Calculation of Eigenmodes in Superconducting Cavities

TECHNISCHE UNIVERSITÄT DARMSTADT

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Status Meeting
December 17, 2012
DESY, Hamburg

Outline

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- Motivation
- Computational model
  - Problem formulation in 3-D
  - Problem formulation in 2-D (boundary condition)
- Numerical examples
  - 1.3 GHz structure, single cavity
  - 3.9 GHz structure, string of four cavities (preliminary,without bellows)
- Summary / Outlook

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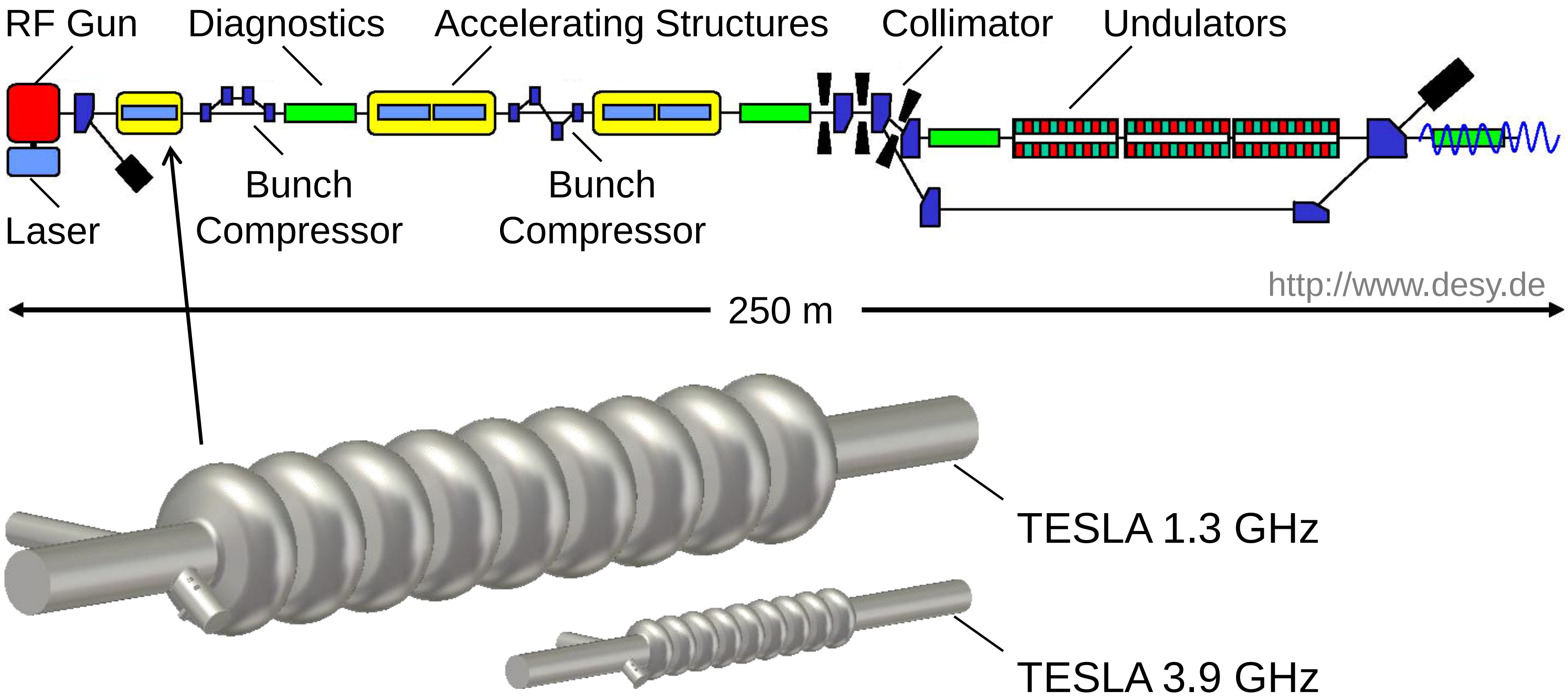
Motivation

- Particle accelerators
  - FLASH at DESY, Hamburg

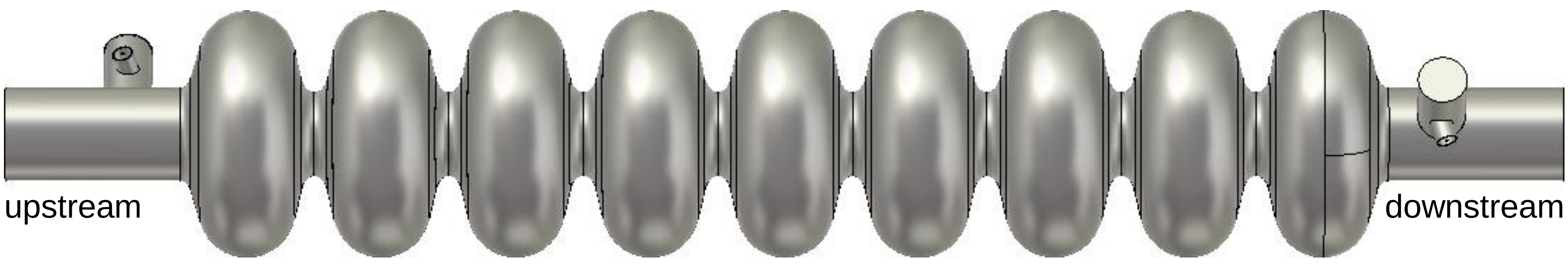


Motivation

- Linac: Cavities
  - Photograph

http://newsline.linearcollider.org

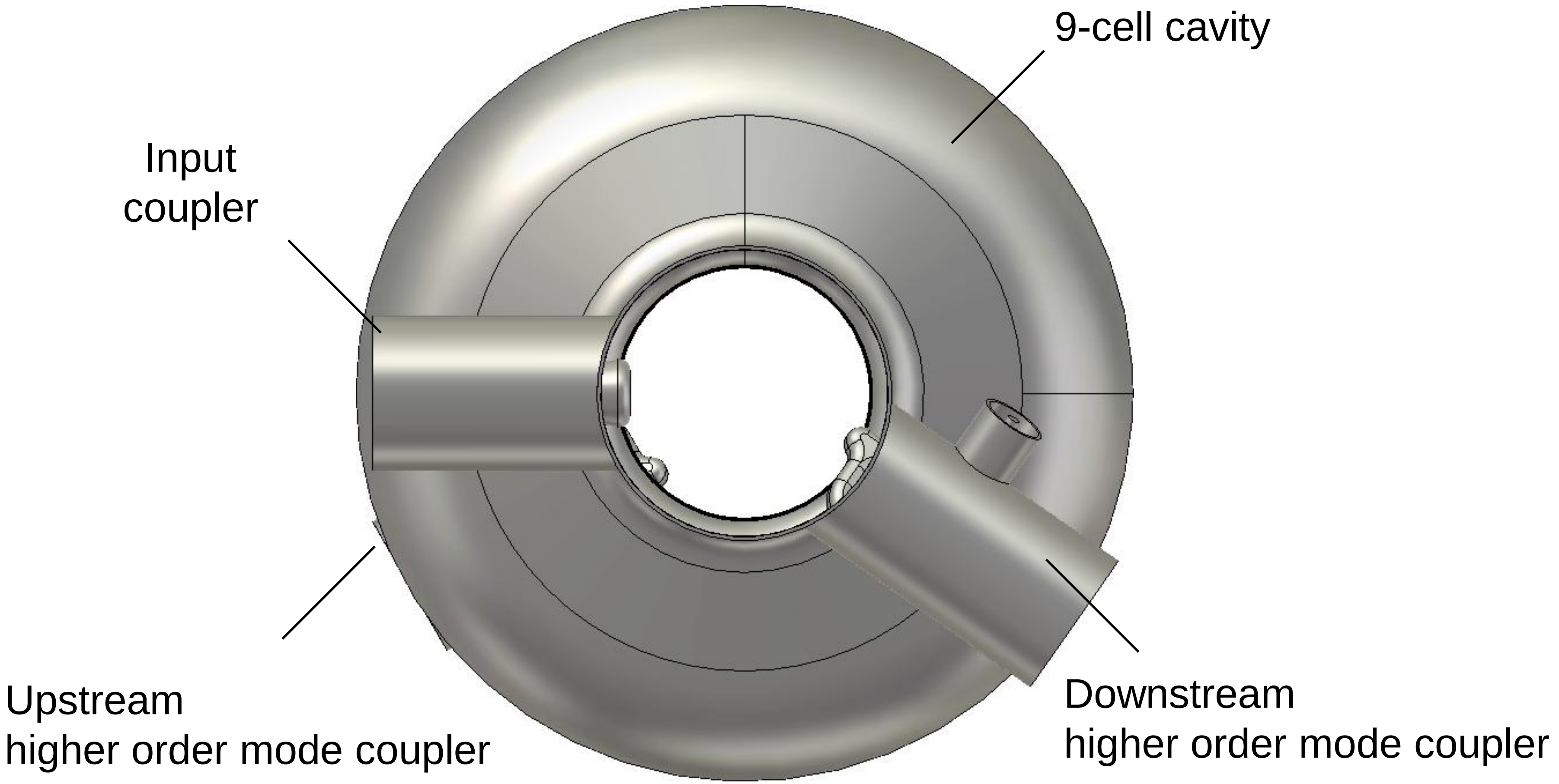
  - Numerical model



CST Studio Suite 2012

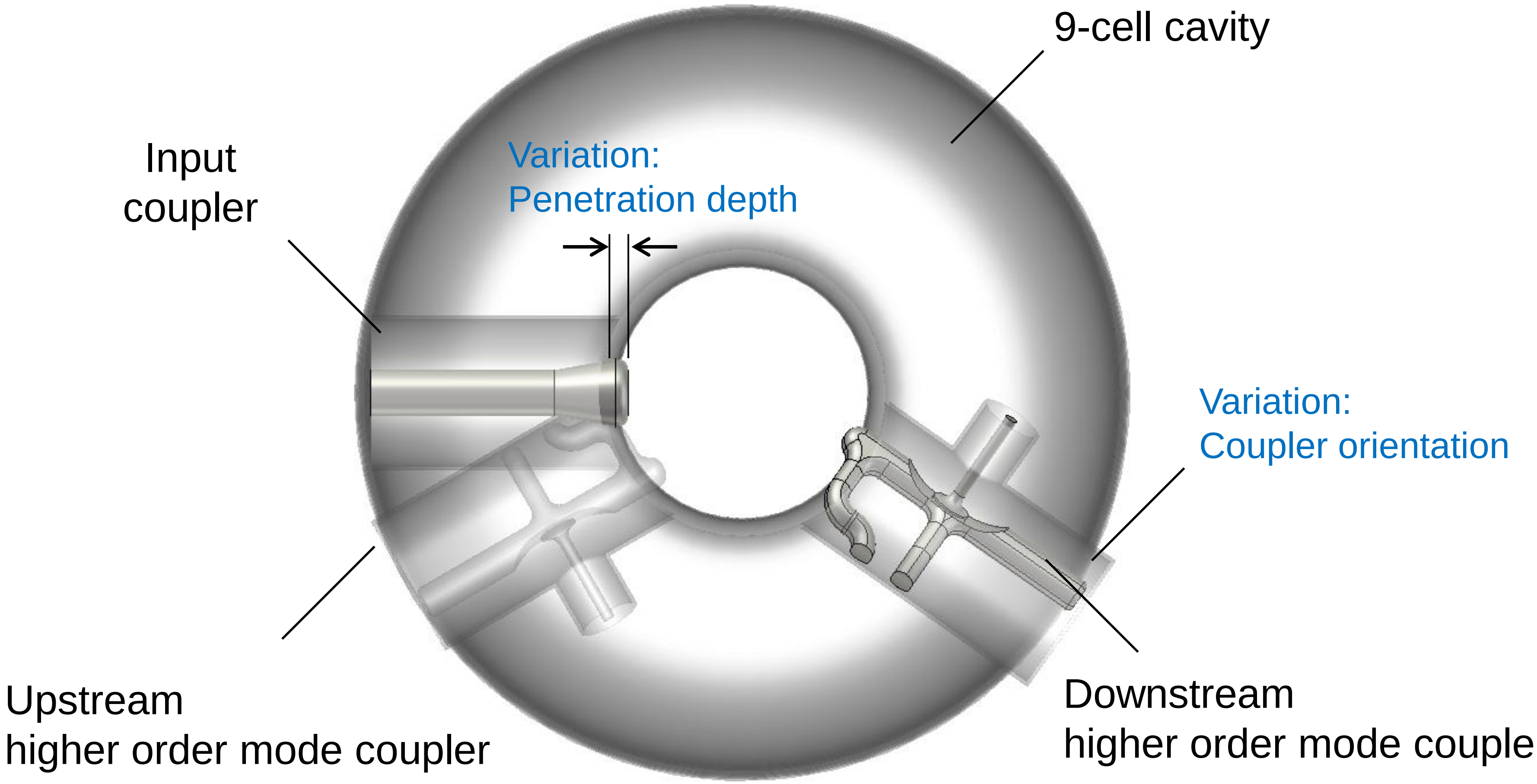
Motivation

- Superconducting resonator



Motivation

- Superconducting resonator



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Computational Model

- Problem formulation
  - Time domain
    - Efficient algorithms available (explicit method, coupled S-parameter) ✓
    - Field excitation to discriminate unknown mode polarizations ✗
  - Frequency domain (driven problem)
    - Efficient algorithms available (coupled S-parameter) ✓
    - Field excitation to discriminate unknown mode polarizations ✗
  - Frequency domain (eigenmode formulation)
    - Expensive algorithms ✗
    - Field distributions available including mode polarization ✓
    - Localized mode patterns with weak coupling naturally included ✓

Computational Model

- 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

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

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

continuous eigenvalue problem

Galerkin

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

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

$$C_{ij} = \iiint_\Omega Z_0\,\sigma\,\vec{w}_i \cdot \vec{w}_j\ \mathrm{d}\Omega$$

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

discrete eigenvalue problem

Computational Model

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- 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 and vector basis functions

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

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

Computational Model

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- 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

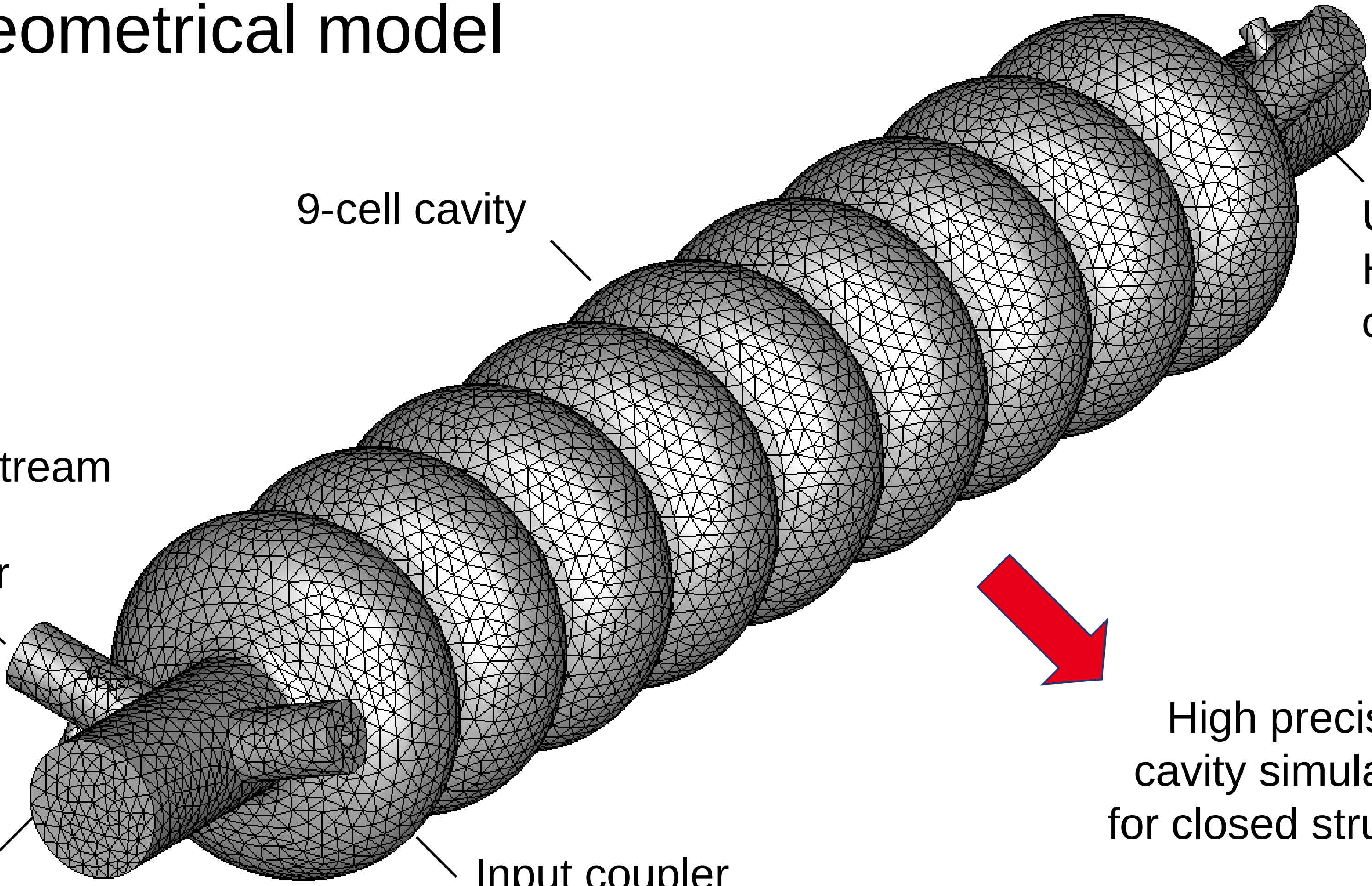
$$A\vec{\alpha} + \lambda C\vec{\alpha} + \lambda^2 B\vec{\alpha} = 0$$

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

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

- Geometrical model



High precision cavity simulations for closed structures

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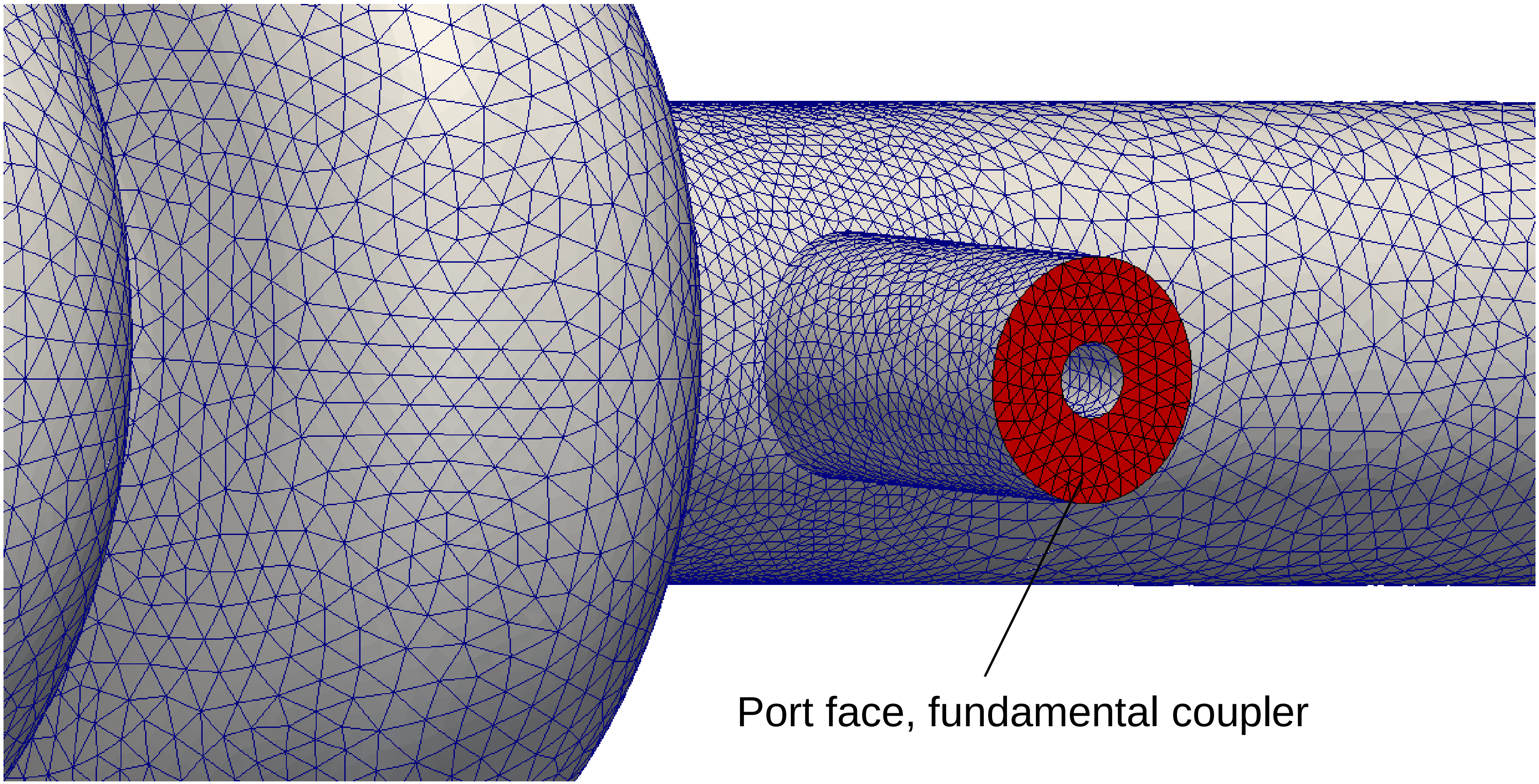
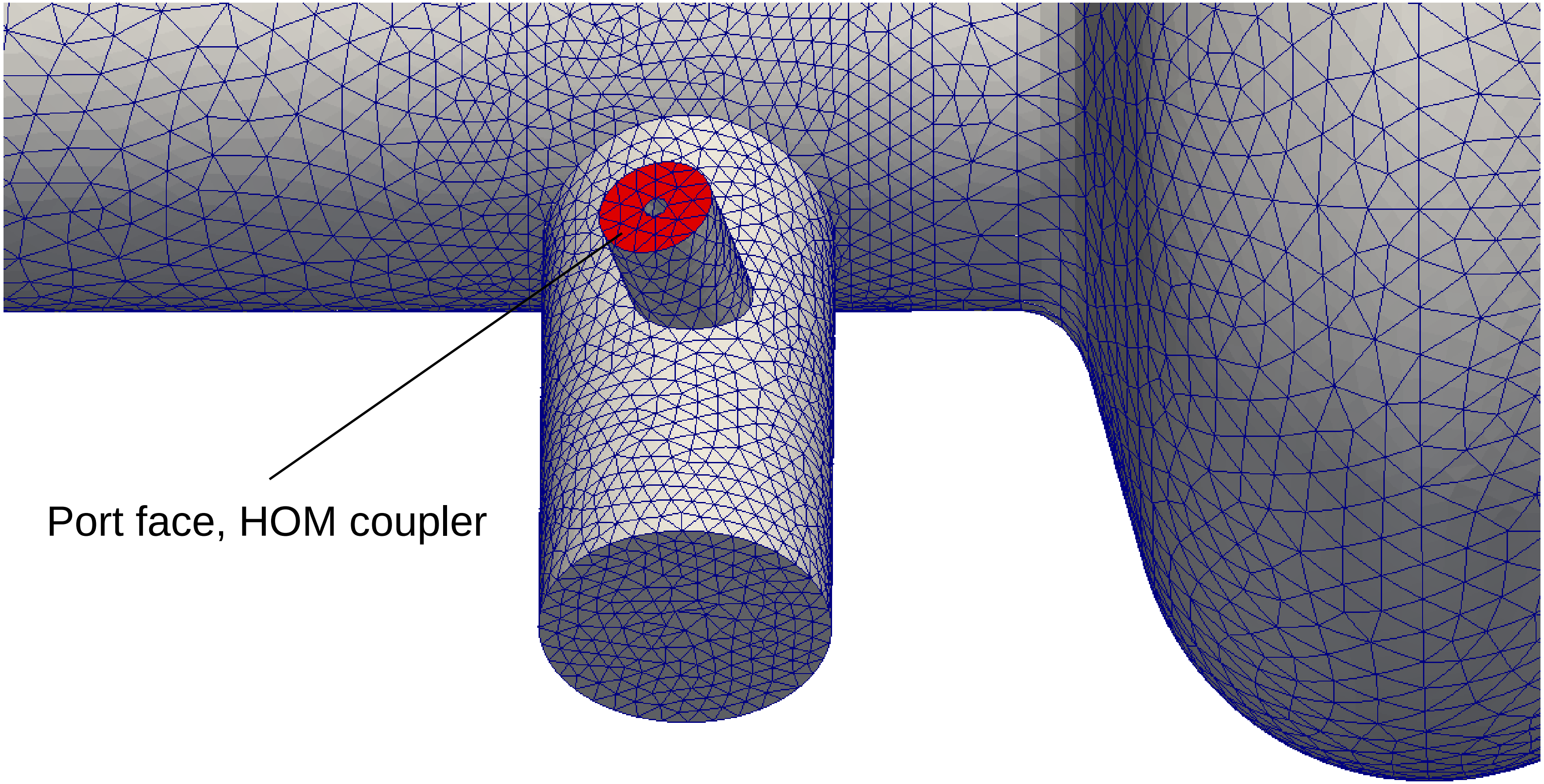
Computational Model

- Port boundary condition



Computational Model

- Port boundary condition



Computational Model

- Problem formulation
  - Local Ritz approach

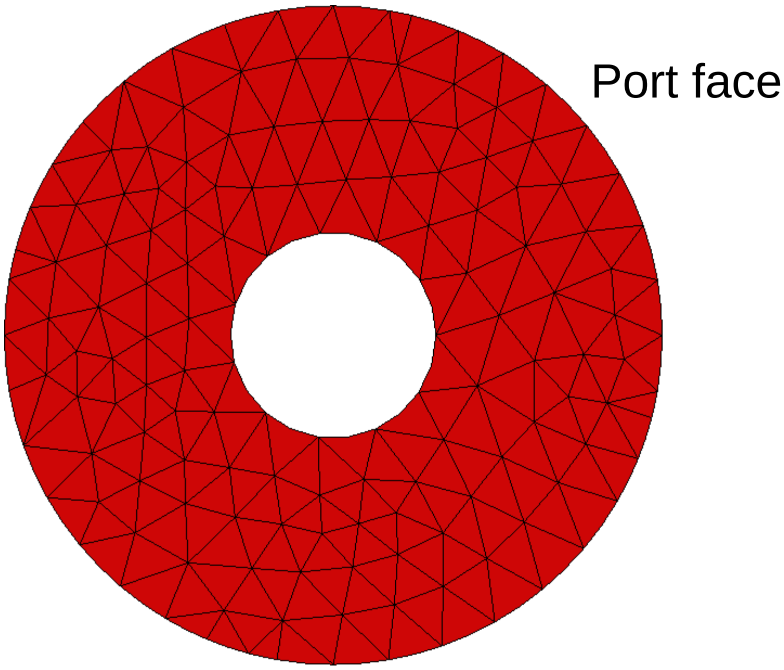
$$\vec{E} = \vec{E}(\vec{r}) = \sum_{i=1}^{n} \alpha_i \, \vec{w}_i(\vec{r})$$

$\vec{w}$ vectorial function

α_i scalar coefficient

i global index

n number of DOFs



Mixed 2-D vector and scalar basis

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

Computational Model

- Problem formulation
  - Local Ritz approach

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

+ boundary conditions

continuous eigenvalue problem, loss-free

Galerkin

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

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

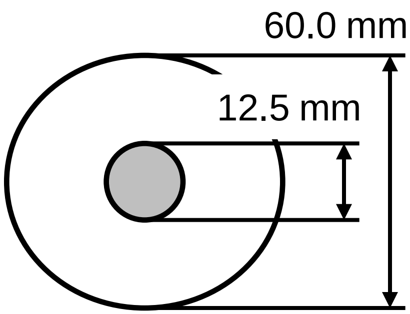
$$\vec{w}_i(x, y, z) = \vec{w}_i(x, y) \cdot e^{-ik_z z}$$

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

discrete eigenvalue problem

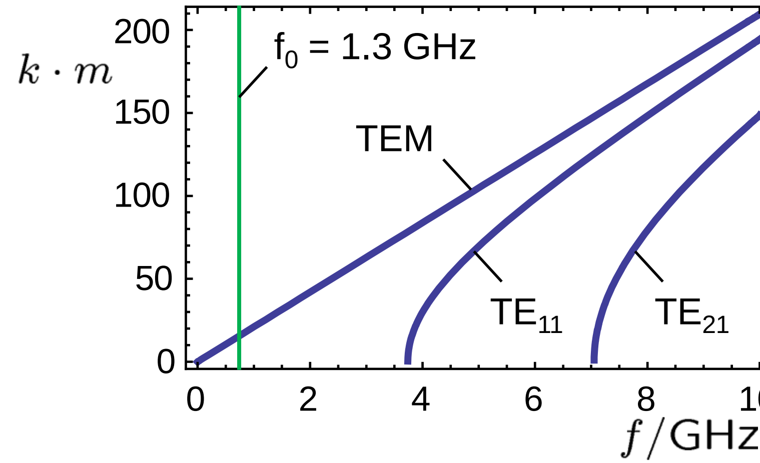
Computational Model

- Wave propagation in the applied coaxial lines
  - Main coupler

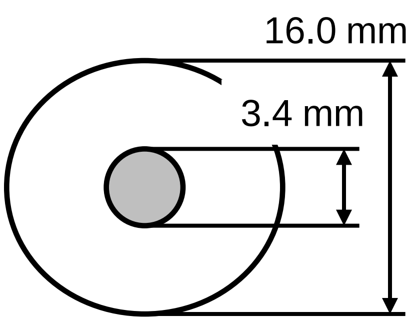


Dispersion relation

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



  - HOM coupler

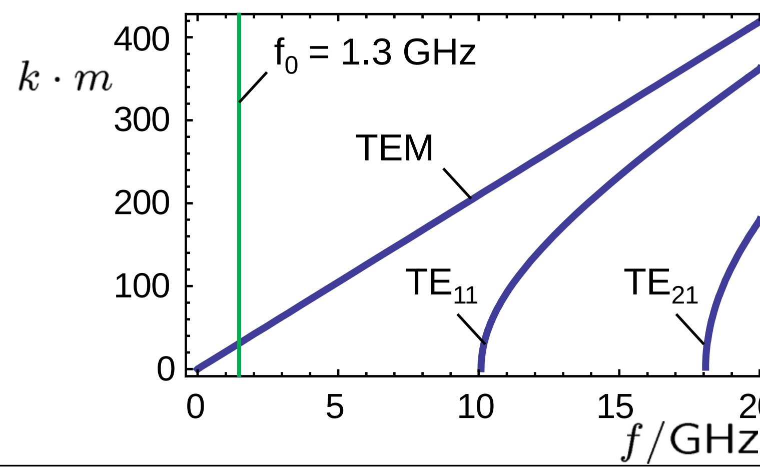


propagation

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

damping

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



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

$$A_{11,ij}^{2\mathrm{D}} = \iint_{A_{\mathrm{port}}} \frac{1}{\mu_r} \, \mathrm{curl}_t \, \vec{\omega}_{t,i}^{2\mathrm{D}} \cdot \mathrm{curl}_t \, \vec{\omega}_{t,j}^{2\mathrm{D}} \, \mathrm{d}\Omega - \omega_{\mathrm{port}}^2 \, \mu_0 \varepsilon_0 \iint_{A_{\mathrm{port}}} \varepsilon_r \, \vec{\omega}_{t,i}^{2\mathrm{D}} \cdot \vec{\omega}_{t,j}^{2\mathrm{D}} \, \mathrm{d}\Omega$$

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

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

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

$$B_{22,ij}^{2\mathrm{D}} = \iint_{A_{\mathrm{port}}} \frac{1}{\mu_r} \, \mathrm{grad}_t \, \omega_{z,i}^{2\mathrm{D}} \cdot \mathrm{grad}_t \, \omega_{z,j}^{2\mathrm{D}} \, \mathrm{d}\Omega - \omega_{\mathrm{port}}^2 \, \mu_0 \varepsilon_0 \iint_{A_{\mathrm{port}}} \varepsilon_r \, \omega_{z,i}^{2\mathrm{D}} \, \omega_{z,j}^{2\mathrm{D}} \, \mathrm{d}\Omega$$

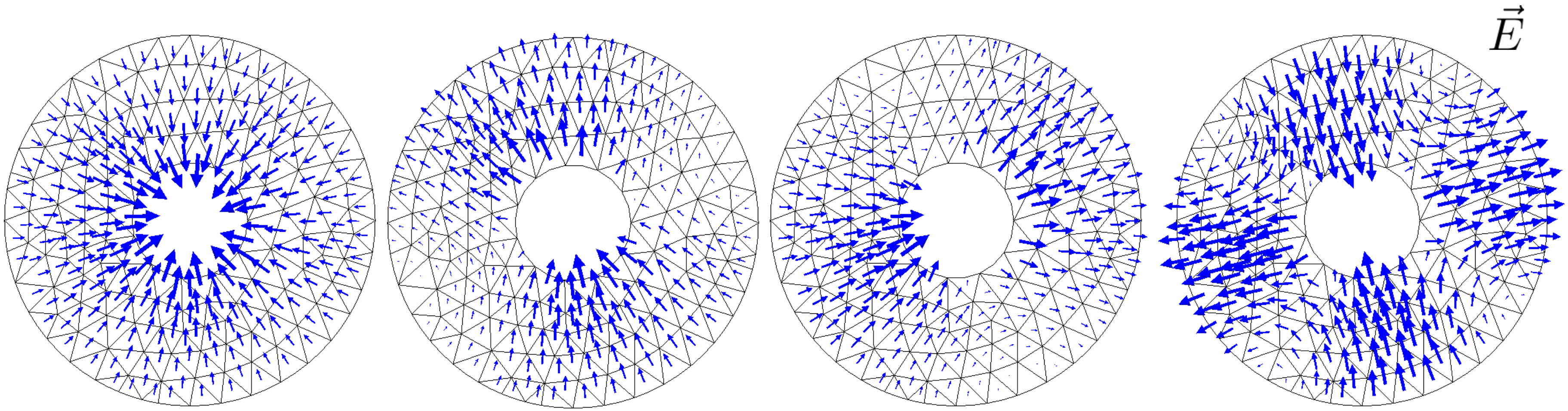
Computational Model

- 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 ...

Computational Model

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- Memory requirement for waveguide formulations
  - Ports with 2-D eigenmodes

$$A_{ij}|_{\text{port}} \propto \iint_{A_{\text{port}}} \frac{1}{\mu_r} \left(\vec{n} \times \operatorname{curl} \vec{E}_{(i)}\right) \cdot \vec{\omega}_j^{\,3\text{D}} \, \mathrm{d}A$$

Port mode series expansion

➡ Projection of the port fields on the set of 3-D basis functions results in a dense matrix block ✘

  - Impedance boundary condition

$$A_{ij}|_{\text{port}} \propto \iint_{A_{\text{port}}} \frac{1}{Z} (\vec{n} \times \vec{\omega}_i^{\,3\text{D}}) \cdot (\vec{n} \times \vec{\omega}_j^{\,3\text{D}}) \, \mathrm{d}A$$

➡ Same population pattern as PMC (natural boundary condition) ✔

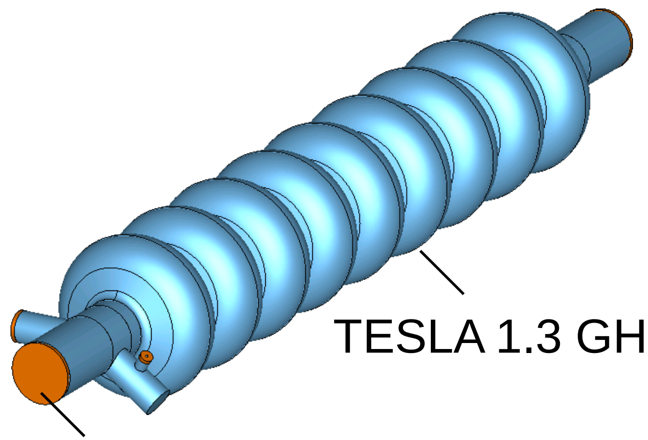
Computational Model

- Memory requirement for waveguide formulations
  - Example 1: 1.119.219 tetrahedrons

$$\frac{\sum \mathrm{NNZ}_{\mathrm{ports}}}{\mathrm{NNZ}_{\mathrm{volume}}} = \frac{4.817.504}{295.093.656} \approx 1,6\ \%$$

  - Example 2: 1.218.296 tetrahedrons

$$\frac{\sum \mathrm{NNZ}_{\mathrm{ports}}}{\mathrm{NNZ}_{\mathrm{volume}}} = \frac{87.845.785}{321.530.896} \approx 27,3\ \%$$



  - General rule:

$$\frac{\mathrm{NNZ}_{\mathrm{port}}}{\mathrm{NNZ}_{\mathrm{volume}}} \propto \frac{1}{b\,h}$$

NNZ = number of non-zero elements

b = mean bandwidth of sparse system matrix
h = mean grid step size

Computational Model

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- Waveguide ports implementation options
  - Standard approach:
    Incorporate dense matrix blocks into sparse system matrix

$$A_{ij}|_{\mathrm{port}} \propto \iint_{A_{\mathrm{port}}} \frac{1}{\mu_r} \left(\vec{n} \times \mathrm{curl}\, \vec{E}_{(i)}\right) \cdot \vec{\omega}_j^{\mathrm{3D}}\, \mathrm{d}A$$

Port mode series expansion

  - Memory-efficient approach:
    Utilize that system matrix is dense but of low rank

$$A_{ij}|_{\mathrm{port}} \propto \sum_{\mathrm{ports}} \sum_{\mathrm{modes}} (\vec{v}\, \vec{v}^{\mathrm{T}})|_{ij}$$

Dyadic product of modified port mode vectors

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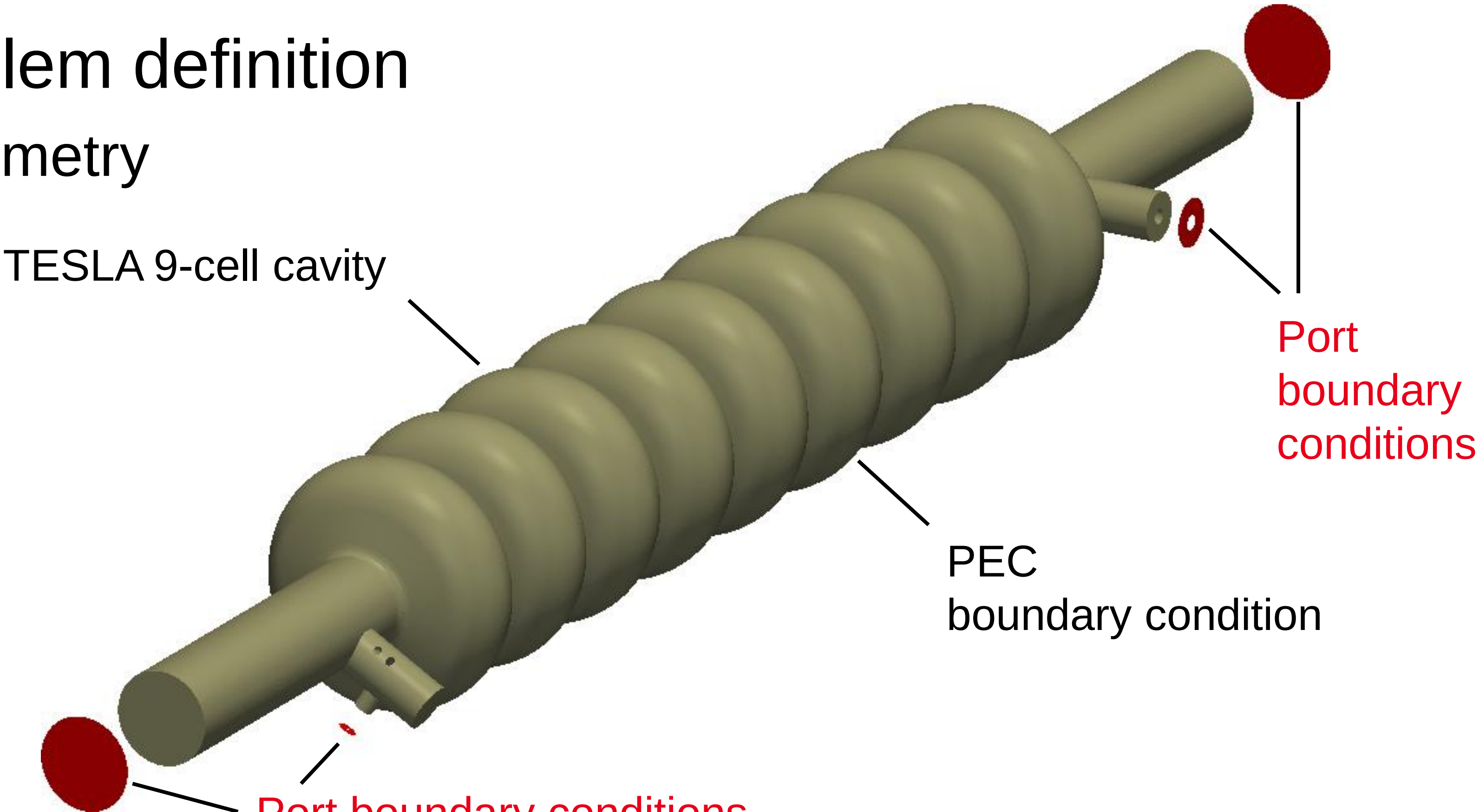
Numerical Examples

- Problem definition
  - Geometry

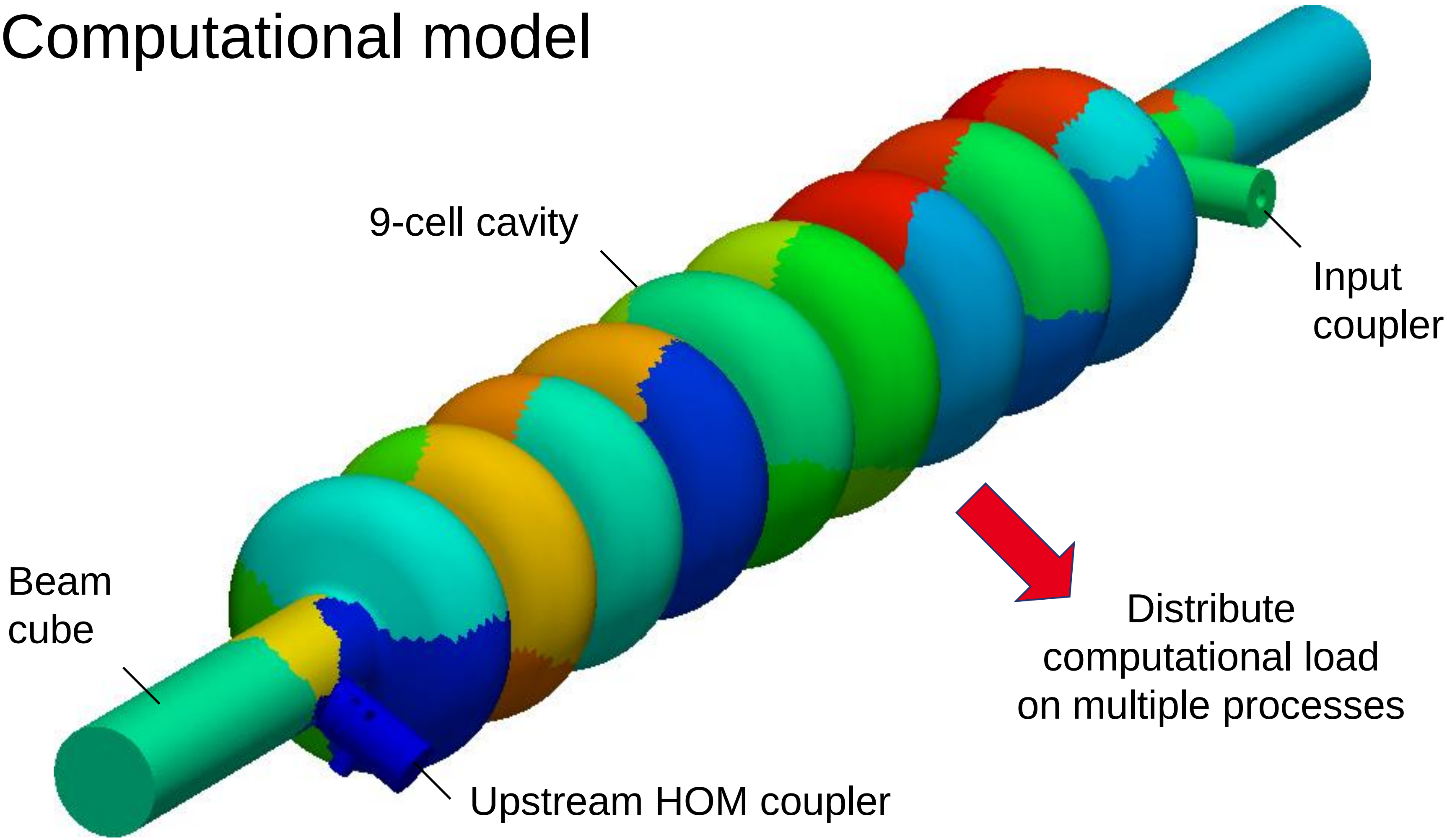


  - Task

    Search for the field distribution, resonance frequency and quality factor

Numerical Examples

- Computational model



Distribute computational load on multiple processes

Numerical Examples

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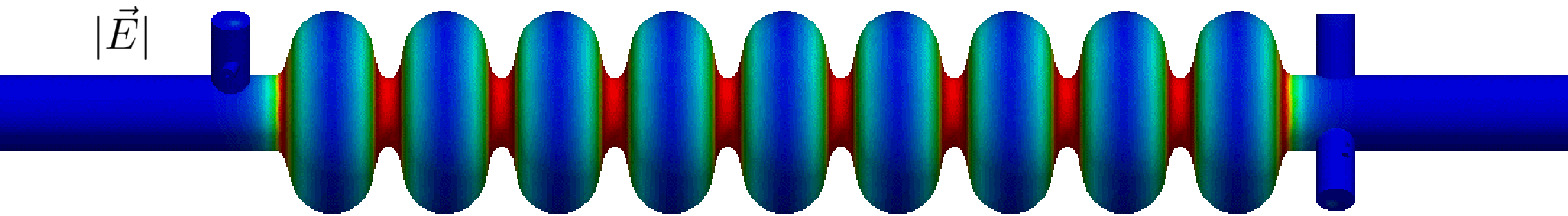
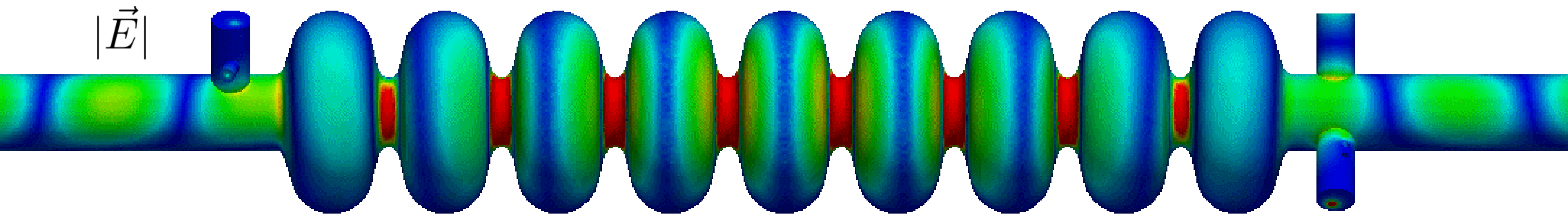
- Simulation results
  - Accelerating mode (monopole #9)

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



  - Higher-order mode (dipole #37)

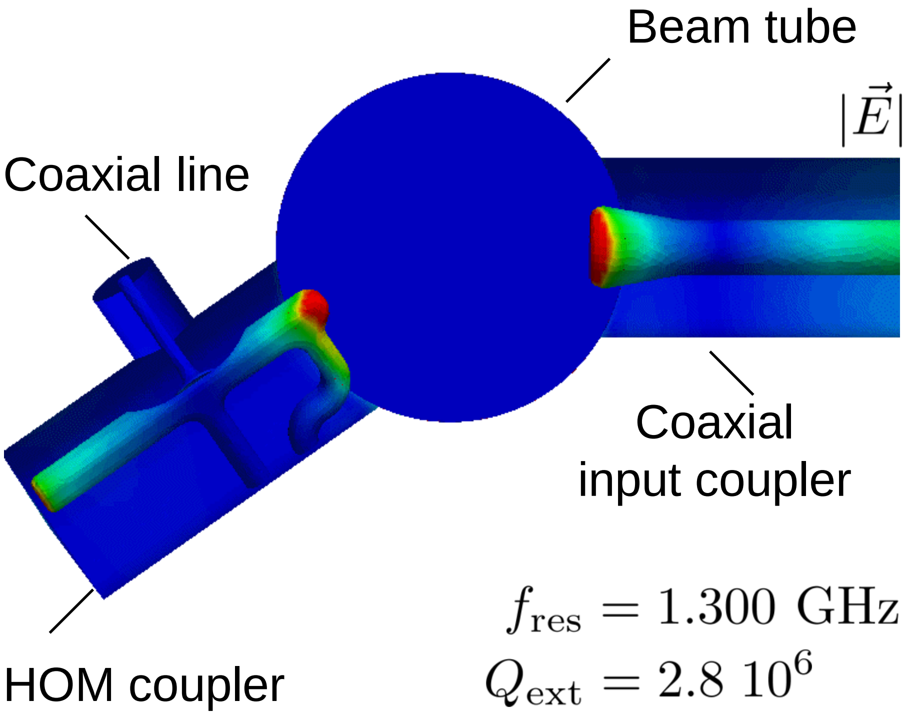
$$f_{\mathrm{res}} = 2.476\ \mathrm{GHz}$$
$$Q_{\mathrm{ext}} = 1.8\ 10^{3}$$



Numerical Examples

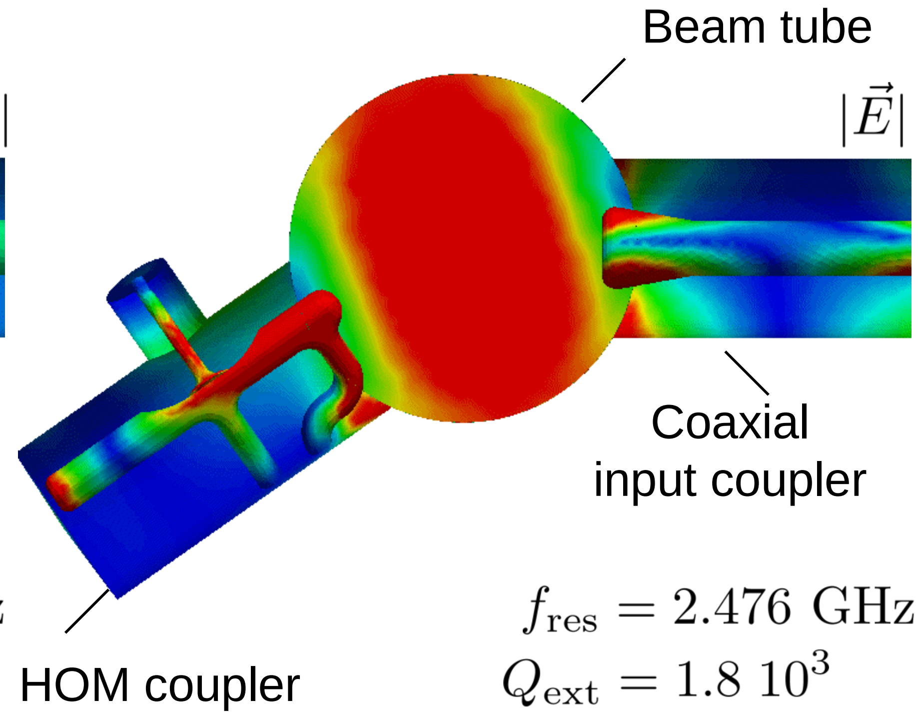
- Simulation results

Accelerating mode (monopole #9)



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

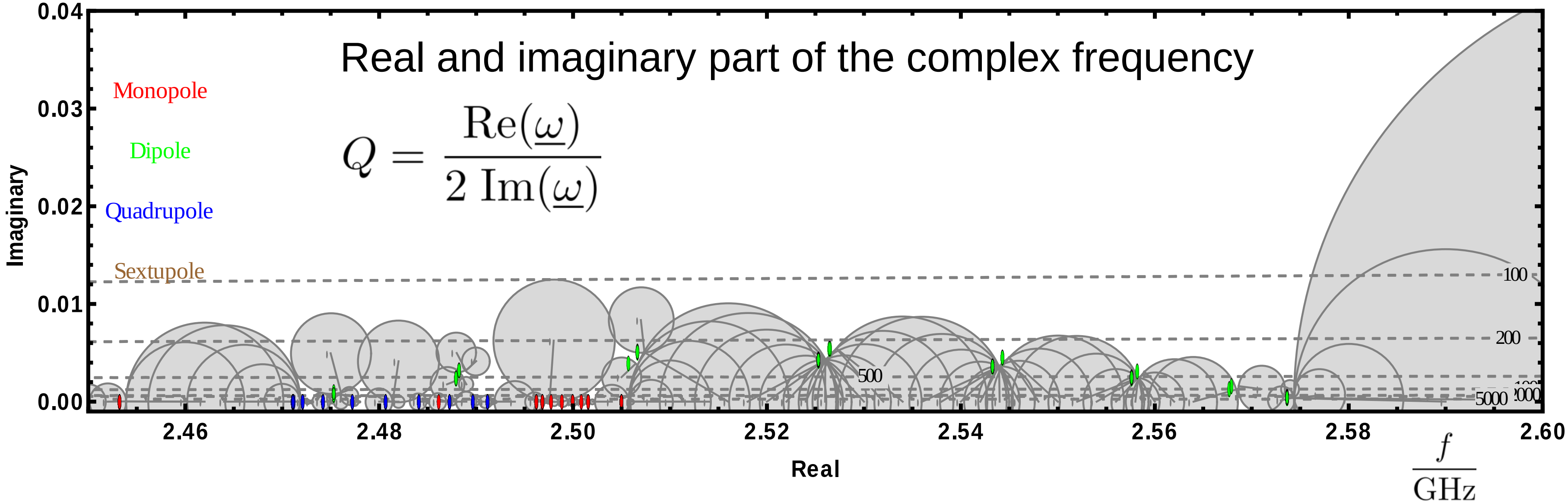
Higher-order mode (dipole #37)



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

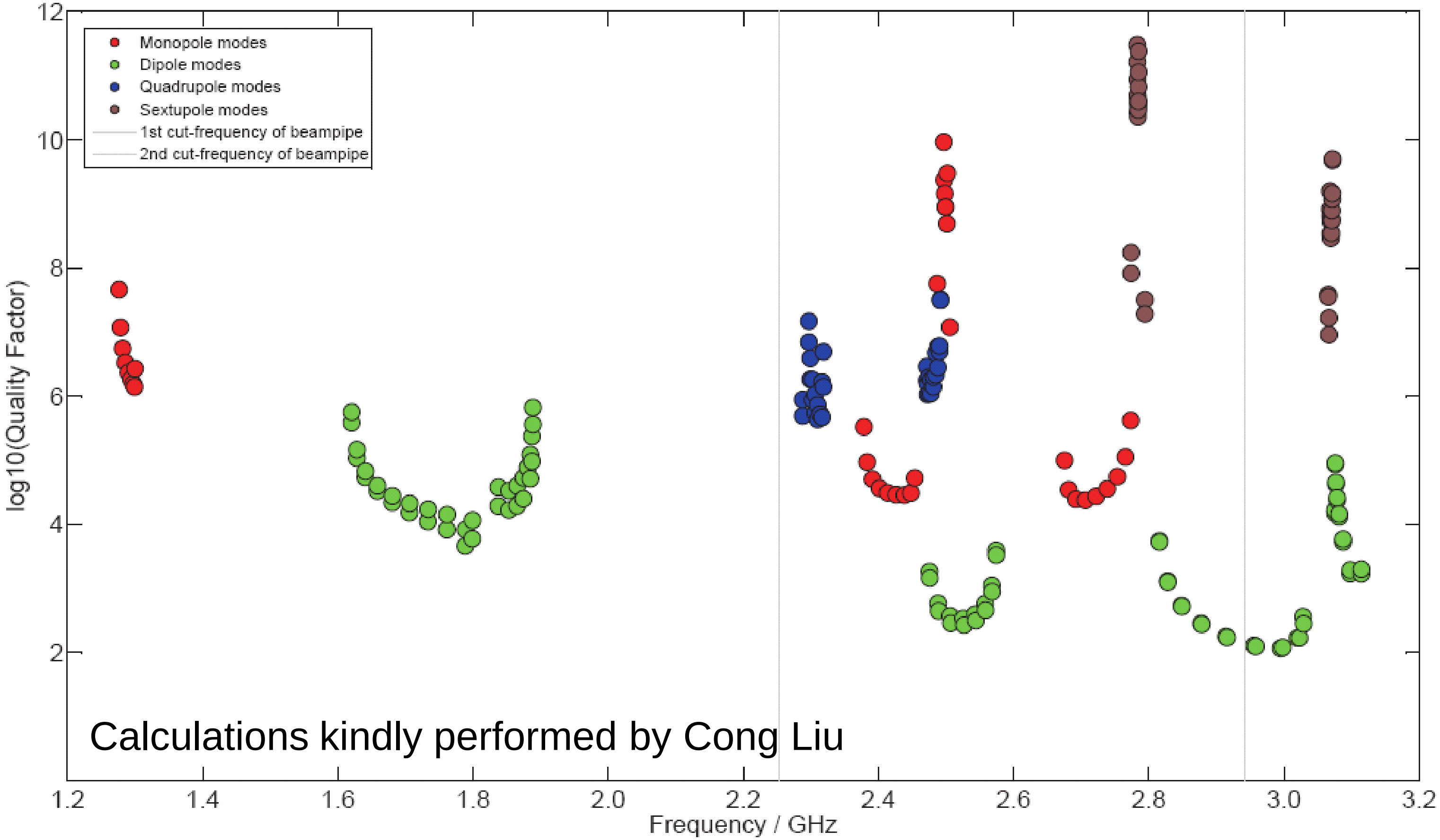
Numerical Examples

- Controlling the Jacobi-Davidson eigenvalue solver
  - Evaluation in the complex frequency plane
  - Select best suited eigenvalues in circular region around user-specified complex target



Numerical Examples

- Quality factor versus frequency



Numerical Examples

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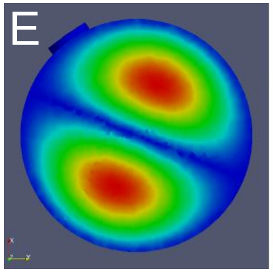
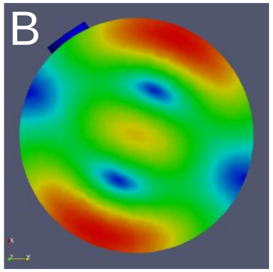
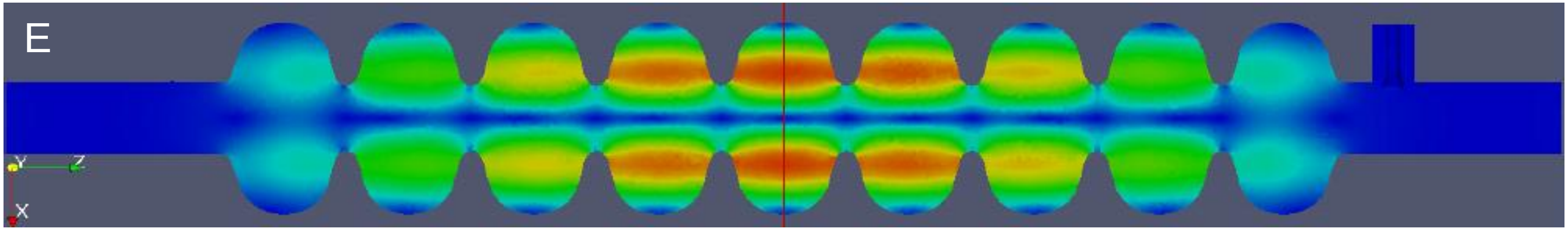
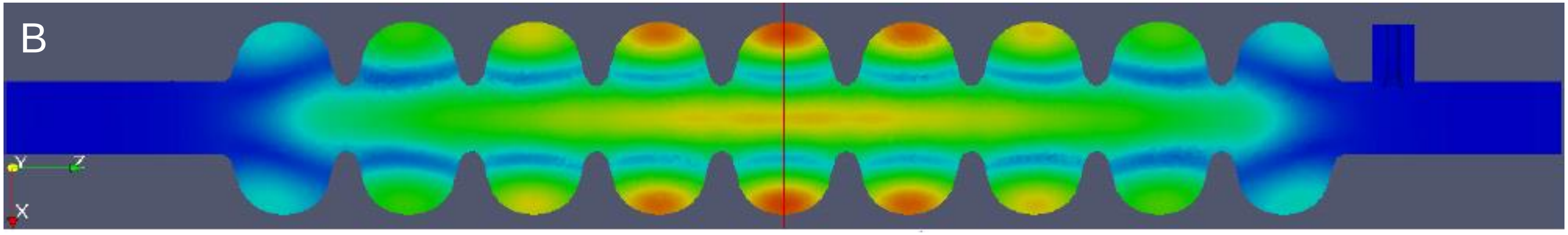
- Field distribution of selected mode
  - First/second dipole passband (mode 17)

Resonance frequency	fres	1.8887 GHz
Quality factor	Q	6.6E+05
Transverse shunt impedance	R/Q	5.10E-02 Ω/m^2
Impedance	R	3.4E+04 Ω









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Numerical Examples (preliminary)

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- 3.9 GHz structure (3rd harmonic cavity)
  - String of four cavities

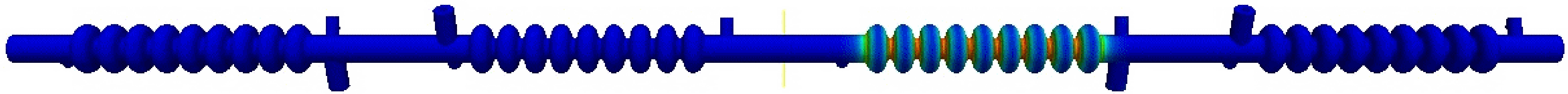
Bellows omitted for the time being

4 main coupler, 8 HOM coupler and 2 beam pipes = 14 ports

- Field distribution for selected modes

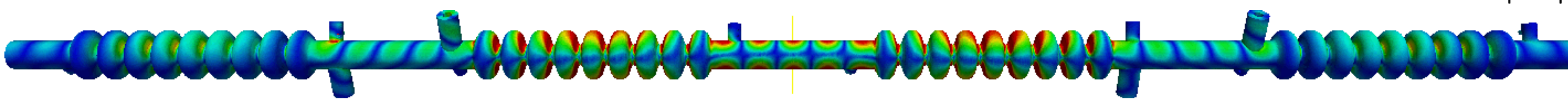
1.040.212 tetrahedrons
6.349.532 complex DOF

$|\vec{E}|$



$f_{\mathrm{res}} = 1.900\ \mathrm{GHz} \qquad Q_{\mathrm{ext}} = 1.0\ 10^{6}$

$|\vec{E}|$



$f_{\mathrm{res}} = 5.351\ \mathrm{GHz} \qquad Q_{\mathrm{ext}} = 2.8\ 10^{3}$

Summary / Outlook

- 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
  - Memory-efficient implementation to evaluate the port fields now available

- Outlook:

  - Application to 1.3 GHz and 3.9 GHz structure and strings