Radboud University

Quantifying the effects of geometric uncertainties

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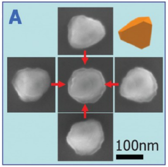
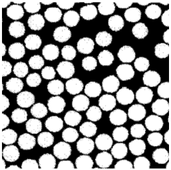
06.10.2022

What are geometric uncertainties?

At the continuum scale, possible variabilities in **boundaries** or **interfaces**.

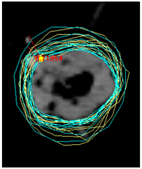


Sannomiya, Diss. ETHZ 18747



Babuška et al. (1999)

serc.carleton.edu



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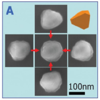
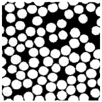
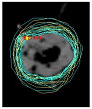
Sources of geometric uncertainties





Intrinsic variability:

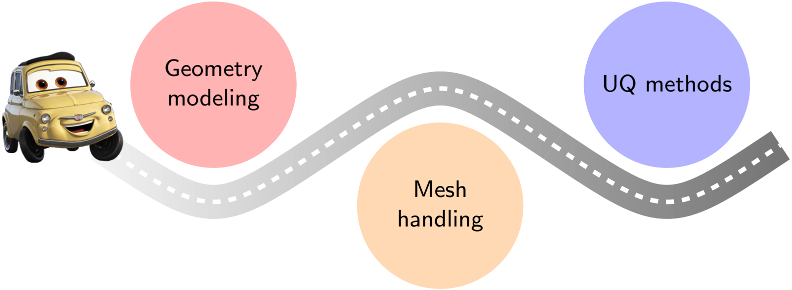
manufacturing defects, randomness in production process, biological variations ...



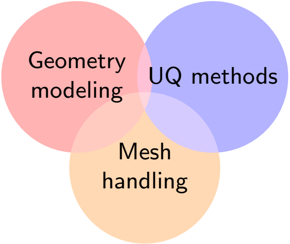
Lack of knowledge:

limited measurements, definition of target volume ...

Roadmap



Applications



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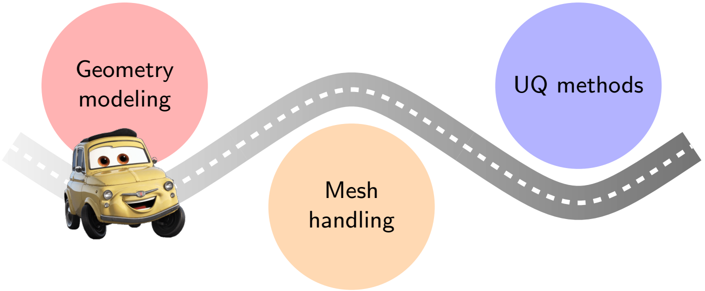


Geometry modeling

Shape variations

Domain mapping

Topology variations

Level set

Point processes

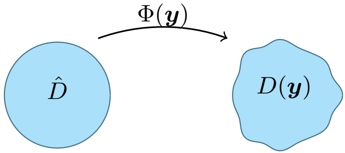
⚠ High dimensionality

Shape variations via domain mapping

Reference domain $\hat{D}$, bounded and Lipschitz

$$\Phi(\boldsymbol{y};\hat{\boldsymbol{x}}) = \hat{\boldsymbol{x}} + \sum_{j=1}^{d} y_j \Phi_j(\hat{\boldsymbol{x}}),\ \boldsymbol{y} \in [-1,1]^d.$$

Set $D(\boldsymbol{y}) := \Phi(\boldsymbol{y};\hat{D})$.



Remark: Given a **boundary parametrization**

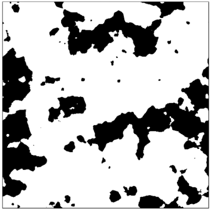
$$\gamma(\boldsymbol{y};s) = \gamma_0(s) + \sum_{j=1}^{d} y_j \psi_j(s),$$

a domain transformation can be obtained by extension.

Topology variations

Level set

Given
$$m(\boldsymbol{y};\boldsymbol{x}) = m_0(\boldsymbol{x}) + \sum_{j=1}^{d} y_j \psi_j(\boldsymbol{x}),$$
with y_j i.i.d., define
$$\Gamma(\boldsymbol{y}) := \{\boldsymbol{x} \in D : m(\boldsymbol{y};\boldsymbol{x}) = \tau\}$$



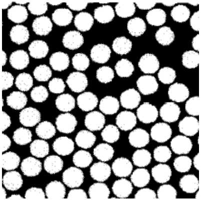
Khristenko et al. (2020)

Point process

A number N of objects

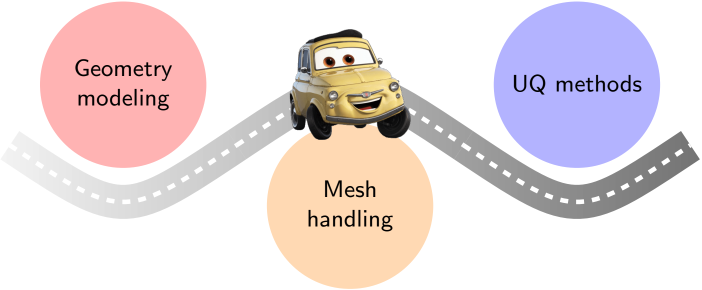
A set $\{\boldsymbol{y}_j\}_{j=1}^{N}$ of points

A shape around each point



Babuška et al. (1999)

Roadmap



Mesh handling

We want to solve

$$\begin{aligned} -\nabla \cdot (a\nabla u) &= f \quad \text{in } D(\boldsymbol{y}), \\ u &= 0 \quad \text{on } \partial D(\boldsymbol{y}) \end{aligned}$$

Possibilities

Fictitious domain approach [Canuto Kozubek 2007]

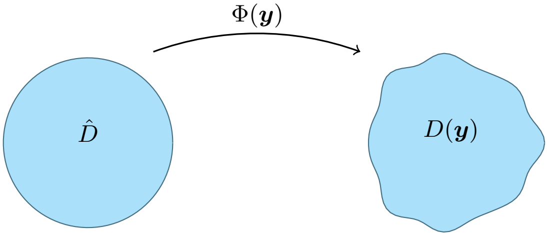
Working on the reference domain [Xiu Tartakovski 2006]

Isogeometric analysis [Dölz et al. 2022]

Moving the mesh / Remeshing

Working on the reference domain

[Xiu Tartakovski 2006]

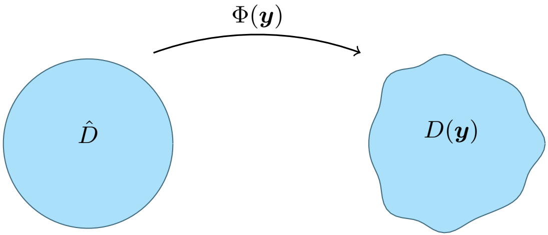


Variational formulation

$$\int_{D(\boldsymbol{y})} a \nabla u(\boldsymbol{y}) \cdot \nabla v \, \mathrm{d}x = \int_{D(\boldsymbol{y})} f v \, \mathrm{d}x$$

Working on the reference domain

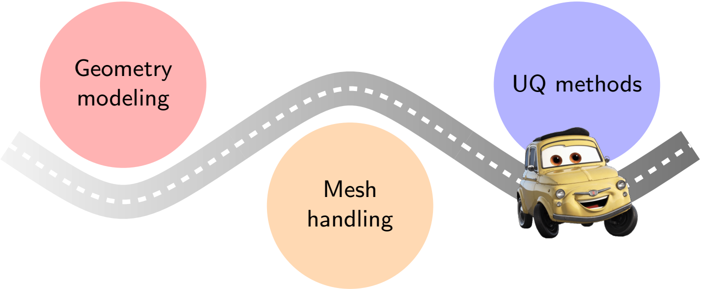
[Xiu Tartakovski 2006]



Variational formulation on **reference domain**

$$\int_{\hat{D}} \underbrace{D\Phi^{-1}(a \circ \Phi) D\Phi^{-\top} \det(D\Phi)}_{\hat{A}(\boldsymbol{y})} \hat{\nabla} \hat{u}(\boldsymbol{y}) \cdot \hat{\nabla} \hat{v} \, \mathrm{d}\hat{x} = \int_{\hat{D}} \underbrace{\det(D\Phi)(f \circ \Phi)}_{\hat{f}(\boldsymbol{y})} \cdot \hat{v} \, \mathrm{d}\hat{x}$$

Roadmap



Non-intrusive UQ methods

$$Q(\boldsymbol{y}),\ \boldsymbol{y} \in [-1,1]^d$$

Moments	Surrogates
Perturbation methods	Reduced Basis
Stochastic collocation	**Stochastic collocation**
(Multilevel) Monte Carlo	**Neural networks**
(High-order) quasi Monte Carlo	Weighted least squares

⚠ High dimensionality

Monte Carlo integration

"Throw the dice" and average:

$$\mathbb{E}[Q] \approx \frac{1}{M} \sum_{m=1}^{M} Q(\boldsymbol{y}_m) := E_M[Q]$$

Error bound

$$\mathbb{E}\left[\|E_M[Q\ \ ] - \mathbb{E}[Q]\|^2\right] \leq \qquad \underbrace{\frac{1}{M}\mathsf{Var}[Q]}_{\text{statistical error}}$$

Monte Carlo integration

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$$\mathbb{E}[Q] \approx \frac{1}{M} \sum_{m=1}^{M} Q(\boldsymbol{y}_m) := E_M[Q] \approx E_M[Q_L]$$

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$$\mathbb{E}\left[\|E_M[Q_L] - \mathbb{E}[Q]\|^2\right] \le \underbrace{\|\mathbb{E}[Q_L - Q]\|^2}_{\text{bias error}} + \underbrace{\frac{1}{M}\mathsf{Var}[Q]}_{\text{statistical error}}$$

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Combine approximations with different accuracy
aka
Compute rough approximation $E_M[Q_1]$ and apply corrections

Multilevel Monte Carlo: definitions

Sequence of approximations

$(Q_l)_{l=1}^{L}$ and $Q_0 := 0$

Multilevel Monte Carlo estimator [Heinrich 2001, Giles 2008]

$$\mathbb{E}\left[Q_L\right] = \sum_{l=1}^{L} \mathbb{E}\left[Q_l - Q_{l-1}\right] \quad \rightsquigarrow \quad \boxed{E^L\left[Q\right] := \sum_{l=1}^{L} E_{M_l}\left[Q_l - Q_{l-1}\right]}$$

Error bound

$$\mathbb{E}\left[\left\|E^L\left[Q\right] - \mathbb{E}\left[Q\right]\right\|^2\right] \leq \underbrace{\left\|\mathbb{E}\left[Q_L - Q\right]\right\|^2}_{\text{bias error}} + \underbrace{\sum_{l=1}^{L} \frac{1}{M_l} \mathrm{Var}\left[Q_l - Q_{l-1}\right]}_{\text{statistical error}}$$

Multilevel Monte Carlo: algorithm

Given a tolerance ε^2:

1. Split $\varepsilon^2 = \varepsilon^2_{bias} + \varepsilon^2_{stat}$

2. Select level L such that $\|\mathbb{E}\left[Q_L - Q\right]\| < \varepsilon_{bias}$

3. Choose $(M_l)_{l=1}^{L}$ s.t. stat error $< \varepsilon^2_{stat}$ at minimum cost

$$\Rightarrow M_l \propto \sqrt{\frac{\mathrm{Var}\left[Q_l - Q_{l-1}\right]}{W_l}}$$

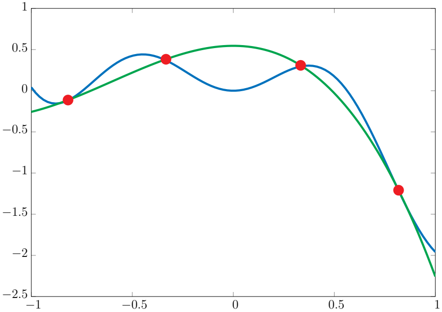
Multilevel Monte Carlo: pros and cons

- **Low regularity** requirements (finite variance)
- **Dimension-independent** convergence rates
- Improvable convergence speed (sometimes)

Stochastic collocation

Collocation: Evaluate $Q(\boldsymbol{y})$ at **deterministic** points $\{\boldsymbol{y}_m\}_{m=1}^{M}$

Stochastic: Choice of points depends on distribution of $\boldsymbol{y}$



Stochastic collocation: sparse grids

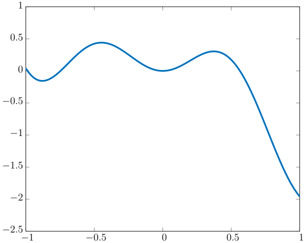
[Gerstner, Griebel 2003 - Schillings, Schwab 2013]

Univariate operators:

$(I_j)_{j\geq 1}$ univariate interpolation operators

$\Delta_j^I := I_j - I_{j-1}$ univariate difference operators.

$$\Rightarrow \qquad \boxed{I_j(Q) = \sum_{i=0}^{j} \Delta_i^I(Q)}$$



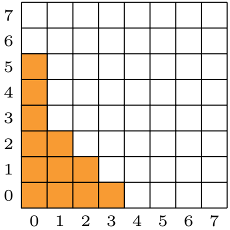
Tensorization and sparse interpolation operators:

$\nu = (\nu_1, \nu_2, \nu_3, 0, \ldots)$ multi-index.

$\Delta_\nu^I := \bigotimes_{j\geq 1} \Delta_{\nu_j}^I$: multivariate operators

Λ downward closed

$$\boxed{Q(\boldsymbol{y}) \approx I_\Lambda(Q)(\boldsymbol{y}) = \sum_{\nu\in\Lambda} \Delta_\nu^I(Q)(\boldsymbol{y})}$$



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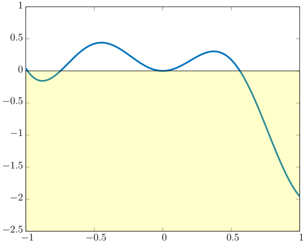

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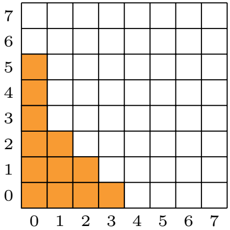

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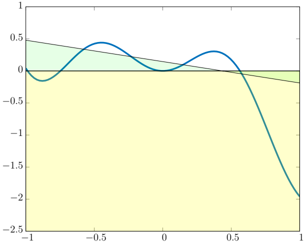

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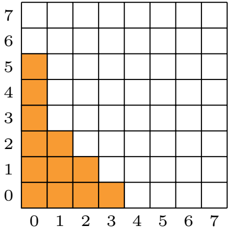

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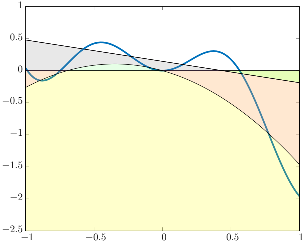

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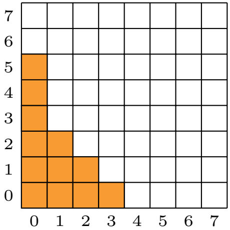

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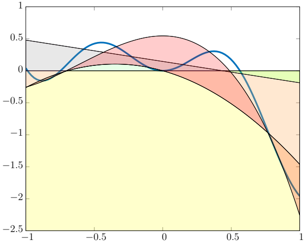

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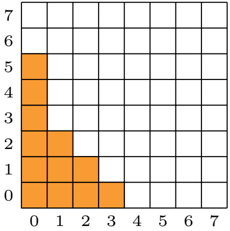


Stochastic collocation: convergence

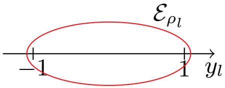
Informal

$$\boxed{\text{smoothness} + \text{sparsity} \Rightarrow \text{fast, dimension-independent convergence}}$$

A bit more formal

(b, p, ε)-holomorphy

$Q = Q(\boldsymbol{y})$ admits uniformly bounded, holomorphic extension to polyellipses in complex plane



Theorem (Chkifa Cohen Schwab 2014)

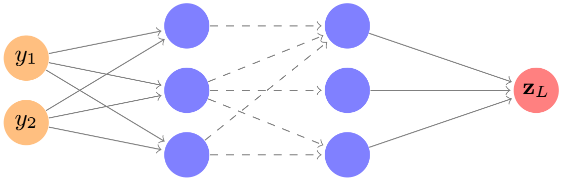
If the $(\boldsymbol{b}, p, \varepsilon)$-*holomorphy assumption holds and* λ_k *grows at most polynomially with* k, *there exists a sequence* $(\Lambda_N)_{N\geq 1}$ *of downward closed sets* Λ_N:

$$\sharp\Lambda_N \leq N \quad \textit{and} \quad \|Q - I_\Lambda(Q)\|_\infty \leq CN^{-s}, \; s = \frac{1}{p} - 1,$$

Stochastic collocation: pros and cons

- 🙂 **High** convergence rates
- 🙂 **Dimension-independent** convergence rates
- 🙁 Needs smoothness and sparsity

Neural network approximation



$R_\rho(\mathcal{N}\mathcal{N})(\boldsymbol{y}) = \mathbf{z}_L$ realization of a neural network

Training set: $\{\boldsymbol{y}_m, Q(\boldsymbol{y}_m)\}_{m=1}^{M}$

Loss: $\mathcal{L}_2(\cdot) := \dfrac{1}{M}\displaystyle\sum_{m=1}^{M} \|Q(\boldsymbol{y}_m) - R_\rho(\mathcal{N}\mathcal{N})(\boldsymbol{y}_m)\|^2.$

Neural networks: pros and cons

- 🙂 **Milder** smoothness requirements
- 🙂 Well-suited for **high-dimensional** approximation
- 🙁 Still a lot of heuristics

Recap UQ methods

$$Q(\boldsymbol{y}),\ \boldsymbol{y} \in [-1,1]^d$$

Moments	Surrogates
Perturbation methods	Reduced Basis
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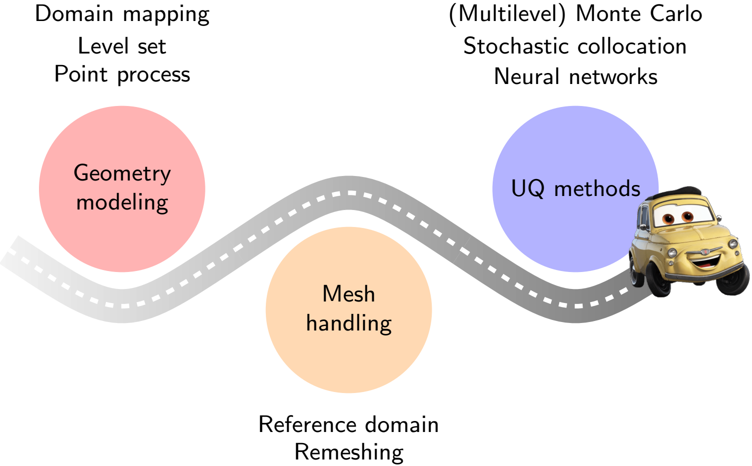
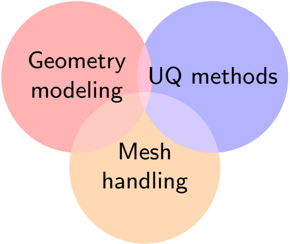
(Multilevel) Monte Carlo	**Neural networks**
(High-order) quasi Monte Carlo	Weighted least squares

Factors of choice: smoothness and sparsity

General recap

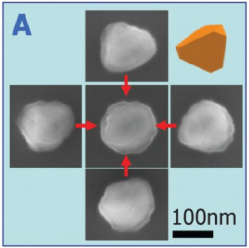


Applications



Helmholtz transmission problem: motivation

Fabrication process of **nano-antennas** introduces **large** shape variations



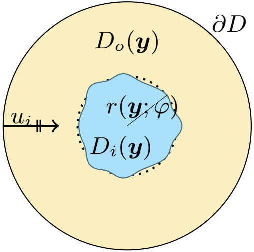
Sannomiya, Diss. ETHZ N.18747.

We consider an **interface problem** on such varying geometry

Helmholtz transmission problem

For every $\boldsymbol{y} \in [-1,1]^d$:

$$\begin{cases} -\nabla \cdot (\alpha \nabla u) - \kappa^2 u = 0 \text{ in } D_i(\boldsymbol{y}) \cup D_o(\boldsymbol{y}) \\ + \text{ continuity conditions at } r(\boldsymbol{y}) \\ + \text{ radiation condition for } (u - u_i) \text{ on } \partial D \end{cases}$$

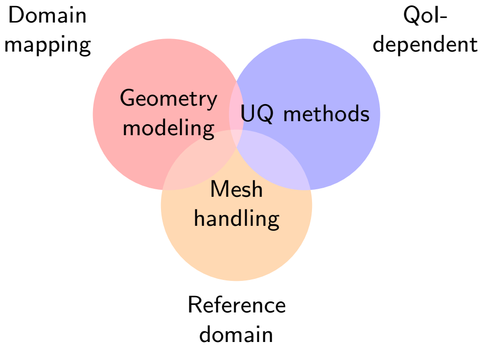


$$\text{with } \alpha = \begin{cases} 1 & \text{in } D_o(\boldsymbol{y}), \\ \alpha_i & \text{in } D_i(\boldsymbol{y}) \end{cases} \quad \text{and} \quad \kappa^2 = \begin{cases} \kappa_o & \text{in } D_o(\boldsymbol{y}), \\ \kappa_i & \text{in } D_i(\boldsymbol{y}). \end{cases}$$

Assumptions

star-shaped scatterer **non-trapping** regime [Moiola, Spence 2019]
low frequency

Helmholtz transmission problem: methods

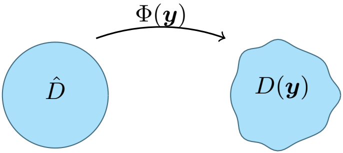


Shape variations via domain mapping

Reference domain $\hat{D}$, bounded and Lipschitz

$$\Phi(\boldsymbol{y};\hat{\boldsymbol{x}}) = \hat{\boldsymbol{x}} + \sum_{j=1}^{d} y_j \Phi_j(\hat{\boldsymbol{x}}),\ \boldsymbol{y} \in [-1,1]^d.$$

Set $D(\boldsymbol{y}) := \Phi(\boldsymbol{y};\hat{D})$.

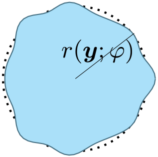


Remark: Given a **boundary parametrization**

$$\gamma(\boldsymbol{y};s) = \gamma_0(s) + \sum_{j=1}^{d} y_j \psi_j(s),$$

a domain transformation can be obtained by extension.

Helmholtz transmission problem: geometry



$$\boxed{r(\boldsymbol{y};\varphi) = r_0(\varphi) + \sum_{j=1}^{d/2} \beta_{2j-1} y_{2j-1} \cos(2\pi\varphi) + \beta_{2j} y_{2j} \sin(2\pi\varphi)}$$

where

$\boldsymbol{y} \in [-1,1]^d$ independent

$\beta_{2j-1}, \beta_{2j} \leq C j^{-\frac{1}{q}}$, $0 < q < 1$

Remark: q associated to interface smoothness.

Helmholtz transmission problem: UQ

$\boxed{\text{QoI: } \hat{u}(\boldsymbol{y})}$

Theorem (Hiptmair et al. 2018)

The (b, p, ε)-holomorphy assumption holds with $\frac{1}{p} = \frac{1}{q} - 1$.

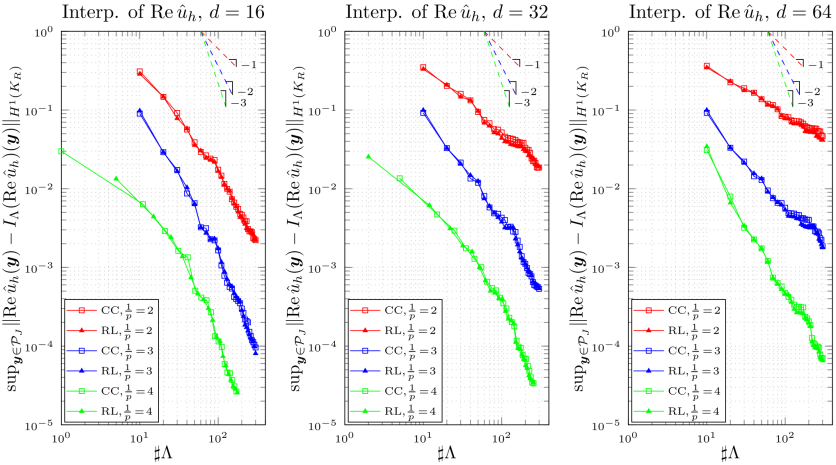
Corollary

If λ_k grows at most polynomially with k, there exists a sequence $(\Lambda_N)_{N \geq 1}$ of downward closed sets:

$$\sharp\Lambda_N \leq N \quad \textit{and} \quad \|\hat{u} - I_\Lambda \hat{u}\|_{L^\infty([-1,1]^\infty, H_0^1(\hat{D}))} \leq CN^{-s}, \; s = \frac{1}{q} - 2.$$

Remark: same holds for the **far field**.

Helmholtz transmission problem: numerics (SC)



Helmholtz transmission problem: UQ

$$\boxed{\text{QoI: } \{u(\boldsymbol{y}; \boldsymbol{x}_i)\}_{i=1}^{N_p}}$$

Helmholtz transmission problem: UQ

$$\boxed{\text{QoI: } \{u(\boldsymbol{y}; \boldsymbol{x}_i)\}_{i=1}^{N_p}}$$

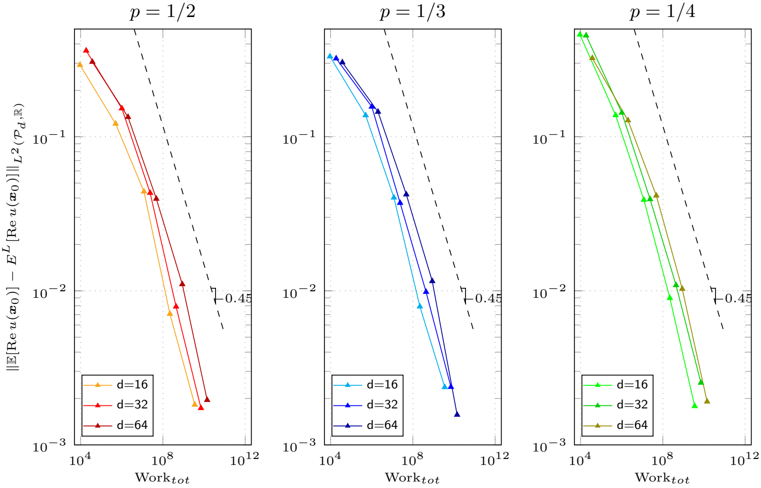
For each evaluation point $\boldsymbol{x}_0$, C^1-discontinuity on *hyperplane*:

$$\mathcal{P}_d^{\Gamma}(\boldsymbol{x}_0) := \left\{ \boldsymbol{y} \in [-1,1]^d : \boldsymbol{x}_0 \in \Gamma(\boldsymbol{y}) \right\}$$

Moments: multilevel Monte Carlo [S. 2019]

Surrogate: ReLU neural networks [S. 2022]

Helmholtz transmission problem: numerics (MLMC)



Helmholtz transmission problem: numerics (NN)

$\alpha_i = 100, \kappa_i/\kappa_o = 0.8,$ 1 point

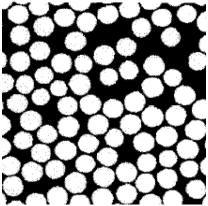
$1/p$ \ d	8	16	32	64
1	0.63‰	1.38‰	1.71‰	2.01‰
2	0.22‰	0.28‰	0.25‰	0.30‰
3	0.12‰	0.13‰	0.15‰	0.13‰

$\alpha_i = 100, \kappa_i/\kappa_o = 0.8,$ 64 points

$1/p$ \ d	8	16	32	64
1	2.15%	3.21%	3.72%	3.75%
2	1.23%	1.31%	1.33%	1.34%
3	0.86%	0.83%	0.89%	0.91%

Mechanics for composites: motivation

Accelerate inference for mechanics of composites with **random microstructure**



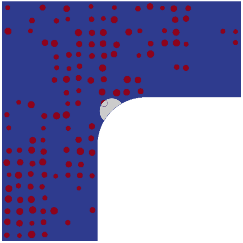
Babuška et al. (1999).

We consider an **elliptic problem** on such varying geometry

Mechanics for composites: model problem

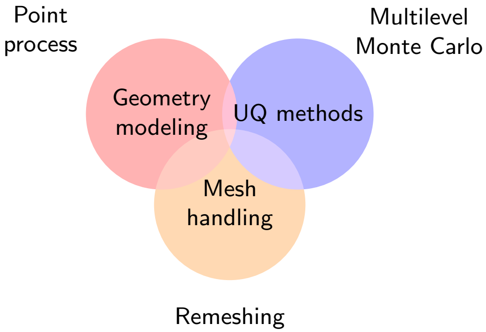
For every $\boldsymbol{y} \in \mathcal{P}$:

$$\begin{cases} \nabla \cdot \mathbf{T}(\boldsymbol{y}; \boldsymbol{u}(\boldsymbol{y})) = \boldsymbol{f} \quad \text{in } D \\ \mathbf{T}(\boldsymbol{y}; \boldsymbol{u}) = 2\mu(\boldsymbol{y})\boldsymbol{\varepsilon}(\boldsymbol{u}) + \lambda(\boldsymbol{y})\mathrm{tr}(\boldsymbol{\varepsilon}(\boldsymbol{u}))\mathbf{I} \\ + \text{ boundary conditions.} \end{cases}$$



$\boxed{Q(\boldsymbol{u}) \text{ local}}$

Mechanics for composites: methods



Mechanics for composites: model-based MLMC

[S. Wohlmuth Oden Faghihi 2019]

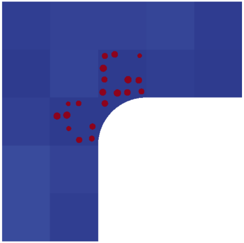
Build sequence of surrogate models for MLMC

Tools

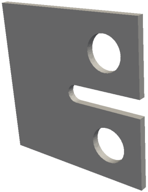
upscaling

goal-oriented, adaptive model selection

model-based multilevel Monte Carlo

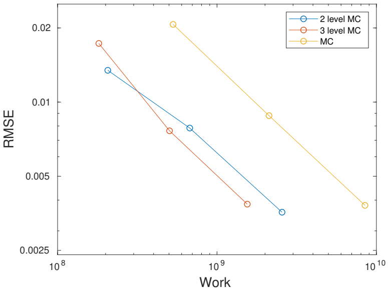


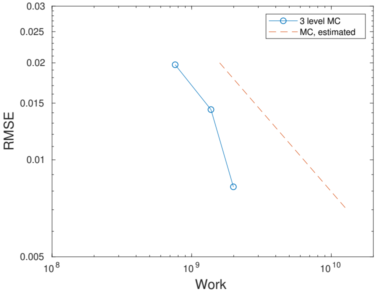
Mechanics for composites: numerics



$Q(\boldsymbol{u})$ = local average of $\mathrm{tr}(\boldsymbol{\varepsilon}(\boldsymbol{u}))$

$Q(\boldsymbol{u})$ = surface average of u_y





Other applications

Linear parabolic PDEs [Djurdjevac 2021, Castrillón-Candás Xu 2021]

Wave equation [Motamed Nobile Tempone 2013, Motamed Nobile Tempone 2015]

Stationary Navier-Stokes [Cohen Schwab Zech 2018]

Maxwell in frequency domain [Jerez-Hanckes Zech 2017, Aylwin Jerez-Hanckes Schwab Zech 2020]

Electrocardiography [Gander Krause Multerer Pezzuto 2021]

Take-home messages

- Uncertainty modeling, mesh handling and UQ method are case-dependent.
- Domain mapping useful to handle shape variations.
- Non-intrusive UQ methods preferred due to highly nonlinear parameter dependence.
- Stochastic collocation efficient upon smoothness and sparsity.
- Multilevel Monte Carlo efficient to compute moments of non-smooth QoIs.
- Neural networks efficient as surrogates of piecewise-smooth QoIs.