Contemporary Challenges in Computational Accelerator Physics

TECHNISCHE UNIVERSITÄT DARMSTADT

Herbert De Gersem, Erion Gjonaj, Wolfgang Ackermann, David Bizzozero, Wolfgang F.O. Müller, Steffen Schmid

Joint DESY and University of Hamburg Accelerator Physics Seminar
Hamburg, Tuesday, 7.07.2020

Collaboration with
Martin Dohlus, Nicoleta Baboi, Dmitry Bazyl, Yong-Chul Chae, Ye Chen, Winfried Decking, Michael Ebert, Mikhail Krasilnikov, Sven Pfeiffer, Holger Schlarb, Jacek Sekutowicz, Frank Stephan, Alexey Sulimov, Rainer Wanzenberg, Igor Zagarodnov

Motivation

simulate electromagnetic fields
in accelerator components
in the presence of

- beam (charged particles)
  - ultra-relativistic, non-relativistic
  - single particles, bunches (bunch shape)
- surrounding structures
  - (complicated) geometry
  - materials (dispersive, lossy, superconducting, permeable)
  - surroundings (waveguides, couplers, (corrugated) walls, diagnostics)

Categorisation : EM Field Simulation

- volumetric meshes
  - structured (hexahedra)
  - unstructured (tetrahedra, possibly +pyramids +bricks)
  - meshless

- volumetric discretisation
  - finite-difference time-domain (FDTD), finite-integration technique (FIT)
  - finite-element methods (FE)
  - discontinuous Galerkin
  - particle-particle models

- discretisation in time
  - time domain
  - frequency domain
  - eigenmodes

Outline

- motivation
- categorisation
- solvers + examples
  - PBCI : e.g. wakefield simulation
  - FD : e.g. impedance simulation
  - CSRDG : e.g. coherent synchrotron radiation
  - PAMASO : e.g. pulsed waveform acceleration
  - REPTIL : e.g. tracking + space charge
  - LW : e.g. radiation in undulators
  - CEM3D : e.g. cavity simulation
- conclusions

Categorisation : EM Field Simulation

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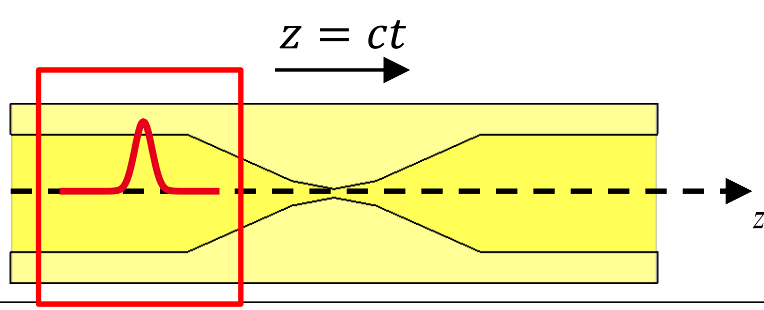
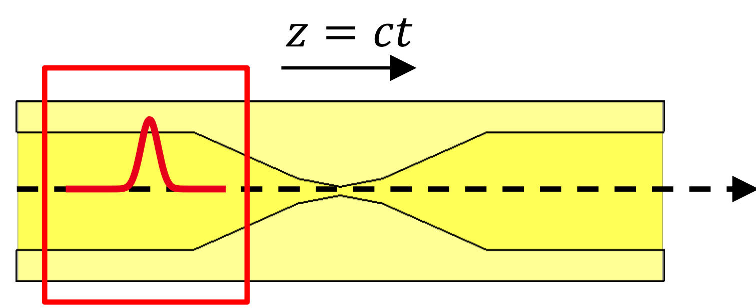
PBCI, e.g., wakefield simulation
main developer: Erion Gjonaj



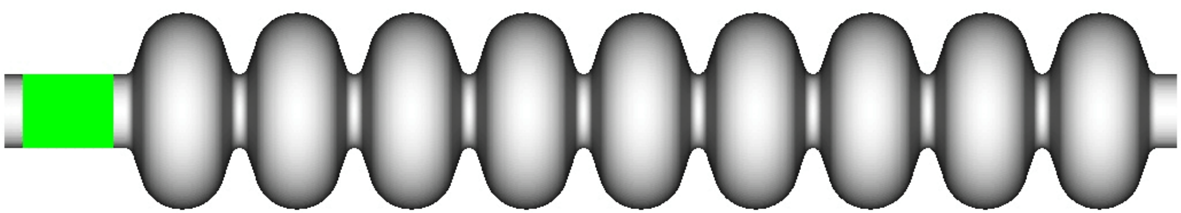
Wake field computation time domain (PBCI)

- Wake fields and wake potentials

$$W_{\parallel}(r,s) = \frac{1}{Q}\int dz\, E_z\big(r,z,t(s,z)\big)$$



- Solve Maxwell's equations in the time domain
  - Dispersion-free Finite Difference / Integration Method*
  - Indirect wake integration
  - Resistive / roughness losses by surface impedance approach
  - Very short ultra-relativistic bunches



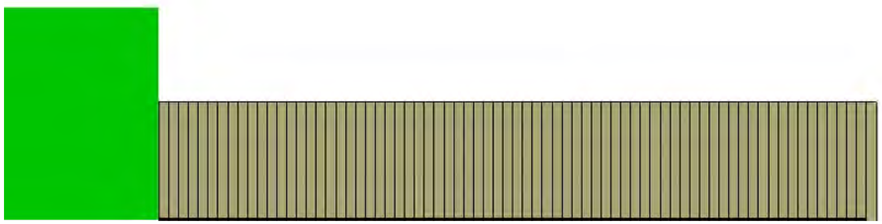
Geometric (longitudinal) wake fields in the TESLA cavity

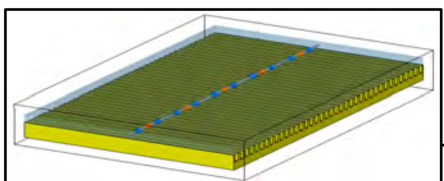
**ICAP 2006*

Erion Gjonaj

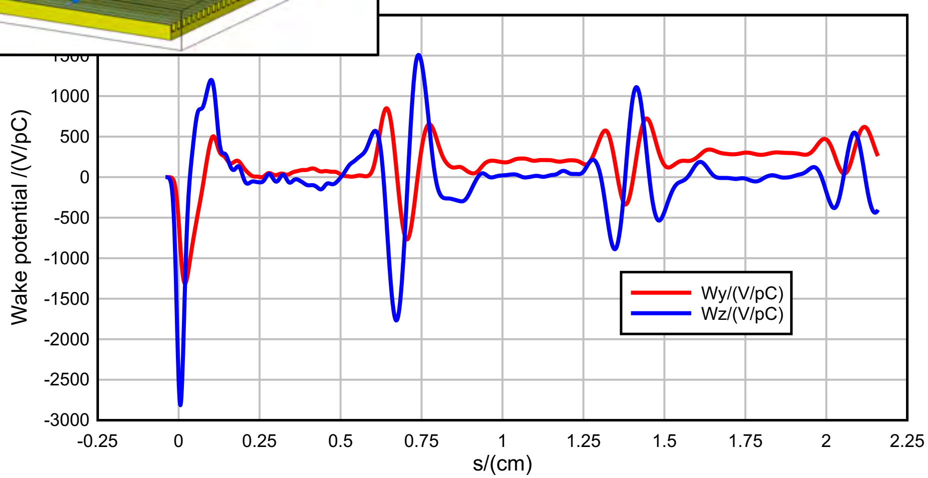
Wake field computation time domain (PBCI)

- Corrugated plate dechirper (XFEL / LCLS II)

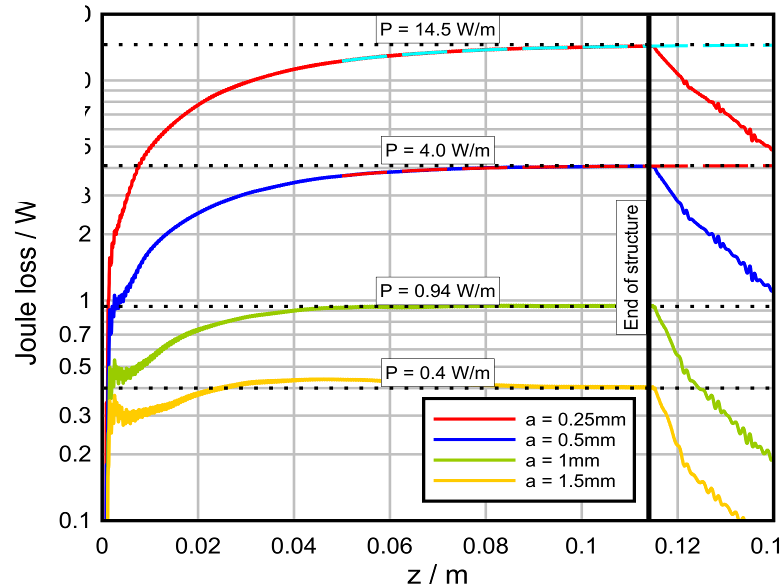




Wake potential ($\sigma_z = 100\mu m$)



Joule losses*



Extremely long-range wake and transient heating times

**Phys. Rev. Accel. Beams 20 (2017)*

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Wake field computation time domain (PBCI)

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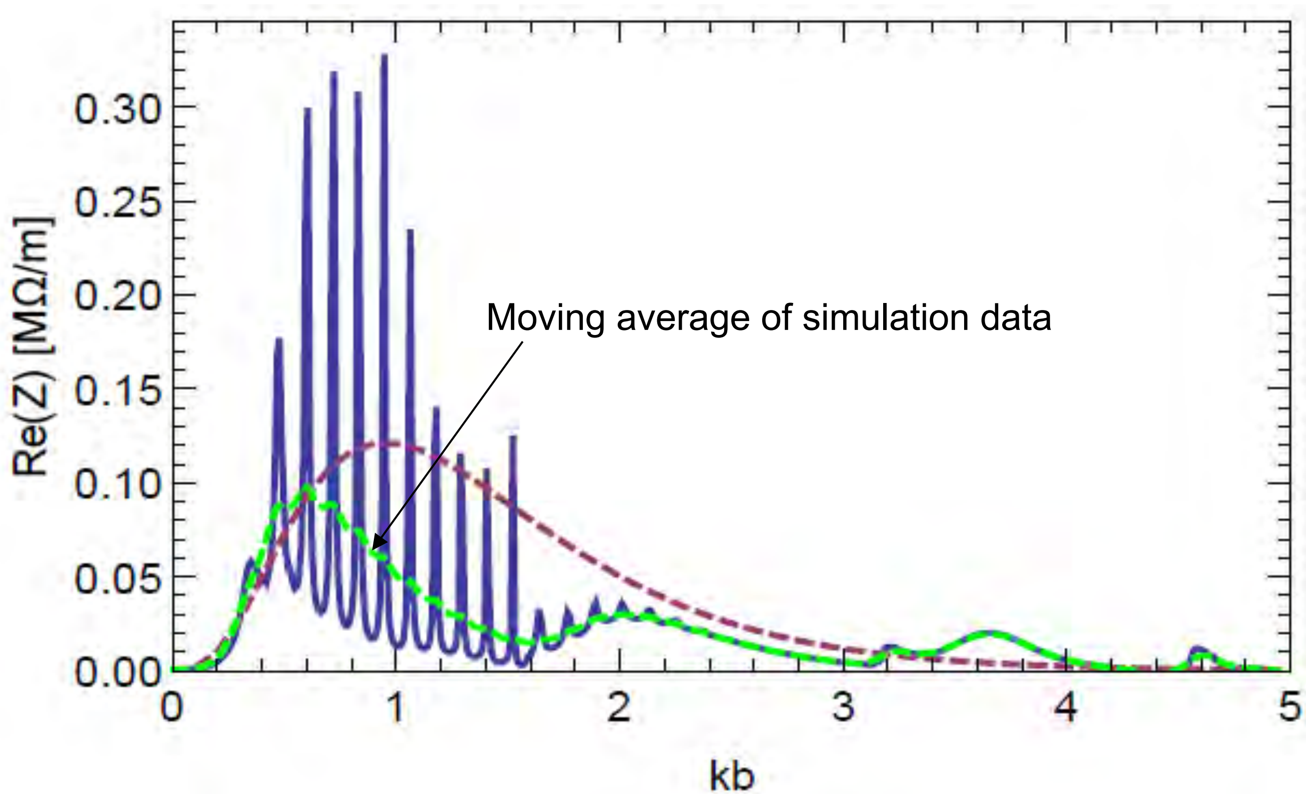
- Corrugated plate dechirper (XFEL / LCLS II)

Comparison of theory vs. simulation for longitudinal impedance (a=1.5mm)



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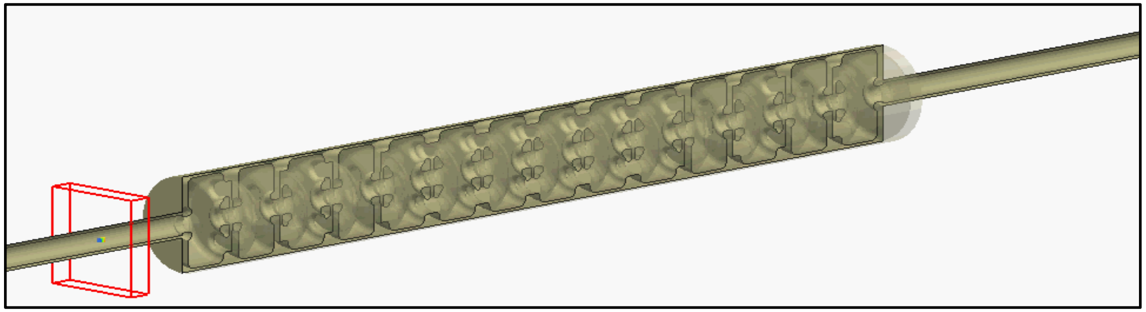
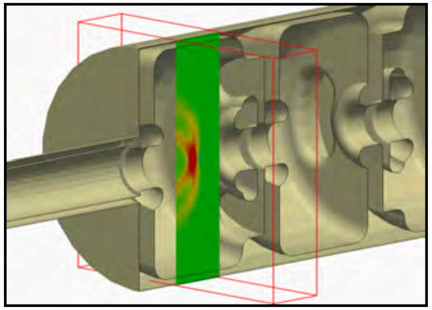
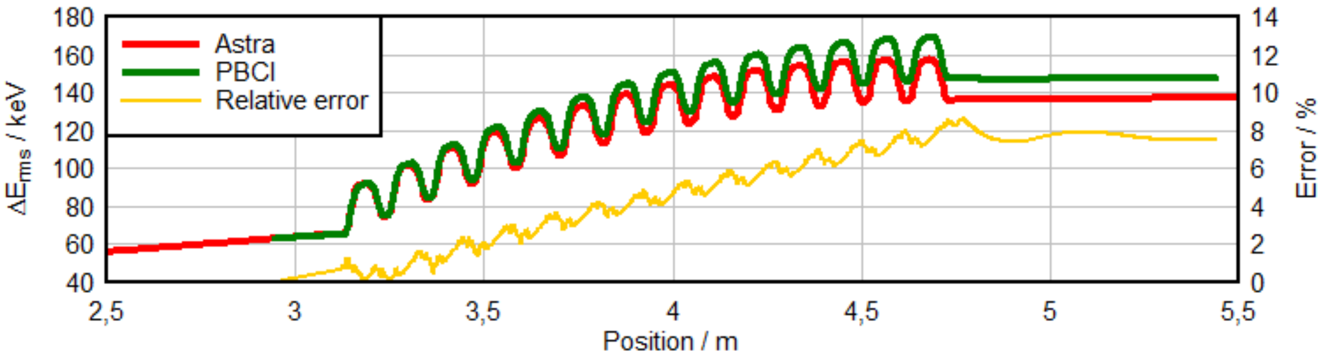
Wake field computation time domain (PBCI)

- CDS Injector Booster Cavity (DESY, PITZ)
  - Effect of wake fields on beam dynamics for soft beams





  - PIC simulations with geometrical wakefields*



Energy spread:

Pure space-charge vs. space-charge + wakefield simulation

***ICAP 2012, DESY 2012**

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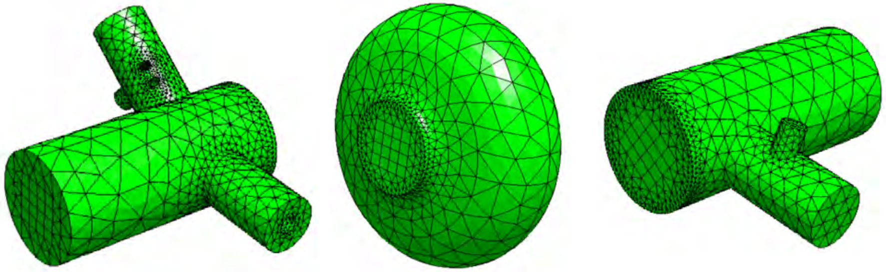
FD, e.g., impedance simulation
main developer: Erion Gjonaj

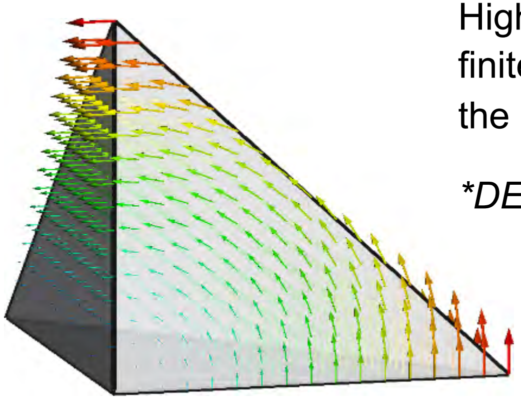


Impedance computation frequency domain

- Wake fields and impedances

$$Z_{\parallel}(r,\omega) = -\frac{1}{c\tilde{\lambda}(\omega)}\int ds W_{\parallel}(r,s)e^{-\frac{i\omega s}{c}} = -\frac{1}{Q\tilde{\lambda}(\omega)}\int dz\tilde{E}_z(r,z,\omega)e^{\frac{i\omega z}{c}}$$

- Solve Maxwell's equations in the frequency domain*
  - High order conforming and hierarchic FE
  - Specialized 3D-beam absorbing boundary condition
  - Long range wakefields
  - Arbitrary geometry
  - Curved beam paths & $\beta < 1$
  - Lossy wall and resistive impedance
  - Hybrid meshes / charge conservation



High order tangential finite element used in the discretization

**DESY 2019*

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Impedance computation frequency domain

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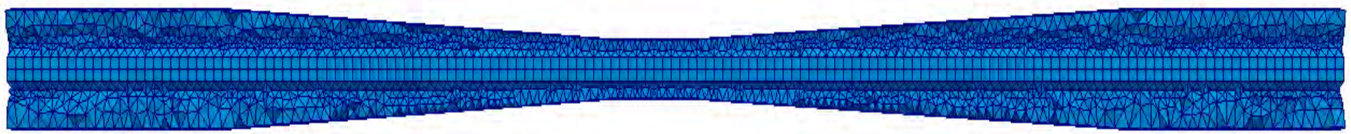
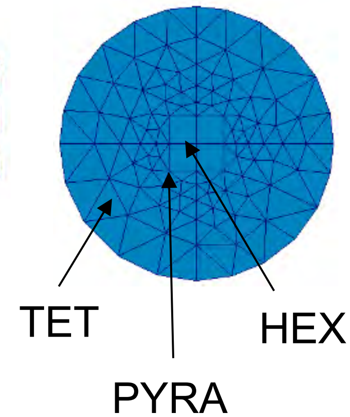
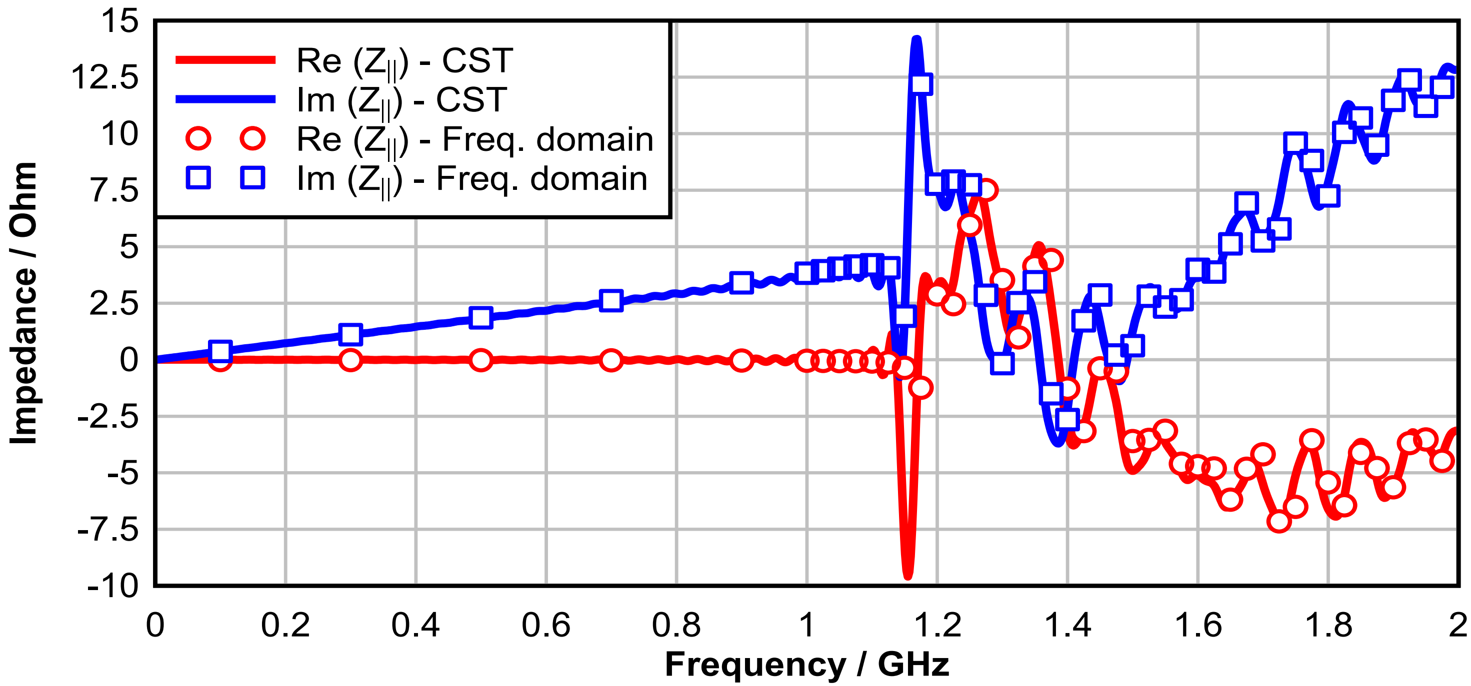
- Tapered collimator example – hybrid meshes







Longitudinal impedance. Frequency domain vs. time domain

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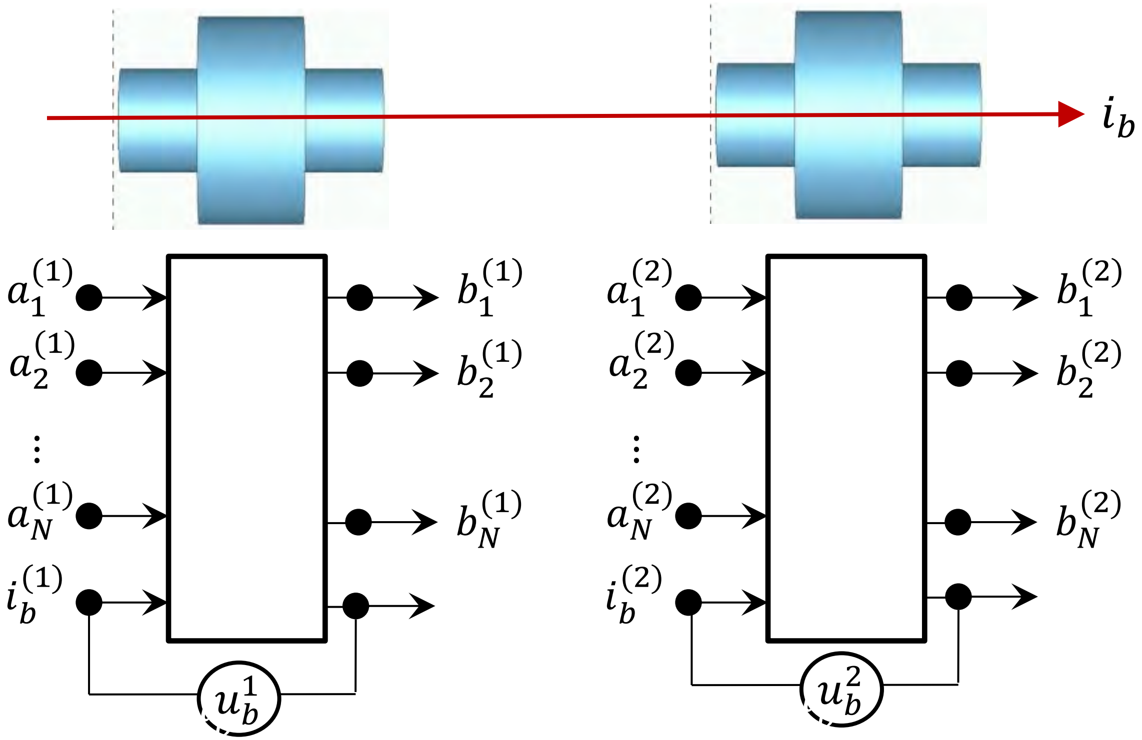
Impedance computation frequency domain

- Concatenation of long accelerator structures*



Matching conditions:

$$b_i^{(n)} = a_i^{(n+1)}$$

$$i_b^{(n)} = i_b^{(n-1)} e^{ik_0 L_{n-1}}$$

$$\sum_n u_b^{(n)} = u_b^{tot}$$

- Generalized S-Matrix*:

$$\begin{pmatrix} S^{tot} & k^{tot} \\ h^{tot} & Z_b^{tot} \end{pmatrix} \begin{pmatrix} a_m \\ i_b \end{pmatrix} = \begin{pmatrix} b_m \\ u_b^{tot} \end{pmatrix}$$

Phys. Rev. Accel. Beams (2020)

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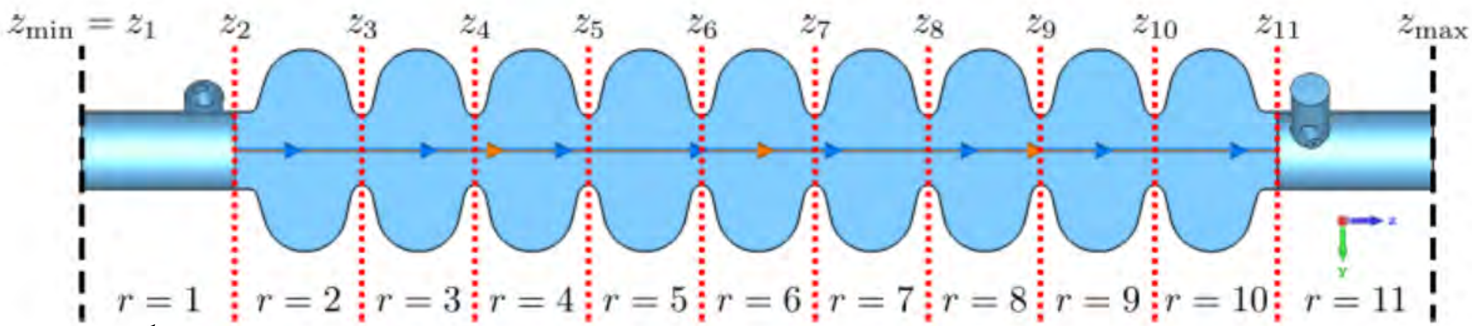
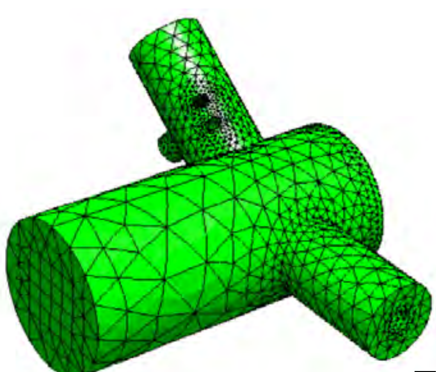
Impedance computation frequency domain

- Tesla 1.3GHz cavity

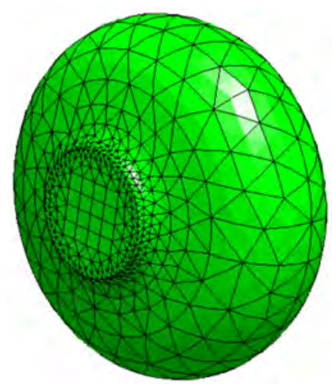


Downstream Cell 1 Cell 2 Cell 3 Upstream



15 TE-Modes
$(f_{max} = 8.2\text{GHz})$
15 TM-Modes
$(f_{max} = 10.6\text{GHz})$

TEM, …



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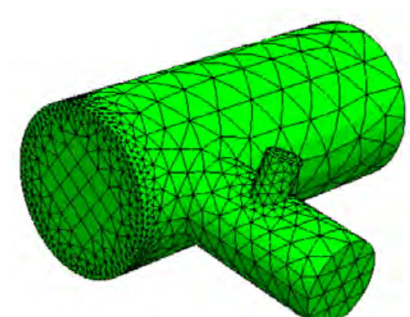

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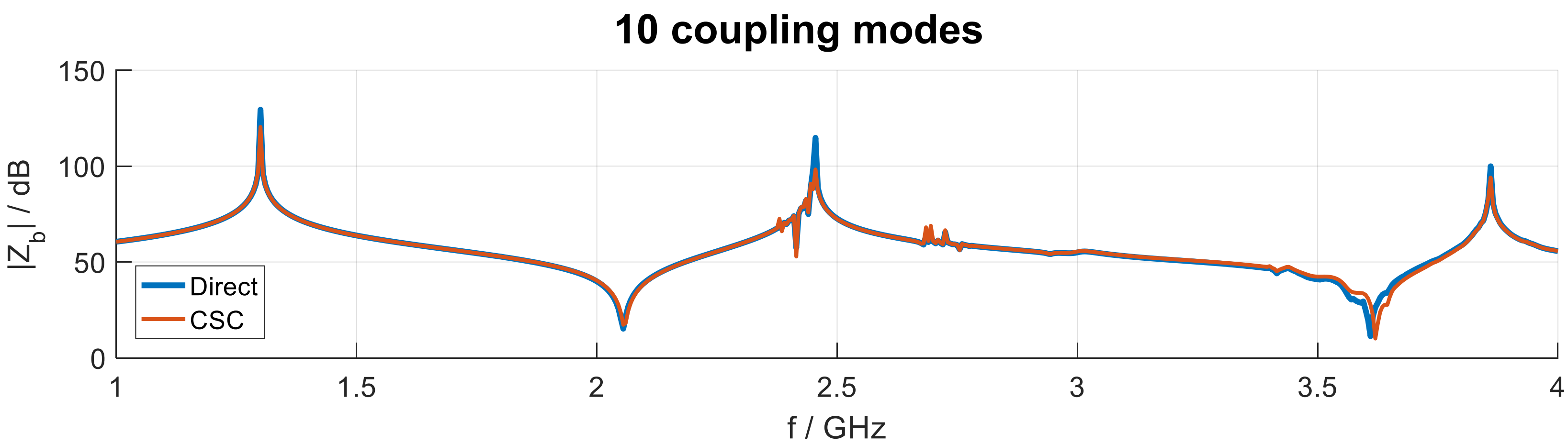
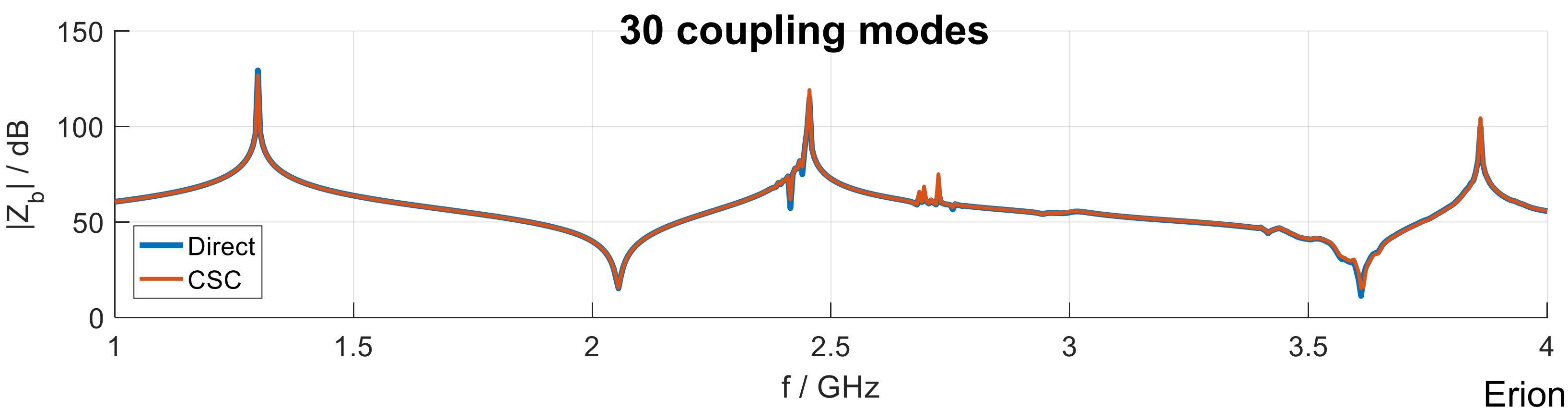
Impedance computation frequency domain

- Tesla 1.3GHz cavity





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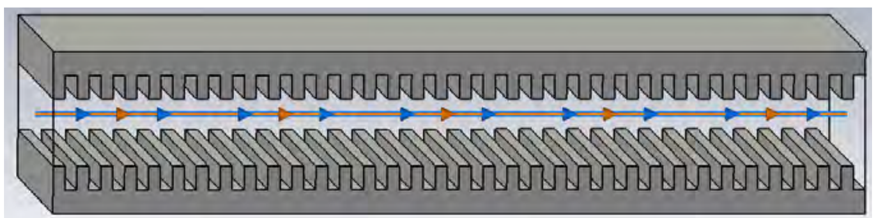
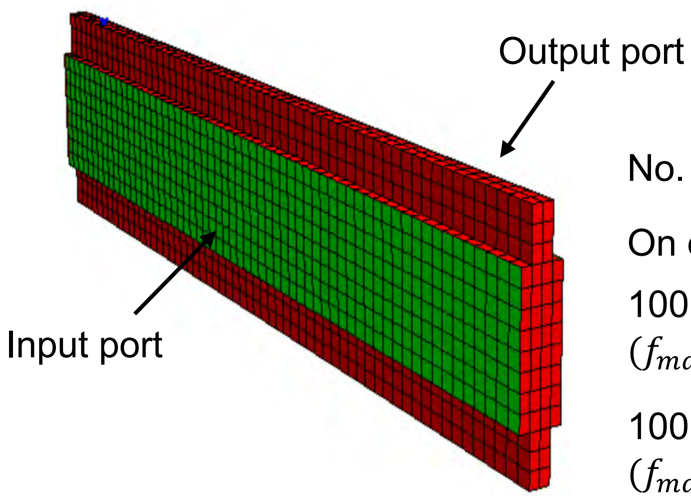
Impedance computation frequency domain

- Other applications - frequency domain impedance solver

(Quasi-) Periodic structures





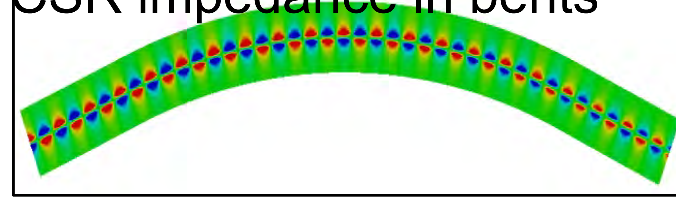
No. elements: 2640

On each port:

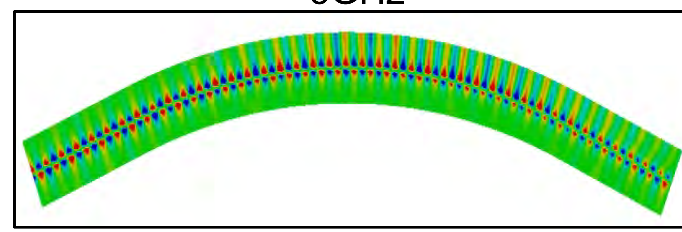
100 TE-Modes
$(f_{max} = 375\text{Ghz})$

100 TM-Modes
$(f_{max} = 448\text{Ghz})$

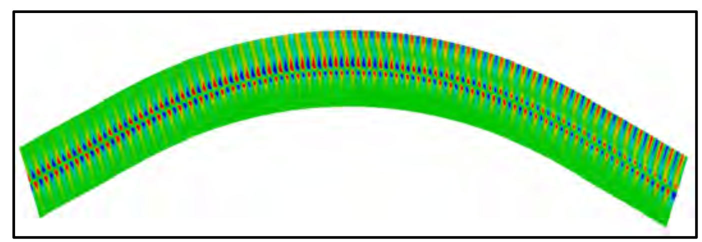
CSR impedance in bents



5GHz



10GHz



15GHz

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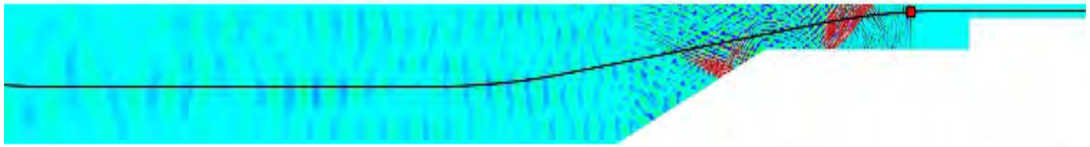
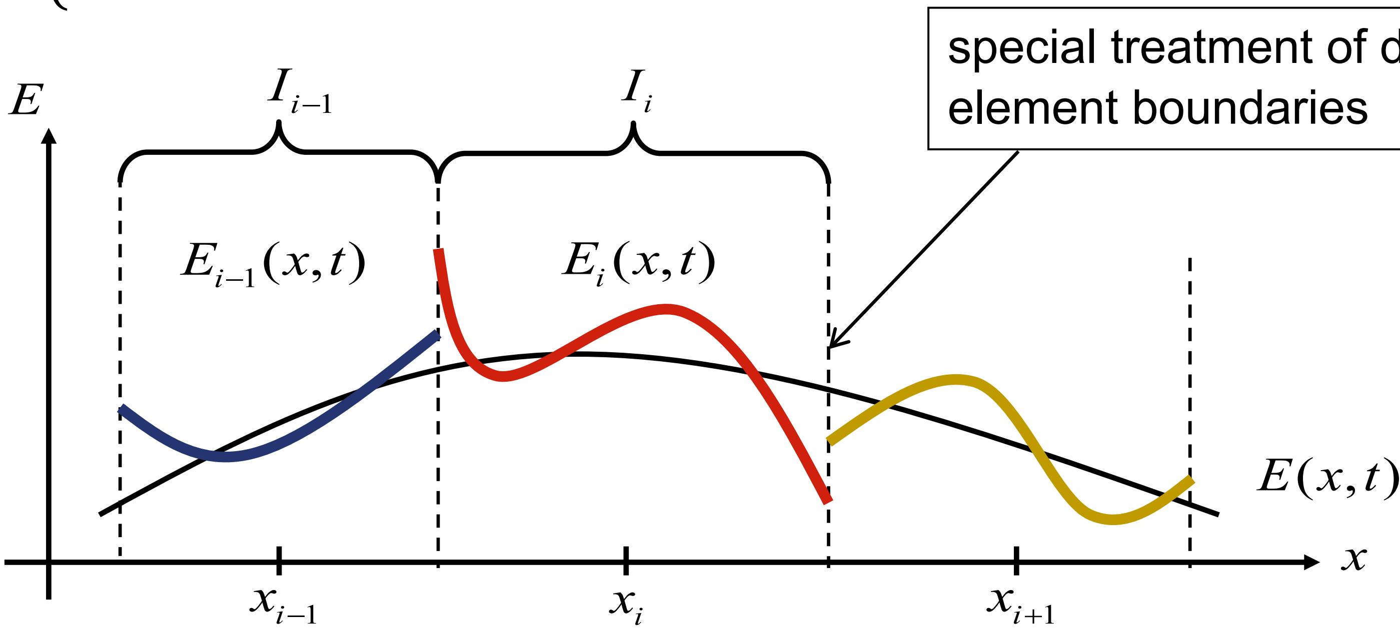
CSRDG, e.g., simulation of coherent synchrotron radiation
main developer: David Bizzozero



High order DG time domain methods

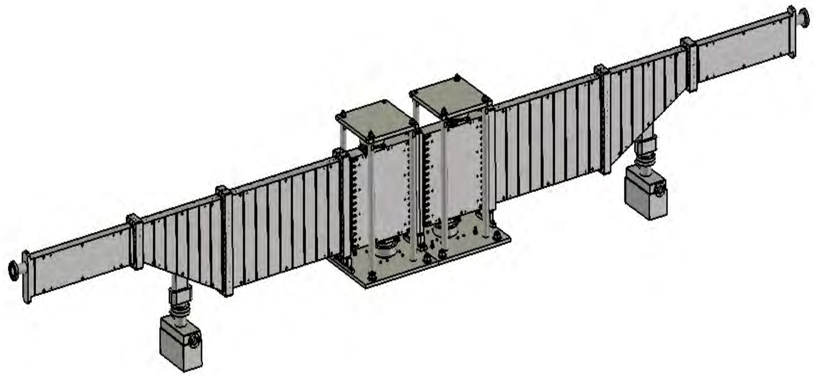
- DG discretization of Maxwell equations

$$\begin{cases} \dfrac{\partial \epsilon \boldsymbol{E}}{\partial t} - \nabla \times \boldsymbol{H} = -\boldsymbol{J} \\ \dfrac{\partial \mu \boldsymbol{H}}{\partial t} + \nabla \times \boldsymbol{E} = 0 \end{cases} \qquad \boldsymbol{E} = \sum_{j,q} \boldsymbol{E}_{j,q}(t)\phi_{j,q}(\boldsymbol{r}) \quad \text{with} \quad \phi_{j,q}(\boldsymbol{r}) \in P^Q(I_j)$$

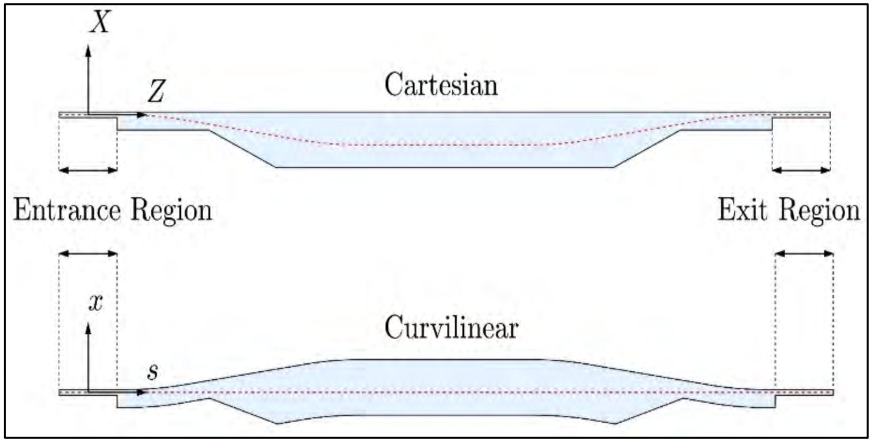


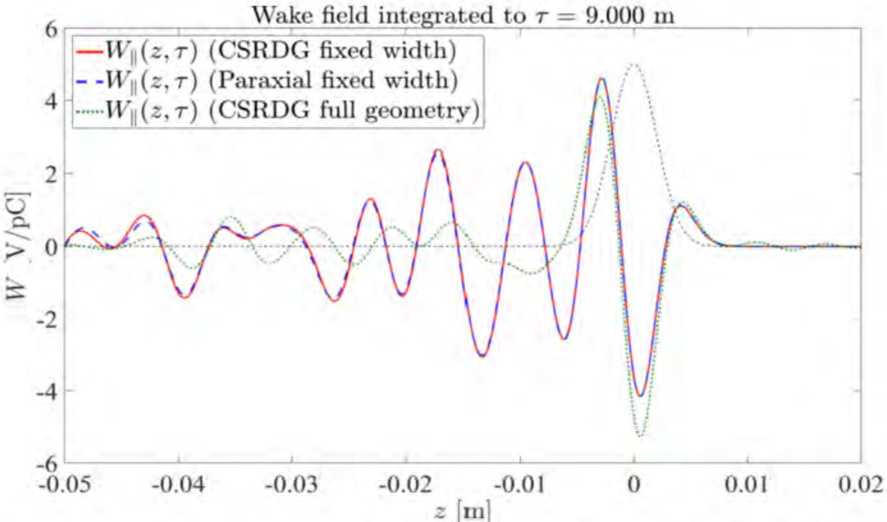
High order DGTD methods (CSRDG)

- CSR wakefields in XFEL BC0 bunch compressor*



  - Transform to Frenet-Serret frame
  - Parallel plate modal decomposition
  - High order DG on the plane





J. Comp. Phys. (2019)

David Bizzozero

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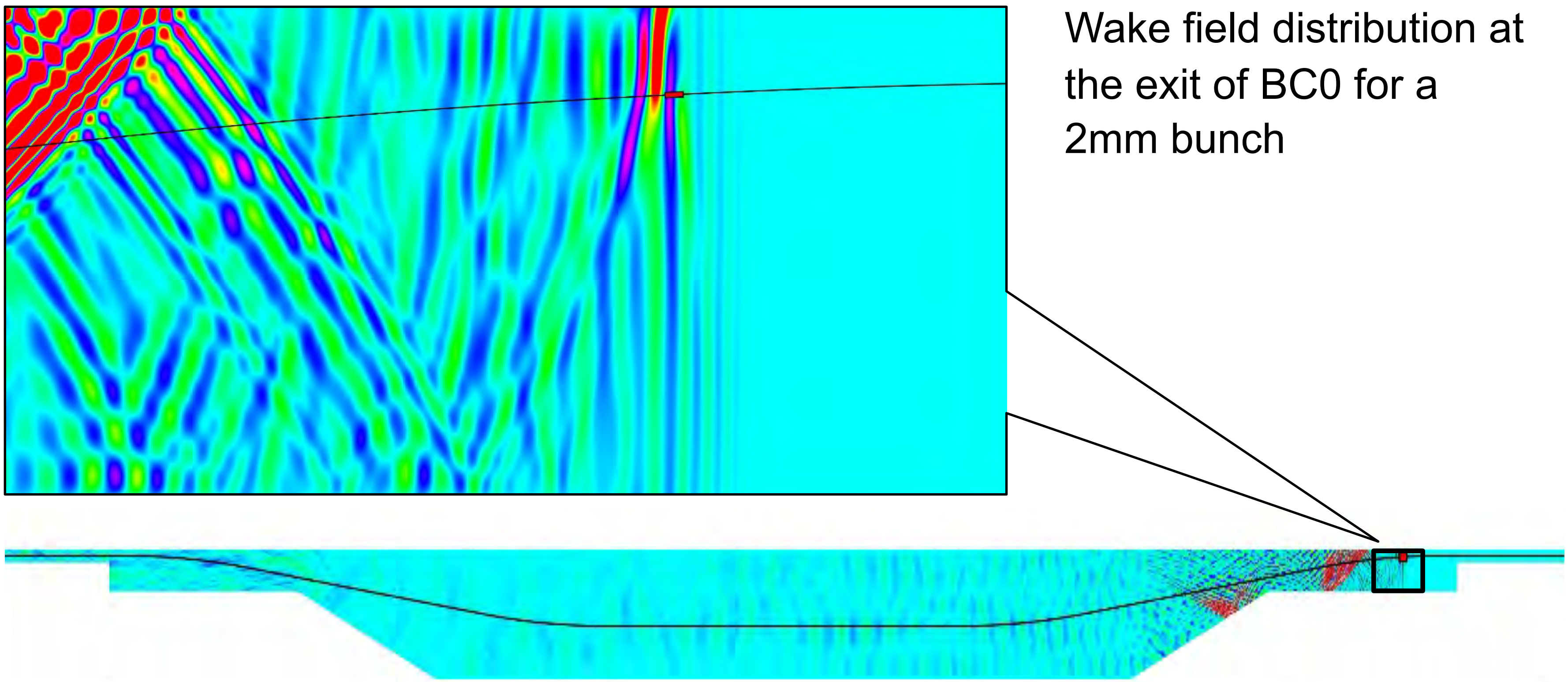

Wake field distribution at the exit of BC0 for a 2mm bunch

**J. Comp. Phys. (2019)*

David Bizzozero

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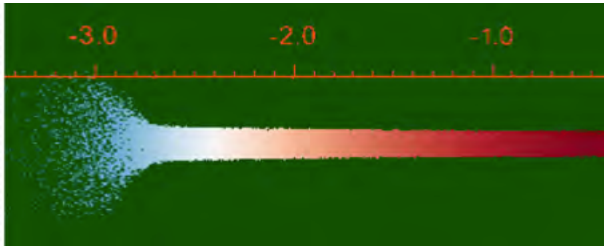
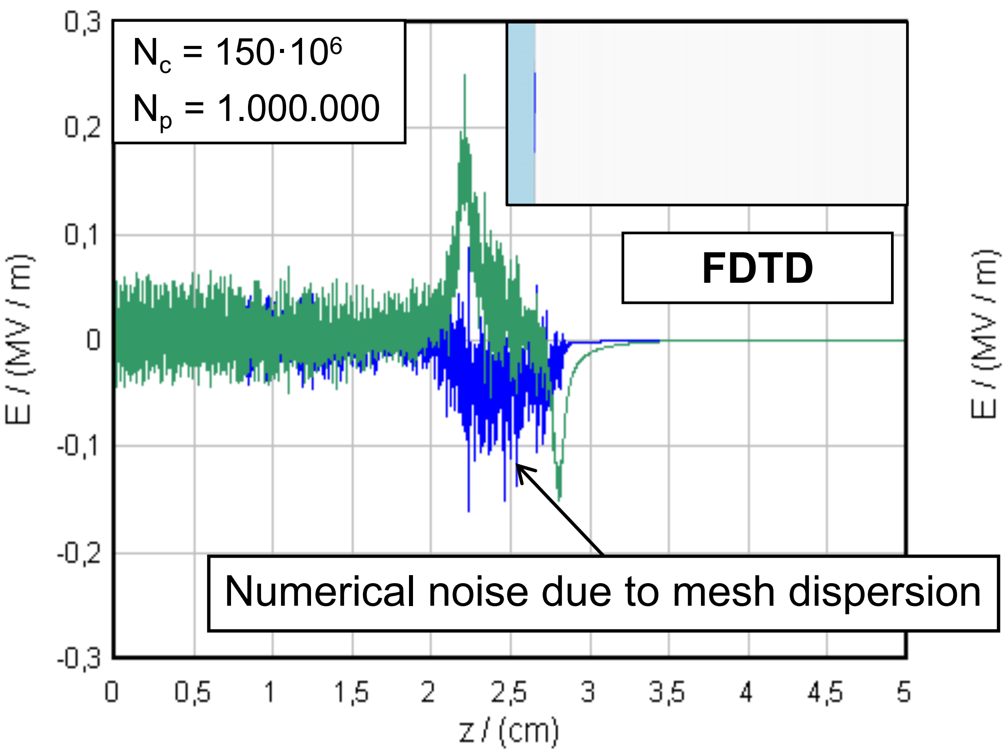
PAMASO, e.g., simulation of pulsed waveform acceleration
main developer: Erion Gjonaj

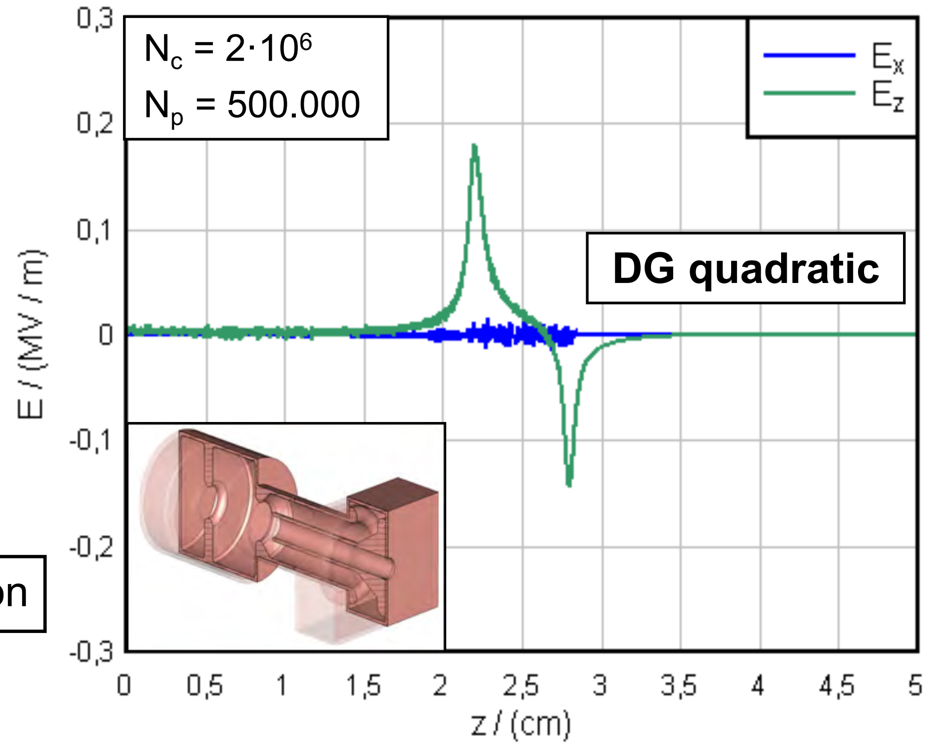


High order DGTD methods (PAMASO)

- Self-consistent beam dynamics using DG

Space charge field on-axis – DESY, PITZ gun





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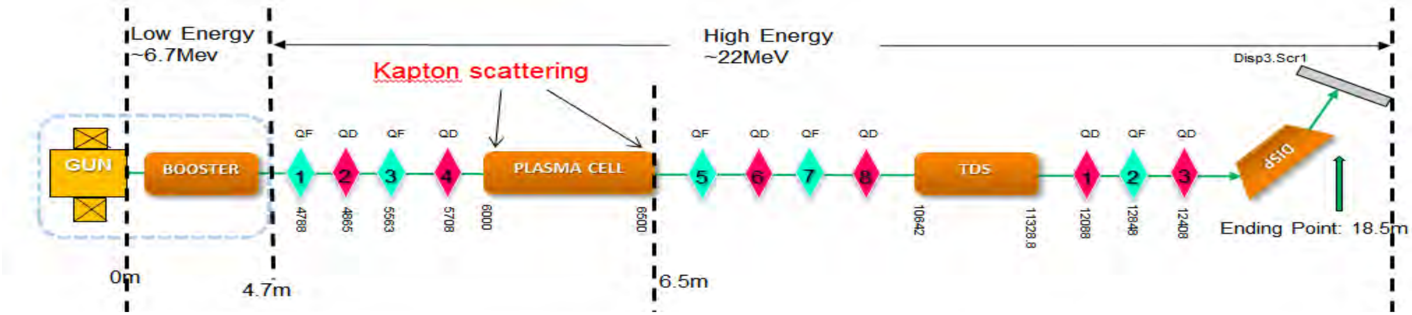
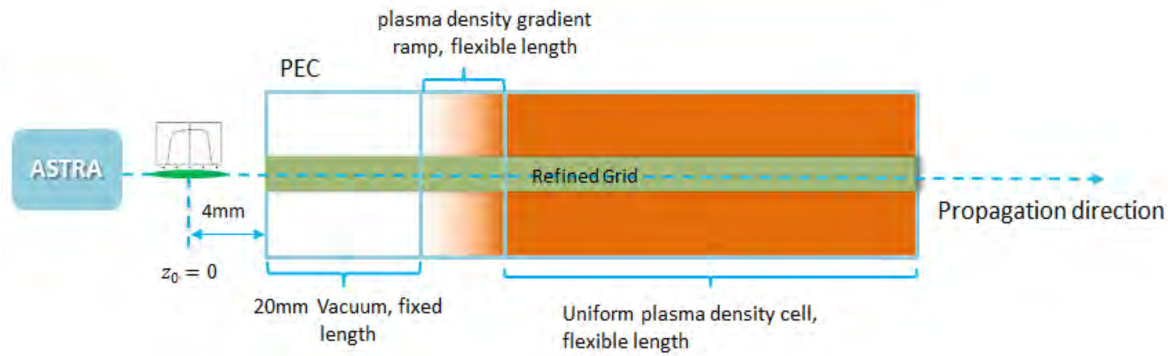
High order DGTD methods (PAMASO)

- Validation studies for beam driven PWFA experiments*
  - PITZ beam line with plasma cell



  - Purpose: validation of the paraxial code (HiPACE) developed at DESY



PAMASO simulation setup for the transformer ratio experiment at PITZ

Phys. Rev. Lett. (2019)

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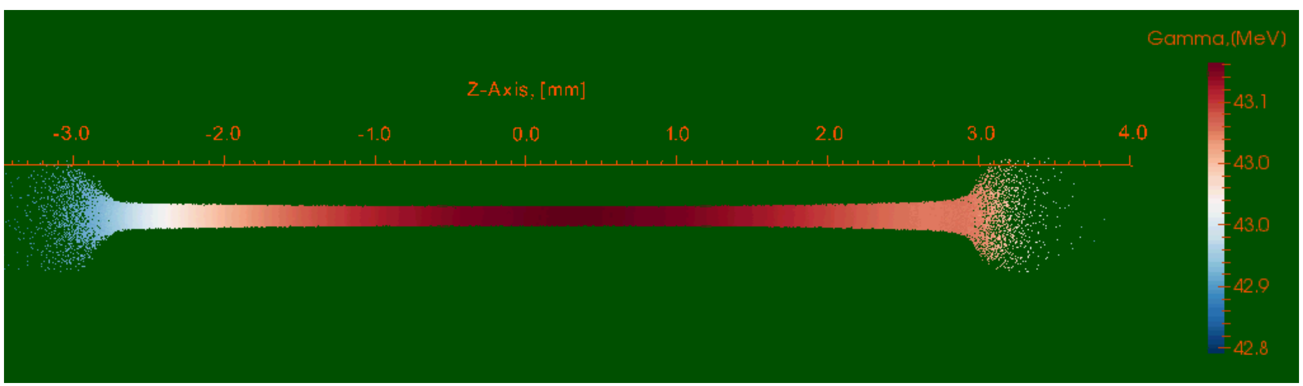
High order DGTD methods (PAMASO)

- Validation studies for beam driven PWFA experiments*

Wake fiels of a PITZ bunch entering the plasma cell



Self modulation of the bunch in the cell

with G. Loisch, Uni Hamburg

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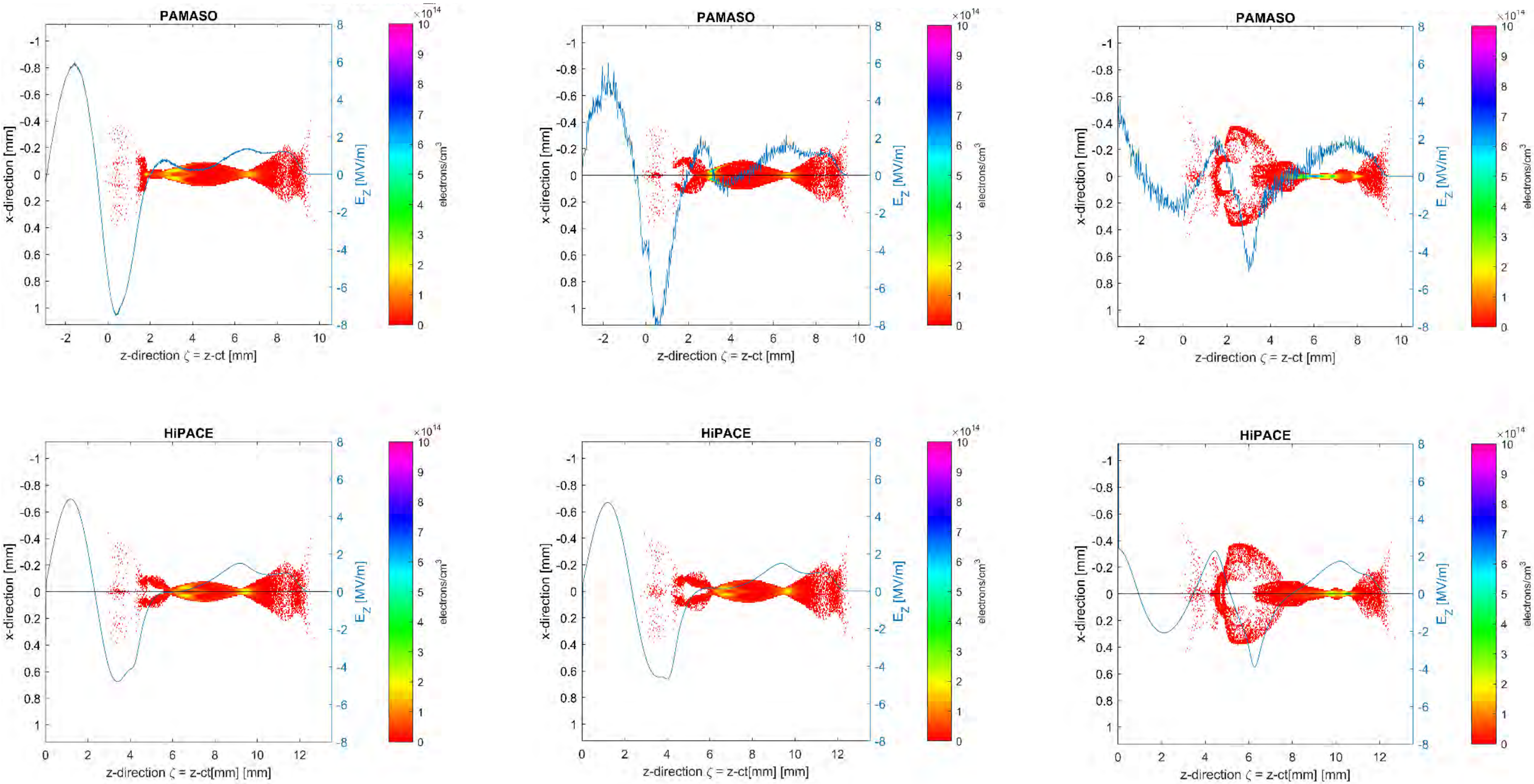
High order DGTD methods (PAMASO)

z = 10mm | z = 16mm | z = 50mm



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REPTIL, e.g., tracking
+ space charge
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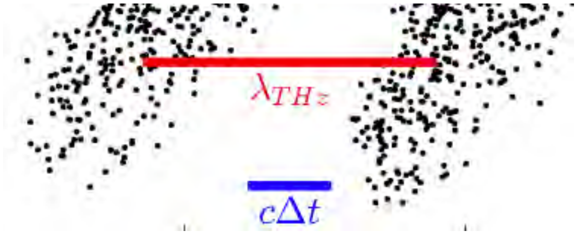

Fast Multipole Method Tracking Simulations

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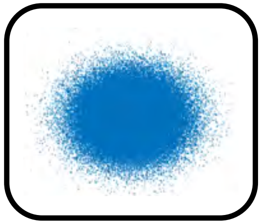
Adaptive FMM for sc-dominated, inhomogeneous, and anisotropic beams



Particles

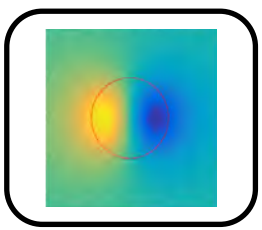
Tree Representation:

+ adaptive resolution
+ full accuracy
+ shape independent

Tree

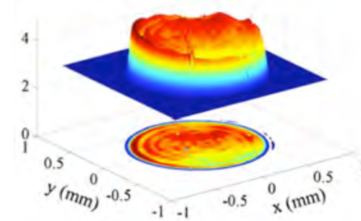
Hierarchical Approx.:

+ $O(N)$ algorithm
+ near field accuracy
+ field resolution



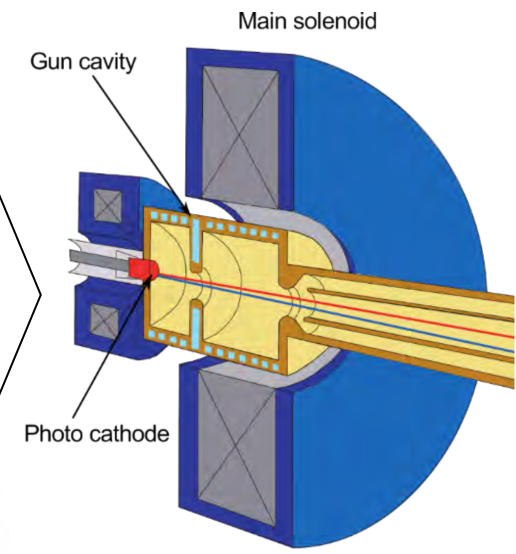
Particle Field

Inhomogeneity

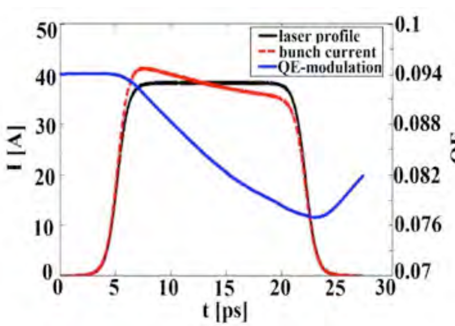


Krasilnikov et al., PRSTAB, **15**, 100701

Photogun Simulations



Emission Modeling



Chen et al., NIMPR A, **889**, p. 129-137

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Fast Multipole Method Tracking Simulations

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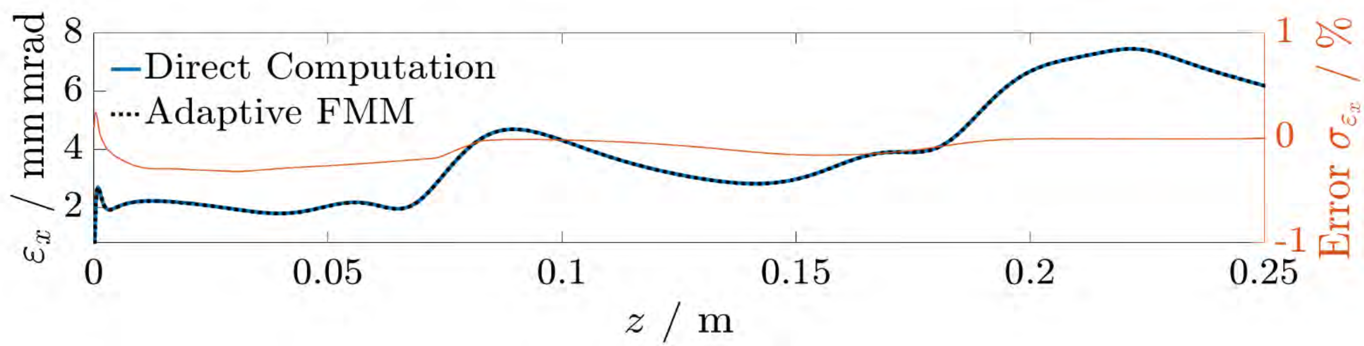
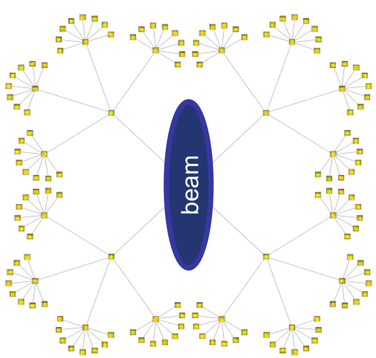
3D FMM Photoinjector Beam Dynamics Simulation

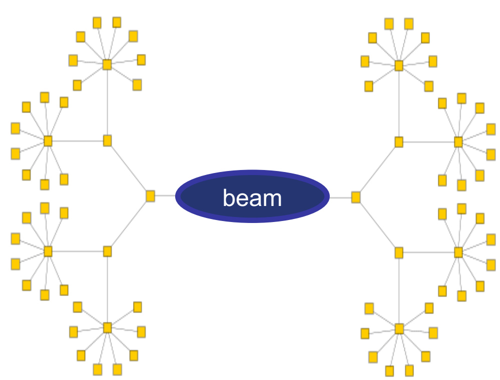


- relativistic, full 3D
- 40 times faster
- deviation $\sigma_{\varepsilon_x} \leq 0.5\%$

Beam Shape Optimized Tree

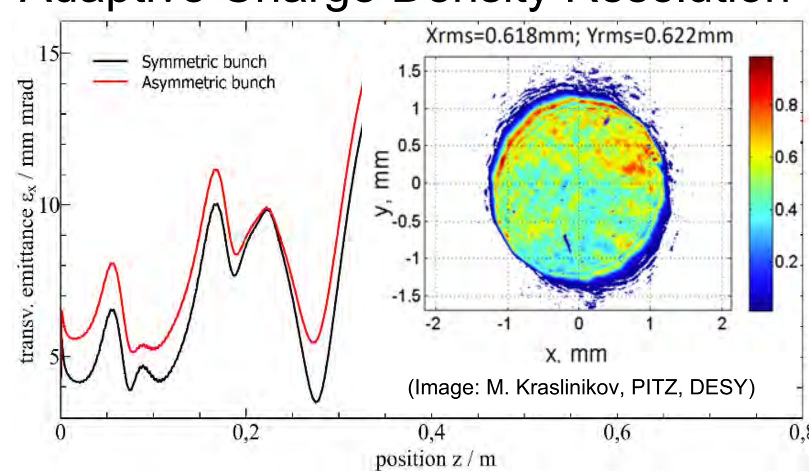


cathode ($\gamma \sim 1$)



gun exit ($\gamma \gg 1$)

Adaptive Charge Density Resolution



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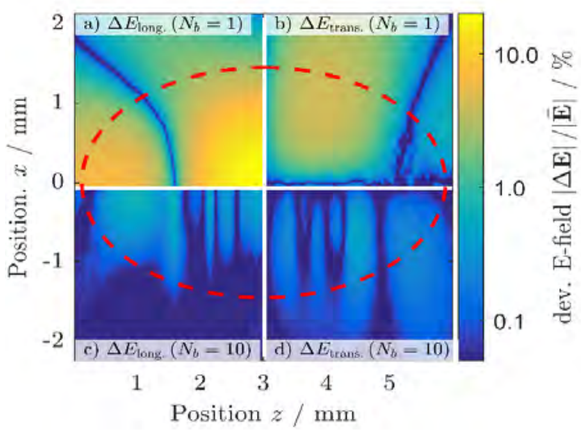
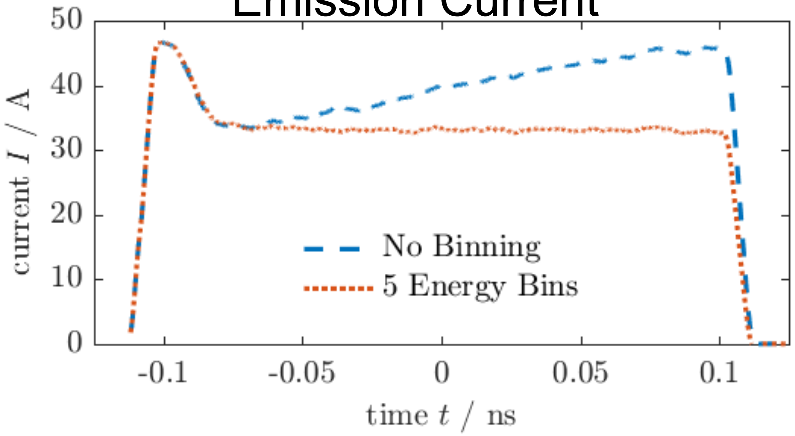
Space Charge Fields of Beams with Large Energy Spread



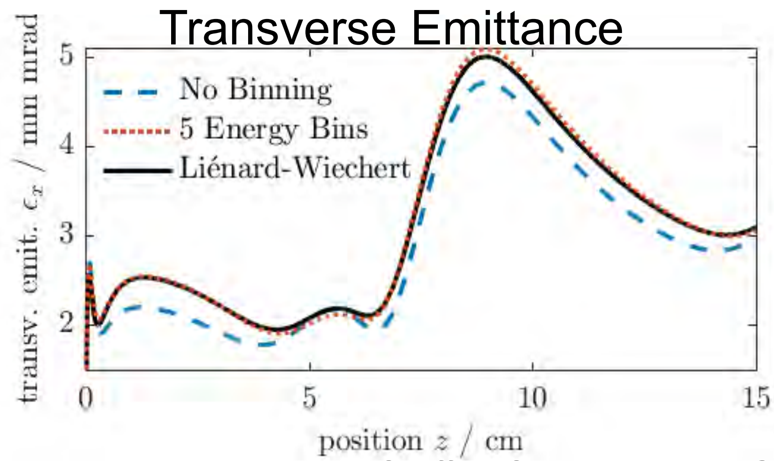
- no binning approach fields deviate by $\frac{\Delta E}{E} > 10\%$
- using 10 energy bins achieves $\frac{\Delta E}{E} \sim 0.5\%$
- $z - p_z$ phase space correlation supports FMM efficiency

$$t_{FMM,10\ bins} \approx 2 \times t_{FMM,\ 1\ bin}$$

Emission Current



Transverse Emittance



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Lienard-Wiechert model for radiation fields

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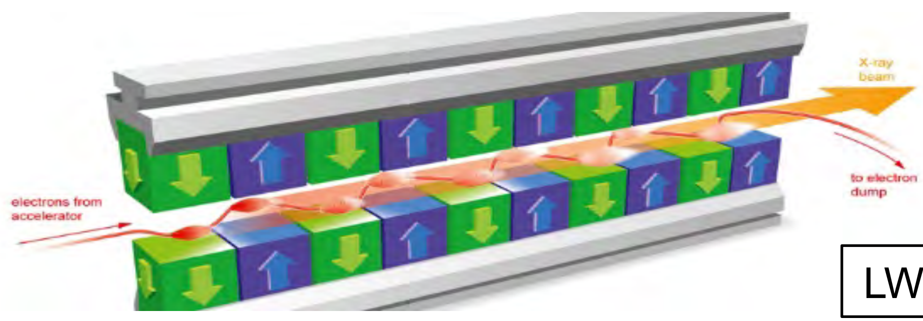
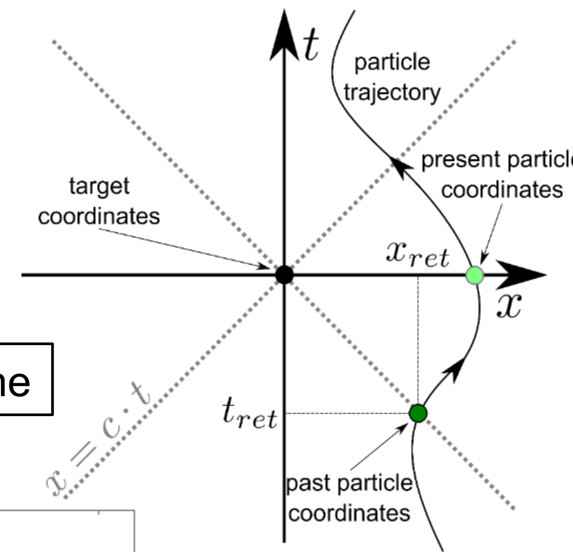
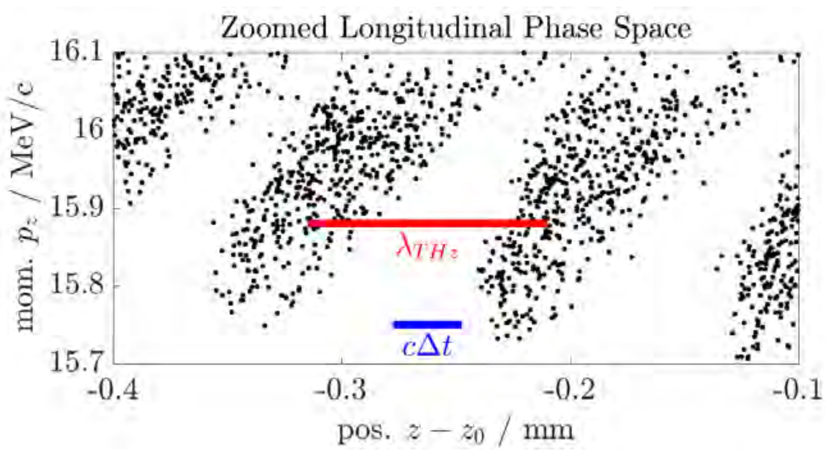
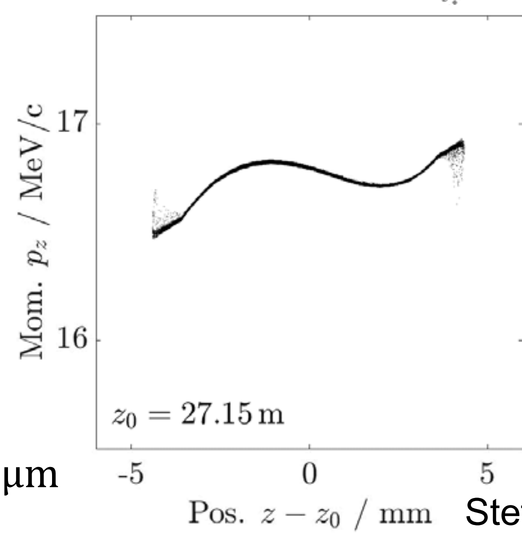
Simulations for DESY-PITZ THz SASE-FEL



LW-Simulation scheme







4 nC bunch

16.7 MeV energy

3.6 m undulator

Micro-bunching: $\lambda_{THz} = \frac{\lambda_U}{2\,\gamma^2}\left(1 + \frac{K^2}{2}\right) \approx 105\ \mu\mathrm{m}$

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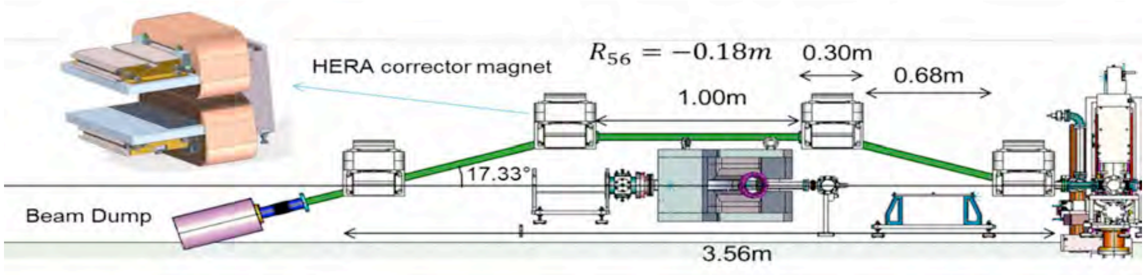
Lienard-Wiechert model for radiation fields

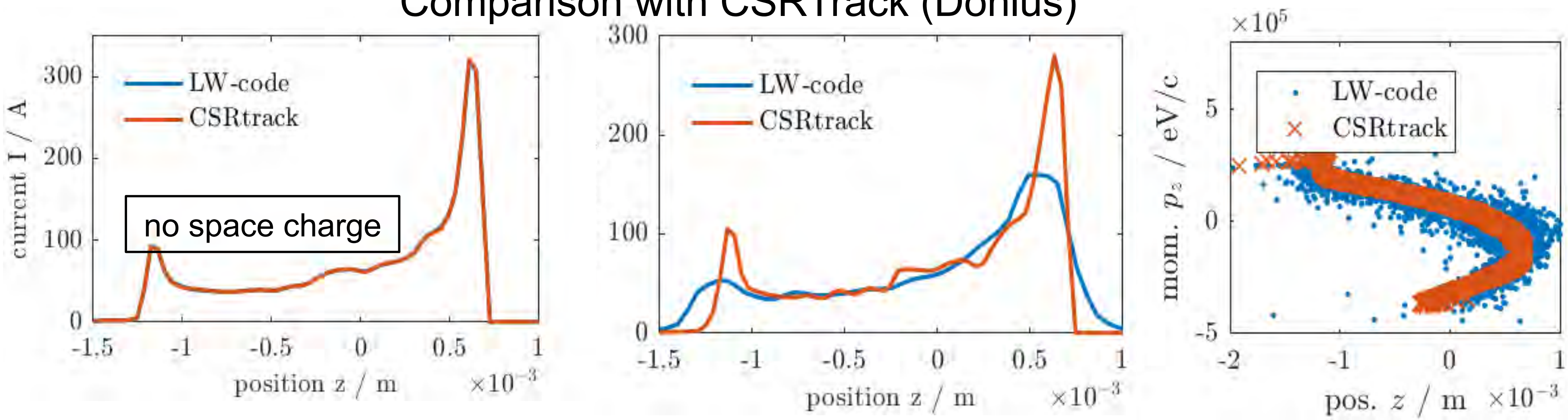
Bunch Compressor for DESY-PITZ THZ FEL



Shaker et al., FEL2019, TUP003

- $I_{peak} \approx 200\text{A}$
- $R_{56} = -0.18\text{ m}$
- $B_{dipole} \sim 50\text{ mT}$

Comparison with CSRTrack (Dohlus)



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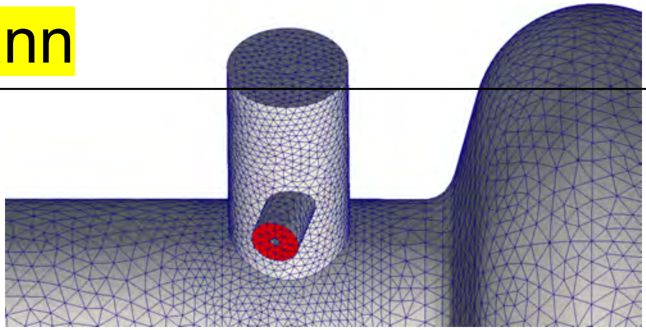
Categorisation : EM Field Simulation

- volumetric meshes
  - structured (hexahedra)
  - unstructured (tetrahedra, possibly +pyramids +bricks)
  - meshless
- volumetric discretisation
  - finite-difference time-domain (FDTD), finite-integration technique (FIT)
  - finite-element methods (FE)
  - discontinuous Galerkin
  - particle-particle models
- discretisation in time
  - time domain
  - frequency domain
  - eigenmodes

CEM3D, e.g., cavity simulation
main developer: Wolfgang Ackermann



3D FE Eigenmode Solver (CEM3D)

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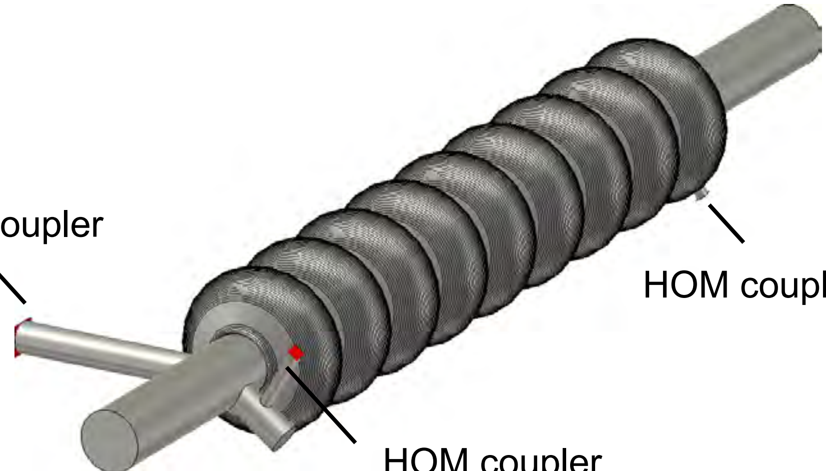
- formulation

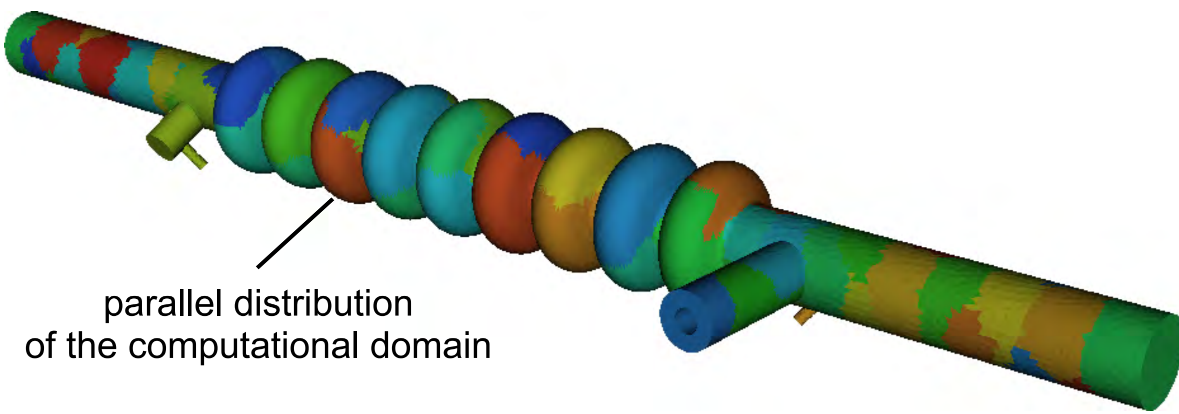
$$\mathrm{curl}\ 1/\mu_r\ \mathrm{curl}\vec{E} = \left(\frac{\omega}{c_0}\right)^2 \varepsilon_r \vec{E}\,\Big|_{\vec{r}\in\Omega}$$

continuous eigenvalue problem

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

discrete eigenvalue problem





parallel computing

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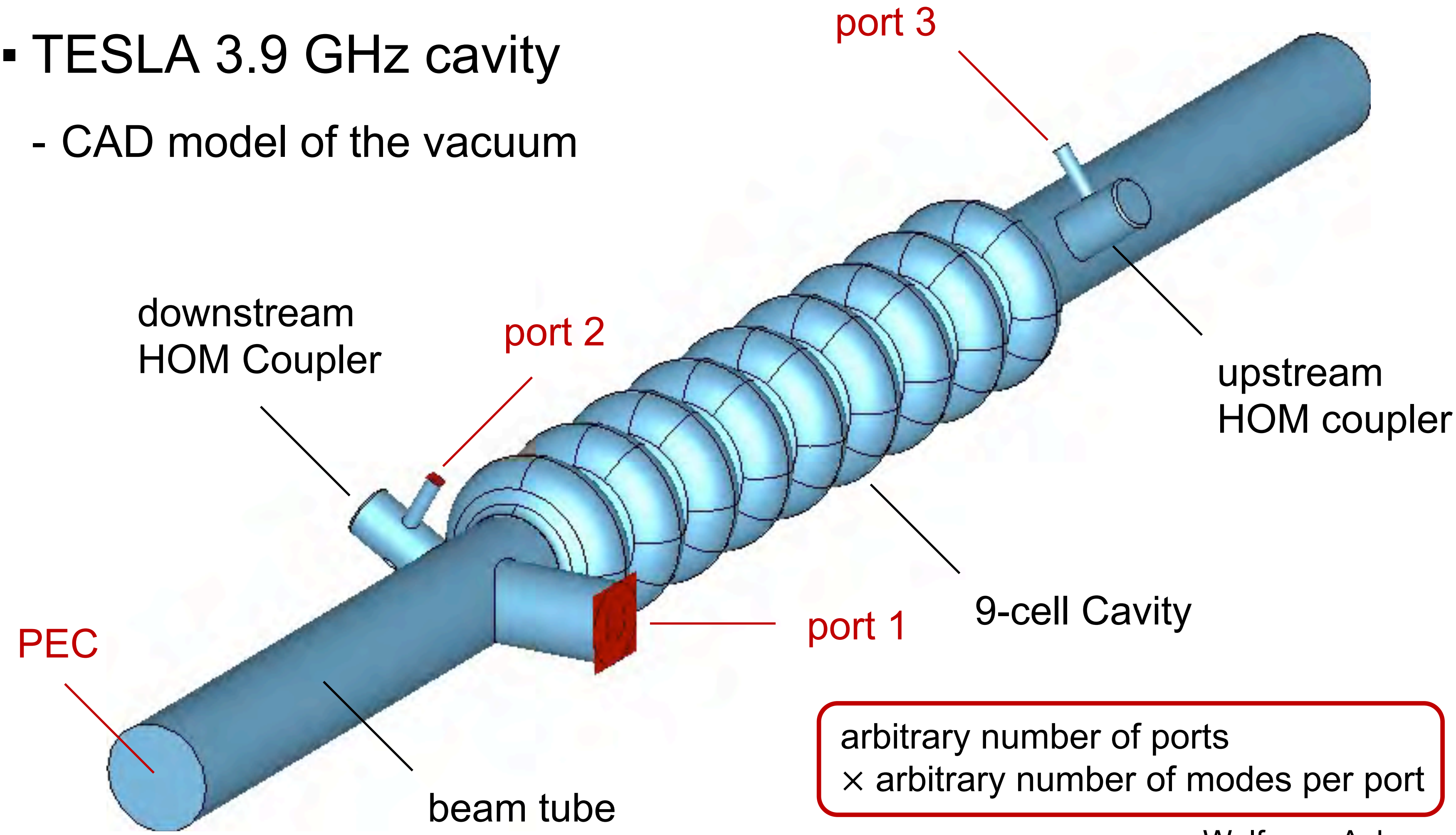
TESLA Resonators

- TESLA 3.9 GHz cavity
  - CAD model of the vacuum



arbitrary number of ports
× arbitrary number of modes per port

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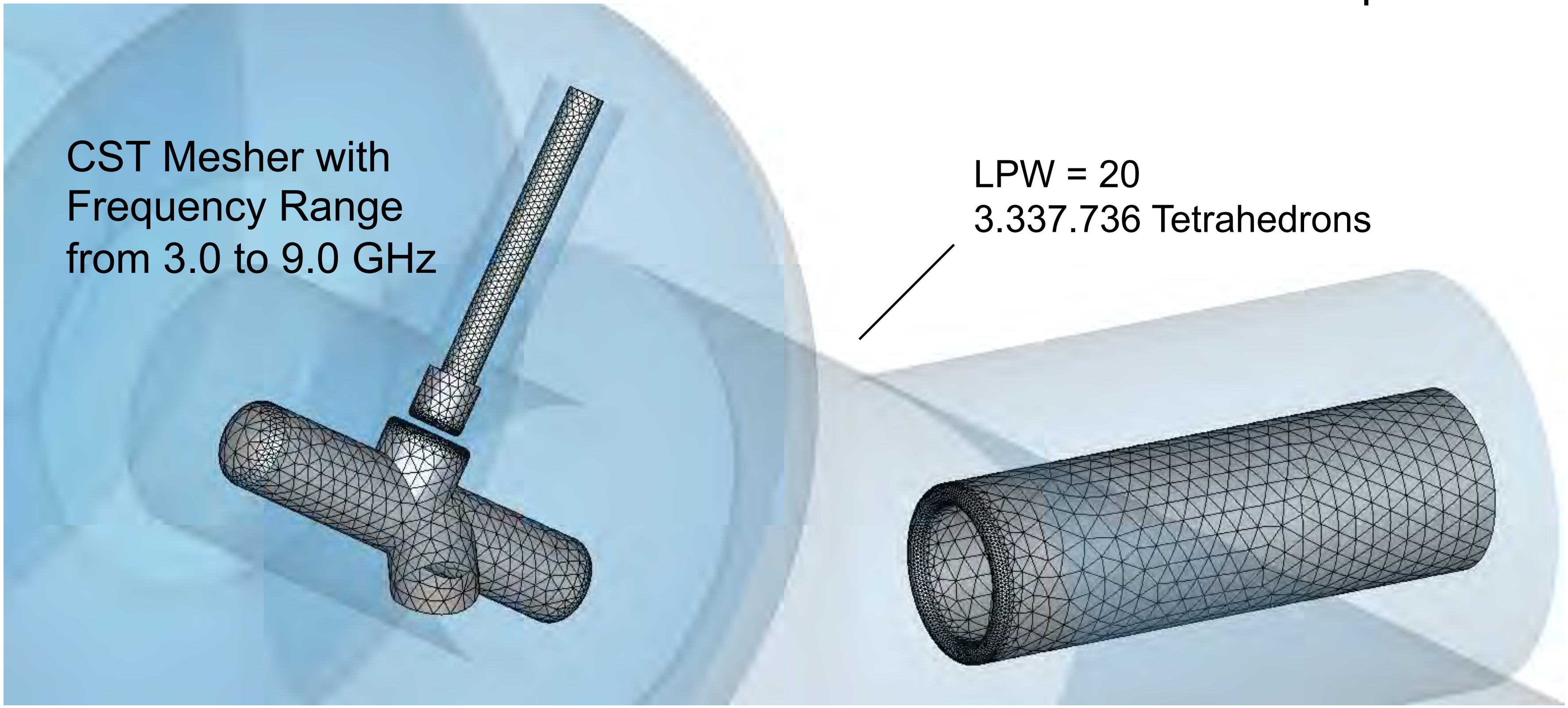
TESLA Resonators

- TESLA 3.9 GHz Cavity
  - CAD Model of the Vacuum with surface mesh on the PEC couplers



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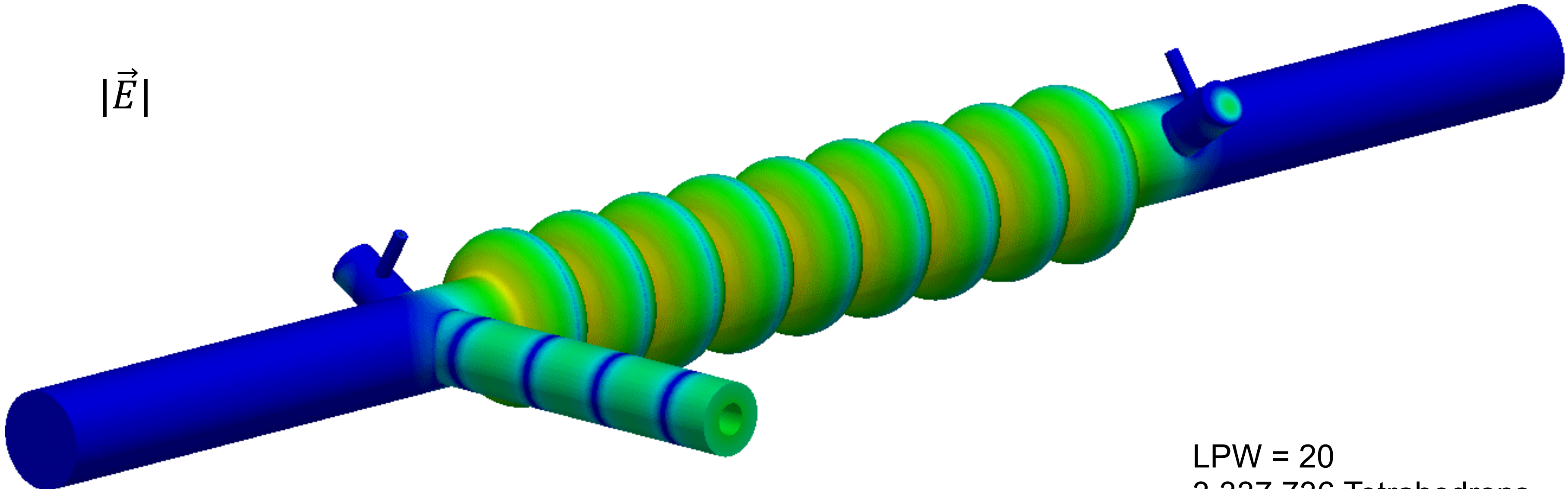
TESLA Resonators

- TESLA 3.9 GHz Cavity
  - Fundamental mode

    Absolute value of the electric field strength

$|\vec{E}|$



LPW = 20
3.337.736 Tetrahedrons

Logarithmic scale from 1e4 to 1e7 V/m

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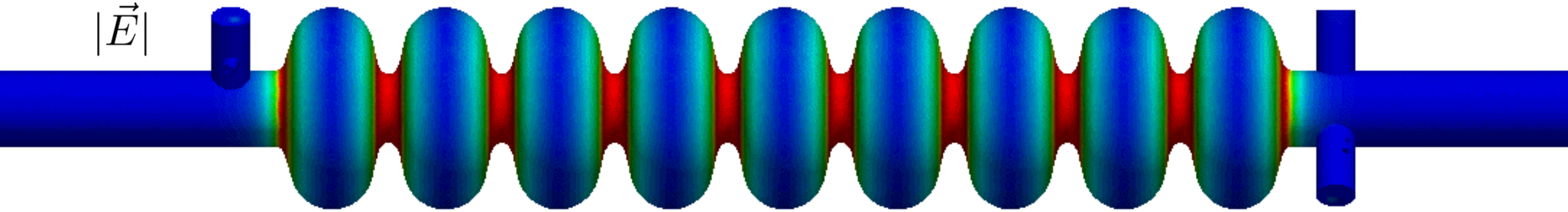
TESLA Resonators

- Simulation results
  - Accelerating mode (monopole #9)

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

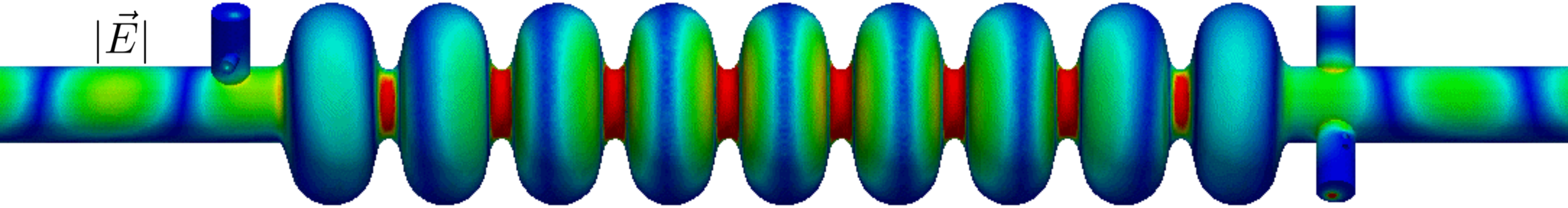
$|\vec{E}|$



  - Higher-order mode (dipole #37)

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

$|\vec{E}|$



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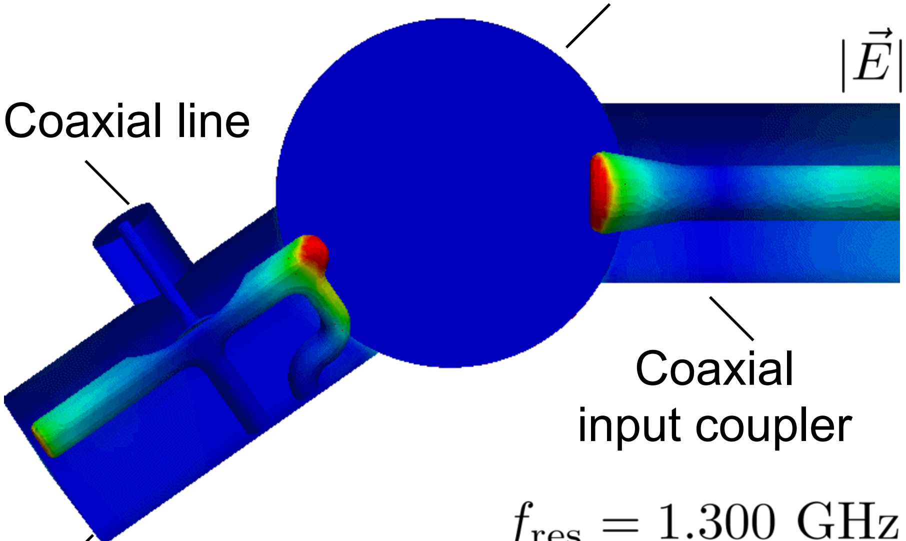
TESLA Resonators

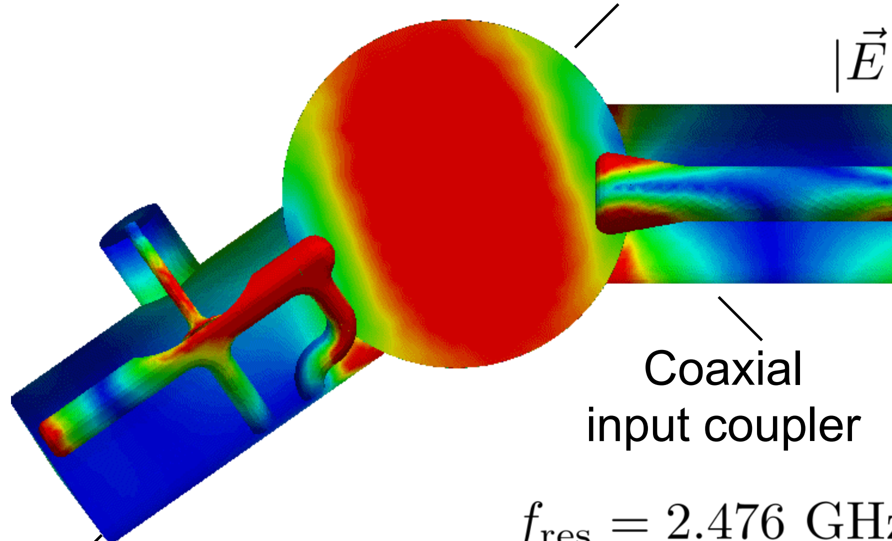
- Simulation results

Accelerating mode (monopole #9)



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

Higher-order mode (dipole #37)



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

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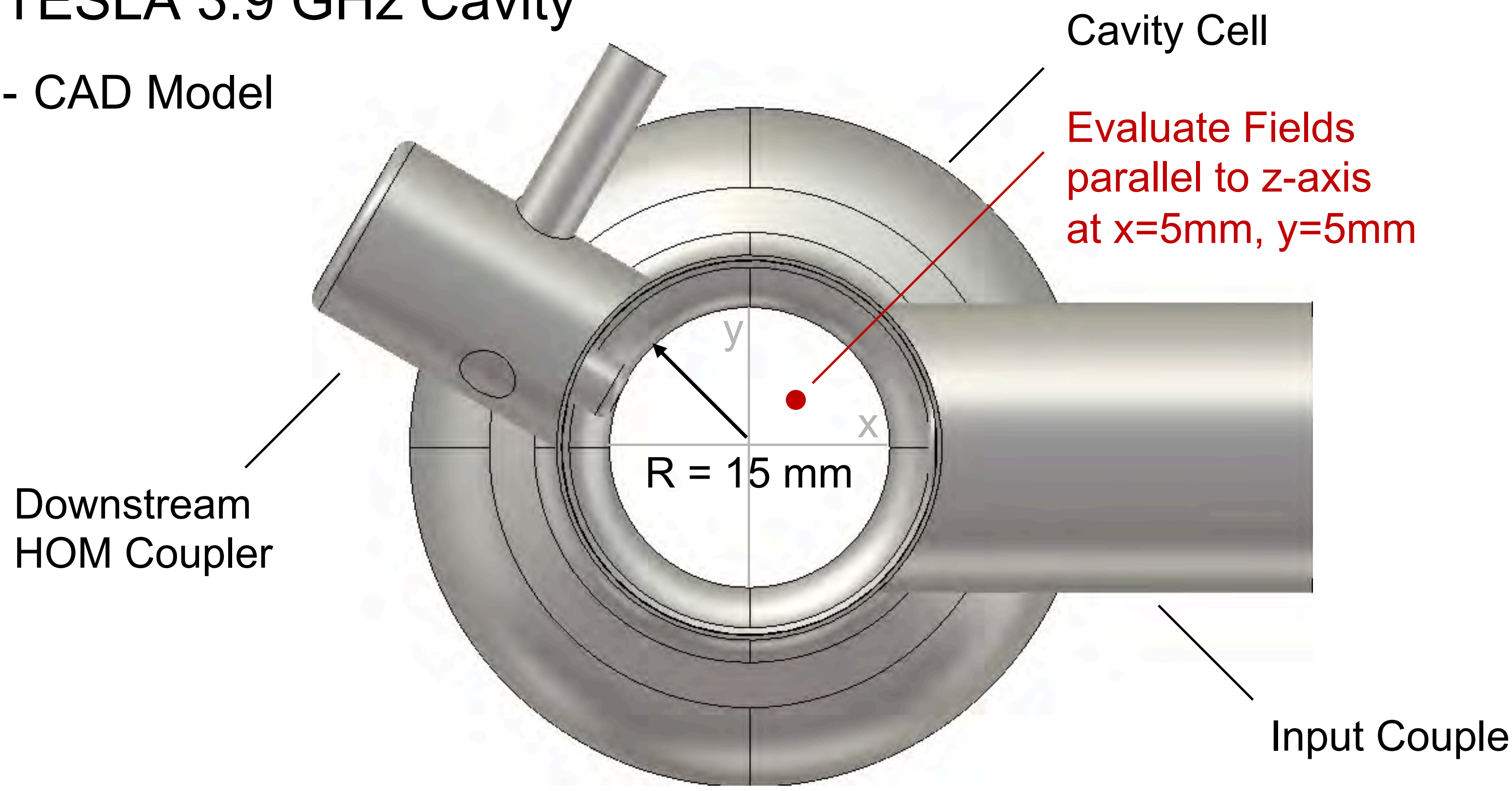
Simulation Results

- TESLA 3.9 GHz Cavity
  - CAD Model



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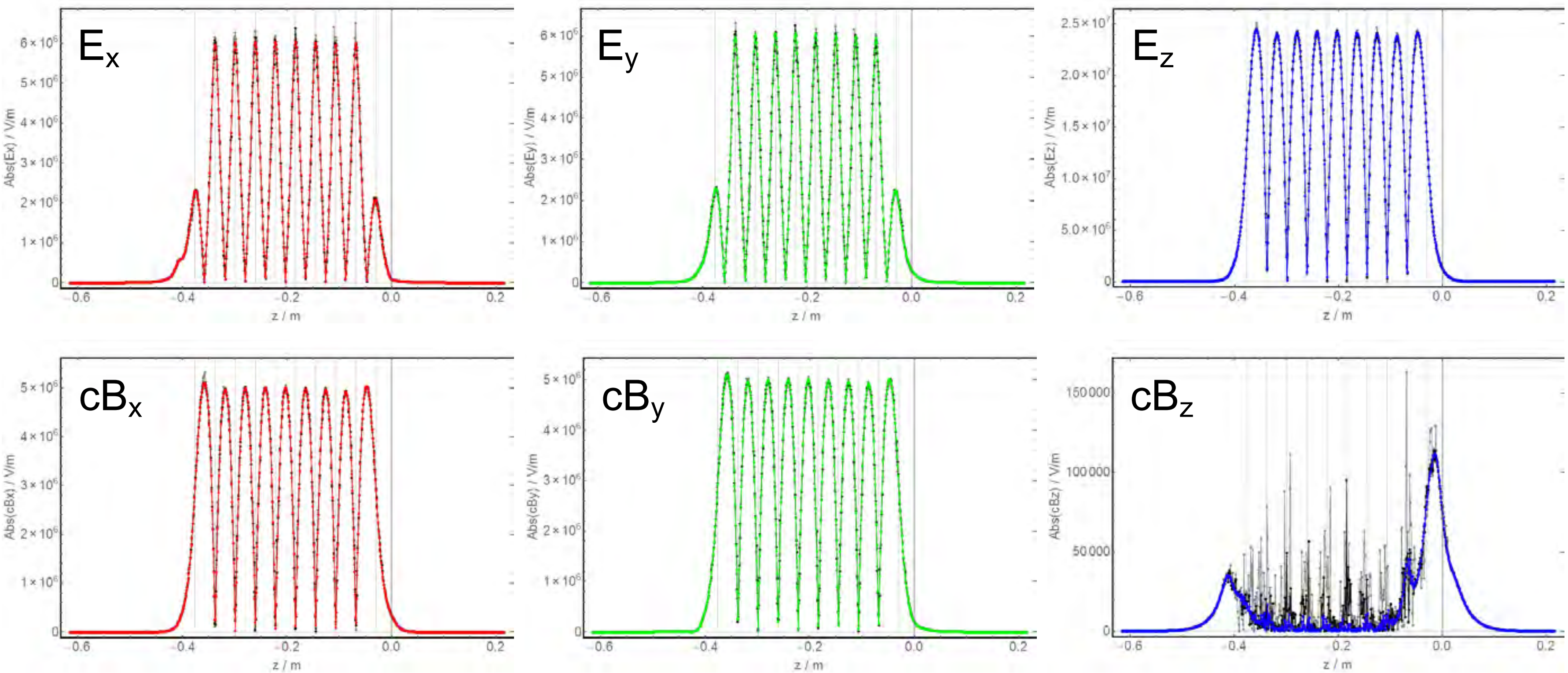
Simulation Results

- Field components parallel to the cavity axis (LPW 4,8,16)
  - Transversal offset at x_0 = 5 mm, y_0 = 5 mm



Wolfgang Ackermann

Simulation Results

- TESLA 3.9 GHz Cavity
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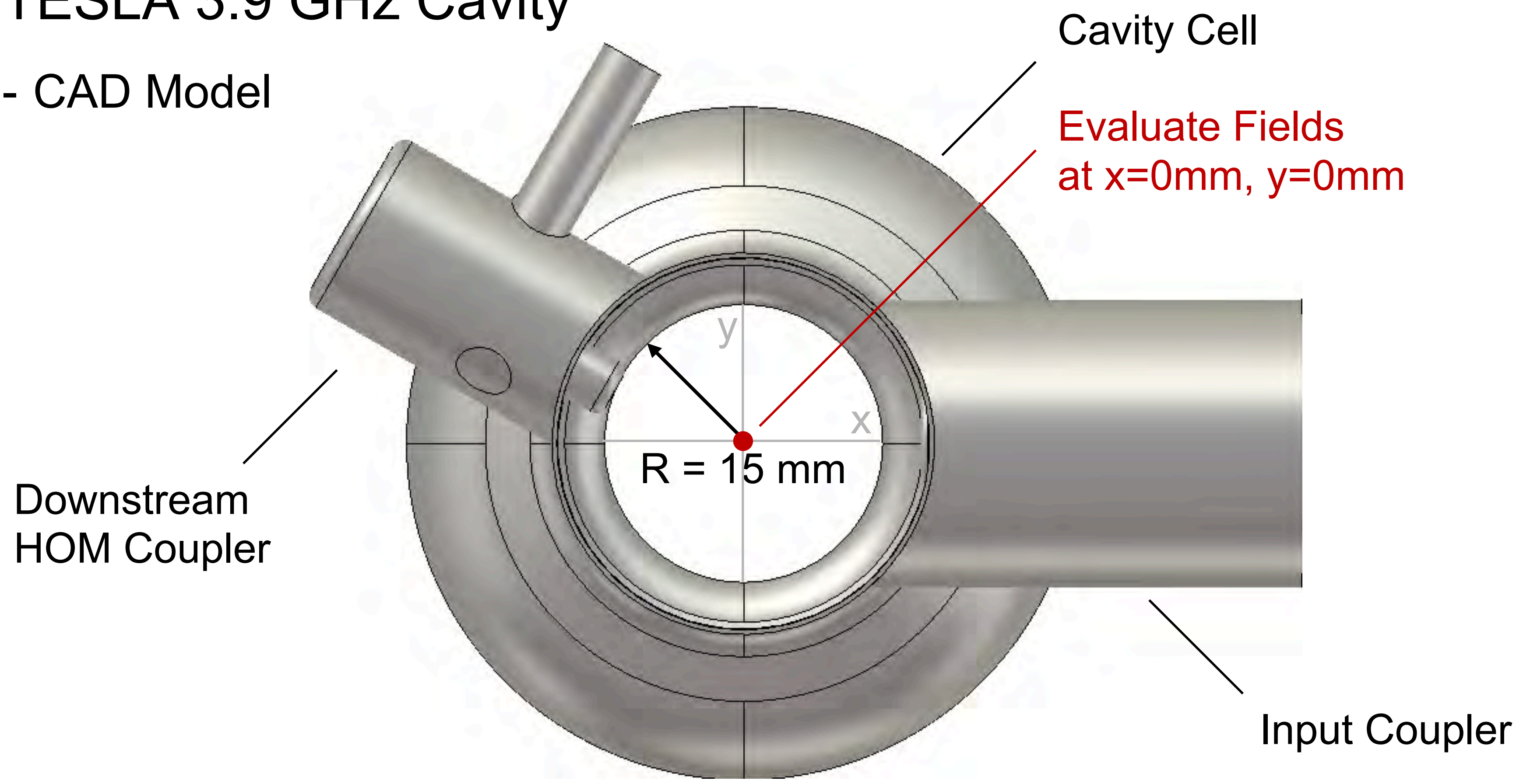

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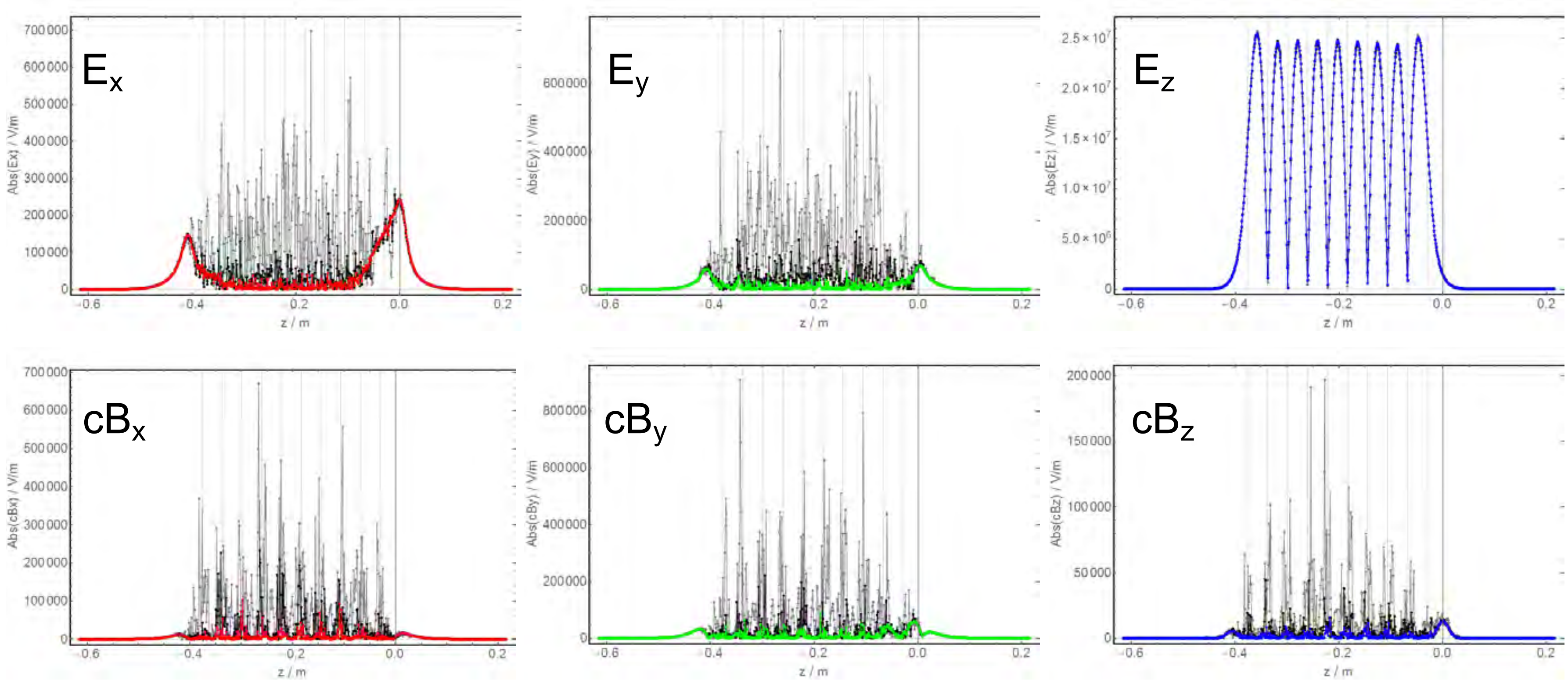
Simulation Results

- Field components parallel to the cavity axis (LPW 4,8,16)
  - Transversal offset at x_0 = 0 mm, y_0 = 0 mm



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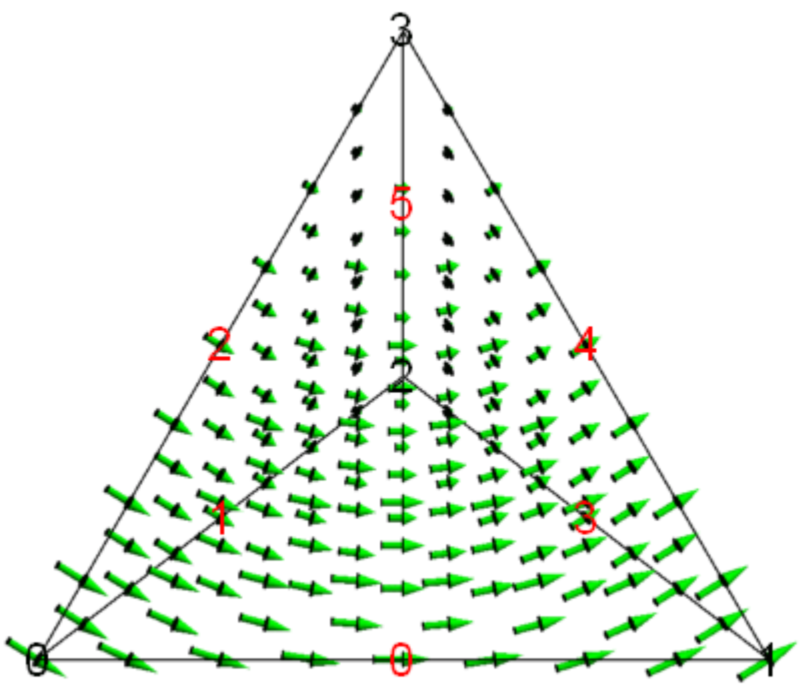
Simulation Results

- Field Representation in the Finite Element Method
  - Vector Basis Funktion $\vec{w}_0(\vec{r})$



Example:
Equilateral tetrahedron

Point	x	y	z
0	0	0	0
1	1	0	0
2	$\frac{1}{2}$	$\frac{1}{2}\sqrt{3}$	0
3	$\frac{1}{2}$	$\frac{1}{2\sqrt{3}}$	$\sqrt{2/3}$

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Simulation Results

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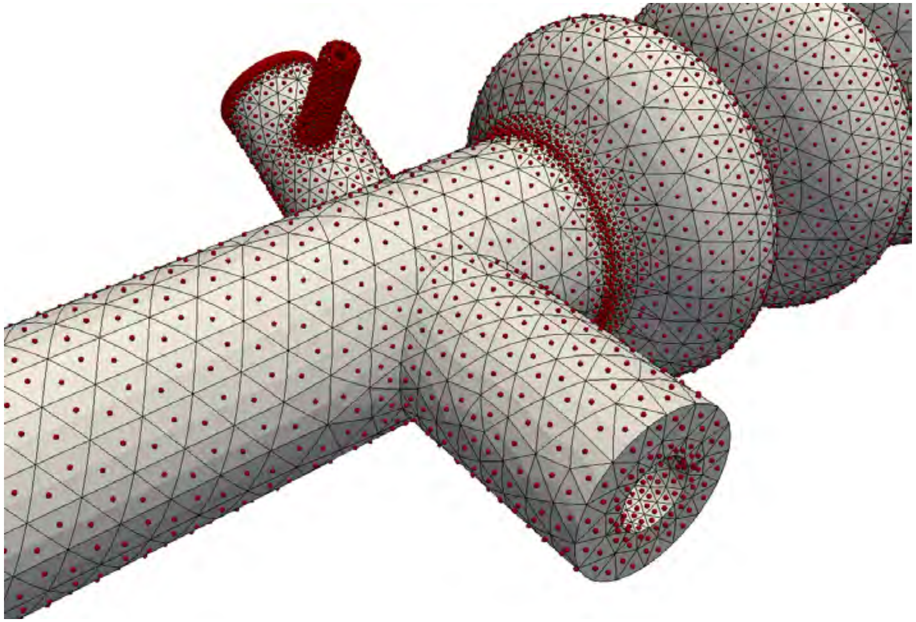
- Field reconstruction using the Kirchhoff integral
  - Field values inside a closed surface can be determined once the surface field components are available
  - Kirchhoff integral



$$G = \frac{e^{-ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|} \qquad k = \frac{2\pi f}{c_0}$$

$$\vec{E}(\vec{r}) = \int \Big(k(\vec{n}' \times ic_0\vec{B}')\, G - (\vec{n}' \times \vec{E}') \times \nabla G - (\vec{n}' \cdot \vec{E}')\, \nabla G \Big)\, \mathrm{d}A'$$

$$ic_0\vec{B}(\vec{r}) = \int \Big(k(\vec{n}' \times \vec{E}')\, G - (\vec{n}' \times ic_0\vec{B}') \times \nabla G - (\vec{n}' \cdot ic_0\vec{B}')\, \nabla G \Big)\, \mathrm{d}A'$$

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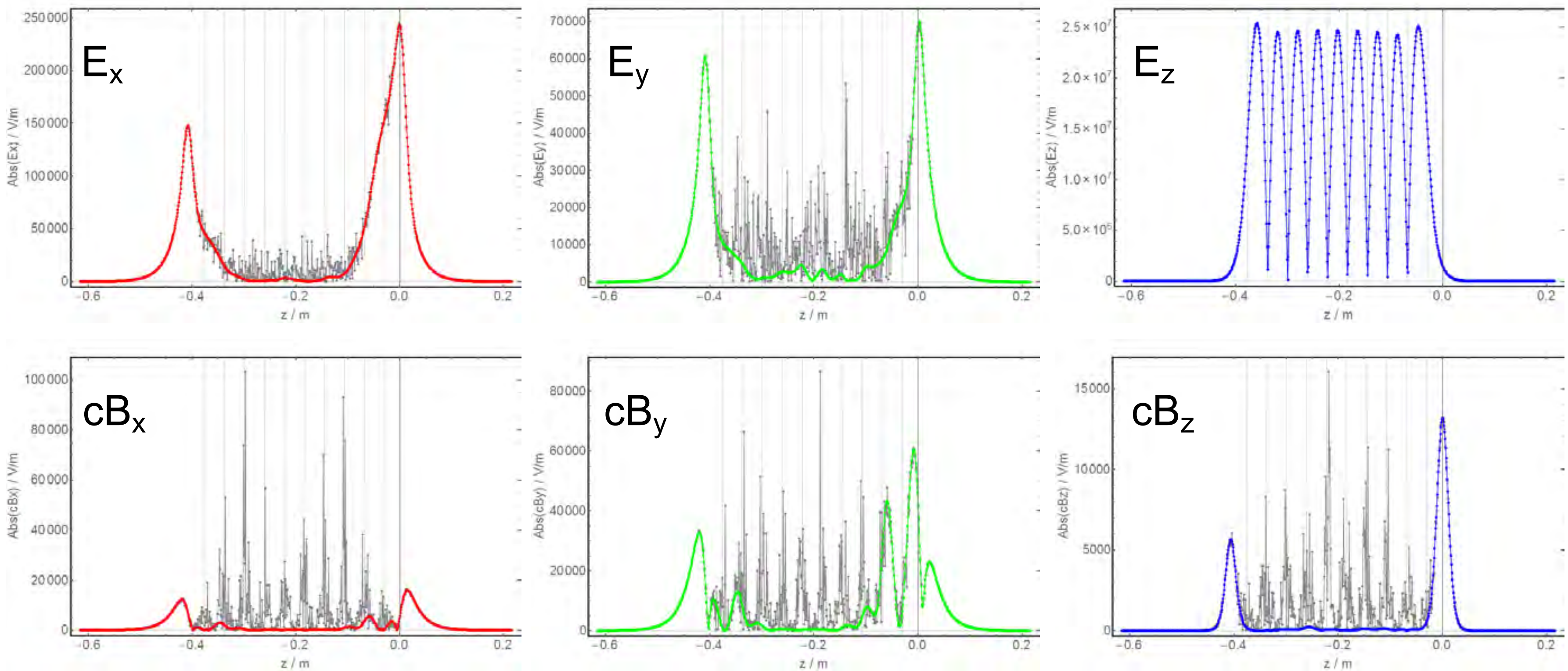
Simulation Results

- Field components parallel to the cavity axis (LPW 16)
  - Transversal offset at x_0 = 0 mm, y_0 = 0 mm



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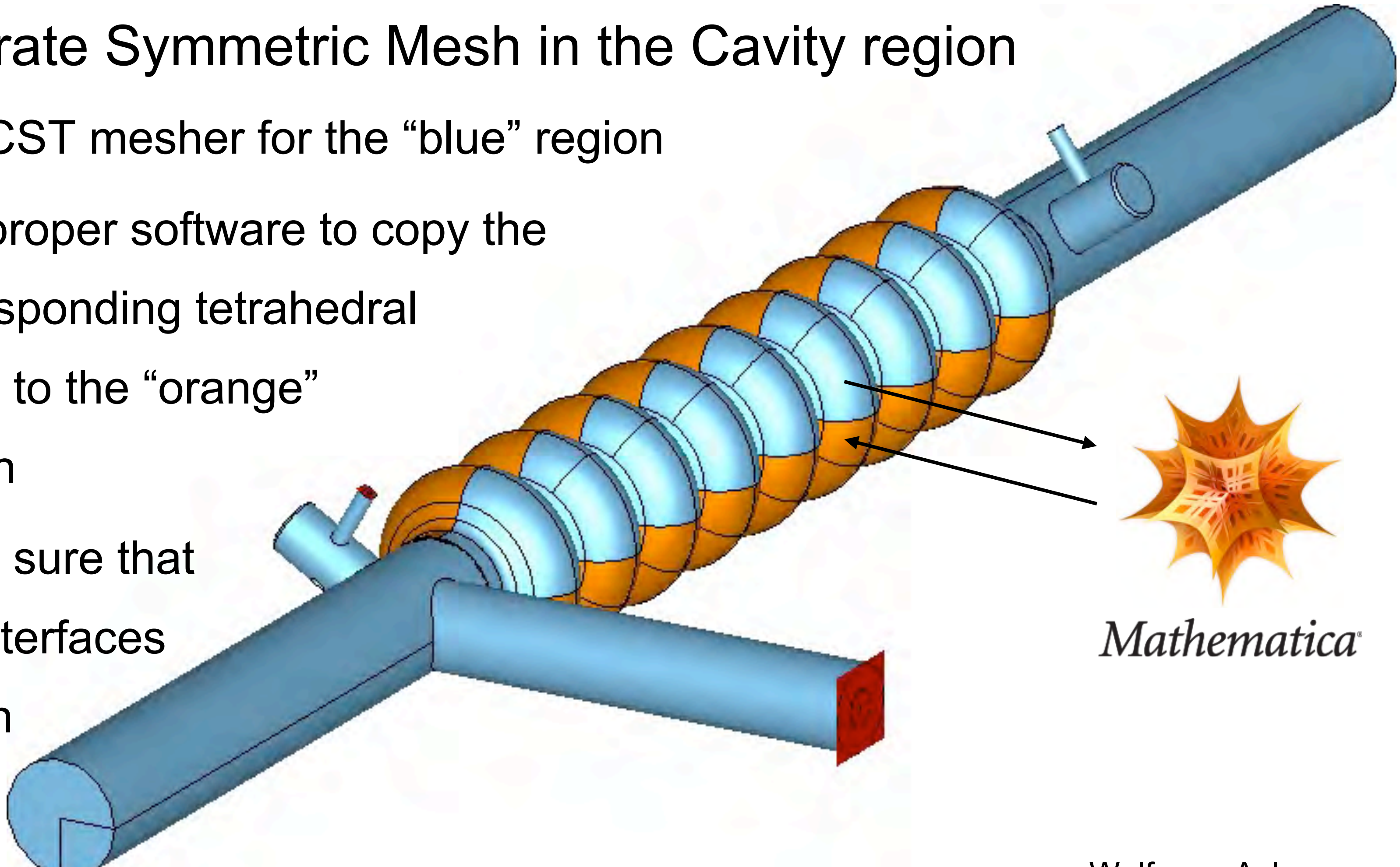
Simulation Results

- Generate Symmetric Mesh in the Cavity region
  - Use CST mesher for the “blue” region
  - Use proper software to copy the corresponding tetrahedral mesh to the “orange” region
  - Make sure that the interfaces match



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Simulation Results

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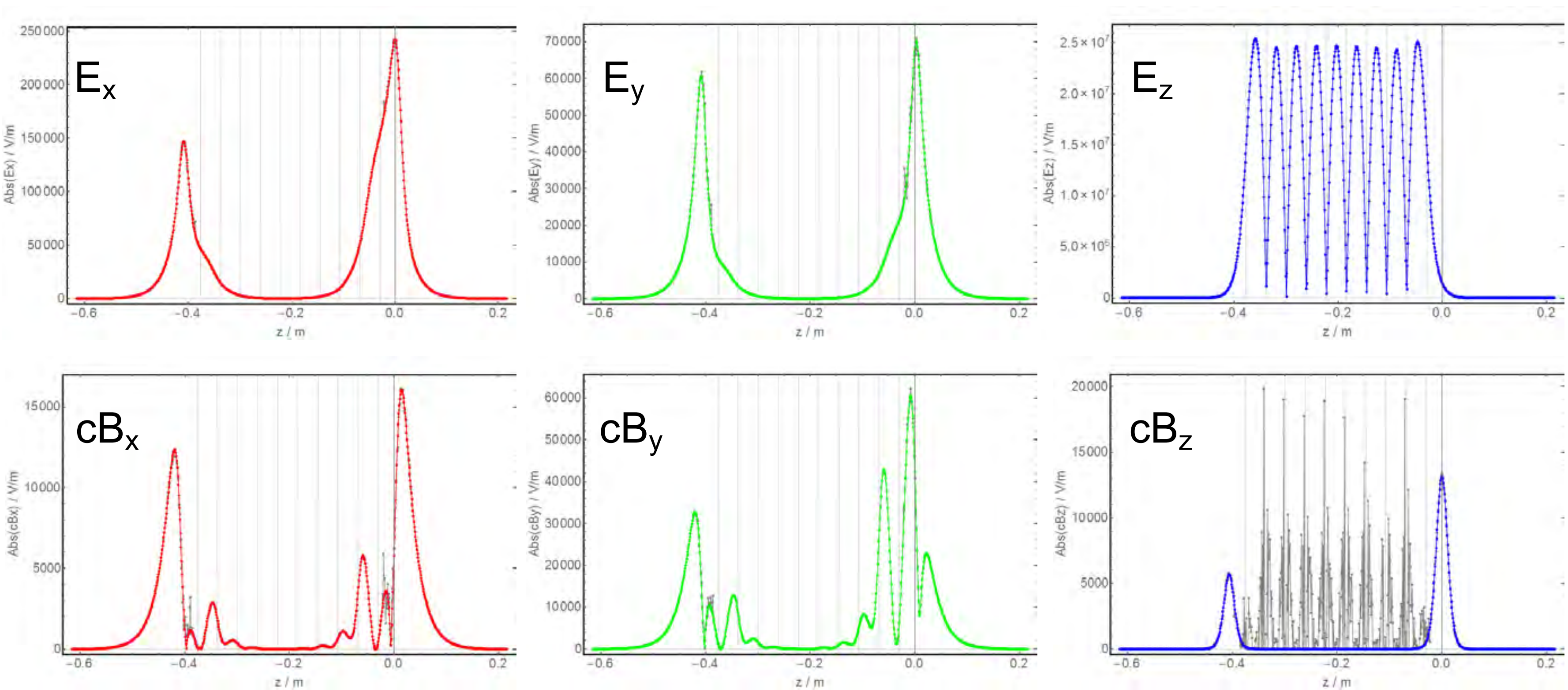
- Field components parallel to the cavity axis (LPW 16)
  - Transversal offset at x_0 = 0 mm, y_0 = 0 mm



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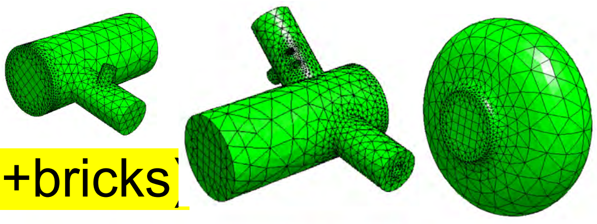
Categorisation : EM Field Simulation

CEM3D | PBCI | FD | CSRDG | PAMASO | REPTIL



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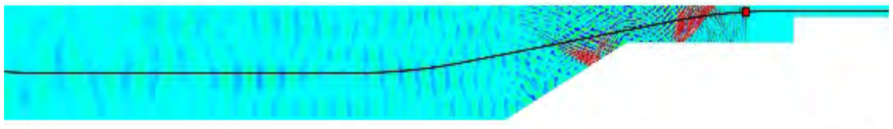
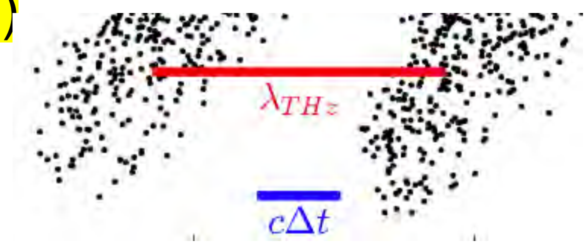
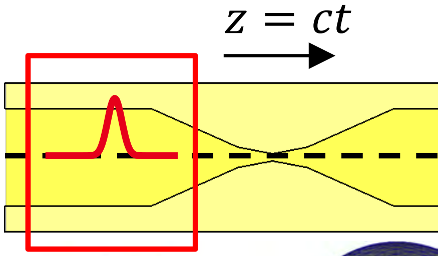
  - structured (hexahedra)
  - unstructured (tetrahedra, possibly +pyramids +bricks)
  - meshless



- volumetric discretisation
  - finite-difference time-domain (FDTD), finite-integration technique (FIT)
  - finite-element methods (FE)
  - discontinuous Galerkin
  - particle-particle models





- discretisation in time
  - time domain
  - frequency domain
  - eigenmodes