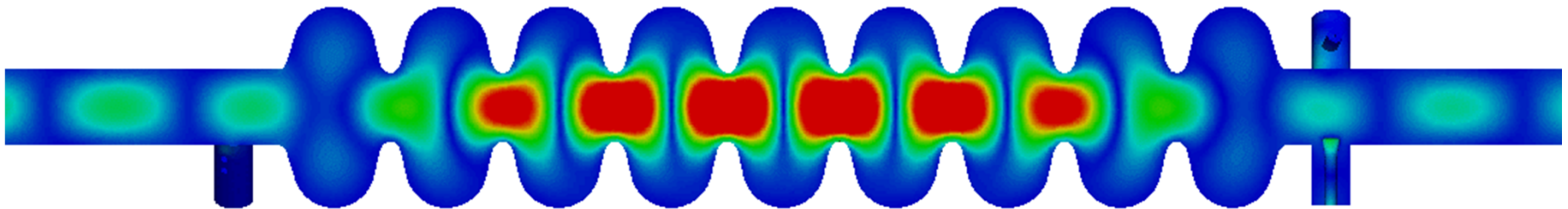


High Precision Cavity Simulations



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Wolfgang Ackermann, Thomas Weiland
Institut Theorie Elektromagnetischer Felder, TU Darmstadt



11th International Computational
Accelerator Physics Conference

ICAP 2012

August 19 - 24, 2012
Warnemünde, Germany

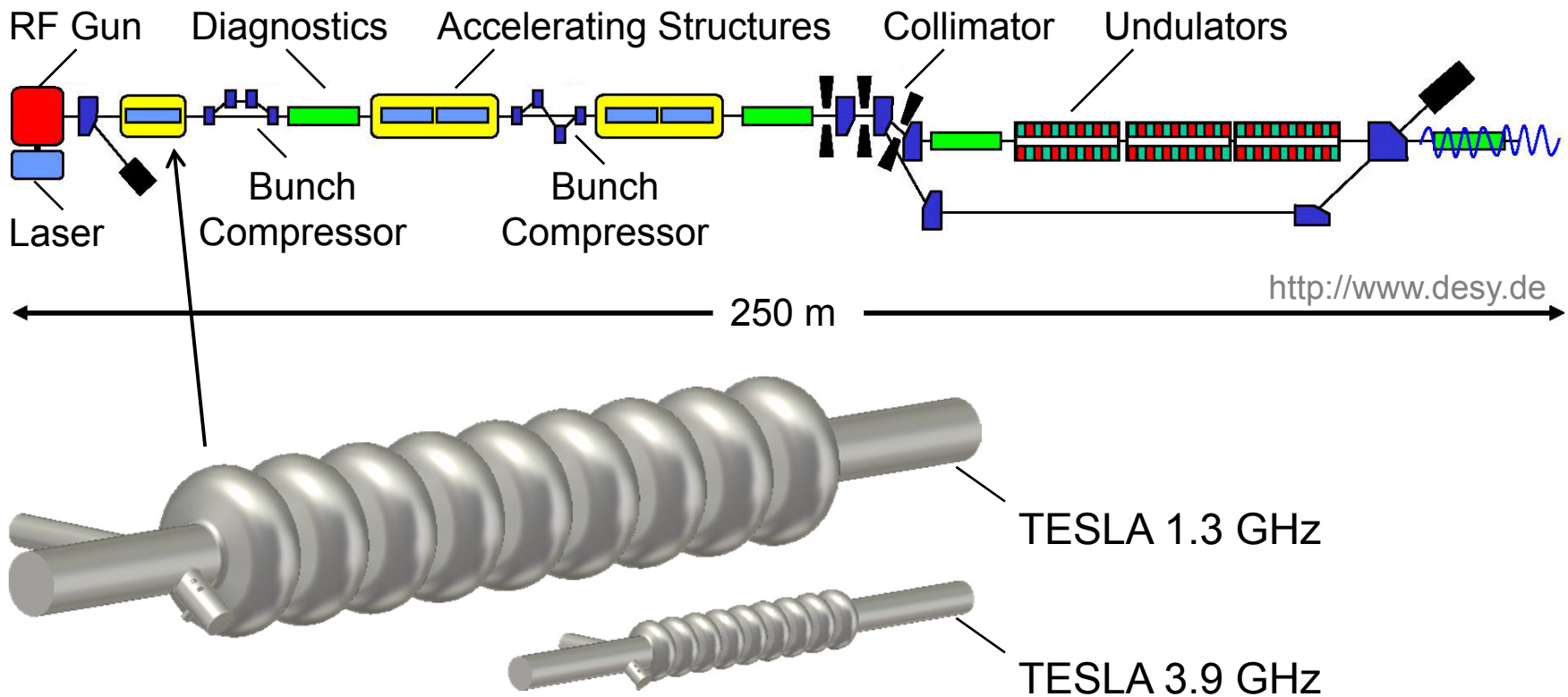
- Motivation
- Computational model
 - Problem formulation in 3-D
 - Problem formulation in 2-D (boundary condition)
- Numerical examples
 - Field patterns for selected modes
 - Resonance frequency and quality factors
- Summary / Outlook



- Motivation
- Computational model
 - Problem formulation in 3-D
 - Problem formulation in 2-D (boundary condition)
- Numerical examples
 - Field patterns for selected modes
 - Resonance frequency and quality factors
- Summary / Outlook

Motivation

- Particle accelerators
 - FLASH at DESY, Hamburg



▪ XFEL: Main parameters of the accelerator

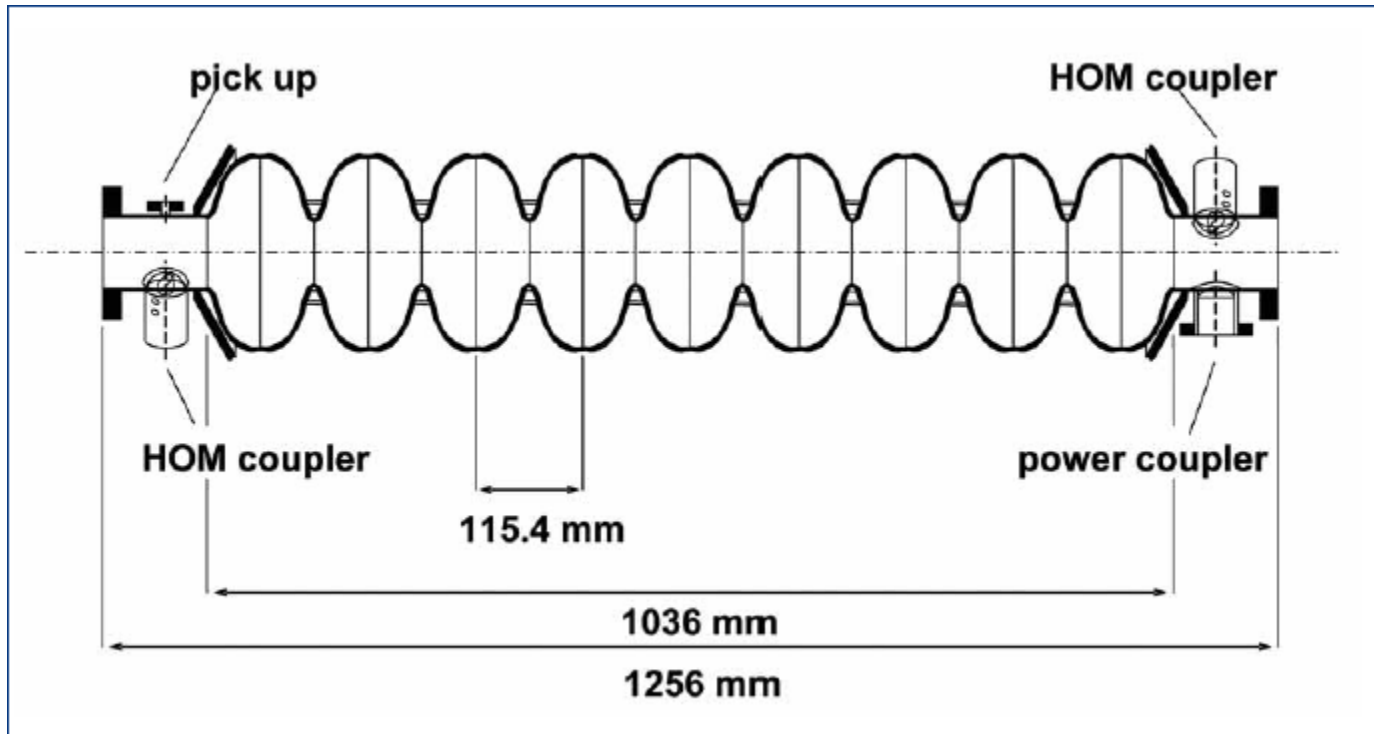
Energy for 0.1nm wavelength (<i>maximum design energy</i>)	17.5 GeV (20 GeV)
Number of installed accelerator modules	116
Number of cavities	928
Acc. gradient (104 active modules) at 20 GeV	23.6 MV/m
Number of installed RF stations	29
Klystron peak power (26 active stations)	5.2 MW
Loaded quality factor Q_{ext}	4.6×10^6
RF pulse length	1.4 ms
Beam pulse length	0.65ms
Repetition rate	10 Hz
Maximum average beam power	600 kW
Unloaded cavity quality factor Q_0	10^{10}
2K cryogenic load (including transfer line losses)	1.7 kW
Maximum number of bunches per pulse (<i>at 20 GeV</i>)	3,250 (3,000) ¹
Minimum bunch spacing	200 ns
Bunch charge	1 nC
Bunch peak current	5 kA
Emittance (slice) at undulator	1.4 mm*mrad
Energy spread (slice) at undulator	1 MeV

▪ Linac: Cavities

XFEL

Type of accelerating structure		standing wave
Accelerating mode		TM010, π -mode
Fundamental frequency	f_{RF} [MHz]	1300
Nominal gradient	E_{acc} [MV/m]	23.6
Quality factor	Q_0	$> 10^{10}$
Active length	L [m]	1.038
Cell-to-cell coupling	k_{cc} [%]	1.87
Iris diameter	[mm]	70
R/Q	$[\Omega]$	1036
E_{peak}/E_{acc}		2.0
B_{peak}/E_{acc}	[mT/MV/m]	4.26
Tuning range	[kHz]	± 300
$\Delta f/\Delta L$	[kHz/mm]	315
Lorentz-force detuning constant	K_{Lor} [Hz/(MV/m) ²]	1
Q_{ext} of input coupler		4.6×10^6
Cavity bandwidth f/Q_{ext}	[Hz] FWHM	283
Fill time	[μ s]	780
Number of HOM couplers		2

▪ Linac: Cavities



Motivation

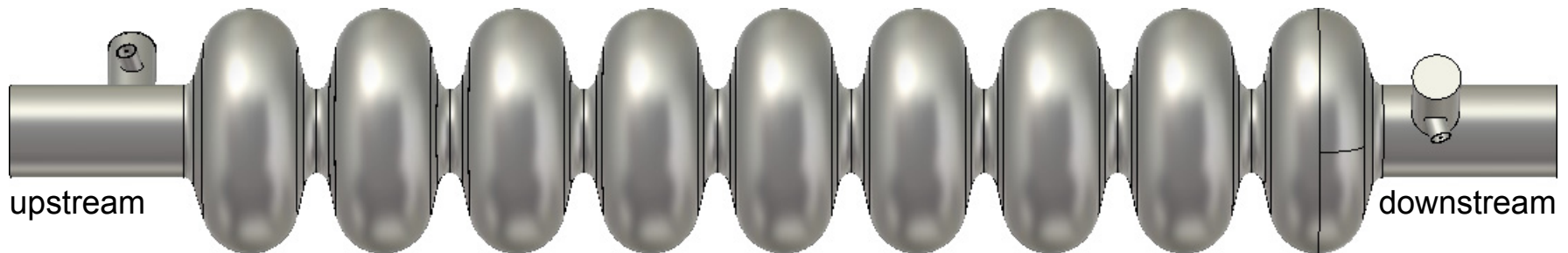
- Linac: Cavities

- Photograph



<http://newsline.linearcollider.org>

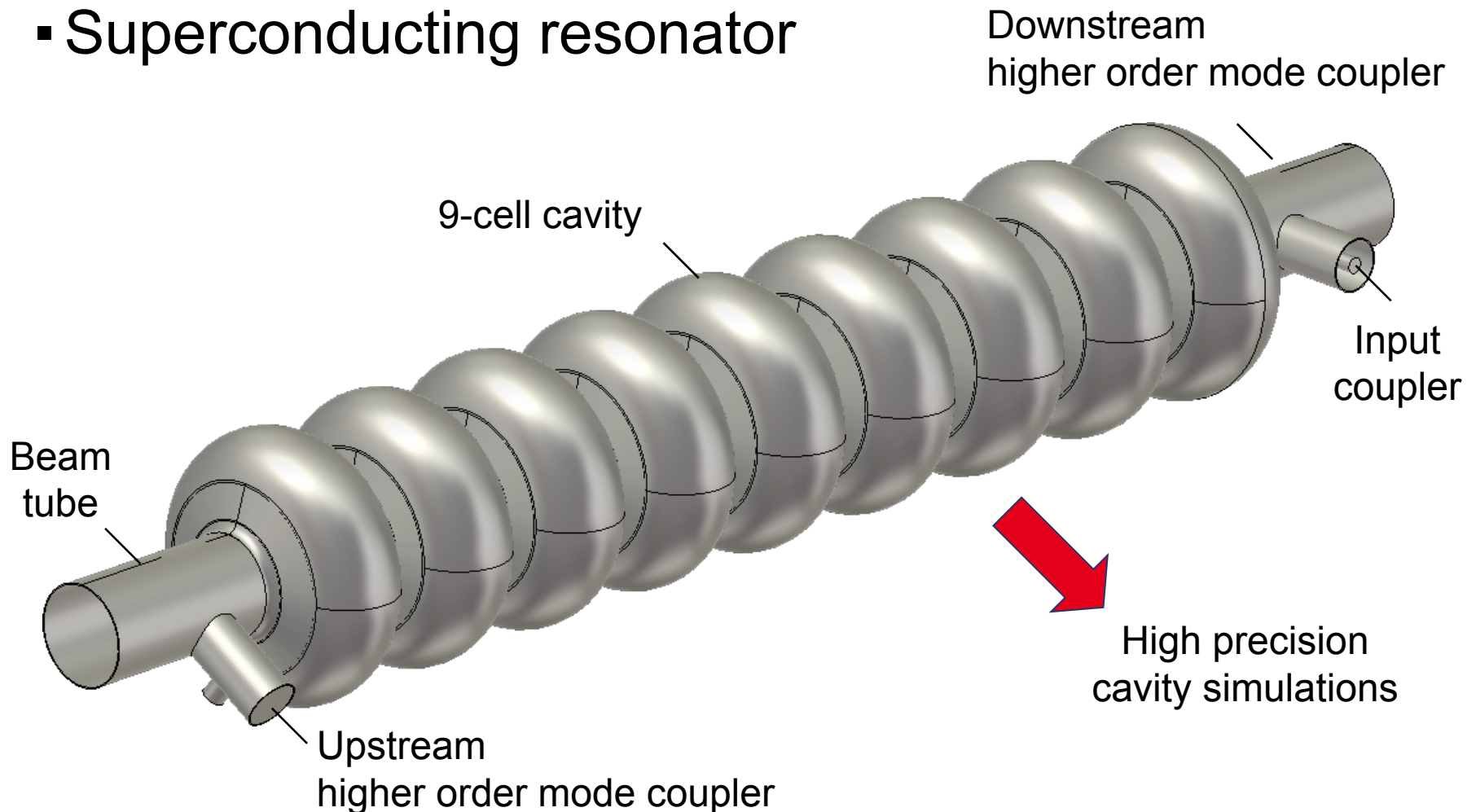
- Numerical model



CST Studio Suite 2012

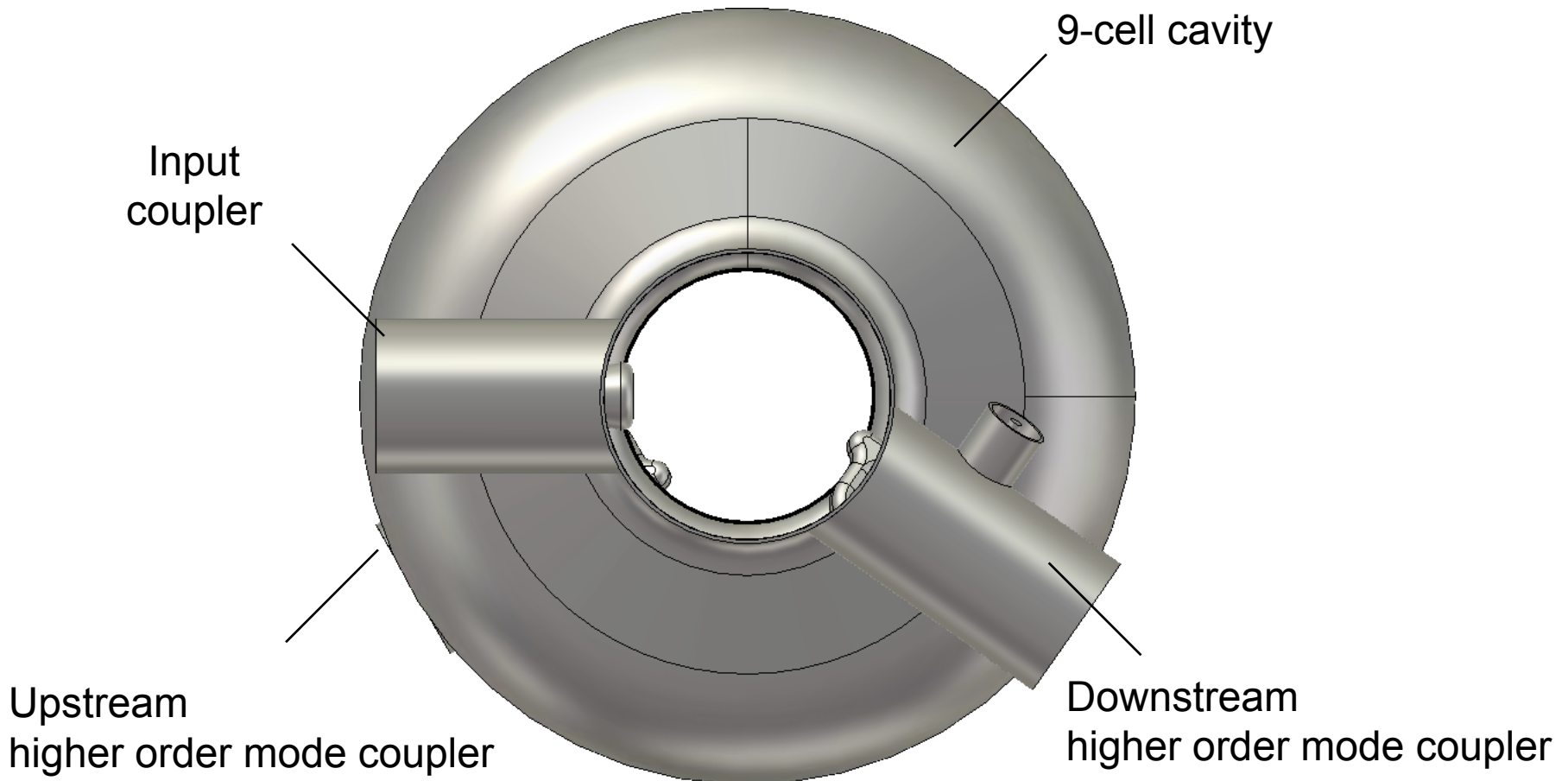
Motivation

- Superconducting resonator



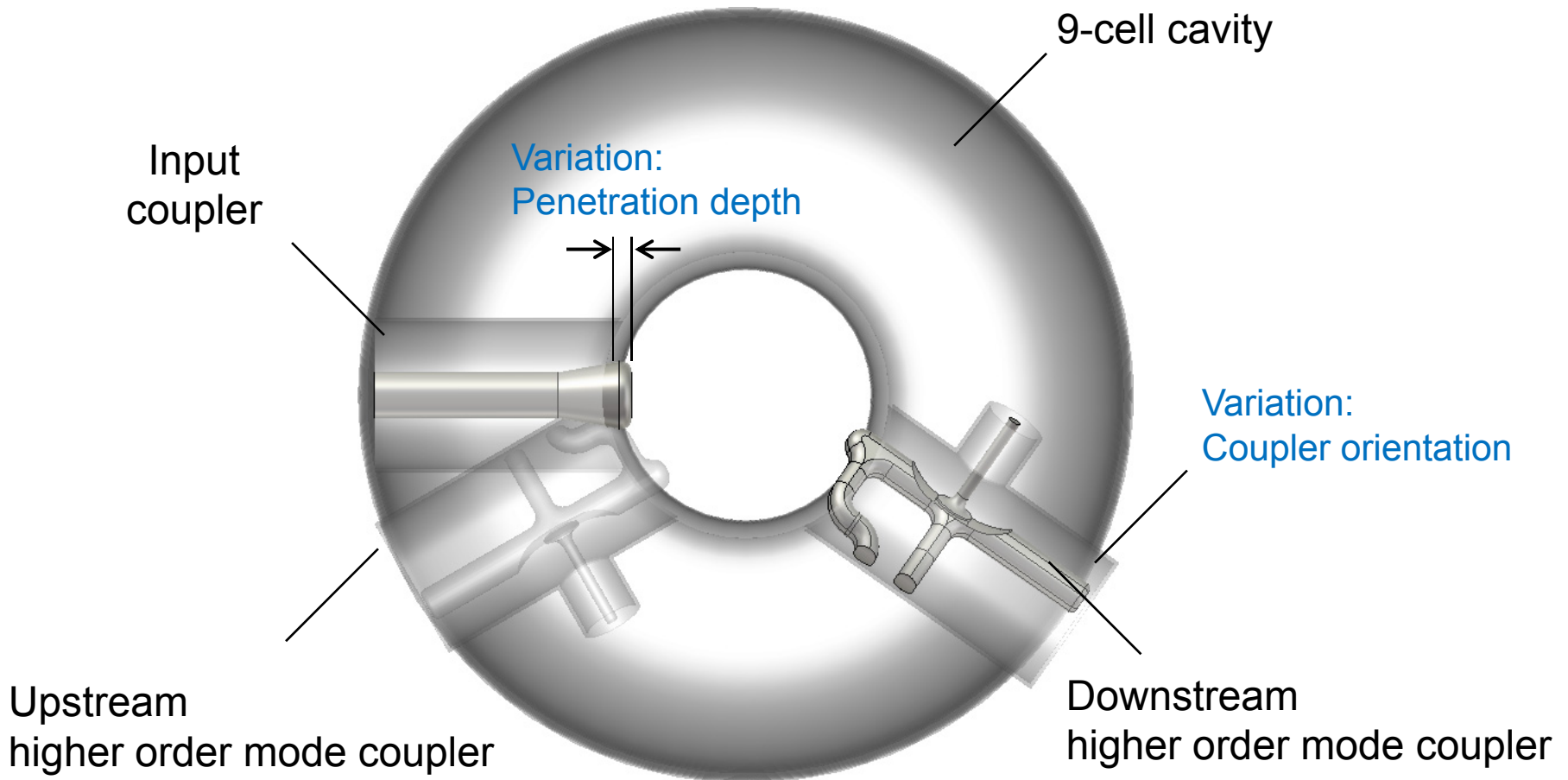
Motivation

- Superconducting resonator



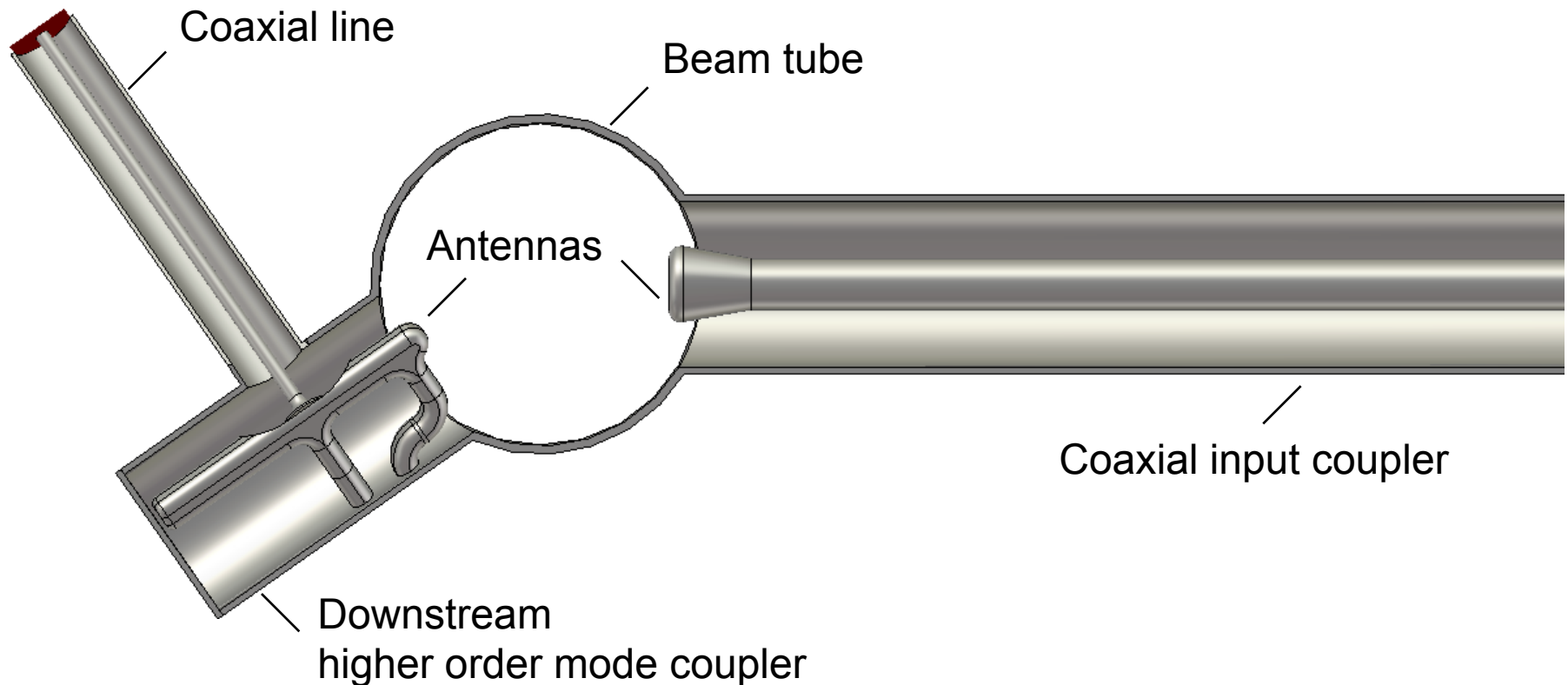
Motivation

- Superconducting resonator



Motivation

- Input coupler and coupler to extract unwanted modes



- Motivation
- Computational model
 - Problem formulation in 3-D
 - Problem formulation in 2-D (boundary condition)
- Numerical examples
 - Field patterns for selected modes
 - Resonance frequency and quality factors
- Summary / Outlook

- Problem formulation
 - Local Ritz approach

$$\begin{aligned}\vec{E} &= \vec{E}(\vec{r}) \\ &= \sum_{i=1}^n \alpha_i \vec{w}_i(\vec{r})\end{aligned}$$

$\vec{w}$ vectorial function

α_i scalar coefficient

i global index

n number of DOFs

Galerkin



$$\begin{aligned}\text{curl } 1/\mu_r \text{ curl } \vec{E} &= \left(\frac{\omega}{c_0}\right)^2 \epsilon_r \vec{E} \Big|_{\vec{r} \in \Omega} \\ \text{div}(\epsilon \vec{E}) \Big|_{\vec{r} \in \Omega} &= 0 \quad + \text{boundary conditions}\end{aligned}$$

continuous eigenvalue problem

$$A_{ij} = \iiint_{\Omega} 1/\mu_r \text{ curl } \vec{w}_i \cdot \text{ curl } \vec{w}_j \, d\Omega$$

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

$$C_{ij} = \iiint_{\Omega} \sigma \vec{w}_i \cdot \vec{w}_j \, d\Omega$$

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

discrete eigenvalue problem

▪ 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

$$AN = CN = 0 \quad \text{for proper chosen scalar and vector basis functions}$$

$$N^T A \vec{x} = \underbrace{(AN)^T}_{0} \vec{\alpha} = \lambda \underbrace{N^T C}_{0} \vec{\alpha} - \lambda^2 N^T B \vec{\alpha} = -\lambda^2 N^T B \vec{\alpha}$$



$$\text{static } \lambda = 0 \quad \text{or} \quad \text{dynamic } N^T B \vec{x} = S\vec{x} = 0$$

▪ Fundamental properties

- Number of eigenvalues

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

Matrix B nonsingular:

- matrix polynomial $Q(\lambda)$ is regular
- $2n$ finite eigenvalues

Notation:

A - stiffness matrix

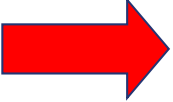
B - mass matrix

C - damping matrix

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

- Orthogonality relation

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


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

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

- Numerical formulation
 - Function definition

FEM06: lowest order approximation
(edge elements, Nedelec)

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

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

- Numerical formulation
 - Function definition

FEM12: higher order approximation

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

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

- Numerical formulation
 - Function definition

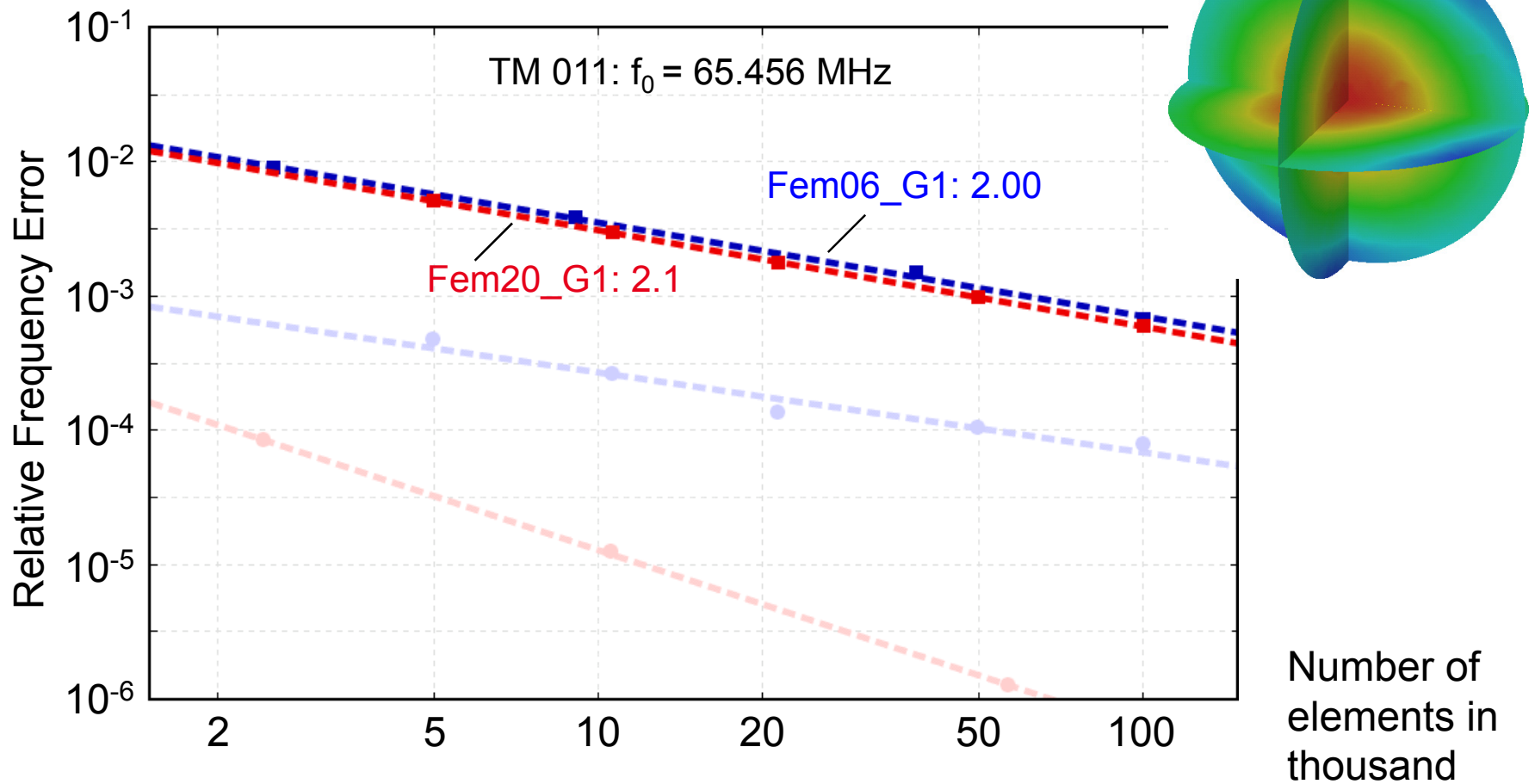
FEM20: higher order approximation

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

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

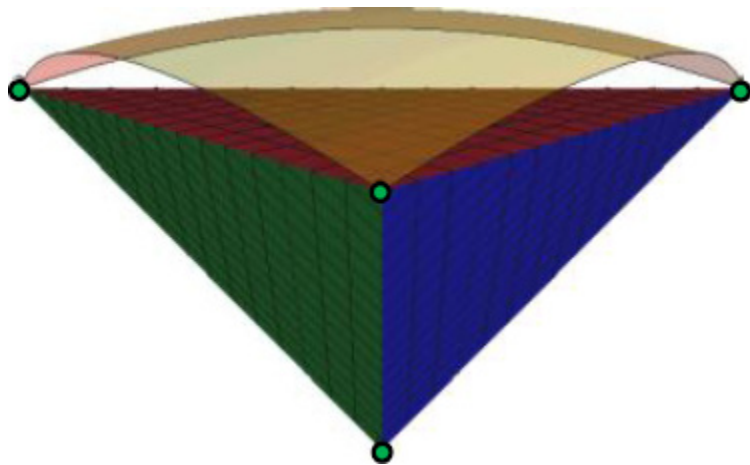
Computational Model

▪ Spherical resonator

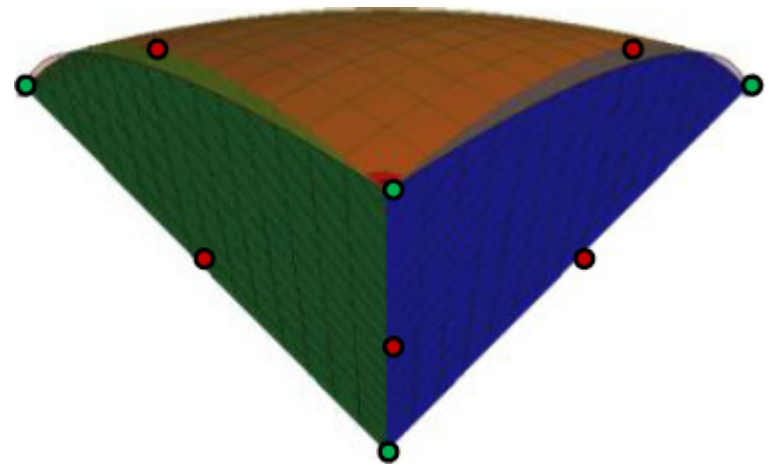


Computational Model

- Geometry approximation
 - Tetrahedral mesh types



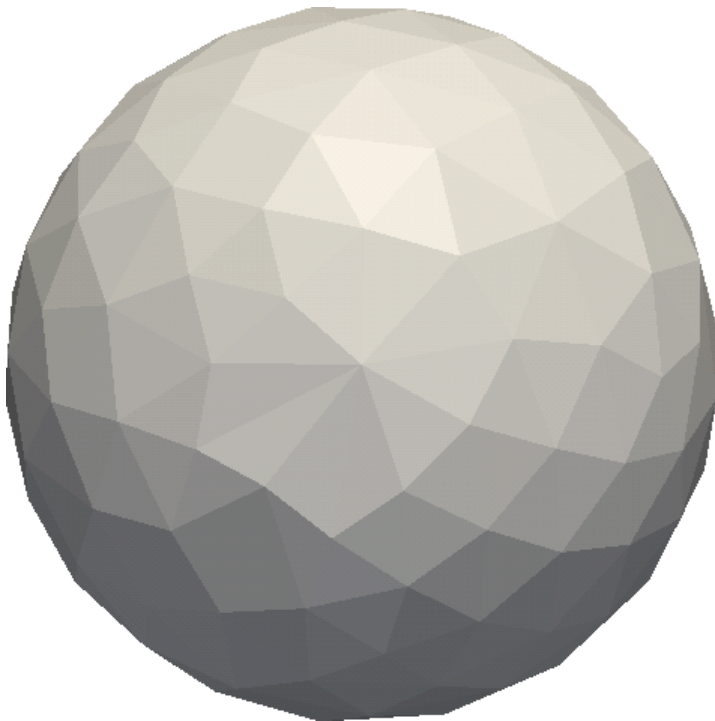
Linear element



Curvilinear element

- Geometry approximation

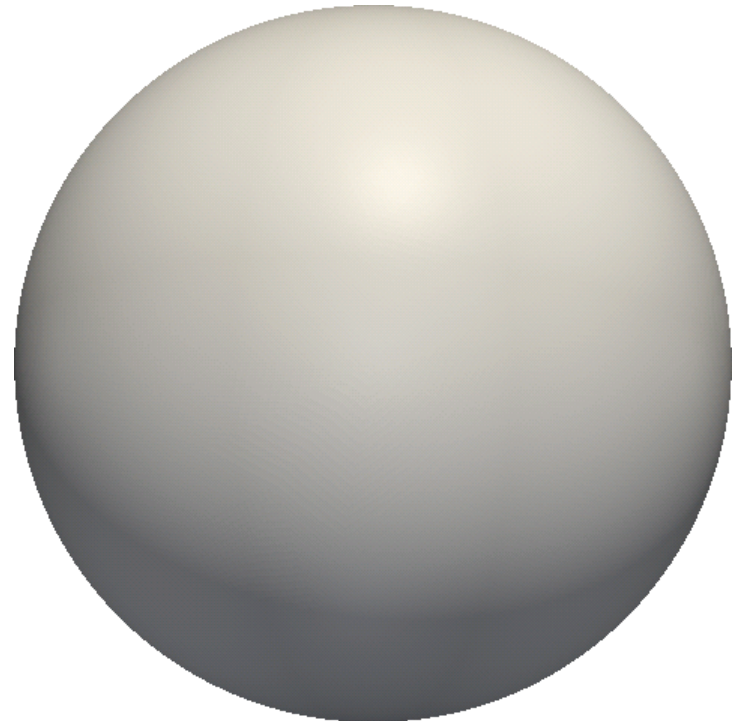
Planar elements



1701 tetrahedrons



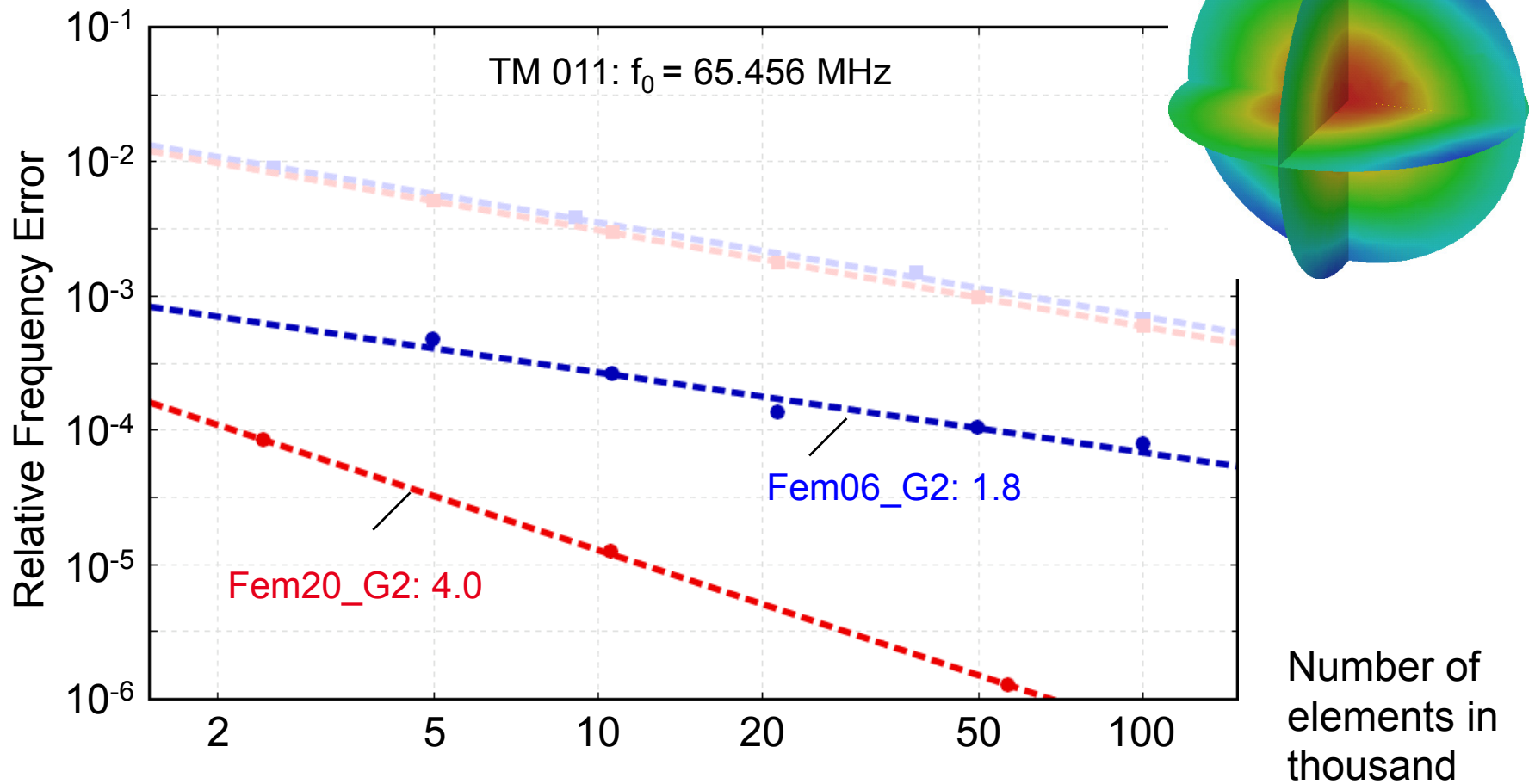
Curvilinear elements



1701 tetrahedrons

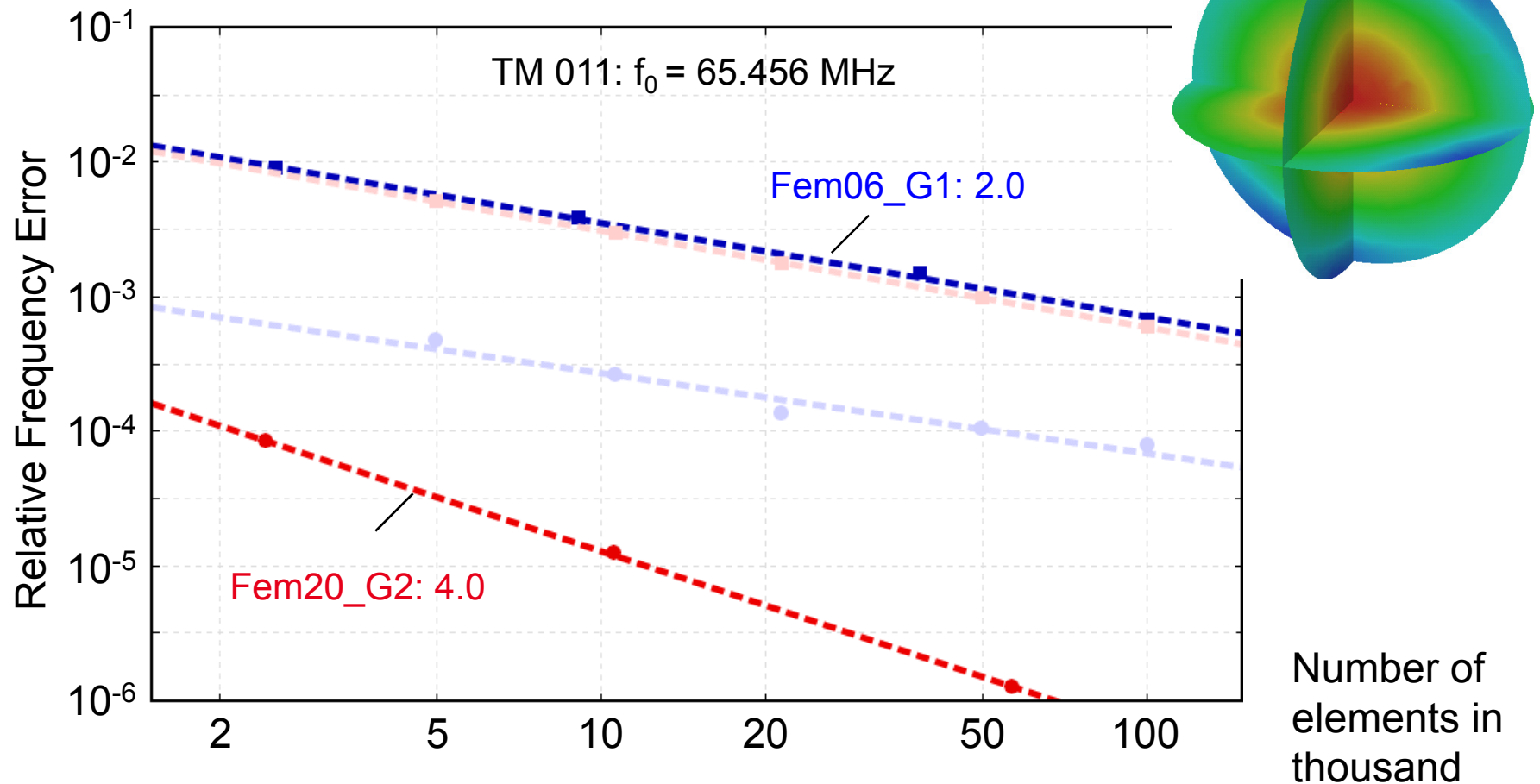
Computational Model

▪ Spherical resonator



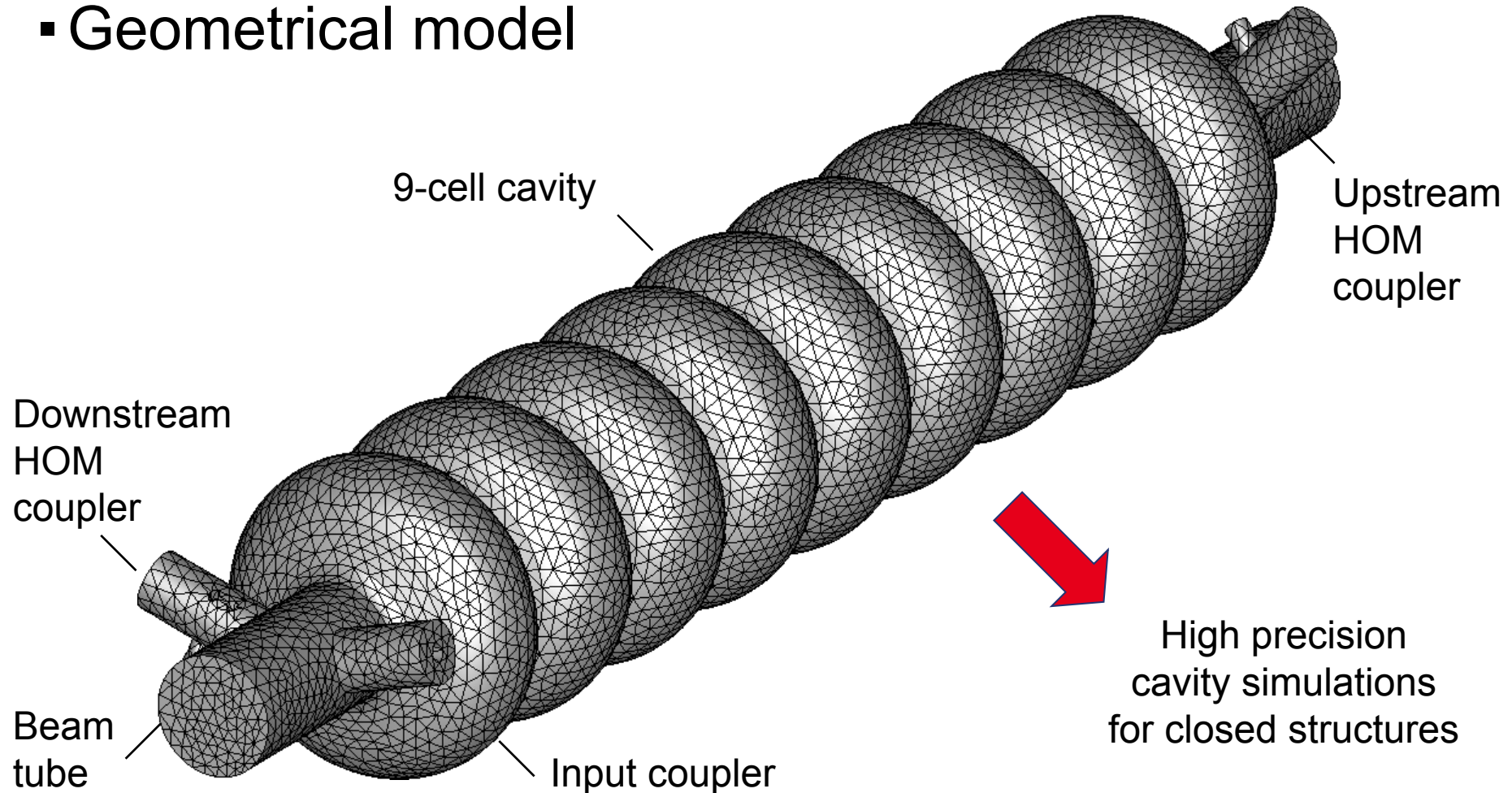
Computational Model

▪ Spherical resonator



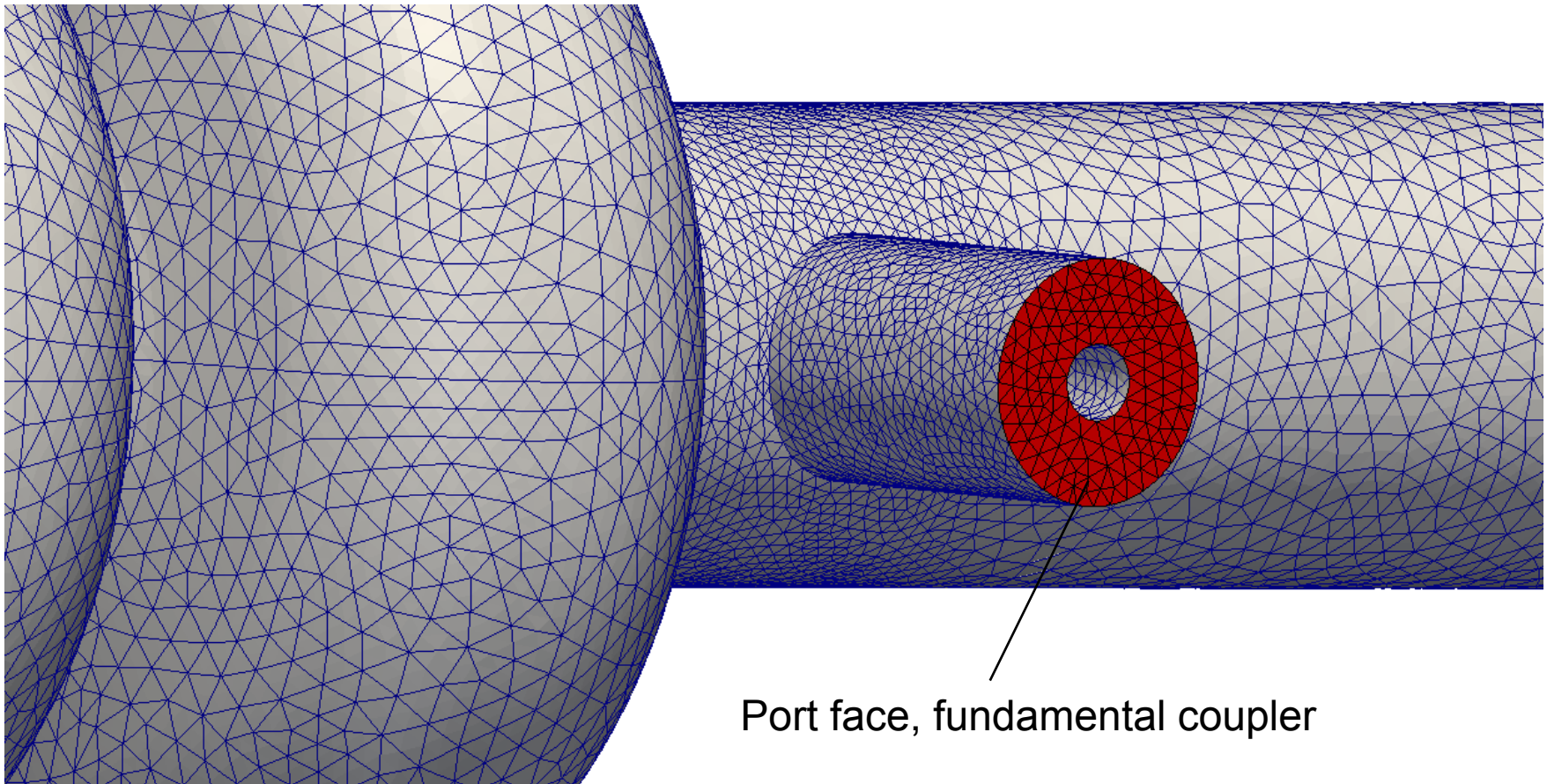
Computational Model

- Geometrical model

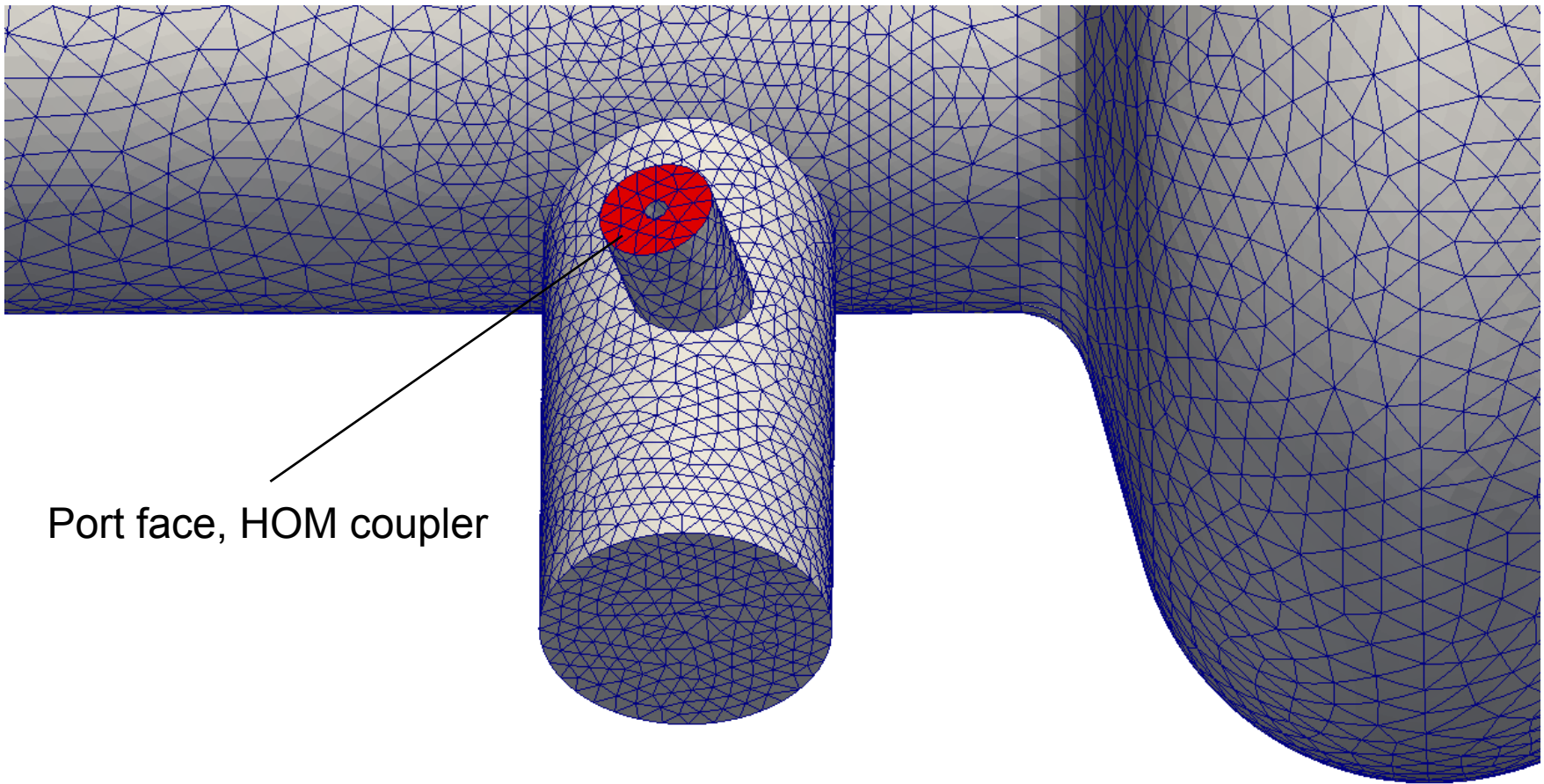


- Motivation
- Computational model
 - Problem formulation in 3-D
 - Problem formulation in 2-D (boundary condition)
- Numerical examples
 - Field patterns for selected modes
 - Resonance frequency and quality factors
- Summary / Outlook

- Port boundary condition



- Port boundary condition



- Problem formulation
 - Local Ritz approach

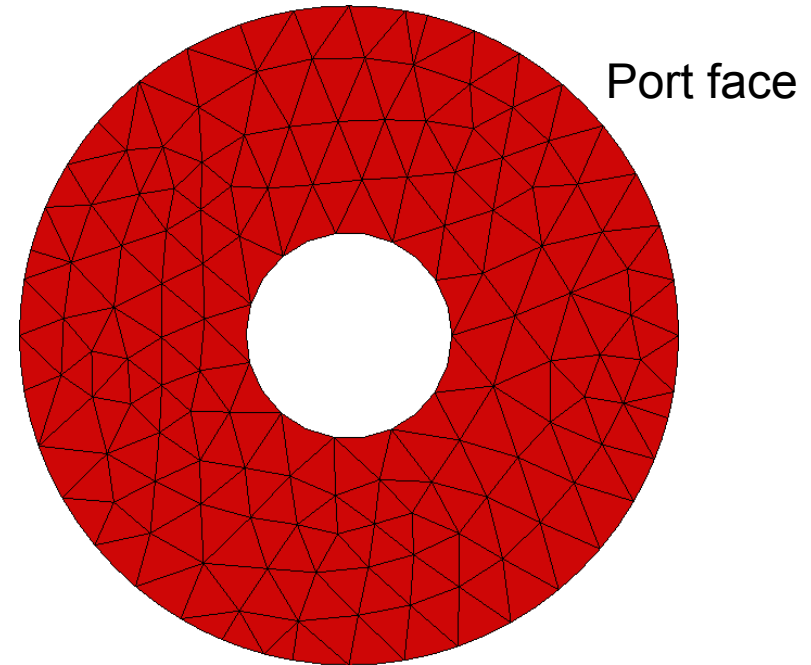
$$\begin{aligned}\vec{E} &= \vec{E}(\vec{r}) \\ &= \sum_{i=1}^n \alpha_i \vec{w}_i(\vec{r})\end{aligned}$$

$\vec{w}$ vectorial function

α_i scalar coefficient

i global index

n number of DOFs



Mixed 2-D vector and scalar basis

$$\vec{w}_i = \begin{cases} \vec{w}_i^{2D} & \text{tangential} \\ \vec{n} \Phi_i & \text{normal} \end{cases}$$

- Problem formulation
 - Local Ritz approach

$$\begin{aligned}\vec{E} &= \vec{E}(\vec{r}) \\ &= \sum_{i=1}^n \alpha_i \vec{w}_i(\vec{r})\end{aligned}$$

Galerkin



$\vec{w}$ vectorial function

α_i scalar coefficient

i global index

n number of DOFs

$$\begin{aligned}\text{curl } 1/\mu_r \text{ curl } \vec{E} &= \left(\frac{\omega}{c_0}\right)^2 \varepsilon_r \vec{E} \Big|_{\vec{r} \in \Omega} \\ \text{div}(\varepsilon \vec{E}) \Big|_{\vec{r} \in \Omega} &= 0 \quad + \text{boundary conditions}\end{aligned}$$

continuous eigenvalue problem, loss-free

$$A_{ij} = \iint_A 1/\mu_r \text{ curl } \vec{w}_i \cdot \text{ curl } \vec{w}_j \, d\Omega$$

$$B_{ij} = \iint_A \varepsilon_r \vec{w}_i \cdot \vec{w}_j \, d\Omega$$

$$\vec{w}_i(x, y, z) = \vec{w}_i(x, y) \cdot e^{-ik_z z}$$

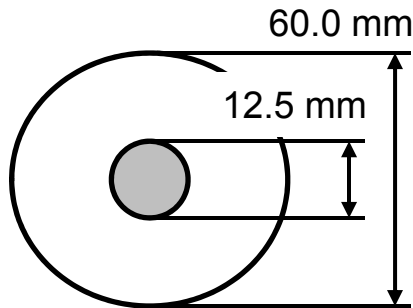
$$A\vec{\alpha} = \left(\frac{\omega}{c_0}\right)^2 B\vec{\alpha}$$

discrete eigenvalue problem

Computational Model

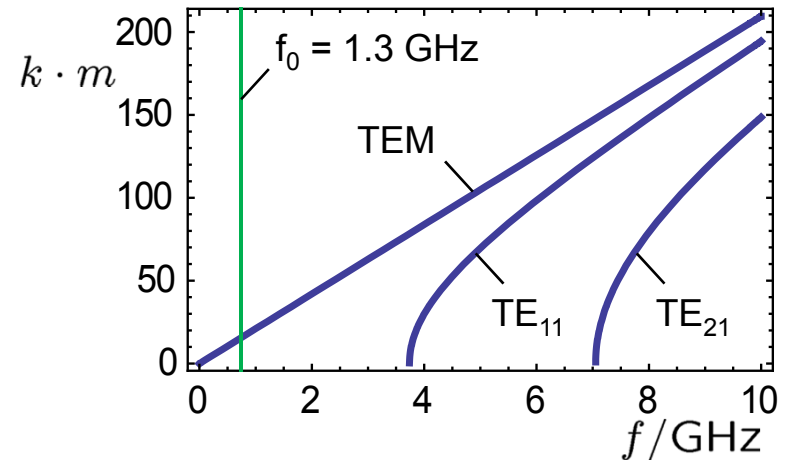
▪ Wave propagation in the applied coaxial lines

- Main coupler

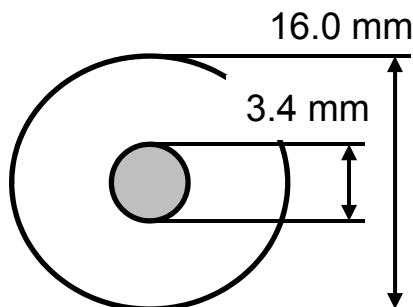


Dispersion relation

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



- HOM coupler

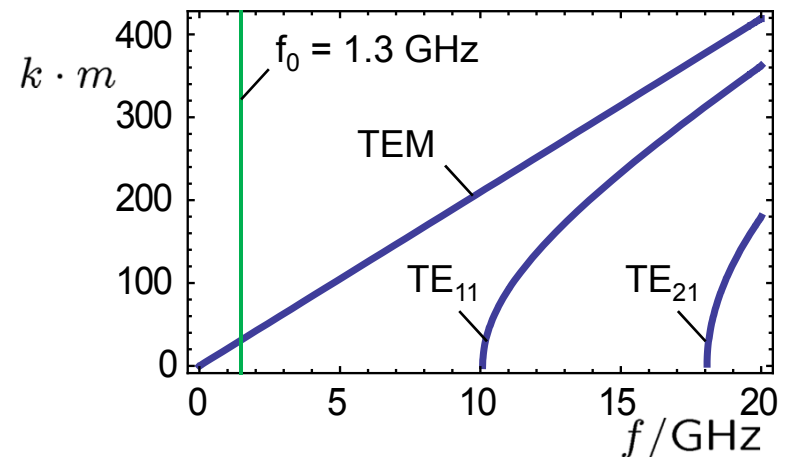


propagation

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

damping

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

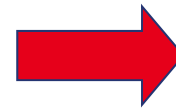


▪ Problem formulation

- Determine propagation constant for a fixed frequency

$$\begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \vec{y}_t \\ \vec{y}_z \end{pmatrix} = -k_z^2 \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} \vec{y}_t \\ \vec{y}_z \end{pmatrix}$$

algebraic eigenvalue problem



eigenvector
and
eigenvalue

$$A_{11,ij}^{2D} = \iint_{A_{\text{port}}} \frac{1}{\mu_r} \text{curl}_t \vec{\omega}_{t,i}^{2D} \cdot \text{curl}_t \vec{\omega}_{t,j}^{2D} d\Omega - \omega_{\text{port}}^2 \mu_0 \epsilon_0 \iint_{A_{\text{port}}} \epsilon_r \vec{\omega}_{t,i}^{2D} \cdot \vec{\omega}_{t,j}^{2D} d\Omega$$

$$B_{11,ij}^{2D} = \iint_{A_{\text{port}}} \frac{1}{\mu_r} \vec{\omega}_{t,i}^{2D} \cdot \vec{\omega}_{t,j}^{2D} d\Omega$$

$$B_{12,ij}^{2D} = \iint_{A_{\text{port}}} \frac{1}{\mu_r} \text{grad}_t \omega_{z,i}^{2D} \cdot \vec{\omega}_{t,j}^{2D} d\Omega$$

$$B_{21,ij}^{2D} = \iint_{A_{\text{port}}} \frac{1}{\mu_r} \vec{\omega}_{t,i}^{2D} \cdot \text{grad}_t \omega_{z,j}^{2D} d\Omega$$

$$B_{22,ij}^{2D} = \iint_{A_{\text{port}}} \frac{1}{\mu_r} \text{grad}_t \omega_{z,i}^{2D} \cdot \text{grad}_t \omega_{z,j}^{2D} d\Omega - \omega_{\text{port}}^2 \mu_0 \epsilon_0 \iint_{A_{\text{port}}} \epsilon_r \omega_{z,i}^{2D} \omega_{z,j}^{2D} d\Omega$$

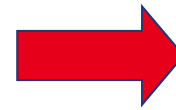
Computational Model

▪ Problem formulation

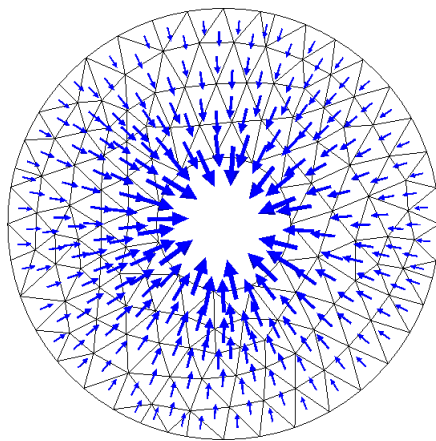
- Determine propagation constant for a fixed frequency

$$\begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \vec{y}_t \\ \vec{y}_z \end{pmatrix} = -k_z^2 \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} \vec{y}_t \\ \vec{y}_z \end{pmatrix}$$

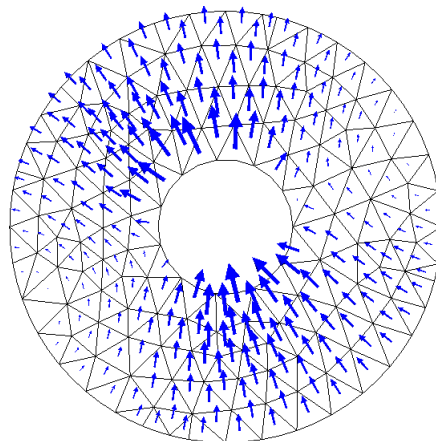
algebraic eigenvalue problem



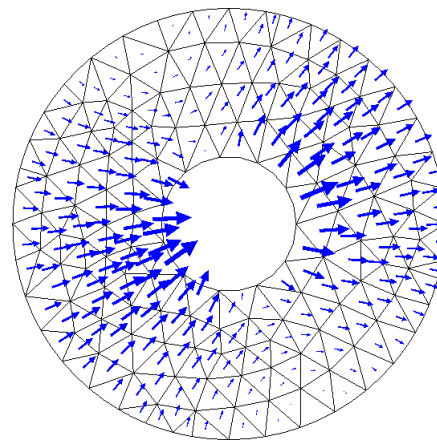
eigenvector
and
eigenvalue



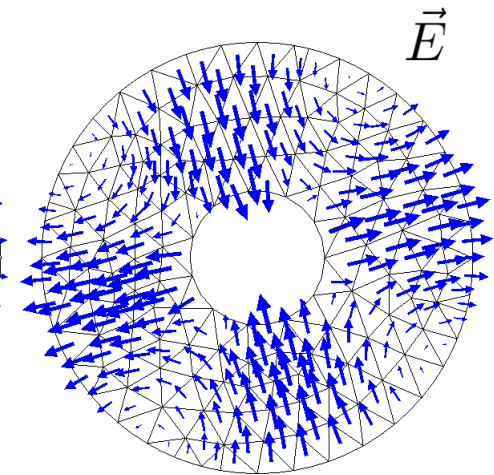
Mode 1



Mode 2



Mode 3



Mode 4

...

Numerical Examples

- Problem definition

- Geometry

TESLA 9-cell cavity

PEC
boundary condition

Port
boundary
conditions

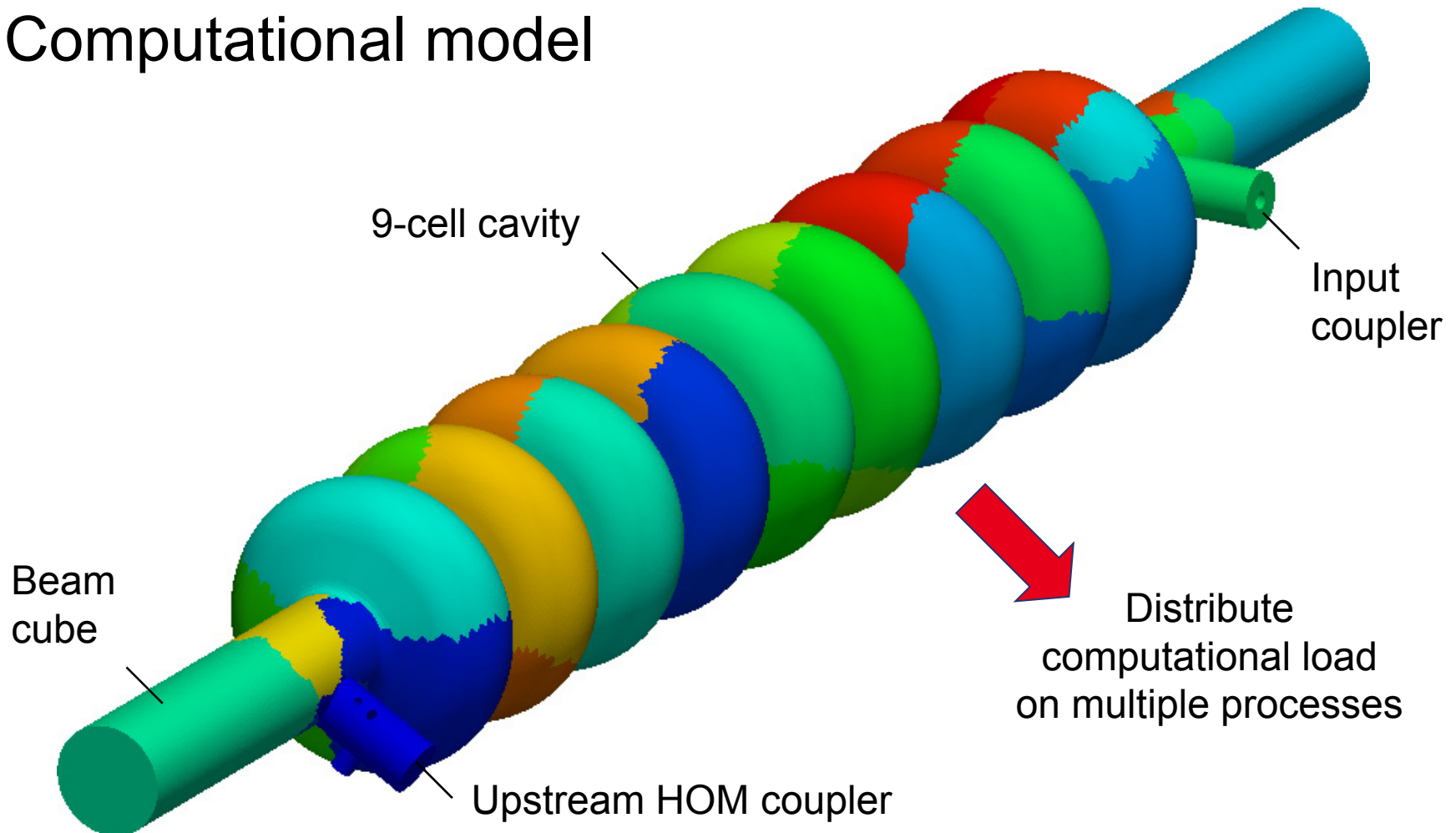
Port boundary conditions

- Task

Search for the field distribution, resonance frequency and quality factor

Numerical Examples

- Computational model



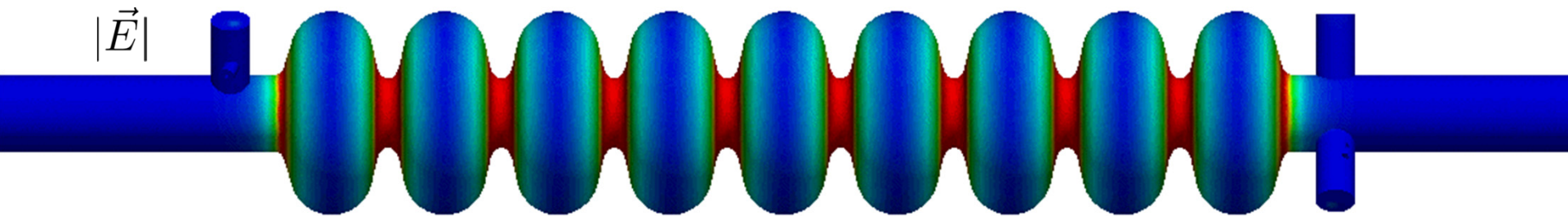
- Motivation
- Computational model
 - Problem formulation in 3-D
 - Problem formulation in 2-D (boundary condition)
- Numerical examples
 - Field patterns for selected modes
 - Resonance frequency and quality factors
- Summary / Outlook

Numerical Examples

- Simulation results

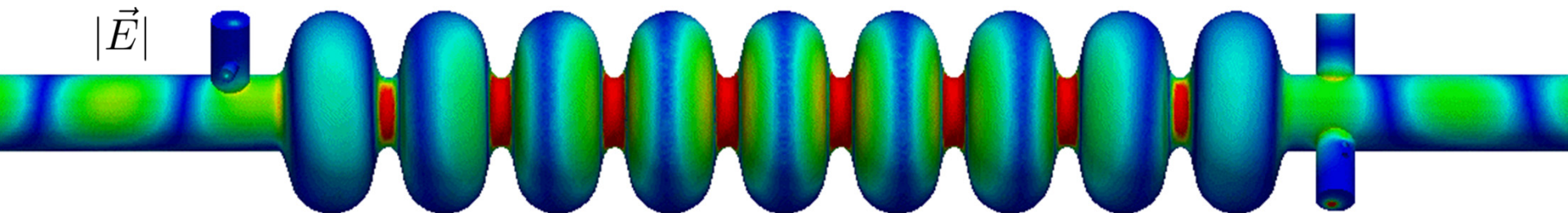
- Accelerating mode (monopole #9)

$$f_{\text{res}} = 1.300 \text{ GHz}$$
$$Q_{\text{ext}} = 2.8 \cdot 10^6$$



- Higher-order mode (dipole #37)

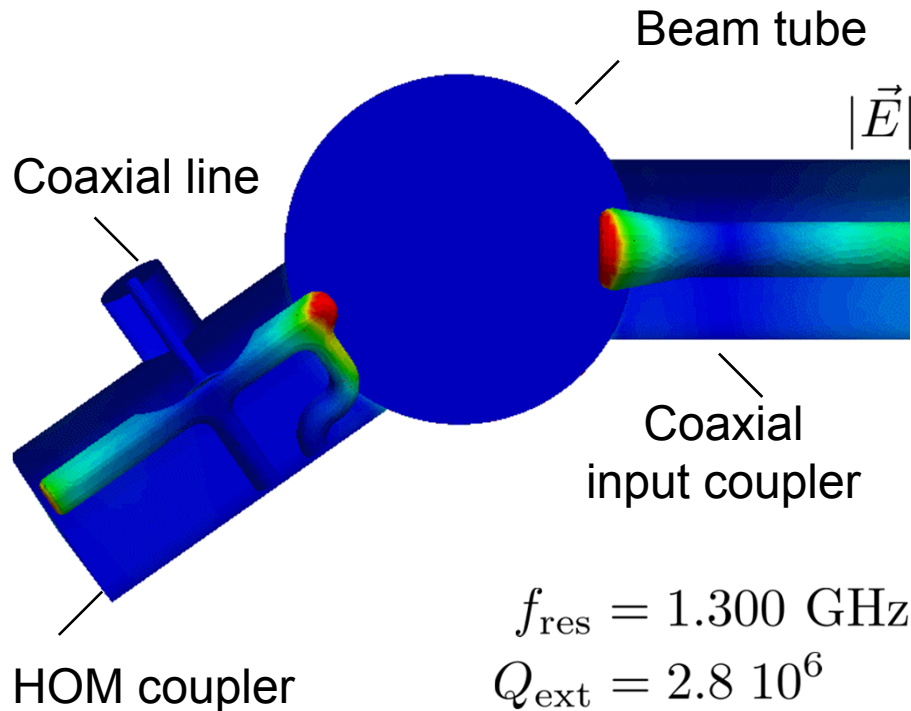
$$f_{\text{res}} = 2.476 \text{ GHz}$$
$$Q_{\text{ext}} = 1.8 \cdot 10^3$$



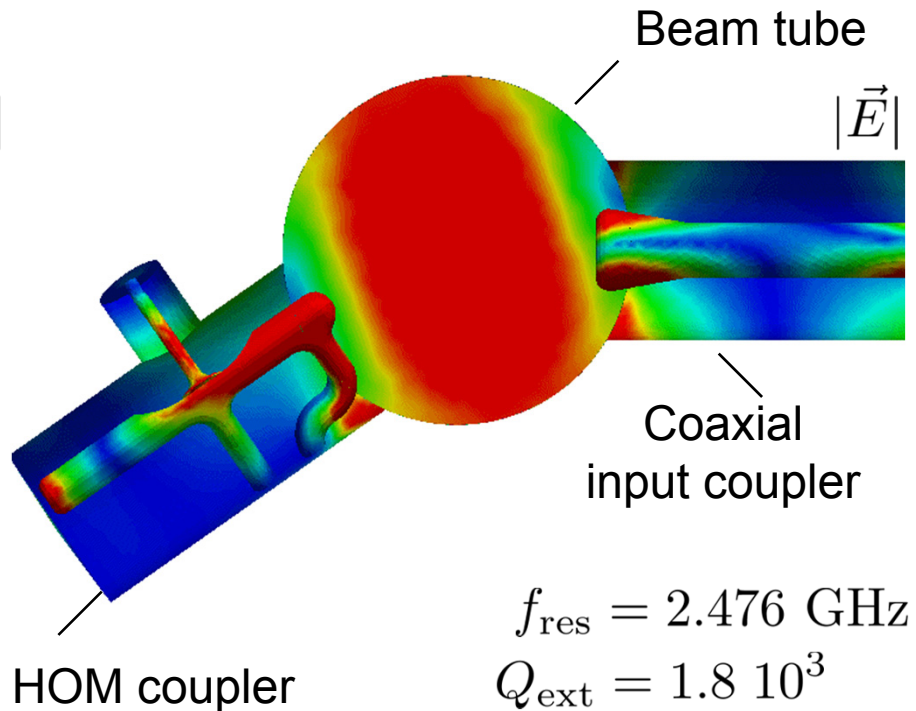
Numerical Examples

- Simulation results

Accelerating mode
(monopole #9)



Higher-order mode
(dipole #37)

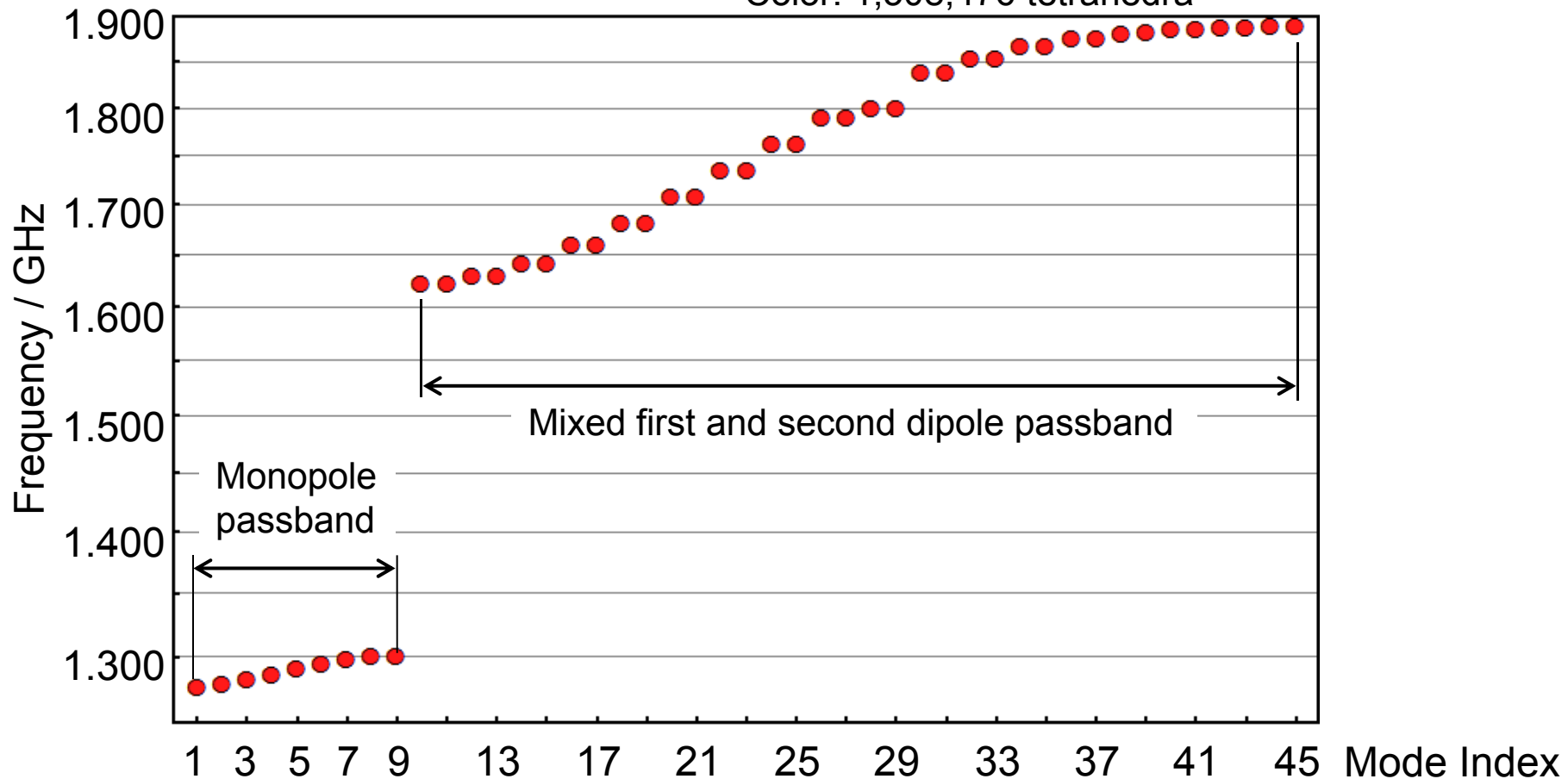


Numerical Examples

■ Simulation results

Black: 283,130 tetrahedra

Color: 1,308,476 tetrahedra

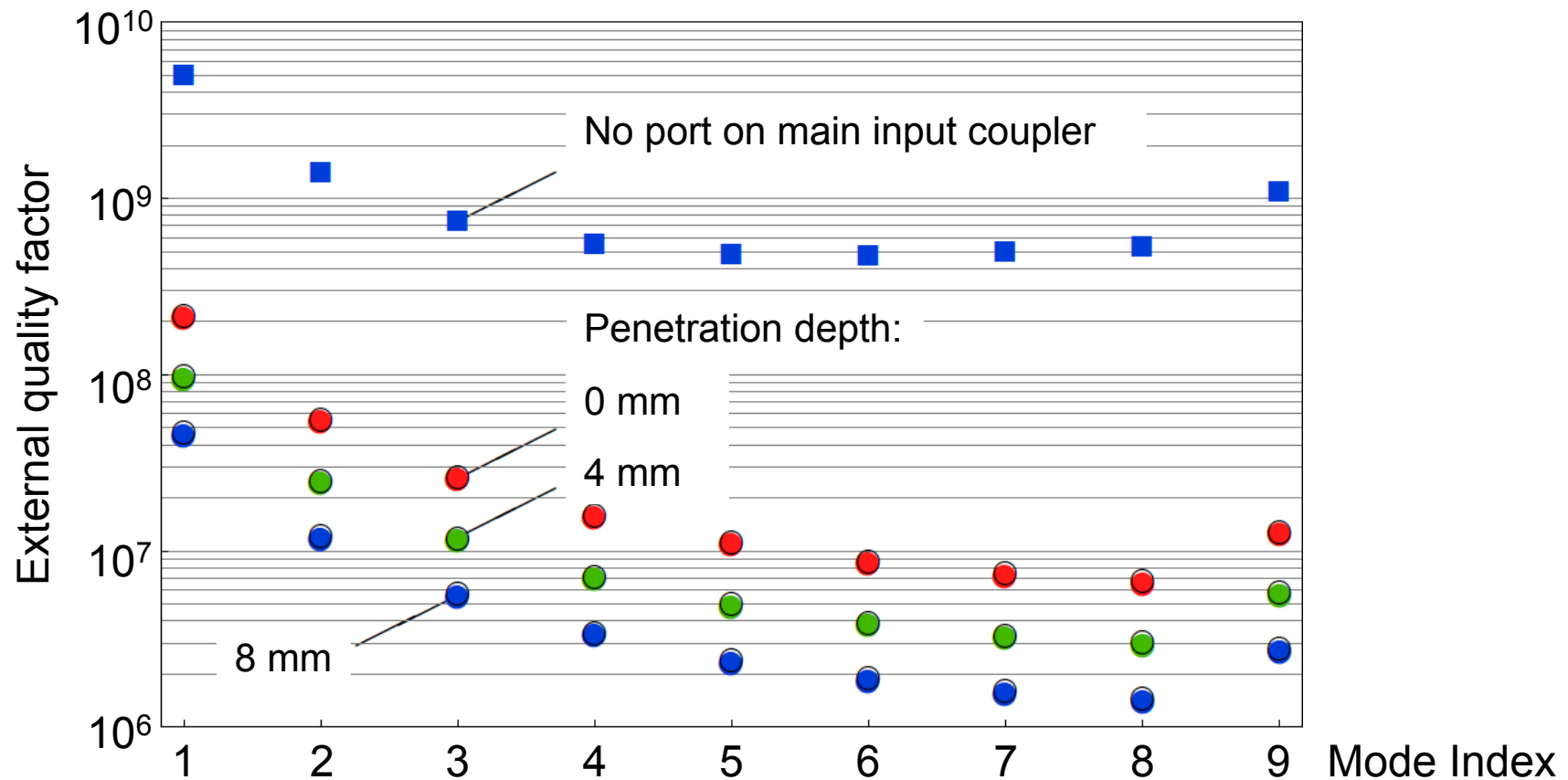


Numerical Examples

■ Simulation results

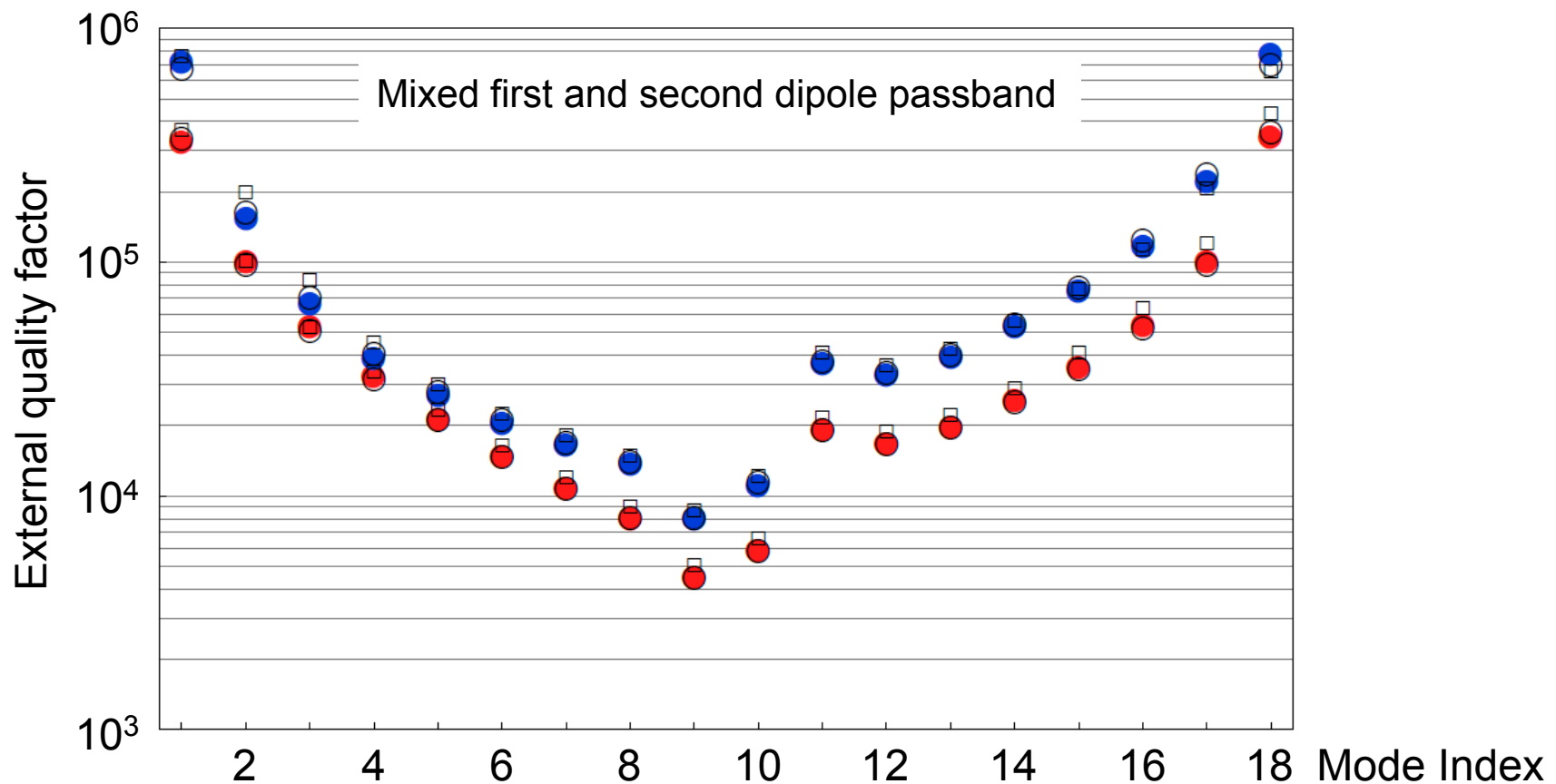
Black: 283,130 tetrahedra

Color: 1,308,476 tetrahedra



Numerical Examples

▪ Simulation results



▪ Summary:

Request for precise modeling of electromagnetic fields within resonant structures including small geometric details:

- Geometric modeling with curved tetrahedral elements
- Port boundary conditions with curved triangles
- Preliminary implementation

▪ Outlook:

- User-friendly parallel implementation