Calculation of Eigenfields for the European XFEL Cavities

TECHNISCHE UNIVERSITÄT DARMSTADT

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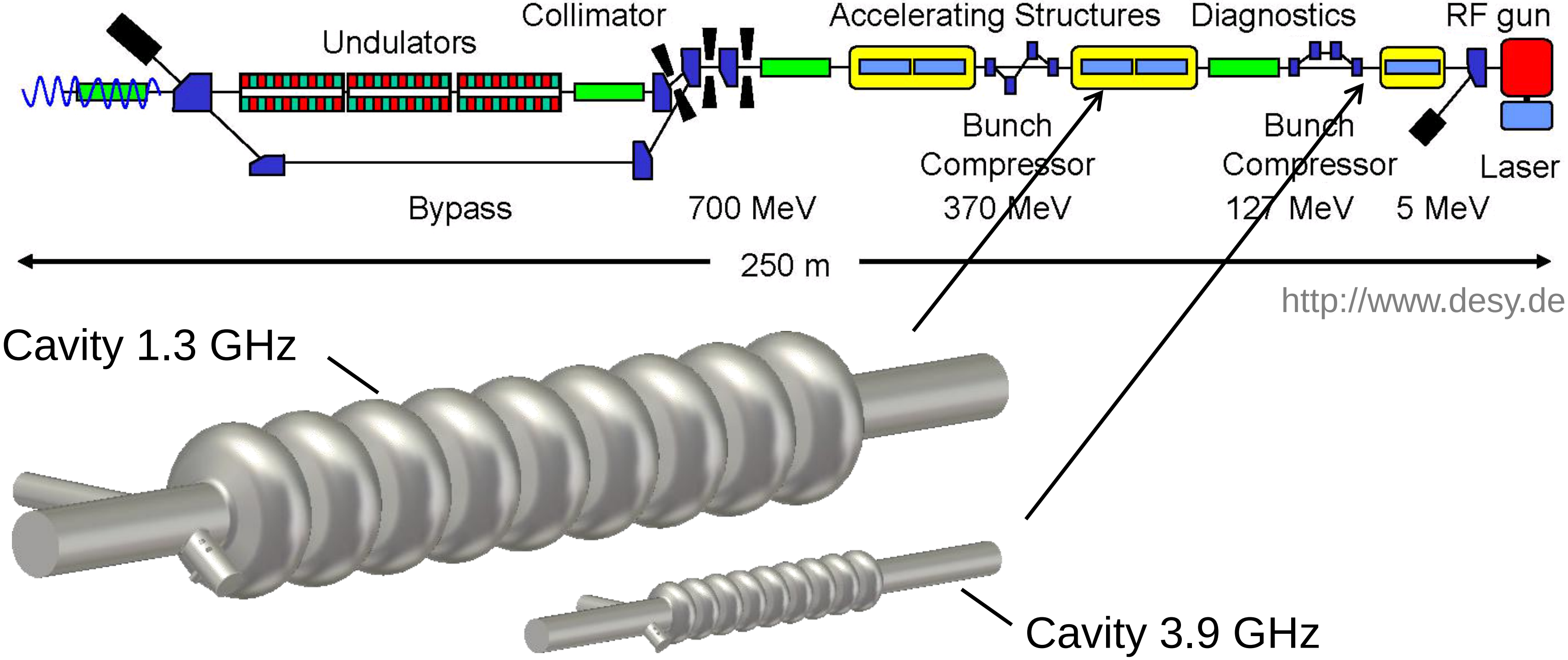
Status Meeting
December 21, 2010
DESY, Hamburg

Overview

- Task
  - Calculation of fields for the European XFEL cavities in 3D considering coupling ports as well as non-ideal geometries
  - Coupling ports:
    - Modeling of ports
    - Include ports in the eigenvalue formulation
    - Implementation for large scale applications
  - Non-ideal geometries
    - Support flexible geometry description in 3D

Motivation

- Particle accelerators
  - Linear accelerator at DESY, Hamburg



Computational Model

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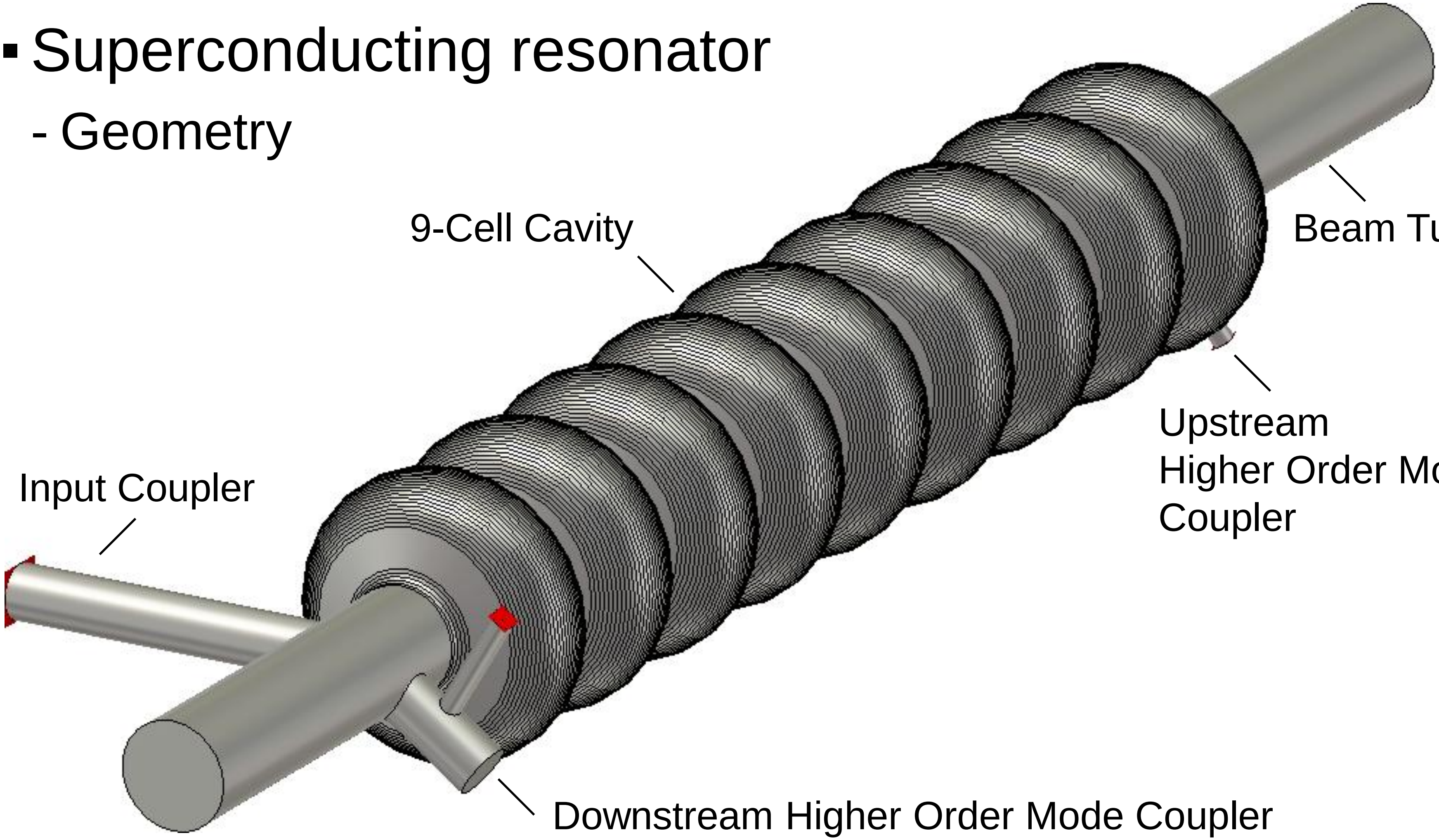
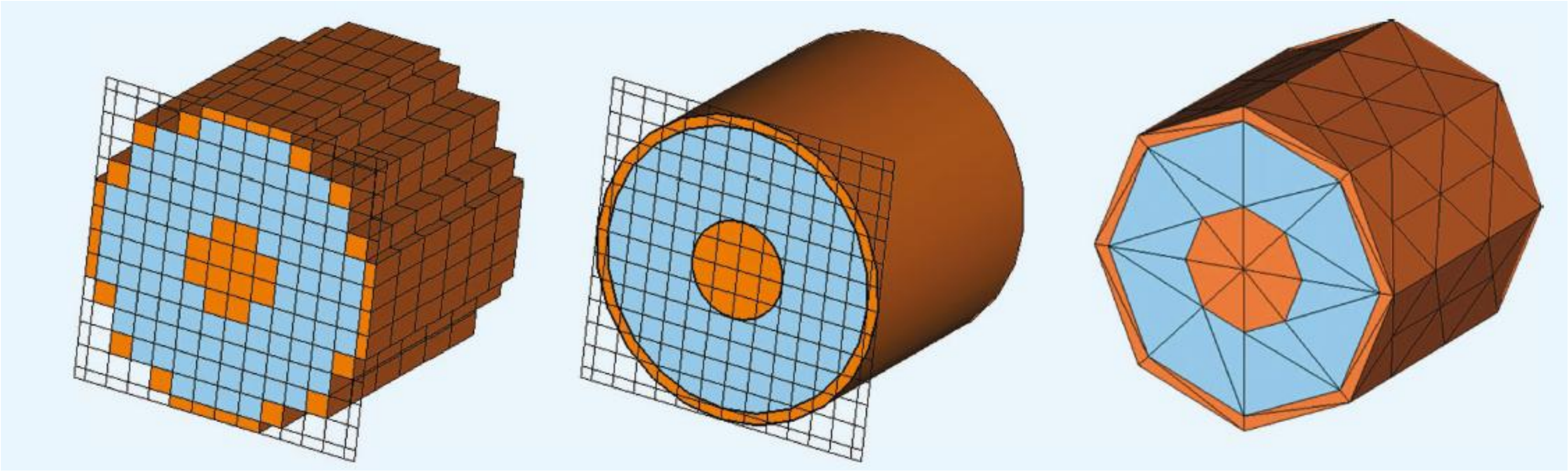
- Superconducting resonator
  - Geometry



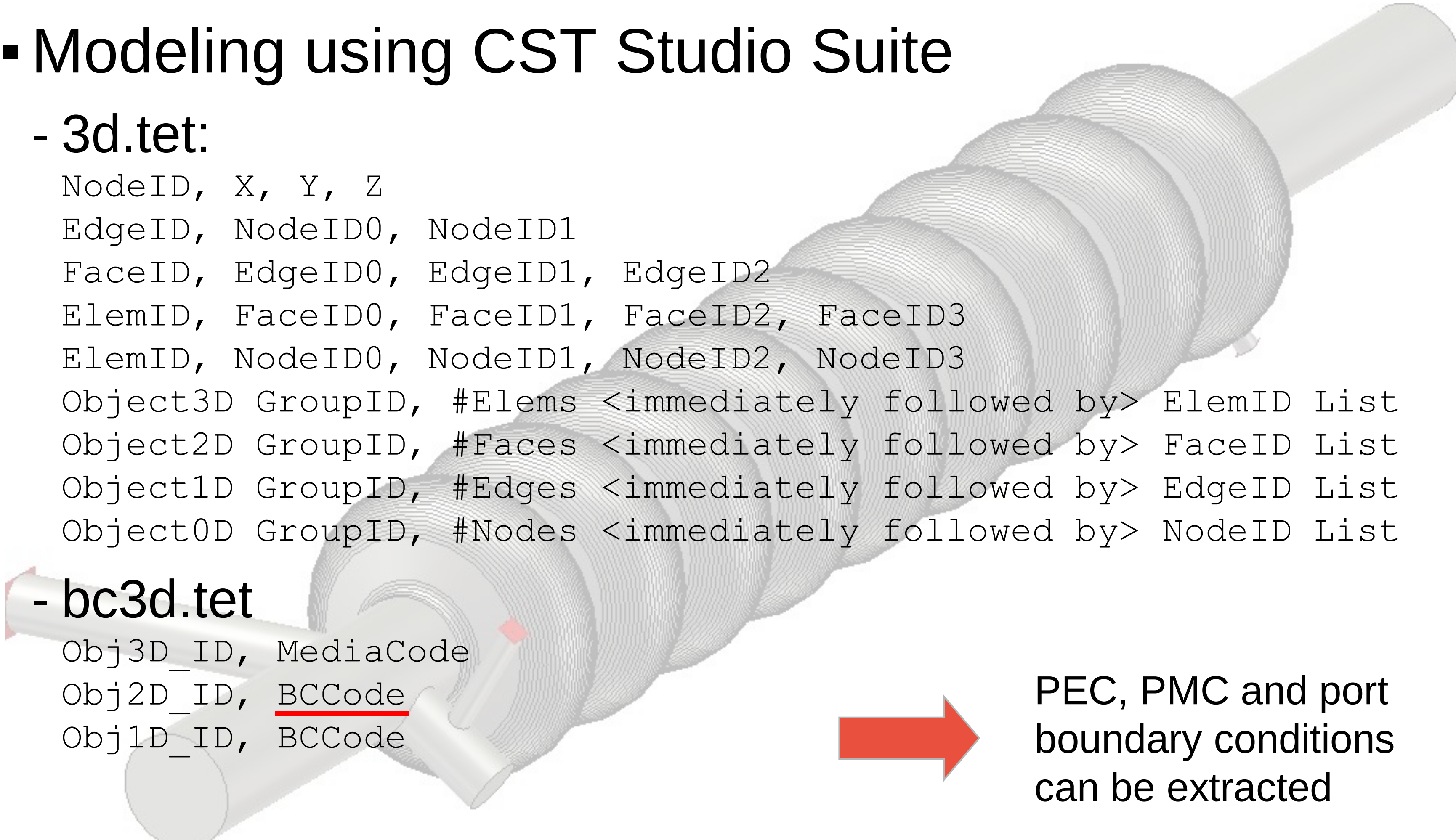
Computational Model

- Available grid structures



‚Staircase'-grid | partially filled cells | tetrahedral mesh

Computational Model



- Modeling using CST Studio Suite
  - 3d.tet:

```
NodeID, X, Y, Z
EdgeID, NodeID0, NodeID1
FaceID, EdgeID0, EdgeID1, EdgeID2
ElemID, FaceID0, FaceID1, FaceID2, FaceID3
ElemID, NodeID0, NodeID1, NodeID2, NodeID3
Object3D GroupID, #Elems <immediately followed by> ElemID List
Object2D GroupID, #Faces <immediately followed by> FaceID List
Object1D GroupID, #Edges <immediately followed by> EdgeID List
Object0D GroupID, #Nodes <immediately followed by> NodeID List
```

  - bc3d.tet

```
Obj3D_ID, MediaCode
Obj2D_ID, BCCode
Obj1D_ID, BCCode
```

→ PEC, PMC and port boundary conditions can be extracted

Computational Model

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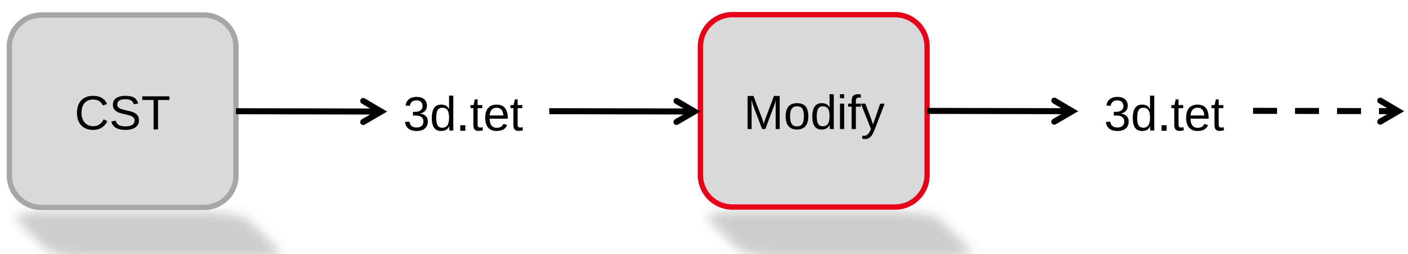
- Modeling using CST Studio Suite
  - 3d.tet:

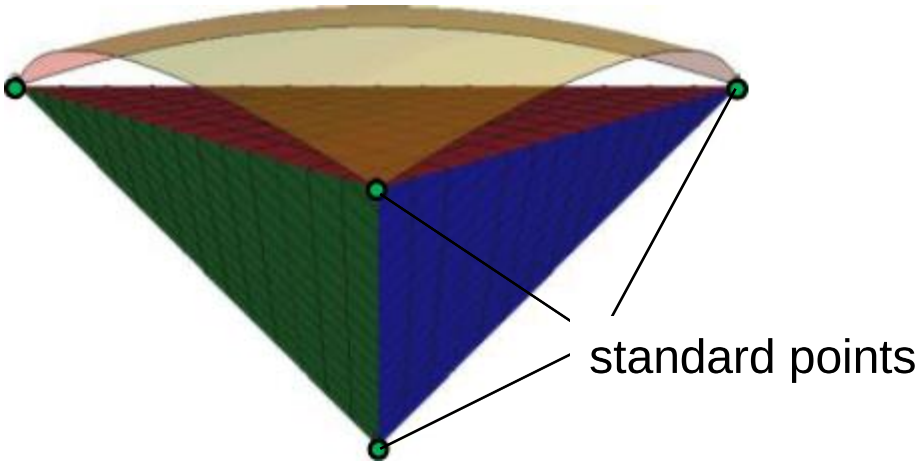
modify point locations but maintain the topology

```
NodeID, X, Y, Z
EdgeID, NodeID0, NodeID1
FaceID, EdgeID0, EdgeID1, EdgeID2
ElemID, FaceID0, FaceID1, FaceID2, FaceID3
ElemID, NodeID0, NodeID1, NodeID2, NodeID3
Object3D GroupID, #Elems <immediately followed by> ElemID List
Object2D GroupID, #Faces <immediately followed by> FaceID List
Object1D GroupID, #Edges <immediately followed by> EdgeID List
Object0D GroupID, #Nodes <immediately followed by> NodeID List
```



Computational Model

- Modeling using CST Studio Suite
  - 3d.tet:



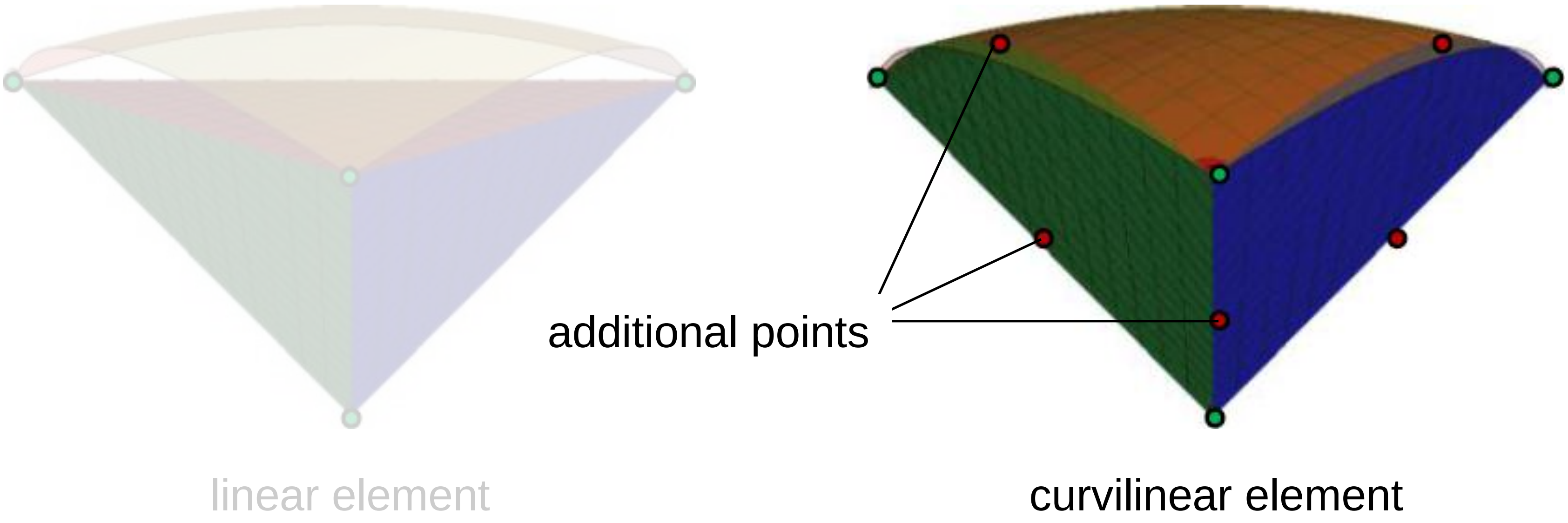
linear element

curvilinear element

only linear geometry transformation available

Computational Model

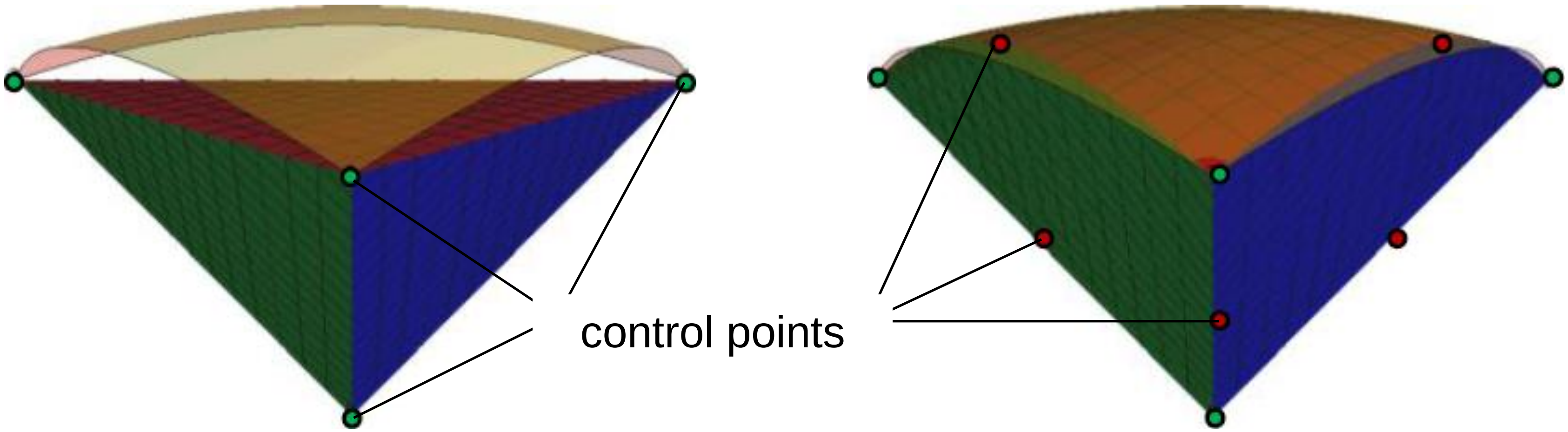
- Modeling using CST Studio Suite
  - 3d.tet:



➡ insert additional control points (at the surface)

Computational Model

- Modeling using CST Studio Suite
  - 3d.slim:



linear element

curvilinear element

→ available in CST but not yet used here… (ToDo)

Motivation

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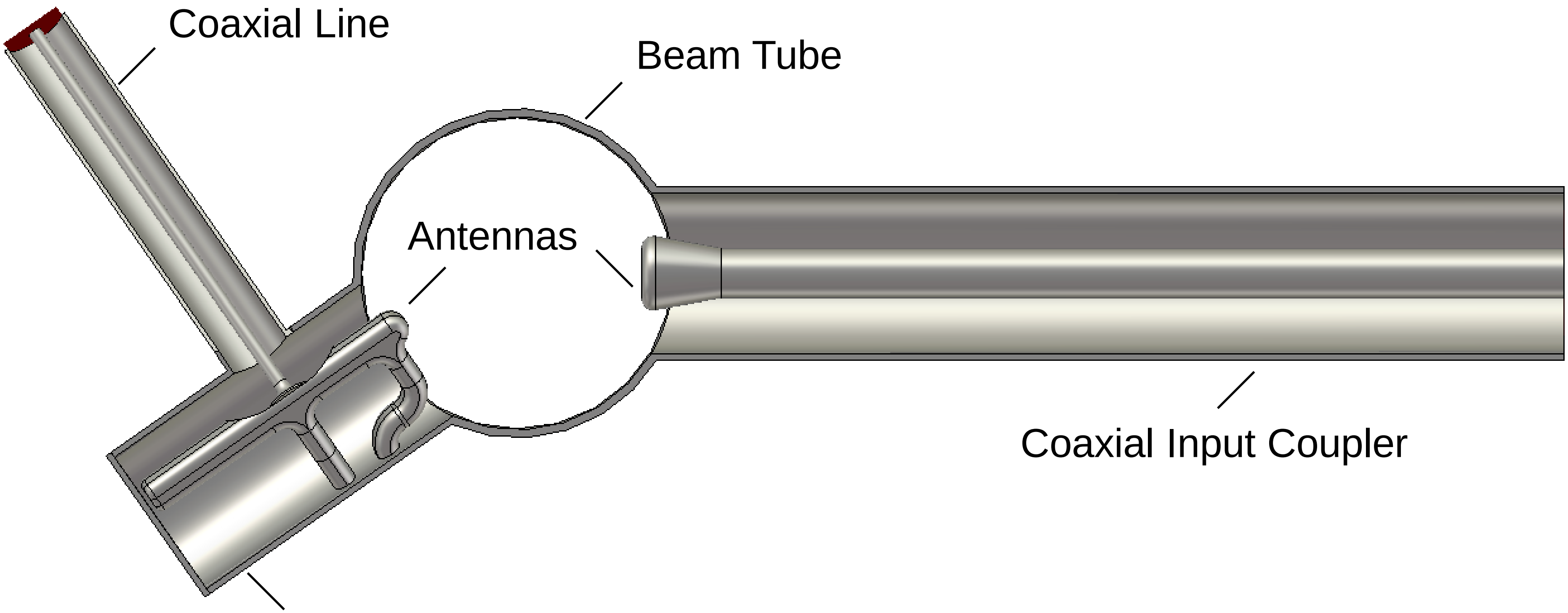
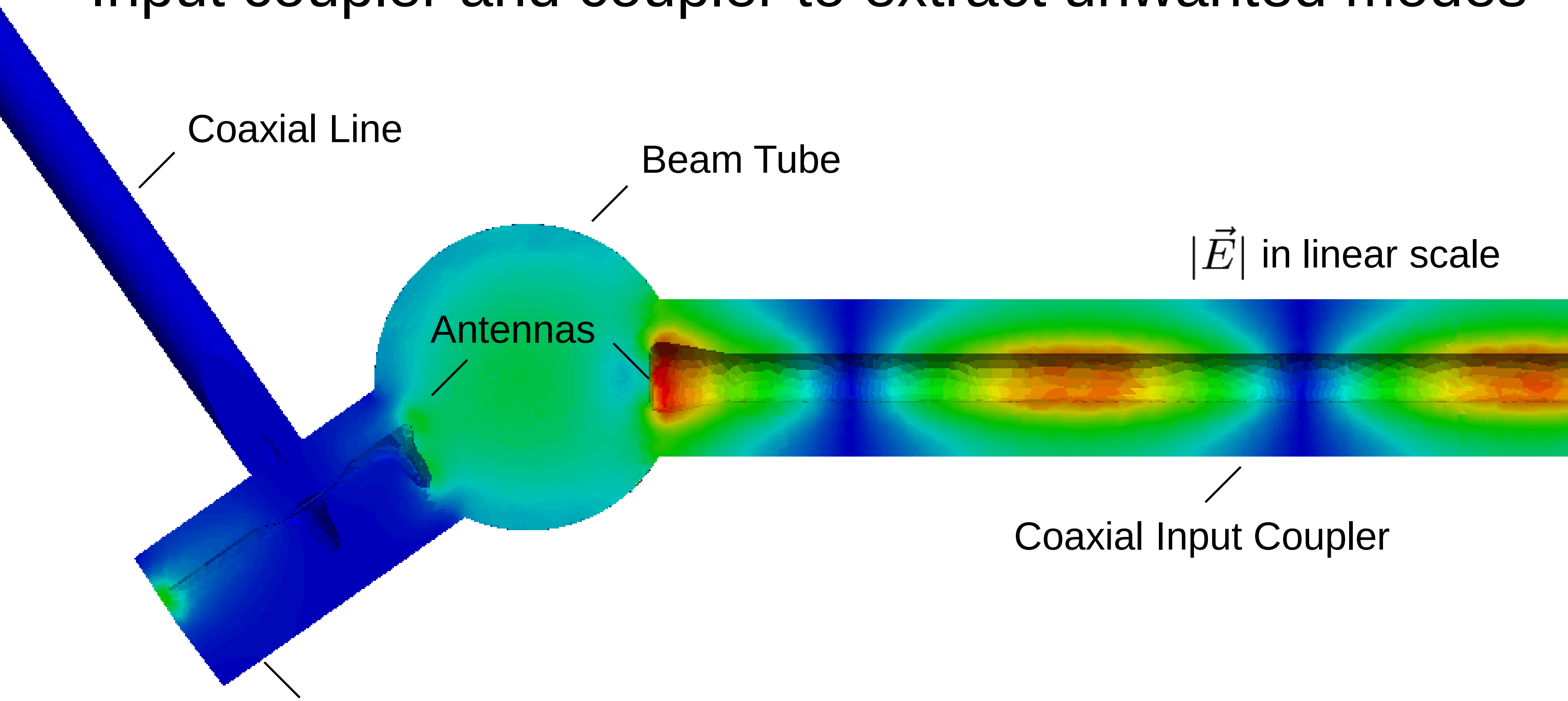
- Input coupler and coupler to extract unwanted modes



Motivation

TECHNISCHE UNIVERSITÄT DARMSTADT

- Input coupler and coupler to extract unwanted modes



$f_0 = 1.300$ GHz

Motivation

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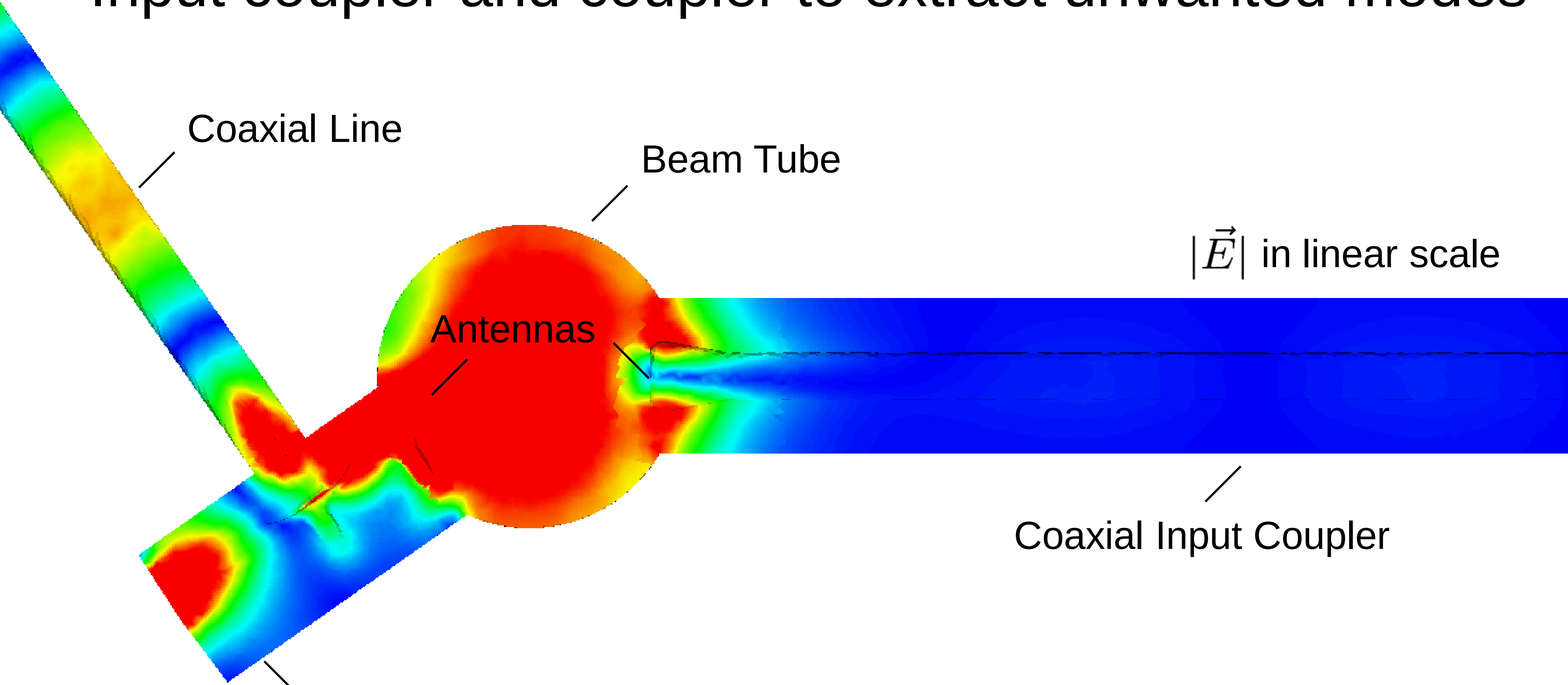
- Input coupler and coupler to extract unwanted modes

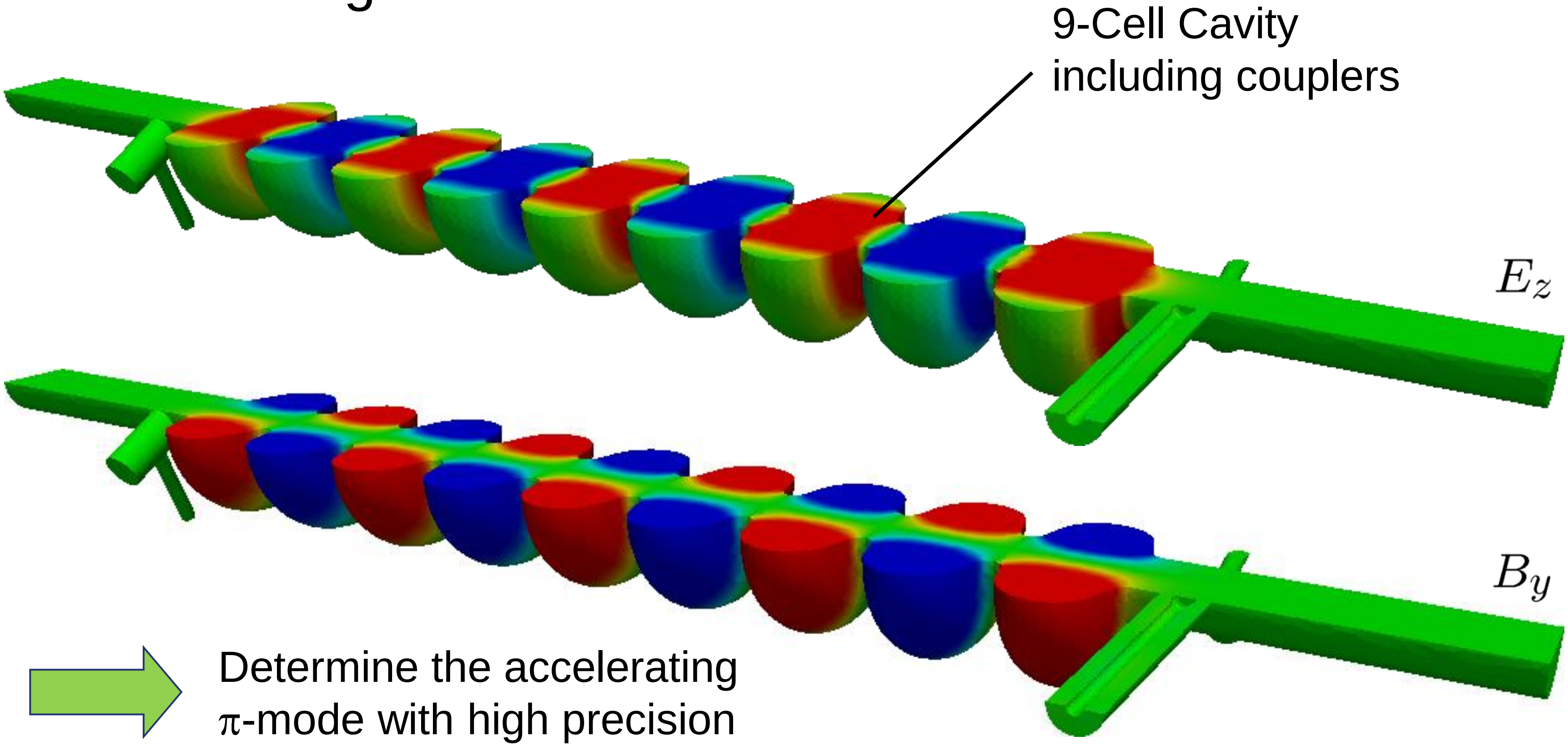


$|\vec{E}|$ in linear scale

$f_0 = 1.709$ GHz

Motivation

- Problem definition
  - Accelerating field



Determine the accelerating π-mode with high precision

Computational Model

- Problem formulation
  - Fundamental equations

$$\mathrm{curl}\ 1/\mu_{\mathrm{r}}\ \mathrm{curl}\vec{E} - \left(\frac{\omega}{c_0}\right)^2 \varepsilon_{\mathrm{r}}\, \vec{E}\,\Big|_{\vec{r}\in\Omega} = 0$$

$$\mathrm{div}(\varepsilon\vec{E})\Big|_{\vec{r}\in\Omega} = 0$$

  - Boundary conditions

$$\vec{n}\times\vec{E}\,\Big|_{\vec{r}\in\partial\Omega_{\mathrm{PEC}}} = 0$$

$$\vec{n}\times\mathrm{curl}\vec{E} + j\frac{\omega}{c_0}\,\vec{n}\times(\vec{n}\times\vec{E})\,\Big|_{\vec{r}\in\partial\Omega_{\mathrm{Port}}} = 0$$

$$\begin{aligned}
\mathrm{curl}\vec{H} &= \partial\vec{D}/\partial t \\
\mathrm{curl}\vec{E} &= -\partial\vec{B}/\partial t \\
\mathrm{div}\vec{D} &= 0 \\
\mathrm{div}\vec{B} &= 0
\end{aligned}$$

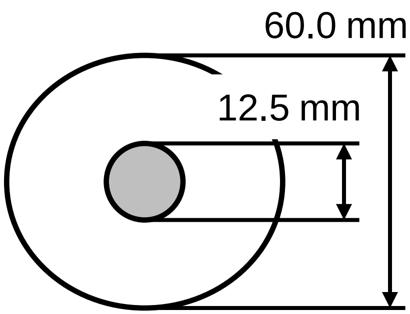
Maxwell‘s equations

$$\begin{aligned}
\vec{D} &= \varepsilon\vec{E} \\
\vec{B} &= \mu\vec{H}
\end{aligned}$$

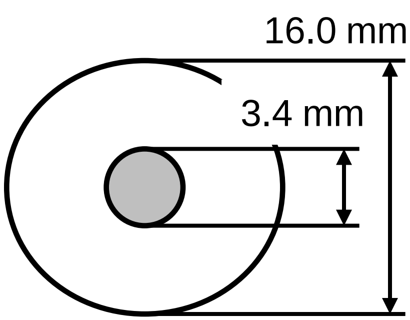
Material relations

Motivation

- Wave propagation in the applied coaxial lines
  - Main coupler



  - HOM coupler



Dispersion relation

$$k = \frac{2\pi}{c_0}\sqrt{f^2 - f_c^2}$$

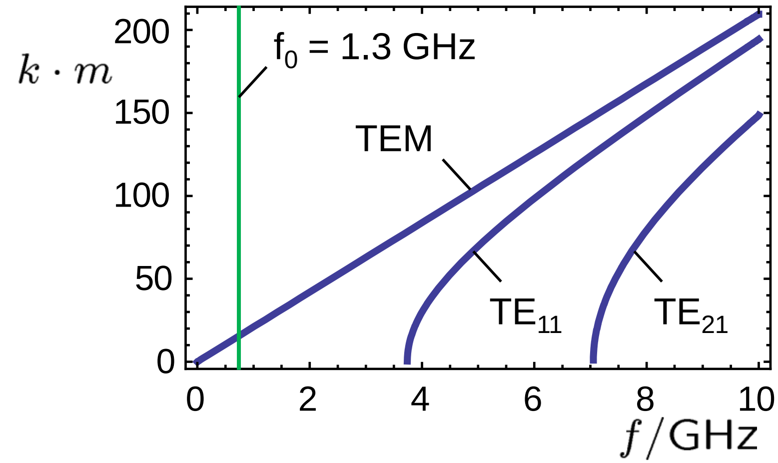
propagation

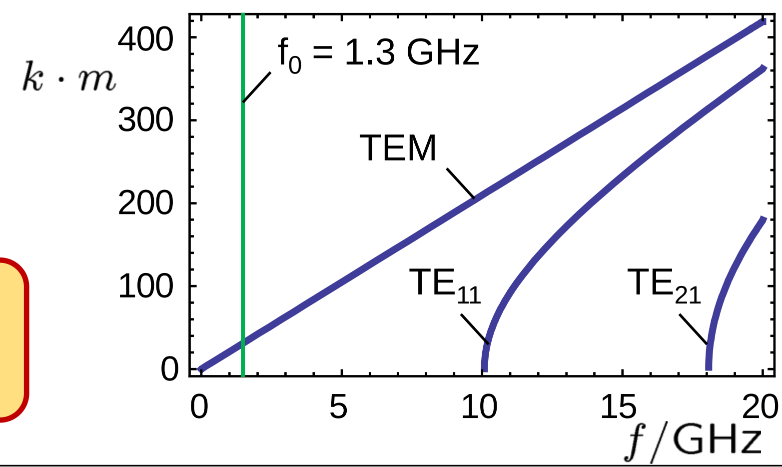
$f > f_c : \quad e^{jkz}$

damping

$f < f_c : \quad e^{-\alpha z}$

$$\alpha_{\text{Main}} = 1/13.6 \text{ mm}$$
$$\alpha_{\text{HOM}} = 1/4.77 \text{ mm}$$





Computational Model

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- Problem formulation
  - Local Ritz approach

$$\vec{E} = \vec{E}(\vec{r}) = \sum_{i=1}^{n} \alpha_i \, \vec{w}_i(\vec{r})$$

$\vec{w}$ vectorial function

α_i scalar coefficient

i global index

n number of DOFs

$$\mathrm{curl}\ 1/\mu_\mathrm{r}\ \mathrm{curl}\vec{E} = \left(\frac{\omega}{c_0}\right)^2 \varepsilon_\mathrm{r}\,\vec{E}\,\Big|_{\vec{r}\in\Omega}$$

$$\mathrm{div}(\varepsilon\vec{E})\Big|_{\vec{r}\in\Omega} = 0 \qquad \text{+ boundary conditions}$$

continuous eigenvalue problem

Galerkin

$$A_{ij} = \iiint_\Omega 1/\mu_\mathrm{r}\,\mathrm{curl}\vec{w}_i \cdot \mathrm{curl}\vec{w}_j \,\mathrm{d}\Omega$$

$$B_{ij} = \iiint_\Omega \varepsilon_\mathrm{r}\,\vec{w}_i \cdot \vec{w}_j \,\mathrm{d}\Omega$$

$$C_{ij} = \iint_{\partial\Omega} \sqrt{\varepsilon_\mathrm{r}/\mu_\mathrm{r}}\,(\vec{n}\times\vec{w}_i)\cdot(\vec{n}\times\vec{w}_j)\mathrm{d}A$$

$$A\vec{\alpha} + j\,\frac{\omega}{c_0}C\vec{\alpha} + (j\,\frac{\omega}{c_0})^2 B\vec{\alpha} = 0$$

discrete eigenvalue problem

Computational Model

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- Numerical formulation
  - Function definition

FEM06: lowest order approximation (edge elements, Nedelec)

	Space	Basis functions	Assoc.
scalar	$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
	$\tilde{\mathcal{V}}_2$	$\phi_i\phi_j$	$\{ij\}$
	$\tilde{\mathcal{V}}_3$	$\phi_i\phi_j(\phi_i - \phi_j)$,	$\{ij\}$
		$\phi_i\phi_j\phi_k$	$\{ijk\}$
vector	$\tilde{\mathcal{A}}_1$	$\phi_i\nabla\phi_j - \phi_j\nabla\phi_i$	$\{ij\}$
	$\tilde{\mathcal{A}}_2$	$3\phi_j\phi_k\nabla\phi_i - \nabla(\phi_i\phi_j\phi_k)$,	$\{ijk\}$
		$3\phi_k\phi_i\nabla\phi_j - \nabla(\phi_i\phi_j\phi_k)$	$\{ijk\}$
	$\tilde{\mathcal{A}}_3$	$4\phi_j\phi_k(\phi_j - \phi_k)\nabla\phi_i - \nabla(\phi_i\phi_j\phi_k(\phi_j - \phi_k))$,	$\{ijk\}$
		$4\phi_k\phi_i(\phi_k - \phi_i)\nabla\phi_j - \nabla(\phi_j\phi_k\phi_i(\phi_k - \phi_i))$,	$\{ijk\}$
		$4\phi_i\phi_j(\phi_i - \phi_j)\nabla\phi_k - \nabla(\phi_k\phi_i\phi_j(\phi_i - \phi_j))$,	$\{ijk\}$
		$4\phi_j\phi_k\phi_l\nabla\phi_i - \nabla(\phi_i\phi_j\phi_k\phi_l)$,	$\{ijkl\}$
		$4\phi_k\phi_l\phi_i\nabla\phi_j - \nabla(\phi_i\phi_j\phi_k\phi_l)$,	$\{ijkl\}$
		$4\phi_l\phi_i\phi_j\nabla\phi_k - \nabla(\phi_i\phi_j\phi_k\phi_l)$	$\{ijkl\}$

Pär Ingelström,
A New Set of H(curl)-Conforming Hierarchical Basis Functions for Tetrahedral Meshes,
IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES,
VOL. 54, NO. 1, JANUARY 2006

Computational Model

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- Numerical formulation
  - Function definition

FEM12: higher order approximation

	Space	Basis functions	Assoc.
scalar	$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
	$\tilde{\mathcal{V}}_2$	$\phi_i \phi_j$	$\{ij\}$
	$\mathcal{V}_3$	$\phi_i \phi_j (\phi_i - \phi_j)$,	$\{ij\}$
		$\phi_i \phi_j \phi_k$	$\{ijk\}$
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		$3\phi_k \phi_i \nabla \phi_j - \nabla(\phi_i \phi_j \phi_k)$	$\{ijk\}$
	$\tilde{\mathcal{A}}_3$	$4\phi_j \phi_k (\phi_j - \phi_k) \nabla \phi_i - \nabla(\phi_i \phi_j \phi_k (\phi_j - \phi_k))$,	$\{ijk\}$
		$4\phi_k \phi_i (\phi_k - \phi_i) \nabla \phi_j - \nabla(\phi_j \phi_k \phi_i (\phi_k - \phi_i))$,	$\{ijk\}$
		$4\phi_i \phi_j (\phi_i - \phi_j) \nabla \phi_k - \nabla(\phi_k \phi_i \phi_j (\phi_i - \phi_j))$,	$\{ijk\}$
		$4\phi_j \phi_k \phi_l \nabla \phi_i - \nabla(\phi_i \phi_j \phi_k \phi_l)$,	$\{ijkl\}$
		$4\phi_k \phi_l \phi_i \nabla \phi_j - \nabla(\phi_i \phi_j \phi_k \phi_l)$,	$\{ijkl\}$
		$4\phi_l \phi_i \phi_j \nabla \phi_k - \nabla(\phi_i \phi_j \phi_k \phi_l)$	$\{ijkl\}$

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VOL. 54, NO. 1, JANUARY 2006

Computational Model

- Numerical formulation
  - Function definition

FEM20: higher order approximation

Space	Basis functions	Assoc.
$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
$\tilde{\mathcal{V}}_2$	$\phi_i \phi_j$	$\{ij\}$
$\tilde{\mathcal{V}}_3$	$\phi_i \phi_j (\phi_i - \phi_j)$,	$\{ij\}$
	$\phi_i \phi_j \phi_k$	$\{ijk\}$
$\tilde{\mathcal{A}}_1$	$\phi_i \nabla \phi_j - \phi_j \nabla \phi_i$	$\{ij\}$
$\tilde{\mathcal{A}}_2$	$3\phi_j \phi_k \nabla \phi_i - \nabla(\phi_i \phi_j \phi_k)$,	$\{ijk\}$
	$3\phi_k \phi_i \nabla \phi_j - \nabla(\phi_i \phi_j \phi_k)$	$\{ijk\}$
$\tilde{\mathcal{A}}_3$	$4\phi_j \phi_k (\phi_j - \phi_k) \nabla \phi_i - \nabla(\phi_i \phi_j \phi_k (\phi_j - \phi_k))$,	$\{ijk\}$
	$4\phi_k \phi_i (\phi_k - \phi_i) \nabla \phi_j - \nabla(\phi_j \phi_k \phi_i (\phi_k - \phi_i))$,	$\{ijk\}$
	$4\phi_i \phi_j (\phi_i - \phi_j) \nabla \phi_k - \nabla(\phi_k \phi_i \phi_j (\phi_i - \phi_j))$,	$\{ijk\}$
	$4\phi_j \phi_k \phi_l \nabla \phi_i - \nabla(\phi_i \phi_j \phi_k \phi_l)$,	$\{ijkl\}$
	$4\phi_k \phi_l \phi_i \nabla \phi_j - \nabla(\phi_i \phi_j \phi_k \phi_l)$,	$\{ijkl\}$
	$4\phi_l \phi_i \phi_j \nabla \phi_k - \nabla(\phi_i \phi_j \phi_k \phi_l)$	$\{ijkl\}$

scalar: $\tilde{\mathcal{V}}_1$–$\tilde{\mathcal{V}}_3$; vector: $\tilde{\mathcal{A}}_1$–$\tilde{\mathcal{A}}_3$

Pär Ingelström,
A New Set of H(curl)-Conforming Hierarchical Basis Functions for Tetrahedral Meshes,
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Computational Model

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- Numerical formulation
  - Implementation

$$a_{ij} = \iiint_\Omega 1/\mu_\mathrm{r}\,\mathrm{curl}\vec{w}_i \cdot \mathrm{curl}\vec{w}_j \,\mathrm{d}\Omega$$

$$b_{ij} = \iiint_\Omega \varepsilon_\mathrm{r}\,\vec{w}_i \cdot \vec{w}_j \,\mathrm{d}\Omega$$

Mathematica

Edge basis elements

- Matrix A

```
(* Element matrix calculation *)
fktA2[i_Integer, j_Integer] :=
  Integrate[(curlW[i].curlW[j]) * jacobi,
   {u1, 0, 1}, {u2, 0, 1 - u1}, {u3, 0, 1 - u1 - u2}];
matA2 = Array[fktA2, {nEdges, nEdges}];
TableForm[Flatten[matA2]]
```

- Matrix B

```
(* Element matrix calculation *)
fktB2[i_Integer, j_Integer] :=
  Integrate[(W[i].W[j]) * jacobi, {u1, 0, 1},
   {u2, 0, 1 - u1}, {u3, 0, 1 - u1 - u2}];
matB2 = Array[fktB2, {nEdges, nEdges}];
TableForm[Flatten[matB2]]
```

contribution of element-matrices ready availabe

Computational Model

- Eigenvalue formulation
  - Fundamental equation

$$A\vec{\alpha} + j\frac{\omega}{c_0}C\vec{\alpha} + (j\frac{\omega}{c_0})^2 B\vec{\alpha} = 0$$

Notation:
A - stiffness matrix
B - mass matrix
C - damping matrix

  - Matrix properties

$$A, B, C \in \mathbb{R}^{n\times n} \quad A = A^T, B = B^T, C = C^T \quad A \geq 0, B > 0, C \geq 0$$

  - Fundamental properties

$AN = CN = 0$ for proper chosen scalar Φ_i and vector basis functions $\vec{\omega}_i$

$$\underbrace{N^T A}_{0}\,\vec{\alpha} + j\frac{\omega}{c_0}\underbrace{N^T C}_{0}\,\vec{\alpha} + (j\frac{\omega}{c_0})^2 N^T B\vec{\alpha} = 0$$

→ static $\omega = 0$ or dynamic $N^T B\,\vec{\alpha} = S\vec{\alpha} = 0$

Computational Model

- Fundamental properties
  - Number of eigenvalues

$$Q(\lambda) = A + \lambda C + \lambda^2 B \qquad \lambda \overset{!}{=} j\,\frac{\omega}{c_0}$$

Matrix B nonsingular:
- matrix polynomial $Q(\lambda)$ is regular
- 2n finite eigenvalues

Notation:
A - stiffness matrix
B - mass matrix
C - damping matrix

$$A \geq 0, B > 0, C \geq 0$$

  - Orthogonality relation

$$A\vec{\alpha} + \lambda C\vec{\alpha} + \lambda^2 B\vec{\alpha} = 0$$

$$\Rightarrow \quad (\lambda_1 - \lambda_2) \cdot [\vec{\alpha}_2^H C\vec{\alpha}_1 + (\lambda_1 + \lambda_2)\vec{\alpha}_2^H B\vec{\alpha}_1] = 0$$

If $C \not\propto B$ the vectors $\vec{\alpha}_1$ and $\vec{\alpha}_2$ are no longer B-orthogonal: $\vec{\alpha}_1 \not\perp_B \vec{\alpha}_2$

Computational Model

- Fundamental properties
  - Orthogonality relation

$$A\vec{\alpha} + \lambda C\vec{\alpha} + \lambda^2 B\vec{\alpha} = 0$$

$$\Rightarrow \quad (\lambda_1 - \lambda_2) \cdot [\vec{\alpha}_2^H C\vec{\alpha}_1 + (\lambda_1 + \lambda_2)\vec{\alpha}_2^H B\vec{\alpha}_1] = 0$$

  - Scalar product

1) $<\alpha\,\vec{x} + \alpha'\,\vec{x}', \vec{y}> = \alpha <\vec{x}, \vec{y}> + \alpha' <\vec{x}', \vec{y}>$

2) $<\vec{y}, \vec{x}> = \overline{<\vec{x}, \vec{y}>}$

3) $\vec{x} \neq 0 \;\rightarrow\; <\vec{x}, \vec{x}> > 0$

$$\Rightarrow \quad <x, y> = 0 \;\rightarrow\; \vec{x} \perp \vec{y}$$

currently not available

Computational Model

- Eigenvalue formulation
  - Fundamental equation

$$A\vec{\alpha} + \lambda C\vec{\alpha} + \lambda^2 B\vec{\alpha} = 0 \qquad \lambda \overset{!}{=} j\,\frac{\omega}{c_0}$$

Notation:
A - stiffness matrix
B - mass matrix
C - damping matrix

→ A, B, C: real symmetric
conjugate complex eigenvalues

  - Companion notation

$$\begin{pmatrix} -A & C \\ 0 & I \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha} \\ \lambda\vec{\alpha} \end{pmatrix} = \lambda \begin{pmatrix} 0 & B \\ I & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha} \\ \lambda\vec{\alpha} \end{pmatrix}$$

→ real asymmetric matrices

$$\begin{pmatrix} -A & 0 \\ 0 & B \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha} \\ \lambda\vec{\alpha} \end{pmatrix} = \lambda \begin{pmatrix} C & B \\ B & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha} \\ \lambda\vec{\alpha} \end{pmatrix}$$

→ real symmetric matrices

Computational Model

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- Eigenvalue solution
  - Fundamental equation

$$A\vec{\alpha} + \lambda C\vec{\alpha} + \lambda^2 B\vec{\alpha} = 0 \qquad \lambda \overset{!}{=} j\,\frac{\omega}{c_0}$$

Notation:
A - stiffness matrix
B - mass matrix
C - damping matrix

  - Subspace projection method

$$\vec{\alpha} = V\vec{\alpha}_\mathrm{V}$$

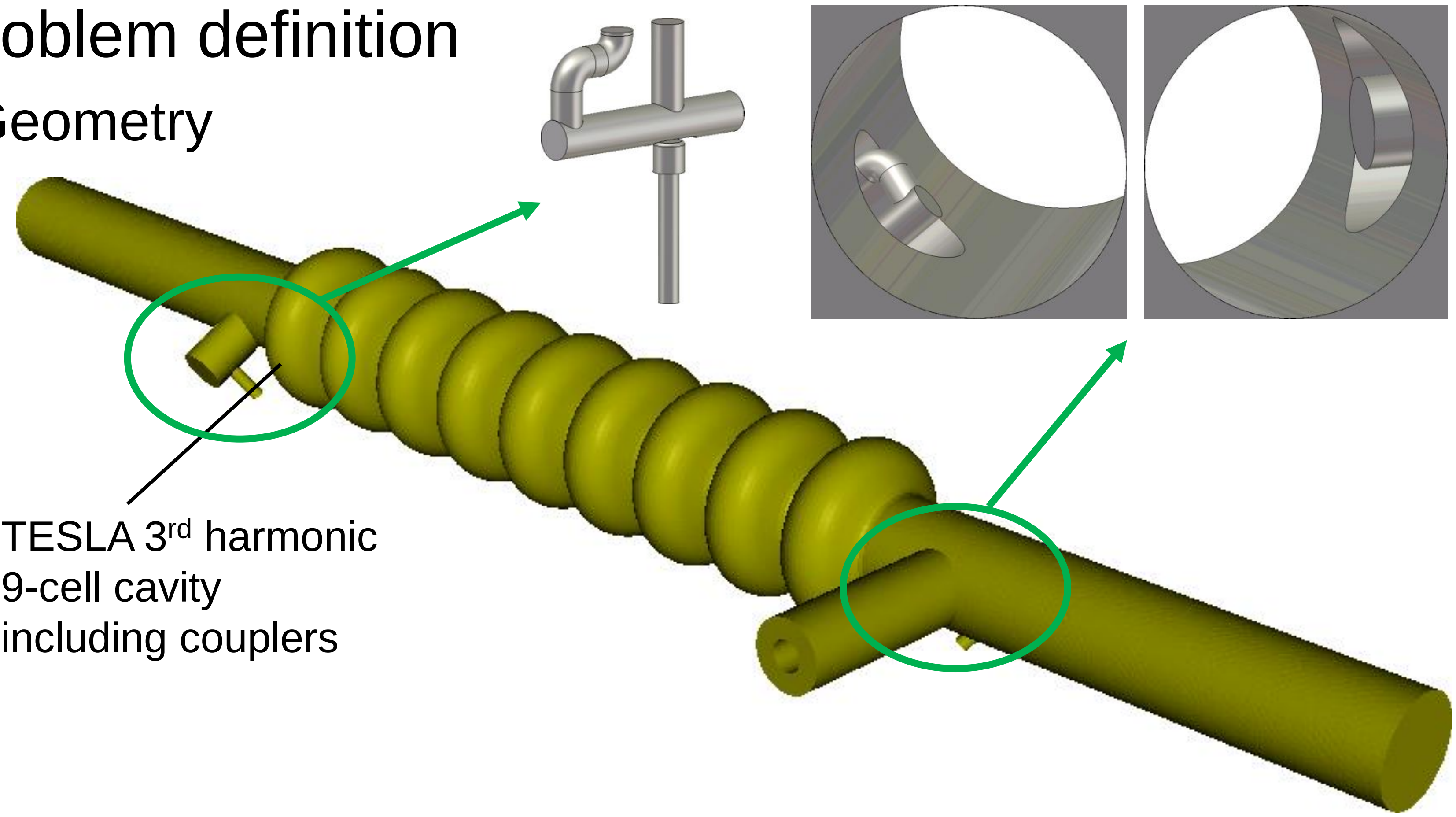
$$V^TAV\vec{\alpha}_\mathrm{V} + \lambda\, V^TCV\vec{\alpha}_\mathrm{V} + \lambda^2 V^TBV\vec{\alpha}_\mathrm{V} = 0$$

  - Companion notation for the projected system

$$\begin{pmatrix} -V^TAV & 0 \\ 0 & V^TBV \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha}_\mathrm{V} \\ \lambda\vec{\alpha}_\mathrm{V} \end{pmatrix} = \lambda \begin{pmatrix} V^TCV & V^TBV \\ V^TBV & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{\alpha}_\mathrm{V} \\ \lambda\vec{\alpha}_\mathrm{V} \end{pmatrix}$$

Numerical Examples

- Problem definition
  - Geometry



Numerical Examples

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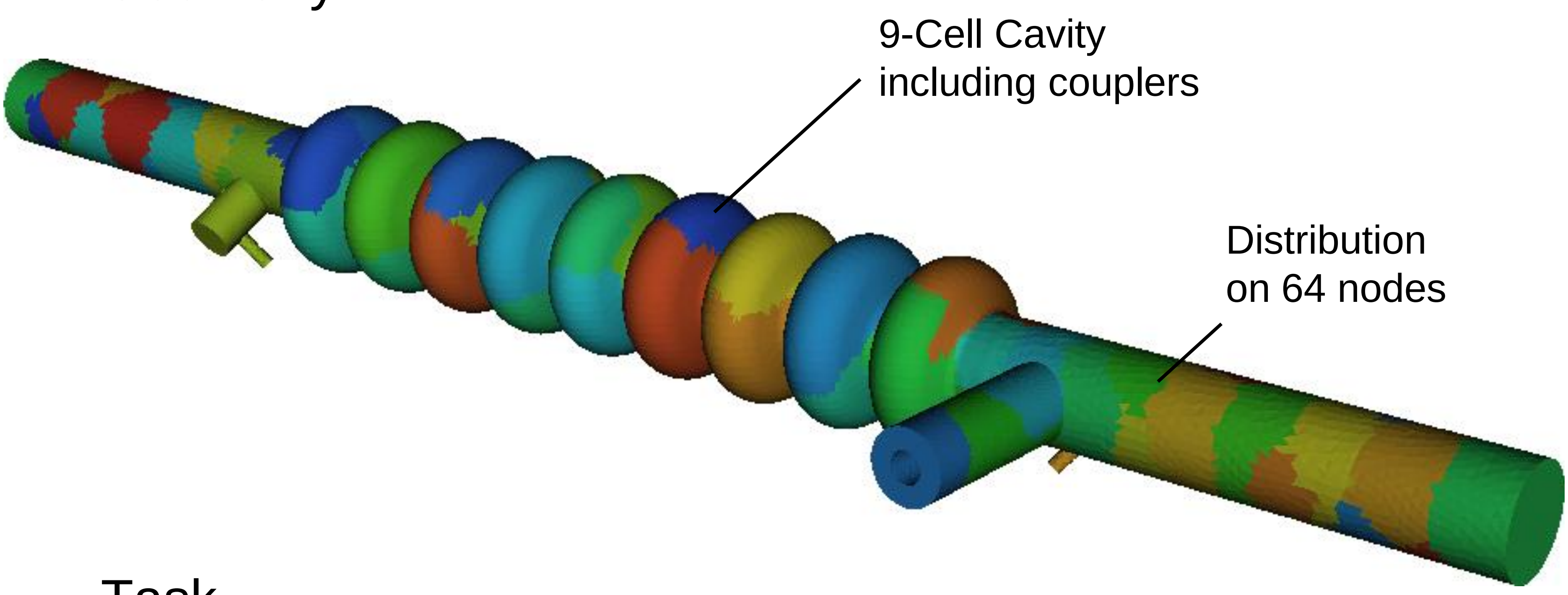
ParMeTiS, VTK and CST - Studio Suite®

- Problem definition
  - Geometry

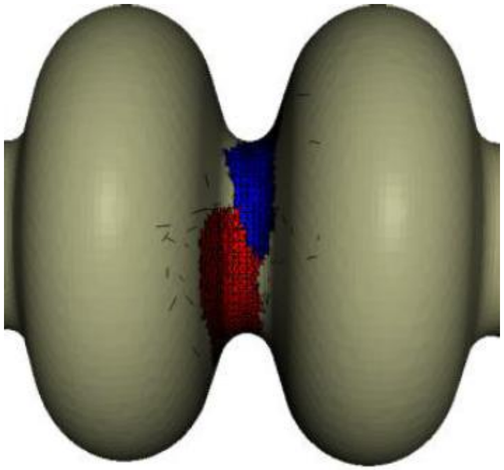


  - Task

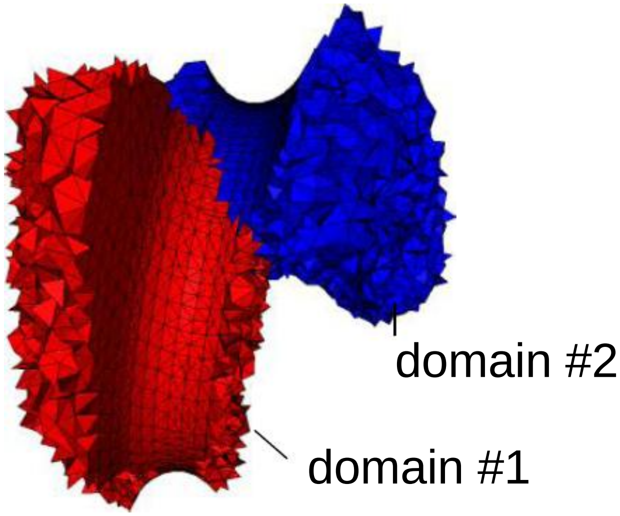
    Search for the π - mode field distribution

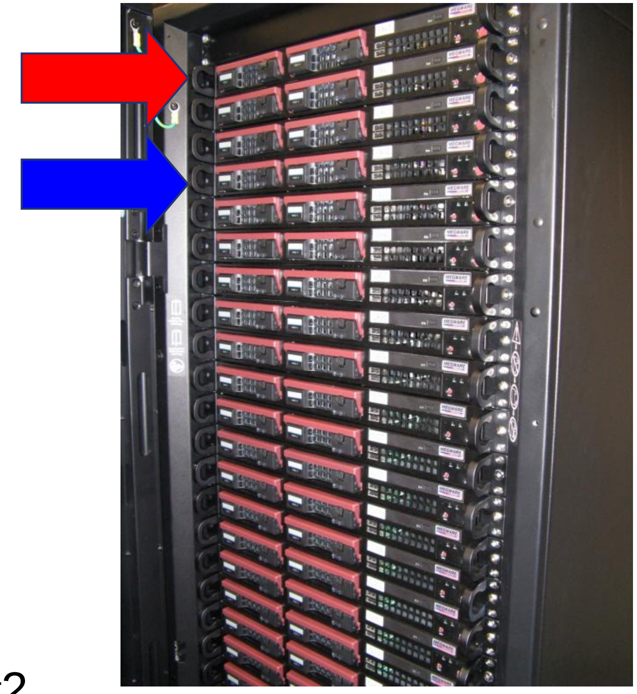
Numerical Examples

- Efficient solution of large problems
  - Domain composition



cavity model

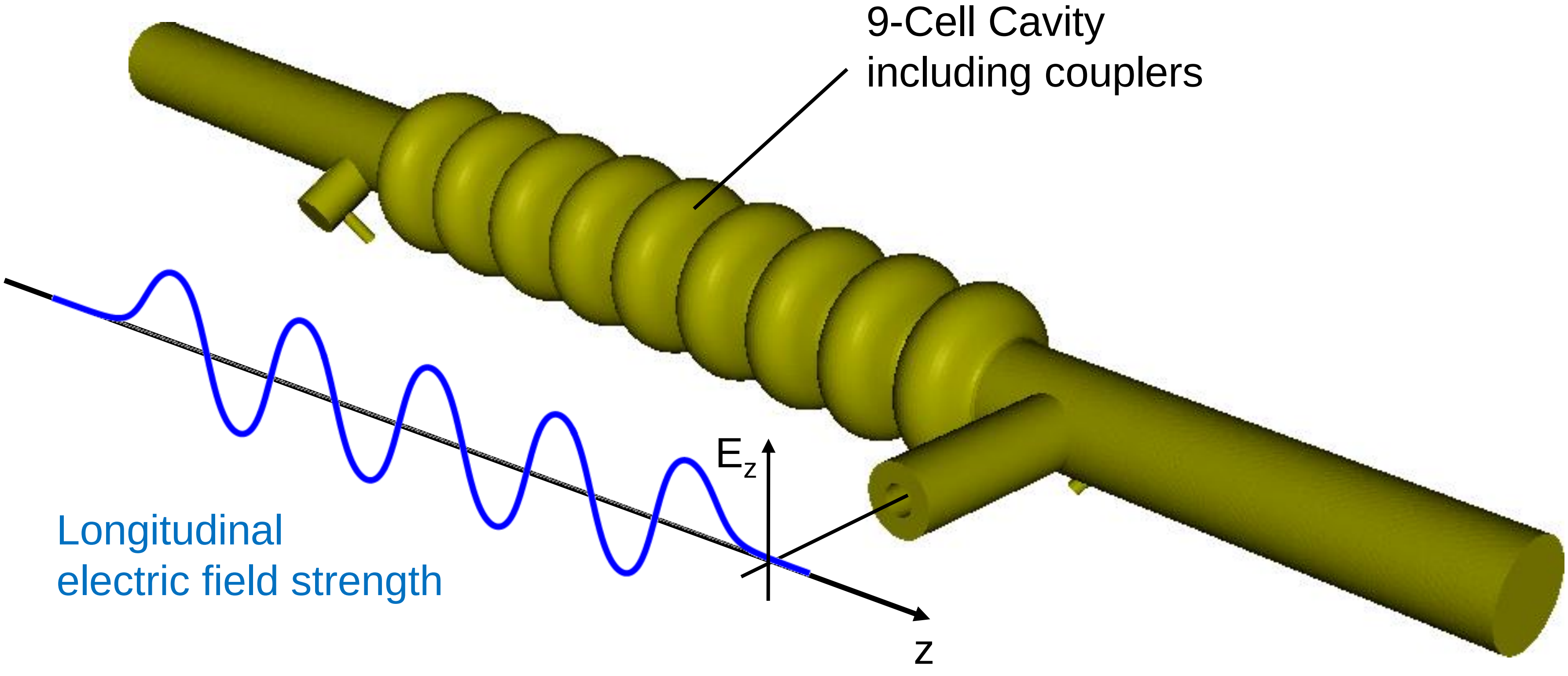




parallel computing

Numerical Examples

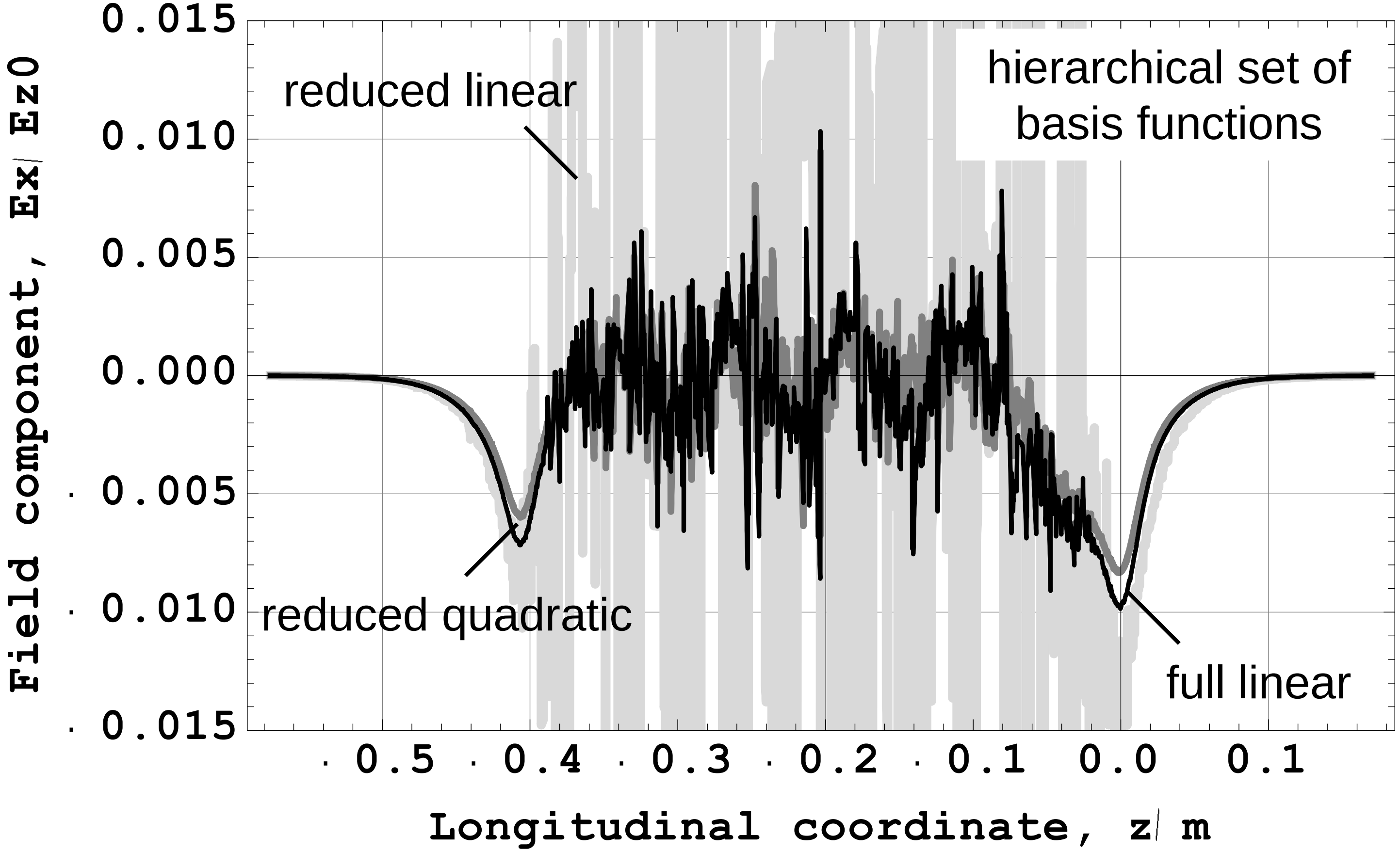
- Fields along the axis of an accelerator cavity



Numerical Examples

- Simulation results

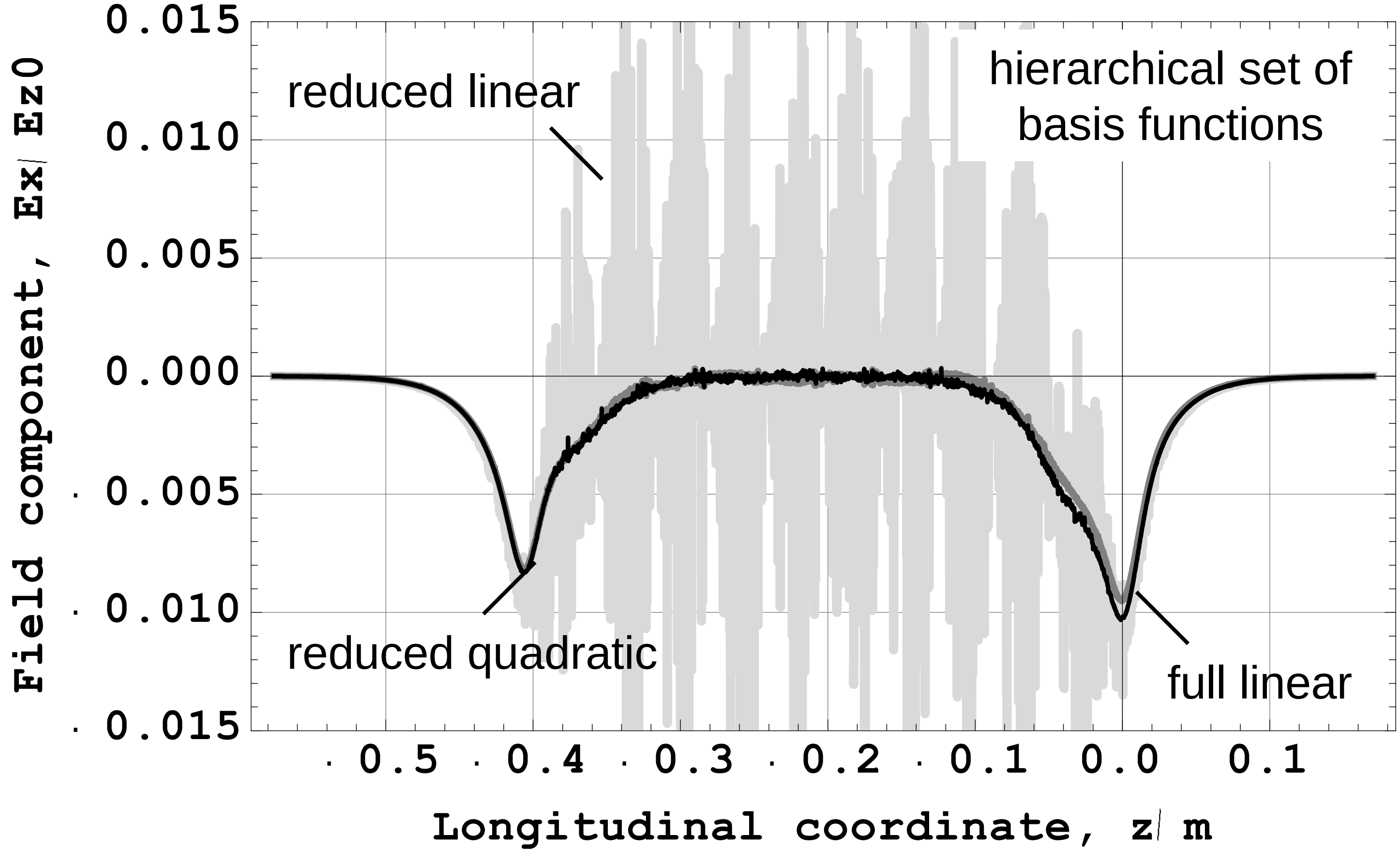
607 576 cells



Numerical Examples

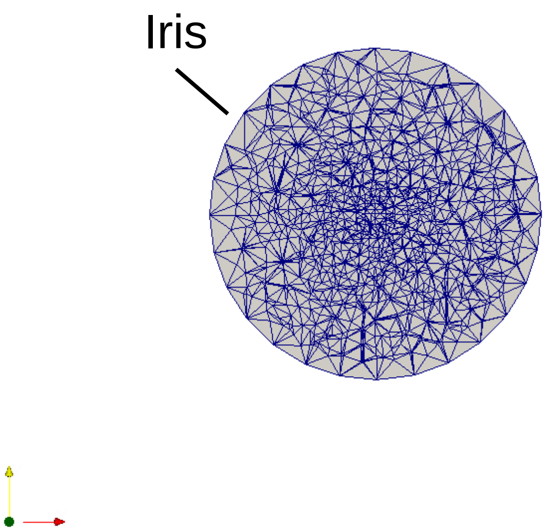
- Simulation results

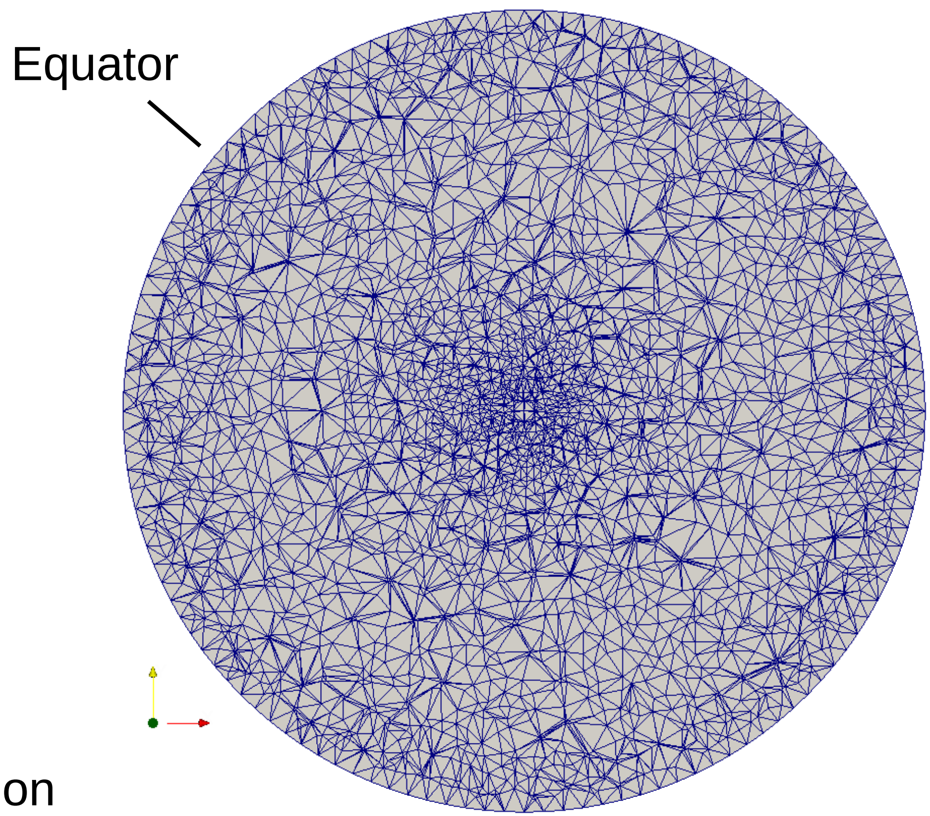
2 064 944 cells



Numerical Examples

- Transversal grid information
  - Cut plane plots





unsymmetric mesh generation

Numerical Examples

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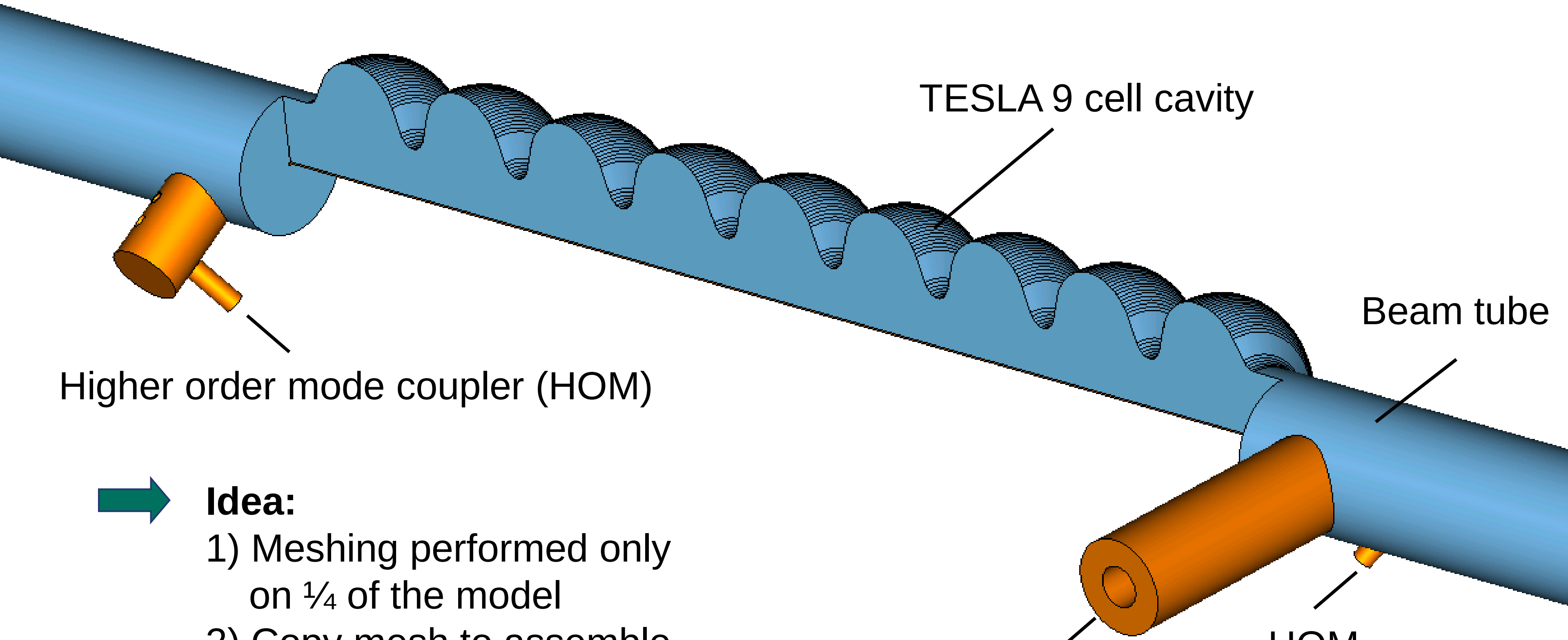
CST – Microwave Studio

- Symmetric mesh generation

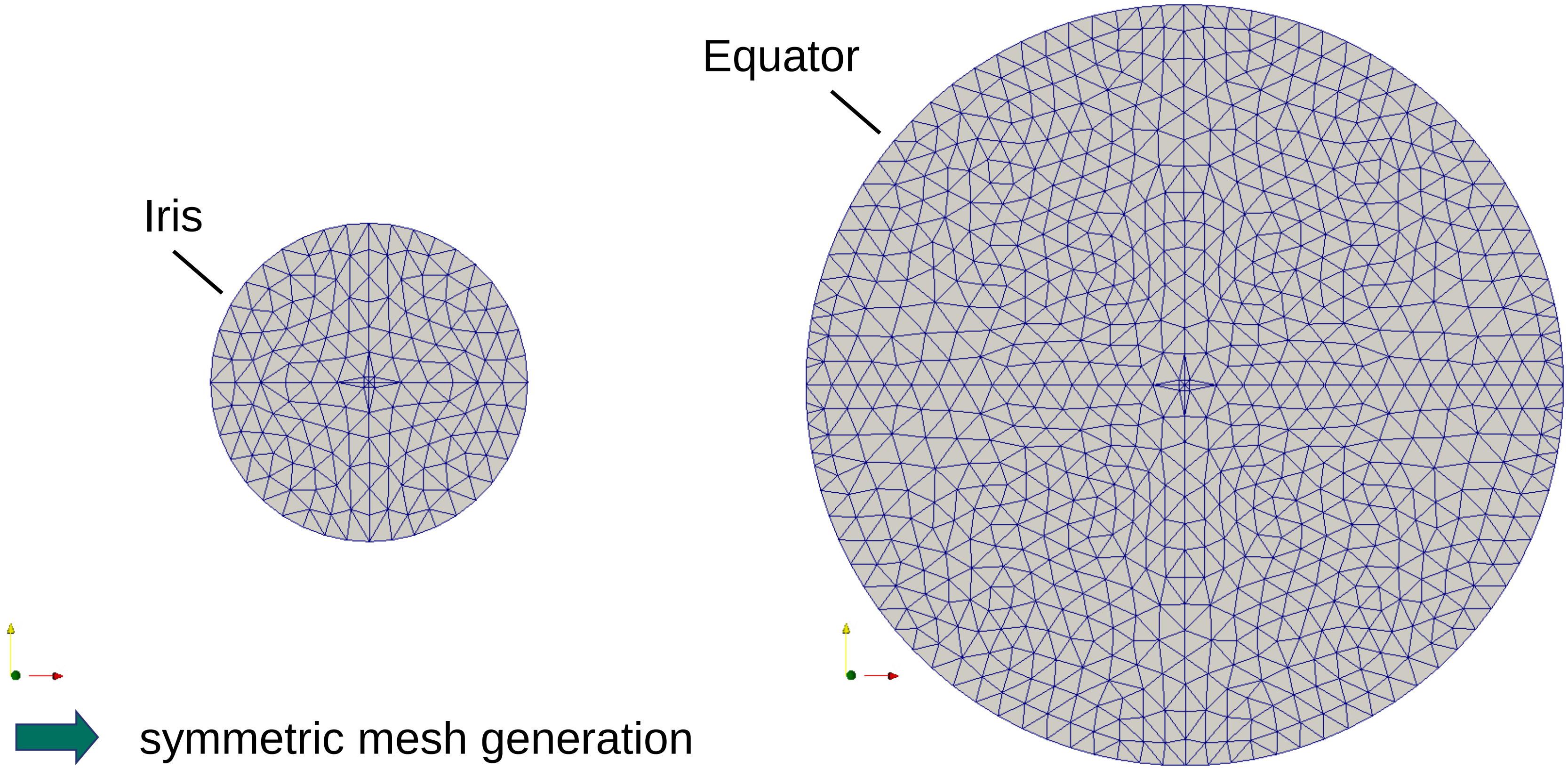


Idea:

1) Meshing performed only on ¼ of the model
2) Copy mesh to assemble the full information

Numerical Examples

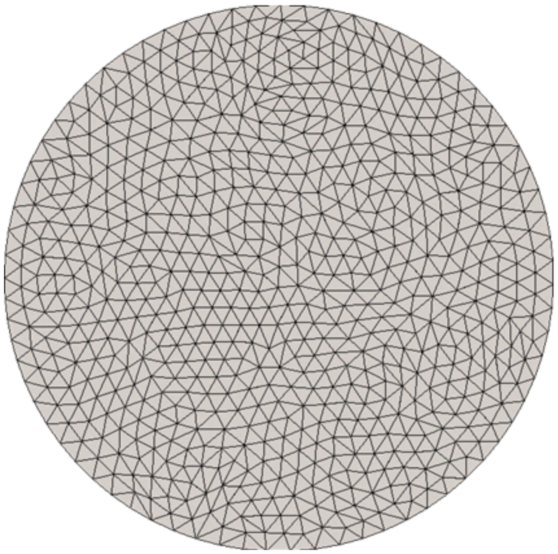
- Transversal grid information
  - Cut plane plots



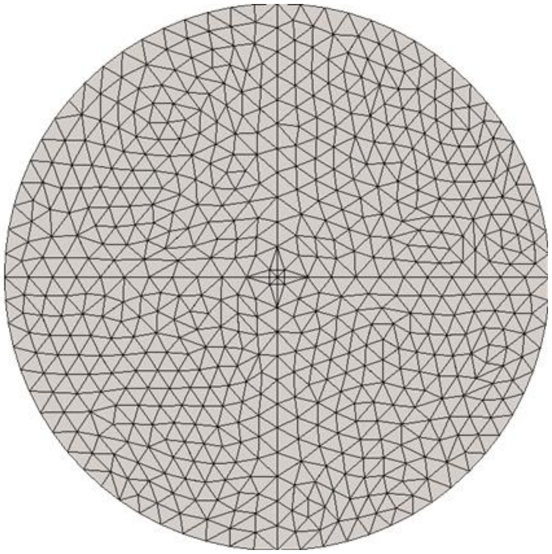
➡ symmetric mesh generation

Numerical Examples

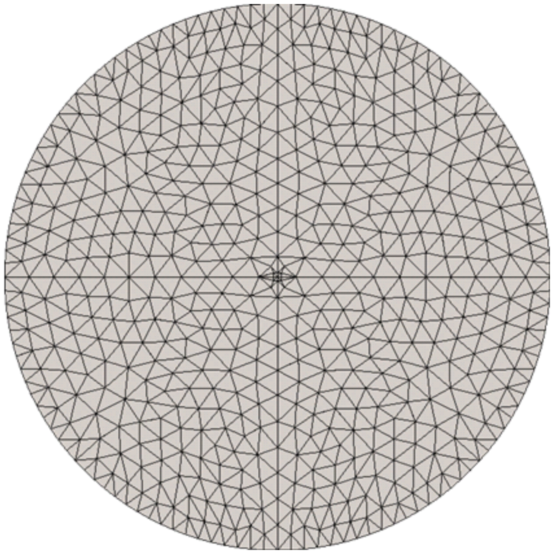
- Simulation results
  - Transverse mesh properties



arbitrary distribution of tetrahedra



tetrahedra faces aligned along coordinate faces

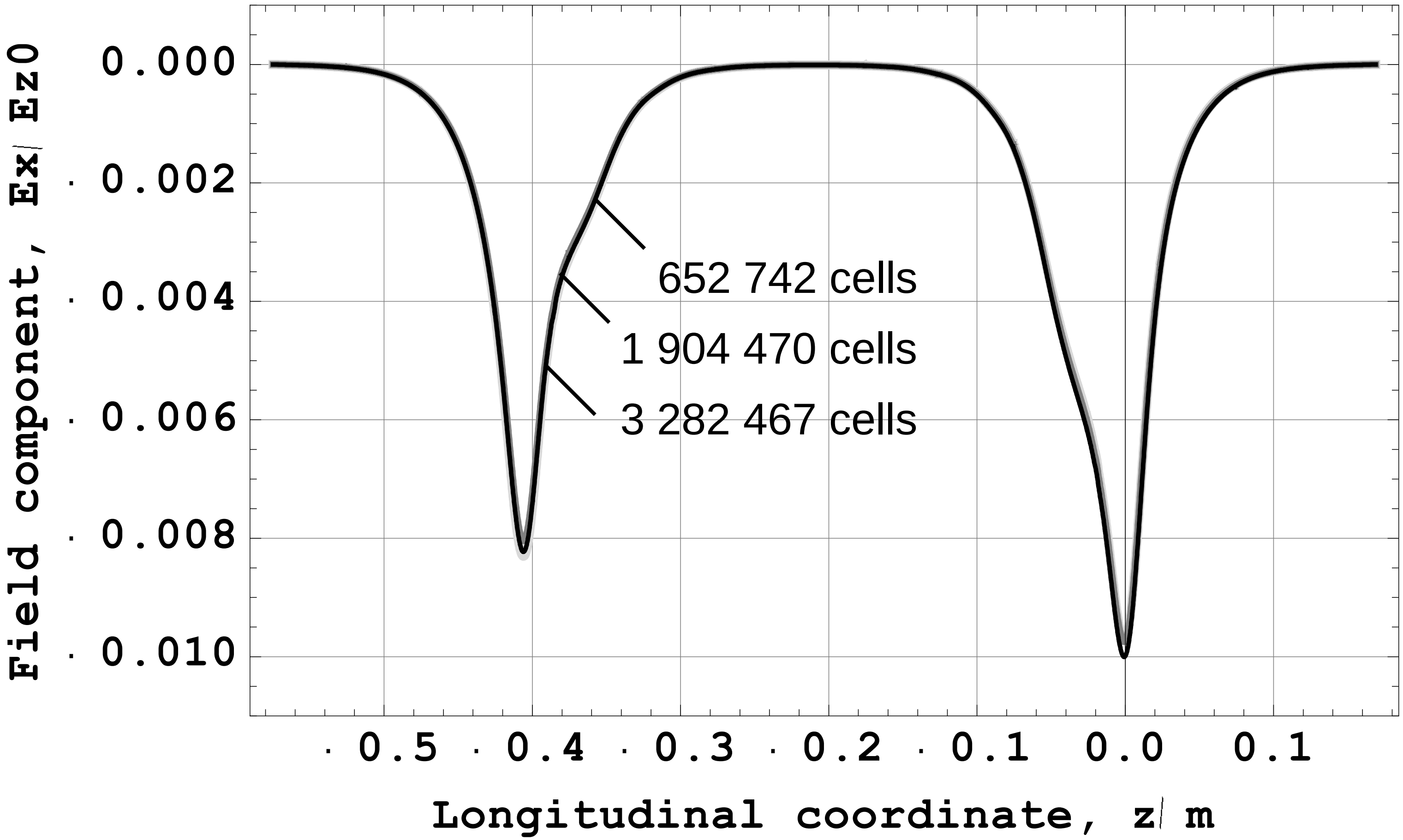


symmetric distribution of tetrahedra

Numerical Examples

- Simulation results

reduced quadratic set of basis functions



Numerical Examples

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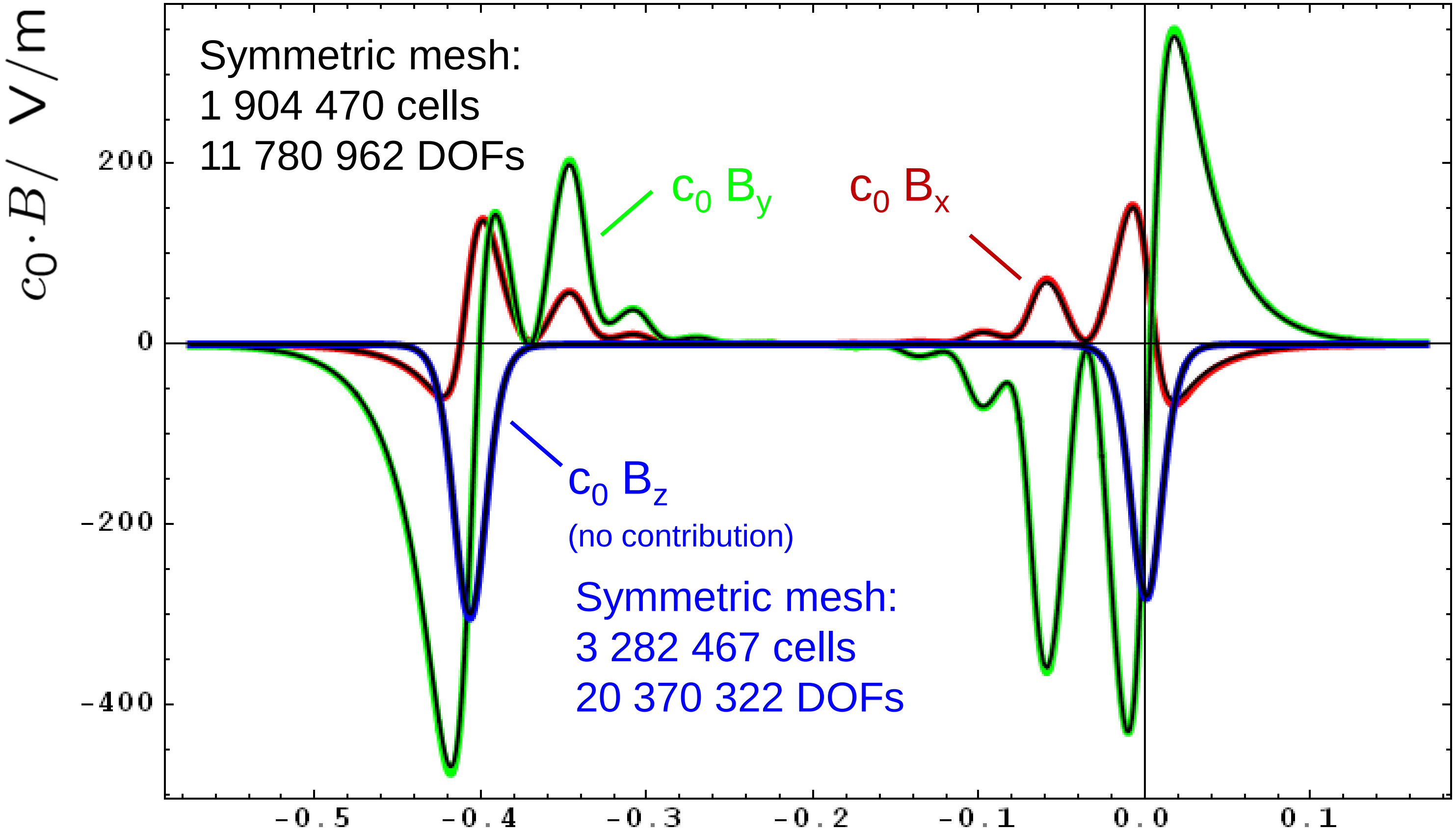
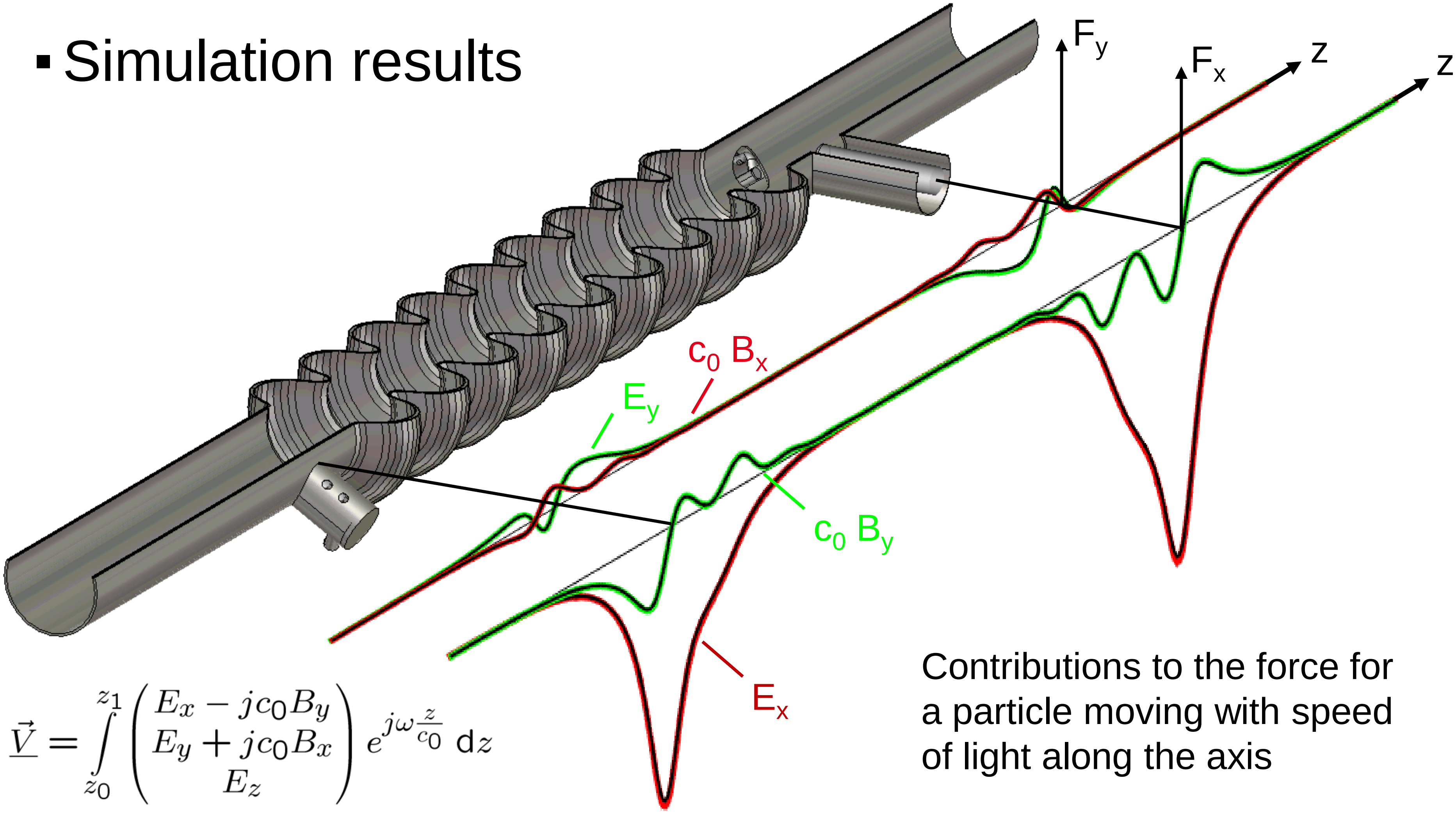
- Simulation results



Numerical Examples

- Simulation results

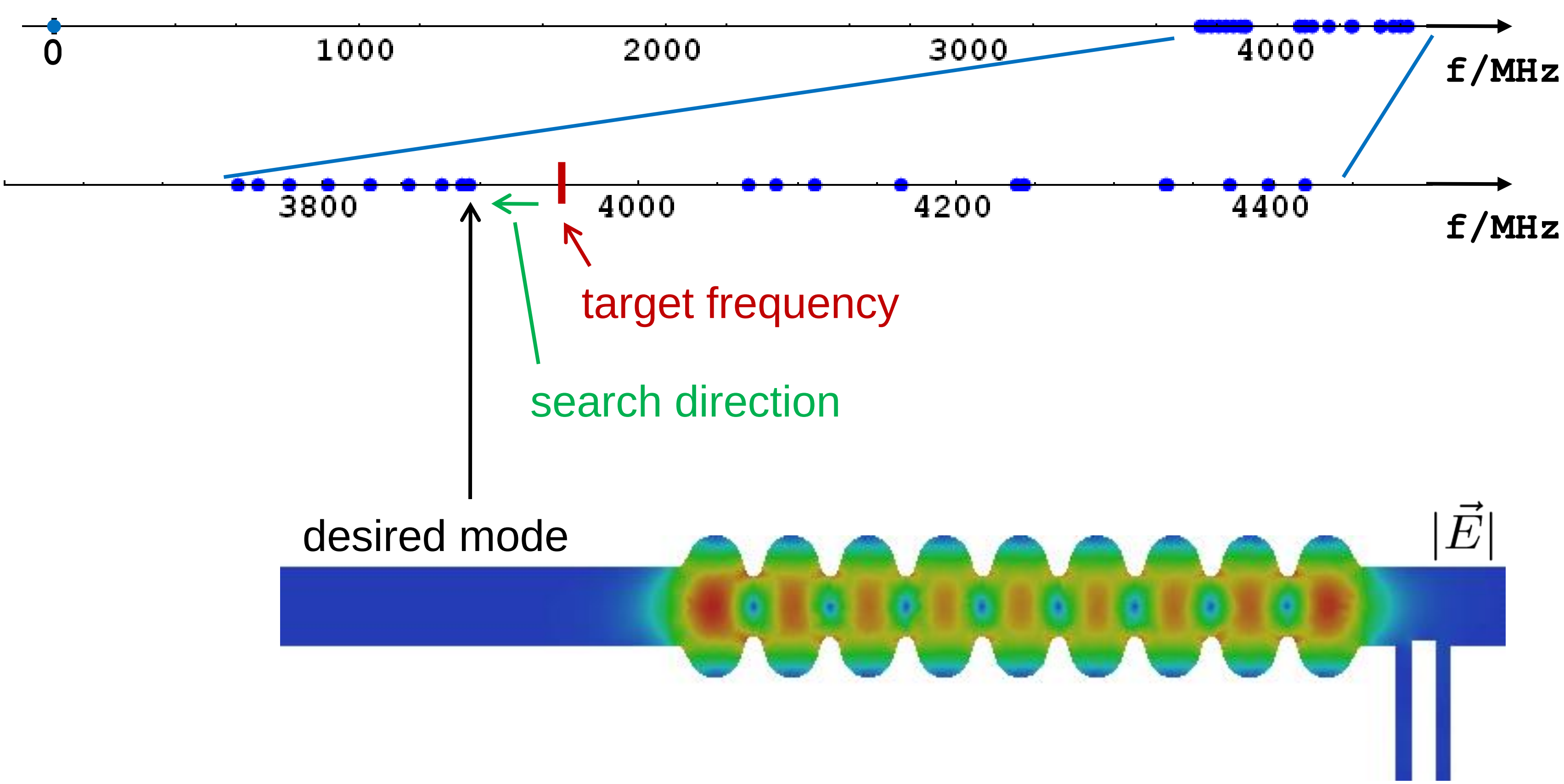


$$\underline{\vec{V}} = \int_{z_0}^{z_1} \begin{pmatrix} E_x - jc_0 B_y \\ E_y + jc_0 B_x \\ E_z \end{pmatrix} e^{j\omega \frac{z}{c_0}} \, \mathrm{d}z$$

Contributions to the force for a particle moving with speed of light along the axis

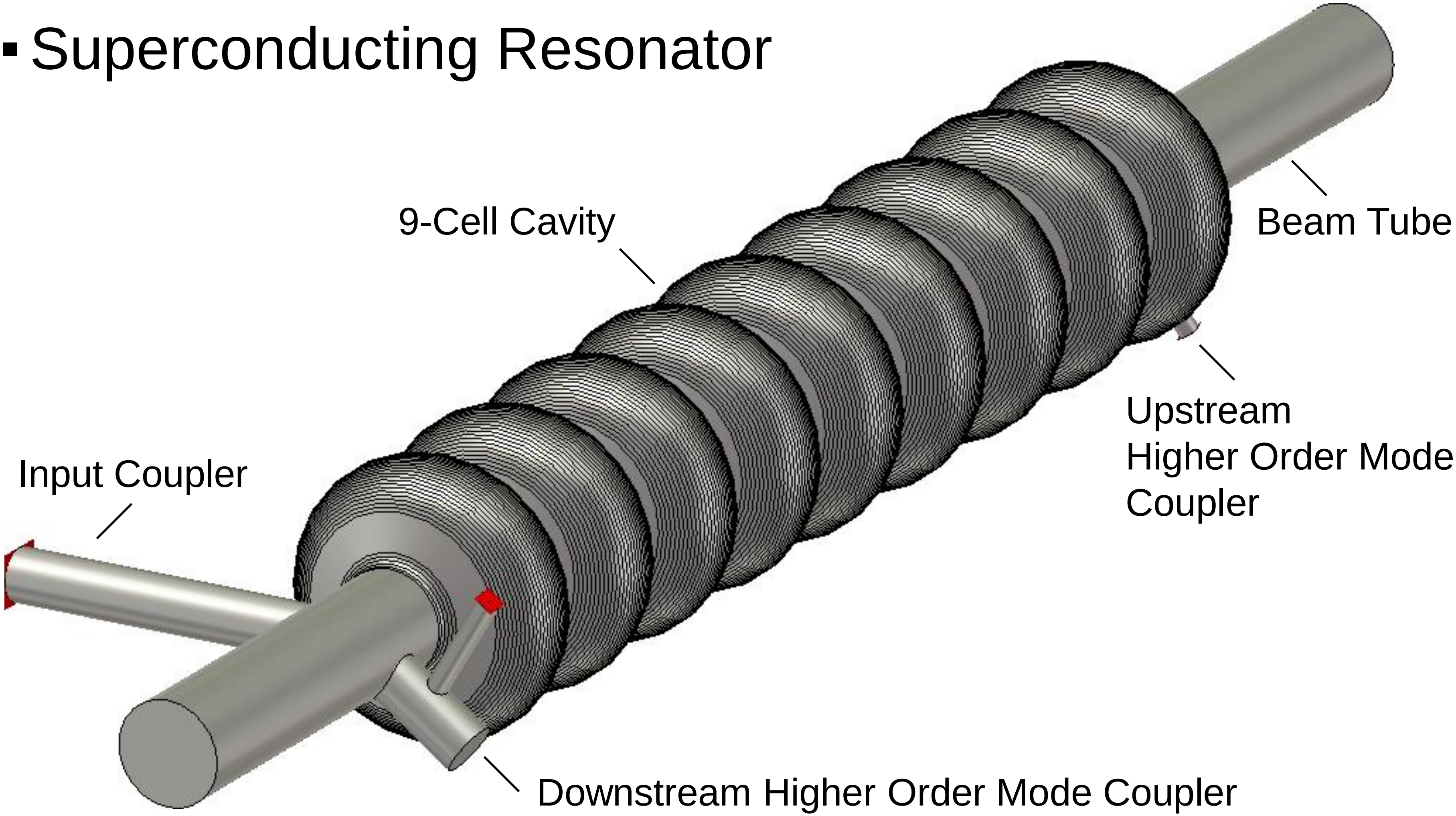
Computational Model

- Eigenvalue distribution



Motivation

- Superconducting Resonator



Numerical Examples

$|\vec{E}|$ in linear scale

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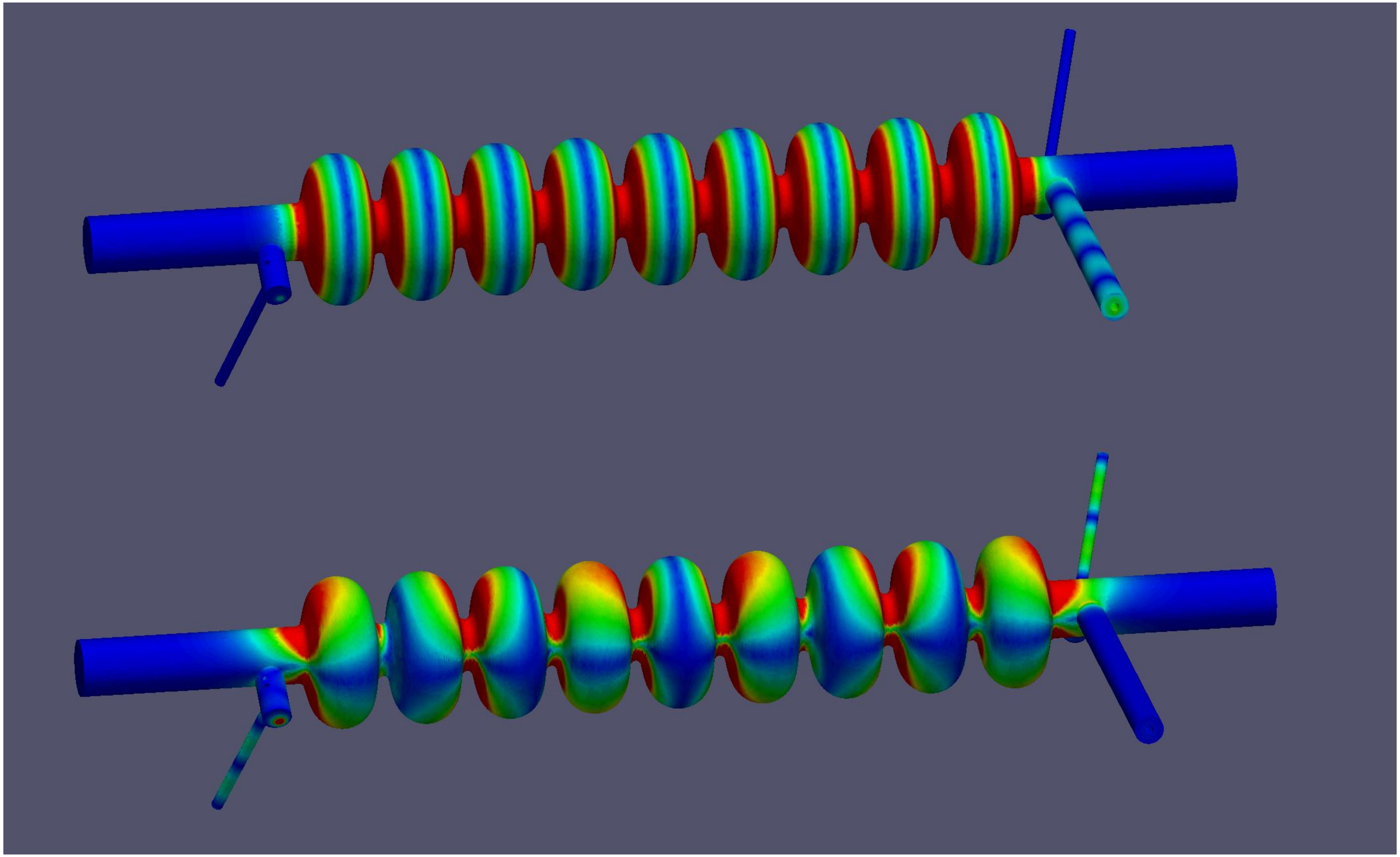
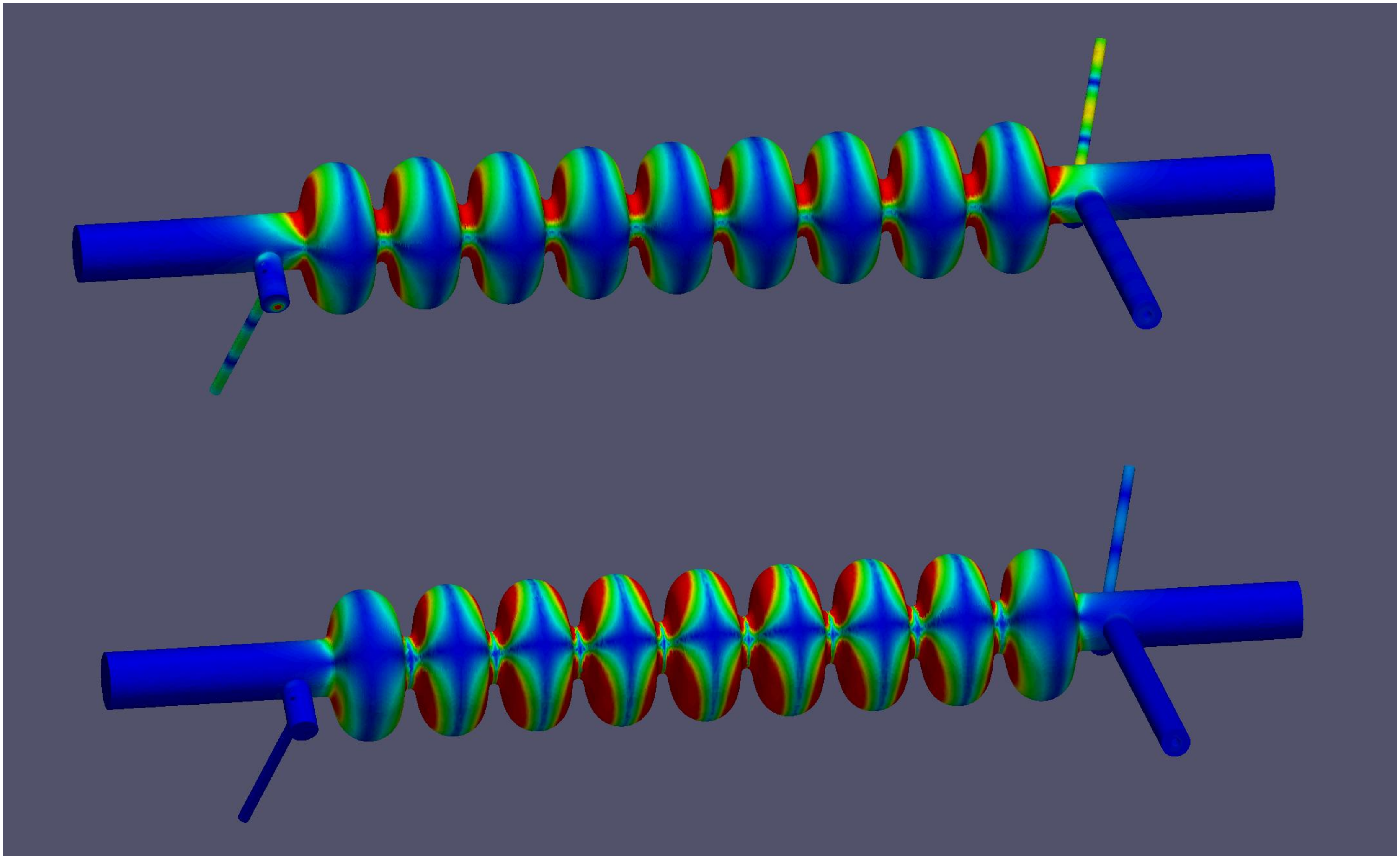


$f_0 = 1.300$ GHz

$f_0 = 1.709$ GHz

Numerical Examples

$|\vec{E}|$ in linear scale



$f_0 = 1.802$ GHz

$f_0 = 1.890$ GHz