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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 Chevreuil² and Anthony Nouy²

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

Context

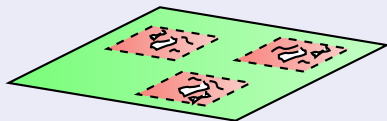
Uncertainty quantification

- 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 Ω 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 Ω 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

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

- 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

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

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

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

- Dedicated strategy to handle high dimensionality and complexity

Challenges

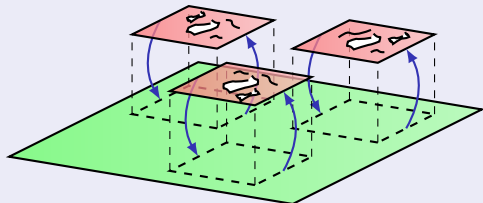
- Develop a multiscale method that exploits the localized side of uncertainties
 - Simple global problem
 - ↔ Traditional solvers / Commercial software packages available in the industry
 - More technical local problems
 - ↔ Specific solvers / In-house research codes

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

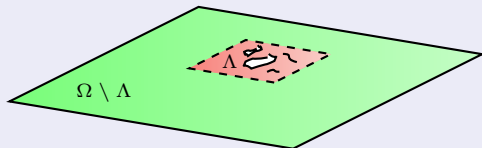
Outline

- 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

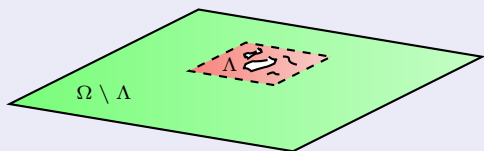
$$\begin{cases} u = 0 & \text{on } \Gamma_D \times I \\ K\nabla u \cdot n = g & \text{on } (\Gamma_N \setminus \Gamma_N^\Lambda) \times I \\ K(\xi)\nabla u \cdot n = g(\xi) & \text{on } \Gamma_N^\Lambda(\xi) \times I \end{cases} \text{ and } \begin{cases} u = u_0 & \text{on } (\Omega \setminus \Lambda) \times \{0\} \\ u = u_0(\xi) & \text{on } \Lambda(\xi) \times \{0\} \end{cases}$$

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

$$m_{\Omega}(\dot{u}(\xi), \delta u; \xi) + a_{\Omega}(u(\xi), \delta u; \xi) = \ell_{\Omega}(\delta u; \xi) \quad \forall \delta u \in \mathcal{V}$$

$$u|_{t=0+}(\xi) = u_0(\xi)$$

with **bilinear** forms $a_{\Omega}(u, v; \xi) = \int_{\Omega} K(\xi) \nabla u \cdot \nabla v + \int_{\Omega} \alpha(\xi) \cdot \nabla u v + \int_{\Omega} R(\xi) uv$,

$m_{\Omega}(u, v; \xi) = \int_{\Omega} c(\xi) uv$ and **linear** form $\ell_{\Omega}(v; \xi) = \int_{\Omega} f(\xi) v + \int_{\Gamma_N} g(\xi) v$.

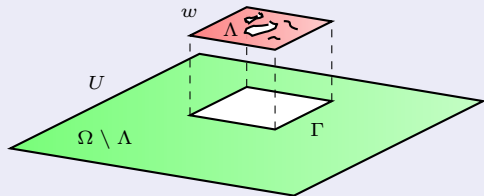
Global-local formulation with patches

Domain decomposition - Introduction of a patch

- Separation of the solution

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

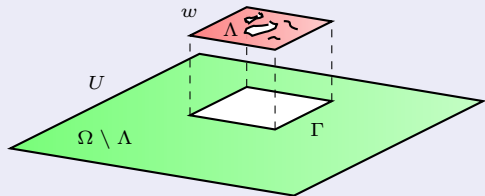
with $U = w$ on Γ (weak sense)



Global-local formulation with patches

Domain decomposition - Introduction of a patch

- **Uncertain** domain Ω
- **Deterministic** subdomain $\Omega \setminus \Lambda$
- **Uncertain** patch Λ
- **Deterministic** interface Γ



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 Λ

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

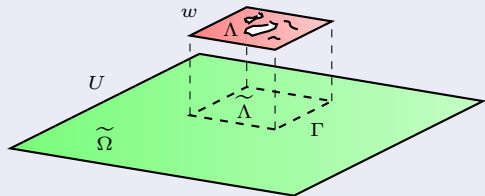
- **Coupling** equation on interface Γ

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

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 Λ
- **Deterministic** interface Γ



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 $\tilde{\Omega} = (\Omega \setminus \Lambda) \cup \tilde{\Lambda}$

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

- **Local** equation on patch Λ

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

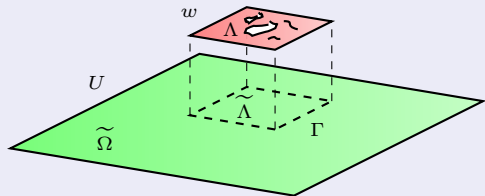
- **Coupling** equation on interface Γ

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

Global-local formulation with patches

Overlapping domain decomposition - Introduction of a fictitious patch

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

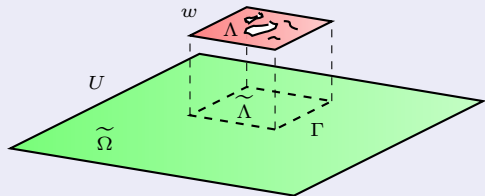
where **bilinear** forms $n_{\mathcal{O}}(U, V; \xi) = \int_{\mathcal{O}} \tilde{c}(\xi) UV$ and

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

Global-local formulation with patches

Overlapping domain decomposition - Introduction of a fictitious patch

- **Deterministic fictitious** domain $\tilde{\Omega}$
- **Deterministic fictitious** patch $\tilde{\Lambda}$
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Reformulation with overlapping domains

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

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

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

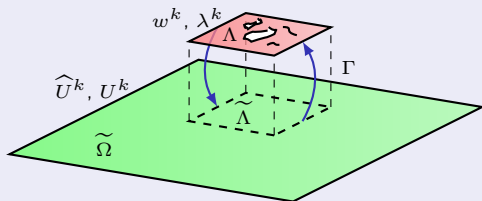
$$c_{\mathcal{O}}(U, V; \xi) = \int_{\mathcal{O}} \tilde{K}(\xi) \nabla U \cdot \nabla V + \int_{\mathcal{O}} \tilde{\alpha}(\xi) \cdot \nabla U V + \int_{\mathcal{O}} \tilde{R}(\xi) UV.$$

Global-local iterative algorithm

Iterative coupling procedure

1

Global step

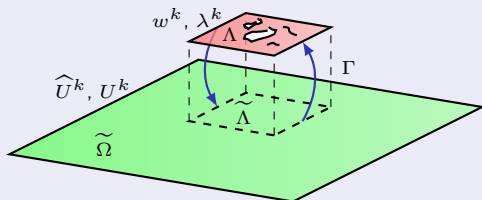
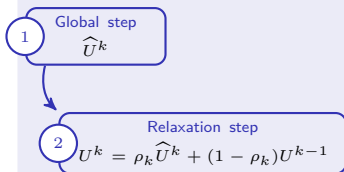
 \hat{U}^k 

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

$$n_{\tilde{\Omega}}(\hat{U}^k(\xi), \delta U) + c_{\tilde{\Omega}}(\hat{U}^k(\xi), \delta U) = n_{\tilde{\Lambda}}(\hat{U}^{k-1}(\xi), \delta U) + c_{\tilde{\Lambda}}(\hat{U}^{k-1}(\xi), \delta U) - b_{\Gamma}(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

Global-local iterative algorithm

Iterative coupling procedure



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

$$n_{\widetilde{\Omega}}(\dot{\widehat{U}}^k(\xi), \delta U) + c_{\widetilde{\Omega}}(\widehat{U}^k(\xi), \delta U) = n_{\widetilde{\Lambda}}(\dot{U}^{k-1}(\xi), \delta U) + c_{\widetilde{\Lambda}}(U^{k-1}(\xi), \delta U) - b_{\Gamma}(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

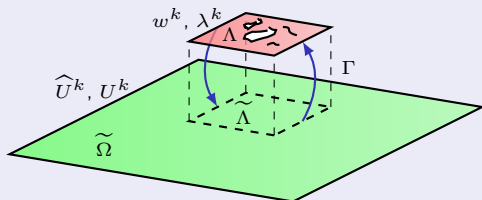
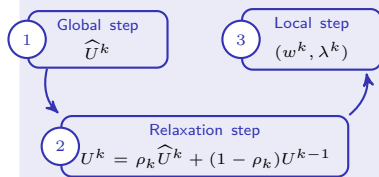
- ② **Relaxation step:** Define $U^k \in \widetilde{U}^\Xi$ by

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

↪ Significant influence on the convergence properties of the algorithm

Global-local iterative algorithm

Iterative coupling procedure



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

$$n_{\widetilde{\Omega}}(\dot{\widehat{U}}^k(\xi), \delta U) + c_{\widetilde{\Omega}}(\widehat{U}^k(\xi), \delta U) = n_{\widetilde{\Lambda}}(\dot{U}^{k-1}(\xi), \delta U) + c_{\widetilde{\Lambda}}(U^{k-1}(\xi), \delta U) - b_{\Gamma}(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

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

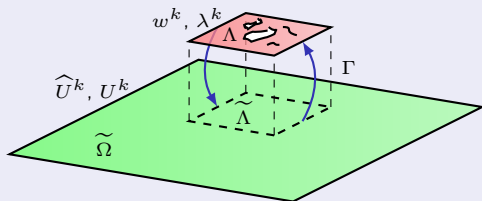
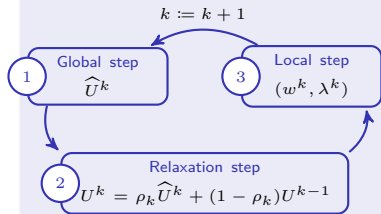
$$U^k(\xi) = \rho_k \widehat{U}^k(\xi) + (1 - \rho_k) U^{k-1}(\xi) \quad \text{with relaxation parameter } \rho_k > 0$$

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

$$\begin{cases} m_{\Lambda}(\dot{w}^k(\xi), \delta w; \xi) + a_{\Lambda}(w^k(\xi), \delta w; \xi) - b_{\Gamma}(\lambda^k(\xi), \delta w) = \ell_{\Lambda}(\delta w; \xi) & \forall \delta w \in \mathcal{W} \\ b_{\Gamma}(\delta \lambda, w^k(\xi)) = b_{\Gamma}(\delta \lambda, U^k(\xi)) & \forall \delta \lambda \in \mathcal{M} \end{cases}$$

Global-local iterative algorithm

Iterative coupling procedure



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

$$n_{\widetilde{\Omega}}(\dot{\widehat{U}}^k(\xi), \delta U) + c_{\widetilde{\Omega}}(\widehat{U}^k(\xi), \delta U) = n_{\widetilde{\Lambda}}(\dot{U}^{k-1}(\xi), \delta U) + c_{\widetilde{\Lambda}}(U^{k-1}(\xi), \delta U) - b_{\Gamma}(\lambda^{k-1}(\xi), \delta U) + \ell_{\Omega \setminus \Lambda}$$

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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 Γ .
- The extended global solution $U \in L^p_\mu(\Xi; \tilde{\mathcal{U}})$, with exponent $2 \leq p \leq +\infty$.

Convergence

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

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

for some strictly positive constants ρ_{inf} and ρ_{sup} independent of ξ and k .

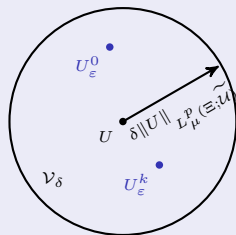
- Then, for ρ_{sup} **sufficiently small**, the sequence $\{(U^k(\xi), w^k(\xi), \lambda^k(\xi))\}_{k \in \mathbb{N}}$ converges almost surely to the unique solution $(U(\xi), w(\xi), \lambda(\xi))$ of the initial global-local problem in $\tilde{\mathcal{U}}_*(\xi) \times \mathcal{W} \times \mathcal{M}$.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

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_ε^k and the unperturbed one U^k at iteration k in a L_μ^p -norm
- Under certain assumptions on the unperturbed and perturbed iteration maps, if the initial global iterate U_ε^0 is in a δ -neighborhood \mathcal{V}_δ of the exact global solution U , then all global iterates U_ε^k remain in \mathcal{V}_δ , 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}_δ of radius $\delta \|U\|_{L_\mu^p(\Xi; \tilde{\mathcal{U}})}$ centered at the exact global solution U and containing all global iterates U_ε^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 α .

- 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:

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

where $\Psi = (\psi_{\alpha}(\xi^l))_{1 \leq l \leq N, \alpha \in \mathcal{A}} \in \mathbb{R}^{N \times \#\mathcal{A}}$ 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 α 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}

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

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

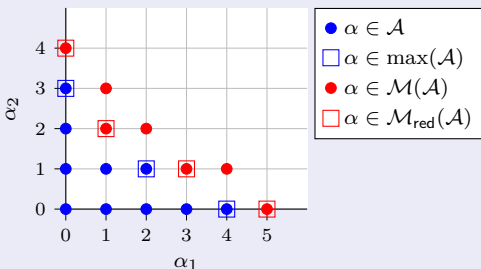


Figure: Monotone multi-index set \mathcal{A} , its maximal elements $\max(\mathcal{A})$, its margin $\mathcal{M}(\mathcal{A})$ and reduced margin $\mathcal{M}_{\text{red}}(\mathcal{A})$

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]

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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 $\varepsilon = (\varepsilon_i)_{i \in \mathcal{I}}$, where ε_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

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

- 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: 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

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

- 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: // 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

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

- 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: // 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 ρ 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 ρ_{opt} defined by [Xu 1992]

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

where λ_{\min} and λ_{\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 [Irons 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; Küttler and Wall 2008; Liu, Sun, and Fan 2014]

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

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

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

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

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]

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

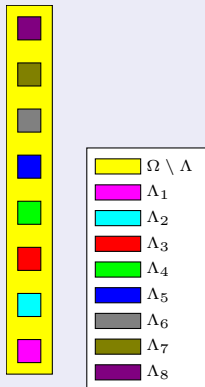
$$u = 0 \quad \text{on } \Gamma_D = \partial\Omega$$

- 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 $\Xi_i = (0, 1)$
- Uniform weights $\gamma_q = 1$



Stationary non-linear diffusion-reaction stochastic problem

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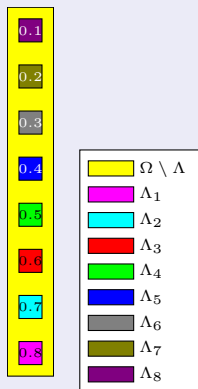
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- **Uniform** random variables $\xi = (\xi_i)_{i=1}^{16}$ on $\Xi_i = (0, 1)$
- **Heterogeneous** weights $\gamma_q = 1 - 0.1(q + 1)$



Stationary non-linear diffusion-reaction stochastic problem

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

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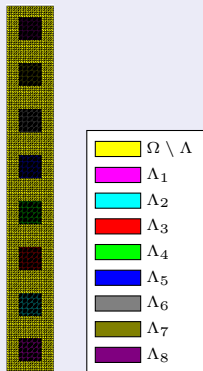
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- **Uniform** random variables $\xi = (\xi_i)_{i=1}^{16}$ on $\Xi_i = (0, 1)$
- **Heterogeneous** weights $\gamma_q = 1 - 0.1(q + 1)$



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 Λ_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^{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^{ref} and approximation spaces $\mathcal{S}_{\mathcal{A}^{\text{ref}}}$ 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^{ref}
 - Anisotropic case:**
 - $N^{\text{ref}} = 491$ samples
 - $\#\mathcal{A}^{\text{ref}} = 173$ for U^{ref}

Stationary non-linear diffusion-reaction stochastic problem

Convergence analysis - Influence of relaxation parameter ρ_k

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

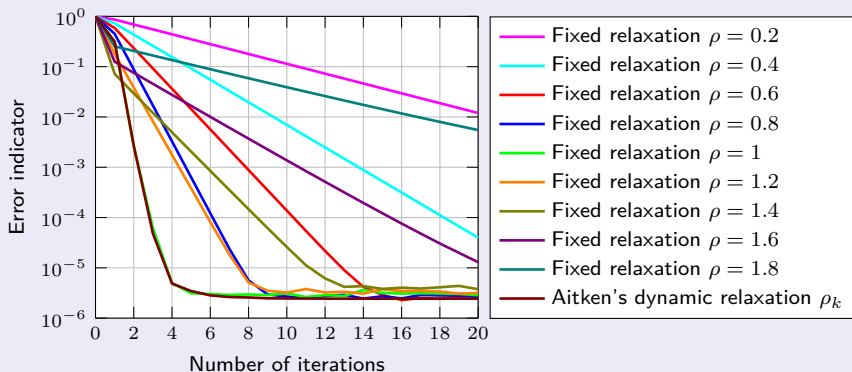


Figure: Isotropic case

↪ Strong influence of relaxation parameter ρ_k on the convergence properties

Stationary non-linear diffusion-reaction stochastic problem

Convergence analysis - Influence of relaxation parameter ρ_k

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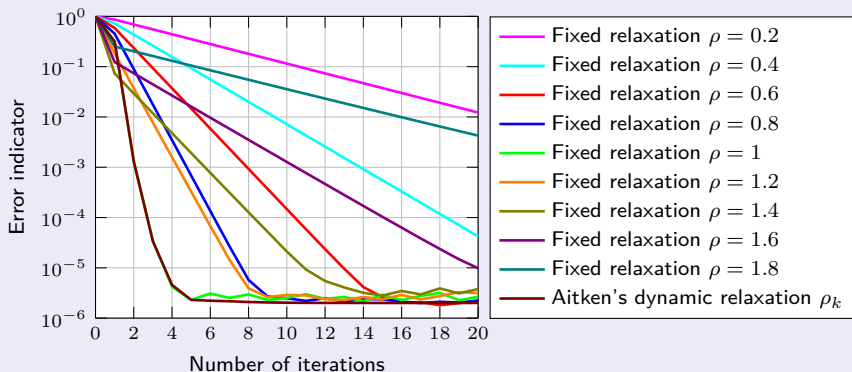


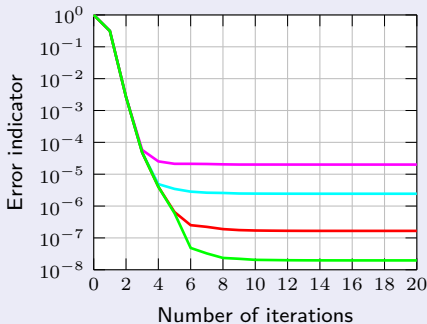
Figure: Anisotropic case

↪ Strong influence of relaxation parameter ρ_k on the convergence properties

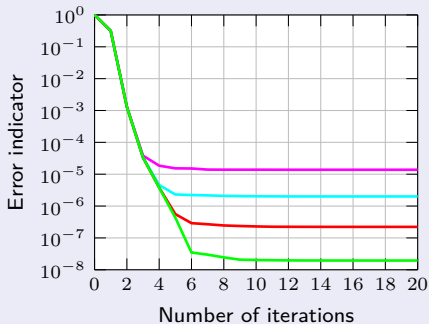
Stationary non-linear diffusion-reaction stochastic problem

Convergence analysis - Influence of cross-validation tolerance ε_{cv}

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



(a) Isotropic case



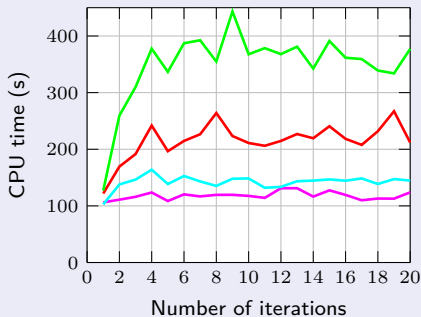
(b) Anisotropic case

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

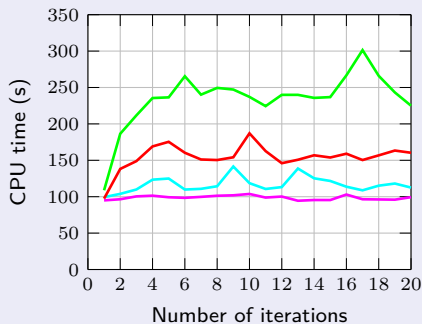
Stationary non-linear diffusion-reaction stochastic problem

Computational efficiency - Influence of cross-validation tolerance ϵ_{cv}

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



(a) Isotropic case



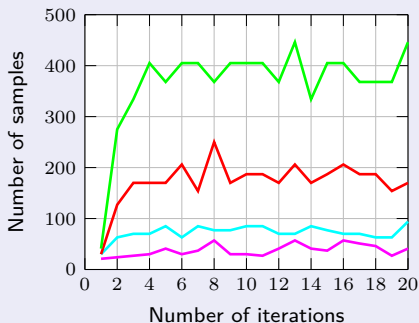
(b) Anisotropic case

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

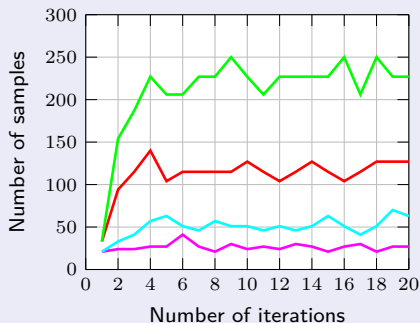
Stationary non-linear diffusion-reaction stochastic problem

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, λ_q^k) within patch Λ_q with respect to iteration $\#k$, for patch $\#q = 4$



(a) Isotropic case



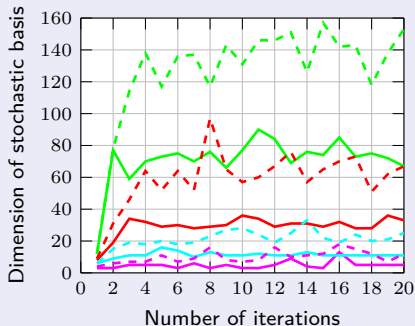
(b) Anisotropic case



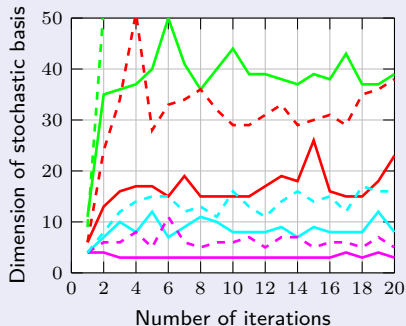
Stationary non-linear diffusion-reaction stochastic problem

Adaptive construction of sparse polynomial approximation spaces

- 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 λ_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 ξ_i) and dimension $\#\mathcal{A}$ of approximation spaces $\mathcal{S}_{\mathcal{A}}$ for global solution U and local solutions (w^q, λ^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	1	0	0	0	0	0	0	0	0	0	0	0	9
λ_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
λ_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
λ_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
λ_4	0	0	0	1	2	2	4	2	2	1	1	1	0	1	1	0	25
w_5	0	0	0	0	0	0	1	1	3	2	1	1	0	0	0	0	11
λ_5	0	0	0	0	0	1	1	2	3	2	2	1	1	1	0	0	20
w_6	0	0	0	0	0	0	0	0	1	1	3	2	1	1	0	0	11
λ_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
λ_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
λ_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 ξ_i) and dimension $\#\mathcal{A}$ of approximation spaces $\mathcal{S}_{\mathcal{A}}$ for global solution U and local solutions (w^q, λ^q)

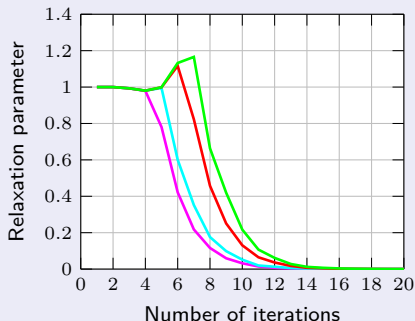
	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}	p_{12}	p_{13}	p_{14}	p_{15}	p_{16}	$\#\mathcal{A}$
U	5	3	3	2	3	2	3	2	3	2	3	1	2	3	2	1	112
w_1	3	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	8
λ_1	4	2	2	1	1	1	1	0	0	0	0	0	0	0	0	0	18
w_2	1	1	2	1	1	1	0	0	0	0	0	0	0	0	0	0	9
λ_2	2	1	3	2	1	1	0	1	0	0	0	0	0	0	0	0	15
w_3	1	0	1	1	2	1	1	2	0	0	0	0	0	0	0	0	13
λ_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
λ_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
λ_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
λ_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
λ_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	0	1	1	1	4
λ_8	0	0	0	0	0	0	0	0	0	0	0	1	1	1	2	1	7

(a) Anisotropic case

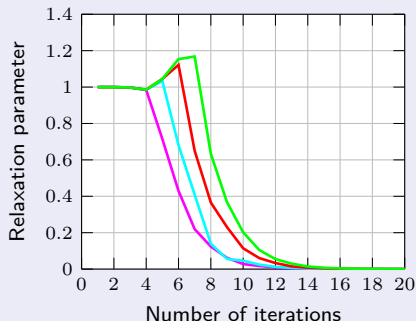
Stationary non-linear diffusion-reaction stochastic problem

Aitken's dynamic relaxation

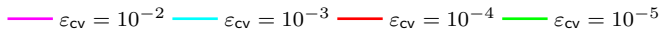
- Evolution of relaxation parameter ρ_k with respect to iteration $\#k$



(a) Isotropic case



(b) Anisotropic case



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

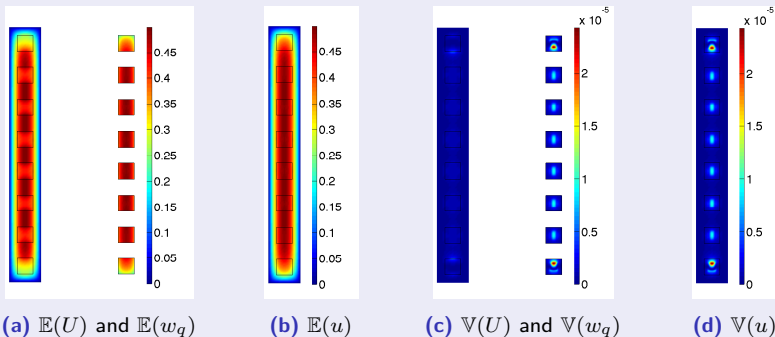


Figure: Isotropic problem

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

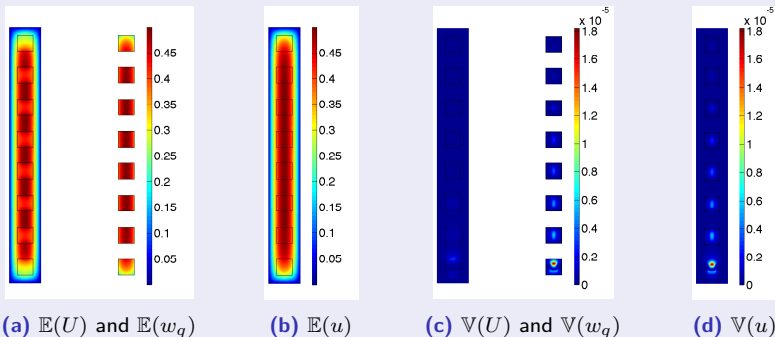


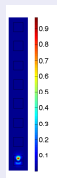
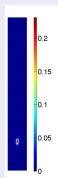
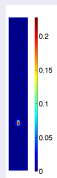
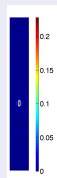
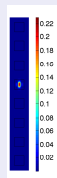
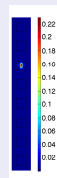
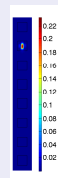
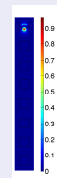
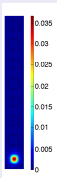
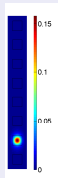
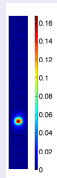
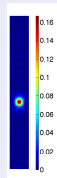
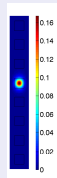
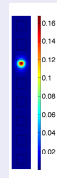
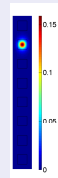
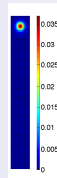
Figure: Anisotropic problem

↔ 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 ξ_i on the variance $\mathbb{V}(u)$ of multiscale solution u

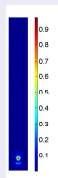
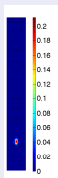
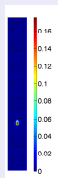
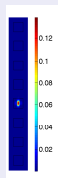
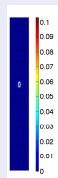
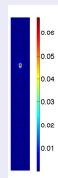
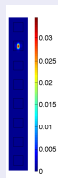
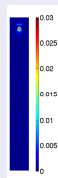
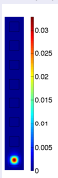
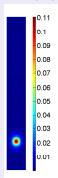
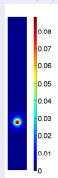
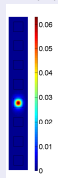
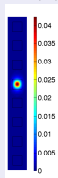
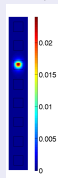
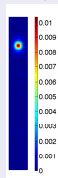
 $\tilde{S}_1(u)$  $\tilde{S}_3(u)$  $\tilde{S}_5(u)$  $\tilde{S}_7(u)$  $\tilde{S}_9(u)$  $\tilde{S}_{11}(u)$  $\tilde{S}_{13}(u)$  $\tilde{S}_{15}(u)$  $\tilde{S}_2(u)$  $\tilde{S}_4(u)$  $\tilde{S}_6(u)$  $\tilde{S}_8(u)$  $\tilde{S}_{10}(u)$  $\tilde{S}_{12}(u)$  $\tilde{S}_{14}(u)$  $\tilde{S}_{16}(u)$

(a) Isotropic case

Stationary non-linear diffusion-reaction stochastic problem

Global sensitivity indices of multiscale solution at convergence

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(a) Anisotropic case

Transient linear advection-diffusion-reaction deterministic problem

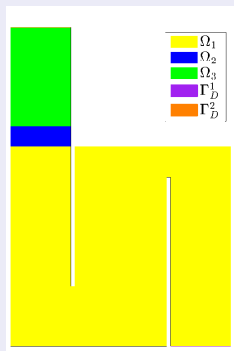
Linear advection-diffusion-reaction problem - Transport of pollutant inside an active carbon filter [Nouy 2010; Parés, Díez, and Huerta 2008]

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

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

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

- 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

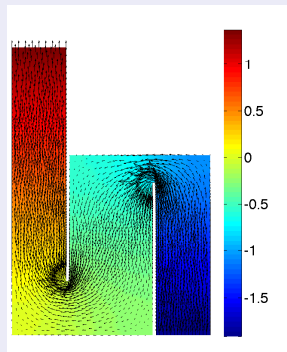
Linear advection-diffusion-reaction problem - Transport of pollutant inside an active carbon filter [Nouy 2010; Parés, Díez, and Huerta 2008]

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



- Potential flow ψ

Transient linear advection-diffusion-reaction deterministic problem

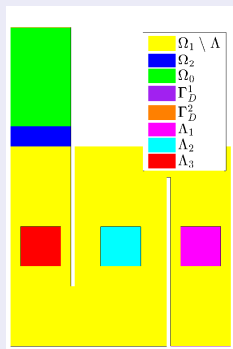
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Transient linear advection-diffusion-reaction deterministic problem

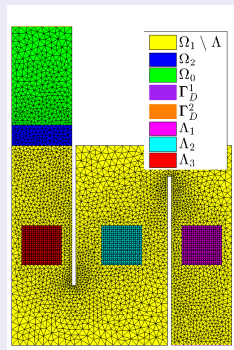
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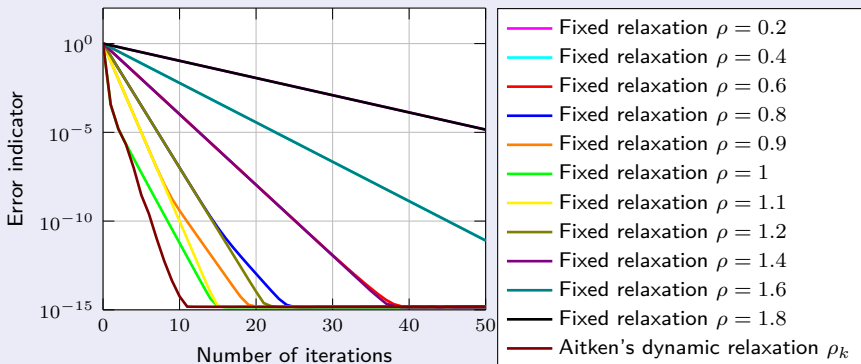
Approximation spaces

- **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 Λ_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 ρ_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 ρ_k on the convergence properties
- ↪ Aitken's acceleration technique provides better 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

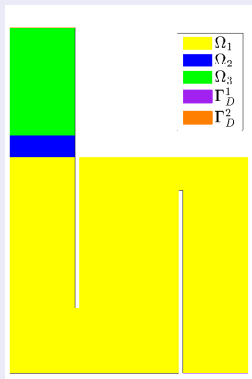
Global, local and multiscale solutions at convergence

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

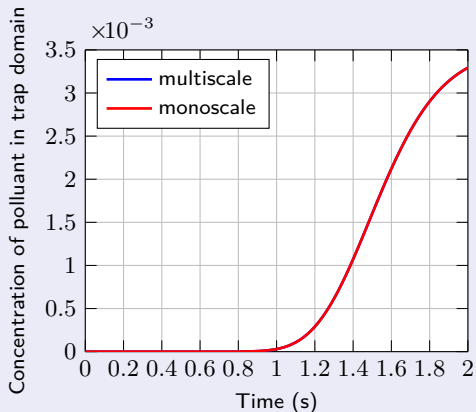
Transient linear advection-diffusion-reaction deterministic problem

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 Ω_2 with respect to time t



(a) Pollutant trap Ω_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 Ω_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, stationary (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 !

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