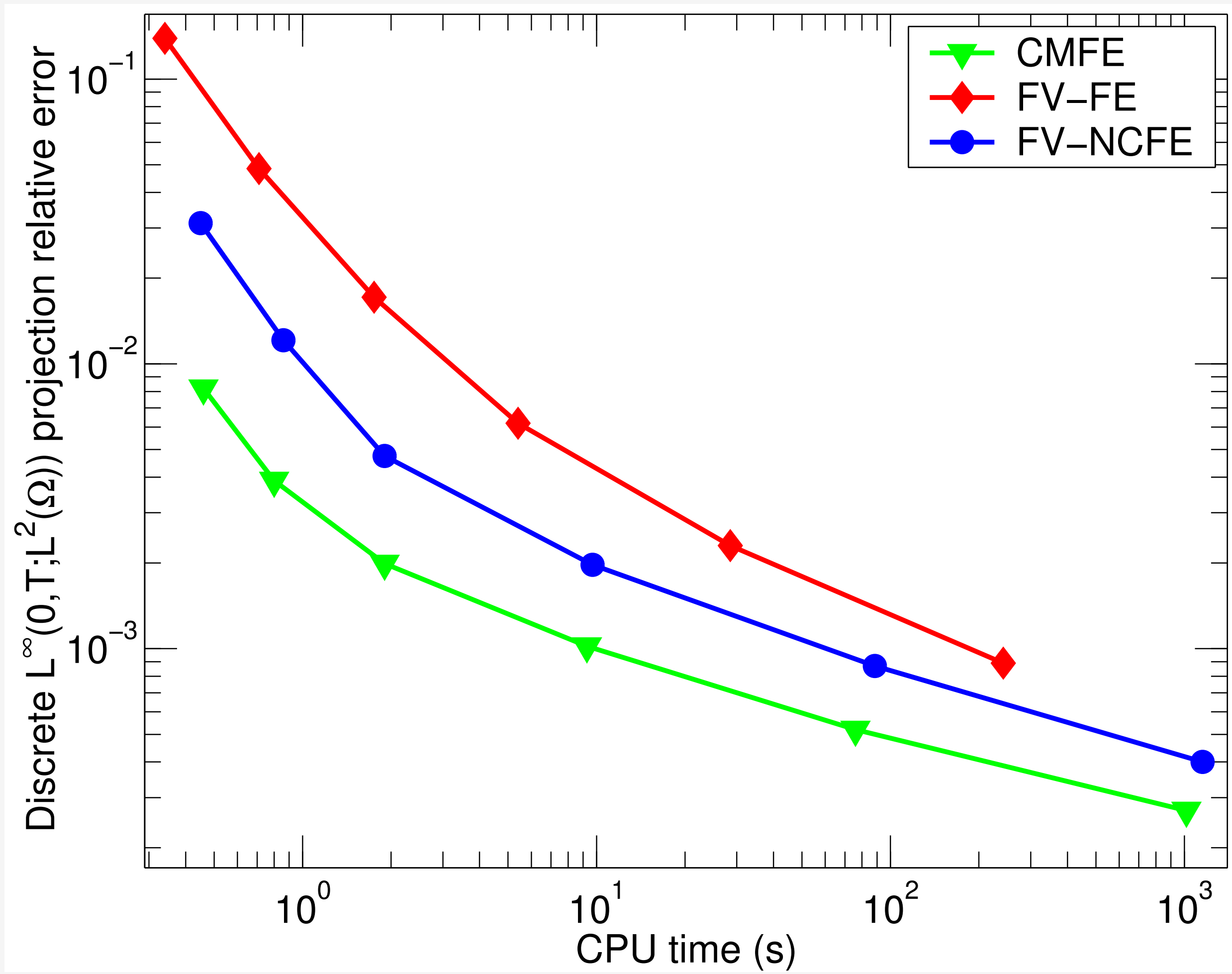
Efficiency comparison of different schemes, case B

Comparison of different schemes, case B



Precision comparison of different schemes (projection), case B

Comparison of different schemes, case B



Efficiency comparison of different schemes (projection), case B

Conclusions and future work

Main idea

- first decompose the problem into scalar and flux unknowns and guarantee the accomplishment of the inf–sup condition

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- then eliminate the added fluxes

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Properties

- reduction of the number of unknowns by 1/3 (1/2 in 3D)
- resulting matrices: very well conditioned, positive definite for not distorted meshes
- substantial savings of CPU time for nonlinear parabolic problems

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Future work

- analysis of the singularities
- extensions to higher-order schemes

Outline

Motivation

Chapter 1, part A: A combined finite volume–nonconforming/mixed-hybrid finite element scheme for degenerate parabolic problems

Chapter 1, part B: A combined finite volume–finite element scheme for contaminant transport simulation on nonmatching grids

Chapter 2: Discrete Poincaré–Friedrichs inequalities

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Chapter 4: Mixed and nonconforming finite element methods on a fracture network

Perspectives and future work

Fracture flow problem

Fracture network

$$\mathcal{S} := \bigcup_{\ell \in L} \alpha_\ell$$

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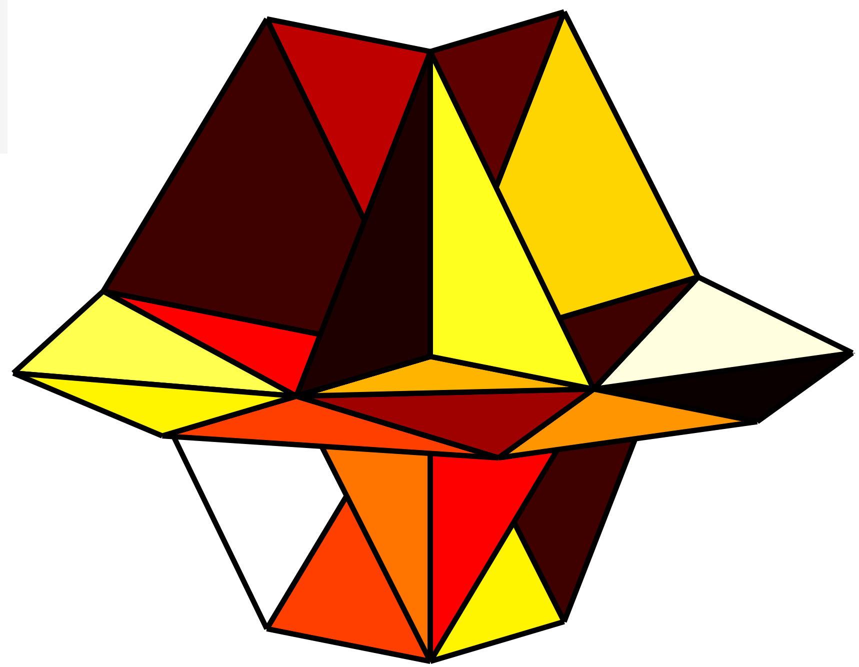
Fracture flow problem

Fracture network

$$\mathcal{S} := \bigcup_{\ell \in L} \alpha_\ell$$



Rock fractures　　Approximation by a system of polygons

Fracture flow problem

Fracture network

$$\mathcal{S} := \bigcup_{\ell \in L} \alpha_\ell$$

Governing equations

$$\begin{aligned} \mathbf{u} &= -\mathbf{K}(\nabla p + \nabla z) \quad \text{in } \alpha_\ell\,,\ \ell \in L\,, \\ \nabla \cdot \mathbf{u} &= q \quad \text{in } \alpha_\ell\,,\ \ell \in L\,, \\ p &= p_D \quad \text{on } \Gamma_D\,, \quad \mathbf{u} \cdot \mathbf{n} = u_N \quad \text{on } \Gamma_N \end{aligned}$$

p pressure head

$\mathbf{u}$ Darcy velocity

$\mathbf{K}$ hydraulic conductivity tensor

z elevation

q sources and sinks

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Fracture flow problem

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p	pressure head	$\mathbf{K}$	hydraulic conductivity tensor
$\mathbf{u}$	Darcy velocity	z	elevation
		q	sources and sinks

Continuity

$$\begin{aligned} p|_{\overline{\alpha_i}} &= p|_{\overline{\alpha_j}} \quad \text{on } f \qquad \forall f \in \mathcal{E}^{\text{int}}\,,\ \forall i, j \in I_f\,, \\ \sum_{i \in I_f} \mathbf{u}|_{\overline{\alpha_i}} \cdot \mathbf{n}_{f,\alpha_i} &= 0 \quad \text{on } f \qquad \forall f \in \mathcal{E}^{\text{int}} \end{aligned}$$

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Known results and our aims

Literature overview

- Baca, Arnett, & King (1984); finite elements
- Koudina, Gonzalez Garcia, Thovert, & Adler (1998); vertex-centered finite volumes
- Reichenberger, Jakobs, Bastian, & Helmig (2004); multi-dimensional vertex-centered finite volumes

Our aims

- definition of mixed finite element methods on fracture networks

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- Arnold & Brezzi (1985)
- Chen (1996)

Our aims

- definition of mixed finite element methods on fracture networks
- relation between the lowest-order mixed and nonconforming finite element methods (theoretical aspects and implementation)

Function spaces

Continuous function spaces

$$L^p(\mathcal{S}) := \prod_{\ell \in L} L^p(\alpha_\ell)\,, \quad \mathbf{L}^p(\mathcal{S}) := L^p(\mathcal{S}) \times L^p(\mathcal{S})$$

$$H^1(\mathcal{S}) \;:=\; \{ v \in L^2(\mathcal{S})\,;\, v|_{\alpha_\ell} \in H^1(\alpha_\ell)\;,$$
$$(v|_{\alpha_i})|_f = (v|_{\alpha_j})|_f \quad \forall f \in \mathcal{E}^{\mathrm{int}}\,, \forall i, j \in I_f \,\}$$

$$\mathbf{H}(\mathrm{div}, \mathcal{S}) \;:=\; \Big\{ \mathbf{v} \in \mathbf{L}^2(\mathcal{S})\,;\, \mathbf{v}|_{\alpha_\ell} \in \mathbf{H}(\mathrm{div}, \alpha_\ell)\,, \sum_{i \in I_f} \langle \mathbf{v}|_{\alpha_i} \cdot \mathbf{n}_{\partial\alpha_i}, \varphi_i \rangle_{\partial\alpha_i} = 0$$
$$\forall \varphi_i \in H^1_{\partial\alpha_i \backslash f}(\alpha_i)\,,\, \varphi_i|_f = \varphi_j|_f \,\forall i, j \in I_f\,,\, \forall f \in \mathcal{E}^{\mathrm{int}} \Big\}$$

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Discrete function spaces

$M^0_{-1}(\mathcal{T}_h)$ constant by elements

$M^0_{-1}(\mathcal{E}_{h,D})$ constant by edges, zero on Γ_D

$X^1_0(\mathcal{E}_{h,D})$ linear by elements, continuous in edge centers, zero on Γ_D

$\mathbf{RT}^0_{-1}(\mathcal{T}_h)$ Raviart–Thomas space, no continuity requirement

$\mathbf{RT}^0_{0,N}(\mathcal{T}_h)$ RT space, normal trace continuity, no flux through Γ_N

Weak mixed solution

Weak mixed solution: functions $\mathbf{u} = \mathbf{u}_0 + \tilde{\mathbf{u}}$, $\mathbf{u}_0 \in \mathbf{H}_{0,N}(\mathrm{div}, \mathcal{S})$, and $p \in L^2(\mathcal{S})$ such that

$$(\mathbf{K}^{-1}\mathbf{u}_0, \mathbf{v})_{0,\mathcal{S}} - (\nabla \cdot \mathbf{v}, p)_{0,\mathcal{S}} = -\langle \mathbf{v} \cdot \mathbf{n}, p_D \rangle_{\partial\mathcal{S}} + (\nabla \cdot \mathbf{v}, z)_{0,\mathcal{S}}$$

$$-\langle \mathbf{v} \cdot \mathbf{n}, z \rangle_{\partial\mathcal{S}} - (\mathbf{K}^{-1}\tilde{\mathbf{u}}, \mathbf{v})_{0,\mathcal{S}} \qquad \forall\, \mathbf{v} \in \mathbf{H}_{0,N}(\mathrm{div}, \mathcal{S})\,,$$

$$-(\nabla \cdot \mathbf{u}_0, \phi)_{0,\mathcal{S}} = -(q, \phi)_{0,\mathcal{S}} + (\nabla \cdot \tilde{\mathbf{u}}, \phi)_{0,\mathcal{S}} \qquad \forall \phi \in L^2(\mathcal{S})$$

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$$-\langle \mathbf{v} \cdot \mathbf{n}, z \rangle_{\partial\mathcal{S}} - (\mathbf{K}^{-1}\tilde{\mathbf{u}}, \mathbf{v})_{0,\mathcal{S}} \qquad \forall\, \mathbf{v} \in \mathbf{H}_{0,N}(\mathrm{div}, \mathcal{S})\,,$$

$$-(\nabla \cdot \mathbf{u}_0, \phi)_{0,\mathcal{S}} = -(q, \phi)_{0,\mathcal{S}} + (\nabla \cdot \tilde{\mathbf{u}}, \phi)_{0,\mathcal{S}} \qquad \forall \phi \in L^2(\mathcal{S})$$

Theorem (Existence and uniqueness of the weak mixed solution) *There exists a unique weak mixed solution.*

- key ingredient: definition of the function spaces
- the fulfillment of the essential inf–sup condition follows from the existence and uniqueness of the primal weak solution

Mixed FEM, relation to the nonconforming FEM

Basis of the dual space to $\mathrm{RT}_0^0(\mathcal{T}_h)$

- There are $|I_f| - 1$ functionals for each interior edge f.

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Mixed FEM, relation to the nonconforming FEM

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Duality

- There are $|I_f| - 1$ dual basis functions for each interior edge f.

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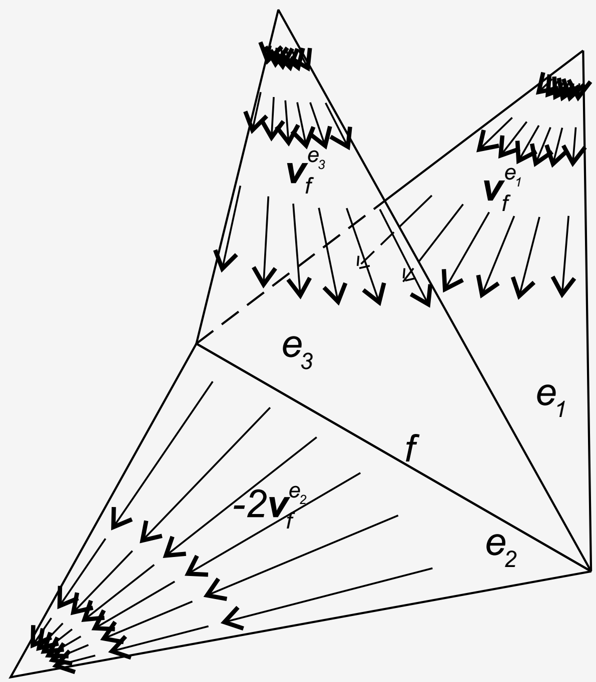

Velocity basis function for $|I_f| = 3$

Mixed FEM, relation to the nonconforming FEM

Basis of the dual space to $\mathrm{RT}^0_0(\mathcal{T}_h)$

- There are $|I_f| - 1$ functionals for each interior edge f.

Duality

- There are $|I_f| - 1$ dual basis functions for each interior edge f.

Theorem (Commuting diagram property)

$$\begin{array}{ccc} \mathbf{H}(\mathrm{grad}, \mathcal{S}) & \xrightarrow{\mathrm{div}} & L^2(\mathcal{S}) \\ \downarrow \pi_h & & \downarrow P_h \\ \mathbf{RT}^0_0(\mathcal{T}_h) & \xrightarrow{\mathrm{div}} & M^0_{-1}(\mathcal{T}_h) \end{array} \quad \Rightarrow$$

Existence and uniqueness of the mixed approximation

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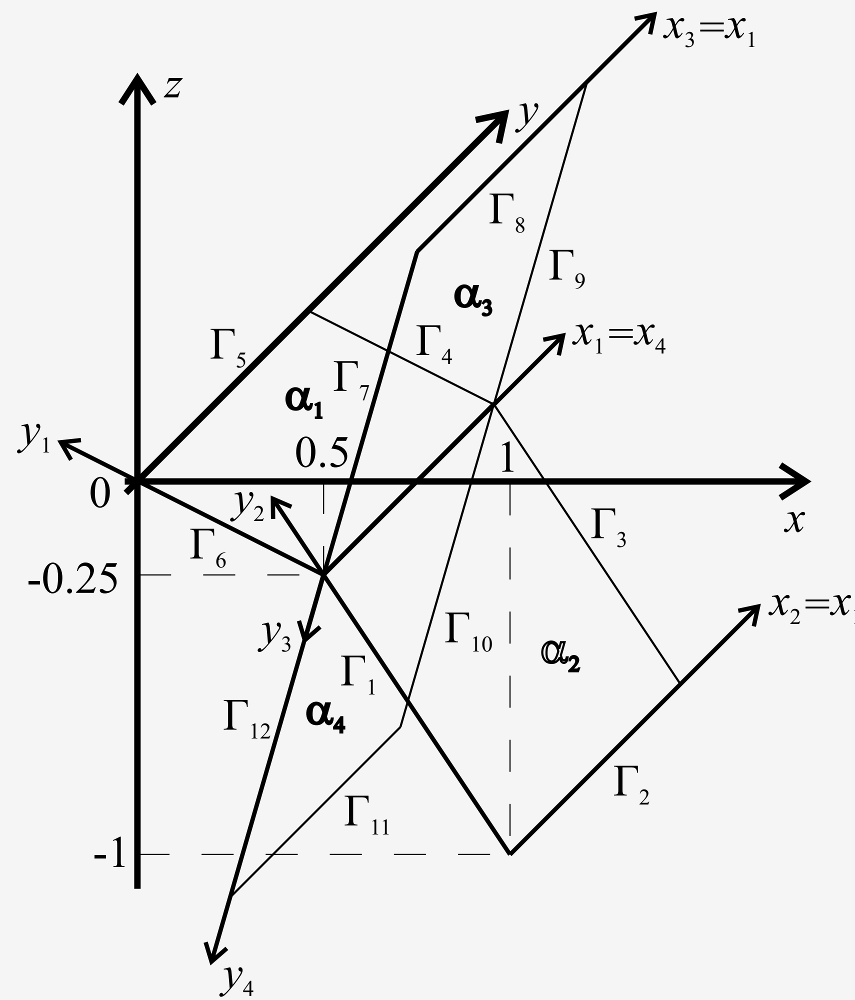
Existence and uniqueness of the mixed approximation

Algebraic reduction of the mixed-hybrid method

- $\mathbf{K}$ pw constant: system matrix, Dirichlet and Neumann BC, and gravity term completely coincide with the nonconforming method
- source term: mixed-hybrid method employs average

Numerical experiment



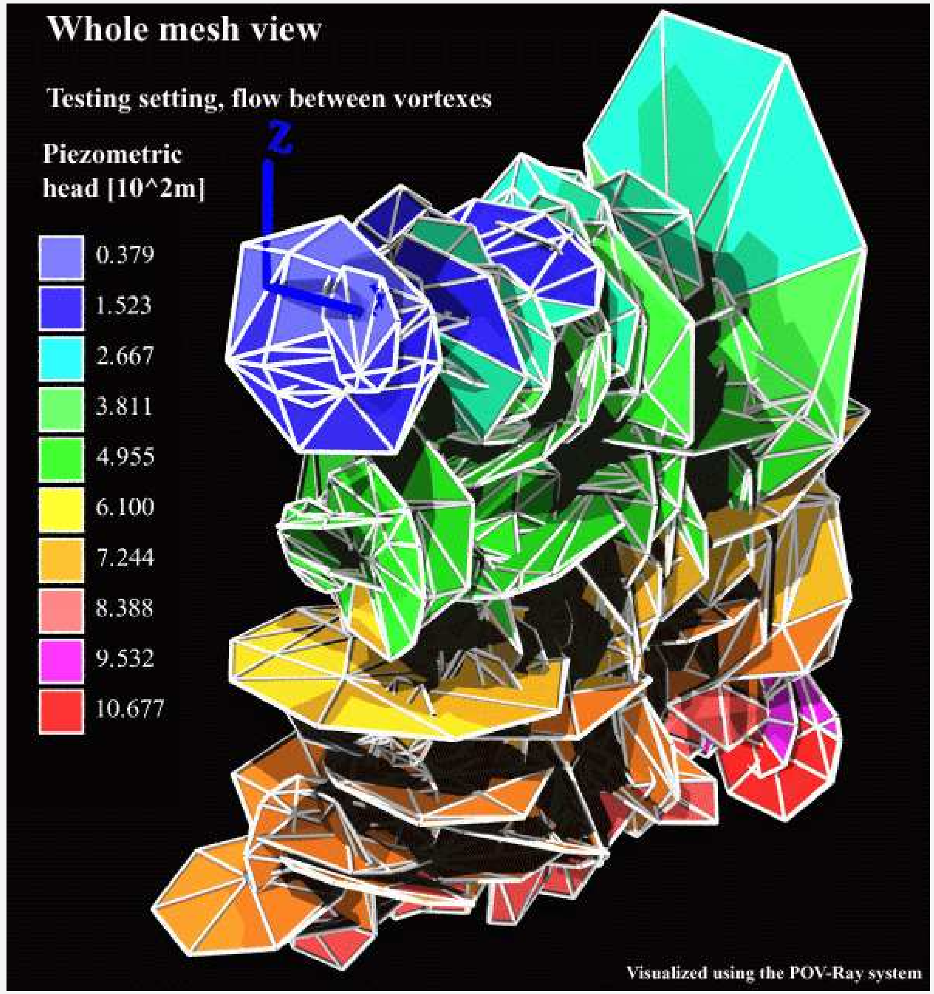
System for a model problem with known solution

Numerical experiment

N	Triangles	$\|p - p_h\|_{0,\mathcal{S}}$	$\|p - \tilde{\lambda}_h\|_{0,\mathcal{S}}$	$\|\mathbf{u} - \mathbf{u}_h\|_{\mathbf{H}(\mathrm{div},\mathcal{S})}$
2	8×4	0.4445	0.1481	1.2247
4	32×4	0.2212	0.0389	0.6263
8	128×4	0.1102	0.0098	0.3150
16	512×4	0.0550	0.0025	0.1577
32	2048×4	0.0275	$6.18 \cdot 10^{-4}$	0.0789
64	8192×4	0.0138	$1.54 \cdot 10^{-4}$	0.0394
128	32768×4	0.0069	$3.87 \cdot 10^{-5}$	0.0197
256	131072×4	0.0034	$9.73 \cdot 10^{-6}$	0.0099

Approximation errors

Fracture flow simulation



Simulation of a nuclear waste repository

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Conclusions and future work

Conclusions

- definition of the mixed finite element method on fracture networks
- relation to the nonconforming method (efficient implementation)

Conclusions and future work

Conclusions

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Future work

- contaminant transport simulation in fracture networks

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Perspectives and future work

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Perspectives and future work

- error estimates for the combined finite volume–finite element schemes
- rigorous study of the combined schemes for nonmatching grids
- analysis of the singularities in the condensation of the mixed finite element method
- extension of the condensation to higher-order schemes
- contaminant transport simulation on fracture networks