Technische Universität Braunschweig

Institute of Dynamics and Vibrations

Simulation of RF and Optical Components with Random Input Data

with N. Georg, D. Loukrezis and S. Schöps (TU Darmstadt);
NACHOS seminar

Ulrich Römer, 5. April 2018

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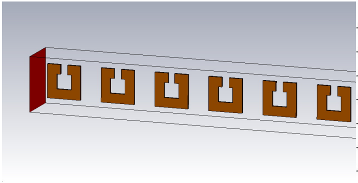
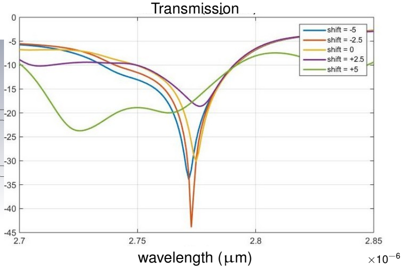
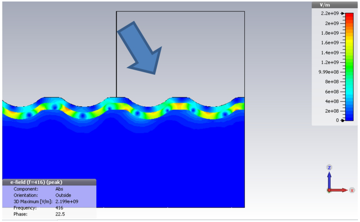
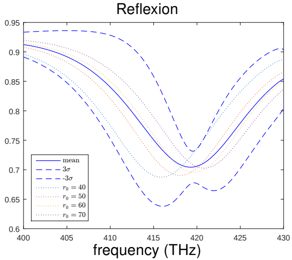
Uncertainties in RF and Optical Components





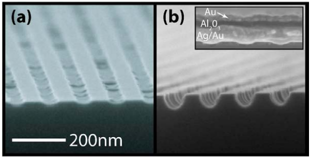
DFG project SIMROCUQ with R. Schuhmann (TU Berlin)





Uncertainties in RF and Optical Components

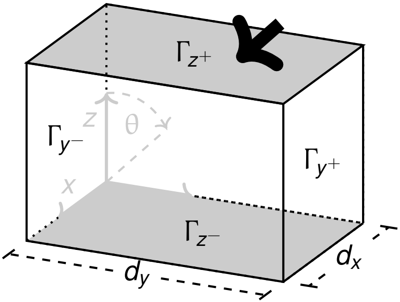
- Uncertainties in materials and geometry
  - Manufacturing tolerances on nano-scales
  - Material properties/geometries are difficult to measure

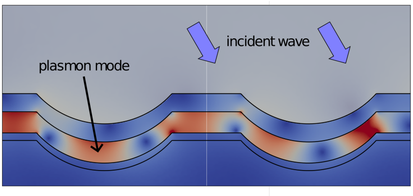


Picture from [Preiner et al. 2008]

- Aims of the project:
  - Systematically model and propagate uncertainties in a stochastic setting
  - Develop and assess performance of methods for time-domain and frequency domain settings
- Application focus: periodic metamaterials, plasmonics

Model Problem





$$\nabla \times \left(\mu_r^{-1} \nabla \times \mathbf{E}\right) - \omega^2 \underline{\epsilon} \mu_0 \mathbf{E} = 0 \qquad \text{in } D$$

$$\mathbf{E}|_{\Gamma_x^+} = \mathbf{E}|_{\Gamma_x^-} e^{j\psi_x} \qquad \text{on } \Gamma_x^+ \cup \Gamma_x^-$$

$$\mathbf{E}|_{\Gamma_y^-} = \mathbf{E}|_{\Gamma_y^+} e^{j\psi_y} \qquad \text{on } \Gamma_y^+ \cup \Gamma_y^-$$

$$\mathbf{n} \times \mathbf{E} = 0 \qquad \text{on } \Gamma_z^-$$

$$(\mu_r^{-1} \nabla \times \mathbf{E}) \times \mathbf{n} + \mathcal{F}(\mathbf{E}) = \mathcal{G}(\mathbf{E}^{\text{inc}}) \qquad \text{on } \Gamma_z^+$$

Model Problem

- Introduce solution space

$$V := \{\mathbf{v} \in H(\mathrm{curl}, D), \quad \text{s.t. Dirichlet and periodic b.c.}\}$$

- Weak formulation: find $\mathbf{E} \in V$ such that

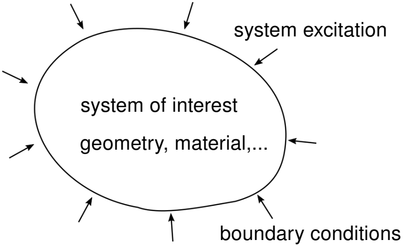
$$\left(\mu_r^{-1}\nabla \times \mathbf{E}, \nabla \times \mathbf{E}'\right)_D - \omega^2\mu_0\left(\underline{\epsilon}\mathbf{E}, \mathbf{E}'\right)_D - \left(\mathcal{F}(\mathbf{E}), \mathbf{E}'\right)_{\Gamma_z^+} = \left(\mathcal{G}(\mathbf{E}^{\mathrm{inc}}), \mathbf{E}'\right)_{\Gamma_z^+} \quad \forall \mathbf{E}' \in V$$

- FEM with Nédélec's elements (2nd order, first kind) leads to

$$\underbrace{\left(\mathbf{K} - \omega^2\mathbf{M}_\varepsilon(\omega) + \mathbf{M}^{\mathrm{port}}(\omega)\right)}_{=:\mathbf{A}}\mathbf{e} = \mathbf{f}(\mathbf{e}^{\mathrm{inc}})$$

Sources of Uncertainty

- Model inputs: constitutive parameters, geometry, initial conditions, boundary conditions, system excitation
  [C.J. Roy, W.L. Oberkampf, 2010]



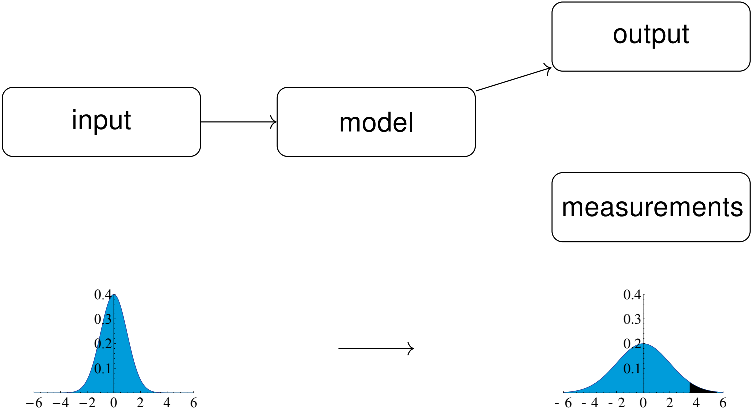
- Numerical approximation errors
- Model-form uncertainty: approximations, abstractions, assumptions on which the model relies

Types of Uncertainties

- Aleatory uncertainty (What is the length of any piece?)
  - Irreducible/stochastic uncertainty
  - Manufacturing process
  - Probabilistic approach
- Epistemic uncertainty (What is the length of a specific piece?)
  - Reducible uncertainty
  - Lack of knowledge
  - Interval/Fuzzy arithmetic vs probabilistic approach (Bayesian)

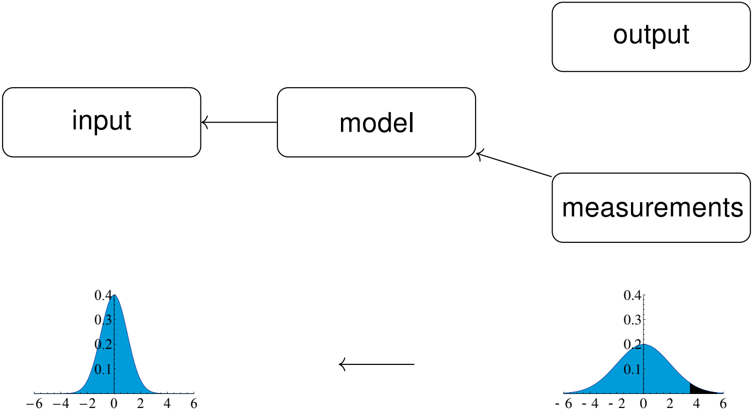
Uncertainty Quantification

- Uncertainty propagation (forward UQ)
- Given density functions of inputs, determine output densities



Inverse Problems in a Bayesian Setting

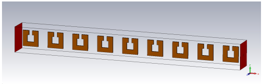
- Inverse UQ in a *Bayesian* setting
- Given measurement data, determine density of inputs



Problem Formulation

Problem Formulation

- **Modeling:** identify a (small) vector of input random variables $\mathbf{Y}$ with joint distribution $f_{\mathbf{Y}}$, capturing the uncertainties under consideration
- **Propagation:** compute probabilities (or moments) of the system output $\mathfrak{Q}$ in an efficient way



input $\mathbf{Y}$ material/geometry parameter → model Maxwell, Navier Stokes eqs. → output $\mathfrak{Q}$ S-parameters, velocity

Contents

Probabilities and Random Variables

- Real continuous random variable

$$Y : \Theta \to \Xi \quad \text{image } \Xi \subseteq \mathbb{R}$$

- Random realization $y = Y(\theta)$
- Probability density function f_Y

$$P(a \leqslant Y \leqslant b) = \int_a^b f_Y(y)\,\mathrm{d}y$$

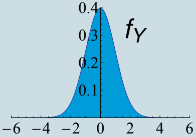
- Moments

$$\mathbb{E}[Y] = \int_\Xi y\, f_Y(y)\,\mathrm{d}y$$

$$\mathrm{Var}[Y] = \int_\Xi (y - \mathbb{E}[Y])^2\, f_Y(y)\,\mathrm{d}y$$

Normal distribution

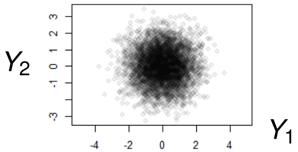
- $Y \sim \mathcal{N}(\mu_Y, \sigma_Y)$



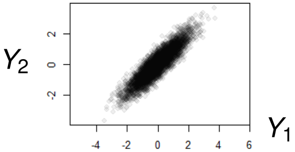
Random Vectors

- Vector of random variables $\mathbf{Y} : \Theta \rightarrow \mathbb{R}^M$ (components are random variables)
- Mean value defined component-wise
- Correlation

$$\operatorname{cov}(Y_i, Y_j) = \mathbb{E}\left[(Y_i - \mathbb{E}[Y_i])(Y_j - \mathbb{E}[Y_j])\right] \text{ (covariance matrix)}$$



uncorrelated $\operatorname{cov}(Y_i, Y_j) = 0$



correlated $\operatorname{cov}(Y_i, Y_j) \neq 0$

- Independence: $f_{\mathbf{Y}} = f_1(y_1) \cdots f_M(y_M)$ (implies no correlation)

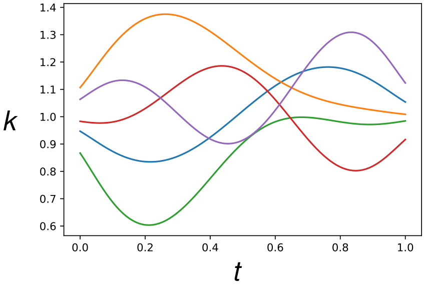
Random Fields

- A stochastic process is a collection of random variables

$$\{k_t \mid t \in T\} \quad \text{interval } T = [a, b]$$

if $T \subset \mathbb{R}$ (random process), if $T \subset \mathbb{R}^n$ (random field)

random paths $k(t, \theta)$



Karhunen-Loève Expansion

- Consider the Fredholm integral equation

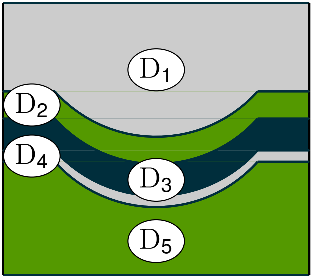
$$\int_0^1 \mathrm{Cov}[k](s,t)\varphi_i(t)\,\mathrm{d}t = \lambda_i \varphi_i(s)$$

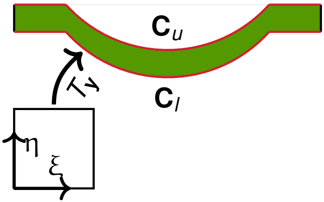
- Karhunen-Loève expansion

$$k(\theta,t) = \mathbb{E}[k](t) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\varphi_i(t) Y_i(\theta)$$

  - For a Gaussian random field: $Y_i \sim \mathcal{N}(0,1)$ i.i.d
  - KLE eigenfunctions are orthonormal (L^2-sense)
  - Eigenvalues are real positive, with zero as only cummulation point
  - Y_i are pairwise uncorrelated with zero mean and unit variance

Uncertainties in the Geometry

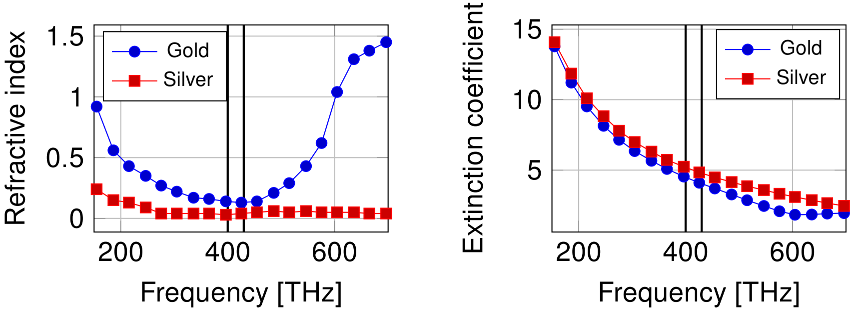




- NURBS curves $\mathbf{C}_{\mathbf{y}}(\xi) = \sum_{j=0}^{n} R_j(\xi)\mathbf{P}_{ij}(\mathbf{y})$
- Domain mapping

$$\mathbf{T}_{\mathbf{y}}(\xi, \eta) = \eta \mathbf{C}_{\mathbf{y}}^{u}(\xi) + (1-\eta)\mathbf{C}_{\mathbf{y}}^{l}(\xi)$$

Uncertainties in the Material



- Parametric model for permittivity

$$\underline{\epsilon}(\omega, \mathbf{y}) = \Big(n(\omega, \mathbf{y})^2 - \kappa(\omega, \mathbf{y})^2 - j(2n(\omega, \mathbf{y})\kappa(\omega, \mathbf{y})) \Big) \epsilon_0$$

Uncertainties in the Material

- Data according to [Johnson et al. 1972]

Index i	Frequency f_i [THz]	Refractive index n_i^{Au}	Extinction coefficient κ_i^{Au}	Refractive index n_i^{Ag}	Extinction coefficient κ_i^{Ag}
0	396.55	0.14 ± 0.02	4.542 ± 0.015	0.03 ± 0.02	5.242 ± 0.015
1	425.57	0.13 ± 0.02	4.103 ± 0.010	0.04 ± 0.02	4.838 ± 0.010
2	454.58	0.14 ± 0.02	3.697 ± 0.007	0.05 ± 0.02	4.483 ± 0.007

- Interpolate with Lagrange polynomials $L_i(\omega)$

$$n(\omega, \mathbf{y}) = \sum_{i=0}^{2} n_i L_i(\omega), \quad k(\omega, \mathbf{y}) = \sum_{i=0}^{2} k_i L_i(\omega)$$

$$\mathbf{y} = (n_0, \ldots, n_2, k_0, \ldots, k_2)$$

- Karhunen-Loève expansion [Römer et al. 2017] can be used instead

Stochastic Problem

- Parameter vector $\mathbf{y} \in \Xi \subset \mathbb{R}^M$, independent with density $f_{\mathbf{Y}}$
- Parametric problem: find $\mathbf{E} \in L^2_{f_{\mathbf{Y}}}(\Xi) \otimes V$ such that almost everywhere (a.e.)

$$\left(\mu_r^{-1}\nabla \times \mathbf{E}, \nabla \times \mathbf{E}'\right)_D - \omega^2\mu_0\left(\underline{\epsilon}(\mathbf{y})\mathbf{E}, \mathbf{E}'\right)_D - \left(\mathcal{F}(\mathbf{E}), \mathbf{E}'\right)_{\Gamma_z^+} = \left(\mathcal{G}(\mathbf{E}^{\mathrm{inc}}), \mathbf{E}'\right)_{\Gamma_z^+} \quad \forall \mathbf{E}' \in V$$

  material and geometric variability entirely represented by $\underline{\epsilon}(\mathbf{y})$

- FEM with Nédélec's elements (2nd order, first kind) leads to

$$\mathbf{A}_{\mathbf{y}}\mathbf{e}(\mathbf{y}) = \mathbf{f}(\mathbf{e}^{\mathrm{inc}})$$

- In the end we compute a quantity of interest (scattering parameter)

$$\mathcal{Q}(\mathbf{y}) := (\mathbf{E}(\mathbf{y}), \mathbf{q})_{\Gamma_z^+}$$

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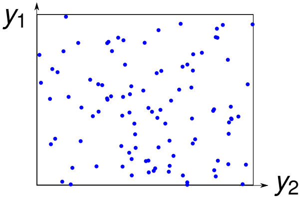
Sampling Strategies

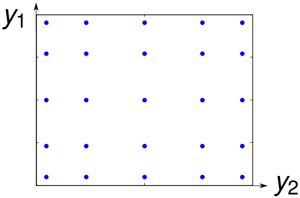
- Systems with random input data require repetitive solution of the model equations

- Monte Carlo



- Random selection of points, no structure

- Collocation



- Deterministic points, points with high probability

- Aim is to improve slow convergence of the Monte Carlo method

Polynomial Surrogate Model

Key Idea

- Compute polynomial surrogate (meta) model

$$\mathcal{Q}(\mathbf{y}) \approx \mathcal{Q}_N(\mathbf{y}) := \sum_{i=1}^{N} q_i \Phi_i(\mathbf{y})$$

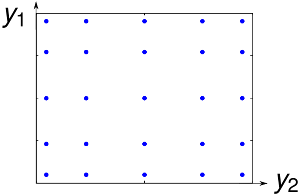
- Φ_i are global polynomial basis functions (spectral method)
- Coefficients q_i are determined by collocation, Galerkin, projection, regression method,...

Stochastic Collocation Method

- Choose points in random domain $\{\mathbf{y}^{(j)}\}_{j=1}^{N}$ and enforce collocation condition

$$\mathcal{Q}(\mathbf{y}^{(j)}) = \sum_{i=1}^{N} q_i \Phi_i(\mathbf{y}^{(j)}), \quad j = 1, \ldots, N$$

- Requirements: solution at collocation points $\mathcal{Q}(\mathbf{y}^{(j)})$
- Call solver with input values $\mathbf{y}^{(j)}$: *non-intrusive* method



Stochastic Collocation Method

- Collocation conditions can be written as

$$\begin{bmatrix} \Phi_1(\mathbf{y}^{(1)}) & \Phi_2(\mathbf{y}^{(1)}) & \cdots & \Phi_N(\mathbf{y}^{(1)}) \\ \Phi_1(\mathbf{y}^{(2)}) & \Phi_2(\mathbf{y}^{(2)}) & \cdots & \Phi_N(\mathbf{y}^{(2)}) \\ \vdots & \vdots & \ddots & \cdots \\ \Phi_1(\mathbf{y}^{(N)}) & \Phi_2(\mathbf{y}^{(N)}) & \cdots & \Phi_N(\mathbf{y}^{(N)}) \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \end{bmatrix} = \begin{bmatrix} \mathcal{Q}(\mathbf{y}^{(1)}) \\ \mathcal{Q}(\mathbf{y}^{(2)}) \\ \vdots \\ \mathcal{Q}(\mathbf{y}^{(N)}) \end{bmatrix}$$

  or in matrix-vector notation $\mathbf{Wq} = \mathcal{Q}$

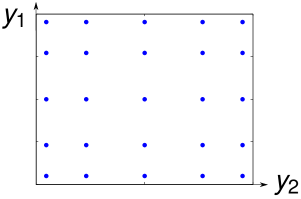
- Choice of collocation points and polynomial basis is crucial
  - Collocation points: Gauß, Clenshaw Curtis, Leja
  - Polynomial basis: polynomial chaos, Lagrange

Collocation Points

- Tensor grid: collocation points are obtained as

$$\{\mathbf{y}^{(i)}\} = \{y_1^{(1)}, \dots, y_1^{(N_1)}\} \times \cdots \times \{y_M^{(1)}, \dots, y_M^{(N_M)}\}$$

Number of points $N = N_1 \cdots N_M$



- Complexity increases exponentially with the dimension: curse-of-dimensionality
- Sparse grids delay the curse-of-dimensionality
  - A priori construction of spare grids, cf. Smolyak
  - Adaptive generation of grid is even more efficient

Adaptive Sparse Collocation

- Polynomial model

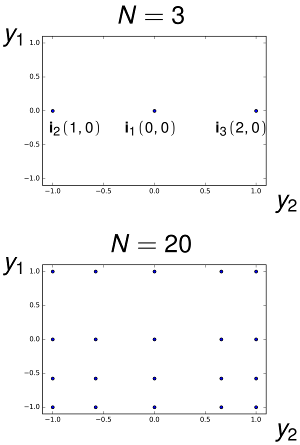
$$\mathcal{Q}_N(\mathbf{y}) = \sum_{n=1}^{N} q_{\mathbf{i}_n} \Phi_{\mathbf{i}_n}(\mathbf{y})$$

  Collocation points
  $\Lambda_N = \cup_n \{\mathbf{y}^{(\mathbf{i}_n)}\}$

- Points and polynomials are one-to-one

- Leja points: hierarchical, one point per degree

  [A. Chkifa, A. Cohen, C. Schwab, 2014]

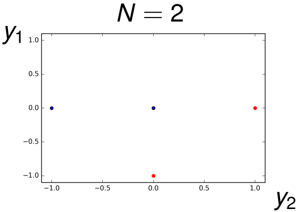


Adaptive Sparse Collocation

- Selection of new points: Greedy strategy
  - Compute solutions for neighbour set $\mathcal{N}(\Lambda_{N-1})$ (red points)
  - Select point satisfying

$$\mathbf{i}_N = \operatorname{argmax}\{|q_{\mathbf{i}_n}|, \mathbf{i}_n \in \mathcal{N}(\Lambda_{N-1})\}$$

  - Update $\Lambda_N = \Lambda_{N-1} \cup \{\mathbf{i}_N\}$



Adjoint Method

- Linear output quantity $\mathcal{Q}(\mathbf{y}) = \mathbf{q}^T \mathbf{e}(\mathbf{y})$

- Primal system

$$\mathbf{A}_{\mathbf{y}} \mathbf{e}(\mathbf{y}) = \mathbf{f}(\mathbf{e}^{\mathrm{inc}})$$

- Adjoint system

$$\mathbf{A}_{\mathbf{y}}^* \mathbf{z}(\mathbf{y}) = \mathbf{q}$$

- Approximate both primal and adjoint problem with adaptive collocation method

- Adjoint error indicator

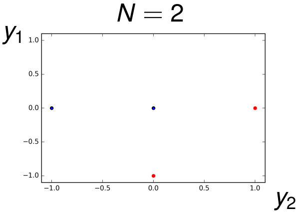
$$\varepsilon(\mathbf{y}) = \left| \mathbf{z}^* \left(\mathbf{A}_{\mathbf{y}} \mathbf{e}_N(\mathbf{y}) - \mathbf{f}(\mathbf{e}^{\mathrm{inc}}) \right) \right| \approx \left| \mathbf{z}_N^* \left(\mathbf{A}_{\mathbf{y}} \mathbf{e}_N(\mathbf{y}) - \mathbf{f}(\mathbf{e}^{\mathrm{inc}}) \right) \right|$$

Adjoint Adaptive Sparse Collocation

- Selection of new points revisited
  - Enlarge the neighbour set $\mathcal{N}(\Lambda_{N-1})$
  - Select point satisfying

$$\mathbf{i}_N = \operatorname{argmax}\{\varepsilon(\mathbf{y}^{(\mathbf{i}_n)}), \mathbf{i}_n \in \mathcal{N}(\Lambda_{N-1})\}$$

  - Update $\Lambda_N = \Lambda_{N-1} \cup \{\mathbf{i}_N\}$



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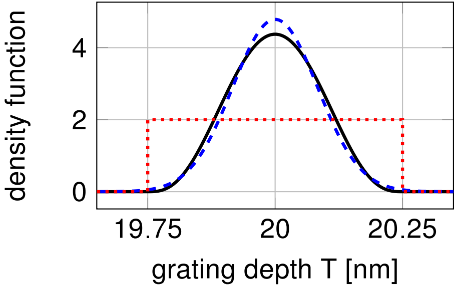
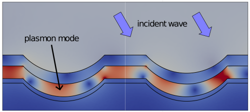
Distributions of Inputs





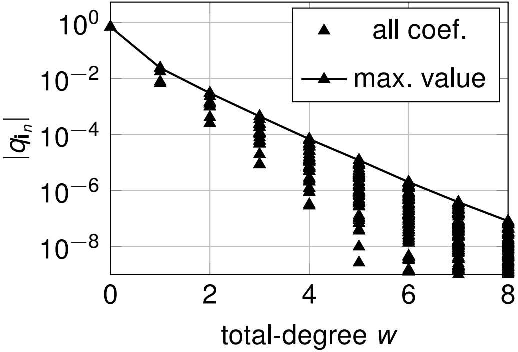
- Absence of large data sets: uniform or Beta dist. are chosen
  - Beta dist.: approximates normal distribution with bounded image
  - Uniform distribution: maximum entropy distribution for random variable in an interval

Convergence of Polynomial Approximation

- Consider polynomial chaos expansion

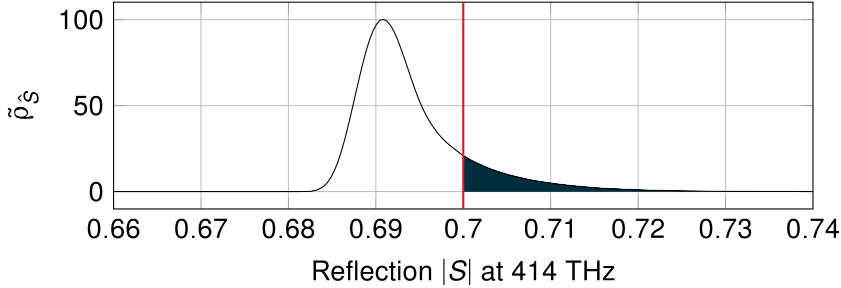
$$\mathcal{Q}(\mathbf{y}) \approx \sum_{n=1}^{N} q_{\mathbf{i}_n} \Phi_{\mathbf{i}_n}(\mathbf{y})$$

- Exponential decay of Fourier coefficients q_i indicates smoothness



Single Frequency Case

- Reconstructed density of reflection coefficient (obtained by sampling the surrogate model)

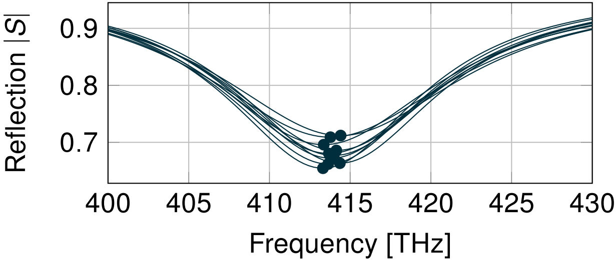


- Moments and failure probabilities

N^{MC}	$\mathbb{E}$	$\sqrt{\mathbb{V}}$	$\mathcal{F}$
10^3	0.6939	6.20×10^{-3}	14.3%
10^4	0.6939	6.48×10^{-3}	13.9%
10^5	0.6940	6.47×10^{-3}	14.1%
10^6	0.6940	6.45×10^{-3}	14.2%

Broadband Results

- Variability of reflection coefficient



- Moments and failure probabilities

	$\mathbb{E}$	$\sqrt{\mathbb{V}}$	$\mathcal{F}_{\text{res}}$
$\lvert S_{\text{res}} \rvert$	0.685	0.017	21.9%
f_{res} [THz]	413.827	0.324	–

Summary

- Uncertainties in material and geometry of optical grating coupler
- Quantify uncertainty of coupling resonance
- Uncertainty propagation with Stochastic Collocation
  - Greedy adaptive method
  - Adjoint error indicator to steer adaptivity
- Fast decay of Fourier coefficients: numerical indicator for smoothness
- Recover density of reflection coefficient and most sensitive parameters

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Thank you for your attention!