

# 3-dimensional Eigenmodal Analysis of Electromagnetic Structures

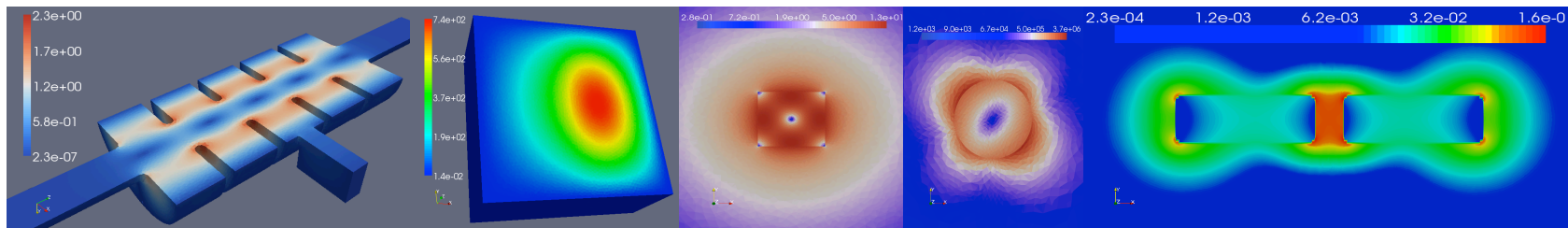
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Swiss Federal Institute of Technology Zurich



# Outline

- Introduction of Femaxx
- Resonant cavities
  - Jacobi-Davidson for linear eigenvalue problems (JDQZ)
- Microwave antennas
  - Jacobi-Davidson for quadratic /nonlinear eigenvalue problems(NLJD)
- Summary

# Introduction of Femaxx

- A large scale software project.
- Developed at ETH Zurich and PSI.
- Simulation tool for electromagnetic structures.
- Parallelized for distributed memory computers.
- Solves electric field vector wave equation.
- Finite element method (FEM).
- 3-dimensional, unstructured tetrahedral mesh.
- Model arbitrary geometry or material property.
- Linear, quadratic and nonlinear eigensolvers.
- Open source software,

<http://amas.web.psi.ch/docs/femaxx-doc/html/> .



Swiss Federal Institute of Technology (ETH Zurich)



Paul Scherrer Institute (PSI)

# Lossless Resonant Cavities

- Time-harmonic electric field *curl-curl* equation

$$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}(\mathbf{x})) - k_0^2 \varepsilon_r \mathbf{E}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Omega.$$

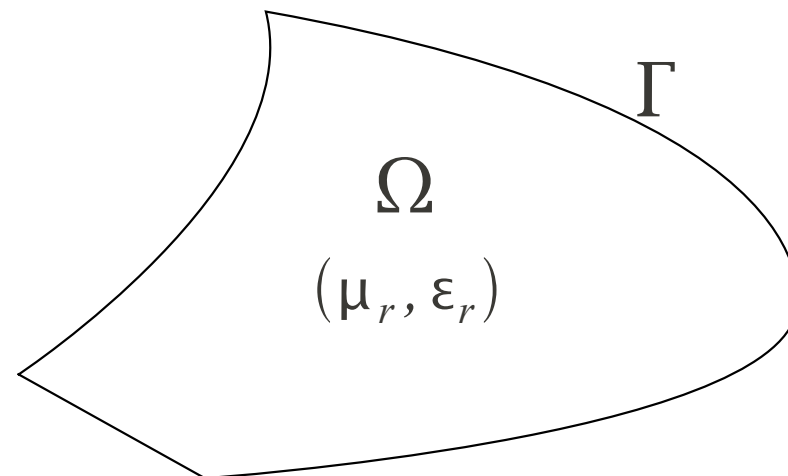
- Divergence free condition

$$\nabla \cdot (\varepsilon_r \mathbf{E}(\mathbf{x})) = \mathbf{0}, \quad \mathbf{x} \in \Omega.$$

- Perfect electric conductor (PEC) boundary condition

$$\mathbf{n} \times \mathbf{E}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Gamma.$$

$k_0$ : wavenumber in free space  
 $\mu_r$ : magnetic relative permeability  
 $\varepsilon_r$ : electric relative permittivity  
 $\Omega$ : computational domain  
 $\Gamma$ : boundary conductor wall



# Lossless Resonant Cavities

- FEM yields a *real-valued linear* eigenvalue problem

$$A \mathbf{x} = \lambda M \mathbf{x}, \quad C^T \mathbf{x} = \mathbf{0}, \quad \lambda = k_0^2.$$

$A$  is positive semi-definite:  $a_{ij} = \int_{\Omega} \mu_r^{-1} (\nabla \times \mathbf{N}_i) \cdot (\nabla \times \mathbf{N}_j) d\mathbf{x}$ .

$M$  is positive definite:  $m_{ij} = \int_{\Omega} \varepsilon_r \mathbf{N}_i \cdot \mathbf{N}_j d\mathbf{x}$ .

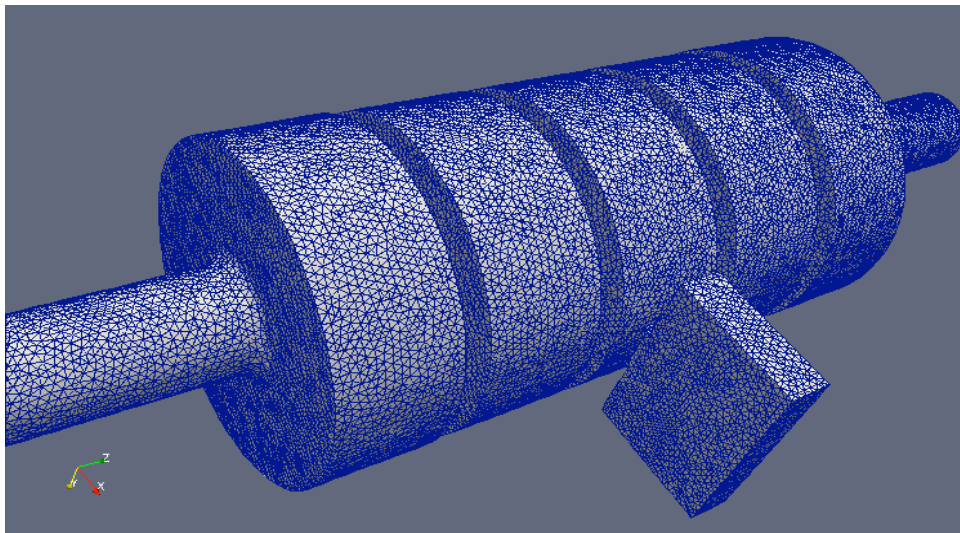
$C$  is a rectangular matrix:  $c_{il} = \int_{\Omega} \varepsilon_r \mathbf{N}_i \cdot \nabla N_l d\mathbf{x}, C = MY$ .

$\mathbf{N}_i$  is Nédélec basis function,  $N_l$  is Lagrange basis function,

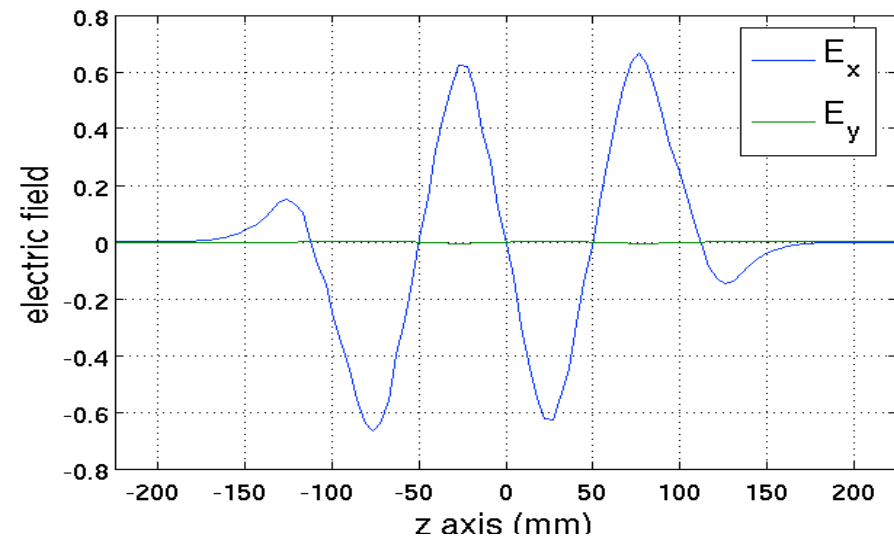
$Y$  is a rectangular matrix of  $y_{jl}$ :  $\nabla N_l = \sum_{j=1}^m y_{jl} \mathbf{N}_j$ .

- JDSYM eigensolver: Jacobi-Davidson method for real-valued symmetric eigenvalue problem.

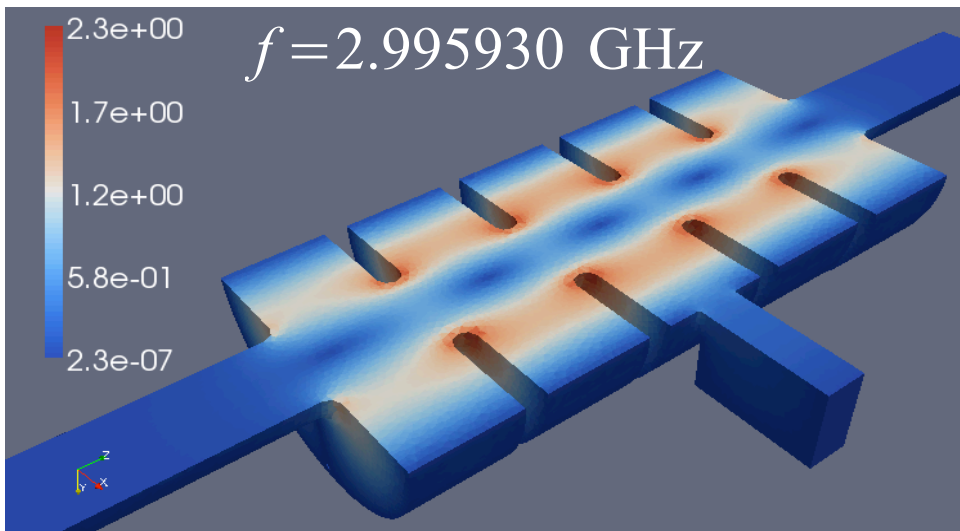
# 5-cells Transverse Deflecting Cavity



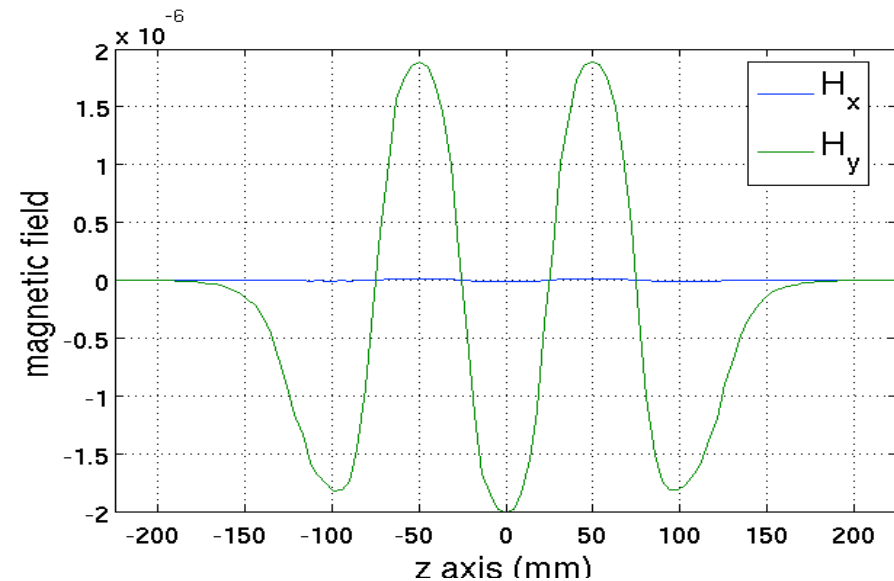
(a) mesh containing 872'261 elements.



(c)  $E_x$  and  $E_y$  over z-axis.



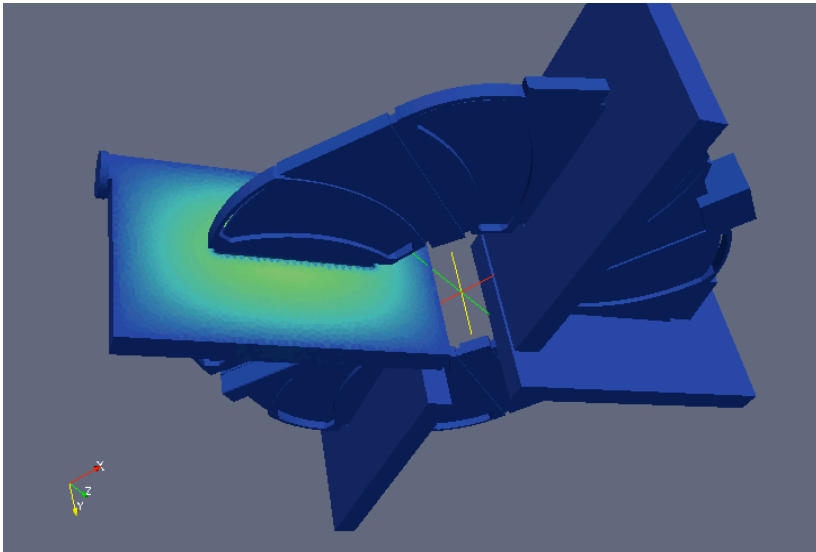
(b) electric field distribution of TM110 mode.



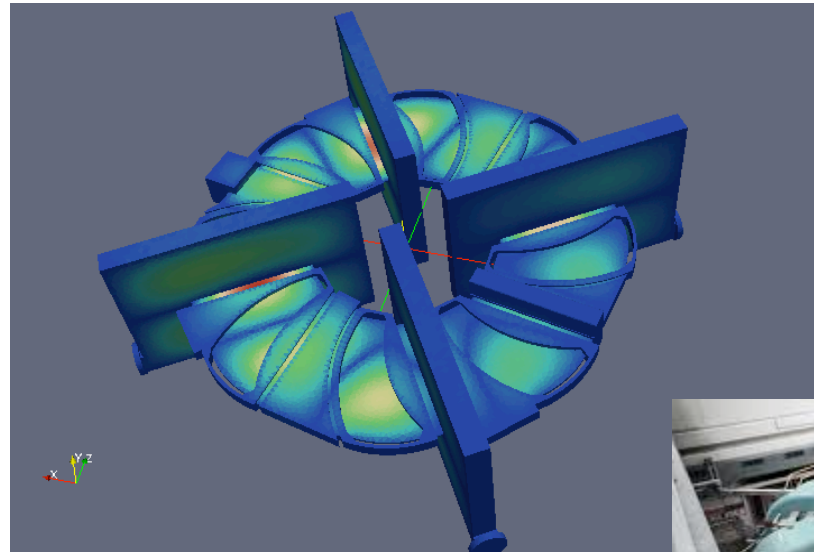
(d)  $H_x$  and  $H_y$  over z-axis.

# Cyclotron at PSI

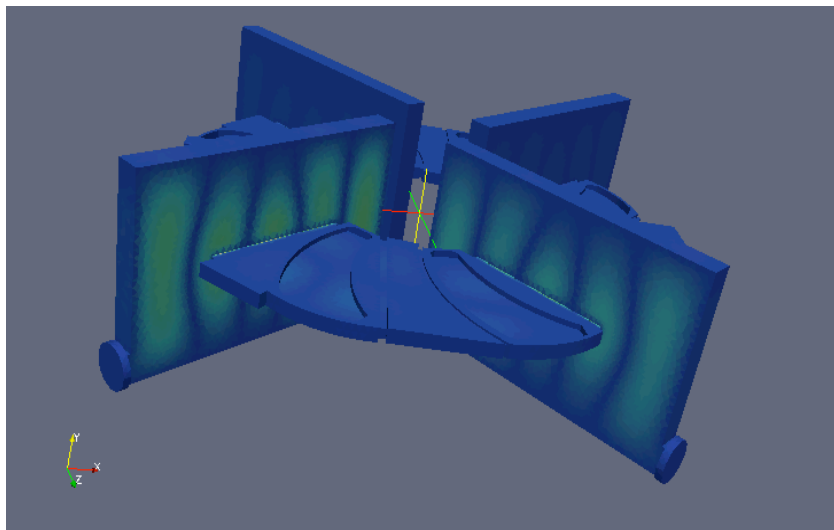
Tetrahedral mesh created from original geometry obtained as STEP file from CAD.



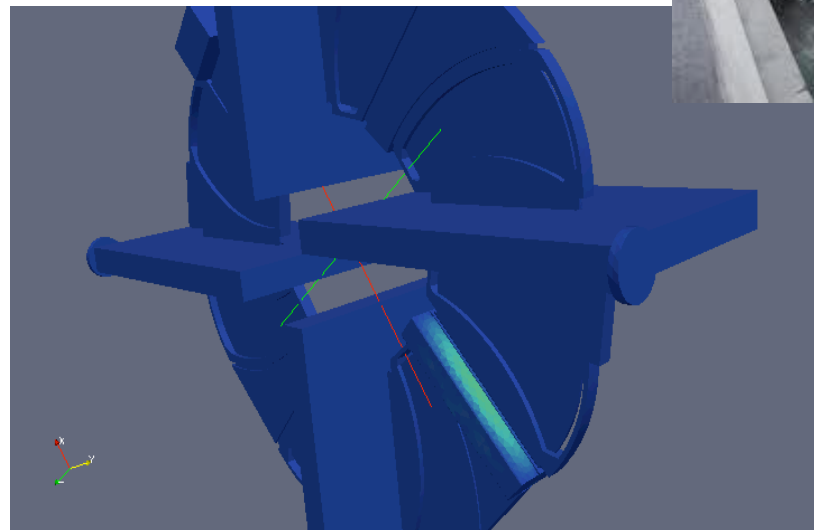
(a) dominant mode: 51.48 MHz



(b) 31st mode: 101.04 MHz

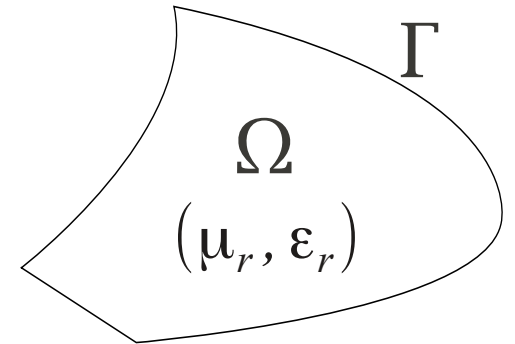


(c) 86th mode: 149.58 MHz



(d) 87th mode: 151.51 MHz

# Dielectric Lossy Material



- Complex-valued relative permittivity

$$\epsilon_r = \text{Re}(\epsilon_r) - i \text{Im}(\epsilon_r).$$

- Perfect electric conductor boundary condition

$$\mathbf{n} \times \mathbf{E}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Gamma.$$

- FEM yields constrained eigenvalue problem

$$\mathbf{A} \mathbf{x} = \lambda \mathbf{M} \mathbf{x},$$

$$\mathbf{C}^T \mathbf{x} = \mathbf{0}.$$

- Entries of M and C depend on  $\epsilon_r$

$$m_{ij} = \int_{\Omega} \epsilon_r \mathbf{N}_i \cdot \mathbf{N}_j d\mathbf{x}, \quad c_{il} = \int_{\Omega} \epsilon_r \mathbf{N}_i \cdot \nabla N_l d\mathbf{x}.$$

$\mathbf{A}$  is *real* symmetric;  $\mathbf{M}$  is *complex* symmetric;  
 $\mathbf{C}$  is a *complex* rectangular matrix.



# Jacobi-Davidson QZ Eigensolver

JDQZ solves generalized *non-Hermitian* eigenvalue problem.

- 1: choose start vector  $\mathbf{x}_0$ ;  $it = 0$ .
- 2: when  $it \leq it_{max}$  do
- 3:     Solve projected eigenproblem with QZ decomposition.
- 4:     Compute an eigenpair closest to target:  $\tau$ .
- 5:     if the associated residual is small enough
- 6:         Accept this eigenpair; deflate search space.
- 7:     end if
- 8:     Restart if necessary.
- 9:     Find an approximate solution  $\mathbf{t}$  of correction equation.
- 10:     Project  $\mathbf{t}$  in null space of  $C^T$ .
- 11:     Orthonormalize  $\mathbf{t}$  against previous search vectors.
- 12:     Expand search space with  $\mathbf{t}$ .  $it++$ .
- 13: end

Krylov solver

Divergence-free condition

Modified Gram-Schmidt

# Implementation of Femaxx

- C++ : object-oriented design pattern
- Gmsh : mesh generator
- ParMETIS : mesh partitioner
- Paraview : visualization of electromagnetic field
- Trilinos : parallel objects

# Trilinos in Femaxx

- Epetra
  - parallel multivectors
  - parallel sparse matrices
  - distribution map
  - uses MPI functionality
- AztecOO
  - Iterative solvers for correction equation
- Ifpack
  - Block Jacobi preconditioners

# Ifpack

- Block Jacobi preconditioner

- Extract diagonal blocks by LU and ILU.

$$\begin{bmatrix} \boxed{A_{11}} & & \\ & \boxed{A_{22}} & \\ & & \boxed{A_{33}} \end{bmatrix} \leftarrow \text{solve each block by LU or ILU}$$

- Ifpack doesn't support Complex arithmetic.

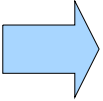
Complex matrix,  $Z = X + iY$ , double-sized =  $\begin{bmatrix} X & Y \\ -Y & X \end{bmatrix}$ .

$$\begin{bmatrix} \boxed{X} & | & Y \\ \hline -Y & | & \boxed{X} \end{bmatrix} \leftarrow \text{Ifpack extracts only real part of } C .$$

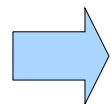
# Construct double-sized real valued matrix

- Alternative approach :

$$Z = X + iY, \quad z_{ij} = x_{ij} + iy_{ij}, \quad Z = \begin{bmatrix} z_{11} & 0 & z_{13} \\ 0 & z_{22} & z_{23} \\ z_{31} & 0 & z_{33} \end{bmatrix}.$$

 double-sized =
 
$$\begin{bmatrix} x_{11} & y_{11} & 0 & 0 & x_{13} & y_{13} \\ -y_{11} & x_{11} & 0 & 0 & -y_{13} & x_{13} \\ 0 & 0 & x_{22} & y_{22} & x_{23} & y_{23} \\ 0 & 0 & -y_{22} & x_{22} & -y_{23} & x_{23} \\ x_{31} & y_{31} & 0 & 0 & x_{33} & y_{33} \\ -y_{31} & x_{31} & 0 & 0 & -y_{33} & x_{33} \end{bmatrix}.$$

- Ifpack can extract block diagonal elements correctly.



Reduction of 5% iterations in JDQZ

# Ifpack

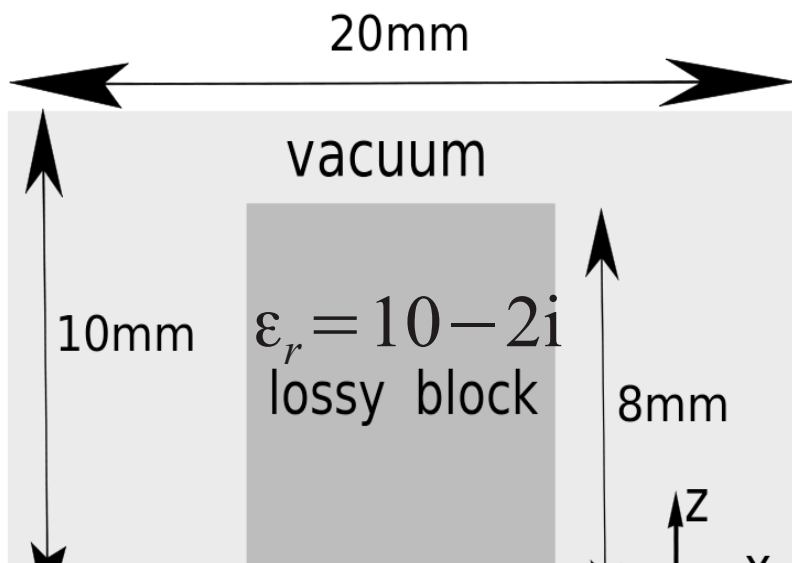
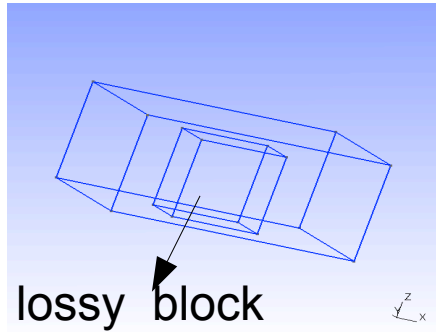
- Construct preconditioners for Krylov solver
  - Block Jacobi AdditiveSchwarz with LU factorization
    - overlap = 0;
    - partitioner : linear;
    - LU solver : Amesos\_Klu;
  - Block Jacobi AdditiveSchwarz with ILU factorization
    - overlap = 0;
    - partitioner : linear
    - ILU solver : Ifpack\_ILU

Ref: Marzio Sala, Michael Heroux, *Robust Algebraic Preconditioners using IFPACK 3.0*, Sandia Report, SAND2005-0662, 2005.

# Example of dielectric lossy material

- **#Tetrahedra : 141'149**
- **Processors : 32**
- **Quadratic element order**
- **Number of eigenvalues : 6**
- **Tolerance : 1.0e-6**
- **Target : [1.0]**
- **Krylov solvers : Bi-CGStab**
- **Preconditioners : Diagonal, Block Jacobi-LU/ILU**
- **Max iteration of correction equation : 50**
- **Jmin : 5, Jmax : 10**

# Lossy Dielectric Block



$$\text{Stored energy: } U = \frac{\epsilon_0}{2} \int_{\Omega} \text{Re}(\epsilon_r) |\mathbf{E}|^2 d\mathbf{x}.$$

$$\text{Dissipated energy: } U_d = \frac{\epsilon_0}{2} \int_{\Omega} \text{Im}(\epsilon_r) |\mathbf{E}|^2 d\mathbf{x}.$$

$$\text{Resonant frequency: } f = \frac{\omega}{2\pi}.$$

$$\text{Quality factor: } Q = \frac{\text{Re}(\lambda)}{2 \times \text{Im}(\lambda)}.$$

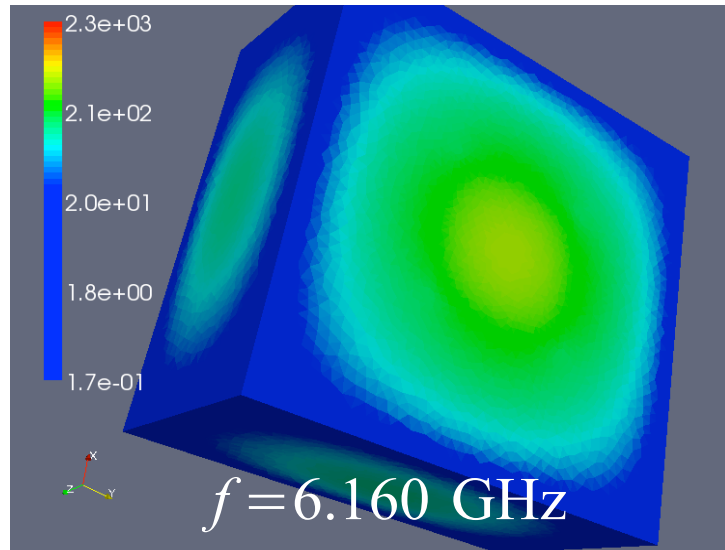
Table : Numerical results of the lossy dielectric block cavity

mode	$f$ (GHz)	Q
1	6.171	11.2
2 3	9.095	5.82
4 5	11.41	7.48
6	11.42	5.49

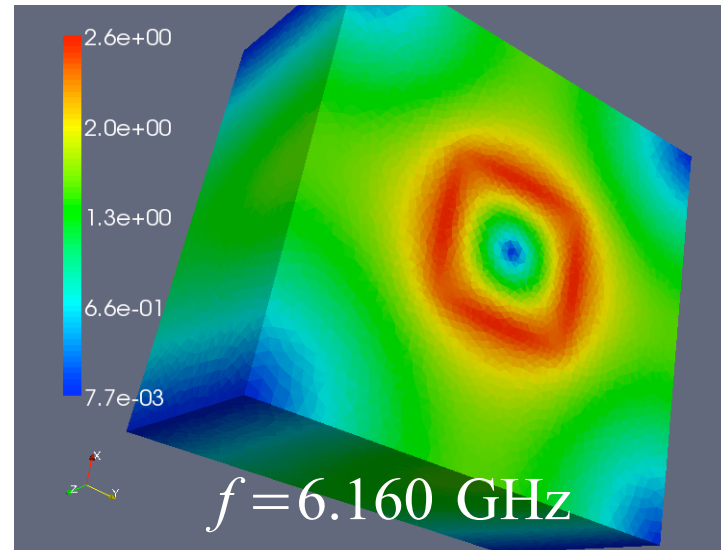
Ref: S.J. Cooke and B. Levush. In 17th Particle Accelerator Conference, pages 2431–2433, May 1997.



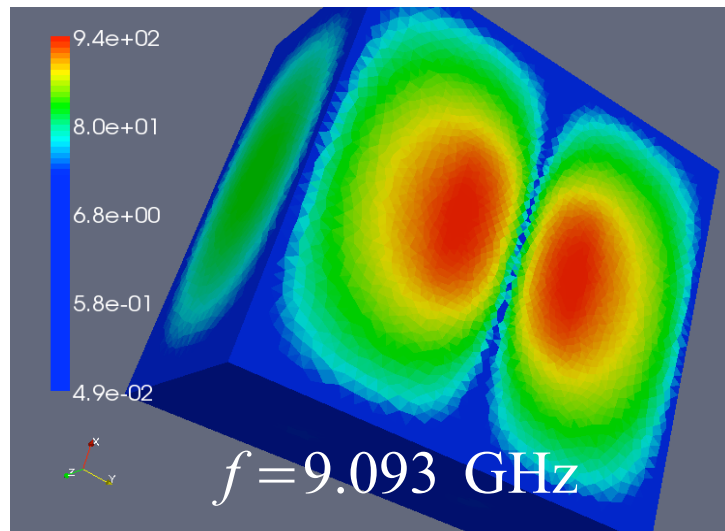
# Lossy Dielectric Block



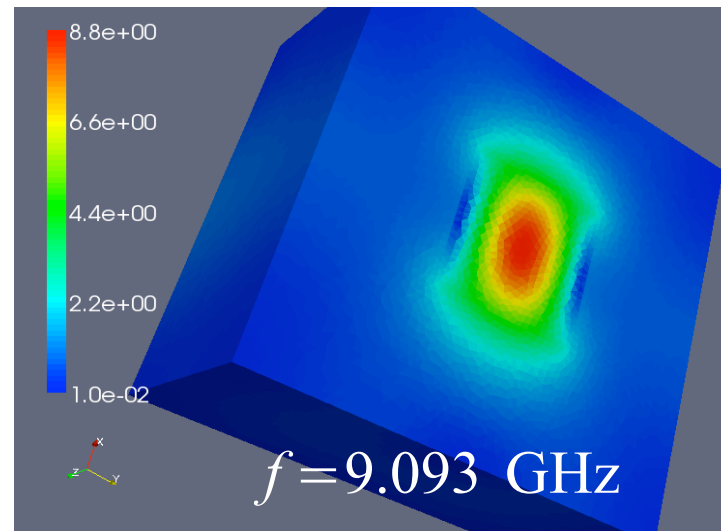
Mode 1: electric field



Mode 1: magnetic field



Mode 2: electric field



Mode 2: magnetic field

# Ohmically Lossy Material

- Considering conduction current density, then time-harmonic electric field vector wave equation is

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}(\mathbf{x})) + i k_0 \sigma Z_0 \mathbf{E} - k_0^2 \varepsilon_r \mathbf{E}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Omega.$$

$\sigma$  is ohmic conductivity.

$Z_0 \approx 377 \Omega$  is characteristic impedance in free space.

- FEM yields a constrained *quadratic* eigenproblem

$$T(\lambda) \mathbf{x} := A \mathbf{x} + \lambda R \mathbf{x} - \lambda^2 M \mathbf{x} = \mathbf{0}, \quad C^T \mathbf{x} = \mathbf{0}.$$

Entry of  $R$ :  $r_{ij} = i \int_{\Omega} \sigma Z_0 \mathbf{N}_i \cdot \mathbf{N}_j d\mathbf{x}.$

# Ohmically Lossy Material

- Linearize the quadratic eigenvalue problem

$$\begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \lambda \begin{bmatrix} -R & M \\ I & 0 \end{bmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix},$$

$$\begin{bmatrix} C & 0 \\ 0 & C \end{bmatrix}^T \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \mathbf{0}.$$



Identity matrix


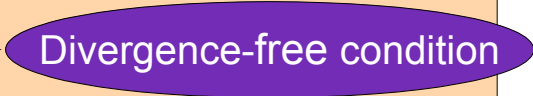

Then it is solved by JDQZ eigensolver.

- Dissipated energy now given as:

$$U_d = \frac{\epsilon_0}{2} \int_{\Omega} \text{Im}(\epsilon_r) |\mathbf{E}|^2 d\mathbf{x} \longrightarrow U_d = \frac{1}{2} \int_{\Omega} \sigma |\mathbf{E}|^2 d\mathbf{x}$$

# Nonlinear Jacobi Davidson method (NLJD)

- Algorithm :

- 1:  $T(\lambda)\mathbf{x}=0$ , choose start vector  $\mathbf{x}_0$ ;  $it=0$ .
- 2: when  $it \leq it_{max}$  do
- 3: Solve projected nonlinear eigenproblem,  $V_k^T T(\lambda_k) V_k \mathbf{y} = 0$ .
- 4: Compute a Ritz pair closest to target.
- 5: if the associated residual is small enough
- 6: Return the Ritz pair.
- 7: end if
- 8: Find an approximate solution  $\mathbf{t}$  of correction equation. 
- 9: Project  $\mathbf{t}$  in null space of  $C^T$ . 
- 10: Orthonormalize  $\mathbf{t}$  against previous search vectors. 
- 11: Expand search space with  $\mathbf{t}$ .  $it++$ .
- 12: end

# AztecOO

- Correction equation in NLJD:

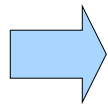
$$\left( \begin{array}{c} I - \frac{p_k u_k^H}{u_k^H p_k} \\ u_k^H p_k \end{array} \right) T(\lambda_k) \left( \begin{array}{c} I - \frac{u_k u_k^H}{u_k^H u_k} \\ u_k^H u_k \end{array} \right) t_k = -r_k, \quad t \perp u_k,$$

where  $\lambda_k$ : approximation of eigenvalue,  $u_k$ : Ritz vector,  $p_k = T'(\lambda_k)u_k$

- Solve by AztecOO

- Epetra\_Operator to calculate projection
- Ifpack preconditioner:  $K \approx T(\tau)$ , tau : target

$$\tilde{T} = \left( \begin{array}{c} I - \frac{p_k u_k^H}{u_k^H p_k} \\ u_k^H p_k \end{array} \right) T(\tau) \left( \begin{array}{c} I - \frac{u_k u_k^H}{u_k^H u_k} \\ u_k^H u_k \end{array} \right), \quad \tilde{K} = \left( \begin{array}{c} I - \frac{p_k u_k^H}{u_k^H p_k} \\ u_k^H p_k \end{array} \right) K \left( \begin{array}{c} I - \frac{u_k u_k^H}{u_k^H u_k} \\ u_k^H u_k \end{array} \right),$$



$$\underline{\tilde{K}^{-1} \tilde{T} t_k = -\tilde{K}^{-1} r_k, \quad t \perp u_k,}$$

# Example of half-filled rectangle cavity

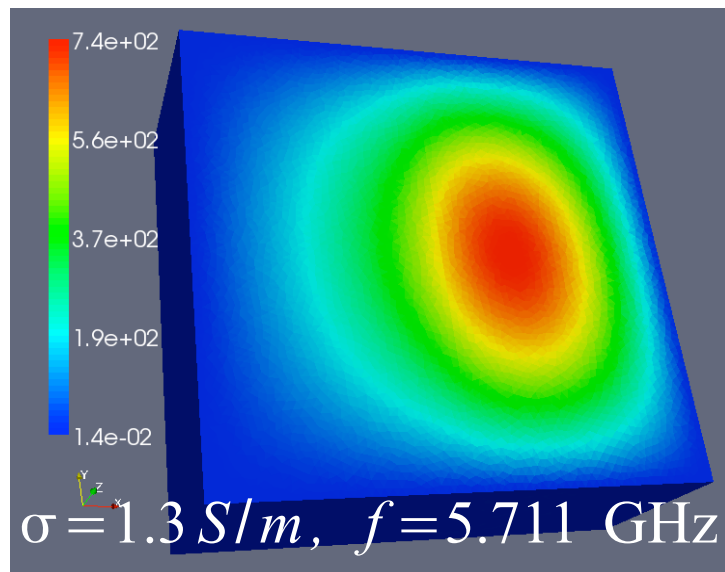
- **#Tetrahedra** : 306'001
- **Processors** : 32
- **Number of eigenvalues** : 1
- **Tolerance** : 1.0e-6(JDQZ), 1.0e-2(NLJD)
- **Target** : [100.0]
- **Krylov solvers** : Bi-CGStab, GMRES(m)
- **Preconditioners** : Diagonal, Block Jacobi-LU/ILU
- **Max iteration of correction equation** : 50
- **Jmin** : 5, **Jmax** : 10

# Half-filled Rectangle Cavity

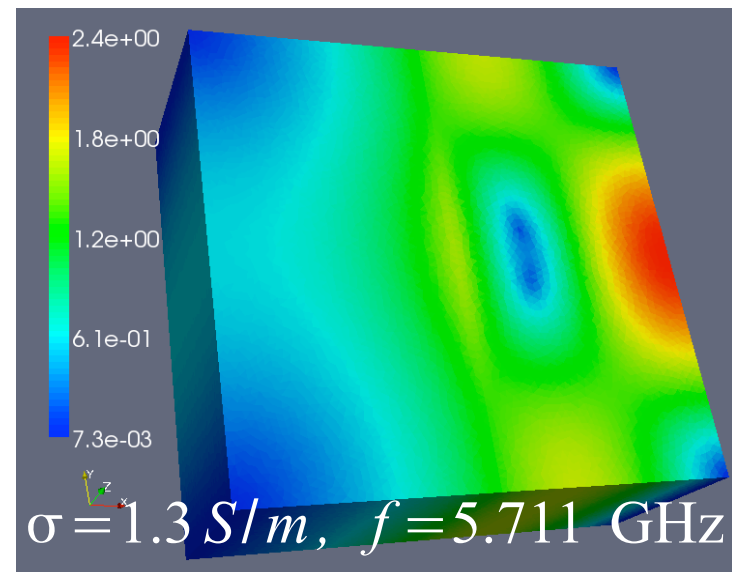
**Table**: dominant mode of a rectangle cavity ( $22.86 \times 22.86 \times 10.16 \text{ mm}^3$ ). Half of the cavity is filled by conductor with  $\epsilon_r = 2.0$  and varying  $\sigma$ .

$\tilde{\omega} = \text{Re}(\sqrt{\lambda})c + i \text{Im}(\sqrt{\lambda})c$ ,  $c$ : the speed of light

$\sigma$ (S/m)	analytical solution for $\tilde{\omega}/(2\pi)$	$\tilde{\omega}/(2\pi)$ computed by Femaxx
0.1	$7.379 + j0.354$	$7.379 + j0.354$
0.5	$7.236 + j1.819$	$7.236 + j1.817$
1.0	$6.579 + j3.864$	$6.579 + j3.864$
1.3	$5.711 + j5.197$	$5.711 + j5.198$



electric field



magnetic field

# Half-filled Rectangle Cavity

- Linear element order
  - JDQZ eigensolver with linearization (dof:664'130)

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	46	667	14.5	67.51	0.01	49.18	
blkj-ilu	34	348	10.24	64.88	1.17	35.9	1.04
blkj-lu	37	276	7.46	141.39	40.19	85.56	0.48

- NLJD eigensolver, Bi-CGStab (dof:332'065)

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	18	597	35.12	39.91	0.01	20.92	
blkj-ilu	17	366	22.88	34.72	1.27	16.18	1.15
blkj-lu	30	69	2.46	81.57	40.64	29.92	0.49



# Half-filled Rectangle Cavity

- Quadratic element order (dof:1'852'810)

- NLJD, Bi-CGStab, 2-level hierarchical basis prec

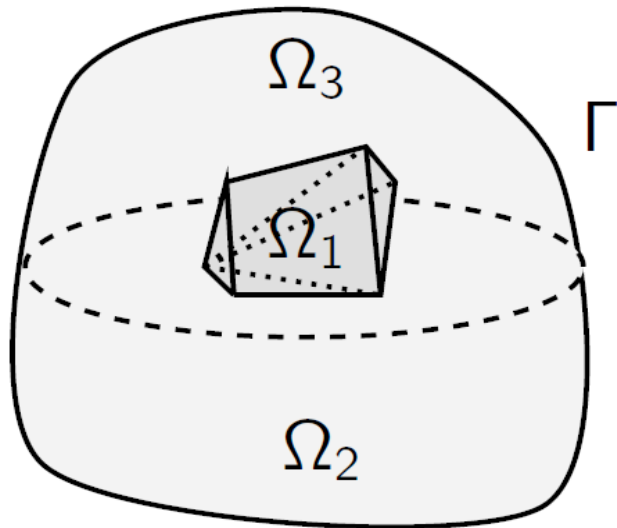
preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	53	1306	24.64	579.78	6.07	496.7	
blkj-ilu	29	366	12.62	261.00	7.3	177.74	2.22
blkj-lu	23	160	6.96	307.44	46.58	183.83	1.89

- NLJD, GMRES(30), 2-level hierarchical basis prec

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	44	852	21.85	384.91	0.05	259.91	
blkj-ilu	26	448	19.48	323.64	7.30	233.31	1.19
blkj-lu	19	202	11.88	360.77	46.30	232.04	1.07

# Microwave Antenna

- *Bounded* computational domain  $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$ .



$\Omega_1$  : antenna device

$\Omega_2$  : substrate

$\Omega_3$  : environment

$\Gamma$  : absorbing boundary

$\Omega$  : arbitrary shape, usually sphere

- 1<sup>st</sup> order absorbing boundary condition (ABC):

$$\mathbf{n} \times \nabla \times \mathbf{E}(\mathbf{x}) = -i k_0 \sqrt{\mu_r \epsilon_r} \mathbf{n} \times (\mathbf{n} \times \mathbf{E}(\mathbf{x})), \quad \mathbf{x} \in \Gamma, k_0 = \sqrt{\lambda}.$$

# Microwave Antenna

- FEM yields a constrained *quadratic* eigenproblem

$$A \mathbf{x} + \lambda R \mathbf{x} - \lambda^2 M \mathbf{x} = \mathbf{0}, \quad C^T \mathbf{x} = \mathbf{0}.$$

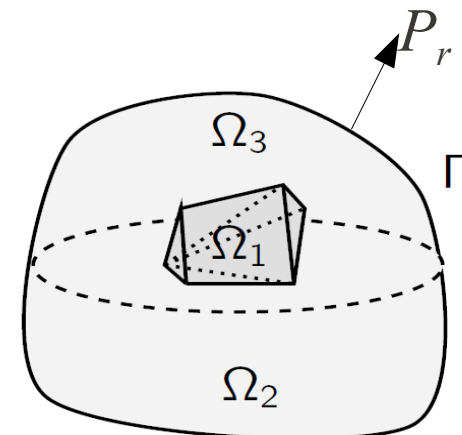
$$a_{ij} = \int_{\Omega} \mu_r^{-1} (\nabla \times \mathbf{N}_i) \cdot (\nabla \times \mathbf{N}_j)$$

$$r_{ij} = i \int_{\Gamma} \sqrt{\epsilon_r / \mu_r} (\mathbf{n} \times \mathbf{N}_i) \cdot (\mathbf{n} \times \mathbf{N}_j)$$

$$m_{ij} = \int_{\Omega} \epsilon_r \mathbf{N}_i \cdot \mathbf{N}_j$$

$$c_{il} = \int_{\Omega} \epsilon_r \mathbf{N}_i \cdot \nabla N_l$$

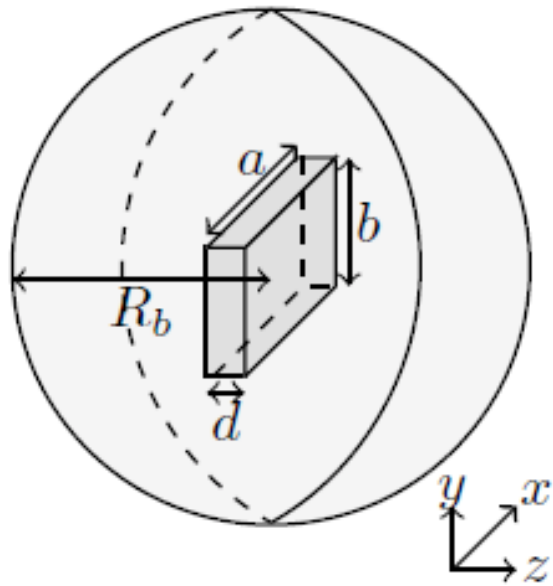
integral on boundary



# Example of microwave antenna

- **#Tetrahedra** : 645'868
- **Processors** : 32
- **Number of eigenvalues** : 1
- **Tolerance** : 1.0e-3(JDQZ), 1.0e-3(NLJD)
- **Target** : [0.1]
- **Krylov solvers**: Bi-CGStab, GMRES(m)
- **Preconditioners** : Diagonal, Block Jacobi-LU/ILU
- **Max iteration of correction equation** : 50
- **Jmin** : 5, **Jmax** : 10

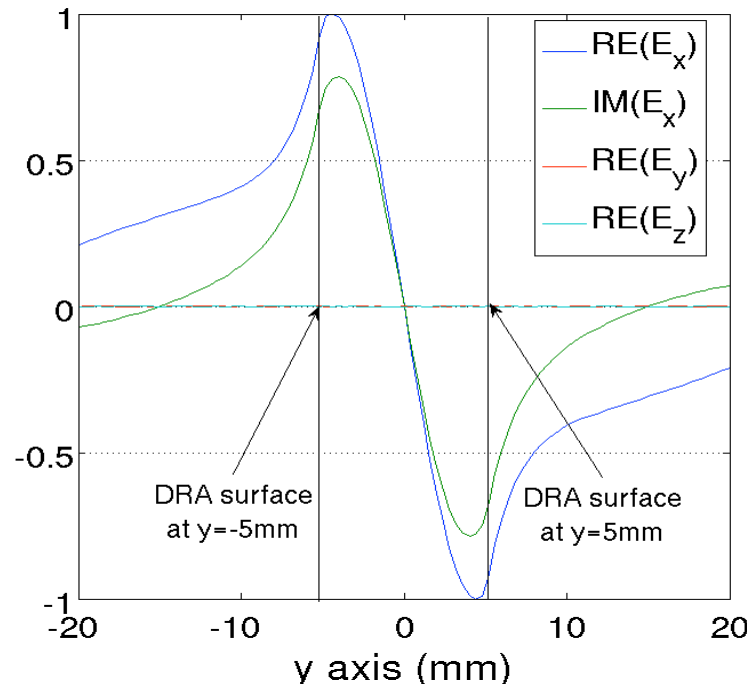
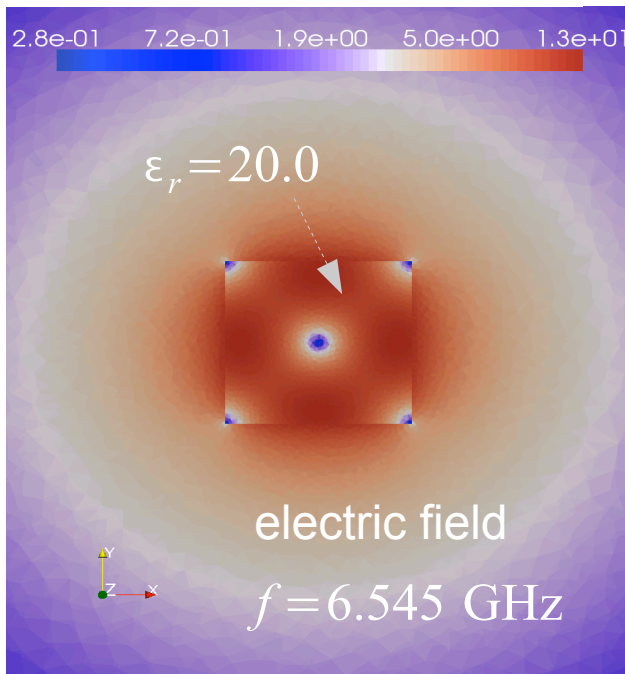
# Dielectric Resonant Antenna (DRA)



**Table:** Dominant mode of several DRA.

$\epsilon_r$	a (mm)	b (mm)	d (mm)	$f$ (GHz)	$f_{MI}$ (GHz)	Diff. (%)	$Q_1$
79.46	7.45	7.45	2.98	4.644	4.346	6.9	176.8
37.84	8.60	8.60	2.58	6.221	5.934	4.8	31.1
37.84	7.45	7.45	3.51	5.614	5.337	5.2	50.8
20.0	10	10	4	6.545	6.409	2.1	13.3

$f$ ,  $Q_1$  and  $Q_2$  are numerical results by using 1st order ABC;  
 $f_{MI}$ ,  $Q_{MI}$  are theoretically determined results by using perfect magnetic conductor (PMC) boundary conditions.



## Remark:

Electric field plotted over y-axis:

$$E_y \approx 0,$$

$$E_x \approx A k_y \sin(k_y y).$$

## Ref:

1, R. K. Mongia and A. Ittipiboon. IEEE Trans. Antennas Propag., 45(9):1348-1356 (1997).

2, H. Guo, B. Oswald, and P. Arbenz, Opt. Express 20, 5481-5500 (2012).

# Microwave Antenna

- Linear element order
  - JDQZ solver with linearization (dof:162'976)

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	20	988	49.78	31.87	0	21.55	
blkj-ilu	18	881	48.94	19.03	0.43	8.93	1.67
blkj-lu	18	259	14.39	22.75	0.3	14.48	1.40

- NLJD solver ,Bi-CGStab(dof:81'488)

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	19	559	29.42	14.44	0	5.35	
blkj-ilu	19	587	30.89	14.60	0.4	5.99	0.99
blkj-lu	20	311	15.55	14.53	0.42	7.01	0.99

# Microwave Antenna

- Quadratic element order(dof:439'188)
  - NLJD solver, Bi-CGStab, 2-level hierarchical basis prec

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	29	745	25.69	47.27	0.04	32.77	
blkj-ilu	17	325	19.12	31.11	0.62	14.31	1.52
blkj-lu	17	223	13.12	36.39	0.81	20.89	1.30

## NLJD, GMRES(30), 2-level hierarchical basis prec

preconditioner	outer iteration	inner iteration	average	overall time	build time	solver time	“speed-up”
diag	35	952	30.71	77.46	0.02	48.78	
blkj-ilu	20	559	31.06	63.90	1.42	37.30	1.76
blkj-lu	33	1035	35.69	149.32	2.96	117.72	0.67

# Summary

- Femaxx: a parallel 3D finite element eigensolver package.
- Simulation tool for advanced electromagnetic structures.

<b>eigensolver</b>	<b>problem type</b>	<b>applications</b>
JDSYM	Generalized real symmetric eigenvalue problem	lossless resonant cavities
JDQZ	Generalized non-Hermitian eigenvalue problem; Quadratic eigenvalue problem	dielectric lossy material; ohmically lossy material; plasmonic nanostructures
NLJD	Nonlinear eigenvalue problem	ohmically lossy material; plasmonic nanostructures