

Schémas de volumes finis à stencil réduit pour approcher des problèmes de diffusion

R. Eymard, in collaboration with
L. Agelas and R. Herbin

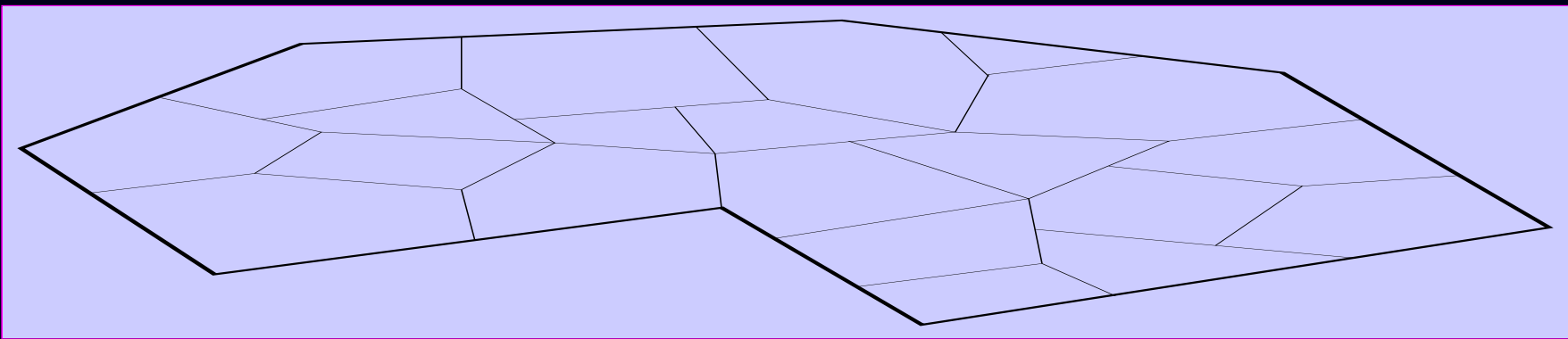
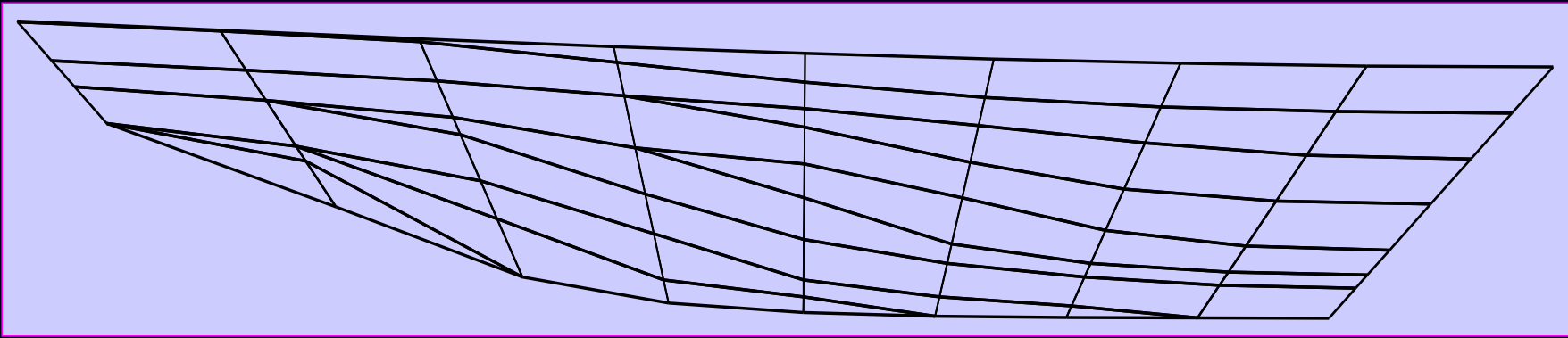
IFP, Paris-Est and Provence universities

Contents

Specifications for the approximation of diffusion terms in industrial codes

Study of one consequence: schemes with reduced stencil

Be valid on 2D and 3D general grids



see 3D benchmark: R. Herbin, F. Hubert

Apply to anisotropic heterogeneous diffusion operators

$$-\operatorname{div}(\Lambda(\boldsymbol{x})\nabla u)$$

examples:

geological data $\Lambda(\boldsymbol{x}) = \lambda_h(\boldsymbol{x}) \boldsymbol{e}_h(\boldsymbol{x}) \otimes \boldsymbol{e}_h(\boldsymbol{x}) + \lambda_v(\boldsymbol{x}) \boldsymbol{e}_v(\boldsymbol{x}) \otimes \boldsymbol{e}_v(\boldsymbol{x})$

diffusion “dispersion” $\Lambda(\boldsymbol{x}) = (\lambda_f + \mu_t|\boldsymbol{v}(\boldsymbol{x})|)\operatorname{Id} + \frac{\mu_l - \mu_t}{|\boldsymbol{v}(\boldsymbol{x})|} \boldsymbol{v}(\boldsymbol{x}) \otimes \boldsymbol{v}(\boldsymbol{x})$

matricial relative permeabilities

Provide conservative fluxes between control volumes

$$F_{KL}(u) + F_{LK}(u) = 0$$

used for transport of species

$$\sum_L w_{KL} F_{KL}(u)$$

examples:

oil engineering

water resources management

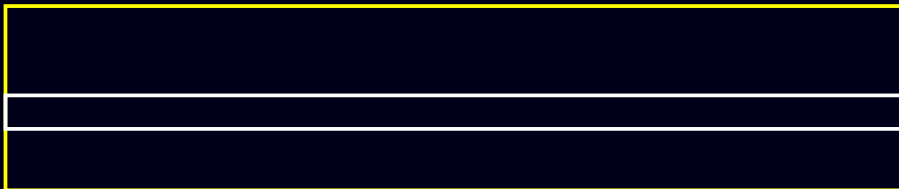
nuclear waste storage simulation

Be exact on coarse mesh with heterogeneous anisotropic diffusion when affine solution

(cf. 2 point flux in 1D problems)

be precise on 2D and 3D meshes with one layer per rock type

with homogeneous control volumes (cf. Vohralik's works)



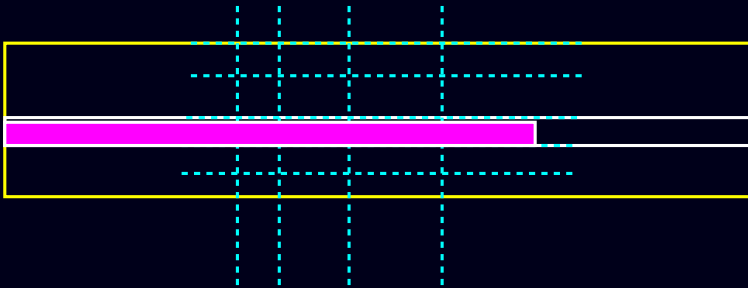
$$\begin{aligned} -\Delta u &= 0 \\ \partial_t w - \operatorname{div}(w \nabla u) &= 0 \end{aligned}$$

Be exact on coarse mesh with heterogeneous anisotropic diffusion when affine solution

(cf. 2 point flux in 1D problems)

be precise on 2D and 3D meshes with one layer per rock type

with homogeneous control volumes (cf. Vohralik's works)



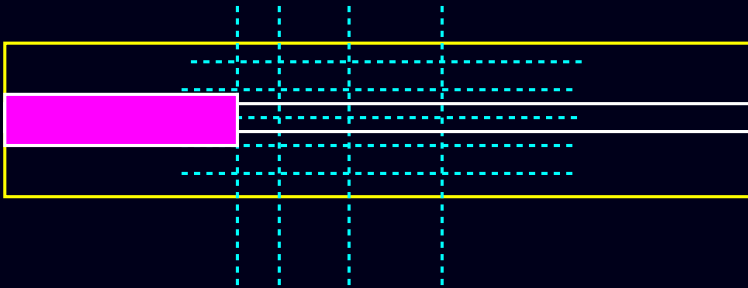
$$\begin{aligned} \sum_L F_{KL}(u) &= 0 \\ |K| \frac{w_K^{n+1} - w_K^n}{\delta t} \\ &+ \sum_L (w_K^n F_{KL}(u)^+ - w_L^n F_{KL}(u)^-) = 0 \end{aligned}$$

Be exact on coarse mesh with heterogeneous anisotropic diffusion when affine solution

(cf. 2 point flux in 1D problems)

be precise on 2D and 3D meshes with one layer per rock type

with homogeneous control volumes (cf. Vohralik's works)



$$\begin{aligned} \sum_L F_{KL}(u) &= 0 \\ |K| \frac{w_K^{n+1} - w_K^n}{\delta t} \\ &+ \sum_L (w_K^n F_{KL}(u)^+ - w_L^n F_{KL}(u)^-) = 0 \end{aligned}$$

Use values $(u_K)_{K \in \mathcal{M}}$ as primary variables

elimination of any $(u_\sigma)_{\sigma \in \mathcal{E}}$

stencil: $\mathcal{M}_K = \{L \in \mathcal{M}, \exists u, F_{KL}(u) \neq 0\}$

for parallel architectures, 9-point in 2D, 27-point in 3D

Ensure convergence properties

$$\sum_L F_{KL}(u) = \int_K f \quad \text{implies} \quad u \text{ converges to continuous solution}$$

resulting from coercivity properties

$$\|u\|_D^2 \leq \alpha \sum_K \sum_L F_{KL}(u)(u_K - u_L)$$

consistency properties

$$\sum_K \sum_L F_{KL}(u)(\varphi_K - \varphi_L) \text{ converges to } \int_{\Omega} \nabla u \cdot \Lambda \nabla \varphi$$

symmetry properties (necessary for “convective nine-point scheme”)

$$\sum_K \sum_L F_{KL}(u)(v_K - v_L) = \sum_K \sum_L F_{KL}(v)(u_K - u_L)$$

Satisfy a local maximum principle

$$\sum_L F_{KL}(u) = 0$$

\Rightarrow

$$\exists \mathcal{M}_K, \min_{L \in \mathcal{M}_K} u_L \leq u_K \leq \max_{L \in \mathcal{M}_K} u_L$$

or less strong properties...

ensured by (non)linear schemes such that

$$F_{KL}(u) = \sum_M T_{KL}^M(u)(u_K - u_M) \text{ with } T_{KL}^M(u) \geq 0$$

cf: Le Potier's works

Review of some linear schemes regarding specifications

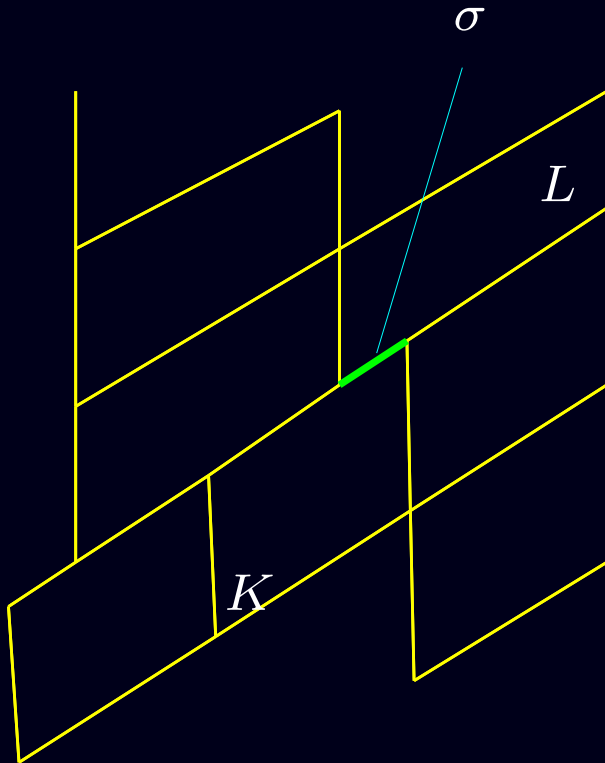
schemes	gen. 2D mesh	gen. 3D mesh	gen. diff. matrix	exact aff. sol.	stencil	coerc. consist. symm.	max.
2-point	N	N	N	Y	Y	Y Y Y	Y
P1 FE	Y/N	Y/N	Y	N	Y	Y Y Y	Y/N
Mix.FE	Y/N	Y/N	Y	Y	N	Y Y Y	N
DG	Y	Y	Y	Y	N	Y Y Y	N
HMM	Y	Y	Y	Y	N	Y Y Y	N
DDFV	Y	Y	Y	Y	N	Y Y Y	N
SUSHI	Y	Y	Y	N/Y	N	Y Y Y	N
MPFA-GEN	Y	Y	Y	Y	Y	N Y N	N
MPFA-REG	N	N	Y	Y	Y	Y Y Y	Y
DIOPTRE	Y	Y/N	Y	Y	Y	Y Y Y	N

no scheme with only "Y"...

Notations for the definition of the schemes

continuous problem: $-\operatorname{div} \Lambda \nabla \bar{u} = f$ in Ω and $\bar{u} = 0$ on $\partial\Omega$

$$\sum_{\sigma \in \mathcal{E}_K} \bar{F}_{K,\sigma}(\bar{u}) = \int_K f(x) dx \text{ with } \bar{F}_{K,\sigma}(\bar{u}) = - \int_{\sigma} \Lambda(x) \nabla \bar{u}(x) \cdot n_{K,\sigma} ds(x)$$



find $u \in X_{\mathcal{D},0}$ s.t. $\sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma}(u) = \int_K f(x) dx$
 and $F_{K,\sigma}(u) + F_{L,\sigma}(u) = 0$ if $\mathcal{M}_\sigma = \{K, L\}$

with

$$X_{\mathcal{D},0} = \{(u_K)_{K \in \mathcal{M}}, (u_\sigma)_{\sigma \in \mathcal{E}}, u_\sigma = 0 \text{ for } \sigma \in \mathcal{E}_{\text{ext}}\}$$

$$\sigma \in \mathcal{E}_{\text{int}} : \mathcal{M}_\sigma = \{K, L\}, \sigma \in \mathcal{E}_{\text{ext}} : \mathcal{M}_\sigma = \{K\}$$

Weak formulation of FV schemes

$$X_{\mathcal{D},0} = \{(u_K)_{K \in \mathcal{M}}, (u_\sigma)_{\sigma \in \mathcal{E}}, u_\sigma = 0 \text{ for } \sigma \in \mathcal{E}_{\text{ext}}\}$$

find $u \in X_{\mathcal{D},0}$ s.t. $\sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma}(u) = \int_K f(x) dx$
and $F_{K,\sigma}(u) + F_{L,\sigma}(u) = 0$ if $\mathcal{M}_\sigma = \{K, L\}$

$$\langle u, v \rangle_{\mathcal{D}} = \sum_{K \in \mathcal{M}} \sum_{\sigma \in \mathcal{E}_K} (v_K - v_\sigma) F_{K,\sigma}(u)$$

$$\Pi_{\mathcal{M}} v(x) = v_K \\ \text{if } x \in K$$

find $u \in X_{\mathcal{D},0}$ s.t.
 $\langle u, v \rangle_{\mathcal{D}} = \int_{\Omega} f(x) \Pi_{\mathcal{M}} v(x) dx, \forall v \in X_{\mathcal{D},0}$

Gradient FV schemes

$$\langle u, v \rangle_{\mathcal{D}} = \sum_{V \in \mathcal{V}} |V| \nabla_V u \cdot \Lambda_V \nabla_V v = \int_{\Omega} \nabla_{\mathcal{D}} u \cdot \Lambda \nabla_{\mathcal{D}} v dx$$

where \mathcal{V} partition of Ω , $V = K$ or particular subset

and $\nabla_{\mathcal{D}} u$, defined by $\nabla_V u = G((u_K), (u_{\sigma}))$ in V , satisfies:

$$\nabla_{\mathcal{D}} P_{\mathcal{D}} \varphi \rightarrow \nabla \varphi \text{ strongly}$$

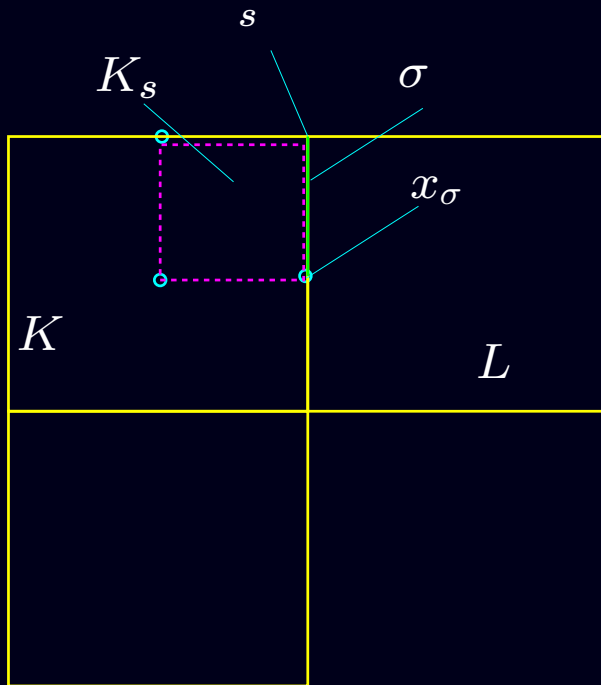
$$\nabla_{\mathcal{D}} u_{\mathcal{D}} \rightarrow \nabla u \text{ weakly if } u_{\mathcal{D}} \rightarrow u \text{ under estimate}$$

sufficient condition for second property:

$$\nabla_V u = \sum_{\epsilon \in \mathcal{E}_V} \frac{|\epsilon|}{|V|} \left(U_{\epsilon}((u_K), (u_{\sigma})) - U_V((u_K), (u_{\sigma})) \right) n_{V,\epsilon} = \sum_{\epsilon \in \mathcal{E}_V} \frac{|\epsilon|}{|V|} U_{\epsilon}((u_K), (u_{\sigma})) n_{V,\epsilon}$$

Multi-Point Flux Approximation on Regular grids

Case of rectangles



$$\mathcal{V} = \{K_s, K \in \mathcal{M}, s \in S_K\}, \quad \mathcal{E} \text{ half-edges}$$

x_σ at center of natural faces

$$\nabla_{K,s} u = \frac{1}{|K_s|} \sum_{\sigma \in \mathcal{E}_{K,s}} |\sigma| (u_\sigma - u_K) n_{K,\sigma}$$

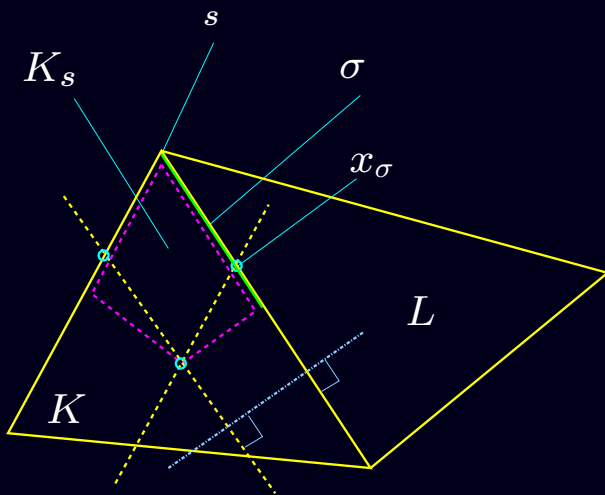
$$\langle u, v \rangle_{\mathcal{D}} = \sum_{K \in \mathcal{M}} \sum_{s \in S_K} |K_s| \nabla_{K,s} u \cdot \Lambda_{K,s} \nabla_{K,s} v$$

gives two-point flux approximation in isotropic cases
elimination of values u_σ by local system for $\sigma \in \mathcal{E}_s$

consistent, coercive, symmetric, nine-point stencil (generalized by MPFA methods)

Multi-Point Flux Approximation on Regular grids

Case of simplices (triangles in 2D, tetrahedra in 3D)



$\mathcal{V} = \{K_s, K \in \mathcal{M}, s \in S_K\}$, \mathcal{E} half-edges

x_σ at 1/3 in 2D

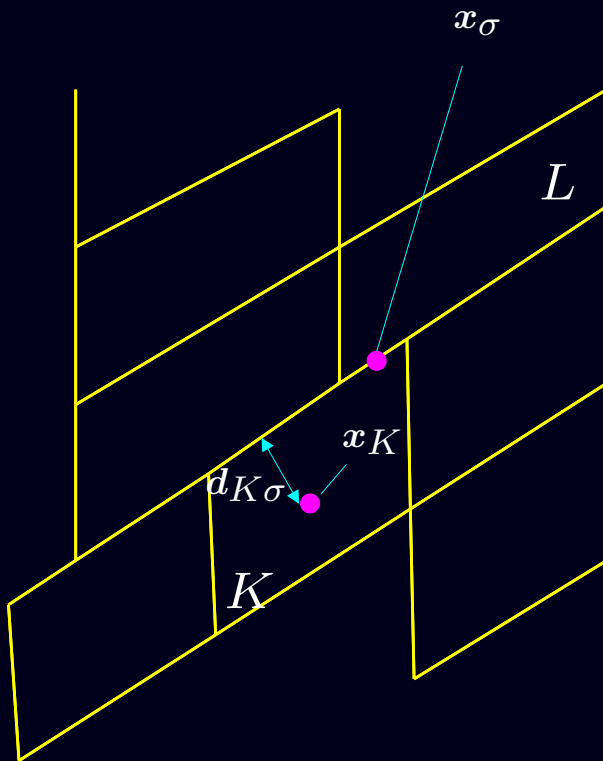
$$\nabla_{K,s} u = \frac{1}{|K_s|} \sum_{\sigma \in \mathcal{E}_{K,s}} |\sigma| (u_\sigma - u_K) n_{K,\sigma}$$

$$\langle u, v \rangle_{\mathcal{D}} = \sum_{K \in \mathcal{M}} \sum_{s \in S_K} |K_s| \nabla_{K,s} u \cdot \Lambda_{K,s} \nabla_{K,s} v$$

elimination of values u_σ by local system for $\sigma \in \mathcal{E}_s$

consistent (remarkable), coercive, symmetric

SUSHI/HMM



$\mathcal{V} = \mathcal{M}$, \mathcal{E} natural edges

$$\nabla_K u = \sum_{\sigma \in \mathcal{E}_K} \frac{|\sigma|}{|K|} (u_\sigma - u_K) n_{K,\sigma}$$

$$(R_K u)_\sigma = \frac{1}{d_{K,\sigma}} (u_\sigma - u_K - \nabla_K u \cdot (x_\sigma - x_K))$$

$$\langle u, v \rangle_{\mathcal{D}} = \sum_{K \in \mathcal{M}} |K| \left(\nabla_K u \cdot \Lambda_K \nabla_K v + (R_K u)^T B_K R_K v \right)$$

where B_K symmetric positive definite matrix with side $\#\mathcal{E}_K$ and bounded eigenvalues
consistent thanks to magical formula

$$\forall G \in \mathbb{R}^d, \forall K \in \mathcal{M}, |K|G = \sum_{\sigma \in \mathcal{E}_K} |\sigma| (x_\sigma - x_K) \cdot G n_{K,\sigma}$$

thm (DEGH2009): HMM coercive consistent symmetric

SUSHI

elimination of selected interfaces unknowns by barycentric averaging

find $u \in X_{\mathcal{B}}$ s.t. $\langle u, v \rangle_{\mathcal{D}} = \int_{\Omega} f(x) \Pi_{\mathcal{M}} v(x) dx, \forall v \in X_{\mathcal{B}}$

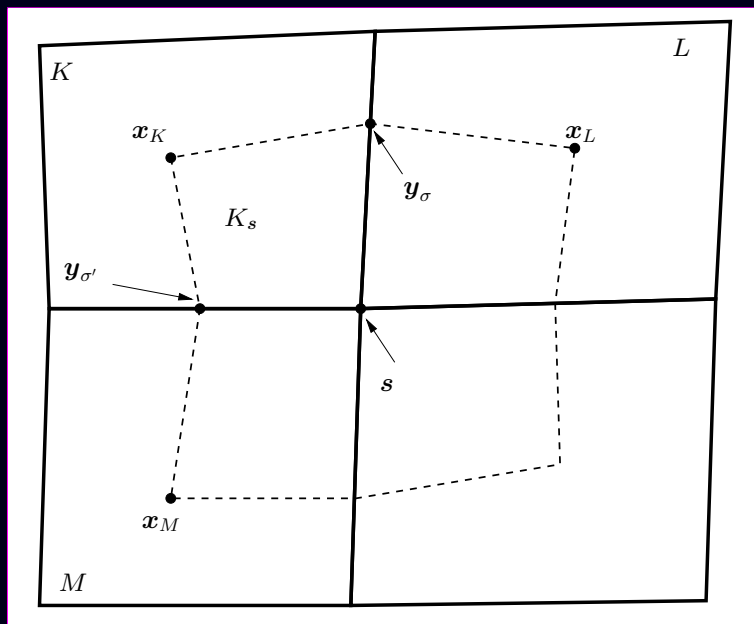
where $X_{\mathcal{B}} = \{u \in X_{\mathcal{D},0}, u_{\sigma} = \sum_K a_{\sigma}^K u_K \text{ for } \sigma \in \mathcal{B}\}$

setting $x_{\sigma} = \sum_K a_{\sigma}^K x_K \text{ for all } \sigma \in \mathcal{B}$

symmetric scheme

DIOP TRE: new scheme inspired by MPFA and SUSHI

Build 9-point scheme on general quadrilateral grid



$$\mathcal{V} = \{K_s, K \in \mathcal{M}, s \in S_K\}$$

values $u_{K,s}^\epsilon$ at centers of edges

$$\epsilon = [x_K, y_{\sigma'}][y_{\sigma'}, s][s, y_\sigma][x_K, y_\sigma]$$

used in
$$|K_s| \nabla_{K,s} u = \sum_{\epsilon \in \mathcal{E}_{K,s}} |\epsilon| (u_{K,s}^\epsilon - u_K) n_{K,s}^\epsilon$$

basic idea:

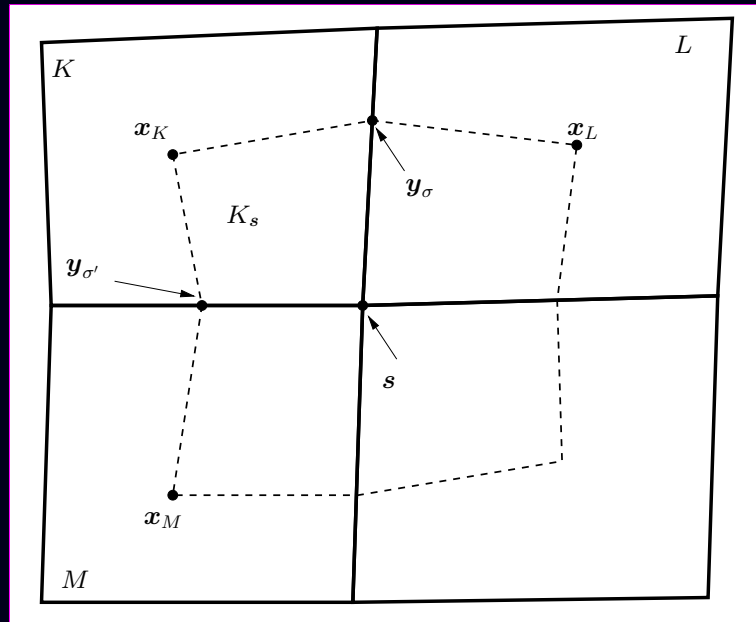
values $u_{K,s}^\epsilon$ for $\epsilon = [y_{\sigma'}, s][s, y_\sigma]$

provided by flux conservation
(as in MPREG and MPFA O-scheme)

values on $u_{K,s}^\epsilon$ for $\epsilon = [x_K, y_{\sigma'}][x_K, y_\sigma]$

provided by averaging expressions

Elimination of interface unknowns



1- MPFA principle

elimination of $u_{K,s}^{\epsilon}$ for $\epsilon = [y_{\sigma'}, s][s, y_{\sigma}]$ provides

$u_{K,s}^{\epsilon}$ lin.comb. of four u_L

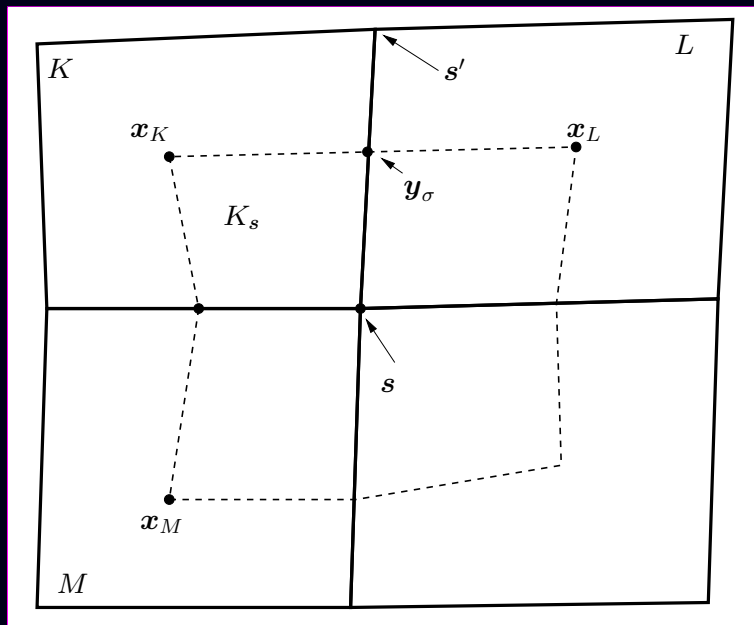
and of eight $u_{K,s}^{\epsilon'}$ for $\epsilon' = [x_K, y_{\sigma}] \dots$

2- Barycentric principle

$$u_{K,s}^{\epsilon'} = \frac{1}{2}(u_K + u_{\sigma})$$

9-point stencil needs $u_{\sigma} = \alpha u_K + (1 - \alpha)u_L \dots$

Averaging on edges



first idea:

$$y_\sigma = [x_K, x_L] \cap [s, s']$$

then barycentric expression

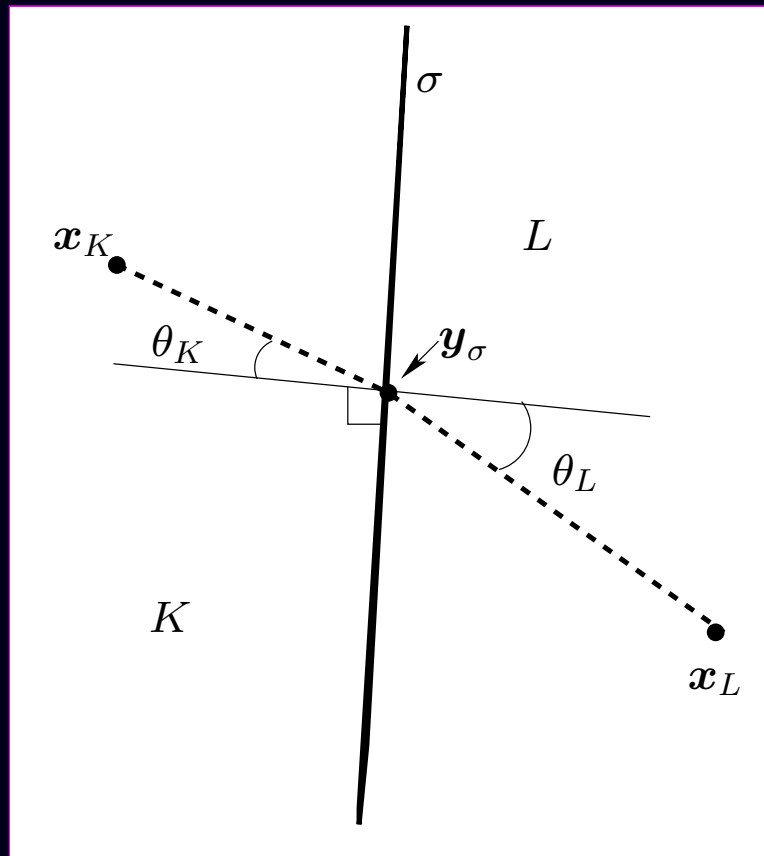
does not respect specification !

second idea:

use “harmonic averaging” instead
of barycentric value...

Need two-point expression in y_σ

A problem which looks like optics...



Problem: find point y_σ

s.t., for all u affine in K and L

continuous at the interface

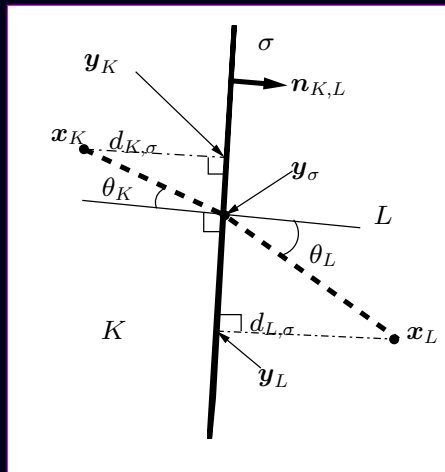
with $\Lambda_K \nabla u|_K \cdot n_{KL} = \Lambda_L \nabla u|_L \cdot n_{KL}$

then $u(y_\sigma)$ given by lin. comb. of $u(x_K)$ and $u(x_L)$

Recall: Snell-Descartes law

$$n_K \sin \theta_K = n_L \sin \theta_L$$

Harmonic averaging points....



$$y_\sigma = \frac{\lambda_L d_{K,\sigma} y_L + \lambda_K d_{L,\sigma} y_K}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}} + \frac{d_{K,\sigma} d_{L,\sigma}}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}} (\lambda_K^\sigma - \lambda_L^\sigma)$$

with

$$\lambda_K = n_{KL} \cdot \Lambda_K n_{KL} \quad \lambda_K^\sigma = (\Lambda_K - \lambda_K \text{Id}) n_{KL}$$

$$\lambda_L = n_{KL} \cdot \Lambda_L n_{KL} \quad \lambda_L^\sigma = (\Lambda_L - \lambda_L \text{Id}) n_{KL}$$

for all continuous function u affine in K and L s.t.

$$\Lambda_K \nabla u|_K \cdot n_{KL} = \Lambda_L \nabla u|_L \cdot n_{KL}$$

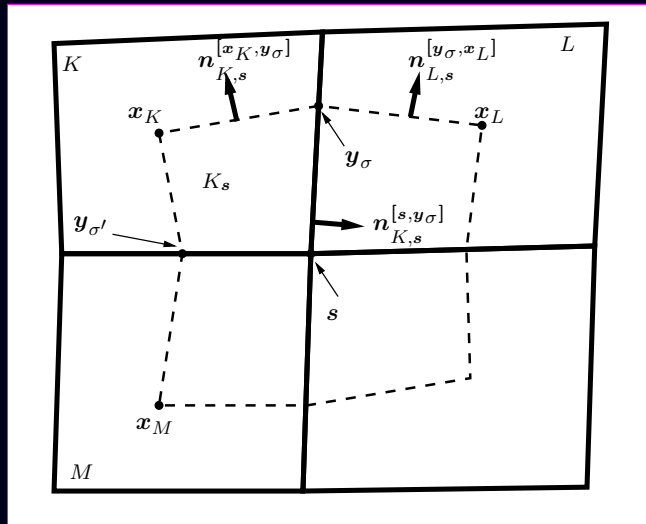
$$u(y_\sigma) = \frac{\lambda_L d_{K,\sigma} u(x_L) + \lambda_K d_{L,\sigma} u(x_K)}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}}$$

Remark:

$$\text{if } \lambda_K^\sigma = \lambda_L^\sigma = 0 \text{ then } \lambda_K \frac{y_K - y_\sigma}{d_{K,\sigma}} = \lambda_L \frac{y_\sigma - y_L}{d_{L,\sigma}} \text{ i.e. } \lambda_K \tan \theta_K = \lambda_L \tan \theta_L$$

... no optics

Resulting construction of $\langle u, v \rangle_{\mathcal{D}}$



$$X_{\mathcal{B}} = \left\{ (u_K)_{K \in \mathcal{M}}, (u_{\sigma})_{\sigma \in \mathcal{E}}, (u_{\sigma,s})_{\sigma \in \mathcal{E}_s, s \in \mathcal{V}} \right. \\ \left. u_{\sigma} \text{ given by harmonic point averaging} \right\}$$

$$u_{K,s}^{\epsilon} = \frac{u_K + u_{\tau}}{2} \text{ if } \epsilon = [x_K, y_{\tau}] \text{ and} \\ u_{K,s}^{\epsilon} = u_{\tau,s} \text{ if } \epsilon = [s, y_{\tau}] \text{ for } \tau = \sigma \text{ and } \sigma'$$

$$|K_s| \nabla_{K,s} u = \sum_{\epsilon \in \mathcal{E}_{K,s}} |\epsilon| (u_{K,s}^{\epsilon} - u_K) n_{K,s}^{\epsilon}$$

$$\langle u, v \rangle_{\mathcal{D}} = \sum_{K \in \mathcal{M}} \sum_{s \in S_K} |K_s| \left(\Lambda_K \nabla_{K,s} u \cdot \nabla_{K,s} v + \sum_{\tau = \sigma, \sigma'} \alpha_{K\tau} R_{K,s}^{\tau} u R_{K,s}^{\tau} v \right)$$

with $\alpha_{K\tau} > 0$, $R_{K,s}^{\tau} u = \frac{1}{d_{K\tau}} (u_{\tau} - u_K - \nabla_{K,s} u \cdot (y_{\tau} - x_K))$, for $\tau = \sigma$ et σ'

properties of scheme: coercive, symmetric, convergent

DIOPTRE: 9-point finite volume scheme

scheme can be expressed by

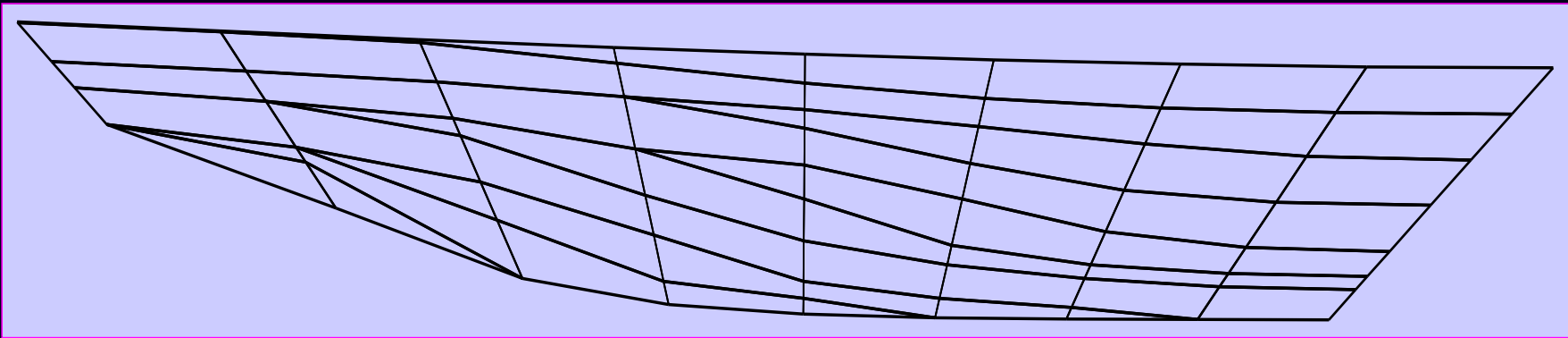
$$\forall K \in \mathcal{M}, \sum_{\substack{\sigma \in \mathcal{E}_K \\ \sigma = K|L}} F_{K,L}(u) + \sum_{\substack{\sigma \in \mathcal{E}_K \\ \sigma \subset \partial\Omega}} F_{K,\sigma}(u) = \int_K f(x) dx$$

where expression of $F_{K,L}(u)$ can be deduced from

$$\langle u, v \rangle_{K,s} = \sum_{\epsilon \in \mathcal{E}_{K,s}} \sum_{\epsilon' \in \mathcal{E}_{K,s}} A_{K,s}^{\epsilon'\epsilon} (u_{K,s}^{\epsilon'} - u_K) (v_{K,s}^{\epsilon} - v_K) = \sum_{\epsilon \in \mathcal{E}_{K,s}} F_{K,s}^{\epsilon}(u) (v_{K,s}^{\epsilon} - v_K)$$

using conservation of fluxes and averaging expressions

Numerical results



$$u(x, y) = \sin(\pi x) \sin(\pi y)$$

	mesh 1	mesh 2	mesh 3	mesh 4	mesh 5
$\#\mathcal{M}$	62	302	1357	5363	21031
# hybrid edges	1	3	6	10	17
L^2 -error	$9.15 \cdot 10^{-3}$	$3.07 \cdot 10^{-3}$	$9.30 \cdot 10^{-4}$	$2.66 \cdot 10^{-4}$	$6.89 \cdot 10^{-5}$

Conclusions

DIOPTRE satisfies a few properties but not easily 3D extension

ideal scheme remains an open problem