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# Multiscale method with patches for the propagation of localized uncertainties in (semi-)linear elliptic and parabolic equations

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joint work with Mathilde Chevreuil<sup>2</sup> and Anthony Nouy<sup>2</sup>

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LMSSC Seminar, June 30, 2017, Conservatoire National des Arts et Métiers  
(CNAM), Paris, France



# Context

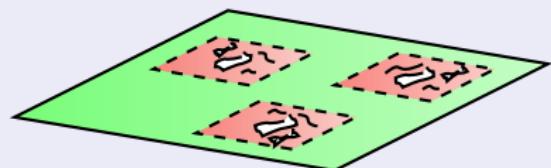
## Uncertainty quantification

- Linear transient model problem

$$c\dot{u} - \nabla \cdot B(u, \nabla u) + C(u, \nabla u) = f \quad \text{on } \Omega$$

with given initial conditions in  $\Omega$  and boundary conditions on  $\partial\Omega$ , and where  $\dot{u} = \frac{\partial u}{\partial t}$

Localized uncertainties  
and non-linearities



- Input variabilities

- Source term  $f$
- Evolution coefficient  $c$  and operators  $B, C$
- Geometrical domain  $\Omega$  and boundary  $\partial\Omega$

- Parametric modeling of uncertainties

- Finite set of random variables  $\xi = (\xi_1, \dots, \xi_m)$
- Finite dimensional probability space  $(\Xi, \mathcal{B}(\Xi), \mu)$  with  $\Xi \subset \mathbb{R}^m$

## Goal

- Propagate the uncertainties through the transient model

$$c(\xi)\dot{u}(\xi) - \nabla \cdot B(u(\xi), \nabla u(\xi); \xi) + C(u(\xi), \nabla u(\xi); \xi) = f(\xi) \quad \text{on } \Omega(\xi)$$

# Context

## Stochastic spectral methods: Functional representation of random variables

- Functional expansion of the solution

$$u(\xi) \approx \sum_{\alpha \in \mathcal{A}} u_\alpha \psi_\alpha(\xi) \in L_\mu^p(\Xi; \mathcal{V})$$

- Stochastic approximation space

- Continuous (generalized) polynomial chaos basis [Ghanem 1999; Ghanem and Spanos 1991; Soize and Ghanem 2004; Xiu and Karniadakis 2002]
- Lagrange interpolation (or collocation) polynomial basis [Babuška, Nobile, and Tempone 2007; Xiu and Hesthaven 2005]
- Piecewise polynomial basis (stochastic finite elements [Babuška, Tempone, and Zouraris 2004, 2005; Deb, Babuška, and Oden 2001; Wan and Karniadakis 2005], multi-wavelets [Le Maître et al. 2004a,b])

## Advantages

- Explicit and accurate prediction of the solution in terms of the random variables
- Quick post-processing / Fast evaluation of quantities of interest
  - Statistical moments
  - Probability of events
  - Quantiles
  - Confidence regions
  - Sensitivity indices
  - ...

# Motivation

Multiscale problems with localized uncertainties on a subdomain called a patch

- Uncertain operators on local subdomains

$$c(\cdot; \xi) = \begin{cases} c(\cdot) & \text{on } \Omega \setminus \Lambda \quad (\text{deterministic}) \\ c(\cdot; \xi) & \text{on } \Lambda(\xi) \quad (\text{uncertain}) \end{cases}$$

$$B(\cdot; \xi) = \begin{cases} B(\cdot) & \text{on } \Omega \setminus \Lambda \\ B(\cdot; \xi) & \text{on } \Lambda(\xi) \end{cases}$$

$$C(\cdot; \xi) = \begin{cases} C(\cdot) & \text{on } \Omega \setminus \Lambda \\ C(\cdot; \xi) & \text{on } \Lambda(\xi) \end{cases}$$

- Dedicated strategy to handle high dimensionality and complexity

## Challenges

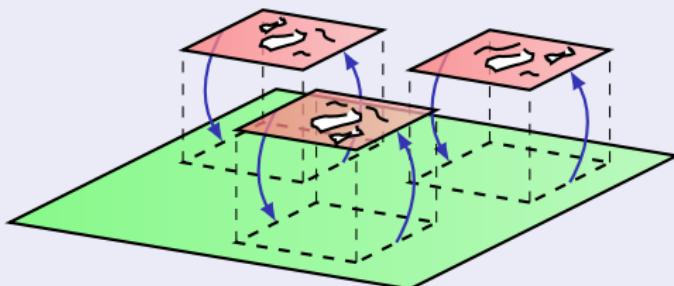
- Develop a multiscale method that exploits the localized side of uncertainties
  - Simple global problem  
→ Traditional solvers / Commercial software packages available in the industry
  - More technical local problems  
→ Specific solvers / In-house research codes

# Motivation

## Multiscale domain decomposition method with patches

- Multiscale method inspired from the Semi-Schwarz-Lagrange method [Chevreuil, Nouy, and Safatly 2013; Gendre, Allix, and Gosselet 2011; Gendre et al. 2009; Hager et al. 2012; Lozinski 2010] that belongs to the class of global-local iterative methods [Whitcomb 1991]

“Numerical zooms”



## Main ingredient - Separation of global and local problems

- Possible refined local solutions with better approximation properties
- Simple global problems
  - Linear
  - No geometrical variabilities
  - Deterministic operator
- Appropriate approximation spaces and solvers to solve efficiently both problems

# Outline

- 1 Context and motivation
- 2 Multiscale domain decomposition method
- 3 Computational aspects
- 4 Numerical illustrations
- 5 Conclusions and outlooks

# Outline

1 Context and motivation

2 Multiscale domain decomposition method

- Global-local formulation with patches
- Global-local iterative algorithm

3 Computational aspects

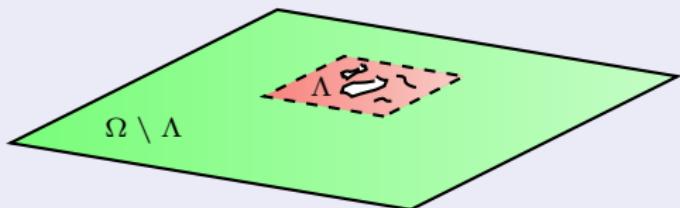
4 Numerical illustrations

5 Conclusions and outlooks

# Initial formulation

Domain featuring localized uncertainties and possible non-linearities

- Partition of **random** domain  $\Omega(\xi)$  into **random** patch  $\Lambda(\xi)$  and **deterministic** complementary subdomain  $\Omega \setminus \Lambda$



Transient linear advection-diffusion-reaction stochastic problem - Formulation

Model problem with **random** material parameters and source terms

$$\begin{cases} c\dot{u} - \nabla \cdot (K\nabla u) + \alpha \cdot \nabla u + Ru = f & \text{on } (\Omega \setminus \Lambda) \times I \\ c(\xi)\dot{u} - \nabla \cdot (K(\xi)\nabla u) + \alpha(\xi) \cdot \nabla u + R(\xi)u = f(\xi) & \text{on } \Lambda(\xi) \times I \end{cases}$$

with possibly **random** boundary and initial conditions

$$\begin{cases} u = 0 & \text{on } \Gamma_D \times I \\ K\nabla u \cdot n = g & \text{on } (\Gamma_N \setminus \Gamma_N^\Lambda) \times I \text{ and } \\ K(\xi)\nabla u \cdot n = g(\xi) & \text{on } \Gamma_N^\Lambda(\xi) \times I \end{cases}$$

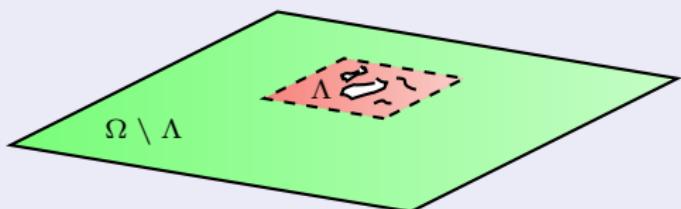
$$\begin{cases} u = u_0 & \text{on } (\Omega \setminus \Lambda) \times \{0\} \\ u = u_0(\xi) & \text{on } \Lambda(\xi) \times \{0\} \end{cases}$$

where  $\dot{u} = \frac{\partial u}{\partial t}$ .

# Initial formulation

Domain featuring localized uncertainties and possible non-linearities

- Partition of **random** domain  $\Omega(\xi)$  into **random** patch  $\Lambda(\xi)$  and **deterministic** complementary subdomain  $\Omega \setminus \Lambda$



Transient linear advection-diffusion-reaction stochastic problem - Space weak formulation

Find  $u \in \mathcal{V}^\Xi$  such that it holds almost surely

$$\begin{aligned} m_\Omega(\dot{u}(\xi), \delta u; \xi) + a_\Omega(u(\xi), \delta u; \xi) &= l_\Omega(\delta u; \xi) \quad \forall \delta u \in \mathcal{V} \\ u|_{t=0^+}(\xi) &= u_0(\xi) \end{aligned}$$

with **bilinear** forms  $a_\Omega(u, v; \xi) = \int_\Omega K(\xi) \nabla u \cdot \nabla v + \int_\Omega \alpha(\xi) \cdot \nabla u v + \int_\Omega R(\xi) u v$ ,  
 $m_\Omega(u, v; \xi) = \int_\Omega c(\xi) u v$  and **linear** form  $l_\Omega(v; \xi) = \int_\Omega f(\xi) v + \int_{\Gamma_N} g(\xi) v$ .

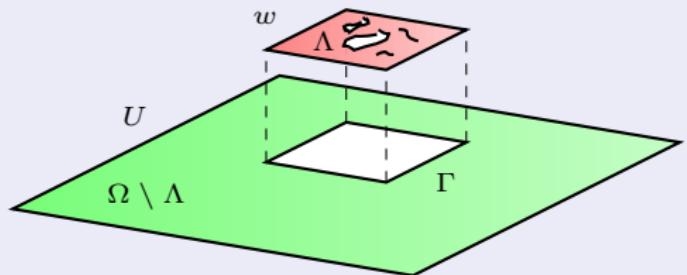
# Global-local formulation with patches

## Domain decomposition - Introduction of a patch

- Separation of the solution

$$u = \begin{cases} U & \text{on } \Omega \setminus \Lambda \\ w & \text{on } \Lambda \end{cases}$$

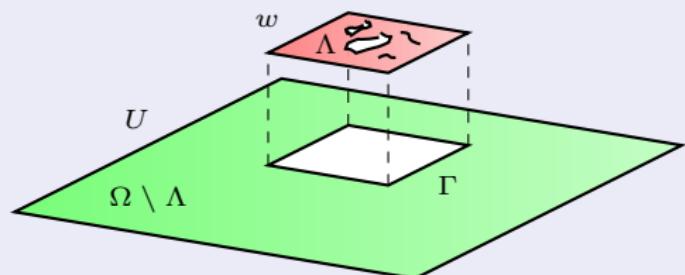
with  $U = w$  on  $\Gamma$  (weak sense)



# Global-local formulation with patches

## Domain decomposition - Introduction of a patch

- **Uncertain** domain  $\Omega$
- **Deterministic** subdomain  $\Omega \setminus \Lambda$
- **Uncertain** patch  $\Lambda$
- **Deterministic** interface  $\Gamma$



## Reformulation using Lagrange multiplier

Find  $(U, w, \lambda) \in \mathcal{U}^\Xi \times \mathcal{W}^\Xi \times \mathcal{M}^\Xi$  such that it holds almost surely

- **Global** equation on subdomain  $\Omega \setminus \Lambda$

$$m_{\Omega \setminus \Lambda}(\dot{U}(\xi), \delta U) + a_{\Omega \setminus \Lambda}(U(\xi), \delta U) + b_\Gamma(\lambda(\xi), \delta U) = \ell_{\Omega \setminus \Lambda}(\delta U; \xi) \quad \forall \delta U \in \mathcal{U}$$

- **Local** equation on patch  $\Lambda$

$$m_\Lambda(\dot{w}(\xi), \delta w; \xi) + a_\Lambda(w(\xi), \delta w; \xi) - b_\Gamma(\lambda(\xi), \delta w) = \ell_\Lambda(\delta w; \xi) \quad \forall \delta w \in \mathcal{W}$$

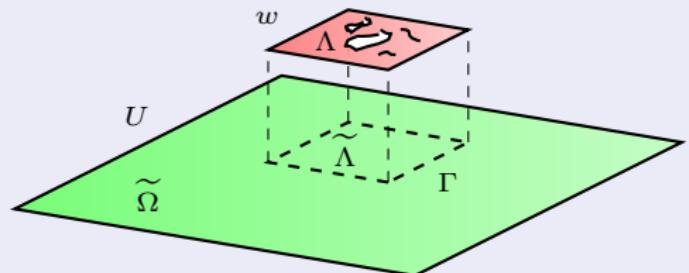
- **Coupling** equation on interface  $\Gamma$

$$b_\Gamma(\delta \lambda, U(\xi)) - b_\Gamma(\delta \lambda, w(\xi)) = 0 \quad \forall \delta \lambda \in \mathcal{M}$$

# Global-local formulation with patches

## Overlapping domain decomposition - Introduction of a fictitious patch

- Deterministic fictitious domain  $\tilde{\Omega}$
- Deterministic fictitious patch  $\tilde{\Lambda}$
- Uncertain patch  $\Lambda$
- Deterministic interface  $\Gamma$



## Reformulation with overlapping domains

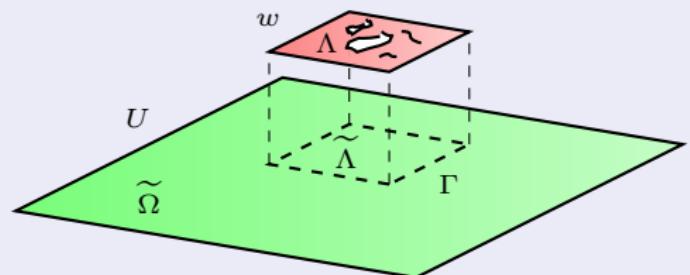
Find  $(U, w, \lambda) \in \tilde{\mathcal{U}}^\Xi \times \mathcal{W}^\Xi \times \mathcal{M}^\Xi$  such that it holds almost surely

- Reformulated global equation on fictitious domain  $\tilde{\Omega} = (\Omega \setminus \Lambda) \cup \tilde{\Lambda}$
  - Local equation on patch  $\Lambda$
  - Coupling equation on interface  $\Gamma$
- $$\mathbf{n}_{\tilde{\Omega}}(\dot{U}(\xi), \delta U; \xi) - \mathbf{n}_{\tilde{\Lambda}}(\dot{U}(\xi), \delta U; \xi) + \mathbf{c}_{\tilde{\Omega}}(U(\xi), \delta U; \xi) - \mathbf{c}_{\tilde{\Lambda}}(U(\xi), \delta U; \xi) + \mathbf{b}_\Gamma(\lambda(\xi), \delta U) = 0 \quad \forall \delta U \in \mathcal{U}$$
- $$\mathbf{m}_\Lambda(\dot{w}(\xi), \delta w; \xi) + \mathbf{a}_\Lambda(w(\xi), \delta w; \xi) - \mathbf{b}_\Gamma(\lambda(\xi), \delta w) = \ell_\Lambda(\delta w; \xi) \quad \forall \delta w \in \mathcal{W}$$
- $$\mathbf{b}_\Gamma(\delta \lambda, U(\xi)) - \mathbf{b}_\Gamma(\delta \lambda, w(\xi)) = 0 \quad \forall \delta \lambda \in \mathcal{M}$$

# Global-local formulation with patches

## Overlapping domain decomposition - Introduction of a fictitious patch

- Deterministic fictitious domain  $\tilde{\Omega}$
- Deterministic fictitious patch  $\tilde{\Lambda}$
- Uncertain patch  $\Lambda$
- Deterministic interface  $\Gamma$



## Reformulation with overlapping domains

Find  $(U, w, \lambda) \in \tilde{\mathcal{U}}^\Xi \times \mathcal{W}^\Xi \times \mathcal{M}^\Xi$  such that it holds almost surely

- Reformulated global equation on fictitious domain  $\tilde{\Omega} = (\Omega \setminus \Lambda) \cup \tilde{\Lambda}$

$$n_{\tilde{\Omega}}(\dot{U}(\xi), \delta U; \xi) - n_{\tilde{\Lambda}}(\dot{U}(\xi), \delta U; \xi) + c_{\tilde{\Omega}}(U(\xi), \delta U; \xi) - c_{\tilde{\Lambda}}(U(\xi), \delta U; \xi) + b_{\Gamma}(\lambda(\xi), \delta U) = 0$$

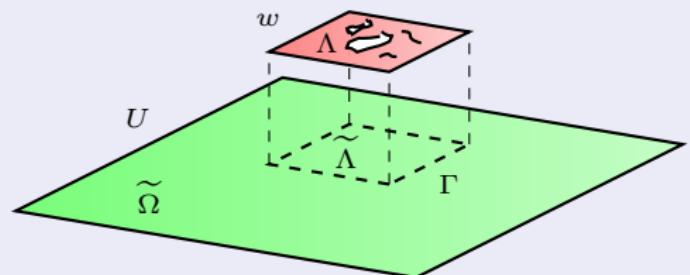
where bilinear forms  $n_{\mathcal{O}}(U, V; \xi) = \int_{\mathcal{O}} \tilde{c}(\xi) UV$  and

$$c_{\mathcal{O}}(U, V; \xi) = \int_{\mathcal{O}} \tilde{K}(\xi) \nabla U \cdot \nabla V + \int_{\mathcal{O}} \tilde{\alpha}(\xi) \cdot \nabla U V + \int_{\mathcal{O}} \tilde{R}(\xi) U V.$$

# Global-local formulation with patches

## Overlapping domain decomposition - Introduction of a fictitious patch

- Deterministic fictitious domain  $\tilde{\Omega}$
- Deterministic fictitious patch  $\tilde{\Lambda}$
- Uncertain patch  $\Lambda$
- Deterministic interface  $\Gamma$



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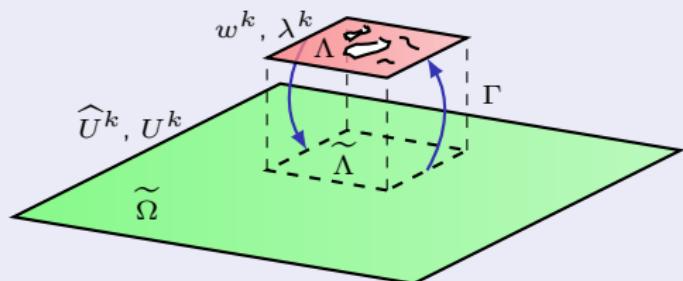
where bilinear forms  $n_{\mathcal{O}}(U, V; \xi) = \int_{\mathcal{O}} \tilde{c}(\xi) UV$  and

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# Global-local iterative algorithm

## Iterative coupling procedure

1 Global step  
 $\widehat{U}^k$

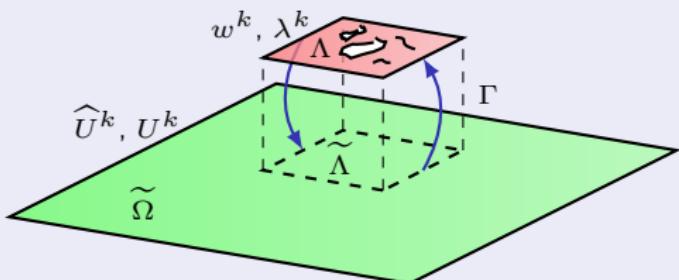
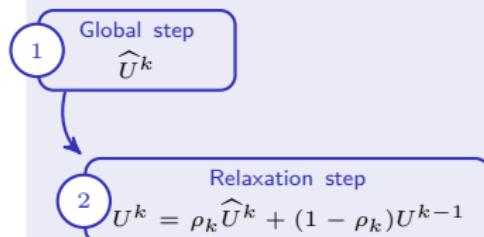


① Global step: Compute  $\widehat{U}^k \in \widetilde{\mathcal{U}}^\Xi$  such that it satisfies almost surely

$$\mathbf{n}_\Omega^\sim(\dot{\widehat{U}}^k(\xi), \delta U) + \mathbf{c}_\Omega^\sim(\widehat{U}^k(\xi), \delta U) = \mathbf{n}_\Lambda^\sim(\dot{U}^{k-1}(\xi), \delta U) + \mathbf{c}_\Lambda^\sim(U^{k-1}(\xi), \delta U) - \mathbf{b}_\Gamma(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

# Global-local iterative algorithm

## Iterative coupling procedure



① **Global step:** Compute  $\hat{U}^k \in \tilde{\mathcal{U}}^\Xi$  such that it satisfies almost surely

$$\mathbf{n}_\Omega^\sim(\dot{\hat{U}}^k(\xi), \delta U) + \mathbf{c}_\Omega^\sim(\hat{U}^k(\xi), \delta U) = \mathbf{n}_\Lambda^\sim(\dot{U}^{k-1}(\xi), \delta U) + \mathbf{c}_\Lambda^\sim(U^{k-1}(\xi), \delta U) - \mathbf{b}_\Gamma(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

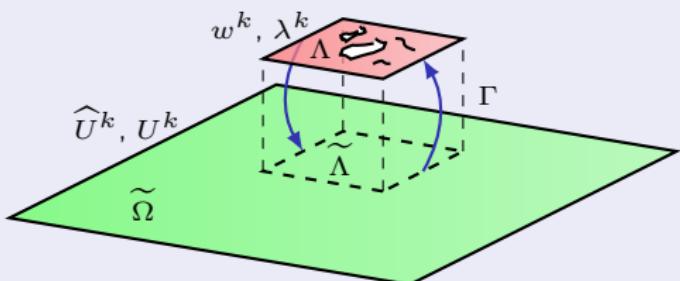
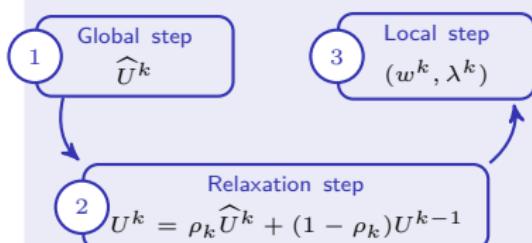
② **Relaxation step:** Define  $U^k \in \tilde{\mathcal{U}}^\Xi$  by

$$U^k(\xi) = \rho_k \hat{U}^k(\xi) + (1 - \rho_k) U^{k-1}(\xi) \quad \text{with relaxation parameter } \rho_k > 0$$

↪ Significant influence on the convergence properties of the algorithm

# Global-local iterative algorithm

## Iterative coupling procedure



**① Global step:** Compute  $\hat{U}^k \in \tilde{\mathcal{U}}^\Xi$  such that it satisfies almost surely

$$\mathbf{n}_\Omega(\dot{\hat{U}}^k(\xi), \delta U) + \mathbf{c}_\Omega(\hat{U}^k(\xi), \delta U) = \mathbf{n}_\Lambda(\dot{U}^{k-1}(\xi), \delta U) + \mathbf{c}_\Lambda(U^{k-1}(\xi), \delta U) - \mathbf{b}_\Gamma(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

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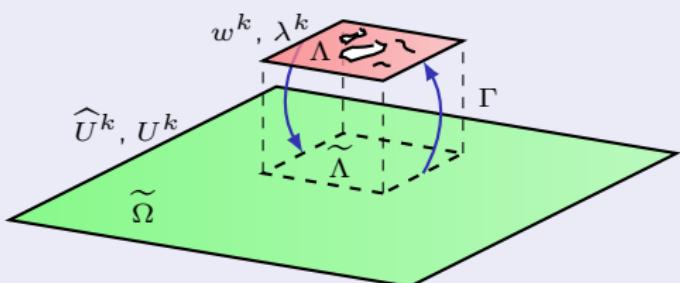
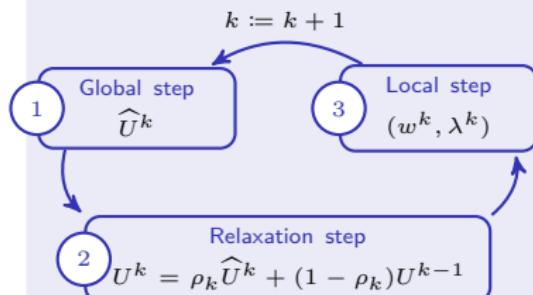
$$U^k(\xi) = \rho_k \hat{U}^k(\xi) + (1 - \rho_k) U^{k-1}(\xi) \quad \text{with relaxation parameter } \rho_k > 0$$

**③ Local step:** Compute  $(w^k, \lambda^k) \in \mathcal{W}^\Xi \times \mathcal{M}^\Xi$  such that it satisfies almost surely

$$\begin{cases} \mathbf{m}_\Lambda(w^k(\xi), \delta w; \xi) + \mathbf{a}_\Lambda(w^k(\xi), \delta w; \xi) - \mathbf{b}_\Gamma(\lambda^k(\xi), \delta w) = \ell_\Lambda(\delta w; \xi) & \forall \delta w \in \mathcal{W} \\ \mathbf{b}_\Gamma(\delta \lambda, w^k(\xi)) = \mathbf{b}_\Gamma(\delta \lambda, U^k(\xi)) & \forall \delta \lambda \in \mathcal{M} \end{cases}$$

# Global-local iterative algorithm

## Iterative coupling procedure



① **Global step:** Compute  $\widehat{U}^k \in \widetilde{\mathcal{U}}^\Xi$  such that it satisfies almost surely

$$\mathbf{n}_\Omega(\dot{\widehat{U}}^k(\xi), \delta U) + \mathbf{c}_{\widetilde{\Omega}}(\widehat{U}^k(\xi), \delta U) = \mathbf{n}_\Lambda(\dot{U}^{k-1}(\xi), \delta U) + \mathbf{c}_\Lambda(U^{k-1}(\xi), \delta U) - \mathbf{b}_\Gamma(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

② **Relaxation step:** Define  $U^k \in \widetilde{\mathcal{U}}^\Xi$  by

$$U^k(\xi) = \rho_k \widehat{U}^k(\xi) + (1 - \rho_k) U^{k-1}(\xi) \quad \text{with relaxation parameter } \rho_k > 0$$

③ **Local step:** Compute  $(w^k, \lambda^k) \in \mathcal{W}^\Xi \times \mathcal{M}^\Xi$  such that it satisfies almost surely

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# Analysis of the algorithm (in the stationary case)

## Consistency

- There exists a **unique extension**  $\tilde{U}(\xi) \in \tilde{\mathcal{U}}_*$  of the global solution  $U(\xi) \in \tilde{\mathcal{U}}$  such that  $\tilde{U}(\xi) = U(\xi)$  on complementary subdomain  $\Omega \setminus \Lambda$  and the restriction of  $\tilde{U}(\xi)$  to fictitious patch  $\tilde{\Lambda}$  is uniquely defined by the trace of  $U(\xi)$  on interface  $\Gamma$ .
- The extended global solution  $U \in L_\mu^p(\Xi; \tilde{\mathcal{U}})$ , with exponent  $2 \leq p \leq +\infty$ .

## Convergence

- Assume that the sequence of relaxation parameters  $\{\rho_k\}_{k \in \mathbb{N}}$  is such that

$$0 < \rho_{\inf} \leq \rho_k \leq \rho_{\sup} < +\infty,$$

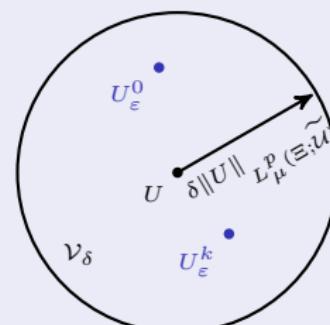
for some strictly positive constants  $\rho_{\inf}$  and  $\rho_{\sup}$  independent of  $\xi$  and  $k$ .

- Then, for  $\rho_{\sup}$  sufficiently small, the sequence  $\{(U^k(\xi), w^k(\xi), \lambda^k(\xi))\}_{k \in \mathbb{N}}$  converges almost surely to the unique solution  $(U(\xi), w(\xi), \lambda(\xi))$  of the initial global-local problem in  $\tilde{\mathcal{U}}_*(\xi) \times \mathcal{W} \times \mathcal{M}$ .  $\hookrightarrow$  **Almost sure convergence**
- Also, the sequence  $\{(U^k, w^k, \lambda^k)\}_{k \in \mathbb{N}}$  converges to  $(U, w, \lambda)$  in  $L_\mu^p(\Xi; \tilde{\mathcal{U}}) \times L_\mu^p(\Xi; \mathcal{W}) \times L_\mu^p(\Xi; \mathcal{M})$ .  $\hookrightarrow$  **Convergence in  $L_\mu^p$**

# Analysis of the algorithm

## Robustness - Impact of approximations

- Analysis of the **sensitivity** of the iterative algorithm with respect to **approximations** introduced at the different steps of the algorithm
- Control of the **approximation error**  $U_\varepsilon^k - U^k$  between the approximate/perturbed global iterate  $U_\varepsilon^k$  and the unperturbed one  $U^k$  at iteration  $k$  in a  $L_\mu^p$ -norm
- Under certain assumptions on the unperturbed and perturbed iteration maps, if the initial global iterate  $U_\varepsilon^0$  is in a  $\delta$ -neighborhood  $\mathcal{V}_\delta$  of the exact global solution  $U$ , then all global iterates  $U_\varepsilon^k$  remain in  $\mathcal{V}_\delta$ , and the **approximate sequence**  $\{U_\varepsilon^k\}_{k \in \mathbb{N}}$  tends to a  $\gamma(\varepsilon)$ -neighborhood of  $U$  in  $L_\mu^p(\Xi; \tilde{\mathcal{U}})$  with  $\gamma(\varepsilon) \rightarrow 0$  as  $\varepsilon \rightarrow 0$ .
- Open ball  $\mathcal{V}_\delta$  of radius  $\delta \|U\|_{L_\mu^p(\Xi; \tilde{\mathcal{U}})}$  centered at the exact global solution  $U$  and containing all global iterates  $U_\varepsilon^k$



# Outline

1 Context and motivation

2 Multiscale domain decomposition method

3 Computational aspects

- Adaptive sampling-based approach
- Relaxation step

4 Numerical illustrations

5 Conclusions and outlooks

# Computational aspects

## Global problem

- Direct computation of global problem by solving a system of uncoupled linear equations with the same deterministic global finite element matrix
- Use of traditional (parallel) solvers available in commercial deterministic finite element codes

## Local problems

- Resolution of stochastic local problems using an adaptive least-squares method
- Sampling-based approaches require evaluations of the solution by standard deterministic codes and are well adapted to massively parallel computation
- Control of the stability of local approximations by increasing the number of samples
- Estimation of the approximation error using cross-validation techniques
- Working sets strategies proposed in [Chkifa, Cohen, and Schwab 2014, 2015; Chkifa et al. 2013] for the construction of an increasing sequence of sparse approximation spaces
- Algorithm with adaptive random sampling and an adaptive selection of approximation spaces for the construction of sparse polynomial approximations of local solutions [Nouy and Pled 2017]

# Least-squares method

## Least-squares approximation in a given subspace

- Least-squares approximation  $\mathbf{v} \in \mathbb{R}^n \otimes \mathcal{S}_{\mathcal{A}}$  of a random vector  $\mathbf{u} \in \mathbb{R}^n \otimes L^2_{\mu}(\Xi)$ :

$$\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_{\alpha} \psi_{\alpha}(\xi)$$

where  $\mathcal{S}_{\mathcal{A}} = \text{span}\{\psi_{\alpha}\}_{\alpha \in \mathcal{A}}$  is a polynomial space for a given subset  $\mathcal{A}$  of multi-indices  $\alpha$ .

- Set of coefficients  $\mathbf{V} = (\mathbf{v}_{\alpha})_{\alpha \in \mathcal{A}} \in \mathbb{R}^{n \times \#\mathcal{A}}$  solution of an unconstrained optimization problem:

$$\begin{aligned} \min_{(\mathbf{v}_{\alpha})_{\alpha \in \mathcal{A}}} \sum_{l=1}^N \|\mathbf{u}(\xi^l) - \sum_{\alpha \in \mathcal{A}} \mathbf{v}_{\alpha} \psi_{\alpha}(\xi^l)\|_2^2 &\iff \min_{\mathbf{V}} \|\mathbf{Y} - \boldsymbol{\Psi} \mathbf{V}^T\|_F^2 \\ &\implies \mathbf{V}^T = (\boldsymbol{\Psi}^T \boldsymbol{\Psi})^{-1} \boldsymbol{\Psi}^T \mathbf{Y} \end{aligned}$$

where  $\boldsymbol{\Psi} = (\psi_{\alpha}(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}} \in \mathbb{R}^{N \times \#\mathcal{A}}$  and  $\mathbf{Y} = (\mathbf{u}(\xi^l))_{1 \leq l \leq N} \in \mathbb{R}^{N \times n}$ .

- In practice, improvement of the stability of the least-squares approximation  $\mathbf{v}$  by increasing the number of samples  $N$

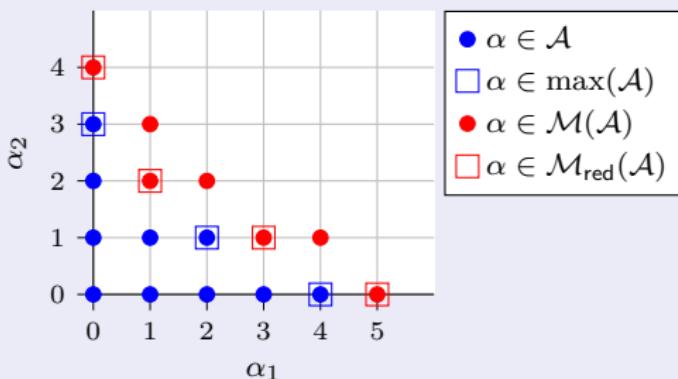
# Working set strategy for adaptive approximation

## Structure of monotone sets

- A finite subset  $\mathcal{A}$  of multi-indices  $\alpha$  is called **monotone** (or **lower** or **downward closed**) if it is such that  $(\beta \in \mathcal{A} \text{ and } \alpha \leq \beta) \implies \alpha \in \mathcal{A}$
- Margin  $\mathcal{M}(\mathcal{A})$  and reduced margin  $\mathcal{M}_{\text{red}}(\mathcal{A})$  of a monotone set  $\mathcal{A}$

$$\mathcal{M}(\mathcal{A}) = \{\alpha \notin \mathcal{A}; \exists i \in \{1, \dots, m\} \text{ such that } \alpha_i \neq 0 \implies \alpha - e_i \in \mathcal{A}\}$$

$$\mathcal{M}_{\text{red}}(\mathcal{A}) = \{\alpha \notin \mathcal{A}; \forall i \in \{1, \dots, m\} \text{ such that } \alpha_i \neq 0 \implies \alpha - e_i \in \mathcal{A}\}$$



**Figure:** Monotone multi-index set  $\mathcal{A}$ , its maximal elements  $\max(\mathcal{A})$ , its margin  $\mathcal{M}(\mathcal{A})$  and reduced margin  $\mathcal{M}_{\text{red}}(\mathcal{A})$

# Working set strategy for adaptive approximation

## Working set strategy - construction of an increasing sequence of monotone sets

- Polynomial function ( $d = 3$ ) [Sudret 2008]

$$u(\xi) = \frac{1}{2^d} \prod_{j=1}^d (3\xi_j^2 + 1)$$

where  $\xi_j \sim \mathcal{U}(0, 1)$  and  $\xi = (\xi_j)_{j=1}^d \in \Xi = (0, 1)^d$

# Working set strategy for adaptive approximation

## Working set strategy - construction of an increasing sequence of monotone sets

- Ishigami function [Blatman and Sudret 2010; Blatman and Sudret 2011;  
Saltelli Andrea and Scott 2000; Sudret 2008]

$$u(\xi) = \sin(\xi_1) + a \sin(\xi_2)^2 + b \xi_3^4 \sin(\xi_1) \quad \text{with } a = 7, b = 0.1$$

where  $\xi_j \sim \mathcal{U}(-\pi, \pi)$  and  $\xi = (\xi_j)_{j=1}^3 \in \Xi = (-\pi, \pi)^3$

# Working set strategy for adaptive approximation

## Working set strategy - construction of an increasing sequence of monotone sets

- Anisotropic function [Chkifa, Cohen, and Schwab 2014]

$$u(\xi) = \xi_3 \sin(\xi_4) + \xi_{16}$$

where  $\xi_j \sim \mathcal{U}(0, 1)$  and  $\xi = (\xi_j)_{j=1}^{16} \in \Xi = (0, 1)^{16}$

# Working set strategy for adaptive approximation

## Working set strategy - construction of an increasing sequence of monotone sets

- Anisotropic function [Chkifa, Cohen, and Schwab 2014]

$$u(\xi) = \xi_3 \sin(\xi_4) + \xi_{16}$$

where  $\xi_j \sim \mathcal{U}(0, 1)$  and  $\xi = (\xi_j)_{j=1}^{16} \in \Xi = (0, 1)^{16}$

# Cross-validation technique

Leave-one-out cross-validation technique: statistical method based on random partitioning of the available sample set [Cawley and Talbot 2004]

**Input:** Coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  of the approximation  $\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_\alpha \psi_\alpha(\xi)$  of  $\mathbf{u}(\xi)$ , and matrices  $\Psi = (\psi_\alpha(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}}$  and  $\mathbf{Y}^T = (\mathbf{u}(\xi^l))_{1 \leq l \leq N}$

**Output:** Vector  $\boldsymbol{\varepsilon} = (\varepsilon_i)_{i \in \mathcal{I}}$ , where  $\varepsilon_i$  is an estimation of the error  $\mathbb{E}((u_i(\xi) - v_i(\xi))^2)$

- 1: **for**  $i = 1, \dots, n$  **do**
- 2:   Compute the set of predicted residuals  $\{\Delta_l^i\}_{l=1}^N$  associated with sample set  $\{\xi^l\}_{l=1}^N$  using Sherman-Morrison-Woodbury formula:

$$\Delta_l^i = \frac{r_{li}}{1 - h_l} \quad \text{with} \quad \begin{cases} r_{li} & \text{the } (l, i)\text{-th entry of matrix } \mathbf{R} = \Psi \mathbf{V}^T - \mathbf{Y} \\ h_l & \text{the } l\text{-th diagonal term in matrix } \mathbf{H} = \Psi (\Psi^T \Psi)^{-1} \Psi^T \end{cases}$$

- 3:   Compute the leave-one-out error  $e_i = \frac{E_i}{\widehat{m}_2(\mathbf{Y}_i)}$ , where  $E_i = \frac{1}{N} \sum_{l=1}^N (\Delta_l^i)^2$  and  $\widehat{m}_2(\mathbf{Y}_i)$  is the empirical second moment of the  $i$ -th column  $\mathbf{Y}_i = (u_i(\xi^l))_{l=1}^N$  of matrix  $\mathbf{Y}$
- 4:   Compute the corrected leave-one-out error  $\varepsilon_i = e_i \times T(\mathcal{A}, N)$ , where  $T(\mathcal{A}, N) = \left(1 - \frac{\#\mathcal{A}}{N}\right)^{-1} \left(1 + \frac{\text{tr}(\widehat{\mathbf{C}}^{-1})}{N}\right)$  is a correction factor allowing to reduce the sensitivity to overfitting [Blatman and Sudret 2011; Chapelle, Vapnik, and Bengio 2002] and where  $\widehat{\mathbf{C}} = \frac{1}{N} \Psi^T \Psi$  is the empirical covariance matrix of  $(\psi_\alpha(\xi))_{\alpha \in \mathcal{A}}$
- 5: **end for**

# Adaptive sparse algorithm

Adaptive sparse least-squares solver with random sampling and working set strategy  
[Nouy and Pled 2017]

**Input:** Initial number of samples  $N \geq 1$ , sampling factor  $p_{\text{add}} > 0$ , parameter  $\theta \in [0, 1]$   
**Output:** Monotone set  $\mathcal{A}$  and coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  of the least-squares approximation

$\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_\alpha \psi_\alpha(\xi)$  of  $\mathbf{u}(\xi)$

- 1: Start with null initial set  $\mathcal{A} = \{0_{\mathcal{F}}\}$
- 2: Generate the initial sample set  $\{\xi^l\}_{l=1}^N$  randomly
- 3: Compute the matrices  $\Psi_{\mathcal{A}} = (\psi_\alpha(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}}$  and  $\mathbf{Y}^T = (\mathbf{u}(\xi^l))_{1 \leq l \leq N}$
- 4: **while** no convergence **do**
- 5:   // Adaptive random sampling
- 6:   **while** no convergence and no stagnation **do**
- 7:     Generate the additional sample set  $\{\xi^{N+l}\}_{l=1}^{N_{\text{add}}}$  randomly, with  $N_{\text{add}} = \text{ceil}(p_{\text{add}} N)$
- 8:     Compute the matrices  $\Psi_{\mathcal{A}, \text{add}}$  and  $\mathbf{Y}_{\text{add}}^T$
- 9:     Update the number of samples  $N \leftarrow N + N_{\text{add}}$  and the matrices  
 $\Psi_{\mathcal{A}}^T \leftarrow (\Psi_{\mathcal{A}}^T, \Psi_{\mathcal{A}, \text{add}}^T)$  and  $\mathbf{Y}^T \leftarrow (\mathbf{Y}^T, \mathbf{Y}_{\text{add}}^T)$
- 10:    Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$
- 11:   **end while**
- 12:   **end while**

# Adaptive sparse algorithm

Adaptive sparse least-squares solver with random sampling and working set strategy  
[Nouy and Pled 2017]

**Input:** Initial number of samples  $N \geq 1$ , sampling factor  $p_{\text{add}} > 0$ , parameter  $\theta \in [0, 1]$   
**Output:** Monotone set  $\mathcal{A}$  and coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  of the least-squares approximation

$$\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_\alpha \psi_\alpha(\xi) \text{ of } \mathbf{u}(\xi)$$

- 1: Start with null initial set  $\mathcal{A} = \{0_{\mathcal{F}}\}$
- 2: Generate the initial sample set  $\{\xi^l\}_{l=1}^N$  randomly
- 3: Compute the matrices  $\Psi_{\mathcal{A}} = (\psi_\alpha(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}}$  and  $\mathbf{Y}^T = (\mathbf{u}(\xi^l))_{1 \leq l \leq N}$
- 4: **while** no convergence **do**
- 5:   // Adaptive random sampling
- 6:   **while** no convergence and no stagnation **do**
- 7:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$   
      by taking into account additional samples
- 8:   **end while**
- 9:   **end while**

# Adaptive sparse algorithm

Adaptive sparse least-squares solver with random sampling and working set strategy  
 [Nouy and Pled 2017]

**Input:** Initial number of samples  $N \geq 1$ , sampling factor  $p_{\text{add}} > 0$ , parameter  $\theta \in [0, 1]$   
**Output:** Monotone set  $\mathcal{A}$  and coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  of the least-squares approximation

$\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_\alpha \psi_\alpha(\xi)$  of  $\mathbf{u}(\xi)$   
 1: Start with null initial set  $\mathcal{A} = \{0_{\mathcal{F}}\}$   
 2: Generate the initial sample set  $\{\xi^l\}_{l=1}^N$  randomly  
 3: Compute the matrices  $\Psi_{\mathcal{A}} = (\psi_\alpha(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}}$  and  $\mathbf{Y}^T = (\mathbf{u}(\xi^l))_{1 \leq l \leq N}$   
 4: **while** no convergence **do**  
 5:   // Adaptive random sampling  
 6:   **while** no convergence and no stagnation **do**  
 7:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$   
      by taking into account additional samples  
 8:   **end while**  
 9:   // Working set strategy  
 10:   **while** no convergence and no overfitting **do**  
 11:     Compute the reduced margin  $\mathcal{M} = \mathcal{M}_{\text{red}}(\mathcal{A})$  of  $\mathcal{A}$  and the set  $\mathcal{T} = \mathcal{A} \cup \mathcal{M}$   
 12:     Compute the matrices  $\Psi_{\mathcal{M}}$  and  $\Psi_{\mathcal{T}} = (\Psi_{\mathcal{A}}, \Psi_{\mathcal{M}})$   
 13:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{T}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{T}}^T \Psi_{\mathcal{T}})^{-1} \Psi_{\mathcal{T}}^T \mathbf{Y}$   
 14:     Define the smallest (monotone) subset  $\mathcal{N}$  of  $\mathcal{M}$  such that  $e(\mathcal{N}) \geq \theta e(\mathcal{M})$ , with  
       $e(\mathcal{N}) = \sum_{\alpha \in \mathcal{N}} \|\mathbf{v}_\alpha\|_2^2$  and  $e(\mathcal{M}) = \sum_{\alpha \in \mathcal{M}} \|\mathbf{v}_\alpha\|_2^2$   
 15:     Update the multi-index set  $\mathcal{A} \leftarrow \mathcal{A} \cup \mathcal{N}$  and the matrix  $\Psi_{\mathcal{A}} \leftarrow (\Psi_{\mathcal{A}}, \Psi_{\mathcal{N}})$   
 16:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$   
 17:   **end while**  
 18: **end while**

# Adaptive sparse algorithm

Adaptive sparse least-squares solver with random sampling and working set strategy  
[Nouy and Pled 2017]

**Input:** Initial number of samples  $N \geq 1$ , sampling factor  $p_{\text{add}} > 0$ , parameter  $\theta \in [0, 1]$   
**Output:** Monotone set  $\mathcal{A}$  and coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  of the least-squares approximation

$\mathbf{v}(\xi) = \sum_{\alpha \in \mathcal{A}} \mathbf{v}_\alpha \psi_\alpha(\xi)$  of  $\mathbf{u}(\xi)$

- 1: Start with null initial set  $\mathcal{A} = \{0_{\mathcal{F}}\}$
- 2: Generate the initial sample set  $\{\xi^l\}_{l=1}^N$  randomly
- 3: Compute the matrices  $\Psi_{\mathcal{A}} = (\psi_\alpha(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}}$  and  $\mathbf{Y}^T = (\mathbf{u}(\xi^l))_{1 \leq l \leq N}$
- 4: **while** no convergence **do**
- 5:   // Adaptive random sampling
- 6:   **while** no convergence and no stagnation **do**
- 7:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$   
     by taking into account additional samples
- 8:   **end while**
- 9:   // Working set strategy
- 10:   **while** no convergence and no overfitting **do**
- 11:     Compute the coefficients  $\mathbf{V} = (\mathbf{v}_\alpha)_{\alpha \in \mathcal{A}}$  such that  $\mathbf{V}^T = (\Psi_{\mathcal{A}}^T \Psi_{\mathcal{A}})^{-1} \Psi_{\mathcal{A}}^T \mathbf{Y}$   
     by updating the approximation basis
- 12:   **end while**
- 13: **end while**

# Relaxation step

## Impact of relaxation step on convergence

- The relaxation step may affect the convergence rate of the iterative algorithm.

## Simplest technique - Fixed relaxation parameter

- A large relaxation parameter may speed up the convergence but can lead to a divergence of the algorithm, while a small relaxation parameter enables to control the convergence but trigger more iterations in return.
- The computation of an optimal relaxation parameter is not obvious in the non-linear framework.
- Even in the linear case, the optimal fixed value of relaxation parameter  $\rho$  is problem-dependent and not known *a priori*.
- In the linear case and under some conditions on the iteration map, an optimal convergent rate of the global-local iterative algorithm can be achieved by computing the optimal relaxation parameter  $\rho_{\text{opt}}$  defined by [Xu 1992]

$$\rho_{\text{opt}} = \frac{2}{\lambda_{\min} + \lambda_{\max}},$$

where  $\lambda_{\min}$  and  $\lambda_{\max}$  are the lowest and largest eigenvalues of the iteration map (see [Chevreuil, Nouy, and Safatly 2013]).

# Relaxation step

## Convergence acceleration technique - Aitken's dynamic relaxation

- Aitken's Delta-Squared method [Iron and Tuck 1969; Macleod 1986]
  - Simple and efficient convergence acceleration technique
  - Improvement of the current solution by using information gained at two previous iterations
- Update Aitken's formula for the relaxation parameter [Duval et al. 2014; Kütller and Wall 2008; Liu, Sun, and Fan 2014]

$$\begin{cases} \rho_1 = \rho_2 = 1 \\ \rho_k = -\rho_{k-1} \frac{\langle \delta^k(\xi) - \delta^{k-1}(\xi), \delta^{k-1}(\xi) \rangle_{\tilde{\mathcal{U}}}}{\|\delta^k(\xi) - \delta^{k-1}(\xi)\|_{\tilde{\mathcal{U}}}^2}, \quad \text{with} \quad \delta^k(\xi) = \widehat{U}^k(\xi) - U^{k-1}(\xi) \end{cases}$$

- Adapted recursive formula to ensure convergence of the algorithm [Nouy and Pled 2017]

$$\rho_k = T_{[\rho_{\inf}, \rho_{\sup}]} \left( -\rho_{k-1} \frac{\langle \delta^k(\xi) - \delta^{k-1}(\xi), \delta^{k-1}(\xi) \rangle_{\tilde{\mathcal{U}}}}{\|\delta^k(\xi) - \delta^{k-1}(\xi)\|_{\tilde{\mathcal{U}}}^2} \right),$$

where  $T_{[\rho_{\inf}, \rho_{\sup}]}(\rho)$  is the projection of  $\rho$  on the interval  $[\rho_{\inf}, \rho_{\sup}]$

# Outline

1 Context and motivation

2 Multiscale domain decomposition method

3 Computational aspects

4 Numerical illustrations

- Stationary non-linear diffusion-reaction stochastic problem
- Transient linear advection-diffusion-reaction deterministic problem

5 Conclusions and outlooks

# Stationary non-linear diffusion-reaction stochastic problem

Non-linear diffusion-reaction problem with localized random material heterogeneities  
[Nouy and Pled 2017]

$$\begin{aligned} -\nabla \cdot (\mathbf{K} \nabla u) + \mathbf{R} u^3 &= 1 \quad \text{on } \Omega = (0, 2) \times (0, 16) \\ u &= 0 \quad \text{on } \Gamma_D = \partial\Omega \end{aligned}$$



- Random diffusion and reaction fields

$$\mathbf{K}(x, \xi) = \begin{cases} 1 & \text{on } \Omega \setminus \left( \bigcup_{q=1}^8 \Lambda_q \right) \\ 1 + \gamma_q \xi_{2q-1} \chi_q(x) & \text{on } \Lambda_q \end{cases}$$

$$\mathbf{R}(x, \xi) = \begin{cases} 0 & \text{on } \Omega \setminus \left( \bigcup_{q=1}^8 \Lambda_q \right) \\ \gamma_q \xi_{2q} \chi_q(x) & \text{on } \Lambda_q \end{cases}$$

- Uniform random variables  $\xi = (\xi_i)_{i=1}^{16}$  on  $\Xi_i = (0, 1)$
- Uniform weights  $\gamma_q = 1$

	$\Omega \setminus \Lambda$
	$\Lambda_1$
	$\Lambda_2$
	$\Lambda_3$
	$\Lambda_4$
	$\Lambda_5$
	$\Lambda_6$
	$\Lambda_7$
	$\Lambda_8$

# Stationary non-linear diffusion-reaction stochastic problem

Non-linear diffusion-reaction problem with localized random material heterogeneities  
[Nouy and Pled 2017]

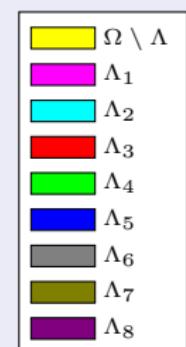
$$\begin{aligned} -\nabla \cdot (K \nabla u) + Ru^3 &= 1 \quad \text{on } \Omega = (0, 2) \times (0, 16) \\ u &= 0 \quad \text{on } \Gamma_D = \partial\Omega \end{aligned}$$



- Random diffusion and reaction fields

$$K(x, \xi) = \begin{cases} 1 & \text{on } \Omega \setminus \left( \bigcup_{q=1}^8 \Lambda_q \right) \\ 1 + \gamma_q \xi_{2q-1} \chi_q(x) & \text{on } \Lambda_q \end{cases}$$

$$R(x, \xi) = \begin{cases} 0 & \text{on } \Omega \setminus \left( \bigcup_{q=1}^8 \Lambda_q \right) \\ \gamma_q \xi_{2q} \chi_q(x) & \text{on } \Lambda_q \end{cases}$$

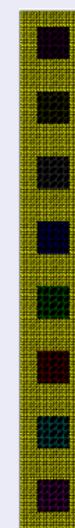


- Uniform random variables  $\xi = (\xi_i)_{i=1}^{16}$  on  $\Xi_i = (0, 1)$
- Heterogeneous weights  $\gamma_q = 1 - 0.1(q + 1)$

# Stationary non-linear diffusion-reaction stochastic problem

Non-linear diffusion-reaction problem with localized random material heterogeneities  
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$$\begin{aligned} -\nabla \cdot (\mathbf{K} \nabla u) + \mathbf{R} u^3 &= 1 \quad \text{on } \Omega = (0, 2) \times (0, 16) \\ u &= 0 \quad \text{on } \Gamma_D = \partial\Omega \end{aligned}$$



	$\Omega \setminus \Lambda$
	$\Lambda_1$
	$\Lambda_2$
	$\Lambda_3$
	$\Lambda_4$
	$\Lambda_5$
	$\Lambda_6$
	$\Lambda_7$
	$\Lambda_8$

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$$\mathbf{K}(x, \xi) = \begin{cases} 1 & \text{on } \Omega \setminus \left( \bigcup_{q=1}^8 \Lambda_q \right) \\ 1 + \gamma_q \xi_{2q-1} \chi_q(x) & \text{on } \Lambda_q \end{cases}$$

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- Uniform random variables  $\xi = (\xi_i)_{i=1}^{16}$  on  $\Xi_i = (0, 1)$
- Heterogeneous weights  $\gamma_q = 1 - 0.1(q + 1)$

## Approximation spaces

- Spatial level: nested global and local finite element approximation spaces
  - $\dim(\tilde{\mathcal{U}}_H) = 3381$  on  $\tilde{\Omega}$
  - $\dim(\mathcal{W}_h^q) = 441$  on  $\Lambda_q$
- Stochastic level: adaptive construction of sparse Legendre polynomial approximation spaces using working sets strategies [Chkifa et al. 2013]

# Stationary non-linear diffusion-reaction stochastic problem

## Convergence analysis

- Control of the accuracy of global approximations  $U^k$  with respect to a global reference solution  $U^{\text{ref}}$  using the relative error indicator

$$\varepsilon_{\Xi, \Omega \setminus \Lambda}(U^k; U^{\text{ref}}) = \frac{\|U^k - U^{\text{ref}}\|_{L^2_\mu(\Xi; L^2(\Omega \setminus \Lambda))}}{\|U^{\text{ref}}\|_{L^2_\mu(\Xi; L^2(\Omega \setminus \Lambda))}}$$

with  $\|U\|_{L^2_\mu(\Xi; L^2(\Omega \setminus \Lambda))}^2 = \mathbb{E}(\|U(\xi)\|_{L^2(\Omega \setminus \Lambda)}^2)$

- Reference solution  $(U^{\text{ref}}, w_q^{\text{ref}}, \lambda_q^{\text{ref}})$  of the full-scale coupled problem obtained using an adaptive sparse least-squares method
  - Spatial level: deterministic non-linear problems solved using a tangent-Newton iterative algorithm with a tolerance  $\epsilon = 10^{-12}$
  - Stochastic level: control of the number of samples  $N^{\text{ref}}$  and approximation spaces  $\mathcal{A}^{\text{ref}}$  using a cross-validation procedure with a tolerance  $\varepsilon_{\text{cv}}^{\text{ref}} = 10^{-6}$
  - Isotropic case:
    - $N^{\text{ref}} = 795$  samples
    - $\#\mathcal{A}^{\text{ref}} = 384$  for  $U^{\text{ref}}$
  - Anisotropic case:
    - $N^{\text{ref}} = 491$  samples
    - $\#\mathcal{A}^{\text{ref}} = 173$  for  $U^{\text{ref}}$

# Stationary non-linear diffusion-reaction stochastic problem

## Convergence analysis - Influence of relaxation parameter $\rho_k$

- Fixed cross-validation tolerance  $\varepsilon_{cv} = 10^{-3}$
- Evolution of relative error indicator  $\varepsilon_{\Xi, \Omega \setminus \Lambda}(U^k; U^{\text{ref}})$  with respect to iteration  $\#k$

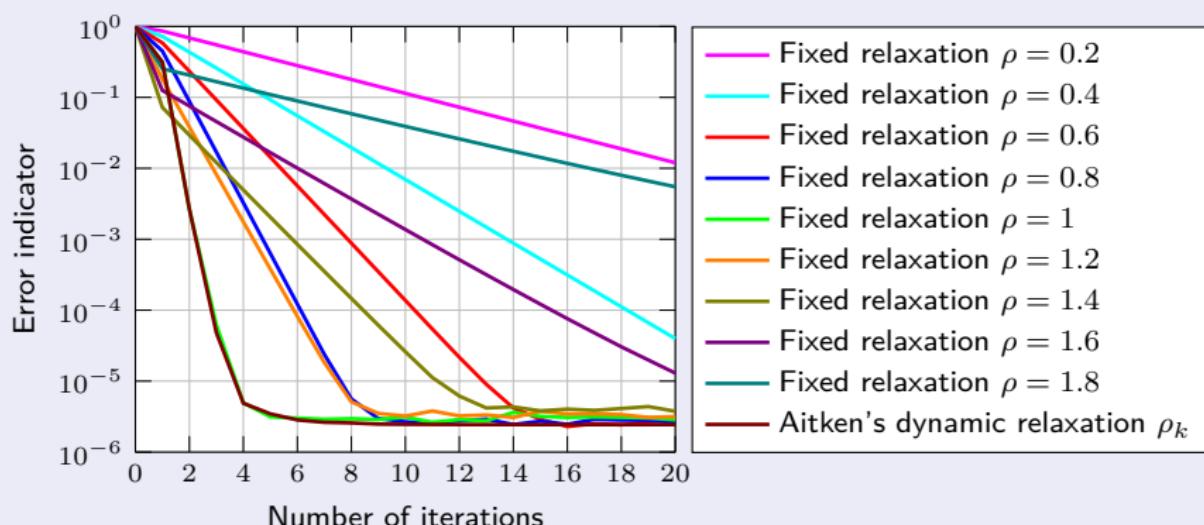


Figure: Isotropic case

→ Strong influence of relaxation parameter  $\rho_k$  on the convergence properties

# Stationary non-linear diffusion-reaction stochastic problem

## Convergence analysis - Influence of relaxation parameter $\rho_k$

- Fixed cross-validation tolerance  $\varepsilon_{cv} = 10^{-3}$
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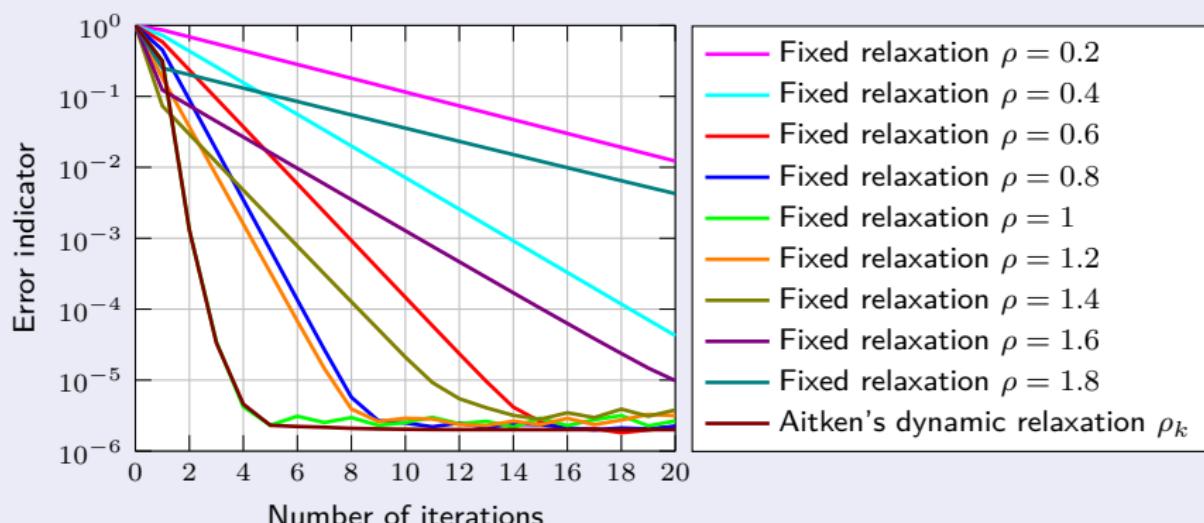


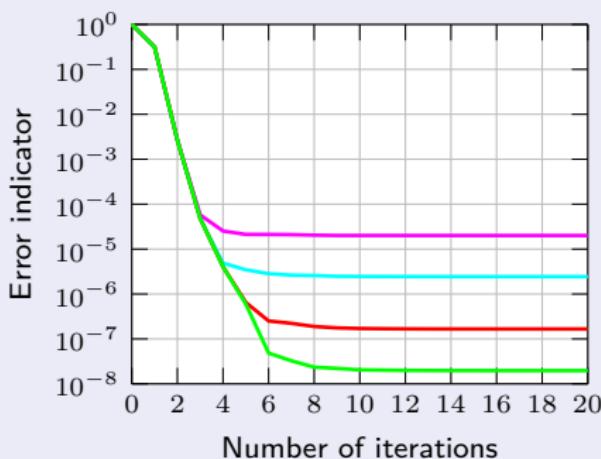
Figure: Anisotropic case

→ Strong influence of relaxation parameter  $\rho_k$  on the convergence properties

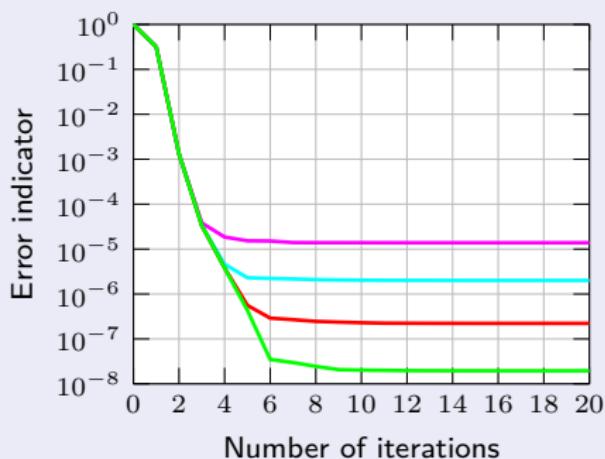
# Stationary non-linear diffusion-reaction stochastic problem

## Convergence analysis - Influence of cross-validation tolerance $\varepsilon_{cv}$

- Relaxation parameter  $\rho_k$  dynamically updated using Aitken's Delta-Squared method
- Evolution of relative error indicator  $\varepsilon_{\Xi, \Omega \setminus \Lambda}(U^k; U^{\text{ref}})$  with respect to iteration  $\#k$



(a) Isotropic case



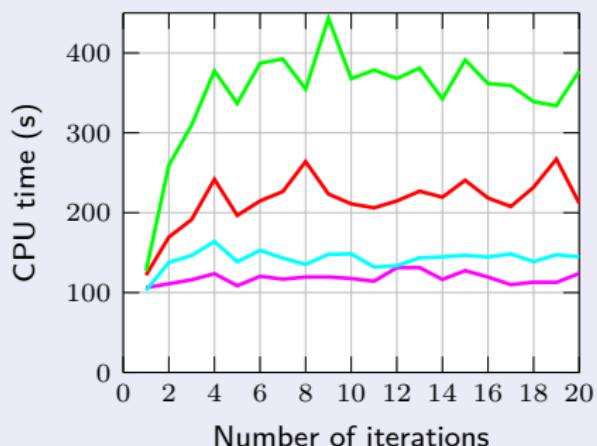
(b) Anisotropic case

—  $\varepsilon_{cv} = 10^{-2}$  —  $\varepsilon_{cv} = 10^{-3}$  —  $\varepsilon_{cv} = 10^{-4}$  —  $\varepsilon_{cv} = 10^{-5}$

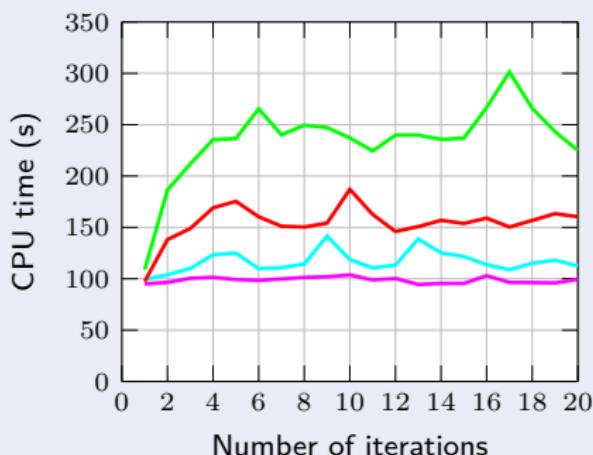
# Stationary non-linear diffusion-reaction stochastic problem

## Computational efficiency - Influence of cross-validation tolerance $\varepsilon_{cv}$

- Relaxation parameter  $\rho_k$  dynamically updated using Aitken's Delta-Squared method
- Evolution of CPU time per iteration with respect to iteration  $\#k$



(a) Isotropic case



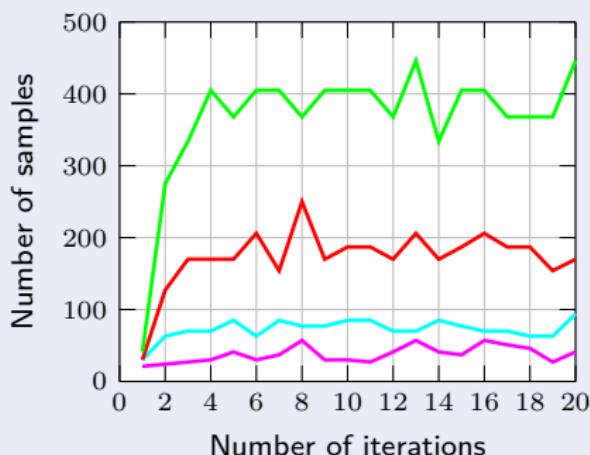
(b) Anisotropic case

—  $\varepsilon_{cv} = 10^{-2}$  —  $\varepsilon_{cv} = 10^{-3}$  —  $\varepsilon_{cv} = 10^{-4}$  —  $\varepsilon_{cv} = 10^{-5}$

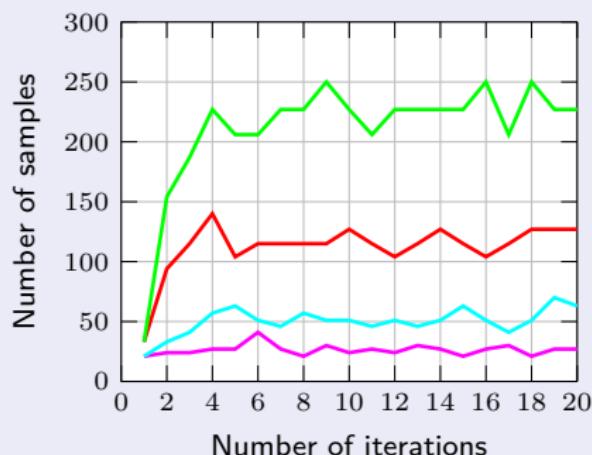
# Stationary non-linear diffusion-reaction stochastic problem

## Adaptive sampling

- Initial sample size  $N = 1$ , Sampling factor  $p_{\text{add}} = 0.1$
- Evolution of sample size  $N_q$  for local solution  $(w_q^k, \lambda_q^k)$  within patch  $\Lambda_q$  with respect to iteration  $\#k$ , for patch  $\#q = 4$



(a) Isotropic case



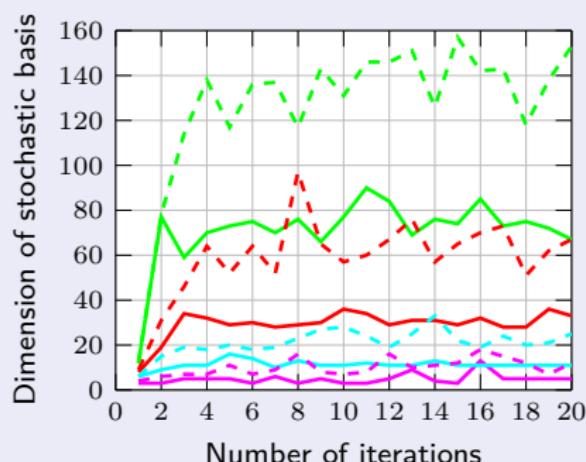
(b) Anisotropic case

—  $\varepsilon_{\text{cv}} = 10^{-2}$  —  $\varepsilon_{\text{cv}} = 10^{-3}$  —  $\varepsilon_{\text{cv}} = 10^{-4}$  —  $\varepsilon_{\text{cv}} = 10^{-5}$

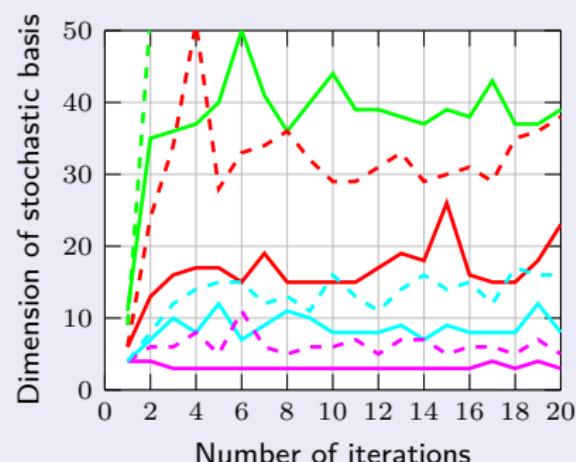
# Stationary non-linear diffusion-reaction stochastic problem

## Adaptive construction of sparse polynomial approximation spaces

- Initial dimension  $\#\mathcal{A}_q = 0$
- Evolution of the dimension  $\#\mathcal{A}_q$  of the stochastic approximation basis for local solution  $w_q^k$  (solid lines) and Lagrange multiplier  $\lambda_q^k$  (dashed lines) with respect to iteration  $\#k$ , for patch  $\#q = 4$



(a) Isotropic case



(b) Anisotropic case



# Stationary non-linear diffusion-reaction stochastic problem

## Adaptive construction of sparse polynomial approximation spaces

- Partial polynomial degrees  $p_i$  (in each random variable  $\xi_i$ ) and dimension  $\#\mathcal{A}$  of approximation spaces  $\mathcal{S}_{\mathcal{A}}$  for global solution  $U$  and local solutions  $(w^q, \lambda^q)$

	$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	$p_6$	$p_7$	$p_8$	$p_9$	$p_{10}$	$p_{11}$	$p_{12}$	$p_{13}$	$p_{14}$	$p_{15}$	$p_{16}$	$\#\mathcal{A}$
$U$	5	2	4	3	4	2	4	3	4	3	4	3	4	2	5	2	192
$w_1$	3	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	9
$\lambda_1$	4	2	2	2	1	1	0	0	0	0	1	0	0	0	0	0	21
$w_2$	2	1	3	2	1	1	0	0	0	0	0	0	0	0	0	0	13
$\lambda_2$	3	1	3	2	2	2	0	1	0	0	0	0	0	0	0	0	19
$w_3$	0	0	1	1	3	2	1	1	0	0	0	0	0	0	0	0	11
$\lambda_3$	1	1	2	1	3	2	2	1	0	1	0	0	0	0	1	1	21
$w_4$	0	0	0	0	1	1	3	2	1	1	0	0	0	0	0	0	11
$\lambda_4$	0	0	0	1	2	2	4	2	2	1	1	0	1	1	0	0	25
$w_5$	0	0	0	0	0	0	1	1	3	2	1	1	0	0	0	0	11
$\lambda_5$	0	0	0	0	0	1	1	2	3	2	2	1	1	0	0	0	20
$w_6$	0	0	0	0	0	0	0	0	1	1	3	2	1	1	0	0	11
$\lambda_6$	0	0	1	0	0	0	1	1	2	2	4	2	2	2	1	1	28
$w_7$	0	0	0	0	0	0	0	0	0	0	1	1	3	2	2	1	13
$\lambda_7$	0	0	0	0	0	0	0	0	1	1	2	2	3	2	3	1	20
$w_8$	0	1	1	0	0	0	0	0	1	0	1	0	1	1	3	1	12
$\lambda_8$	0	1	1	0	0	0	0	0	1	1	1	1	3	2	5	2	26

(a) Isotropic case

# Stationary non-linear diffusion-reaction stochastic problem

## Adaptive construction of sparse polynomial approximation spaces

- Partial polynomial degrees  $p_i$  (in each random variable  $\xi_i$ ) and dimension  $\#\mathcal{A}$  of approximation spaces  $\mathcal{S}_{\mathcal{A}}$  for global solution  $U$  and local solutions  $(w^q, \lambda^q)$

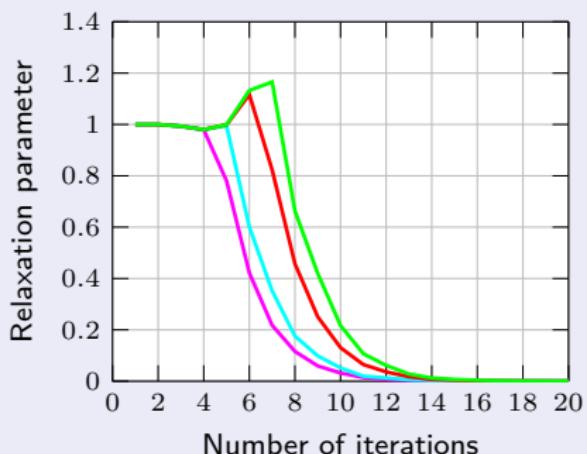
	$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	$p_6$	$p_7$	$p_8$	$p_9$	$p_{10}$	$p_{11}$	$p_{12}$	$p_{13}$	$p_{14}$	$p_{15}$	$p_{16}$	$\#\mathcal{A}$
$U$	5	3	3	2	3	2	3	2	3	2	3	1	2	3	2	1	112
$w_1$	3	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	8
$\lambda_1$	4	2	2	1	1	1	1	0	0	0	0	0	0	0	0	0	18
$w_2$	1	1	2	1	1	1	0	0	0	0	0	0	0	0	0	0	9
$\lambda_2$	2	1	3	2	1	1	0	1	0	0	0	0	0	0	0	0	15
$w_3$	1	0	1	1	2	1	1	2	0	0	0	0	0	0	0	0	13
$\lambda_3$	1	1	2	1	3	2	1	2	0	1	0	0	0	0	0	0	18
$w_4$	0	0	0	0	1	1	2	1	1	1	0	0	0	0	0	0	8
$\lambda_4$	0	0	0	1	1	1	2	2	1	2	0	1	0	0	1	0	16
$w_5$	0	0	0	0	0	0	1	1	2	1	0	1	0	0	0	0	7
$\lambda_5$	0	0	0	0	0	1	1	1	2	2	1	1	0	0	0	0	11
$w_6$	0	0	0	0	0	0	0	0	1	1	2	1	0	1	0	0	7
$\lambda_6$	0	0	0	0	0	0	0	0	1	1	2	1	1	1	0	0	8
$w_7$	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	5
$\lambda_7$	0	0	0	0	0	0	0	0	0	0	1	1	2	1	1	1	8
$w_8$	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	4
$\lambda_8$	0	0	0	0	0	0	0	0	0	0	1	1	2	1	1	1	7

(a) Anisotropic case

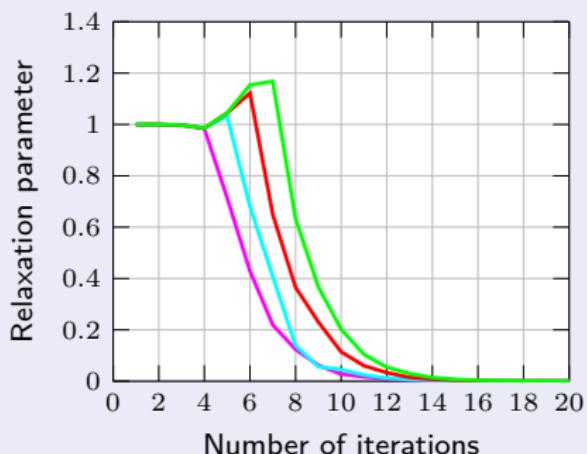
# Stationary non-linear diffusion-reaction stochastic problem

## Aitken's dynamic relaxation

- Evolution of relaxation parameter  $\rho_k$  with respect to iteration  $\#k$



(a) Isotropic case



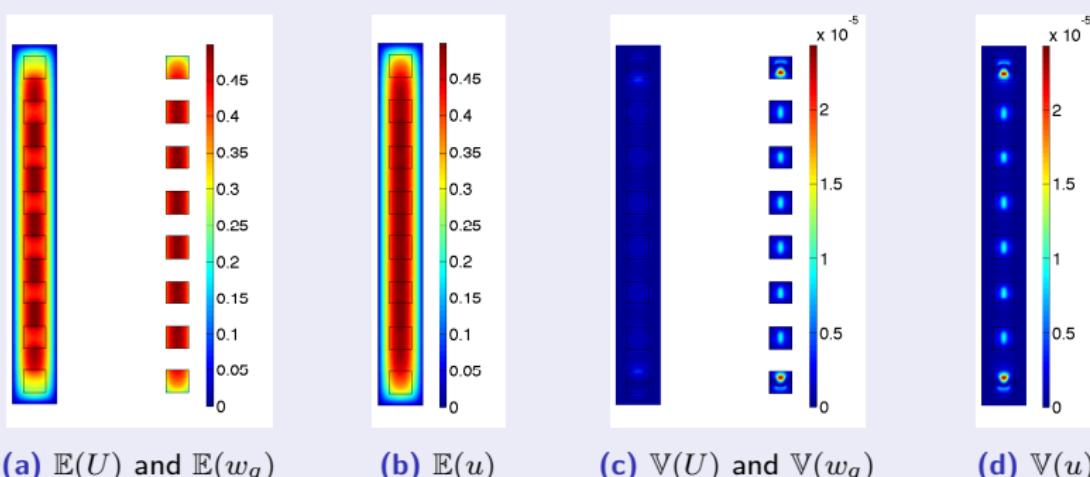
(b) Anisotropic case

Legend:  
—  $\varepsilon_{cv} = 10^{-2}$  —  $\varepsilon_{cv} = 10^{-3}$  —  $\varepsilon_{cv} = 10^{-4}$  —  $\varepsilon_{cv} = 10^{-5}$

# Stationary non-linear diffusion-reaction stochastic problem

## Statistical moments of global, local and multiscale solutions at convergence

- Mean  $\mathbb{E}$  and variance  $\mathbb{V}$  of global solution  $U$ , local solutions  $w_q$  and multiscale solution  $u$



**Figure:** Isotropic problem

↪ The highest spatial contributions to the variance  $\mathbb{V}(u)$  are captured by the local solution  $w_q$  within every patch  $\Lambda_q$

# Stationary non-linear diffusion-reaction stochastic problem

## Statistical moments of global, local and multiscale solutions at convergence

- Mean  $\mathbb{E}$  and variance  $\mathbb{V}$  of global solution  $U$ , local solutions  $w_q$  and multiscale solution  $u$

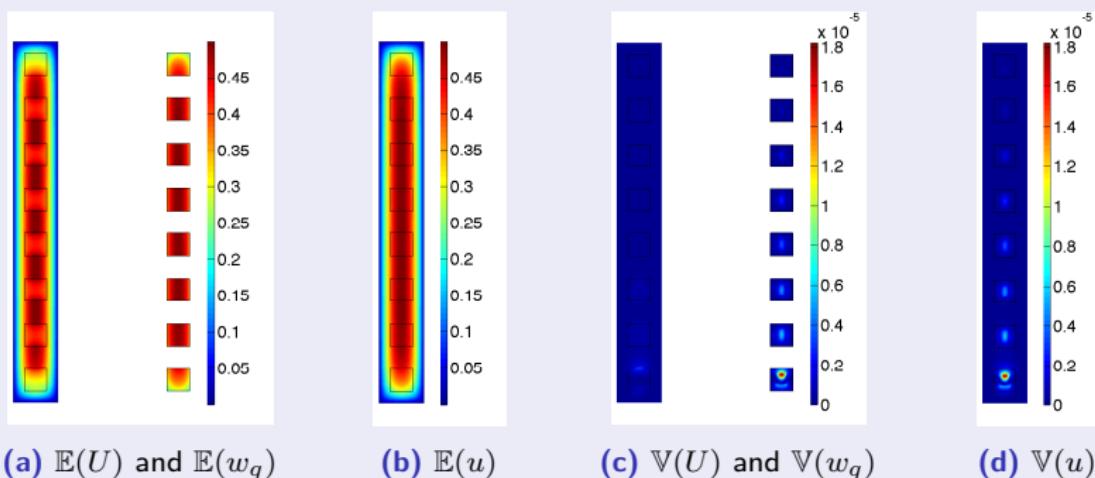


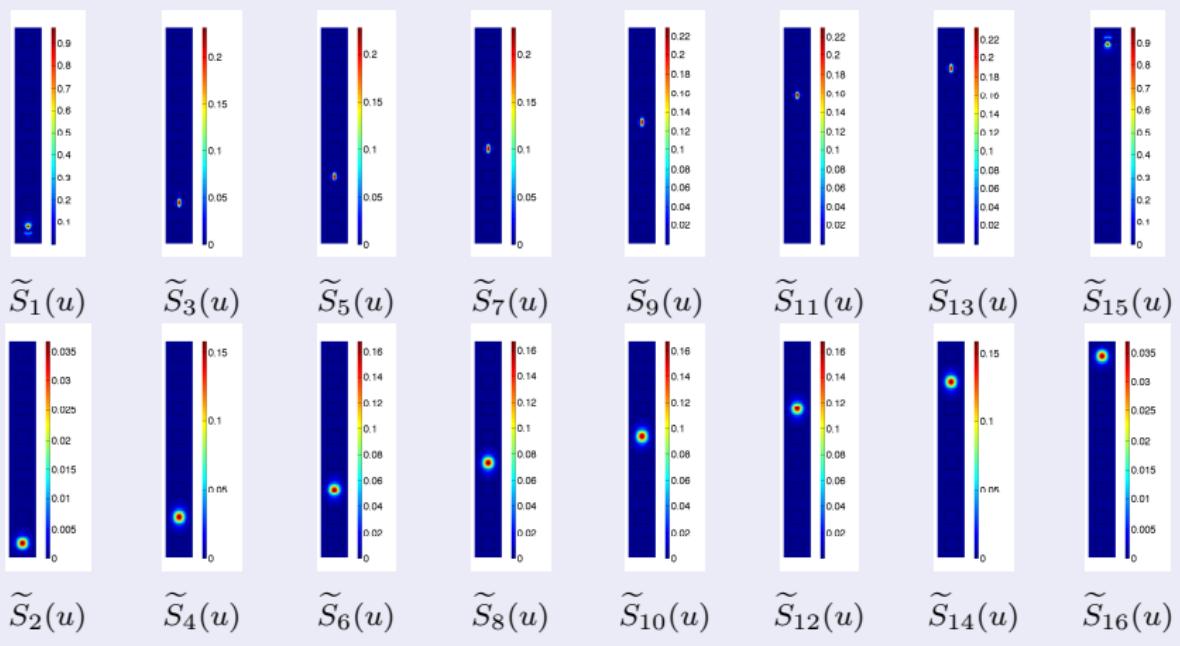
Figure: Anisotropic problem

→ The highest spatial contributions to the variance  $\mathbb{V}(u)$  are localized in the patches exhibiting the highest input variabilities

# Stationary non-linear diffusion-reaction stochastic problem

## Global sensitivity indices of multiscale solution at convergence

- Sensitivity indices  $\tilde{S}_i(u) = \frac{\mathbb{V}(\mathbb{E}(u|\xi_i))}{\max_{x \in \Omega} \mathbb{V}(u)}$  quantifying the **impact** of each **random variable**  $\xi_i$  on the **variance**  $\mathbb{V}(u)$  of multiscale solution  $u$

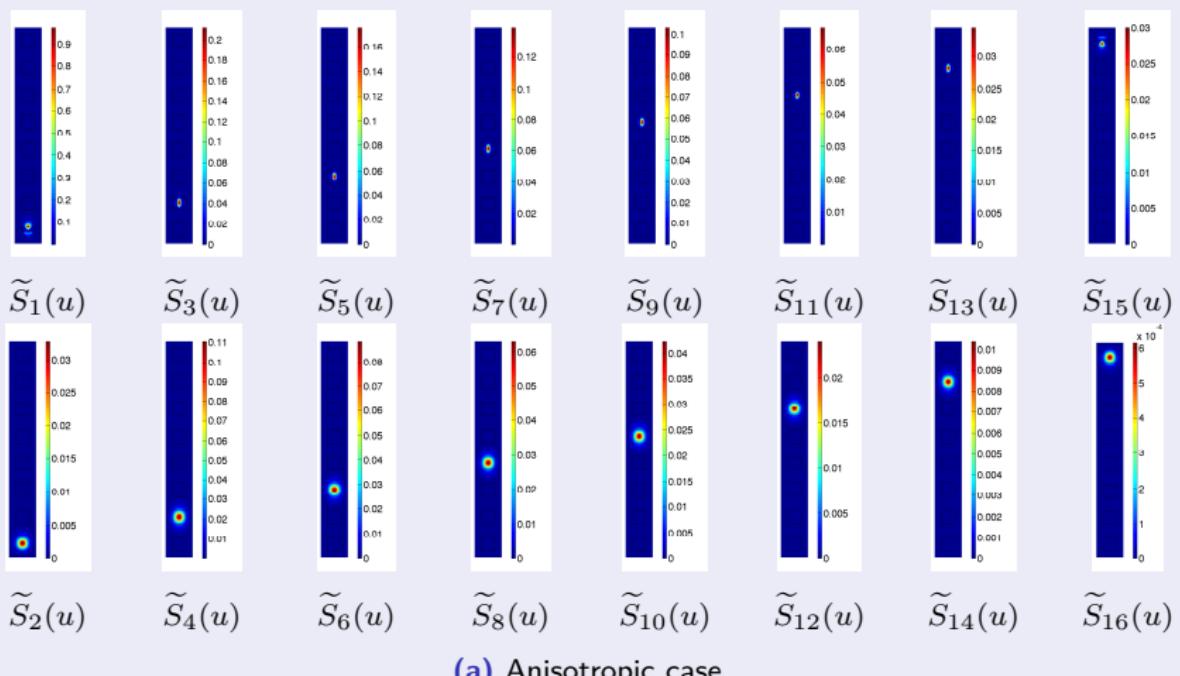


**(a) Isotropic case**

# Stationary non-linear diffusion-reaction stochastic problem

## Global sensitivity indices of multiscale solution at convergence

- Sensitivity indices  $\tilde{S}_i(u) = \frac{\mathbb{V}(\mathbb{E}(u|\xi_i))}{\max_{x \in \Omega} \mathbb{V}(u)}$  quantifying the **impact** of each **random variable**  $\xi_i$  on the **variance**  $\mathbb{V}(u)$  of multiscale solution  $u$



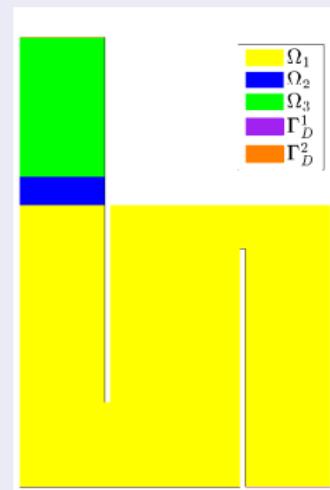
# Transient linear advection-diffusion-reaction deterministic problem

Linear advection-diffusion-reaction problem - Transport of pollutant inside an active carbon filter [Nouy 2010; Parés, Díez, and Huerta 2008]

$$c\dot{u} - \nabla \cdot (K \nabla u) + \alpha \cdot \nabla u + Ru = 0 \quad \text{on } \Omega \times [0, T]$$

$$u = 1 \text{ on } \Gamma_D^1, \quad u = 0 \text{ on } \Gamma_D^2, \quad u = 0 \quad \text{elsewhere on } \partial\Omega$$

$$u_0 = 1 \text{ on } \Gamma_D^1, \quad u_0 = 0 \quad \text{elsewhere on } \Omega$$



- Space domain  $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$
- Time interval  $I = [0, T]$  with  $T = 2 \text{ s}$
- Thermal capacity  $c = 1$
- Diffusion coefficient  $K = 0.01$
- Reaction parameter  $R = \begin{cases} 0.1 & \text{on } \Omega_1 \\ 10 & \text{on } \Omega_2 \cup \Omega_3 \end{cases}$
- Piecewise linear advection field  $\alpha = \nabla \psi$

# Transient linear advection-diffusion-reaction deterministic problem

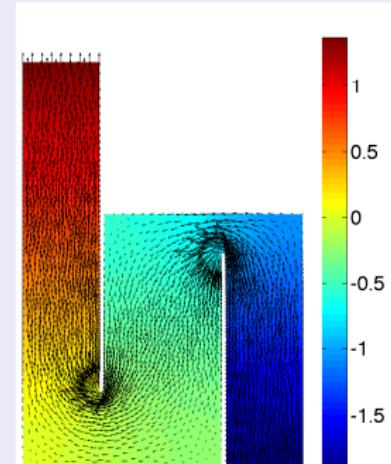
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- Piecewise linear advection field  $\alpha = \nabla\psi$



• Potential flow  $\psi$

# Transient linear advection-diffusion-reaction deterministic problem

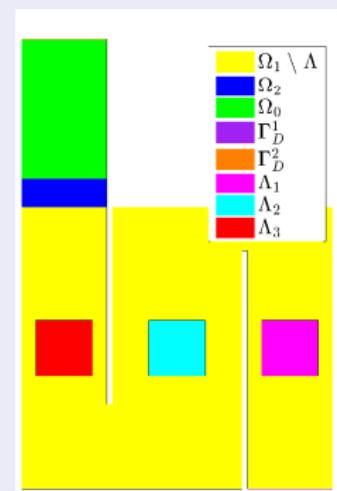
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# Transient linear advection-diffusion-reaction deterministic problem

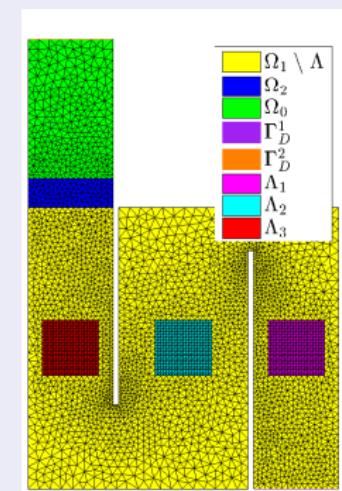
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- Thermal capacity  $c = 1$
- Diffusion coefficient  $K = 0.01$
- Reaction parameter  $R = \begin{cases} 0.1 & \text{on } \Omega_1 \\ 10 & \text{on } \Omega_2 \cup \Omega_3 \end{cases}$
- Piecewise linear advection field  $\alpha = \nabla \psi$



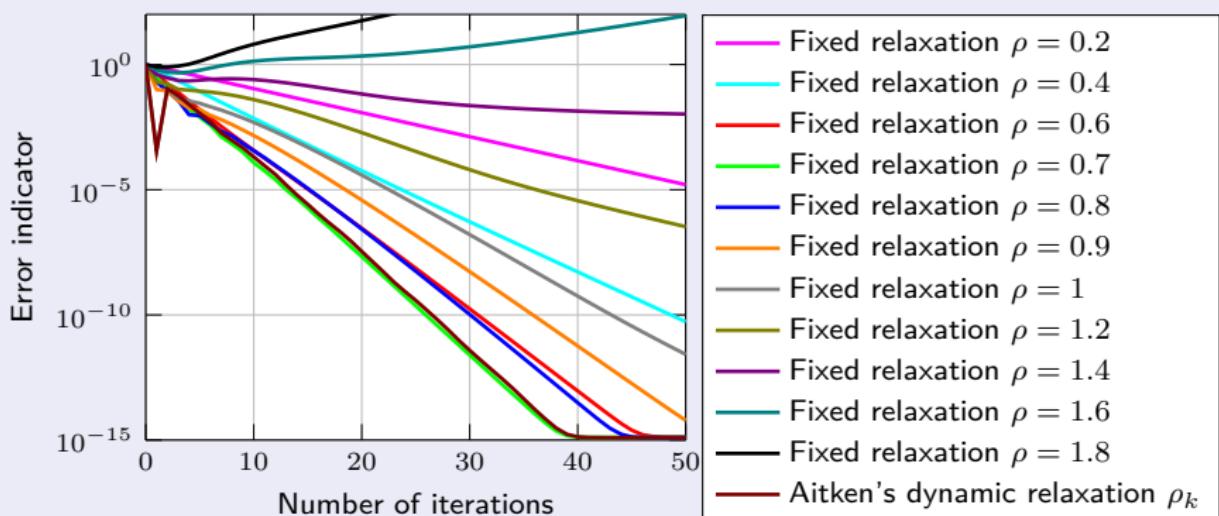
## Approximation spaces

- **Spatial level:** coarse global and fine local finite element approximation spaces
  - $\dim(\tilde{\mathcal{U}}_H) = 3416$  on  $\tilde{\Omega}$
  - $\dim(\mathcal{W}_h^q) = 441$  on  $\Lambda_q$
- **Time level:** implicit Euler time scheme with  $N_t = 100$  time steps

# Transient linear advection-diffusion-reaction deterministic problem

## Convergence analysis - Influence of relaxation parameter $\rho_k$

- Evolution of relative error indicator  $\varepsilon_{\Omega \setminus \Lambda, I}(U^k; U^{\text{ref}})$  with respect to iteration  $\#k$



- Strong influence of relaxation parameter  $\rho_k$  on the convergence properties
- Aitken's acceleration technique provides similar results as those obtained with an optimal fixed relaxation parameter

# Transient linear advection-diffusion-reaction deterministic problem

## Global, local and multiscale solutions at convergence

- Time evolutions of global solution  $U$ , local solutions  $w_q$  and multiscale solution  $u$ 
  - Local solutions  $w_q$

Global solution  $U$

# Transient linear advection-diffusion-reaction deterministic problem

## Global, local and multiscale solutions at convergence

- Time evolutions of **global** solution  $U$ , **local** solutions  $w_q$  and **multiscale** solution  $u$   
**Multiscale** solution  $u$

# Transient linear advection-diffusion-reaction deterministic problem

## Global, local and multiscale solutions at convergence

- Time evolutions of **global** solution  $\dot{U}$ , **local** solutions  $\dot{w}_q$  and **multiscale** solution  $\dot{u}$   
Local solutions  $\dot{w}_q$

Global solution  $\dot{U}$

# Transient linear advection-diffusion-reaction deterministic problem

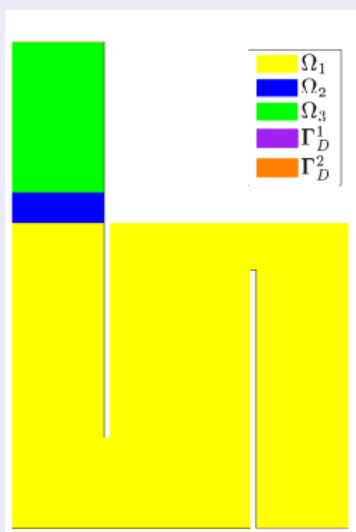
## Global, local and multiscale solutions at convergence

- Time evolutions of **global** solution  $\dot{U}$ , **local** solutions  $\dot{w}_q$  and **multiscale** solution  $\dot{u}$   
**Multiscale** solution  $\dot{u}$

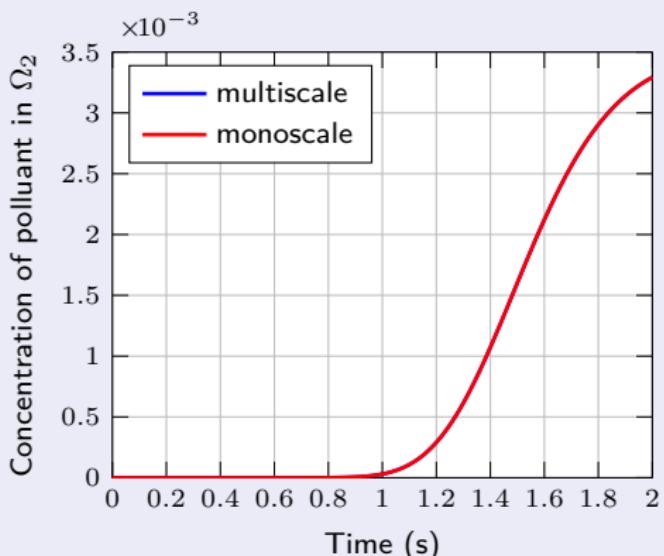
# Transient linear advection-diffusion-reaction deterministic problem

Quantity of interest: concentration of pollutant captured by the trap domain

- Evolution of the concentration of pollutant  $\ell_2(u; t) = \int_{\Omega_2} u(x, y, t) d\Omega$  captured by the trap domain  $\Omega_2$  with respect to time  $t$



(a) Pollutant trap  $\Omega_2$



(b) Concentration of pollutant  $\ell_2(u; t)$

# Transient linear advection-diffusion-reaction deterministic problem

Quantity of interest: concentration of pollutant captured by the trap domain

- Total concentration of pollutant captured by the trap domain  $\Omega_2$  along the complete time evolution  $I = [0, T]$ :

$$L_2(u) = \int_0^T \ell_2(u; t) dt = \int_0^T \int_{\Omega_2} u(x, y, t) d\Omega dt = 1.60876 \times 10^{-3}$$

$$L_2(u^{\text{ref}}) = \int_0^T \ell_2(u^{\text{ref}}; t) dt = \int_0^T \int_{\Omega_2} u^{\text{ref}}(x, y, t) d\Omega dt = 1.60876 \times 10^{-3}$$

with a relative error

$$\varepsilon_L = \frac{L_2(u) - L_2(u^{\text{ref}})}{L_2(u^{\text{ref}})} \approx 3 \times 10^{-15} \quad (\text{machine precision})$$

- The canister is considered to work properly if  $L_2(u)$  is small enough.
- If the outcome of pollutant exceeds a threshold value, the canister breaks and the design is not admissible.

# Outline

- 1 Context and motivation
- 2 Multiscale domain decomposition method
- 3 Computational aspects
- 4 Numerical illustrations
- 5 Conclusions and outlooks

# Conclusions and outlooks

## Conclusions

- A multiscale method dedicated to **localized uncertainties** and possible **localized non-linearities**
  - Domain decomposition method with patches
  - Global-local iterative algorithm with proven convergence properties
- **Analysis** of the **consistency**, **convergence** and **robustness** properties of the algorithm under general assumptions
- Application to a broad class of problems
  - linear [Chevreuil, Nouy, and Safatly 2013] and semi-linear [Nouy and Pled 2017] elliptic equations (linear elasticity, stationnary (non-)linear diffusion-reaction)
  - linear **parabolic** equations (transient linear advection-diffusion-reaction)

## On-going works

- Extension to linear **hyperbolic** equations (linear elasticity structural dynamics)
- Validation on **industrial applications** with 3D complex geometry
- Extension to **non-linear dynamic problems** by incorporating **non-linear effects**
  - geometrical or material non-linearities
  - contact with friction (see [Hager et al. 2012] for a 3D dynamic tire problem with non-linear material and frictional contact)
- Improved sampling-based methods for solving time-dependent local problems

Thanks for your attention !

 Nouy, A. & F. Pled [2017]. "A multiscale method for semi-linear elliptic equations with localized uncertainties and non-linearities". In: *ESAIM: M2AN (submitted)*. 37 pages.

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