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Implementational Aspects of Eigenmode Computation based on Perturbation Theory

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Overview

- Introduction
- Perturbation Theory
  - Basics
  - Introduction of two different Perturbative Methods
  - Analytical Proof of Principle
- Numerical Implementation
- Results
- Conclusion & Outlook

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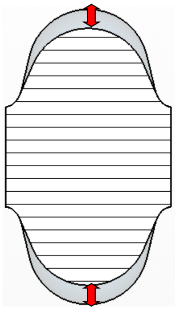
Introduction

Geometrical Perturbations of a Cavity

- Geometrical shape of a cavity determines
  - Eigenmodes inside the cavity
  - Cavity characteristics

→ Perturbation of the cavity shape changes its characteristics



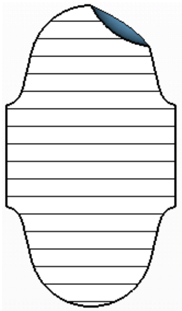
- Forms of perturbations:
  - Desired modification

    → Optimization of cavity characteristics (E_{acc}/E_{peak} ,Q,…)

  - Undesired perturbation: Deviation of desired geometry due to manufacturing tolerances and operational demands

    → Impairment of accelerating performance (π-Mode)

    → Beam deflection / wakefield excitation



➡ Need to assess perturbation effects

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Motivation for Using Perturbation Theory

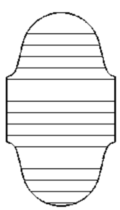
- Parameter studies to investigate perturbation effects

→ Computation of eigenmodes for numerous different cavity geometries

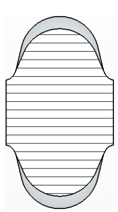
- Common numerical solvers:

  Perform a full computation even if geometry is only slightly changed

  → Computationally extensive and inefficient



Geometry 1 → Eigenmode Computation → Eigenmodes 1



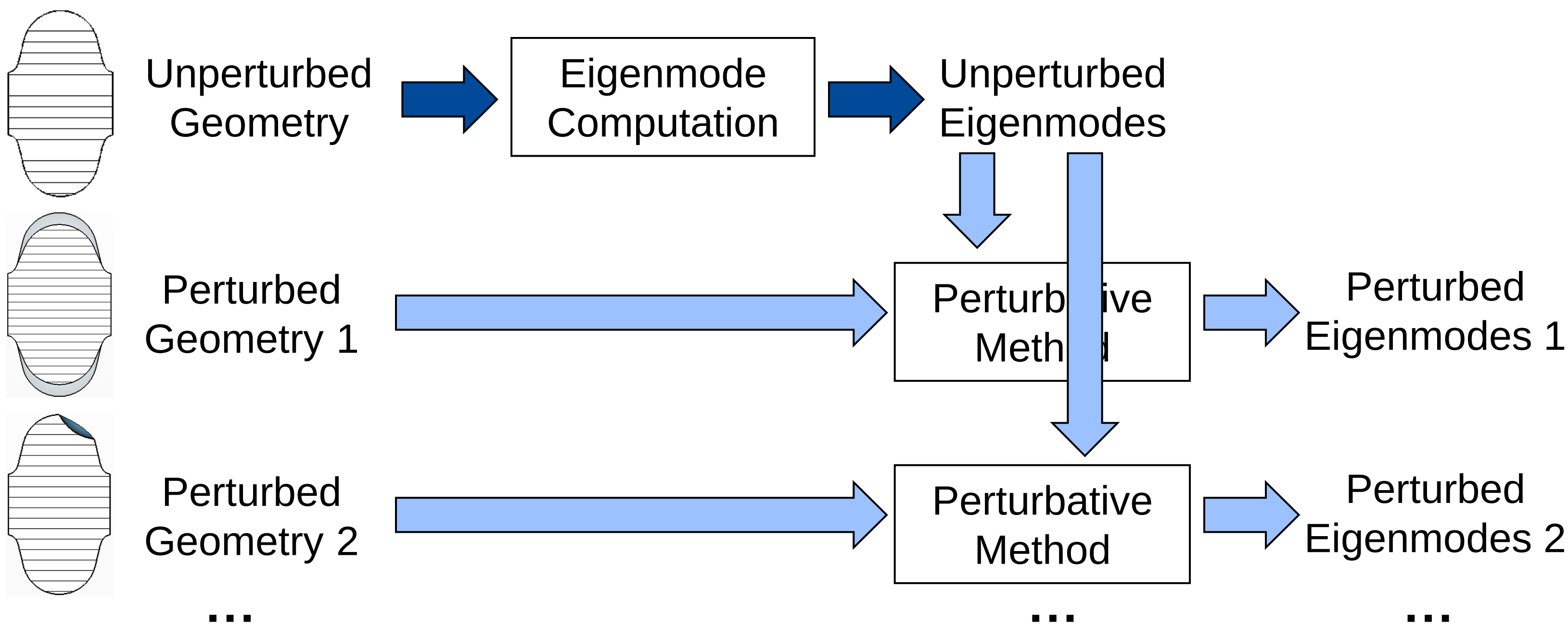
Geometry 2 → Eigenmode Computation → Eigenmodes 2

... ...

Motivation for Using Perturbation Theory

- Perturbative methods:
  - Perform full eigenmode computation <u>solely for one</u> geometry
  - Derive eigenmodes of every other geometry from these eigenmodes

    → Significant reduction of computational effort



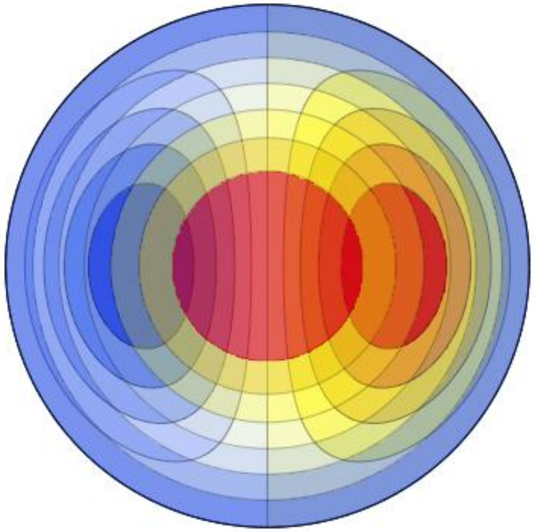
Basics of Perturbation Theory

Orthogonality of Eigenmodes

The integral of the product of the stationary fields of two different modes over the complete cavity volume is always zero

$$\frac{\epsilon}{2U_\mathrm{i}} \iiint\limits_V \mathbf{E}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{E}_\mathrm{k}(\mathbf{r})\,\mathrm{d}V = \delta_\mathrm{ik} = \begin{cases} 1 & \mathrm{i} = \mathrm{k} \\ 0 & \mathrm{i} \neq \mathrm{k} \end{cases}$$

$$\frac{\mu}{2U_\mathrm{i}} \iiint\limits_V \mathbf{H}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{H}_\mathrm{k}(\mathbf{r})\,\mathrm{d}V = \delta_\mathrm{ik} = \begin{cases} 1 & \mathrm{i} = \mathrm{k} \\ 0 & \mathrm{i} \neq \mathrm{k} \end{cases}$$



Cross section of cylindrical cavity

E_z of TM_{01} and TM_{11} mode

V : Volume of the unperturbed cavity

U_i : Energy stored in unperturbed mode i

Orthogonality of Eigenmodes → Series Expansion

Fields of unperturbed eigenmodes

=

System of mutually orthogonal functions

↓

Field pattern of perturbed eigenmodes:

Expansion as a series of the unperturbed modes

$$\begin{aligned} \widetilde{\mathbf{E}}_\mathrm{i}(\mathbf{r}) &= \sum_{\mathrm{k}=1}^{N} e_\mathrm{ik} \cdot \mathbf{E}_\mathrm{k}(\mathbf{r}) \\ \widetilde{\mathbf{H}}_\mathrm{i}(\mathbf{r}) &= \sum_{\mathrm{k}=1}^{N} h_\mathrm{ik} \cdot \mathbf{H}_\mathrm{k}(\mathbf{r}) \end{aligned}$$

Condition: Perturbed volume has to be part of unperturbed volume

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How to determine the perturbed eigenmodes

- Key aspect:
  Interaction of each unperturbed mode with every other unperturbed mode inside the volume ΔV that is removed by the perturbation

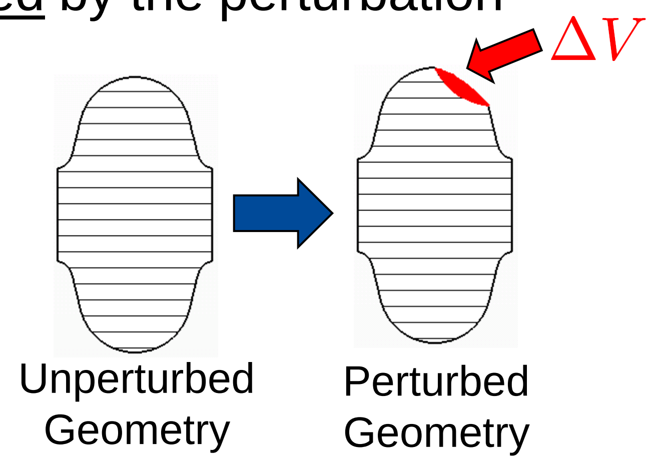
$$IT_{E(\mathrm{ik})} = \iiint_{\Delta V} \mathbf{E}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{E}_\mathrm{k}(\mathbf{r})\, \mathrm{d}V$$

$$IT_{H(\mathrm{ik})} = \iiint_{\Delta V} \mathbf{H}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{H}_\mathrm{k}(\mathbf{r})\, \mathrm{d}V$$

↓

Volume integral matrices

$IT_E\,,\; IT_H$



Basic Operations of Perturbation Theory

	Method 1: GST Generalisation of Slater's Theorem	Method 2
Computation of unperturbed modes	Analytical computation or Use of numerical eigenmode solver	Analytical computation or Use of numerical eigenmode solver
Computation of volume integral matrices	$IT_E \, , \, IT_H$	IT_E
Computation of interaction term matrix	$\frac{\omega_\mathrm{k}}{U_\mathrm{i}}\left(\omega_\mathrm{i}\epsilon \cdot IT_{E(\mathrm{ik})} - \omega_\mathrm{k}\mu \cdot IT_{H(\mathrm{ik})}\right)$	$\frac{\epsilon}{2U_\mathrm{i}} \cdot IT_{E(\mathrm{ik})}$
Arithmetic operations (e.g. eigensystem computation)	Operations 1	Operations 2 (more complex)
Perturbed eigenmodes (Frequencies, weighting factors for series expansion)	Perturbed eigenmodes	Perturbed eigenmodes

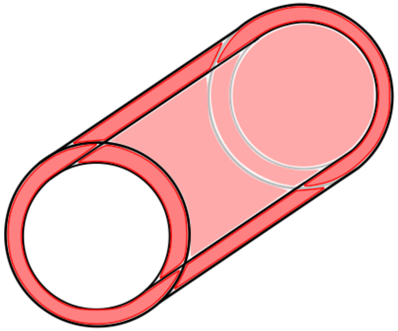
Proof of Principle I

- Analytically evaluable cavity shape
  - Use of <u>analytically</u> computed unperturbed and eigenmodes

  → Any desired number of unperturbed modes usable for series expansion

  → Very high precision for implementation

  → Very low effort



- Computation example
  - cylindrical cavity
  - subject to radial perturbation of 5%
  - Investigation of TM_{0n0} modes (n: radial mode index)

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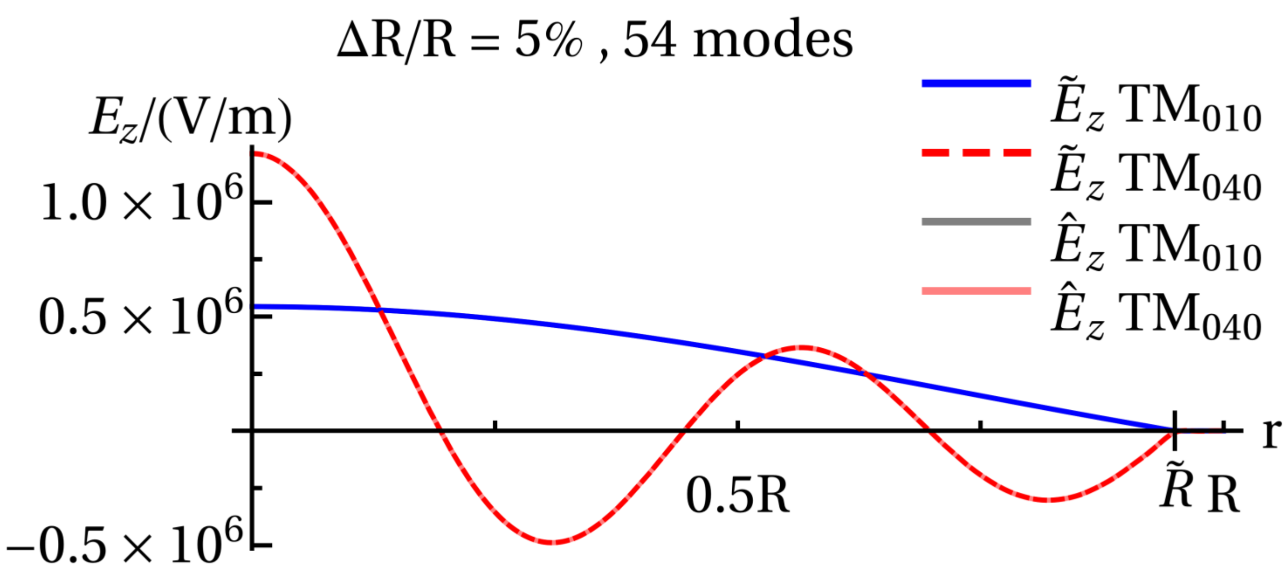
Proof of Principle II:

- Using only a small number of unperturbed modes $TM_{0.1.0}$ to $TM_{0.54.0}$
- Relative error of perturbed frequencies < 10^{-3}
- Longitudinal electric field along the radius r



Fields coincide very well

$\tilde{E}_z$: perturbed longitudinal E-field (GST)

$\hat{E}_z$: perturbed longitudinal E-field (analytical)

Proof of Principle II:

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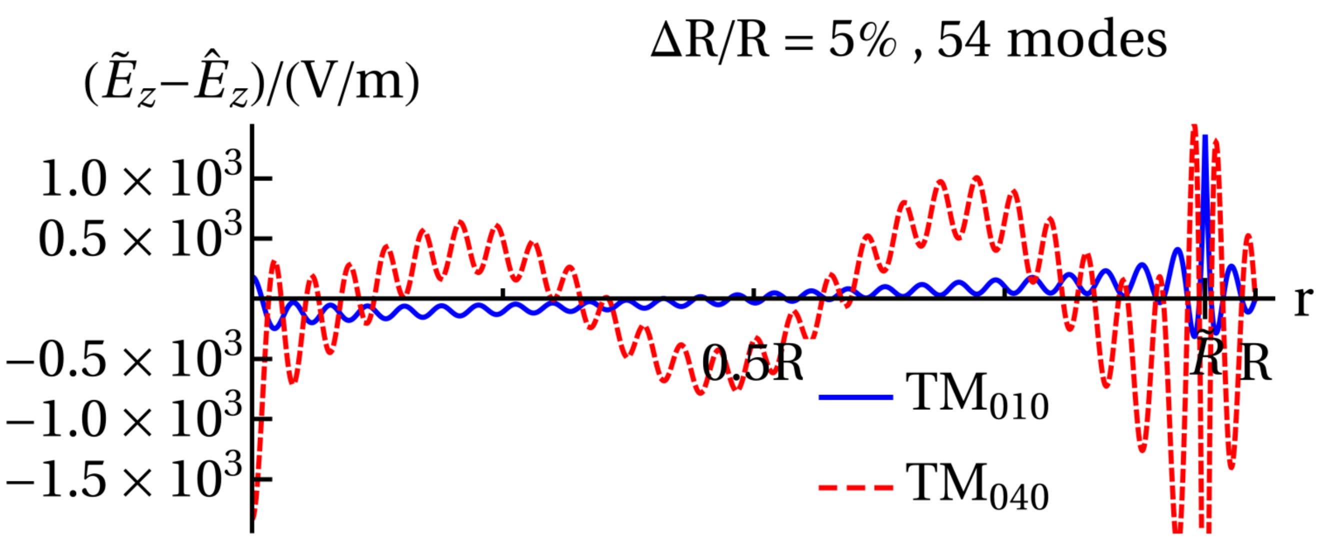


Deviation is less than 10^{-3} of maximal value

➡ Very accurate results

$\tilde{E}_z$: perturbed longitudinal E-field (GST)

$\hat{E}_z$: perturbed longitudinal E-field (analytical)

Numerical Implementation

Basic Operations of Numerical Implementation

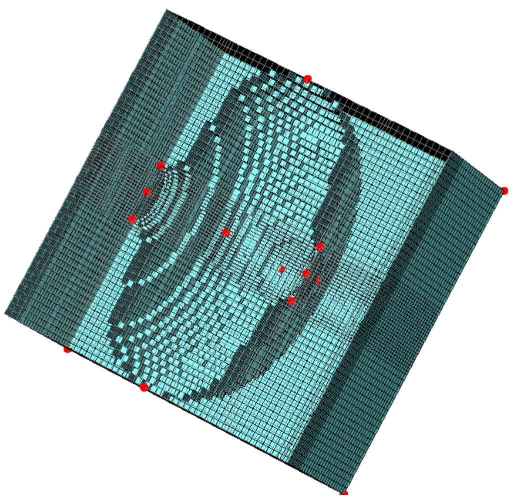
- Computation of unperturbed eigenmodes
  → Unperturbed frequencies and fields
- Computation of volume integrals
- Computation of interaction terms
- Evaluation of arithmetic operations
  → Perturbed frequencies and weighting factors

}
- Simple & Low effort
- Equal for analytical and numerical implementation

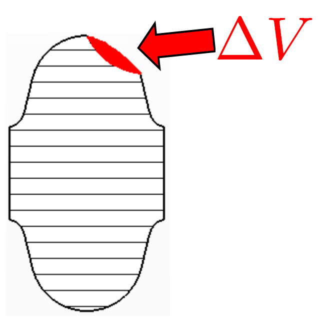
- Series expansion in terms of unperturbed fields
  → Perturbed fields

Numerical computation of unperturbed eigenmodes

- Result relevant parameters
  - Mesh density
  - Exactness of boundary discretization
  - → Accuracy of unperturbed frequencies and fields



- Depends on
  - Cavity geometry
  - Frequency range / minimal wavelength
  - → Computation method



→ Accuracy of boundary fields very important

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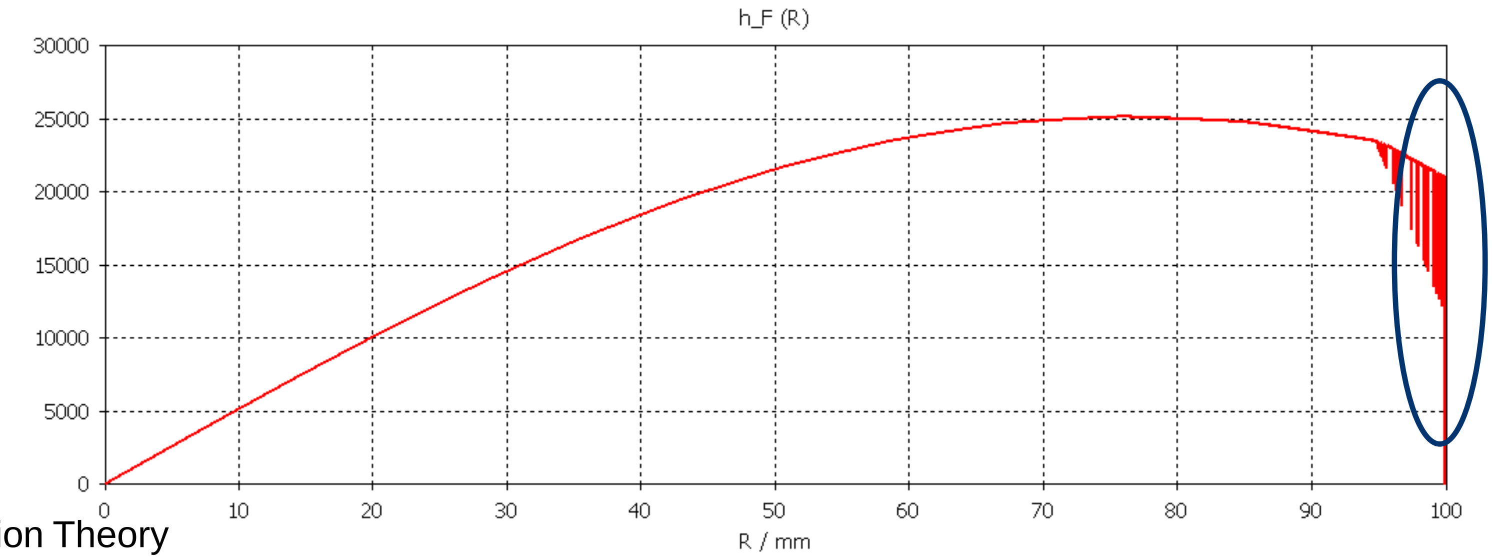
FIT*-based Eigenmode-Computation (CST-MicrowaveStudio©)

- Dual grid with hexahedral cells and PBA (partially filled cells)
  - Inner fields: Good approximation
  - Fields near to the boundary: abrupt transition to zero

Magnetic field along the radius (R=100 mm)



* Finite Integration Theory

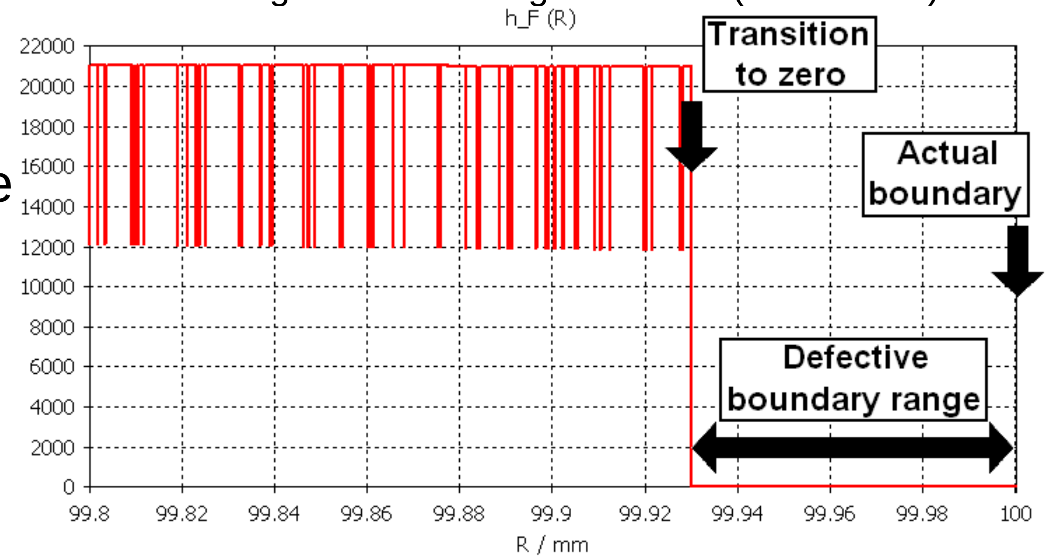
FIT*-based Eigenmode-Computation (CST-MicrowaveStudio©)

- Dual grid with hexahedral cells and PBA (partially filled cells)
  - Inner fields: Good approximation
  - Fields near to the boundary: abrupt transition to zero
- Boundary fields are of crucial importance for volume integrals

Defective boundary range must be as small as possible

FIT not appropriate for Perturbation Theory

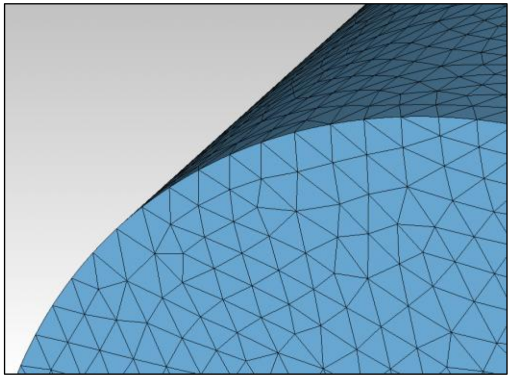
Magnetic field along the radius (R=100 mm)

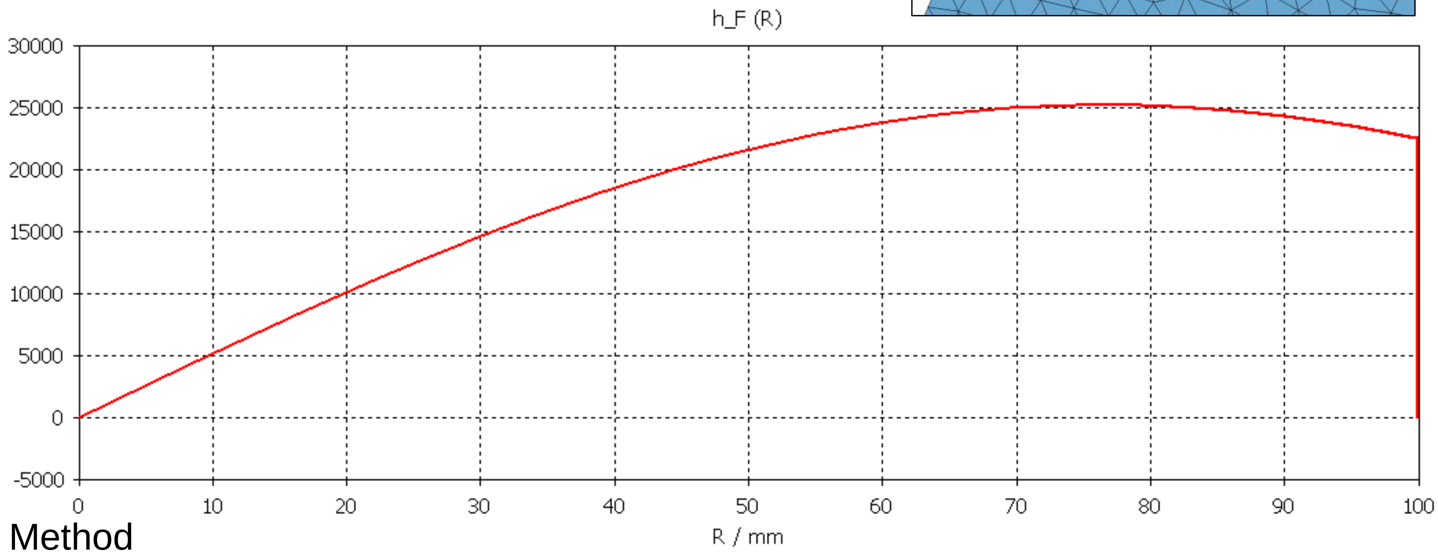


* Finite Integration Theory

FEM*-based Eigenmode-Computation (CST-MicrowaveStudio©)

- Tetraeder-Grid with Curved Elements
  - Better approximation of boundary curve
  - No oscillations





* Finite Elements Method

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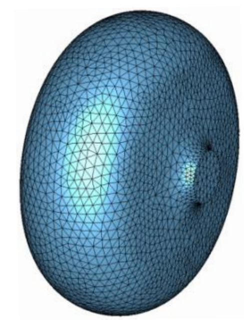
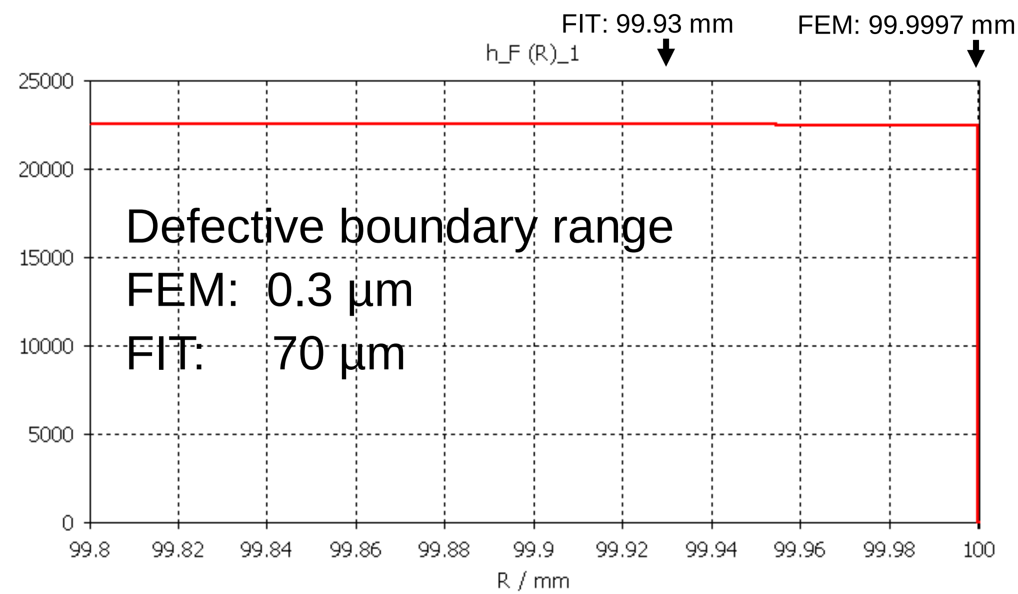
FEM*-based Eigenmode-Computation (CST-MicrowaveStudio©)

- Tetraeder-Grid with Curved Elements
  - Better approximation of boundary curve
  - No oscillations
  - Defective boundary range <u>essentially</u> smaller

→ Especially for elliptical cavities more accurate results



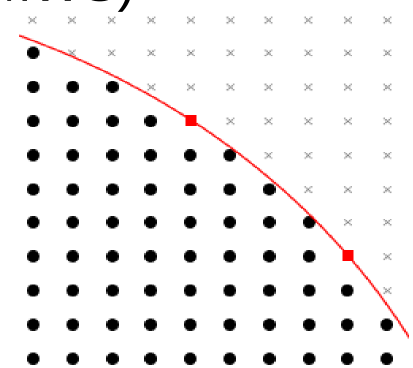


FEM more suitable for boundary fields

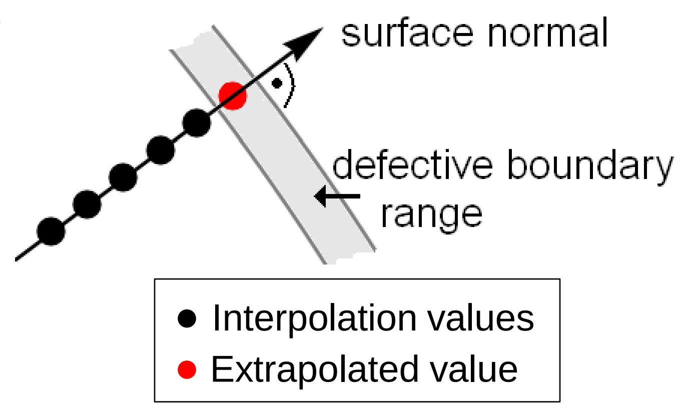
* Finite Elements Method

Extrapolation of Boundary Field Values

- After computation of unperturbed eigenmodes (CST MWS)
  - Fields have to be exported as discrete field points
- But still: Field points inside defective boundary range
  → Incorrect field values of zero
  → Impairment of volume integrals



- Simple but effective solution
  Extrapolation of defective field value from set of correct values along surface normal vector
  → 1D interpolation



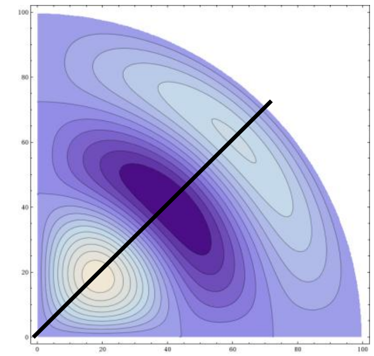
Computation of Volume Integrals: Approach 1

- Interpolation of discrete field data
  → Continuous 3D IP-functions for integration

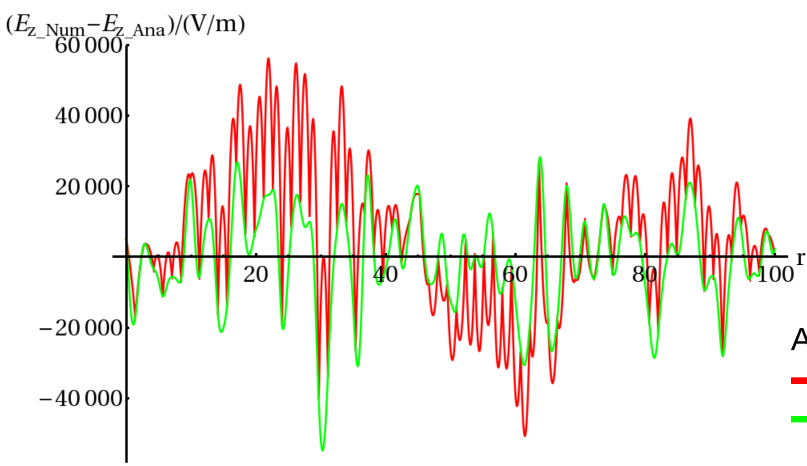
$$IT_{E(\mathrm{ik})} = \iiint\limits_{\Delta V} \mathbf{E}_{\mathrm{i}}(\mathbf{r}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r})\ \mathrm{d}V$$

- For very accurate results
  - IP-functions with polynomial degree > 1 needed

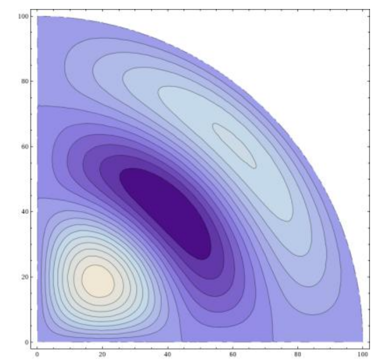
Cylindrical cavity
E_z-Field of TM_{232}



Analytical



Absolute error of field along radius:
Interpolation (degree of 1)
Interpolation (degree of 3)



Interpolation

Computation of Volume Integrals: Approach 1

- Interpolation of discrete field data

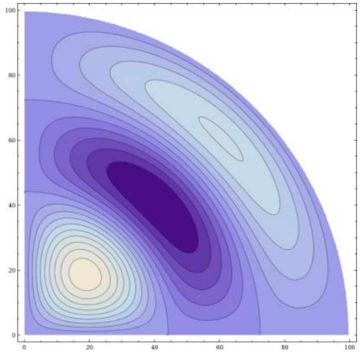
  → Continuous 3D IP-functions for integration

$$IT_{E(\mathrm{ik})} = \iiint\limits_{\Delta V} \mathbf{E}_{\mathrm{i}}(\mathbf{r}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r}) \, \mathrm{d}V$$

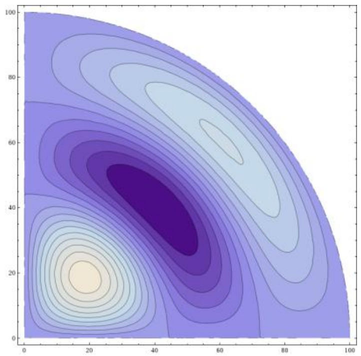
- For very accurate results
  - IP-functions with polynomial degree > 1 needed
  - Only realizable on a structured grid

  → Very large number of field points

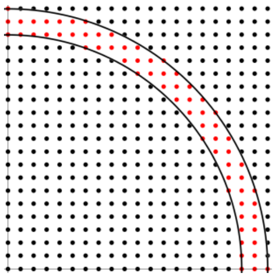
Cylindrical cavity
E_z-Field of TM_{232}



Analytical



Interpolation



Radial perturbation

Enormous effort

- Export of field values
- 3D Interpolation of degree > 1

Computation of Volume Integrals: Approach 2

- Numerical integration: Summation of products of discrete fields and discrete volume

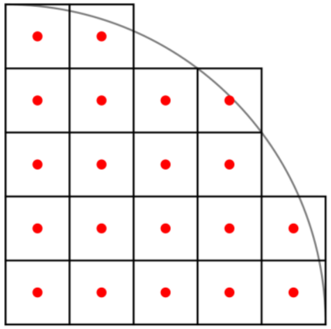
$$\iiint\limits_{\Delta V} \mathbf{E}_{\mathrm{i}}(\mathbf{r}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r})\, \mathrm{d}V \quad \rightarrow \quad \sum_{\mathrm{m}=1}^{M} \mathbf{E}_{\mathrm{i}}(\mathbf{r}_{\mathrm{m}}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r}_{\mathrm{m}}) \cdot \Delta V_{\mathrm{m}}$$

- Partitioning of ΔV into volume elements

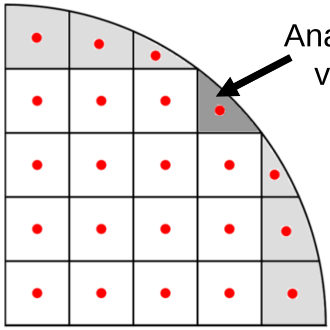
  Commonly used cubic elements: very inaccurate for boundary elements

- Solution: Analytical volume elements

  If boundary of ΔV and element intersect: analytical computation of volume and center



Cubic elements



Cubic elements (analytical)

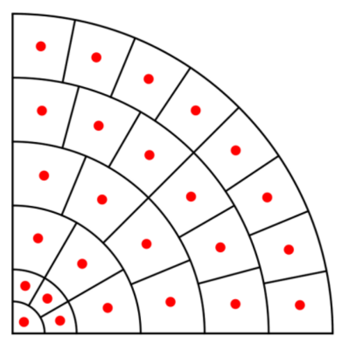
Computation of Volume Integrals: Approach 2

- Numerical integration: Summation of products of discrete fields and discrete volume

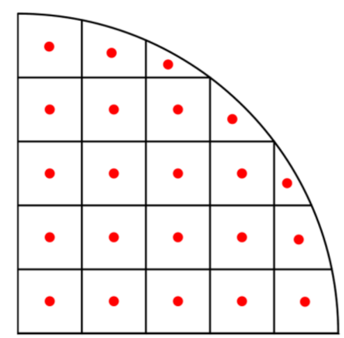
$$\iiint\limits_{\Delta V} \mathbf{E}_{\mathrm{i}}(\mathbf{r}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r})\ \mathrm{d}V \quad \rightarrow \quad \sum_{\mathrm{m}=1}^{M} \mathbf{E}_{\mathrm{i}}(\mathbf{r}_{\mathrm{m}}) \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r}_{\mathrm{m}}) \cdot \Delta V_{\mathrm{m}}$$

- Partitioning of ΔV into volume elements
  - Commonly used cubic elements: very inaccurate for boundary elements
- Solution: <u>Analytical volume elements</u>
  - If boundary of ΔV and element intersect: analytical computation of volume and center

⇒
- Precise discretization
- Low effort



Cylindrical elements (analytical)



Cubic elements (analytical)

Computation of perturbed fields

- Final arithmetic operations yield
  - Perturbed frequencies
  - Weighting factors for series expansion
- Series expansion of perturbed fields

$$\widetilde{\mathbf{E}}_{\mathrm{i}}(\mathbf{r}) = \sum_{\mathrm{k}=1}^{N} e_{\mathrm{ik}} \cdot \mathbf{E}_{\mathrm{k}}(\mathbf{r})$$
$$\widetilde{\mathbf{H}}_{\mathrm{i}}(\mathbf{r}) = \sum_{\mathrm{k}=1}^{N} h_{\mathrm{ik}} \cdot \mathbf{H}_{\mathrm{k}}(\mathbf{r})$$

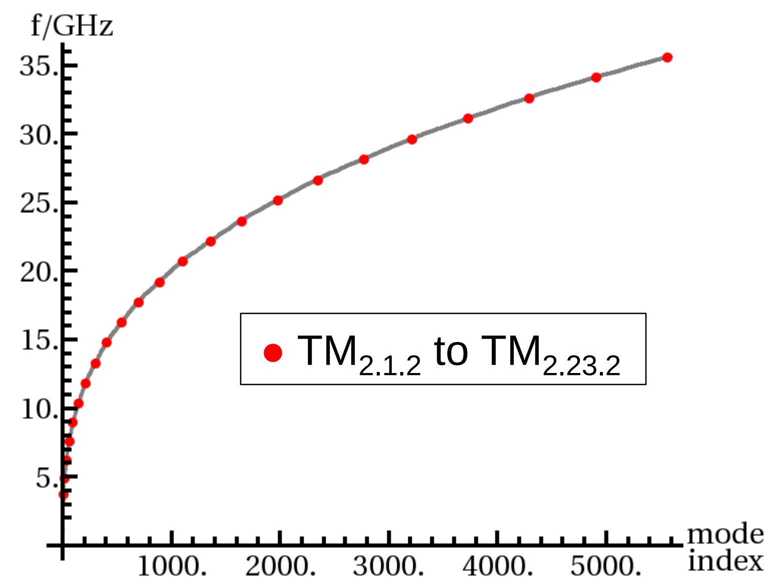
  - CST MWS post processing: Summation of unperturbed fields multiplied by weighting factors
  - External program: Export of unperturbed fields
    → Summation of discrete field values

Results

Numerical computation of unperturbed eigenmodes

- Computation example
  - Cylindrical cavity (R=100 mm, L=100 mm, fundamental mode: 1.15 GHz)
  - Investigation of TM_{2n2} modes subject to radial perturbations

- Eigenmodes computable in a very large frequency range
  - Up to 35.71 GHz



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Numerical computation of unperturbed eigenmodes

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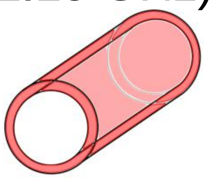
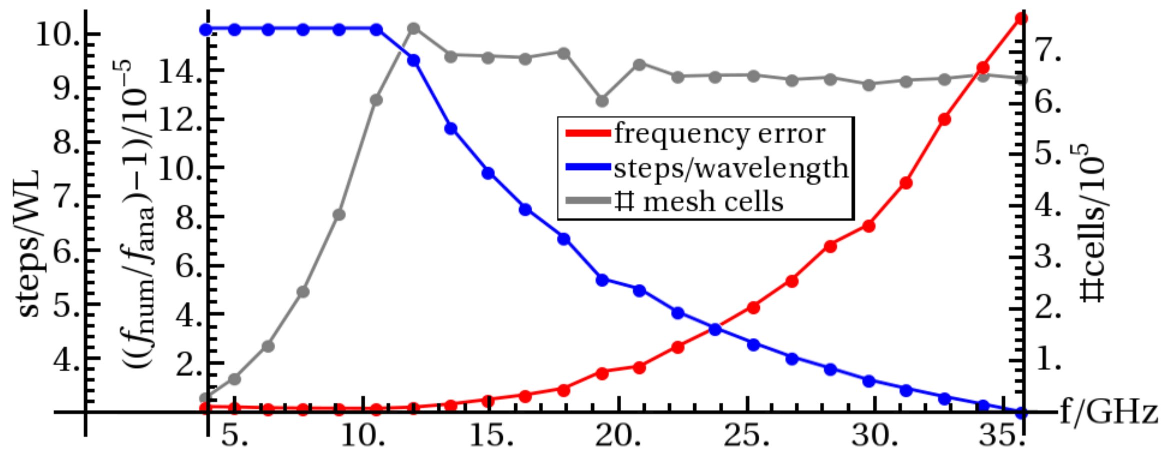


- Eigenmodes computable in a very large frequency range
  - Up to 35.71 GHz
  - Frequency error < $1.6 \cdot 10^{-4}$

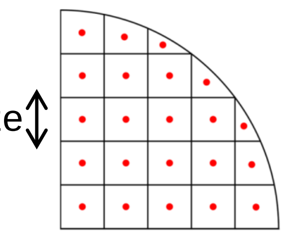
Very accurate in a large frequency range

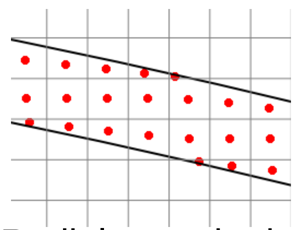


  K. Brackebusch

Computation of Volume Integrals: Size of elements

- Necessary step size depends on
  - Frequency / wave length
  - Extent of perturbation

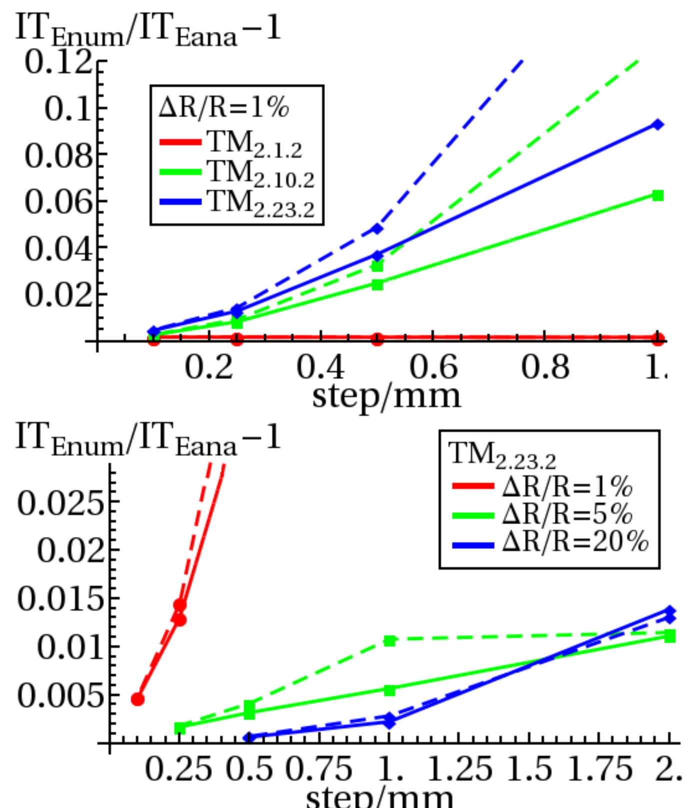
Step size



Radial perturbation

ΔR/R	ΔR	Step size	# elements
1 %	1 mm	0.25 mm	500000
5 %	5 mm	0.5 mm	306000
20 %	20 mm	1 mm	150000

⇒ **Reasonable number of mesh cells**

Relative deviation of volume integrals



— Cubic elements
··· Cylindrical elements

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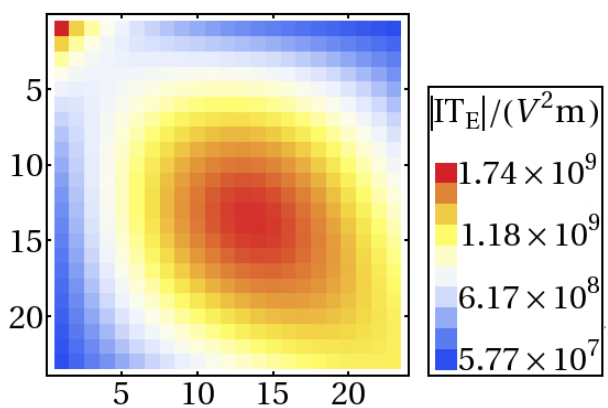
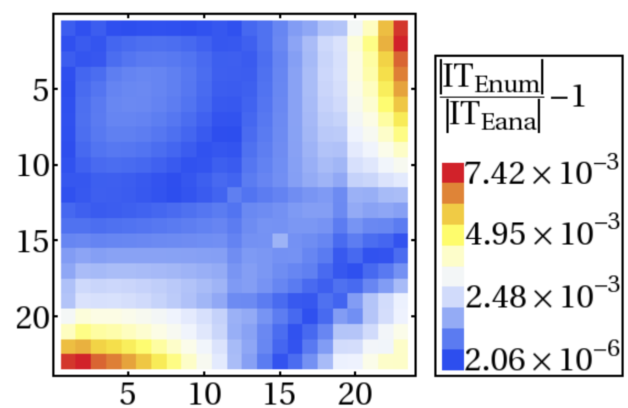
Computation of Volume Integrals: Accuracy

- IT_E (electric fields) : Very accurate
  - Relative error mainly < $2 \cdot 10^{-3}$
  - Only for small values of IT_E larger error

Absolute values



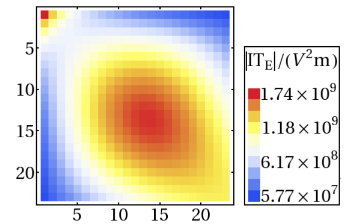
Relative deviation

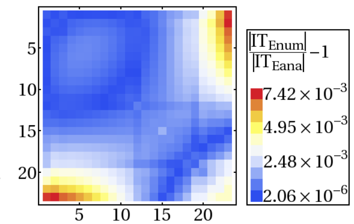


Radial perturbation: 5% (5 mm)
Step size: 0.5 mm

Computation of Volume Integrals: Accuracy

- IT_E (electric fields) : Very accurate
  - Relative error mainly < $2 \cdot 10^{-3}$
  - Only for small values of IT_E larger error

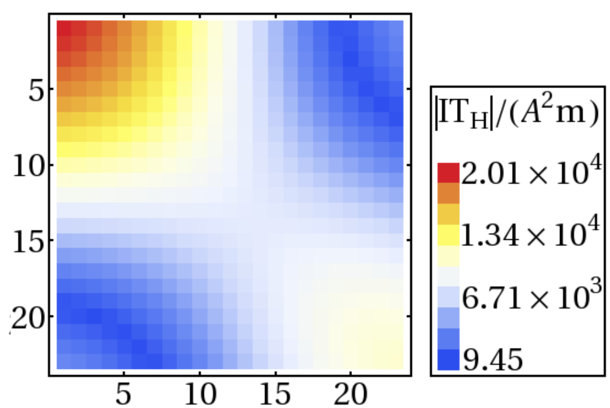




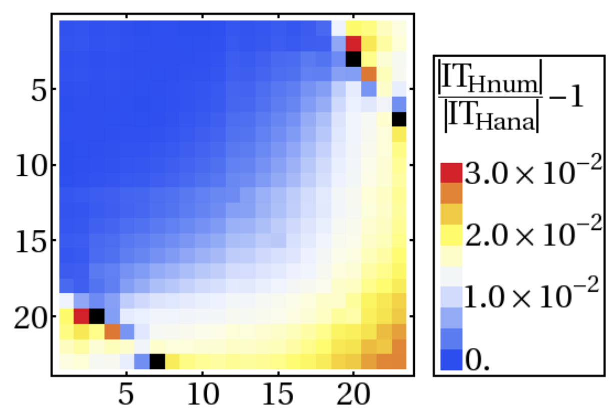
- IT_H (magnetic fields) : Very accurate for limited frequency range
  - Up to 21 GHz (13th mode): Relative error < $7 \cdot 10^{-3}$
  - Increases up to $3 \cdot 10^{-2}$ for frequencies

IT_E: very accurate
IT_H: accurate

Absolute values



Relative deviation



Radial perturbation: 5% (5 mm)
Step size: 0.5 mm

Interaction Terms & Final Results

- Accuracy depends on perturbative method

Method 1

$$\frac{\omega_{\mathrm{k}}}{U_{\mathrm{i}}}\left(\omega_{\mathrm{i}}\epsilon\cdot IT_{E(\mathrm{ik})}-\omega_{\mathrm{k}}\mu\cdot IT_{H(\mathrm{ik})}\right)$$

$\mu/\varepsilon \approx 10^5$

Absolute error of IT_H scaled up

Depending on ratio of $\omega_i\cdot\varepsilon\cdot IT_{E(ik)}$ to $\omega_k\cdot\mu\cdot IT_{H(ik)}$

Error of resulting interaction term may increase

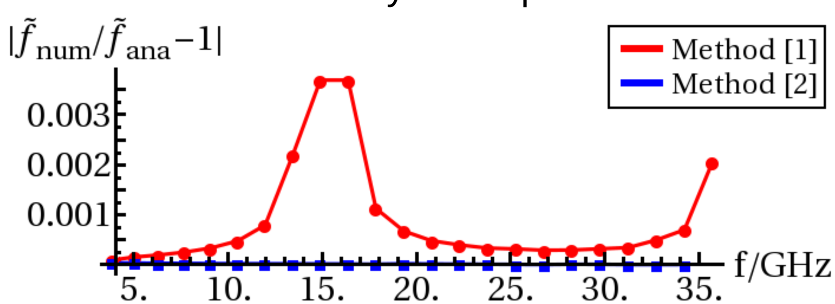
Method 2

$$\frac{\epsilon}{2U_{\mathrm{i}}}\cdot IT_{E(\mathrm{ik})}$$

Same relative error as IT_E

Very accurate

Relative deviation between numerical and analytical implementation



Error of perturbed frequencies

- Method 2: Extremely small
- Method 1: Increased but still very small

Conclusion & Outlook

Conclusion

- Perturbation Theory: Efficient method to compute perturbed eigenmodes of cavities in the context of parameter studies
- Numerical implementation
  - Feasible with commonly used standard software
  - (Very) accurate results over a large frequency range
  - Reasonable computational effort
  - Differences in error propagation depending on perturbative method

  → Application to arbitrary cavity geometries

Outlook

- Application to real cavities (elliptical cavities)
- Improvement of algorithm of perturbative methods

References

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