Uncertainty Quantification for the Fundamental Mode Spectrum of the European XFEL Cavities

N. Georg[1,2,3,*], J. Corno[2,3], H. De Gersem[2,3], S. Gorgi Zadeh[4],
U. Römer[1], S. Schöps[2,3], A. Sulimov[5], U. van Rienen[4]

[1] Institute of Dynamics and Vibrations, TU Braunschweig
[2] Institut für Theorie Elektromagnetischer Felder, TU Darmstadt
[3] Centre for Computational Engineering, TU Darmstadt
[4] Theoretical Electrical Engineering, Universität Rostock
[5] Deutsches Elektronen-Synchroton DESY

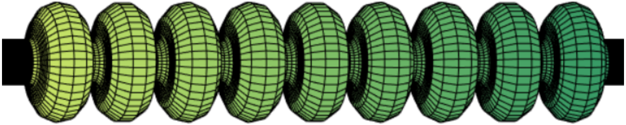
[*] n.georg@tu-bs.de

TECHNISCHE UNIVERSITÄT DARMSTADT

Institut für Theorie Elektromagnetischer Felder
Computational Electromagnetics Research Group at GSCE

Introduction

9-cell TESLA cavities @ DESY



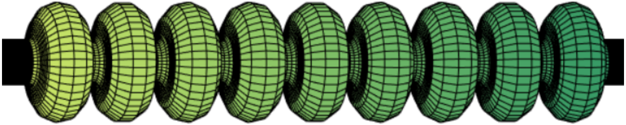
geometry
(parameters)

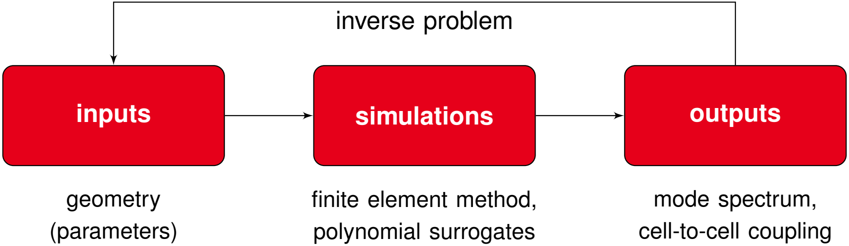
finite element method,
polynomial surrogates

mode spectrum,
cell-to-cell coupling

Introduction

9-cell TESLA cavities @ DESY

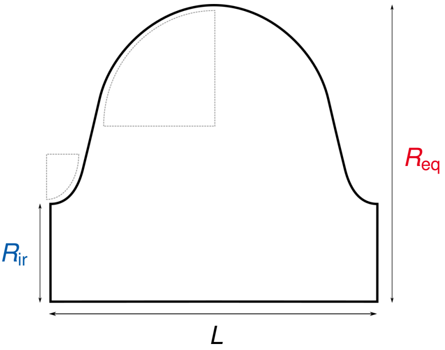




Outline of the Talk

1. Introduction
2. Inputs
3. Simulations
4. Outputs
5. Inverse problem
6. Conclusion

INPUTS
Uncertain geometry



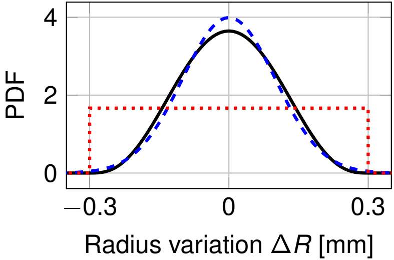
Geometrical shape of an elliptical cell.

- Random event θ
- 10 uncertain parameters: equatorial radii $R_{eq}^{(i)}(\theta)$, $i = 1, \ldots, 9$ of each cell and iris radius $R_{ir}(\theta)$

INPUTS

Uncertainty modelling

- Changes in the radii are modelled as beta distributed random variables
  - Shape parameters are chosen such that normal distribution is approximated
  - Probability density function (PDF) has bounded support
- Constraints due to manufacturing (e.g. sorting) lead to correlation



- Black: PDF of beta distribution with support in [-0.3 mm, 0.3 mm].
- Blue, dashed: PDF of normal distribution with $\mu = 0$ mm and $\sigma = \frac{0.2}{2}$ mm.
- Red, dotted: PDF of uniform distribution with support in [-0.3 mm, 0.3 mm].

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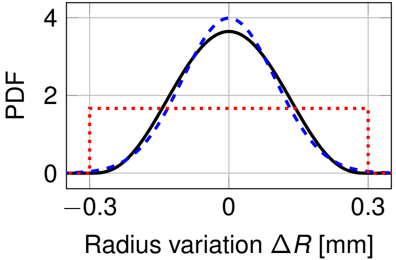

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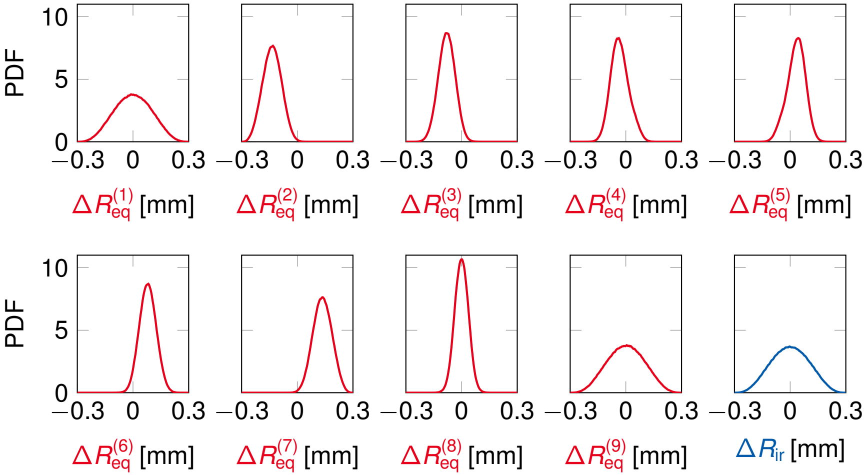
INPUTS

Kernel density estimates of correlated random variables



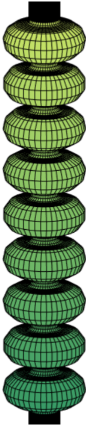
SIMULATIONS
Maxwell's eigenproblem

- We solve Maxwell's eigenproblem

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{E}_i \right) = (2\pi f_i)^2 \, \epsilon_0 \mathbf{E}_i$$

with PEC boundary conditions.

- Using the finite element method in 2D, a high accuracy can easily be achieved (error $\approx \pm 0.001$ MHz)



SIMULATIONS
Tuning

- Each cell whose $R_{\mathrm{eq}}^{(i)}$ or R_{ir} is changed, is tuned independently by solving for the unknown length $L^{(i)}$

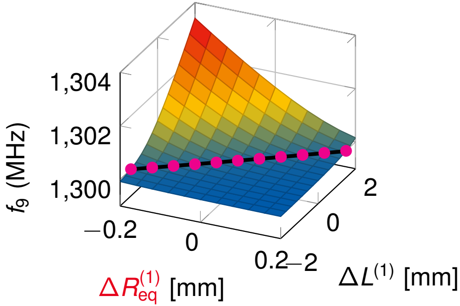
$$f_9\left(L^{(i)}\right) - 1.3\,\mathrm{GHz} = 0.$$

- E.g. the effect of a change in

$$R_{\mathrm{eq}}^{(1)} = R_{\mathrm{design}}^{(1)} + \Delta R_{\mathrm{eq}}^{(1)}$$

on the accelerating frequency f_9 is compensated by changes in

$$L^{(1)} = L_{\mathrm{design}}^{(1)} + \Delta L^{(1)}.$$



The black line is the 1.3 GHz contour line. The magenta points are the tuning values for $\Delta L^{(1)}$ obtained for a given value of $\Delta R_{\mathrm{eq}}^{(1)}$ (unique solution).

SIMULATIONS
Polynomial Surrogate Model

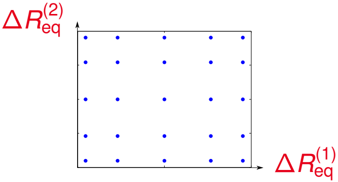
- Quantities of interest
  - Fundamental eigenfrequencies f_i, $i = 1, \dots, 9$
  - Cell-to-cell coupling

$$k_{cc} = 2\frac{f_9 - f_1}{f_9 + f_1} \cdot 100\%.$$

Key Idea

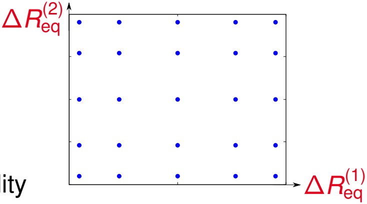
- Compute polynomial surrogate (meta) model of mapping from inputs $\Delta R_{ir}, \Delta R_{eq}^{(i)}$, $i = 1, \dots, 9$ to outputs k_{cc}, f_i, $i = 1, \dots, 9$.

- Global polynomial basis functions (Lagrange polynomials)
- Interpolation on collocation points (Leja nodes)



Simulations
Collocation Points

- Tensor grid: Number of points
  $N = N_{\Delta R_{\text{eq}}^{(1)}} \cdots N_{\Delta R_{\text{eq}}^{(9)}} N_{\Delta R_{\text{ir}}}$
- Complexity increases exponentially with the dimension: curse-of-dimensionality
- Sparse grids delay the curse-of-dimensionality
  - A priori construction of sparse grids, cf. Smolyak
  - **Adaptive** generation of grid is even more efficient[1]



- 500 (non-intrusive) model evaluations $\rightarrow$ suitable accuracy
- Evaluation of polynomials is almost for free

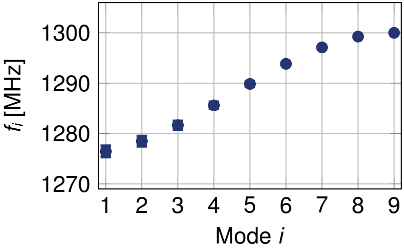
[1] Narayan, Akil, and John D. Jakeman. *Adaptive Leja sparse grid constructions for stochastic collocation and high-dimensional approximation.* SIAM Journal on Scientific Computing 36.6 (2014): A2952-A2983.

Outputs
Fundamental mode spectrum

Using $N^{\mathrm{MC}} = 815983$ random samples $\{f_i^{(m)}\}_{m=1}^{N^{\mathrm{MC}}}$, we compute

$$\mathbb{E}_{\mathrm{MC}}[f_i] = \frac{1}{N^{\mathrm{MC}}} \sum_{m}^{N^{\mathrm{MC}}} f_i^{(m)}$$

$$\mathrm{var}_{\mathrm{MC}}[f_i] = \frac{1}{N^{\mathrm{MC}} - 1} \sum_{m}^{N^{\mathrm{MC}}} \left(f_i^{(m)} - \mathbb{E}_{\mathrm{MC}} \right)^2$$



Mode i	Mean [MHz]	Std. dev. [MHz]
1	1,276.46	0.36
2	1,278.49	0.32
3	1,281.64	0.28
4	1,285.60	0.22
5	1,289.85	0.15
6	1,293.84	0.09
7	1,297.11	0.04
8	1,299.25	0.01
9	1,300.00	0.00

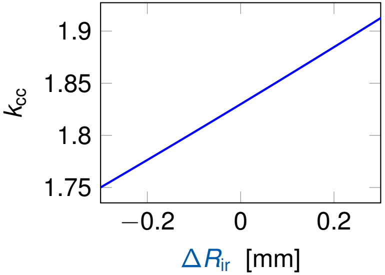
OUTPUTS
Cell-to-cell coupling coefficient

- Statistical moments of cell-to-cell coupling coefficient k_{cc}
  - Mean $\mathbb{E}[k_{cc}] \approx 1.828$
  - Standard deviation $\sqrt{\text{var}[k_{cc}]} \approx 0.019$

- Analysis of variance-based sensitivity indices (Sobol) yields

$$\frac{\text{var}_{R_{ir}}[k_{cc}]}{\text{var}[k_{cc}]} > 96\%.$$

- k_{cc} is heavily influenced by iris radius R_{ir} while equatorial radii $R_{eq}^{(i)}$ have significantly less impact $\rightarrow$ we neglect those parameters (use nominal values)



INVERSE PROBLEM

- Collect measurements of the fundamental mode spectra for $M \approx 400$ cavities (manufactured by the same vendor) from the XFEL cavity database
- From measurements, calculate for each cavity j the cell-to-cell coupling coefficient $k_{cc,j}$
- For each $k_{cc,j}$, we then calculate the deformation in the iris radius by solving

$$\Delta R_{ir,j} = f^{-1}(k_{cc,j})$$

- For $j \in [1, \ldots, M]$

$\mathbb{E}\left[k_{cc,j}\right]$	$\text{Std}\left[k_{cc,j}\right]$	$\mathbb{E}\left[\Delta R_{ir,j}\right]$	$\text{Std}\left[\Delta R_{ir,j}\right]$
1.854	0.016	0.087 mm	0.057 mm

- Majority of considered cavities is within specification $|\Delta R_{ir,j}| \leq 0.2\,\text{mm}$

Conclusion

- Incorporation of manufacturing imperfections into numerical simulations
- Modelling of manufacturing process (constraints and tuning)
- Dimension-adaptive sparse grid approximation to significantly reduce computational cost of repeated model evaluations
- Variance-based sensitivity analysis $\rightarrow$ first steps towards inverse problems

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