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Uncertainty Quantification for order reduced Maxwell's equations

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Motivation

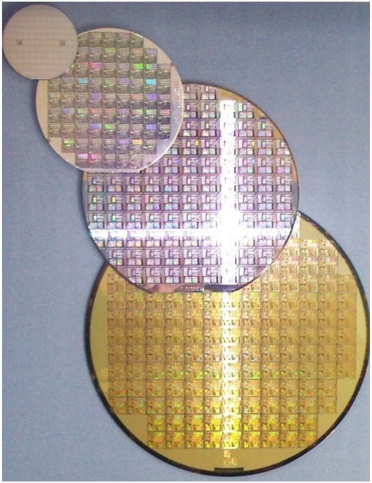
- Expensive production of semiconductor prototypes

$\Rightarrow$ Simulation necessary for design process

- High number of circuit elements

$\hookrightarrow$ High system dimension ($\mathcal{O}(10^6)$)

$\Rightarrow$ Model Order Reduction (MOR)



Wafer from 2 to 8 inches. (Source: wikipedia.org)

Motivation

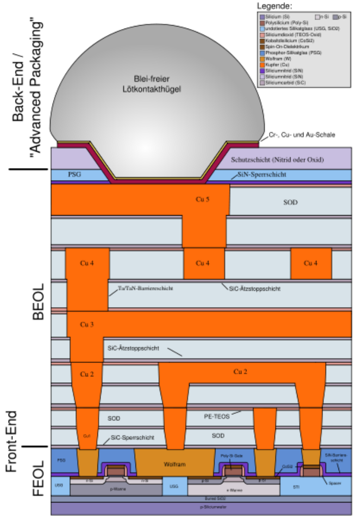
- Ongoing miniaturization
- Increase of working frequencies

⇒ Parasitic effects like crosstalk

- Uncertain materials and geometries

↪ Uncertainties in state and output

⇒ Uncertainty Quantification (UQ)



Chip layer structure. (Source: wikipedia.org)

Maxwell's Equations

On $G \subset \mathbb{R}^3$ we consider

$$
\begin{aligned}
\partial_t(\epsilon \mathbf{E}) &= \nabla \times \mathbf{H} - \sigma \mathbf{E} - \mathbf{J}, \\
\partial_t(\mu \mathbf{H}) &= -\nabla \times \mathbf{E}, \\
\nabla \cdot (\epsilon \mathbf{E}) &= \rho, \\
\nabla \cdot (\mu \mathbf{H}) &= 0,
\end{aligned}
$$

with

- electric field intensity $\mathbf{E}$,
- magnetic field intensity $\mathbf{H}$,
- charge density ρ,
- impressed current source $\mathbf{J}$,
- permittivity $\epsilon = \epsilon_r \cdot \epsilon_0$,
- permeability $\mu = \mu_r \cdot \mu_0$,
- electrical conductivity σ.

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material dependent

The Setting

- Consider time-harmonic Maxwell's equations

$$\nabla \times ((\mu_0 \mu_r)^{-1} \nabla \times \mathbf{E}) + i\,\omega\,\sigma\,\mathbf{E} - \omega^2\,\epsilon_0 \epsilon_r\,\mathbf{E} = i\,\omega\,\mathbf{J}$$

  with uncertain material parameters μ_r, σ, and ϵ_r.
- Parameters need to be positive ⇒ Use log-normal distribution.

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- Task: Approximate expectation value and standard deviation of the quantities of interest.

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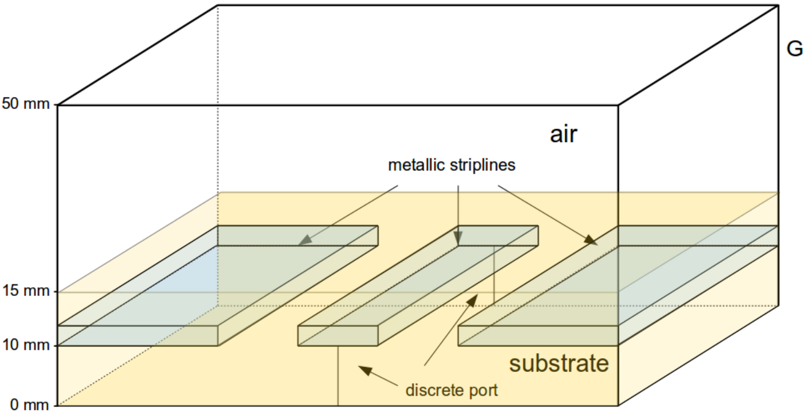
- Expensive for many evaluations of high dimensional systems.

⇒ MOR

Coplanar Waveguide



- Perfect electric conductor (PEC) boundary conditions.
- Two different materials with a different physical behavior.
- Five uncertain parameters ϵ_r^s, ϵ_r^a, μ_r, σ^s, σ^a.

Discretized Time-Harmonic Maxwell's Equations

To obtain an affine form of the PDE, the system is rewritten

$$\nabla \times ((\mu_r \mu_0)^{-1} \nabla \times \mathbf{E}) + i\omega(\sigma^s \mathbb{1}_{substrate} + \sigma^a \mathbb{1}_{air})\mathbf{E}$$
$$-\omega^2 \epsilon_0 (\epsilon_r^s \mathbb{1}_{substrate} + \epsilon_r^a \mathbb{1}_{air})\mathbf{E} = i\omega \mathbf{J}.$$

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Affine discretized system on G_h (18755 dofs)

$$\mu_r A_{\mu_0} \mathbf{e} + i\omega(\sigma^s A^s + \sigma^a A^a)\mathbf{e} - \omega^2(\epsilon_r^s A^s_{\epsilon_0} + \epsilon_r^a A^a_{\epsilon_0})\mathbf{e} = Bu, \\ y = C\mathbf{e},$$

with

- current u, induced at the discrete port,
- output y, the integral over the voltage along the port,
- associated matrices B, C.

Stochastic Collocation

Given

- a probability space $(\Omega, \mathcal{F}, \mathcal{P})$,
- a square integrable random variable $Y : \Omega \to \Gamma$, with probability density function f
- an arbitrary function $g : \Gamma \to \mathbb{C}^d$ for a natural number d.

Idea: Approximate expectation value $\mathbb{E}\left(g(Y)\right)$, by quadrature rule

$$\mathbb{E}\left(g(Y)\right) = \int_\Gamma g(x) f(x) dx \approx \sum_{i=1}^{n} g(\xi_i) w_i,$$

with

- realization $(\xi_1, \ldots, \xi_n)$, later called sample points $\{\xi_i\}_{i=1}^n$,
- weights $\{w_i\}_{i=1}^n$,

both determined by the probability density function f.

Application to the Coplanar Waveguide

- Use stochastic collocation for $g = \mathbf{e}$ and $g = y$

$$\mathbb{E}(\mathbf{e}) \approx \sum_{i=1}^{n} \mathbf{e}(\xi^i) w_i, \quad std(\mathbf{e}) \approx \sqrt{\sum_{i=1}^{n} |\mathbf{e}(\xi^i)|^2 w_i - |\mathbb{E}(\mathbf{e})|^2},$$

$$\mathbb{E}(y) \approx \sum_{i=1}^{n} y(\xi^i) w_i, \quad std(y) \approx \sqrt{\sum_{i=1}^{n} |y(\xi^i)|^2 w_i - |\mathbb{E}(y)|^2}.$$

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- Solve the discretized time-harmonic Maxwell's equations

$$\xi_3^i A_{\mu_0} \mathbf{e} + i\omega(\xi_4^i A^s + \xi_5^i A^a)\mathbf{e} - \omega^2(\xi_1^i A_{\epsilon_0}^s + \xi_2^i A_{\epsilon_0}^a)\mathbf{e} = Bu,$$
$$y = C\mathbf{e},$$

for sampling vectors $\boldsymbol{\xi}^i = (\xi_1^i, \ldots, \xi_5^i)^T$, $i = 1, \ldots, n$.

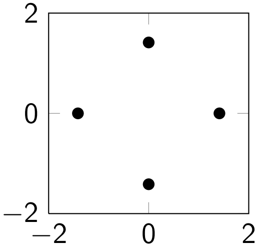
Stroud Points

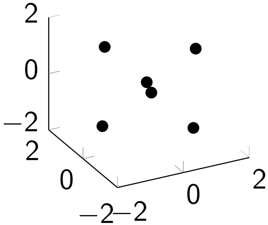
- $2N$ normally distributed interpolation points for system with N parameters.
- k-th component $x_k^i = \boldsymbol{\sigma}_k \cdot z_k^i + \boldsymbol{\mu}_k$, where

$$z_k^{2r-1} = \sqrt{2}\cos\left(\frac{(2r-1)k\pi}{N}\right),$$

$$z_k^{2r} = \sqrt{2}\sin\left(\frac{(2r-1)k\pi}{N}\right),$$

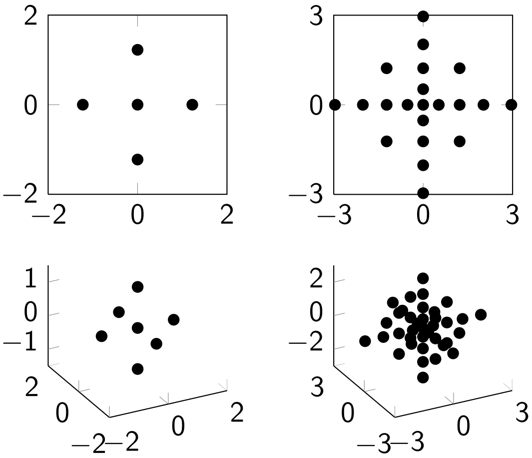
for $r = 1, 2, \ldots, \lfloor N/2 \rfloor$.
If N odd, then $z_k^N = (-1)^k$.
- No refinement possible.





Hermite-Genz-Keister Sparse Grids

- Smolyak algorithm.
- Points are
  - normally distributed,
  - computed on infinite regions,
  - refinable,
  - and nested.
- SGMGA MATLAB® library.



Monte Carlo (MC) Simulation

- Independent from the number of parameters.
- Slow convergence: Need 1 million sample points for good approximation.
- Computation time for our system (18755 dofs): **10 days** (on a 64-bit server with CPU type Intel®Xeon®X5650 @2.67GHz, with 2 CPUs, 12 Cores (6 Cores per CPU) and 48 GB main memory available).

⇒ Combination with MOR.

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⇒ Combination with MOR.

Idea: Use a reduced order model for the (various) expensive system evaluations $\mathbf{e}(\xi^i)$ to save computation time.
We use Proper Orthogonal Decomposition (POD).

Coplanar Waveguide

- Discretized in FEniCS by Nédélec finite elements $\rightarrow$ 18755 dofs.
- Induced current $u = 1$ Ampère, working frequency $\omega = 0.6 \cdot 10^9$ Hertz.

Coplanar Waveguide

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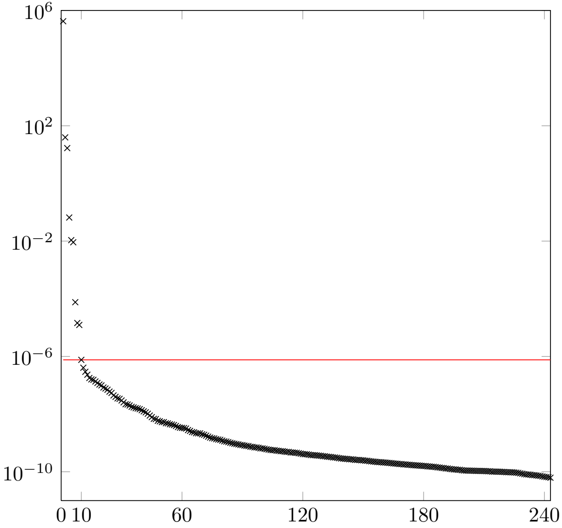
- Induced current $u = 1$ Ampère, working frequency $\omega = 0.6 \cdot 10^9$ Hertz.
- Parameter vector $\boldsymbol{\xi}$ is log-normally distributed $\sim \mathcal{LN}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2)$

j	ξ_j	$\mathbb{E}(\xi_j)$	$std(\xi_j)$	μ_j	σ_j
1	ϵ_r^1	4.40	10^{-2}	1.4816	0.0023
2	ϵ_r^2	1.07	10^{-2}	0.0676	0.0093
3	μ_r	1.00	10^{-2}	0.0000	0.0100
4	σ^1	0.02	10^{-4}	-3.9120	0.0005
5	σ^2	0.01	10^{-4}	-4.6052	0.0100

Singular Value Decay for POD with 3^5 snapshots



Overview

Affine discretized time-harmonic Maxwell's equations

$$\mu_r A_{\mu_0}\mathbf{e} + i\omega(\sigma^s A^s + \sigma^a A^a)\mathbf{e} - \omega^2(\epsilon_r^s A_{\epsilon_0}^s + \epsilon_r^a A_{\epsilon_0}^a)\mathbf{e} = Bu,$$
$$y = C\mathbf{e}.$$

Find: Statistic quantities of $\mathbf{e}$ and y.
Methods:

- MC for full model with 10^6 sample points $\rightarrow$ reference solution.
- Stochastic collocation for full model with n sample points computed via
  - Stroud rule ($n = 10$),
  - HGK sparse grids ($n = 11, 81$).
- MC and stochastic collocation for POD-reduced model of dimension 10.

Error computation

Compute the following errors for all methods ($\mathbf{x} \in G_h$)

$$err^{rel}_{\mathbb{E}(\mathbf{e})} := \left| \frac{\mathbb{E}(\mathbf{e}(\mathbf{x})) - \mathbb{E}_{MC}(\mathbf{e}(\mathbf{x}))}{\mathbb{E}_{MC}(\mathbf{e}(\mathbf{x}))} \right|,$$

$$err^{rel}_{std(\mathbf{e})} := \left| \frac{std(\mathbf{e}(\mathbf{x})) - std_{MC}(\mathbf{e}(\mathbf{x}))}{std_{MC}(\mathbf{e}(\mathbf{x}))} \right|,$$

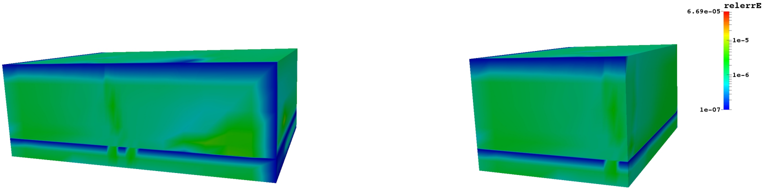
$$err^{rel}_{\mathbb{E}(y)} := \left| \frac{\mathbb{E}(y) - \mathbb{E}_{MC}(y)}{\mathbb{E}_{MC}(y)} \right|,$$

$$err^{rel}_{std(y)} := \left| \frac{std(y) - std_{MC}(y)}{std_{MC}(y)} \right|.$$

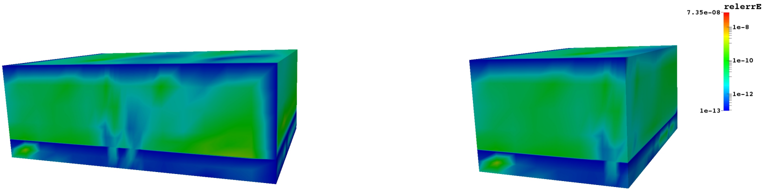
Errors for e

Method	$\|err^{rel}_{\mathbb{E}(\mathbf{e})}\|_2$	$\|err^{rel}_{\mathbb{E}(\mathbf{e})}\|_\infty$	$\|err^{rel}_{std(\mathbf{e})}\|_2$	$\|err^{rel}_{std(\mathbf{e})}\|_\infty$
Stroud	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.12 \cdot 10^{-2}$	$1.06 \cdot 10^{-3}$
HGK 1	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.64 \cdot 10^{-2}$	$1.11 \cdot 10^{-3}$
HGK 2	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.55 \cdot 10^{-2}$	$1.10 \cdot 10^{-3}$
MC-POD	$8.79 \cdot 10^{-8}$	$7.35 \cdot 10^{-8}$	$1.83 \cdot 10^{-7}$	$3.04 \cdot 10^{-8}$
Stroud-POD	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.12 \cdot 10^{-2}$	$1.06 \cdot 10^{-3}$
HGK 1-POD	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.64 \cdot 10^{-2}$	$1.11 \cdot 10^{-3}$
HGK 2-POD	$1.13 \cdot 10^{-3}$	$6.69 \cdot 10^{-5}$	$7.55 \cdot 10^{-2}$	$1.10 \cdot 10^{-3}$

Error plots for $\mathbb{E}(\mathbf{e})$



(a) $err^{rel}_{\mathbb{E}(\mathbf{e})}$ for Stroud collocation



(b) $err^{rel}_{\mathbb{E}(\mathbf{e})}$ for MC-POD

Errors for y

Method	$err^{rel}_{\mathbb{E}(y)}$	$err^{rel}_{std(y)}$
Stroud	$8.76 \cdot 10^{-6}$	$4.03 \cdot 10^{-4}$
HGK 1	$8.76 \cdot 10^{-6}$	$4.51 \cdot 10^{-4}$
HGK 2	$8.76 \cdot 10^{-6}$	$4.52 \cdot 10^{-4}$
MC-POD	$6.96 \cdot 10^{-12}$	$4.10 \cdot 10^{-11}$
Stroud-POD	$8.76 \cdot 10^{-6}$	$4.03 \cdot 10^{-4}$
HGK 1-POD	$8.76 \cdot 10^{-6}$	$4.51 \cdot 10^{-4}$
HGK 2-POD	$8.76 \cdot 10^{-6}$	$4.52 \cdot 10^{-4}$

Time Comparison

Computation time for the POD 10: 4 minutes and 35 seconds.

Method \ Model	FOM (18755 dofs)	ROM (10 dofs)
Stroud ($n = 10$)	00 : 00 : 00 : 13	00 : 00 : 00 : 04
HGK 1 ($n = 11$)	00 : 00 : 00 : 14	00 : 00 : 00 : 04
HGK 2 ($n = 81$)	00 : 00 : 01 : 15	00 : 00 : 00 : 04
MC ($n = 10^6$)	10 : 06 : 58 : 34	00 : 00 : 07 : 44

Table: Computation time in *days* : *hours* : *minutes* : *seconds*.

Computations are done on a 64-bit server with CPU type Intel®Xeon®X5650 @2.67GHz, with 2 CPUs, 12 Cores (6 Cores per CPU) and 48 GB main memory available.

Conclusion

- Stroud points and HGK 1 sparse grids lead to comparable good results.
- MC for the POD-reduced system yields even better results but is also more expensive.
- Combining collocation and POD, the collocation error is the dominant one.
- For small examples like the coplanar waveguide, a combination of POD and collocation does not save time.

Outlook

- Higher dimensional examples.
- Geometric parameters.

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