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

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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:

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

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  to compute $k_{eff} = 1\,/\,\min_\lambda \lambda$.
- Physical assumptions on the set of parameters:

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

$\rightarrow$ Σ_f may vanish on some regions of $\mathcal{R}$.

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

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- Context
- *Low-regularity solutions*

Source problem and a priori regularity

- The *source problem* with data $S_f \in L^2(\mathcal{R})$ writes:
  Find $(\mathbf{p}, \phi) \in \boldsymbol{H}(\mathrm{div}\,, \mathcal{R}) \times H^1_0(\mathcal{R})$ such that:

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

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- cf. [Costabel-Dauge-Nicaise'99] and [Bonito-Guermond-Luddens'13].
  `Proposition` Suppose $D \in \mathcal{P}\mathbb{W}^{1,\infty}(\mathcal{R})$, $\Sigma_a \in \mathcal{P}W^{1,\infty}(\mathcal{R})$, 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:

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

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

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

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$\rightarrow$ If $S_f \in \mathcal{P}H^s(\mathcal{R})$ for some $s \in (0,1]$, then $\mathrm{div}\,\mathbf{p} \in \mathcal{P}H^s(\mathcal{R})$.

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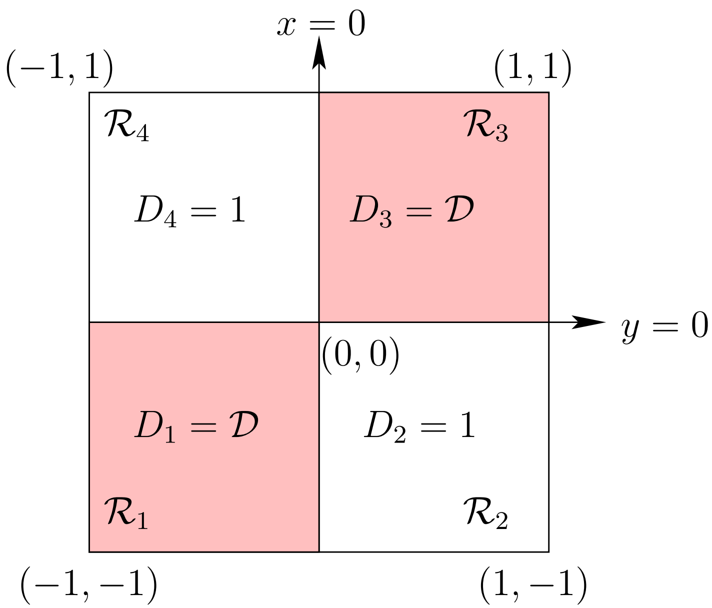
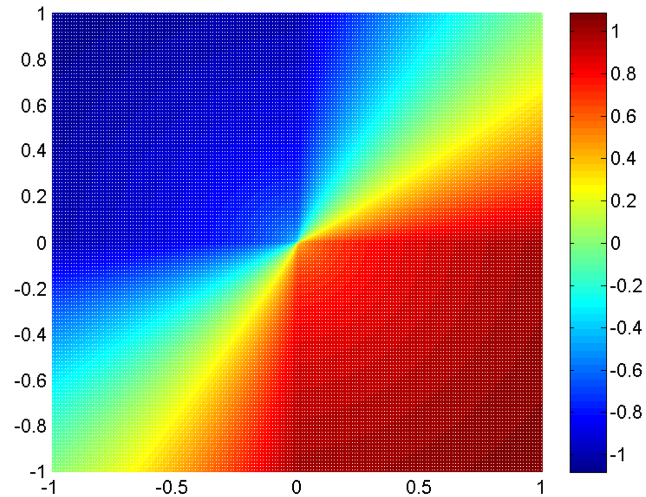
Checkerboard singular solution-1

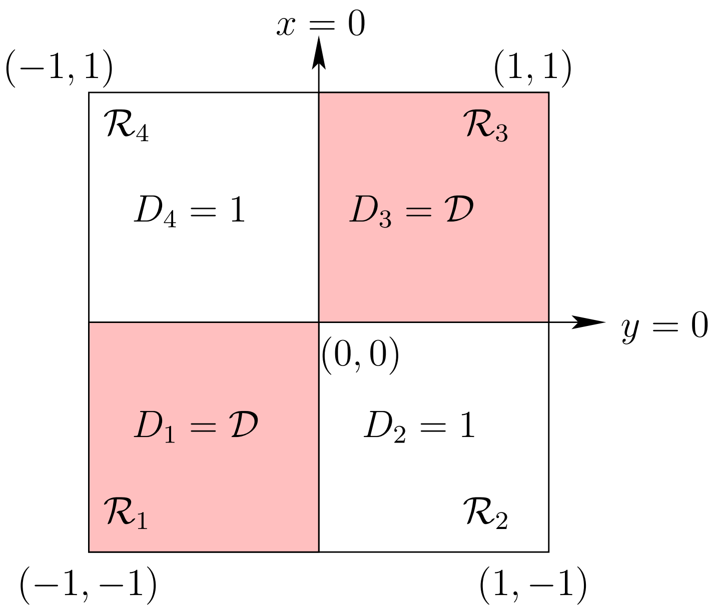




- Consider the "toy" problem:
  Find $\phi \in H^1(\mathcal{R}) \mid -\operatorname{div} D\, \mathbf{grad}\, \phi = 0 +$ BC.

- A solution in polar coordinates is: $\phi(\rho, \theta) = \rho^\beta (c \cos(\beta\theta) + s \sin(\beta\theta))$, with $\beta = \frac{2}{\pi} \arccos\left(\frac{\mathcal{D}-1}{\mathcal{D}+1}\right)$, 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]: $\phi(\rho, \theta) = \rho^{\beta}(c\cos(\beta\theta) + s\sin(\beta\theta)) \in \mathcal{P}H^{1+\beta-\epsilon}(\mathcal{R})$.
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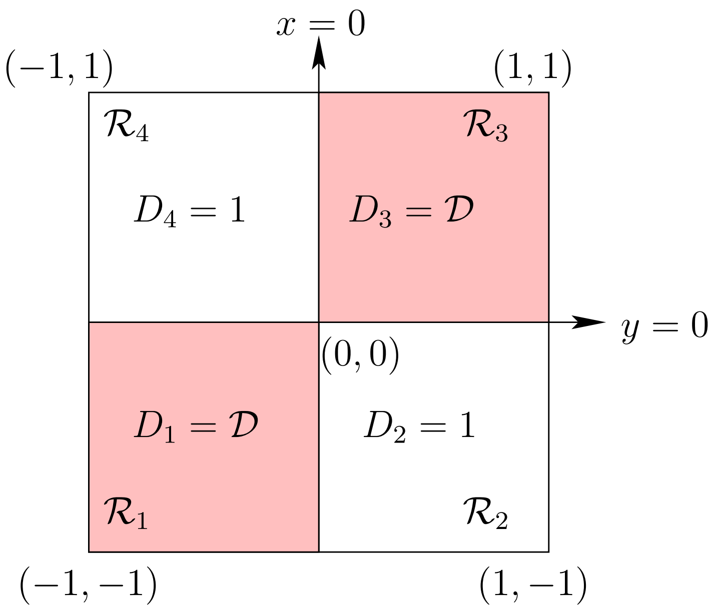

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$\rightarrow$ The Proposition holds with $r_{max} = \beta$.

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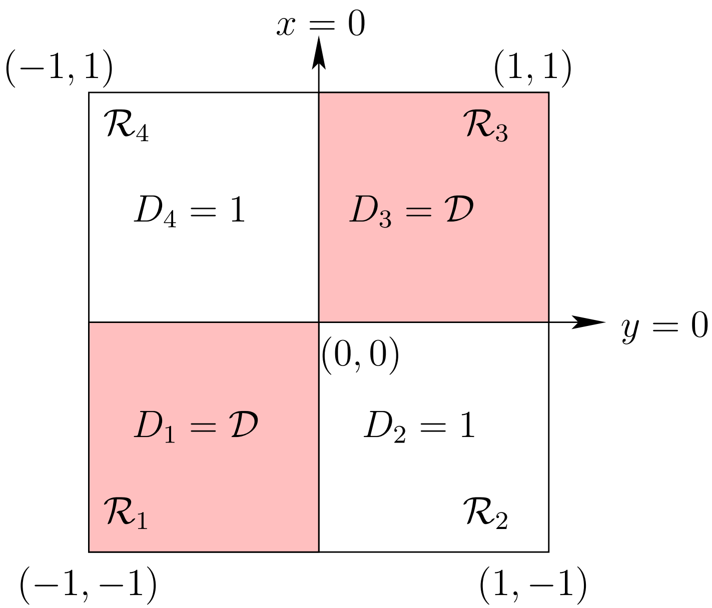

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- Difficulty (1): more generally, one deals with *low-regularity solutions* in neutronics.

Eigenproblem and a priori regularity

- The generalized eigenvalue problem, or *eigenproblem*, writes:
  Find $(\mathbf{p}, \phi, \lambda) \in \boldsymbol{H}(\mathrm{div}\,, \mathcal{R}) \times (H^1_0(\mathcal{R}) \setminus \{0\}) \times \mathbb{R}$ such that:

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\text{(Eigen)} \qquad \left\{ \begin{array}{rcll} D^{-1}\,\mathbf{p} + \mathbf{grad}\,\phi & = & 0, & \text{in } \mathcal{R}, \\ \mathrm{div}\,\mathbf{p} + \Sigma_a\,\phi & = & \lambda\,\nu\Sigma_f\phi, & \text{in } \mathcal{R}. \end{array} \right.
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- In the *low-regularity case* $(r_{max} < 1/2)$:

$$(\mathbf{p},\phi) \in \bigcap_{0\le r<r_{max}} \mathcal{P}\boldsymbol{H}^r(\mathcal{R}) \times \bigcap_{0\le r<r_{max}} \mathcal{P}H^{1+r}(\mathcal{R})\,;$$
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$\rightarrow$ Which abstract tool to study the eigenproblem?

- Use the mixed setting for eigenvalue problems, cf. [Boffi-Brezzi-Gastaldi’97] or [Boffi-Brezzi-Fortin’13].

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- Study the operator $\phi \mapsto (\nu\Sigma_f)^{-1}(\mathrm{div}\,\mathbf{p} + \Sigma_a\,\phi)$ (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}) .

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

Variational formulation

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

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

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- Recall the *Banach-Nečas-Babuška conditions*:
  - (inf-sup) $\exists \kappa > 0 \,|\, \forall (\mathbf{p},\phi) \in \mathbf{X},\ \exists (\mathbf{q},\psi) \in \mathbf{X}$:
    $$|c((\mathbf{p},\phi),(\mathbf{q},\psi))| \geq \kappa ||(\mathbf{p},\phi)||_{\mathbf{X}}\, ||(\mathbf{q},\psi)||_{\mathbf{X}}\,;$$
  - (solv) $\{(\mathbf{q},\psi) \in \mathbf{X} \,|\, \forall (\mathbf{p},\phi) \in \mathbf{X},\ c((\mathbf{p},\phi),(\mathbf{q},\psi)) = 0\} = \{0\}$.

  `Theorem` $\exists!\,(\mathbf{p},\phi)$ 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 $(\mathbf{Q}_h)_h \subset \boldsymbol{H}(\mathrm{div}\,,\mathcal{R})$ and $(L_h)_h \subset L^2(\mathcal{R})$ with the *approximability property*:

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

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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: Find $(\mathbf{p}_h, \phi_h) \in \mathbf{X}_h \,|\, \forall(\mathbf{q}_h, \psi_h) \in \mathbf{X}_h$:

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- This is a *conforming discretization*, so one can use Strang's Lemmas if

$$\boxed{\text{a } \textit{discrete inf-sup condition} \text{ holds}}.$$

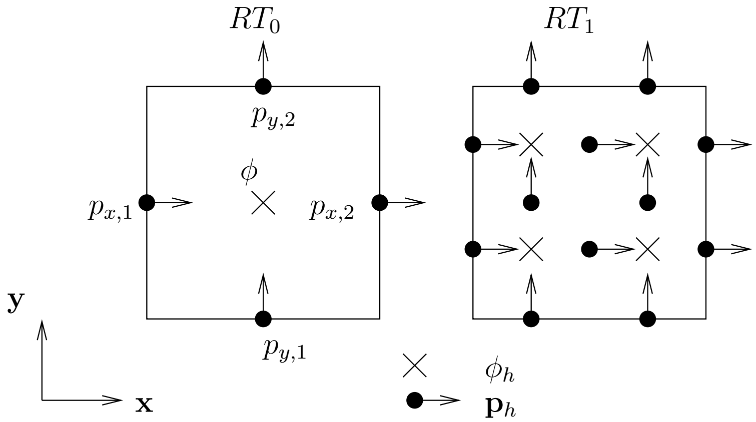
Error estimates-1

- Introduce $(\mathbf{Q}_h)_h \subset \boldsymbol{H}(\mathrm{div}\,, \mathcal{R})$ and $(L_h)_h \subset L^2(\mathcal{R})$ with an *approximability property*. We require that $\mathrm{div}\, \mathbf{Q}_h \subset L_h$, and that L_h includes piecewise constant functions.

- 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: Find $(\mathbf{p}_h, \phi_h) \in \mathbf{X}_h \mid \forall (\mathbf{q}_h, \psi_h) \in \mathbf{X}_h$:

$$c((\mathbf{p}_h, \phi_h), (\mathbf{q}_h, \psi_h)) = \int_{\mathcal{R}} S_f\, \psi_h.$$

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 $\mathbf{q} \in \boldsymbol{H}^r(\mathcal{R})$, 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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→ *Aubin-Nitsche estimate for* $||\phi - \phi_h||_0$*:* no improvement when the solution is *smooth* ; however one can adapt [Falk-Osborn'80] for low-regularity solutions.

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

Error estimates-3

- Theorem [PC-Giret-Jamelot-Kpadonou'17] Let $0 < s < r_{max}$.
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- *Optimal convergence rate*. We follow [Boffi-Gallistl-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])

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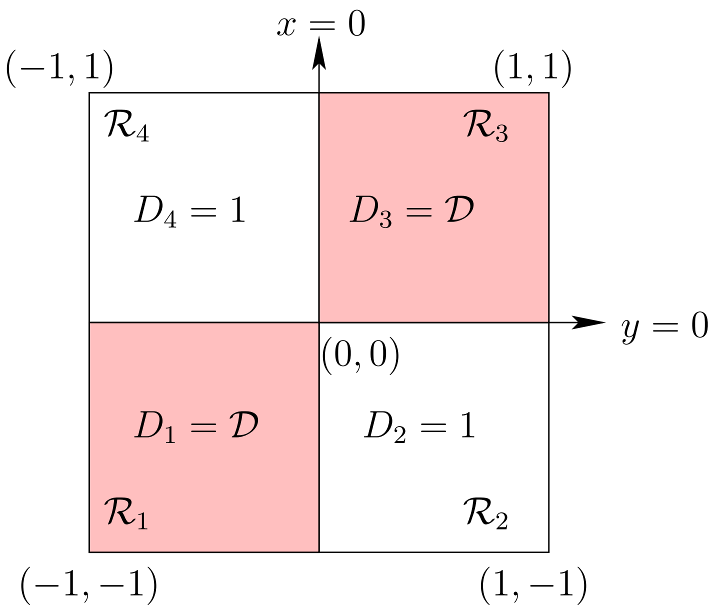
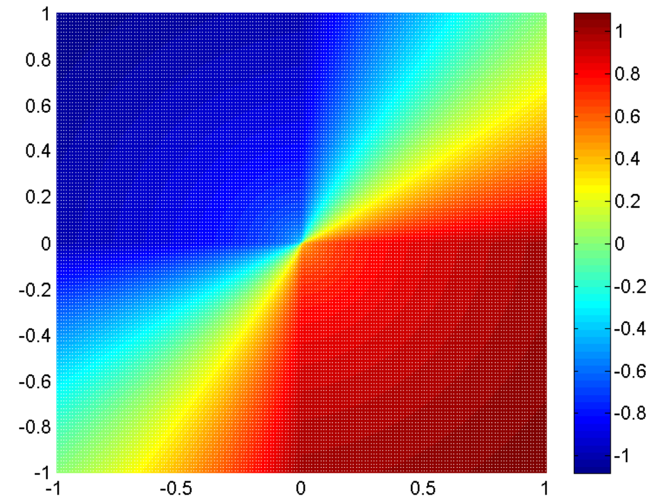
Numerical results - Source problem





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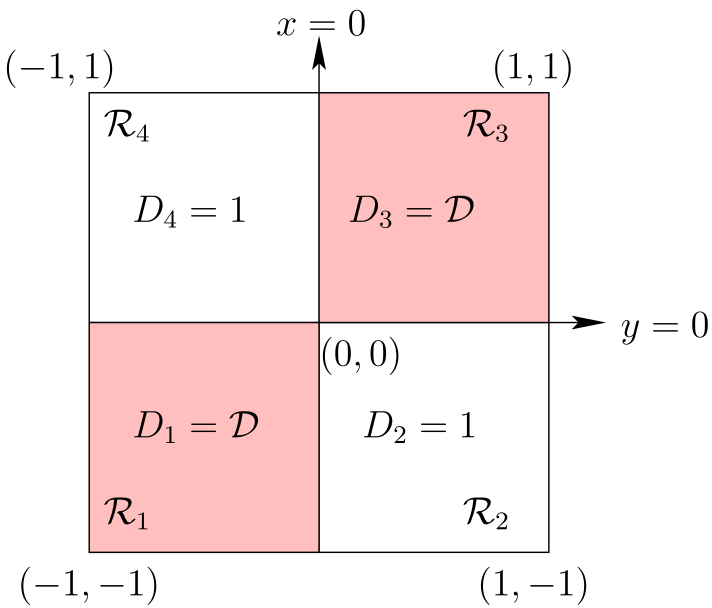

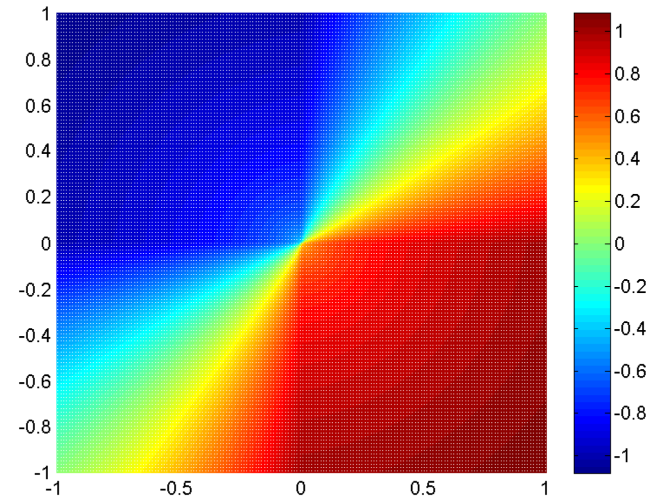

Nested grids with 4 subdomains, $h_1 = h_3 = 1/2\,h$, $h_2 = h_4 = h$:

	$r_{max} = 0.45$ ($\mathcal{D} \approx 7.35$)		$r_{max} = 0.20$ ($\mathcal{D} \approx 39.9$)	
$1/h$	$\|\|\phi - \phi_h\|\|_0$	$\|\|\mathbf{p} - \mathbf{p}_h\|\|_0$	$\|\|\phi - \phi_h\|\|_0$	$\|\|\mathbf{p} - \mathbf{p}_h\|\|_0$
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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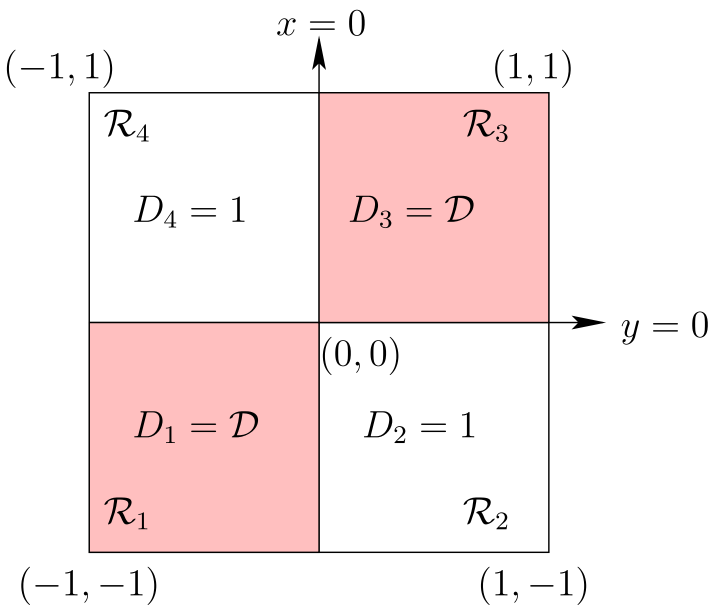
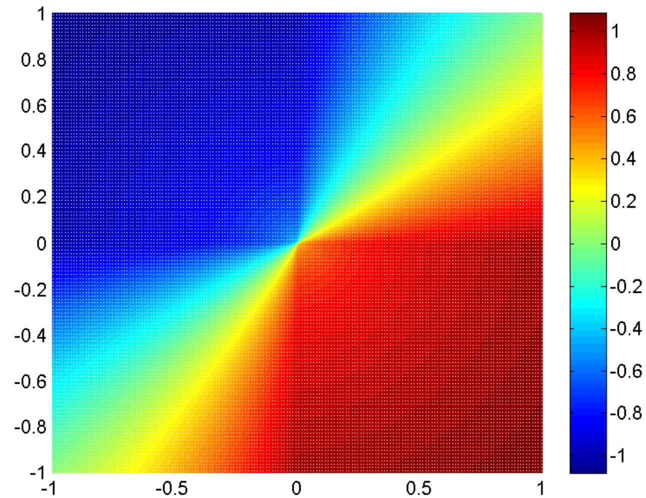
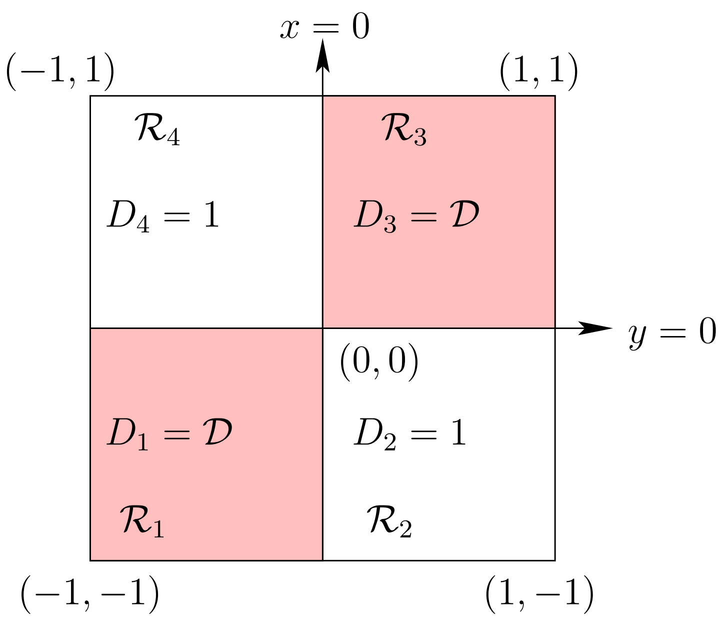




Non-nested grids with 4 subdomains, $h_1 = h_3 = 2/3\,h$, $h_2 = h_4 = h$:

	$r_{max} = 0.45$ ($\mathcal{D} \approx 7.35$)		$r_{max} = 0.20$ ($\mathcal{D} \approx 39.9$)	
$1/h$	$\|\|\phi - \phi_h\|\|_0$	$\|\|\mathbf{p} - \mathbf{p}_h\|\|_0$	$\|\|\phi - \phi_h\|\|_0$	$\|\|\mathbf{p} - \mathbf{p}_h\|\|_0$
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	$1.44\,e^{-3}$	$5.12\,e^{-2}$	$1.80\,e^{-2}$	$3.29\,e^{-1}$
rate	$h^{0.92}$	$h^{0.46}$	$h^{0.38}$	$h^{0.20}$

Numerical results - Eigenproblem

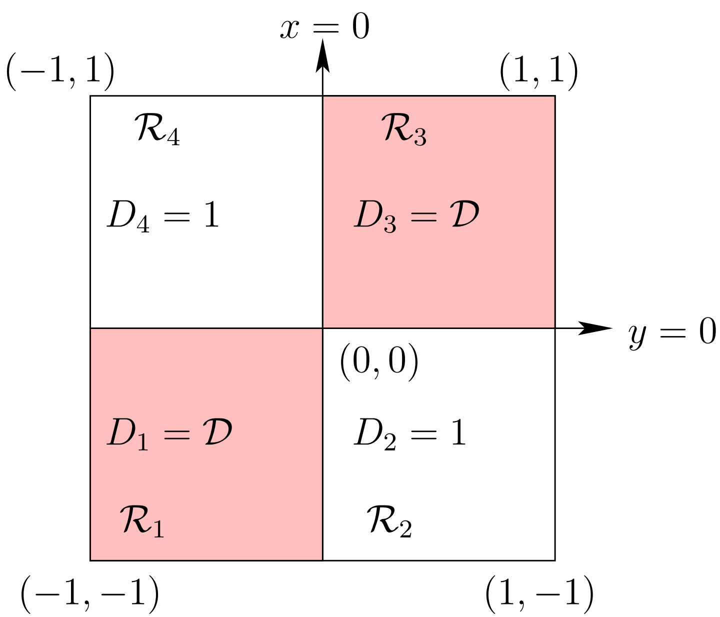


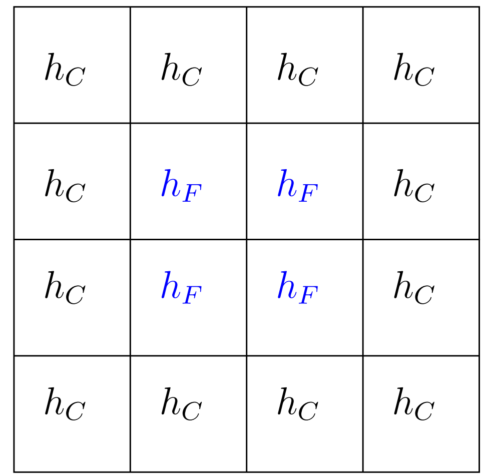
h_C	h_C	h_C	h_C
h_C	h_F	h_F	h_C
h_C	h_F	h_F	h_C
h_C	h_C	h_C	h_C

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

Outline

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- *Concluding remarks*

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Conclusion/Perspectives

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