Deterministic uncertainty quantification in Nano Optics

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Motivation

Aim: to investigate

defects in fabrication process	←– – – – –→	optical response of nano structures

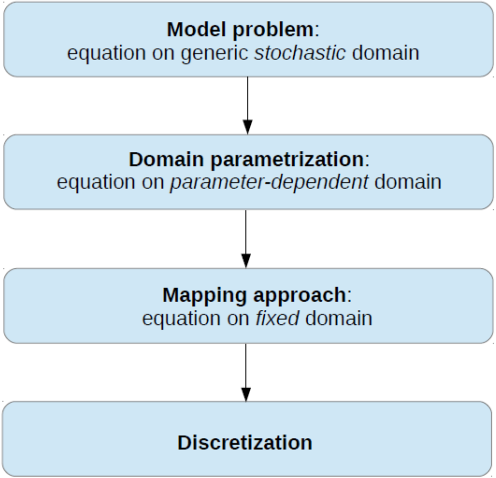
How to perform uncertainty quantification?

- not 'small' stochastic variations of the domain:
  ~~perturbative method~~
- low convergence rate of Monte Carlo sampling

$\Rightarrow$ **deterministic** uncertainty quantification

Quantities of interest:
statistics (mean, variance, ...) of solution / linear output functionals.

Outline

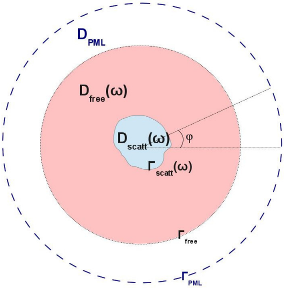

Model problem:
equation on generic *stochastic* domain
Domain parametrization:
equation on *parameter-dependent* domain
Mapping approach:
equation on *fixed* domain
Discretization

Model problem

plane wave interacting with a scatterer
TE / TM symmetry $\Bigg\} \Rightarrow$ **2d Helmholtz equation**

$$\Gamma_{\textbf{scatt}} = \Gamma_{\textbf{scatt}}(\omega), \quad \omega \in \Omega \qquad \Rightarrow \quad u = u(\omega)$$

$$\begin{cases} -\Delta u - k_1^2 u &= 0 \quad \text{in} \quad \mathrm{D}_{\text{free}}(\omega) \cup \mathrm{D}_{\text{PML}} \\ -\Delta u - k_2^2 u &= 0 \quad \text{in} \quad \mathrm{D}_{\text{scatt}}(\omega) \\ [\![u]\!] &= 0 \quad \text{on } \Gamma_{\text{scatt}}(\omega) \\ \dfrac{\partial u}{\partial \mathbf{n}}\Big|_{\text{out}} - \mu_d \dfrac{\partial u}{\partial \mathbf{n}}\Big|_{\text{in}} &= 0 \quad \text{on } \Gamma_{\text{scatt}}(\omega) \end{cases}$$



with

$\mu_d = \dfrac{\epsilon_{\text{scatt}}}{\epsilon_{\text{free}}}$ for TE case,

$\mu_d = \dfrac{\mu_{\text{scatt}}}{\mu_{\text{free}}} = 1$ for TM case.

Incident plane wave from the left: $u_i(x) = e^{ik_1 x}$.

Domain parametrization

Assumption: star-shaped scatterer.
$\Rightarrow$ to each angle $\varphi \in [0, 2\pi)$, associate a stochastic radius:

$$0 < \rho_{\text{min}} \leq \rho(\omega, \varphi) \leq \rho_{\text{max}}, \qquad \omega \in \Omega$$

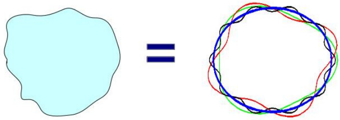
Problem: How to discretize the probability space Ω?

Parametrization of Ω:

$$\rho(\omega, \varphi) = \bar{\rho}(\varphi) + \sum_{k \geq 1} c_k Y_{2k}(\omega) \cos(k\varphi) + s_k Y_{2k+1}(\omega) \sin(k\varphi)$$

$Y_l : \Omega \to \Gamma_l$ real-valued random variables, i.i.d.

- Parameter space: $\Gamma = \mathsf{X}_{l \in \mathbb{N}} \Gamma_l$
- Define $\mathbf{Y} : \Omega \to \Gamma$ as $\mathbf{Y} = (Y_l)_{l \in \mathbb{N}}$
- $D(\omega)$ replaced by $D(\mathbf{y})$, $\mathbf{y} = \mathbf{Y}(\omega) \in \Gamma$



Assumption: $Y_l \sim U[-1, 1] \Rightarrow \Gamma = [-1, 1]^{\infty}$

Mapping approach (1)

The variational formulation for the model problem is:

Find $u(\mathbf{y}) \in H^1(D(\mathbf{y})) \cap H^1(D_{\text{PML}})$ s.t.:

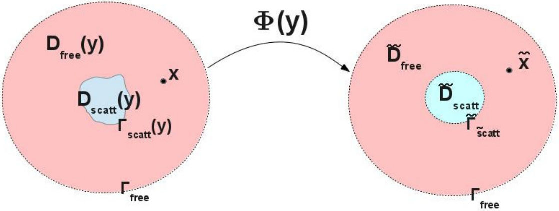
$$\int_{D(\mathbf{y})} \mu \nabla u \cdot \nabla v \, d\mathbf{x} - \int_{D(\mathbf{y})} k^2 u \, v \, d\mathbf{x} = \int_{\Gamma_{\text{free}}} \frac{\partial u_i}{\partial \mathbf{n}} v \, d\mathbf{x} \qquad \forall v \in H_0^1(D(\mathbf{y})) \cap H_0^1(D_{\text{PML}})$$

for P-a.e. $\mathbf{y} \in \Gamma$.

y-dependent integration!

with:

- $D(\mathbf{y}) = D_{\text{scatt}}(\mathbf{y}) \cup D_{\text{free}}(\mathbf{y})$
- $\mu = \begin{cases} \mu_d & \text{in} D_{\text{scatt}} \\ 1 & \text{in} D_{\text{free}} \end{cases}$
- $k = \begin{cases} \mu_d k_2^2 & \text{in} D_{\text{scatt}} \\ k_1^2 & \text{in} D_{\text{free}} \end{cases}$



Variational formulation after the mapping:

Find $u(\mathbf{y}) \in H^1(\tilde{D}) \cap H^1(D_{\text{PML}})$ s.t.:

$$\int_D a_1(\mathbf{y}) \tilde{\nabla} u \cdot \tilde{\nabla} v \, d\hat{\mathbf{x}} - \int_D a_2(\mathbf{y}) u \, v \, d\hat{\mathbf{x}} = \int_{\Gamma_{\text{free}}} \mathrm{f}(\mathbf{y}) \, d\hat{\mathbf{x}} \qquad \forall v \in H_0^1(\tilde{D}) \cap H_0^1(D_{\text{PML}})$$

for P-a.e. $\mathbf{y} \in \Gamma$.

integration over a FIXED domain!

with $\tilde{D} = \tilde{D}_{\text{scatt}} \cup \tilde{D}_{\text{free}}$ and

$$a_1(\mathbf{y}) = \mu \, (D\Phi^{-1})(D\Phi^{-T}) \, |\det D\Phi| \,, \qquad a_2(\mathbf{y}) = k^2 \, |\det D\Phi|$$

$$f(\mathbf{y}) = \frac{\tilde{\partial} u_i}{\tilde{\partial} \mathbf{n}} \, |\det D\Phi|$$

Regularity of the solution

Regularity in the physical space (P-a.e. $\mathbf{y} \in \Gamma$)

Notation: $\rho^K(\mathbf{y}, \varphi) = \bar{\rho}(\varphi) + \sum_{k=1}^{K} c_k y_{2k} \cos(k\varphi) + s_k y_{2k+1} \sin(k\varphi)$

- $(c_k)_k,\ (s_k)_k \ \in l^p(\mathbb{N}) \Rightarrow \rho^K \in C^s_{\text{per}}([0, 2\pi])$ **uniformly in** K, with $s \to \infty$ as $p \downarrow 0$
- $\Rightarrow \Phi^K(\mathbf{y}),\ \Phi^K(\mathbf{y})^{-1} \in C^s_{\text{per}}$,
- $\Rightarrow a_1(\mathbf{y}), a_2(\mathbf{y}), f(\mathbf{y}) \in C^{s-1}_{\text{per}}$
- $\Rightarrow u(\mathbf{y}) \in H^{s+1}$

Remark: if Karhunen-Loève expansion for ρ:
smoothness of $\rho \longleftrightarrow$ smoothness of covariance kernel

Regularity in the parameter space

Conjecture: analytic dependence of u on $y \in \Gamma$

Discretization

Two discretizations are needed:

- discretization of the parameter space Γ: **stochastic collocation** (**nonintrusive**)
- discretization of the physical reference domain: **finite element** discretization

generalized Lagrange polynomials

$$u_{\Lambda,L}(\mathbf{y}) = \sum_{\nu \in \Lambda} u_{\nu,L} L_\nu(\mathbf{y})$$

choose a finite subset Λ of indices $\leftrightarrow$ of collocation points $\mathbf{y}_\nu \in \Gamma$

for each collocation point $\mathbf{y}_\nu$, compute the FE solution to the PDE

Stochastic collocation: sparse adaptive Smolyak algorithm (1)

Aim: choose the **index set** for collocation points

$$\Lambda \subset \mathcal{F} = \left\{ \nu \in \mathbb{N}_0^{\mathbb{N}} : \sharp \mathrm{supp} \nu < \infty \right\}$$

in order to achieve an optimal convergence rate for **moments** of the solution $u = u(\mathbf{y})$

$$\Rightarrow \textbf{quadrature rule} \text{ on } \Gamma.$$

Strategy:

1. start from $\Lambda = \{0\}$
2. consider 'neighborhood' $\mathcal{N}(\Lambda)$
3. choose the index in $\mathcal{N}(\Lambda)$ with highest estimated error contribution
4. update Λ and repeat 2 and 3 iteratively

Stochastic collocation: sparse adaptive Smolyak algorithm (2)

Definitions:

univariate quadrature operator:

$$Q^k(u) = \sum_{i=0}^{n_k} w_i^k \cdot u(y_i^k)$$

univariate quadrature difference operator:

$$\Delta_j = Q^j - Q^{j-1}$$

$$\Rightarrow Q^k = \sum_{j=0}^{k} \Delta_k$$

for $\nu \in \mathcal{F}$, tensorized multivariate operators (inductively defined):

$$Q_\nu = \bigotimes_{j \geq 1} Q^{\nu_j} \quad \Delta_\nu = \bigotimes_{j \geq 1} \Delta^{\nu_j}$$

sparse quadrature operator:

$$Q_\Lambda = \sum_{\nu \in \Lambda} \Delta_\nu$$

Stochastic collocation: sparse adaptive Smolyak algorithm (2)

function ASG
    Set $\Lambda_1 = \{0\}, k = 1$ and compute $\Delta_0(\mathcal{X})$.
    Determine the set of reduced neighbors $N(\Lambda_1)$.
    Compute $\Delta_\nu(\mathcal{X}), \forall \nu \in N(\Lambda_1)$.
    while $\sum_{\nu \in N(\Lambda_k)} \|\Delta_\nu(\mathcal{X})\|_\mathcal{S} > tol$ **do**
        Select ν from $N(\Lambda_k)$ with largest $\|\Delta_\nu\|_\mathcal{S}$ and set $\Lambda_{k+1} = \Lambda_k \cup \{\nu\}$.
        Determine the set of reduced neighbors $N(\Lambda_{k+1})$.
        Compute $\Delta_\nu(\mathcal{X}), \forall \nu \in N(\Lambda_{k+1})$.
        Set $k = k + 1$.
    end while
end function

for $\nu \in \mathcal{F}$, tensorized multivariate operators (inductively defined):

$$Q_\nu = \bigotimes_{j \geq 1} Q^{\nu_j} \quad \Delta_\nu = \bigotimes_{j \geq 1} \Delta^{\nu_j}$$

sparse quadrature operator:

$$Q_\Lambda = \sum_{\nu \in \Lambda} \Delta_\nu$$

Stochastic collocation: sparse adaptive Smolyak algorithm (3)

Convergence of adaptive Smolyak algorithm:

If the solution to the PDE depends **analytically** on $\mathbf{y}$

$\Downarrow$

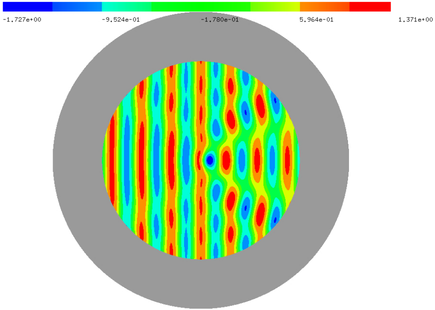
convergence weights depend only on the **sparsity class**[1] of the unknown,

not on the number of dimensions activated [Schillings,Schwab 2012]

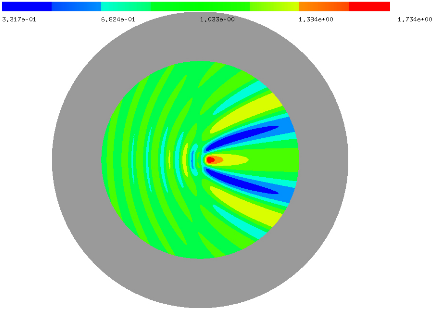
(**dimension-robust** algorithm)

[1] **sparsity class** = decay of Taylor coefficients

Numerical results: physical setting (TM case)

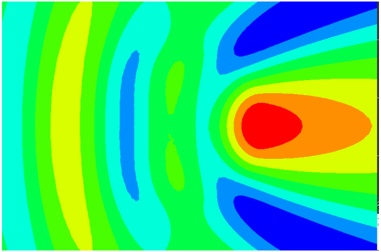


Total field, real part

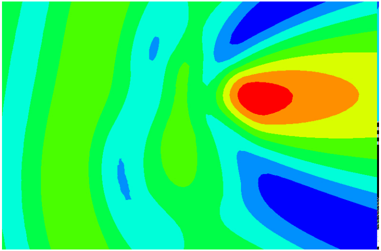


Total field, absolute value

Numerical results: stochastic outputs comparison



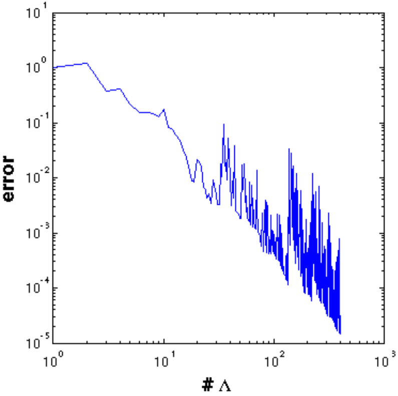
Deterministic case:
$s_k, c_k = 0 \quad \forall k \geq 1$



Stochastic case:
$s_1 \neq 0$

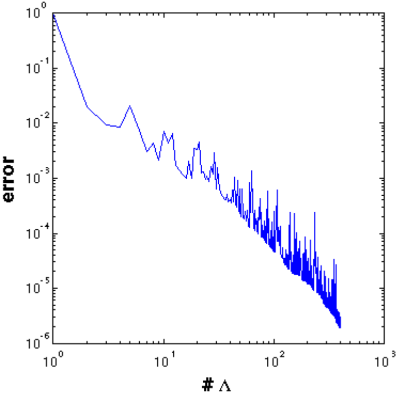
Numerical results: convergence (1)

Quantity considered: total field point value in the center of the scatterer.



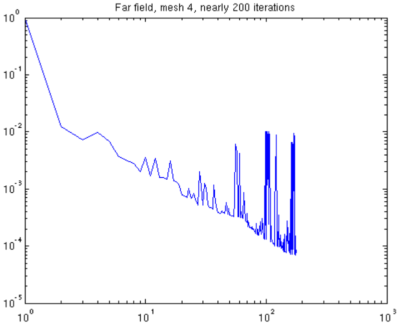
Numerical results: convergence (2)

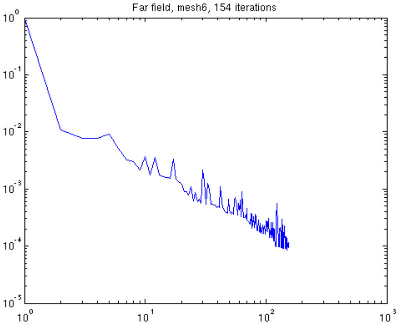
Quantity considered: total field point value in far field region.



Numerical results: convergence (3)

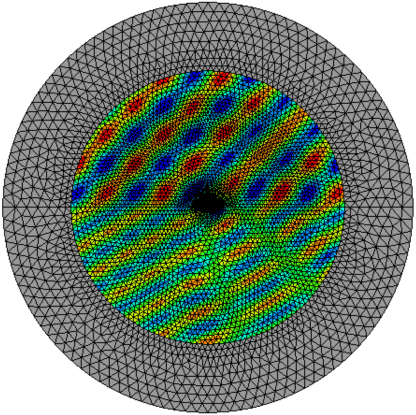
Quantity considered: far field Fourier coefficients.



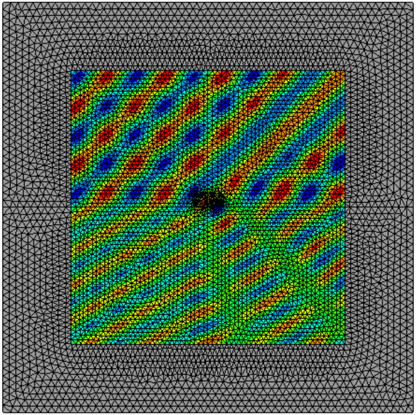


$\Rightarrow$ **Multilevel strategy**:
for each collocation point, FE discretization capable to resolve the oscillations in the parameter-dependent coefficients.

Ongoing work: particle on a substrate



Half-circular scatterer



Rectangular scatterer

Conclusions

- parametrization of the shape using an angle-dependent stochastic radius can be used to describe a wide range of domains;
- the sparse adaptive Smolyak algorithm produced promising preliminary results;
- proof of *analyticity* of the solution with respect to $\mathbf{y}$ is crucial to apply the theoretical convergence results;
- a *multilevel* approach (FE space - collocation point coupling) is important to improve the convergence and reduce the computational effort.