

Analysis of the mathematical tools to perform nuclear core reactor simulations

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Outline

- Context
- Low-regularity solutions
- Mixed formulation and error estimates
- Numerical illustrations (with $DD+L^2$ -jumps)
- Concluding remarks

Outline

 *Context*

Context: the model

- Let \mathcal{R} be a domain of \mathbb{R}^d , $d = 1, 2, 3$.
(for practical applications, the domain \mathcal{R} is a rectangular cuboid).

- Goal: solve the *eigenproblem*
Find $(\phi, \lambda) \in (H_0^1(\mathcal{R}) \setminus \{0\}) \times \mathbb{R}$ such that:

$$-\operatorname{div} (D \mathbf{grad} \phi) + \Sigma_a \phi = \lambda \nu \Sigma_f \phi, \text{ in } \mathcal{R}$$

to compute $k_{eff} = 1 / \min_{\lambda} \lambda$.

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- Physical assumptions on the set of parameters:

$$(\text{Param}) \quad \begin{cases} "D > 0", & D, D^{-1} \in \mathbb{L}_{sym}^{\infty}(\mathcal{R}); \\ \Sigma_a, \Sigma_f \geq 0, & \Sigma_a, \Sigma_f \in L^{\infty}(\mathcal{R}), \Sigma_a + \Sigma_f \geq \Sigma_0 > 0; \\ \nu = \nu_0 > 0. \end{cases}$$

→ Σ_f **may vanish** on some regions of \mathcal{R} .

- In *mixed form*: one introduces $\mathbf{p} := -D \mathbf{grad} \phi \in \mathbf{H}(\operatorname{div}, \mathcal{R})$.

Outline

- Context
- *Low-regularity solutions*

Source problem and a priori regularity

- The *source problem* with data $S_f \in L^2(\mathcal{R})$ writes:
Find $(\mathbf{p}, \phi) \in \mathbf{H}(\text{div}, \mathcal{R}) \times H_0^1(\mathcal{R})$ such that:

$$\text{(Source)} \quad \begin{cases} D^{-1} \mathbf{p} + \mathbf{grad} \phi & = 0, & \text{in } \mathcal{R}, \\ \text{div } \mathbf{p} + \Sigma_a \phi & = S_f, & \text{in } \mathcal{R}. \end{cases}$$

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- cf. [Costabel-Dauge-Nicaise'99] and [Bonito-Guermond-Luddens'13].
Proposition Suppose $D \in \mathcal{PW}^{1,\infty}(\mathcal{R})$, $\Sigma_a \in \mathcal{PW}^{1,\infty}(\mathcal{R})$, satisfy (Param).
The problem (Source) is well-posed and moreover there exists $r_{max} \in (0, 1]$, called the *regularity exponent*, such that $\forall S_f \in L^2(\mathcal{R})$, the solution satisfies:

$$(\mathbf{p}, \phi) \in \bigcap_{0 \leq r < r_{max}} \mathcal{PH}^r(\mathcal{R}) \times \bigcap_{0 \leq r < r_{max}} \mathcal{PH}^{1+r}(\mathcal{R}) \quad (r_{max} < 1).$$

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$$(\mathbf{p}, \phi) \in \mathcal{PH}^1(\mathcal{R}) \times \mathcal{PH}^2(\mathcal{R}) \quad (r_{max} = 1).$$

Moreover, the solution depends continuously on the data in the corresponding norms.

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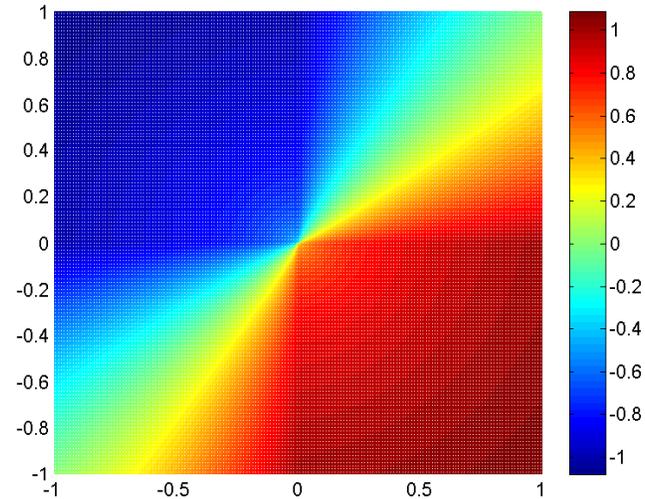
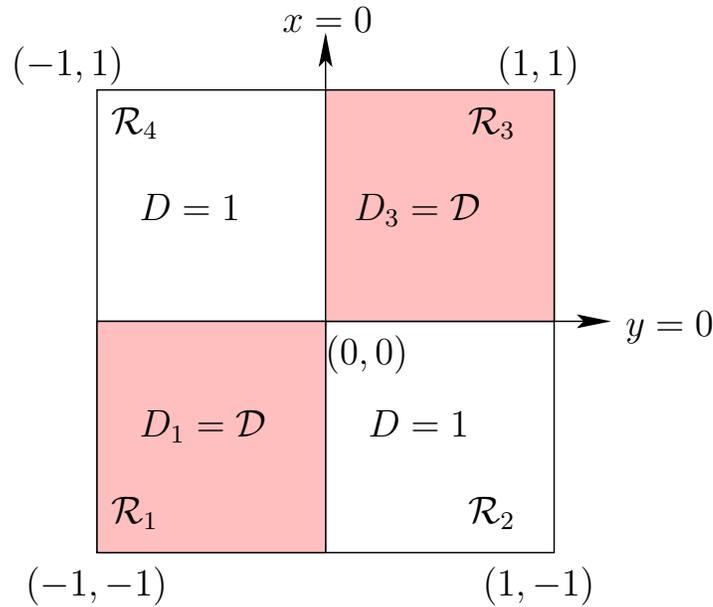
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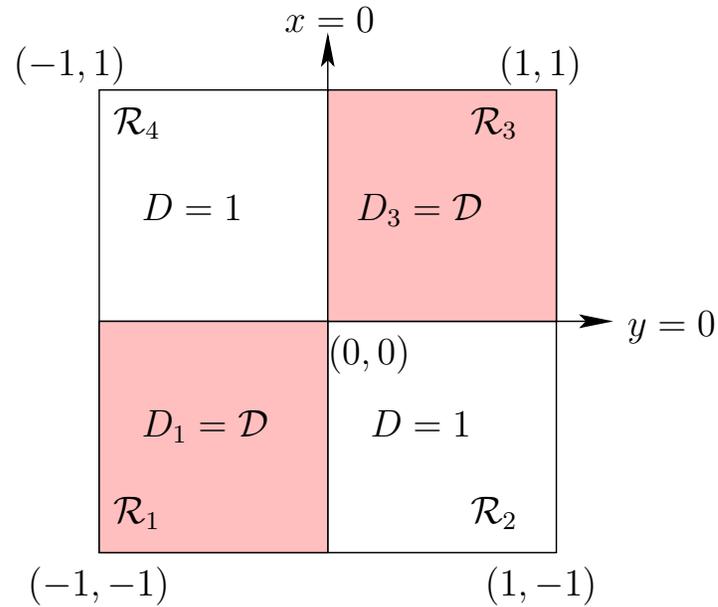
- The *low-regularity case* corresponds to $r_{max} < 1/2$.
→ If $S_f \in \mathcal{PH}^s(\mathcal{R})$ for some $s \in (0, 1]$, then $\text{div } \mathbf{p} \in \mathcal{PH}^s(\mathcal{R})$.

Checkerboard singular solution-1



- Consider the problem:
Find $\phi \in H^1(\mathcal{R}) \mid -\operatorname{div} D \operatorname{grad} \phi = 0 + \text{BC}$.
- A solution in polar coordinates is: $\phi(\rho, \theta) = \rho^\beta (c \cos(\beta\theta) + s \sin(\beta\theta))$, with $\beta = \frac{2}{\pi} \arccos\left(\frac{D-1}{D+1}\right)$, c and s piecewise constant.

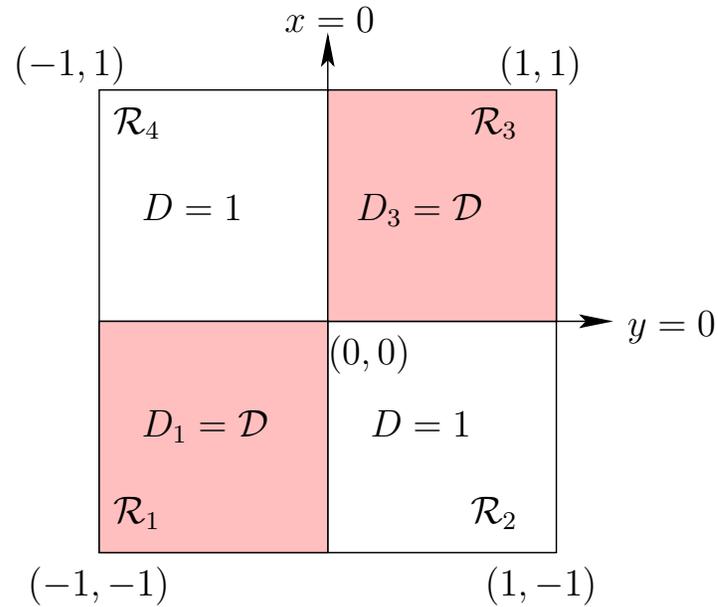
Checkerboard singular solution-2



\mathcal{D}	5	7	10	15	30	100
r_{max}	0.54	0.46	0.39	0.32	0.23	0.13

- One has [Grisvard'92]: $\phi(\rho, \theta) = \rho^\beta (c \cos(\beta\theta) + s \sin(\beta\theta)) \in \mathcal{P}H^{1+\beta-\epsilon}(\mathcal{R})$.
- $\mathbf{p} = -D \mathbf{grad} \phi \in \mathcal{P}H^{\beta-\epsilon}(\mathcal{R})$.

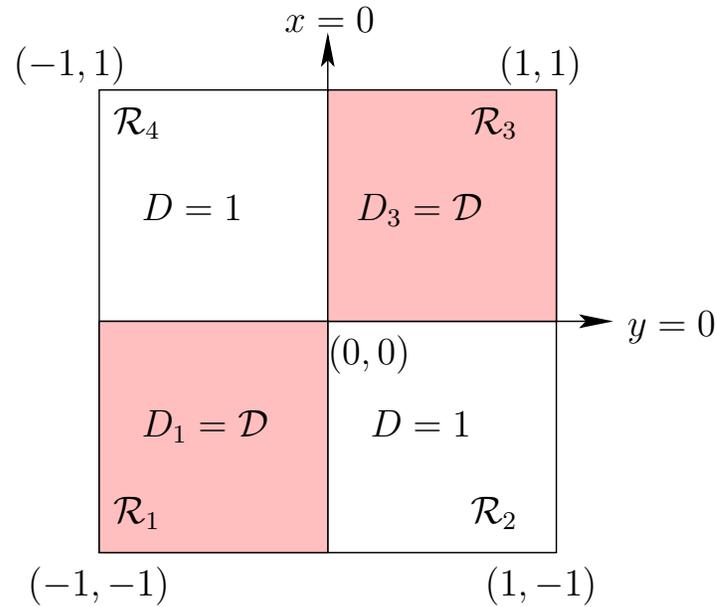
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- The Proposition holds with $r_{max} = \beta$.

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→ The Proposition holds with $r_{max} = \beta$.

● Difficulty (1): in neutronics, one deals with *low-regularity solutions* ($r_{max} < 1/2$).

Eigenproblem and a priori regularity

- The generalized eigenvalue problem, or *eigenproblem*, writes:
Find $(\mathbf{p}, \phi, \lambda) \in \mathbf{H}(\text{div}, \mathcal{R}) \times (H_0^1(\mathcal{R}) \setminus \{0\}) \times \mathbb{R}$ such that:

$$\text{(Eigen)} \quad \begin{cases} D^{-1} \mathbf{p} + \mathbf{grad} \phi & = 0, & \text{in } \mathcal{R}, \\ \text{div } \mathbf{p} + \Sigma_a \phi & = \lambda \nu \Sigma_f \phi, & \text{in } \mathcal{R}. \end{cases}$$

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- In the *low-regularity case* ($r_{max} < 1/2$):

$$\begin{aligned} (\mathbf{p}, \phi) &\in \bigcap_{0 \leq r < r_{max}} \mathcal{P}H^r(\mathcal{R}) \times \bigcap_{0 \leq r < r_{max}} \mathcal{P}H^{1+r}(\mathcal{R}); \\ \text{div } \mathbf{p} &\in \mathcal{P}H^1(\mathcal{R}). \end{aligned}$$

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- Use the mixed setting for eigenvalue problems, cf. [\[Boffi-Brezzi-Gastaldi'97\]](#) or [\[Boffi-Brezzi-Fortin'13\]](#).

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- Study the operator $\phi \mapsto (\nu \Sigma_f)^{-1}(\text{div } \mathbf{p} + \Sigma_a \phi)$ (eigenvalue is λ).

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● Given $S_f (:= \nu \Sigma_f \phi)$, solve the problem (Source): $S_f \mapsto \phi$ (eigenvalue is λ^{-1}) .

Outline

- Context
- Low-regularity solutions
- *Mixed formulation and error estimates*

Variational formulation

- The mixed form of the problem (Source) can be rewritten in $\mathbf{H}(\text{div}, \mathcal{R}) \times L^2(\mathcal{R})$:
Find $(\mathbf{p}, \phi) \in \mathbf{H}(\text{div}, \mathcal{R}) \times L^2(\mathcal{R}) \mid \forall (\mathbf{q}, \psi) \in \mathbf{H}(\text{div}, \mathcal{R}) \times L^2(\mathcal{R})$:

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- Notations: let $\mathbf{X} := \mathbf{H}(\text{div}, \mathcal{R}) \times L^2(\mathcal{R})$. The VF writes:
Find $(\mathbf{p}, \phi) \in \mathbf{X} \mid \forall (\mathbf{q}, \psi) \in \mathbf{X}$:

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- Recall the *Banach-Nečas-Babuška conditions*:

- (inf-sup) $\exists \kappa > 0 \mid \forall (\mathbf{p}, \phi) \in \mathbf{X}, \exists (\mathbf{q}, \psi) \in \mathbf{X}$:

$$|c((\mathbf{p}, \phi), (\mathbf{q}, \psi))| \geq \kappa \|(\mathbf{p}, \phi)\|_{\mathbf{X}} \|(\mathbf{q}, \psi)\|_{\mathbf{X}};$$

- (solv) $\{(\mathbf{q}, \psi) \in \mathbf{X} \mid \forall (\mathbf{p}, \phi) \in \mathbf{X}, c((\mathbf{p}, \phi), (\mathbf{q}, \psi)) = 0\} = \{0\}$.

Theorem $\exists!$ (\mathbf{p}, ϕ) solution with continuous dependence on S_f iff (inf-sup)+(solv) hold.

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Proposition The VF is well-posed and its solution solves (Source).

Error estimates-1

- Introduce $(\mathbf{Q}_h)_h \subset \mathbf{H}(\text{div}, \mathcal{R})$ and $(L_h)_h \subset L^2(\mathcal{R})$ with the *approximability property*:

$$\forall \mathbf{q} \in \mathbf{H}(\text{div}, \mathcal{R}), \lim_{h \rightarrow 0} \left(\inf_{\mathbf{q}_h \in \mathbf{Q}_h} \|\mathbf{q} - \mathbf{q}_h\|_{\mathbf{H}(\text{div}, \mathcal{R})} \right) = 0,$$
$$\forall \psi \in L^2(\mathcal{R}), \lim_{h \rightarrow 0} \left(\inf_{\psi_h \in L_h} \|\psi - \psi_h\|_0 \right) = 0.$$

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- Define $\mathbf{X}_h = \{(\mathbf{q}_h, \psi_h) \in \mathbf{Q}_h \times L_h\}$, endowed with $\|\cdot\|_{\mathbf{X}}$. The discrete VF writes:
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- This is a *conforming discretization*, so one can use Strang's Lemmas if

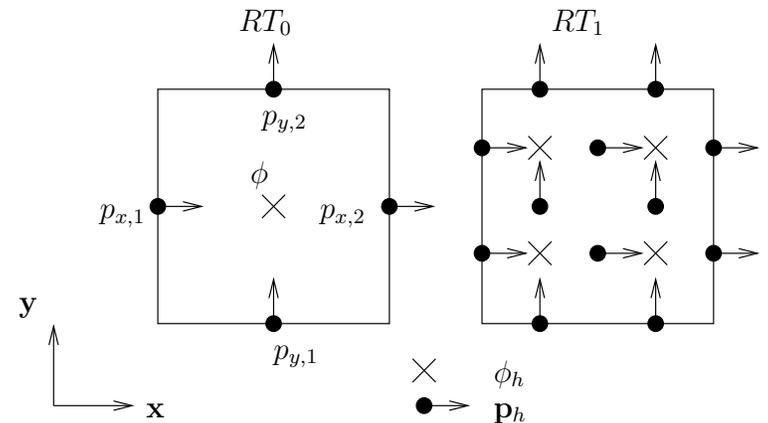
a *discrete inf-sup condition* holds.

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We choose the Raviart-Thomas FE, defined (for instance) on rectangular cuboids. The order of the FE is denoted by m .



Error estimates-2

- *Approximability of low-regularity solutions* ($r_{max} < 1/2$):
 - Let $\mathbf{q} \in \mathbf{H}^r(\mathcal{R})$, such that $\operatorname{div} \mathbf{q} \in H^s(\mathcal{R})$, $0 < r, s < r_{max}$ and $\Pi_{RT} \mathbf{q}$ be its RT interpolant [Bermudez-Gamallo-Nogueiras-Rodriguez'06]:

$$\begin{aligned} \|\mathbf{q} - \Pi_{RT} \mathbf{q}\|_0 &\lesssim h^r |\mathbf{q}|_r + h \|\operatorname{div} \mathbf{q}\|_0, \\ \|\operatorname{div} (\mathbf{q} - \Pi_{RT} \mathbf{q})\|_0 &\lesssim h^s |\operatorname{div} \mathbf{q}|_s. \end{aligned}$$

- Let $\psi \in H^1(\mathcal{R})$ and $\Pi^0 \psi$ be its L^2 -orthogonal projection on piecewise constant functions [Ern-Guermond 04]: $\|\psi - \Pi^0 \psi\|_0 \lesssim h |\psi|_1$.

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- Derive error estimates for the operator $B_s : H^s(\mathcal{R}) \rightarrow H^s(\mathcal{R})$ for $s > 0$.

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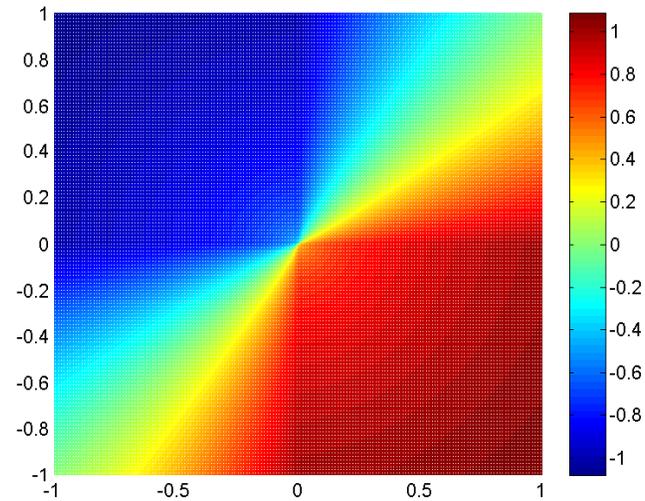
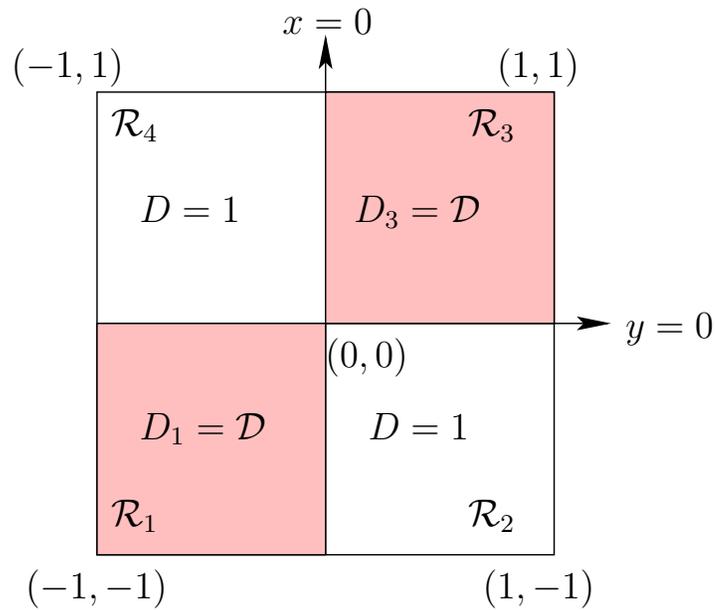
- *Optimal convergence rate.* We follow [Boffi-Gallisti-Gardini-Gastaldi'17].
 - λ is a simple eigenvalue, with $E_\lambda \subset \bigcap_{0 \leq s < \omega_\lambda} \mathcal{P}H^{1+s}(\mathcal{R})$.
 - Let $\omega := \min(\omega_\lambda, m + 1)$ (we use RT finite elements of order m).
 - It holds:

$$|\lambda - \lambda_h| \lesssim h^{2\omega}.$$

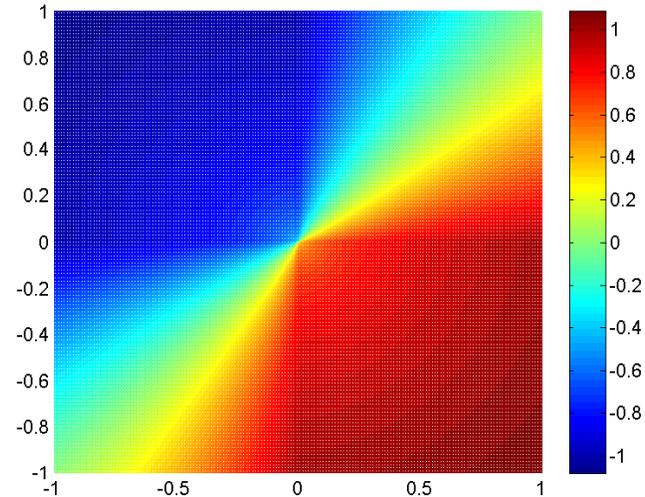
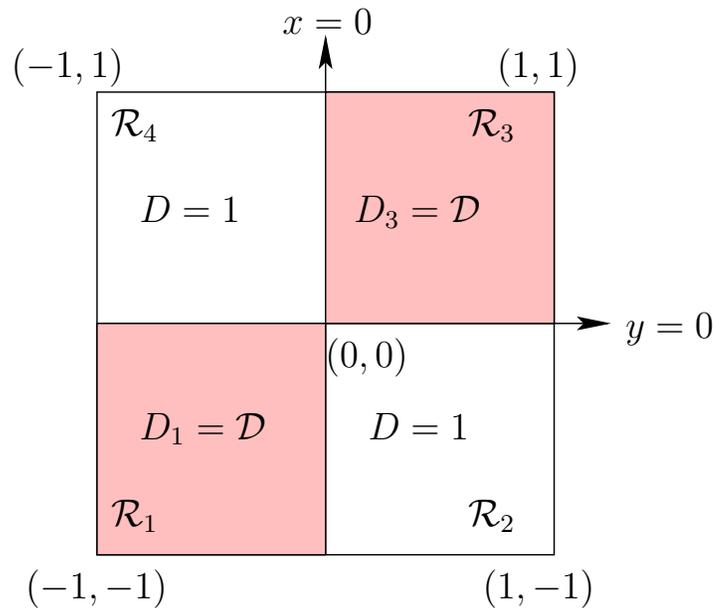
Outline

- Context
- Low-regularity solutions
- Mixed formulation and error estimates
- Numerical illustrations (with $DD+L^2$ -jumps, *à la* [PC-Jamelot-Kpadonou'17])

Numerical results - Source problem



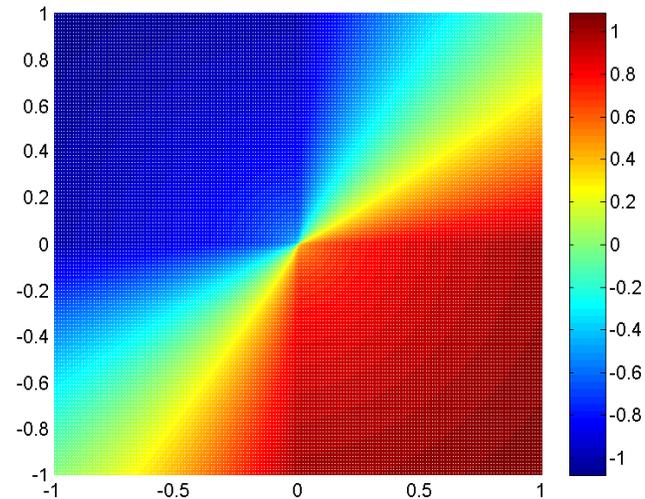
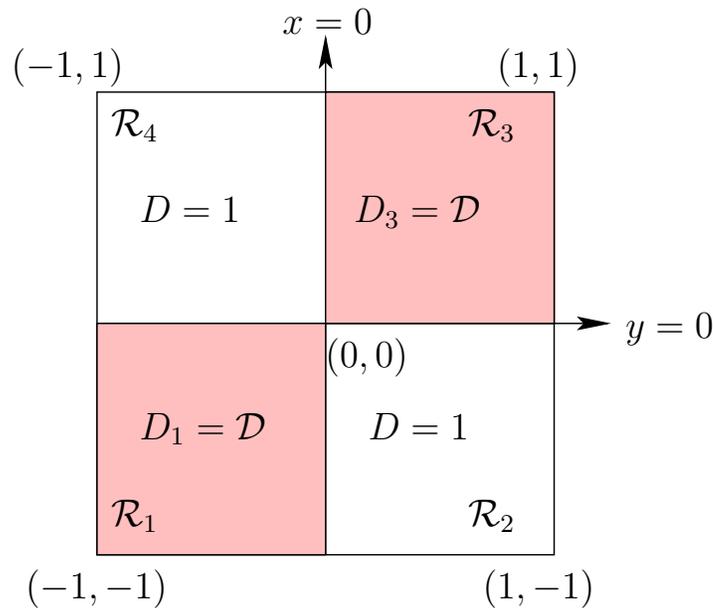
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Nested grids with 4 subdomains, $h_1 = h_3 = 1/2 h$, $h_2 = h_4 = h$:

	$r_{max} = 0.45$ ($\mathcal{D} \approx 7.35$)		$r_{max} = 0.20$ ($\mathcal{D} \approx 39.9$)	
$1/h$	$\ \phi - \phi_h\ _0$	$\ \mathbf{p} - \mathbf{p}_h\ _0$	$\ \phi - \phi_h\ _0$	$\ \mathbf{p} - \mathbf{p}_h\ _0$
25	$5.25 e^{-3}$	$8.92 e^{-2}$	$3.06 e^{-2}$	$4.29 e^{-1}$
50	$2.81 e^{-3}$	$6.49 e^{-2}$	$2.37 e^{-2}$	$3.72 e^{-1}$
100	$1.51 e^{-3}$	$4.73 e^{-2}$	$1.83 e^{-2}$	$3.21 e^{-1}$
rate	$h^{0.90}$	$h^{0.46}$	$h^{0.36}$	$h^{0.21}$

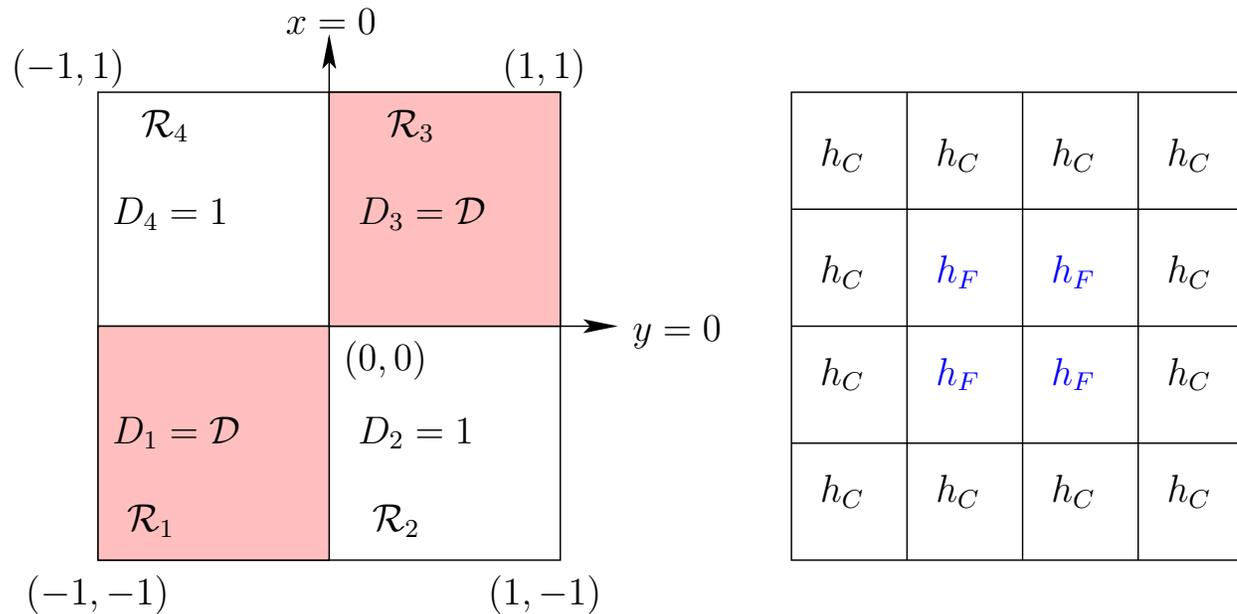
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Non-nested grids with 4 subdomains, $h_1 = h_3 = 2/3 h$, $h_2 = h_4 = h$:

	$r_{max} = 0.45 (\mathcal{D} \approx 7.35)$		$r_{max} = 0.20 (\mathcal{D} \approx 39.9)$	
$1/h$	$\ \phi - \phi_h\ _0$	$\ \mathbf{p} - \mathbf{p}_h\ _0$	$\ \phi - \phi_h\ _0$	$\ \mathbf{p} - \mathbf{p}_h\ _0$
48	$5.11 e^{-3}$	$9.63 e^{-2}$	$3.04 e^{-2}$	$4.39 e^{-1}$
96	$2.71 e^{-3}$	$7.02 e^{-2}$	$2.34 e^{-2}$	$3.80 e^{-1}$
192	$1.44 e^{-3}$	$5.12 e^{-2}$	$1.80 e^{-2}$	$3.29 e^{-1}$
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Numerical results - Eigenproblem



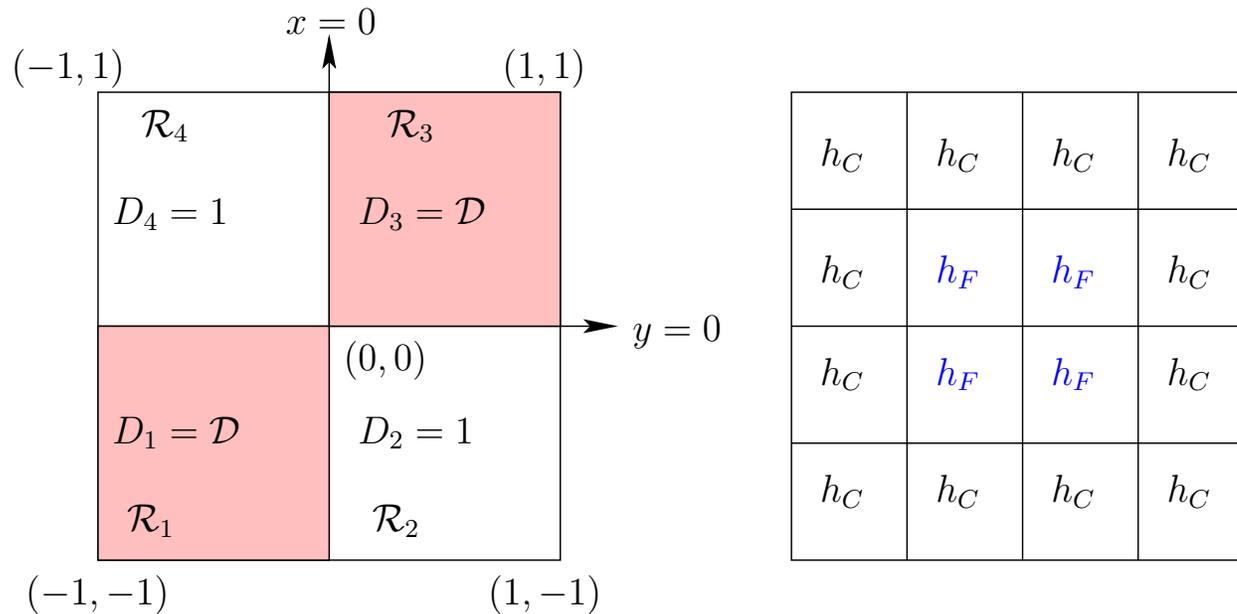
Solve the diffusion equation with *Neumann bc*, $r_{max} \approx 0.39$ ($\mathcal{D} = 0.1$).

Compare the computed eigenvalues to **M. Dauge's benchmark**.

Error on the first eigenvalues, *excluding the first – trivial – one*:

$$\epsilon_{\lambda_i} = \frac{|\lambda_{h,i} - \lambda_i|}{\lambda_i}.$$

Numerical results - Eigenproblem



Nested grids with 16 subdomains, $h_F = 1/2 h$, $h_C = h$ ($r_{max} \approx 0.39$):

$1/h$	ϵ_{λ_1}	ϵ_{λ_2}	ϵ_{λ_3}	ϵ_{λ_4}
8	$8.82e^{-4}$	$2.74e^{-2}$	$1.57e^{-3}$	$5.22e^{-3}$
16	$2.21e^{-4}$	$1.62e^{-2}$	$3.93e^{-4}$	$1.31e^{-3}$
24	$9.83e^{-5}$	$1.19e^{-2}$	$1.75e^{-4}$	$5.05e^{-4}$
rate	h^2	$h^{0.74}$	h^2	h^2

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- *Concluding remarks*

Conclusion/Perspectives

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 - Classical and DD + L^2 -jumps methods OK for low-regularity solutions ; for DD + L^2 -jumps method, crosspoints are allowed [PC-Jamelot-Kpadonou'17].
 - Parallelization OK [PC-Jamelot'13].

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- Extension (3): *post-doc proposal*
 - Computations using numerical homogenization (MS-FEM or HMM).