Recent developments in wakefield computation

E. Gjonaj, D. Bizzozero, H. De Gersem
Computational Elektromagnetics Lab, Technische Universität Darmstadt, Germany

ICAP 2018

October 20 — 24, 2018, Key West, Florida, USA

Contents

- Wakefield simulation in the time domain
- CSR wakefield computations with high order DG
- Calculation of wakefields in the frequency domain
- Summary

* S. Schmid, *REPTIL - A relativistic 3D space charge particle tracking code based on the fast multipole method* (Wed, 9:15)

Wakefield simulation in the time domain

TECHNISCHE UNIVERSITÄT DARMSTADT

- Wakefield codes based on the solution of Maxwell's equations in the time domain

$$\frac{\partial B}{\partial t} = -\nabla \times E,$$

$$\frac{\partial \varepsilon E}{\partial t} = \nabla \times \frac{1}{\mu} B - j,$$

$$\boxed{j = qc\rho(x, y, z - ct)}$$ rigid, ultra-relativistic bunch

- Wake potentials and coupling impedances by post processing simulated field data

$$W_z(r_\perp, s) = -\frac{1}{q} \int_{-\infty}^{\infty} dz\, E_z\left(r_\perp, z, t = \frac{z+s}{c}\right)$$

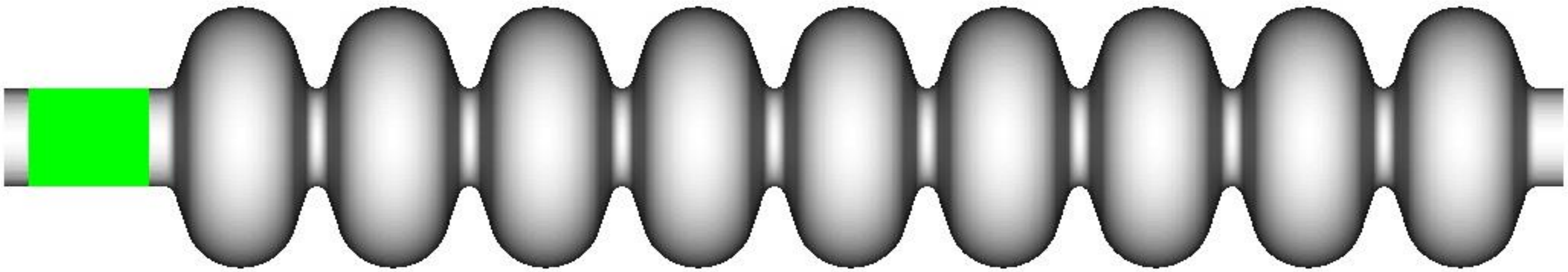
$$\underbrace{\frac{\partial}{\partial s} W_\perp(r_\perp, s) = -\nabla_\perp W_s(r_\perp, s)}_{\text{Panofsky-Wenzel theorem}}$$

Panofsky-Wenzel theorem

$$Z_z(r_\perp, \omega) = \frac{1}{c\rho(r_\perp, \omega)} \int_{-\infty}^{\infty} dz W_z(r_\perp, s)\, e^{-\frac{i\omega s}{c}}$$

The moving window

- Fields are calculated within a small computational frame which is co-mowing with the bunch
  - Numerically efficient for large structures
  - Can handle complicated 3D-geometry by on-the-fly meshing
  - Can handle very short bunches



Wakefield (E_z) in a TESLA cavity computed with PBCI

Dispersion-free methods

- Exact propagation in z-direction by splitting of the FDTD operators

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ e \end{pmatrix} = \begin{pmatrix} 0 & -C \\ C^T & 0 \end{pmatrix} \cdot \begin{pmatrix} h \\ e \end{pmatrix}$$

PBCI	ECHO
LT	TE/TM
$e^{A\cdot\Delta t} = R_T\left(\frac{\Delta t}{2}\right)R_L(\Delta t)R_T\left(\frac{\Delta t}{2}\right)$	$e^{A\cdot\Delta t} = R_L\left(\frac{\Delta t}{2}\right)R_T(\Delta t)R_L\left(\frac{\Delta t}{2}\right)$

update equations

PBCI:

$$\begin{cases} H\_XY(\Delta t/4) \\ E\_XY(\Delta t/2) \leftarrow J_z \\ H\_XY(\Delta t/4) \end{cases}$$
$$\begin{cases} H\_Z(\Delta t/2) \\ E\_Z(\Delta t) \\ H\_Z(\Delta t/2) \end{cases}$$
$$\begin{cases} H\_XY(\Delta t/4) \\ E\_XY(\Delta t/2) \leftarrow J_z \\ H\_XY(\Delta t/4) \end{cases}$$

ECHO:

$$\begin{cases} H\_Z(\Delta t/4) \\ E\_Z(\Delta t/2) \\ H\_Z(\Delta t/4) \end{cases}$$
$$\begin{cases} H\_XY(\Delta t/2) \\ E\_XY(\Delta t) \leftarrow J_z \\ H\_XY(\Delta t/2) \end{cases}$$
$$\begin{cases} H\_Z(\Delta t/4) \\ E\_Z(\Delta t/2) \\ H\_Z(\Delta t/4) \end{cases}$$

number of operations: no = 30 (PBCI), no = 24 (ECHO)

numerical stability

PBCI:

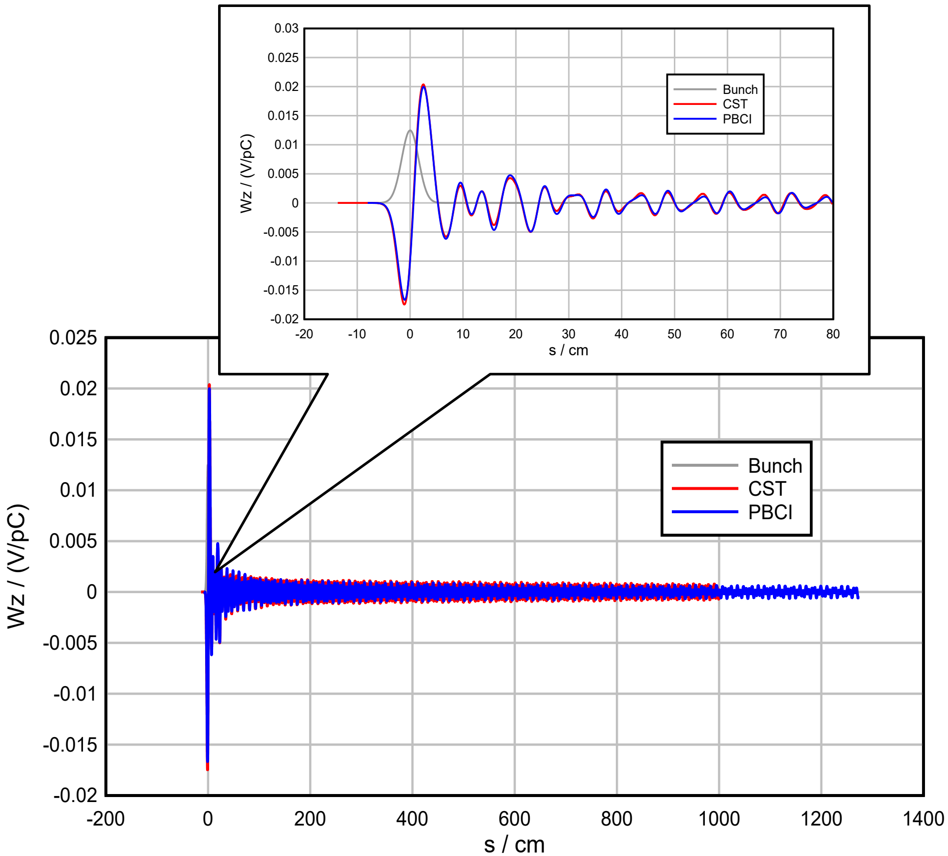
$$\begin{cases} c\,\Delta t \le 2\left(\frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2}\right)^{-1/2} \\ c\,\Delta t \le \Delta_z \end{cases}$$

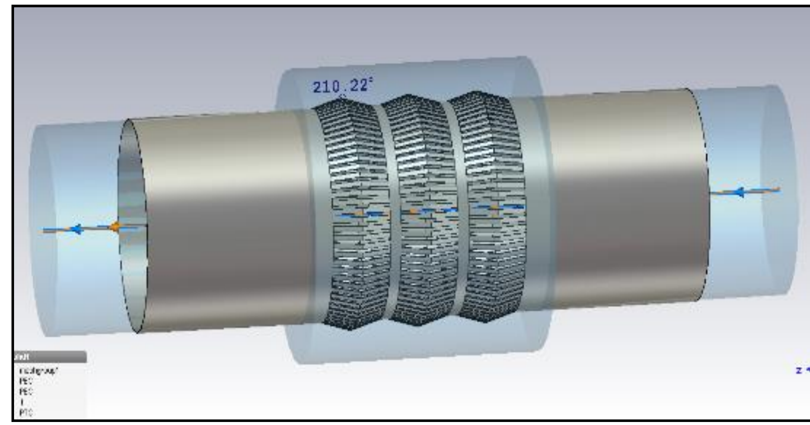
ECHO:

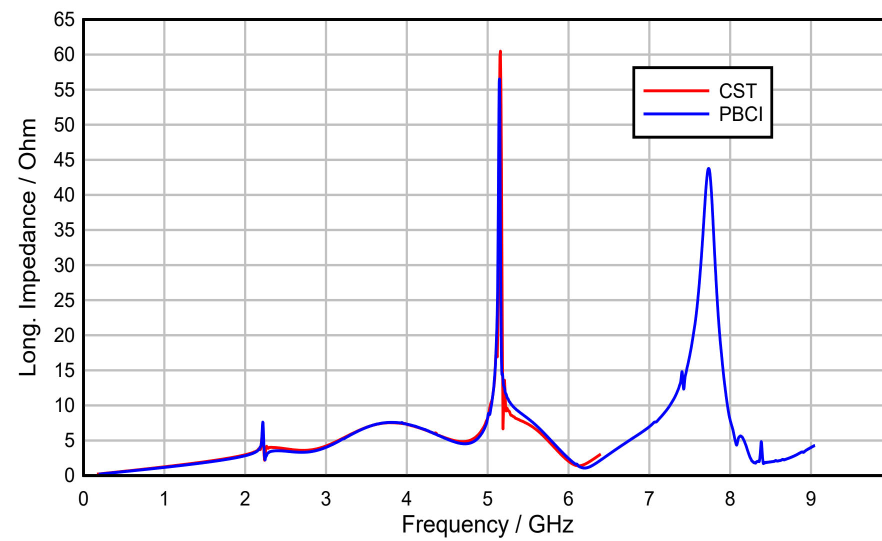
$$\begin{cases} c\,\Delta t \le \left(\frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2}\right)^{-1/2} \\ c\,\Delta t \le \Delta_z \end{cases}$$

Electrically large structures

- LHC RF-Fingers







Resistive wall wakefields

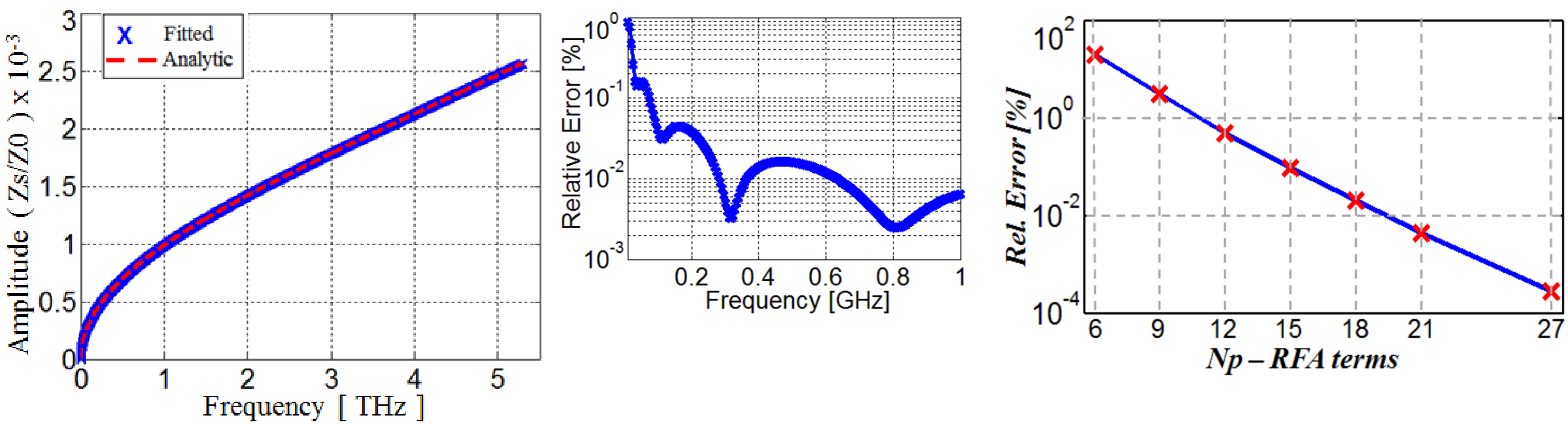
- Generalized surface impedance functions

$$\vec{E}_\tau(\omega) = Z_s(\omega)\,[\vec{n} \times \vec{H}_\tau(\omega)] \;\Rightarrow\; Z_s(\omega) = j\omega L + \alpha_0 + \sum_{i=1}^{Np} \frac{\alpha_i}{j\omega + \beta_i}$$

Pole-residue approximation

- "Vector fitting" of resistive wall impedance: $Z_s(\omega) \cong \sqrt{\frac{j\omega\mu}{\sigma(\omega) + j\omega\varepsilon}}$

Example : Cu – N=21, ~ 10MHz-5THz, Δf~5MHz



Resistive wall wakefields

- Auxiliary Differential Equation (ADE) formulation

$$\vec{n}\times\vec{E}(t) = L\cdot\frac{d}{dt}\left[\vec{n}\times\vec{n}\times\vec{H}(t)\right] + \sum_{i=0}^{Np}\vec{n}\times\vec{G}_i(t)$$

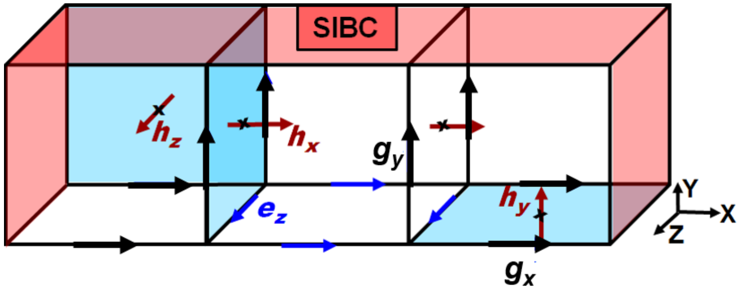
$$\vec{n}\times\vec{G}_0 = \alpha_0\,[\vec{n}\times\vec{n}\times\vec{H}]$$

$$\frac{d}{dt}\vec{n}\times\vec{G}_i + \beta_i\vec{n}\times\vec{G}_i = \alpha_i\,[\vec{n}\times\vec{n}\times\vec{H}]$$

set of ADE for magnetic “surface currents” (Woyna, Gjonaj, 2014)

- Modified discrete Maxwell’s equations:

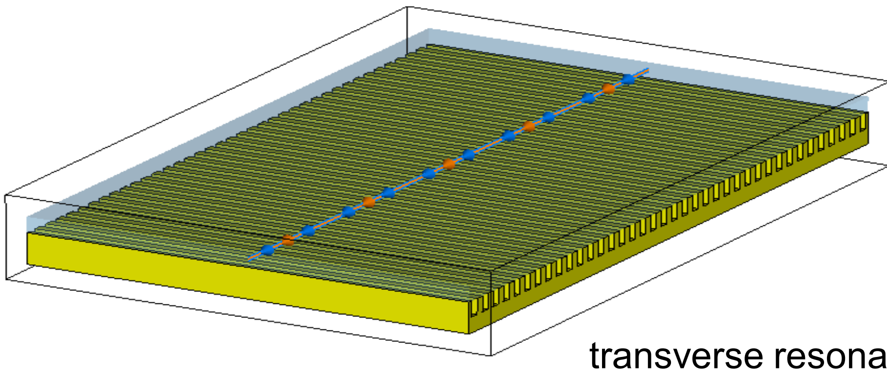
$$\frac{d}{dt}\begin{pmatrix}\widehat{e}\\ \widehat{h}\\ 0\\ g_0\\ \vdots\\ g_N\end{pmatrix} = \begin{pmatrix} 0 & M_\varepsilon^{-1}C^T & 0 & 0 & \cdots & 0\\ -M_\mu^{-1}C & 0 & C_B & C_B & \cdots & C_B\\ 0 & \alpha_0 & 1 & 0 & \cdots & 0\\ 0 & -\alpha_1 & 0 & \beta_1 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & -\alpha_N & 0 & 0 & \cdots & \beta_N\end{pmatrix}\begin{pmatrix}\widehat{e}\\ \widehat{h}\\ g_0\\ g_1\\ \vdots\\ g_N\end{pmatrix}$$



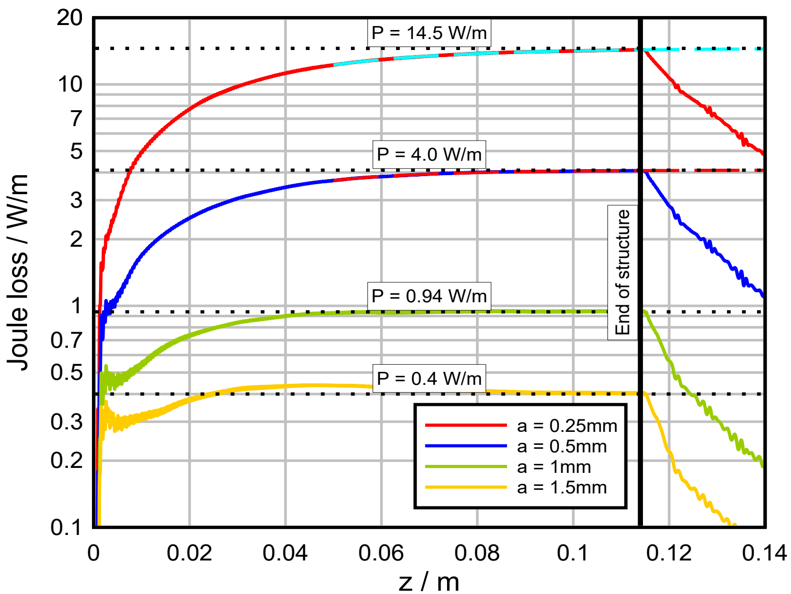
allocation of SIBC currents on grid

Open structures

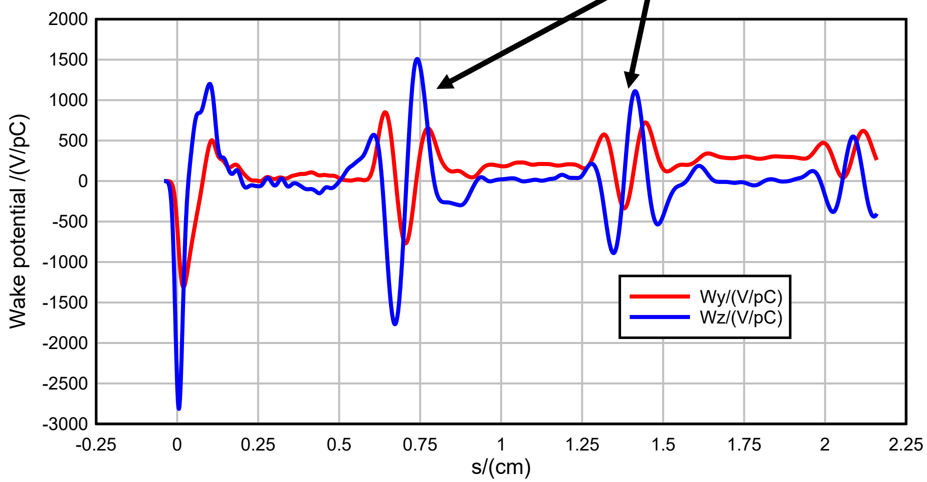
- Single plate dechirper (with Bane, Stupakov)



Joule losses



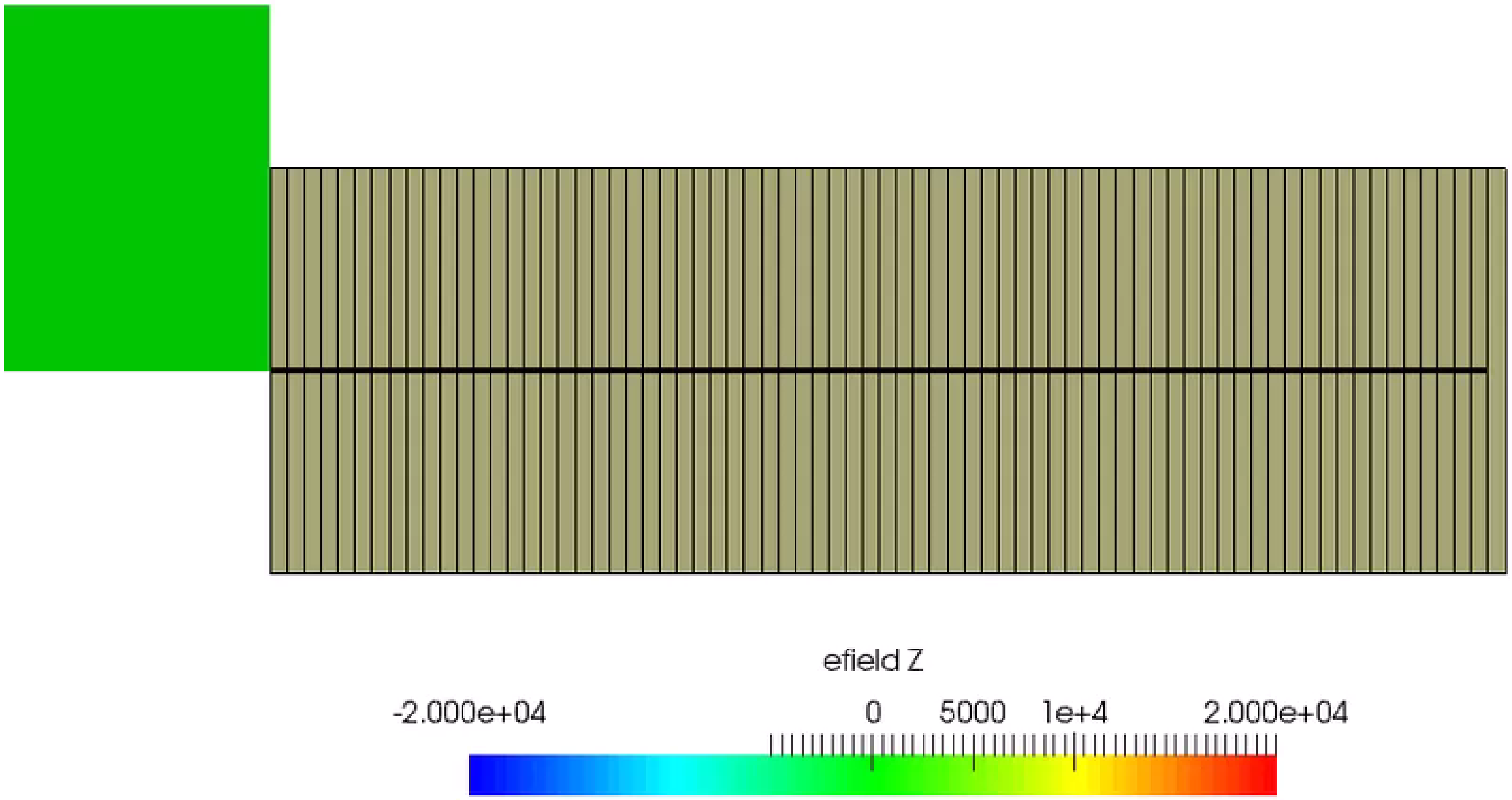
transverse resonances



Wake potentials for a 100um bunch

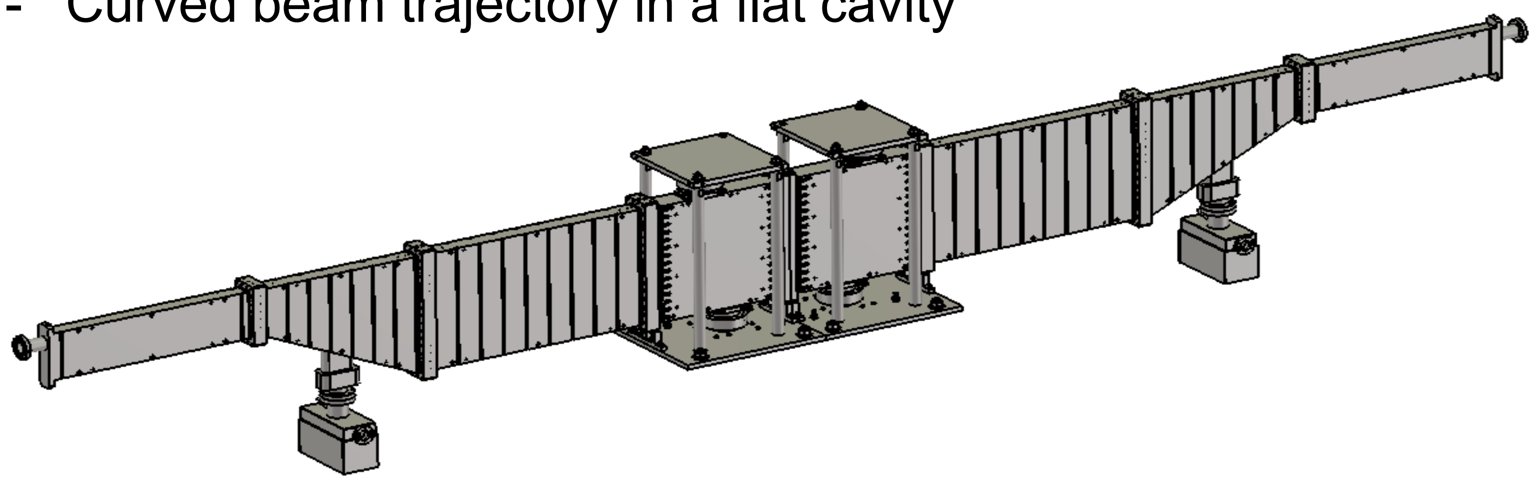
Open structures

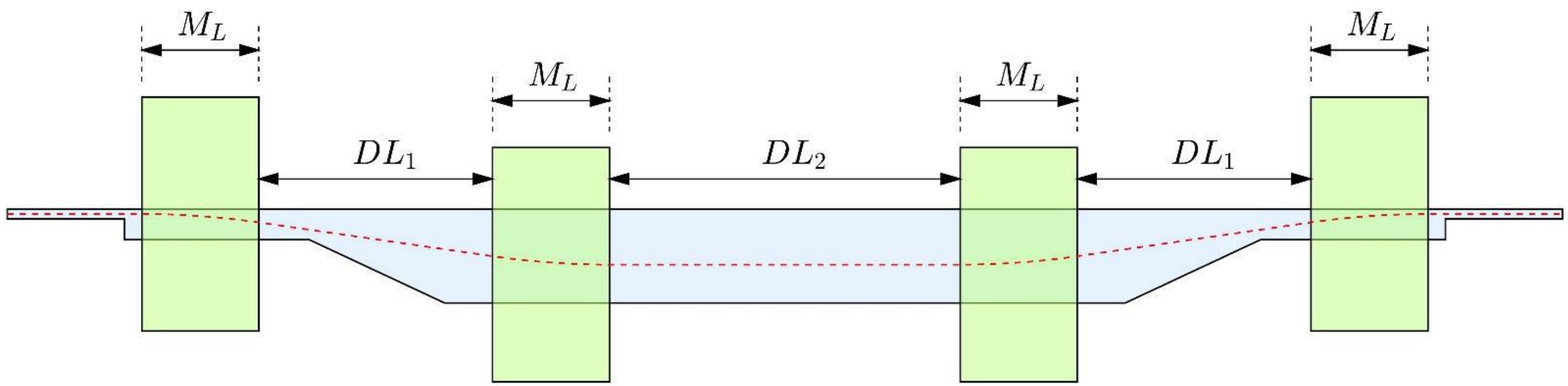
- Single plate dechirper (with Bane, Stupakov)



CSR computations with high order DG

- DESY XFEL bunch compressor (BC0)
  - Curved beam trajectory in a flat cavity





CSR computations with high order DG

- CSRDG code (Bizzozero, Ellison, Warnock)
  1. Transform Maxwell's equations to Frenet-Serret coordinates
  2. Apply a Fourier mode decomposition in the y-direction

$$\frac{1}{Z_0}\frac{\partial E_{sp}}{\partial \tau} = \frac{\partial \widetilde{H}_{yp}}{\partial x} + \alpha_p H_{xp}$$

$$\frac{1}{Z_0}\frac{\partial E_{xp}}{\partial \tau} = -\alpha_p H_{sp} - \frac{1}{\eta}\frac{\partial \widetilde{H}_{yp}}{\partial s} - \frac{1}{\eta} qcG_p\lambda'(s-\tau)\Theta(x)$$

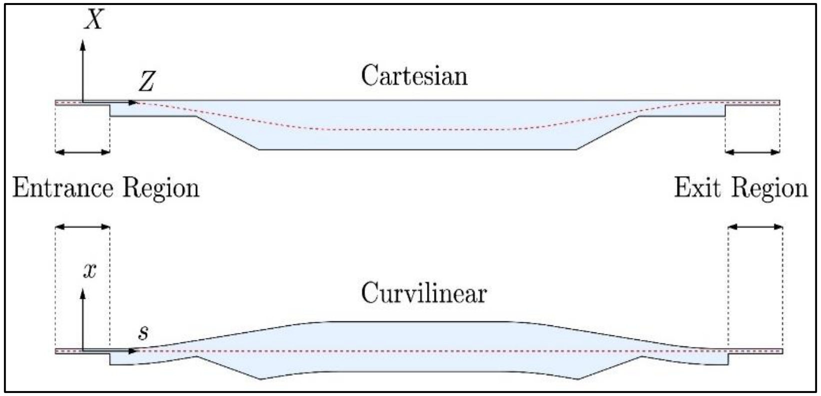
$$\frac{1}{Z_0}\frac{\partial E_{yp}}{\partial \tau} = \frac{1}{\eta}\frac{\partial H_{xp}}{\partial s} - \frac{\partial H_{sp}}{\partial x} - \frac{\kappa}{\eta}H_{sp}$$

$$Z_0\frac{\partial H_{sp}}{\partial \tau} = \alpha_p E_{xp} - \frac{\partial E_{yp}}{\partial x}$$

$$Z_0\frac{\partial H_{xp}}{\partial \tau} = \frac{1}{\eta}\frac{\partial E_{yp}}{\partial s} - \alpha_p E_{sp}$$

$$Z_0\frac{\partial \widetilde{H}_{yp}}{\partial \tau} = \frac{\partial E_{sp}}{\partial x} + \frac{\kappa}{\eta}E_{sp} - \frac{1}{\eta}\frac{\partial E_{xp}}{\partial s} + qZ_0cG_p\lambda'(s-\tau)\Theta(x)$$

Transformation of geometry



CSR computations with high order DG

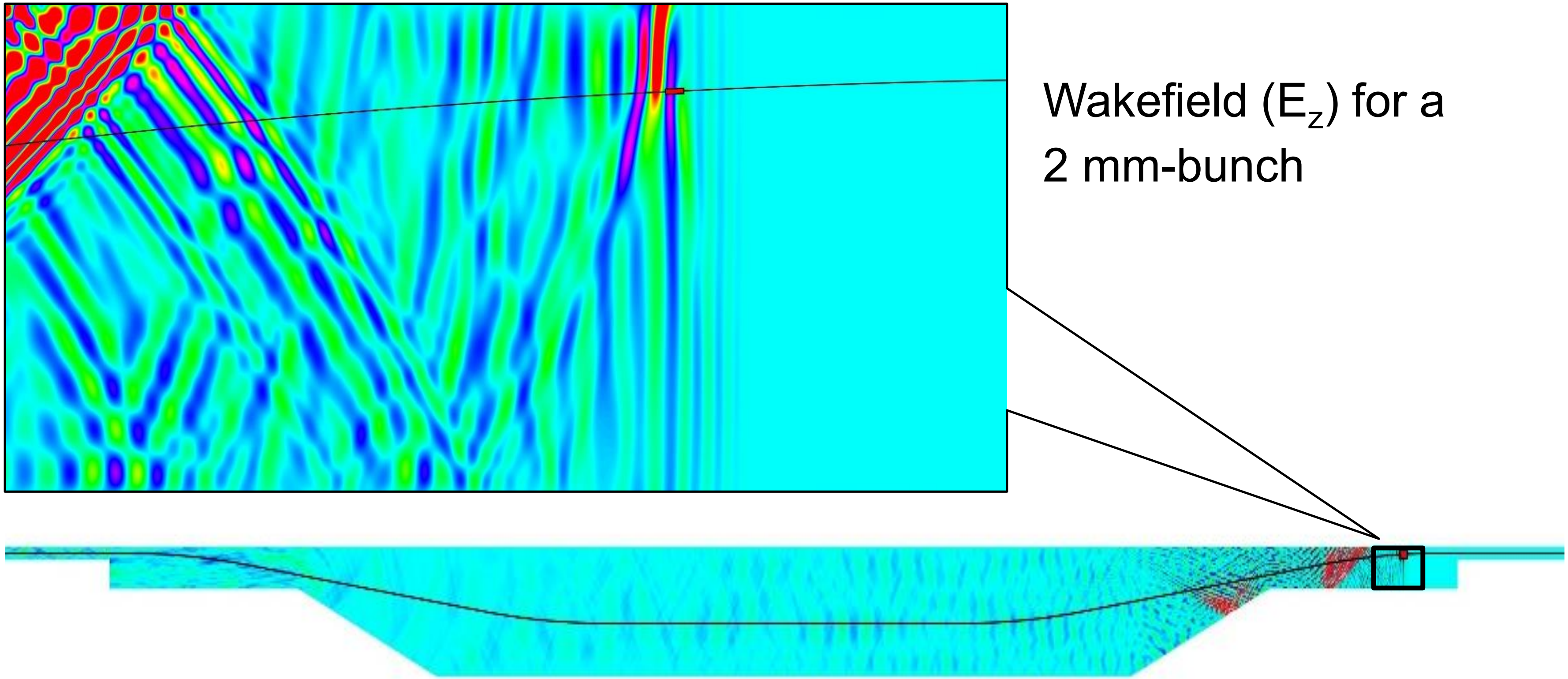
- CSRDG code (Bizzozero, Ellison, Warnock)
  3. Discretize the 2D-equations for each mode using the high order nodal discontinuous Galerkin method

$$
\begin{aligned}
\frac{dE_{sp}}{d\tau} =& Z_0 \mathcal{D}_x \widetilde{H}_{yp} + Z_0 \alpha_p H_{xp} \\
&+ \frac{1}{2}(J\mathcal{M})^{-1}\Big(- Z_0 \mathbf{n}_x [\![\widetilde{H}_{yp}]\!] - [\![E_{sp}]\!] + \mathbf{n}_s(\mathbf{n}_s [\![E_{sp}]\!] + \mathbf{n}_x [\![E_{xp}]\!])\Big) \\
\frac{dE_{xp}}{d\tau} =& - Z_0 \alpha_p H_{sp} - \frac{Z_0}{1+\kappa x}\mathcal{D}_s \widetilde{H}_{yp} - \frac{Z_0}{1+\kappa x} qcG_p \lambda'(s-\tau)\Theta(x) \\
&+ \frac{1}{2}(J\mathcal{M})^{-1}\Big(\frac{Z_0}{1+\kappa x}\mathbf{n}_s [\![\widetilde{H}_{yp}]\!] - [\![E_{xp}]\!] + \mathbf{n}_x(\mathbf{n}_s [\![E_{sp}]\!] + \mathbf{n}_x [\![E_{xp}]\!])\Big) \\
\frac{dE_{yp}}{d\tau} =& \frac{Z_0}{1+\kappa x}\mathcal{D}_s H_{xp} - Z_0 \mathcal{D}_x H_{sp} - \frac{Z_0 \kappa}{1+\kappa x} H_{sp} \\
&+ \frac{1}{2}(J\mathcal{M})^{-1}\Big(- \frac{Z_0}{1+\kappa x}\mathbf{n}_s [\![H_{xp}]\!] + Z_0 \mathbf{n}_x [\![H_{sp}]\!] - [\![E_{yp}]\!]\Big)
\end{aligned}
$$

…and similarly for the magnetic components

CSR computations with high order DG

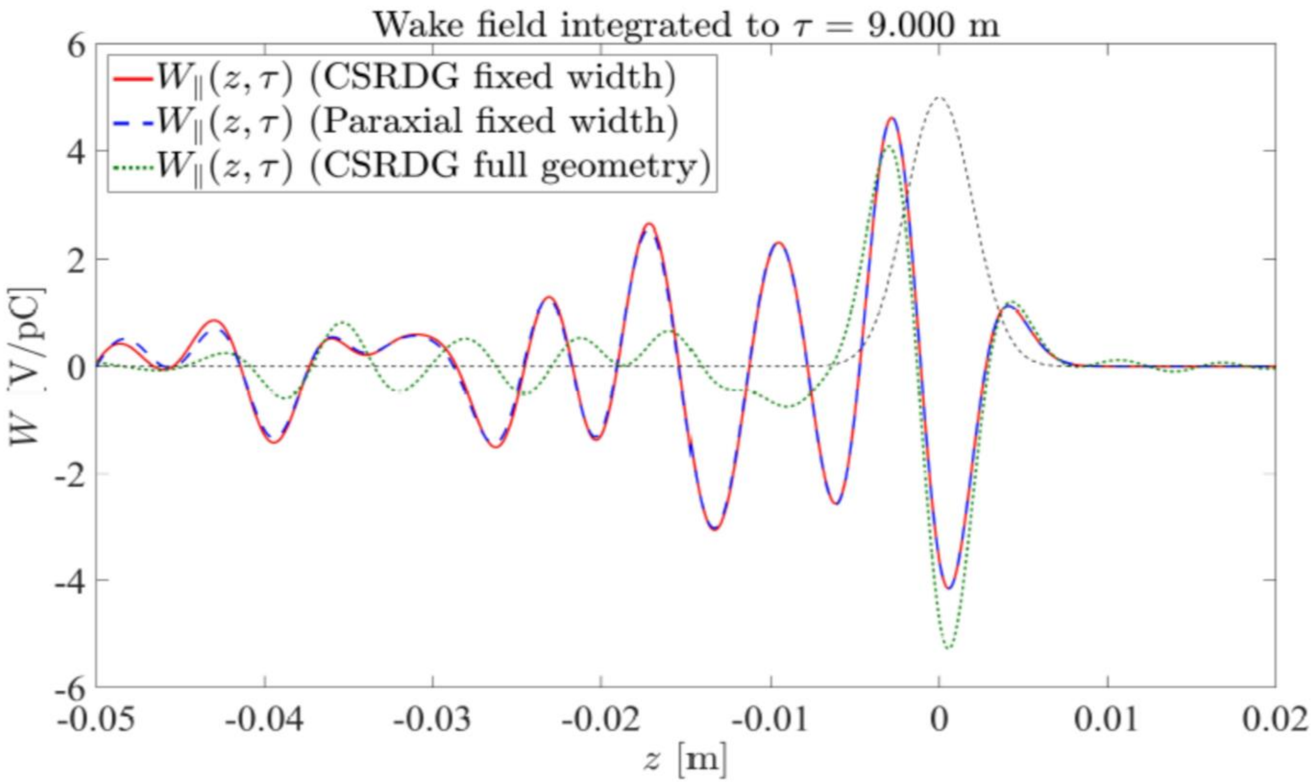
- CSRDG code (Bizzozero, Ellison, Warnock)



Wakefield (E_z) for a 2 mm-bunch

CSR computations with high order DG

- CSRDG code (Bizzozero, Ellison, Warnock)



* D. Bizzozero, *Exploring the validity of the paraxial approximation for coherent synchrotron radiation wake fields* (Mo., 11:45)

Wakefields in the Frequency Domain

TECHNISCHE UNIVERSITÄT DARMSTADT

- Long range wakefields are needed
  - Low frequency, long bunches (ion, proton accelerators), bunch trains and/or high repetition rate
  - Wall heating (in resonant structures)
- Approximation of complicated geometry
  - Geometrical details smaller than bunch length
  - Smooth tapering etc. – Cartesian mesh approx. not sufficient
- Beams with $\beta < 1$
  - TD: Restriction in the choice of time step (M. Balk et al.)
  - TD: Expensive convolution for waveguide boundary conditions
- Curved beam trajectories
  - Moving window in the time domain not possible/complicated

Wakefields in the Frequency Domain

TECHNISCHE UNIVERSITÄT DARMSTADT

- The frequency domain problem

$$\nabla \times \mu^{-1} \nabla \times E - k_0^2 \varepsilon E = -jk_0 Z_0 J_s \qquad J_s(x,y,z,\omega) = \rho(x,y) e^{-i\frac{\omega}{v}z}$$

- Weak FE formulation: find $E \in H(curl)$ such that:

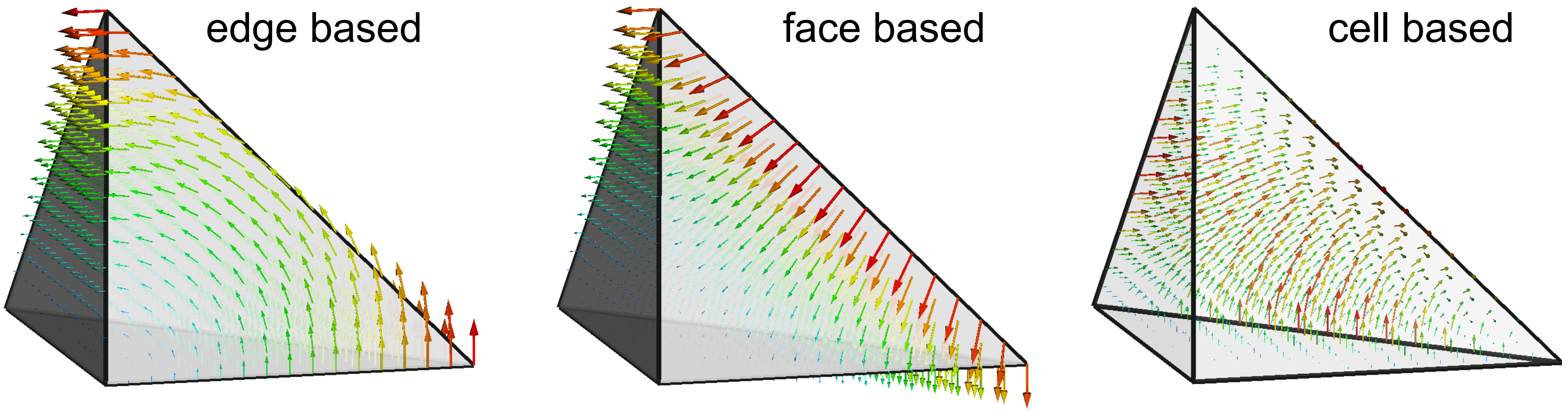
$$\int dV \mu^{-1}\, \nabla \times E \cdot \nabla \times v_h - k_0^2 \int dV \varepsilon\, E \cdot v_h =$$

$$-jk_0 Z_0 \int dV\, J_s \cdot v_h + \oint_S dS\ n \cdot [v_h \times \mu^{-1}\, \nabla \times E] \qquad \forall\, v_h \in H(curl)$$

$$\begin{array}{ccccccc}
H_1 & \xrightarrow{grad} & H(curl) & \xrightarrow{curl} & H(div) & \xrightarrow{div} & L_2 \\
\cup & & \cup & & \cup & & \cup \\
w_h^{p+1} & \xrightarrow{grad} & v_h^p & \xrightarrow{curl} & q_h^{p-1} & \xrightarrow{div} & s_h^{p-2}
\end{array}$$

Wakefields in the Frequency Domain

- High-order hierarchic basis functions*



  - Allows for simple hp-adaption
  - **Supports mesh elements of different type + hybrid meshes**

**M. Ainsworth, J. Coyle: Int. J. of Numerical Methods in Eng., 2003.*

**J. Schöberl, S. Zaglmayr: Int. J. Comp. and Math. in Electrical and Electronic Eng., 2005.*

Wakefields in the Frequency Domain

TECHNISCHE UNIVERSITÄT DARMSTADT

- Treatment of boundary surfaces

$$\int dV \mu^{-1} \nabla \times E \cdot \nabla \times v_h - k_0^2 \int dV \varepsilon \, E \cdot v_h =$$

$$-jk_0 Z_0 \int dV \, J_s \cdot v_h \; + \underbrace{\int_{S_{SIBC}} \boldsymbol{dS\, n \cdot [v_h \times \mu^{-1} \nabla \times E]}}_{\text{resistive walls}} + \underbrace{\int_{S_{WG}} dS n \cdot [v_h \times \mu^{-1} \nabla \times E]}_{\text{in \& outgoing pipes}}$$

resistive walls **in & outgoing pipes**

- SIBC boundaries

$$\oint_{S_{SIBC}} dS \;\, n \cdot [v_h \times \mu^{-1} \nabla \times E] = \cdots = j\omega \boldsymbol{Y_S(\omega)} \oint_{S_{SIBC}} dS \;\, v_h \cdot E$$

Simple modification of the system matrix on SIBC surfaces

No fitting of the surface impedance function or ADE/convolution is needed

Wakefields in the Frequency Domain

TECHNISCHE UNIVERSITÄT DARMSTADT

- Treatment of boundary surfaces

$$\int dV \mu^{-1}\, \nabla \times E \cdot \nabla \times v_h - k_0^2 \int dV \varepsilon\, E \cdot v_h =$$

$$-jk_0 Z_0 \int dV\, J_s \cdot v_h + \underbrace{\int_{S_{SIBC}} dS\, n \cdot [v_h \times \mu^{-1}\, \nabla \times E]}_{\text{resistive walls}} + \underbrace{\int_{S_{WG}} \boldsymbol{dSn} \cdot [\boldsymbol{v_h} \times \boldsymbol{\mu^{-1}}\, \boldsymbol{\nabla} \times \boldsymbol{E}]}_{\text{in \& outgoing pipes}}$$

- Beam pipe boundaries

$$n \times \nabla \times E = n \times \nabla \times E^{inc} + \sum_m a_m^{TE} \gamma_m^{TE} e_m^{TE} + \sum_m a_m^{TM} \gamma_m^{TM} e_m^{TM}$$

$$a_m^{TE} = \int_{S_{WG}} dS e_m^{TE} \cdot [E - E^{inc}]$$

Reflection coefficients for each mode

$$a_m^{TM} = \int_{S_{WG}} dS e_m^{TM} \cdot [E - E^{inc}]$$

Wakefields in the Frequency Domain

- Beam pipe boundary conditions

$$\int dV \mu^{-1}\, \nabla \times E \cdot \nabla \times v_h - k_0^2 \int dV \varepsilon\, E \cdot v_h + \sum_m \boldsymbol{P_m^{TE}(E)} + \sum_m \boldsymbol{P_m^{TM}(E)} =$$

$$-jk_0 Z_0 \int dV\, J_s \cdot v_h \;+ \oint_{S_{WG}} \boldsymbol{dS\; n \cdot \left[v_h \times \mu^{-1}\, \nabla \times E^{inc}\right]} + \sum_m \boldsymbol{U_m^{TE}} + \sum_m \boldsymbol{U_m^{TM}}$$

with $P_m^{TE}(E) = -\gamma_m^{TE}\left(\int_{S_{WG}} dS\; v_h \cdot e_m^{TE}\right)\left(\int_{S_{WG}} dS\; e_m^{TE} \cdot E\right), \qquad P_m^{TM}(E) = \cdots$

and matrix representation (TE):

$$\boxed{P_m^{TE}(E) \;\rightarrow\; \mathbf{P}_m^{TE} \cdot \mathbf{e} = -\gamma_m^{TE} \mathbf{R}^T \cdot \mathbf{M}_m^{TE} \cdot \mathbf{R} \cdot \mathbf{e}}$$

$$[\mathbf{R}\,]_{ij} = \underbrace{\int_{S_{WG}} dS\; \varphi_i^{2D} \cdot \varphi_j^{3D}}_{\text{3D-to-2D projection matrix}}$$

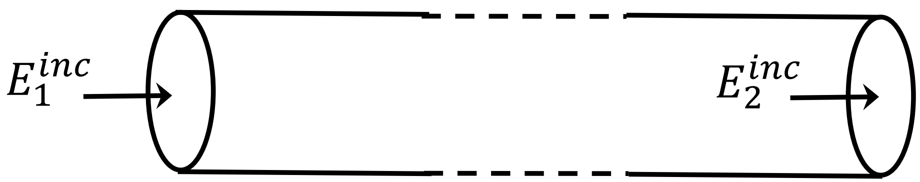
$$\boxed{\mathbf{M}_m^{TE} = \mathbf{e}_m^{TE} \otimes \mathbf{e}_m^{TE}}$$ small but dense modal dyadic

Wakefields in the Frequency Domain

- Beam pipe boundary excitation
  - For an ultra-relativistic bunch (same idea for β < 1):

$$\nabla_t \cdot E^{inc} = \frac{1}{\varepsilon_0}\rho(x,y)e^{-ik_0 z_0}$$

$$\nabla \times E^{inc} = 0$$



2D-electrostatic problem at both ends of the pipe

  - Modal contribution to the RHS

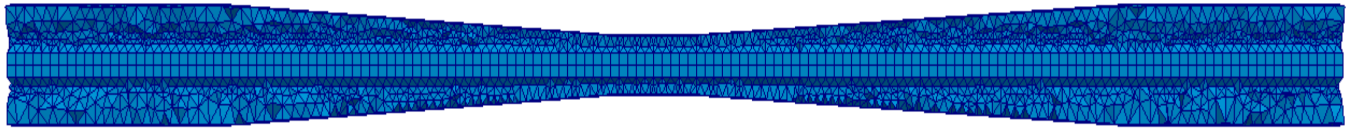
$$U_m^{TE}\left(E^{inc}\right) = -\gamma_m^{TE}\left(\int_{S_{WG}} dS\, v_h \cdot e_m^{TE}\right)\left(\int_{S_{WG}} dS\, e_m^{TE} \cdot E^{inc}\right)$$

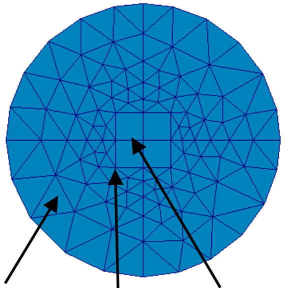
$$\boxed{U_m^{TE}\left(E^{inc}\right) \;\rightarrow\cdot\; \mathbf{U}_m^{TE}\cdot \mathbf{e}^{inc} = -\gamma_0^{TE}\mathbf{R}^T \cdot \mathbf{M}_m^{TE}\cdot \mathbf{R}^{2D} \cdot \mathbf{e}^{inc}}$$

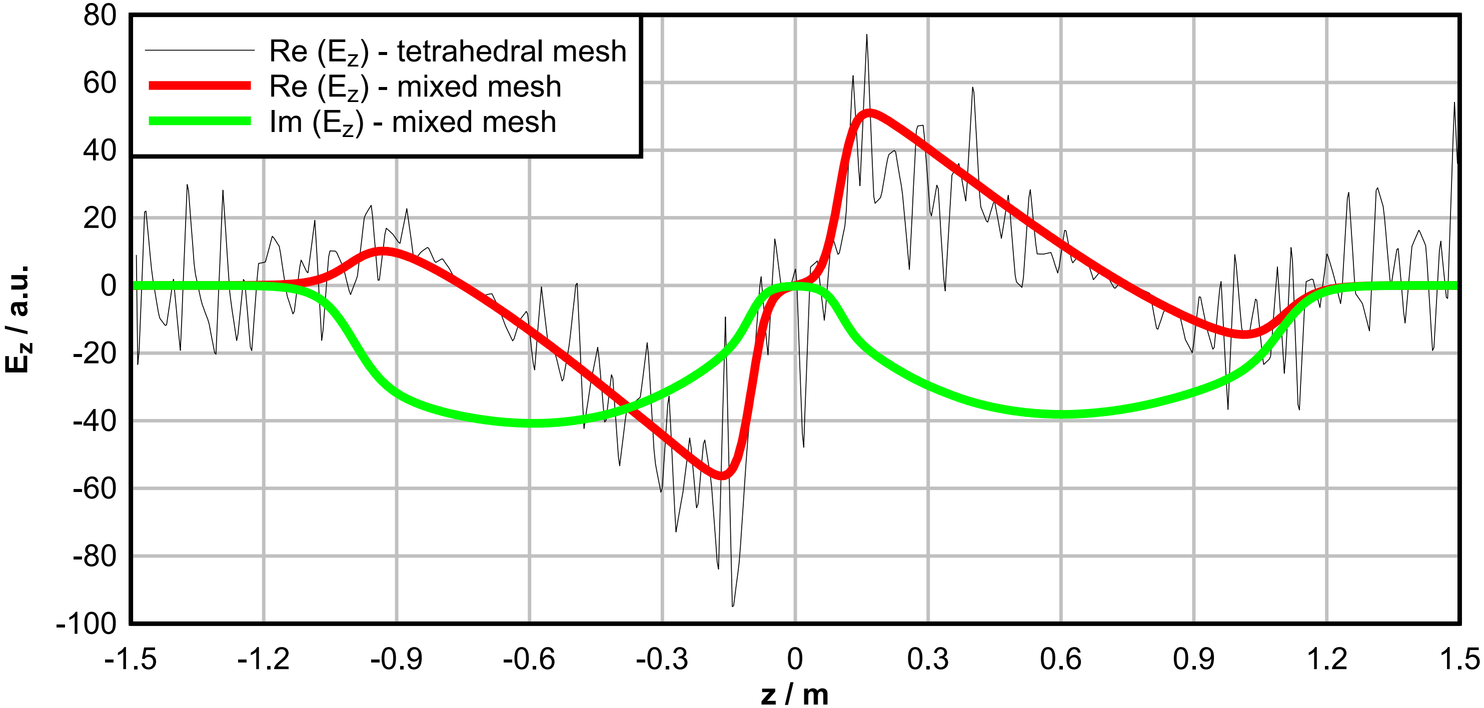
…for all waveguide modes supported in the pipe

Wakefields in the Frequency Domain

- Collimator example – use of hybrid meshes



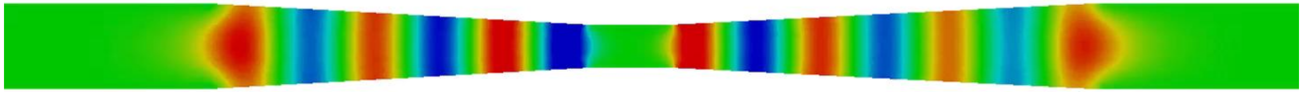




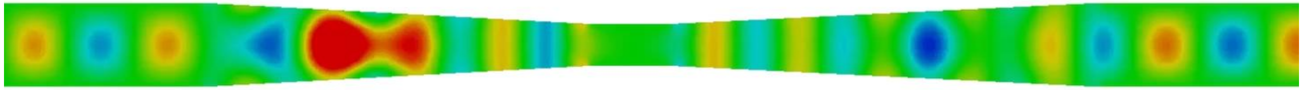
Longitudinal wakefield on axis at 100MHz

Wakefields in the Frequency Domain

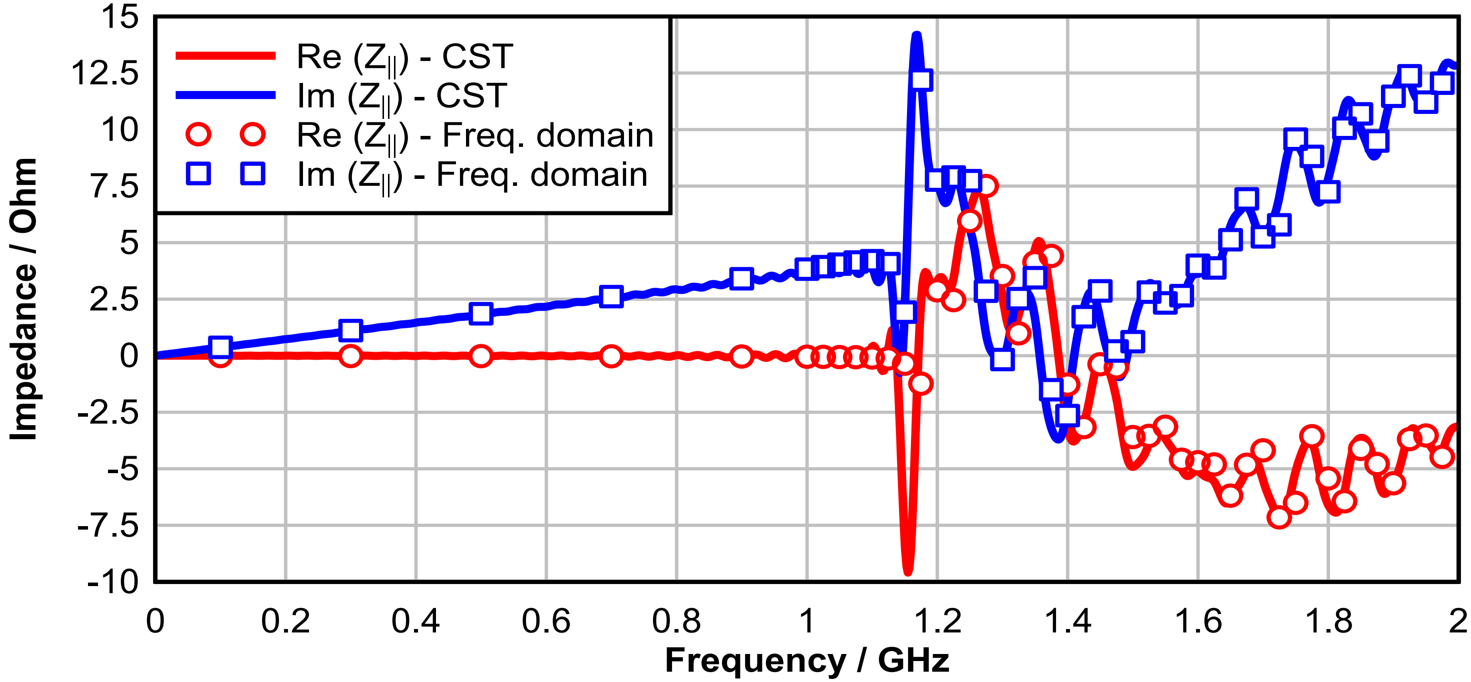
- Collimator example – impedance



E_z – 1GHz



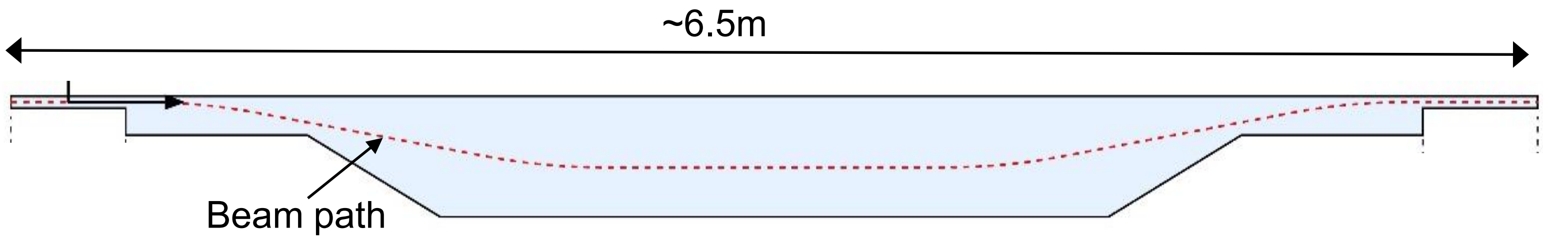
E_z – 1.5GHz

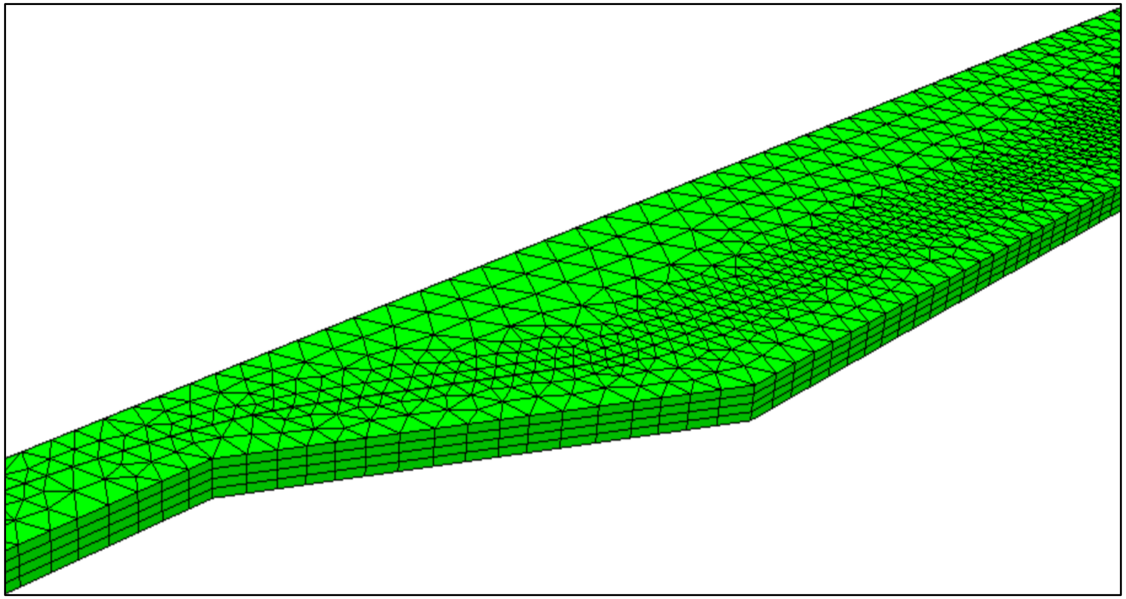


Comparison with CST PS (time domain)

Wakefields in the Frequency Domain

- Bunch compressor of XFEL, DESY



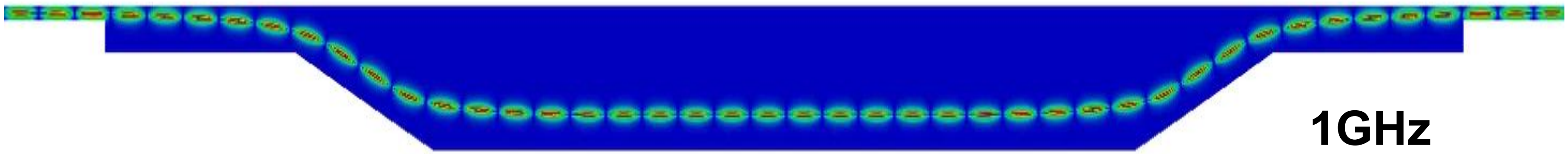


Prismatic element mesh:
$\Delta \approx 5$mm
600k cells
4^{th} order FEM

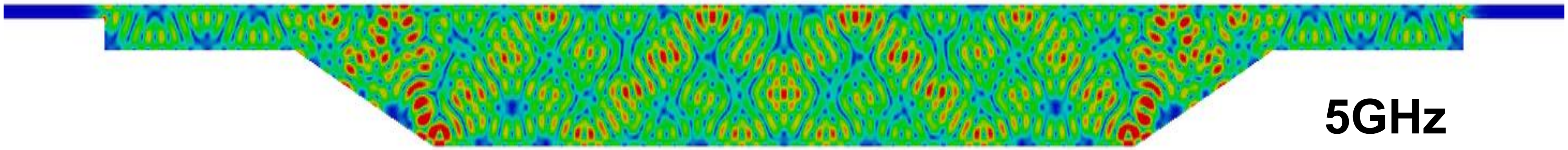
Wakefields in the Frequency Domain

TECHNISCHE UNIVERSITÄT DARMSTADT

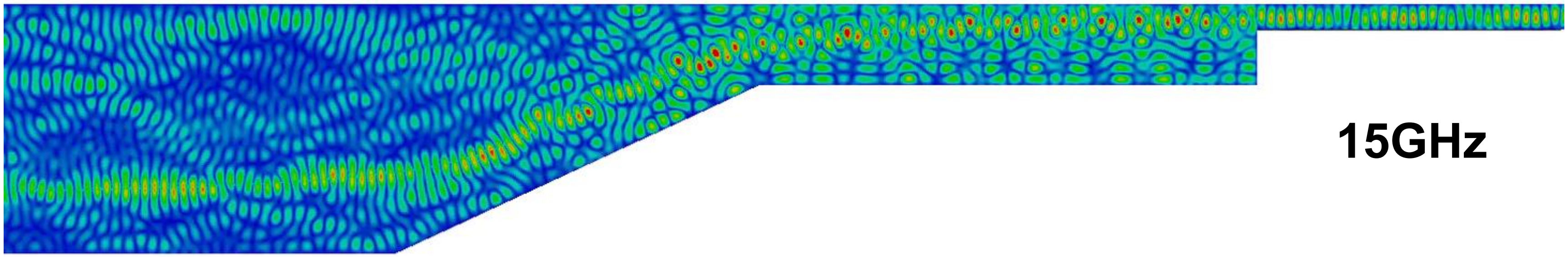
- Bunch compressor of XFEL, DESY



1GHz



5GHz



15GHz

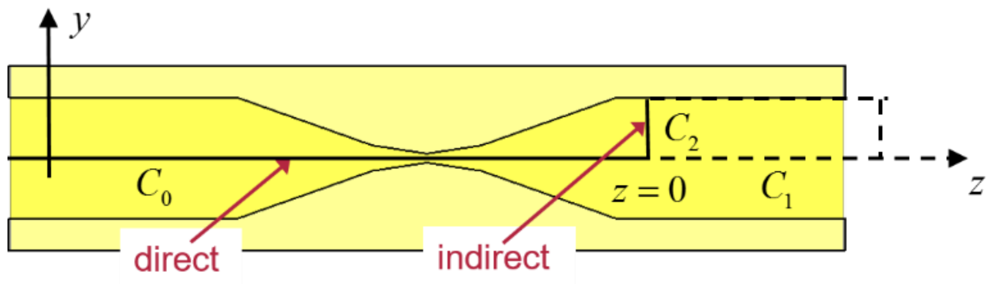
Summary & Conclusions

- **Wakefield codes in the time domain**
  - Moving window – not always applicable
  - Conformal boundary techniques – not always accurate
  - Resistive wall wakefields – ADE, expensive convolution
  - Electrically large structures – numerical efficiency
  - Long wake transients – numerical efficiency
- **CSR wakes**
  - CSRDG code using DG in the time domain
- **Frequency domain approach**
  - May be filling the gap for a number of applications
  - Difficult for very high frequency problems
  - Efficient solvers for large system of equations are needed

Thank You for your attention

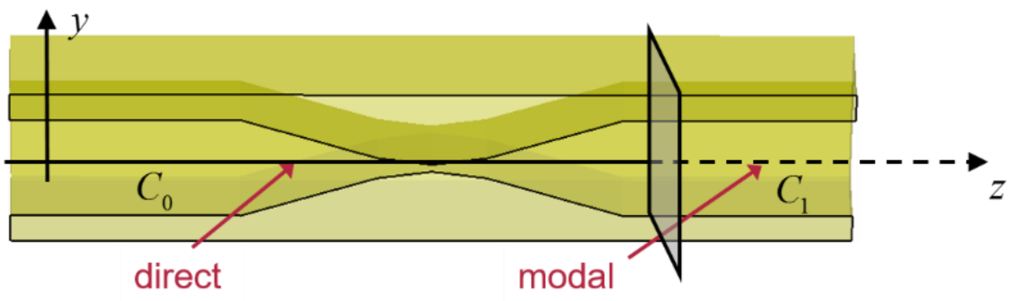
Indirect integration

- Indirect integration based on wake path deformation



- Weiland 1983, Napoly 1993
- A. Henke, W. Bruns, EPAC'06

- Indirect integration using modal decomposition

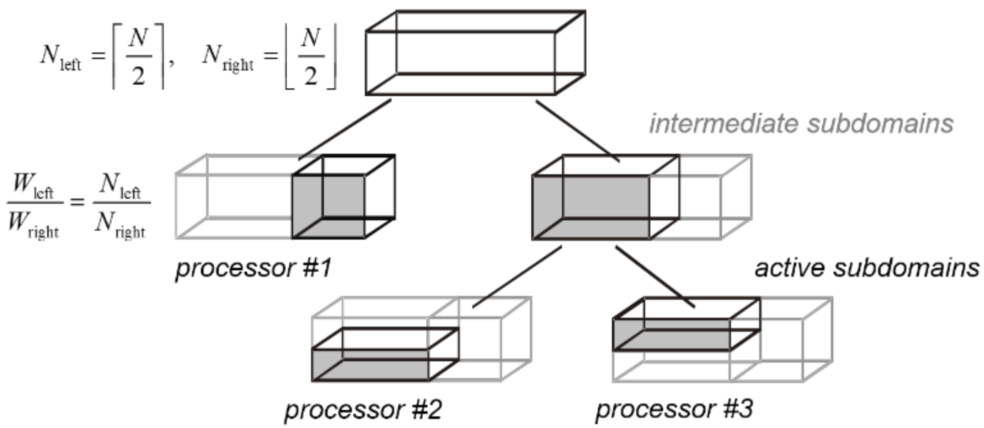


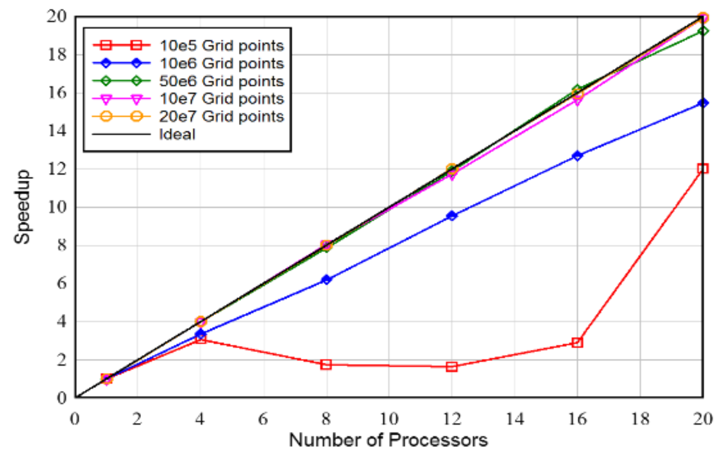
- I. Zagorodnov, PRSTAB 2006
- X. Dong, E. Gjonaj, ICAP'06

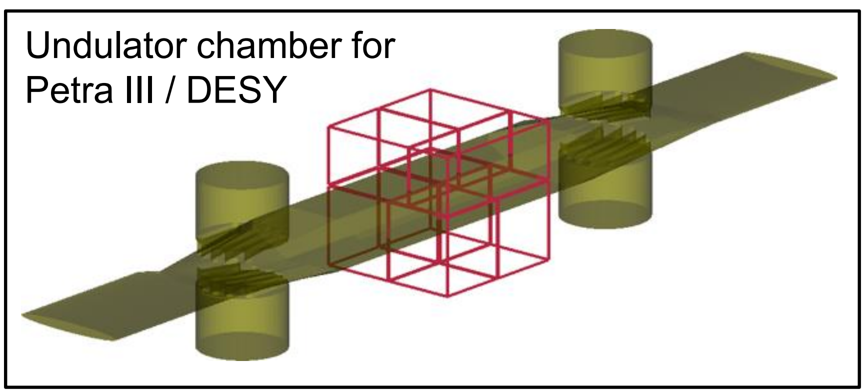
$$W_z(s) = -\frac{1}{Q}\int_{-\infty}^{\infty} dz\, E_z(z, t=\frac{z+s}{c}) = -\frac{1}{Q}\int_{C_0} dz\, E_z(z, t=\frac{z+s}{c}) - \frac{1}{Q}\sum_n e_z^n(x,y) W_n(s)$$

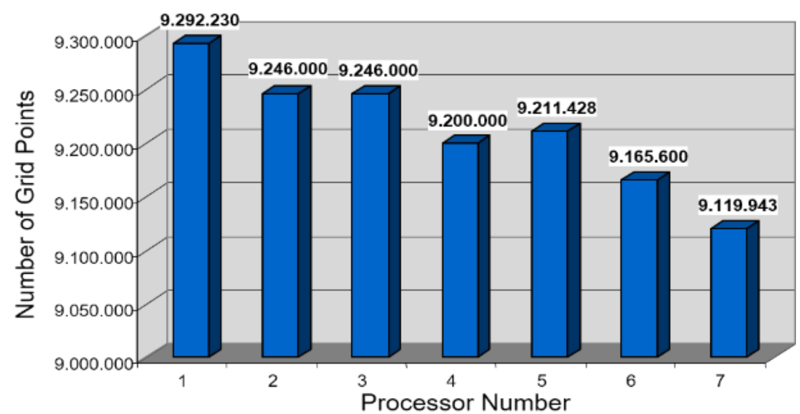
Parallelization

- Domain decomposition approach on large HPC-Clusters







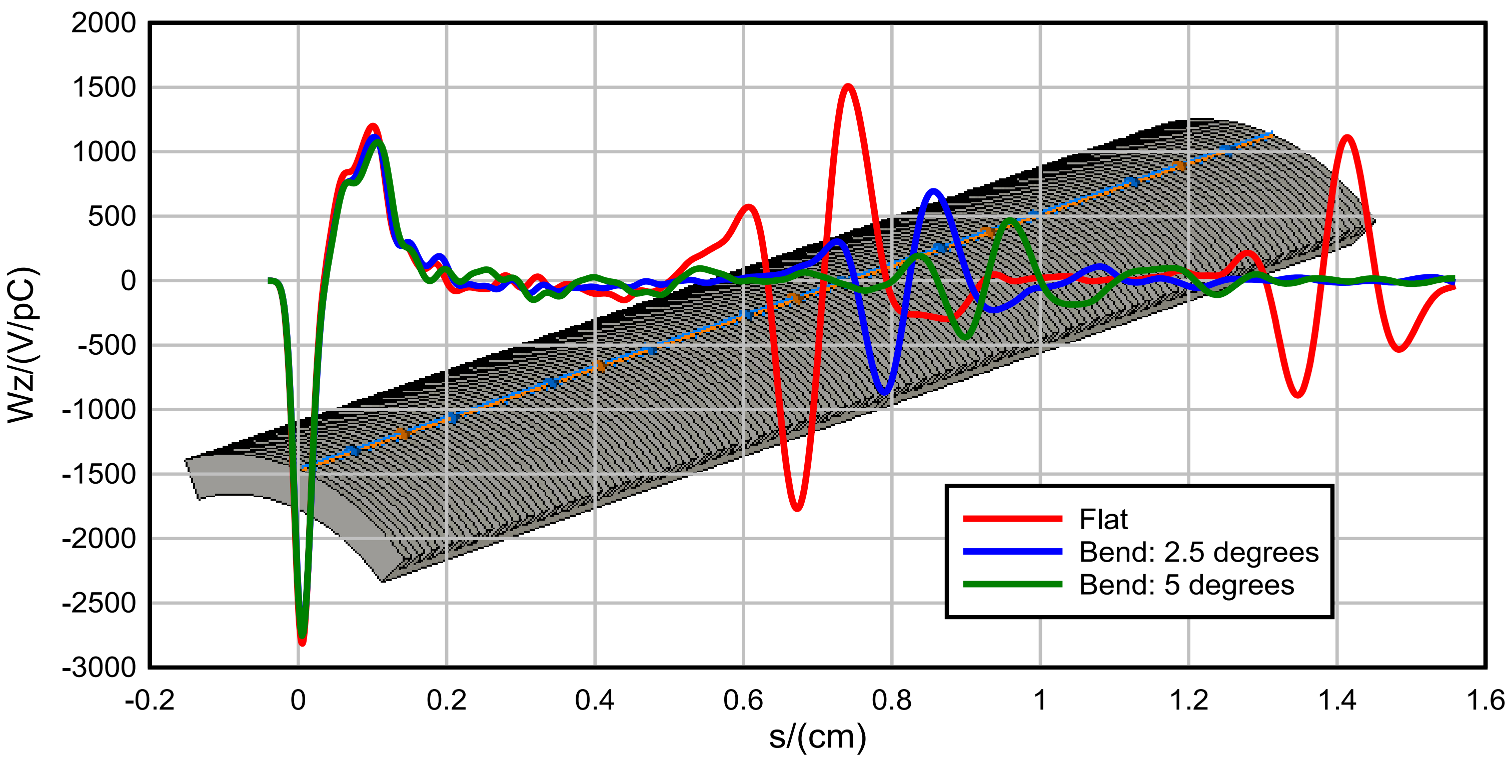


Open structures

TECHNISCHE UNIVERSITÄT DARMSTADT

- Single plate dechirper (with Bane, Stupakov)

Bend dechirper to minimize side end reflections



Wakefield simulation in the time domain

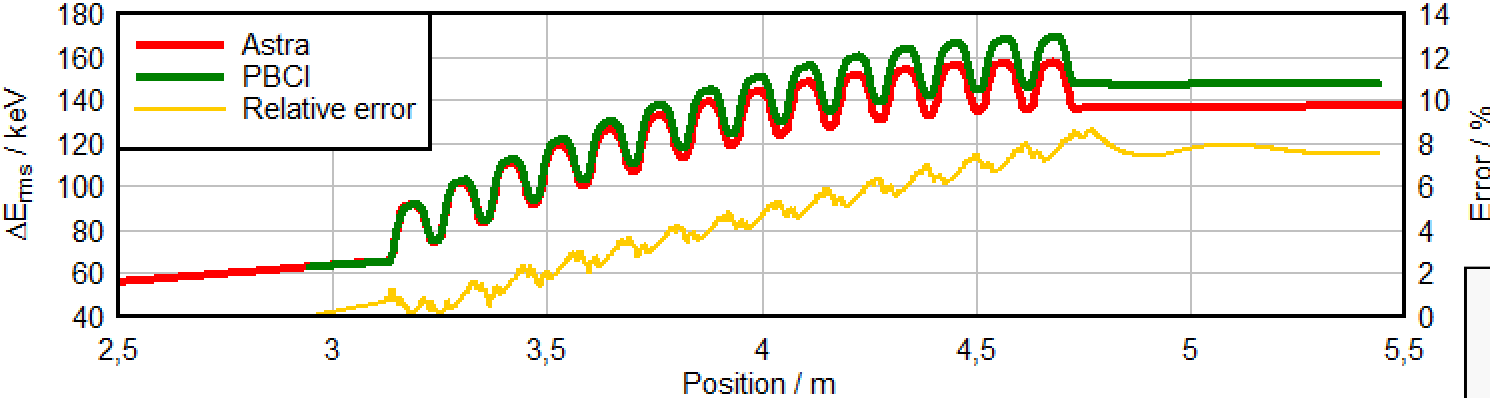
TECHNISCHE UNIVERSITÄT DARMSTADT

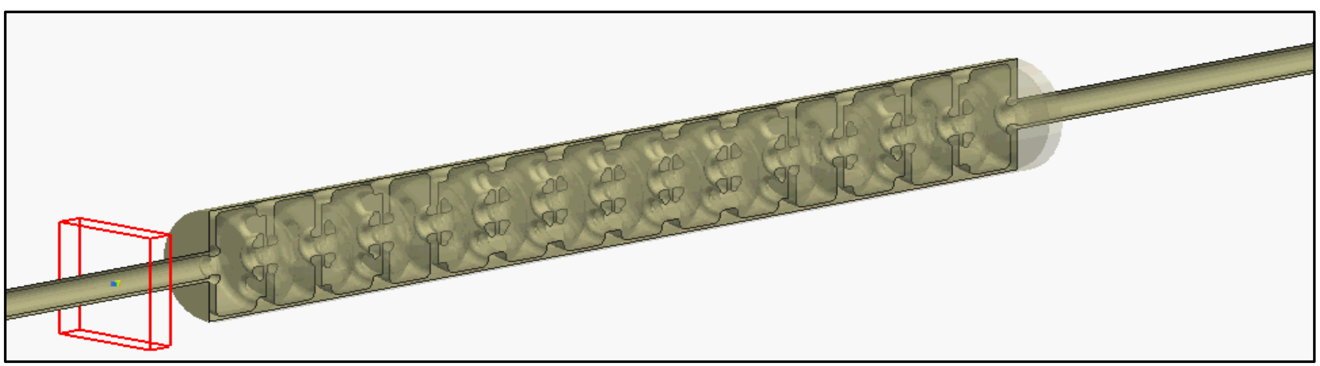
- Different approaches for the solution of Maxwell's equations
  - Fixed window codes
    - ABCI – FDTD
    - CST Particle Studio – FIT
    - Tech-X VSim – FDTD
    - T3P (SLAC) – high order FEM
    - GdfidL – FDTD/FIT
    - …
  - Moving window and dispersion-free codes
    - GdfidL – FDTD/FIT
    - Echo2D, Echo3D (DESY) – FDTD/FIT
    - Parallel Beam Cavity Interaction PBCI (TEMF) – FDTD/FIT
    - …

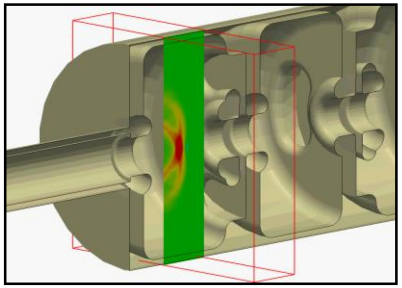
Particle tracking with wakefields

- Incorporate a particle tracker into the wakefield code

Influence of geometrical wakefields in the booster of the XFEL injector (PITZ, DESY)



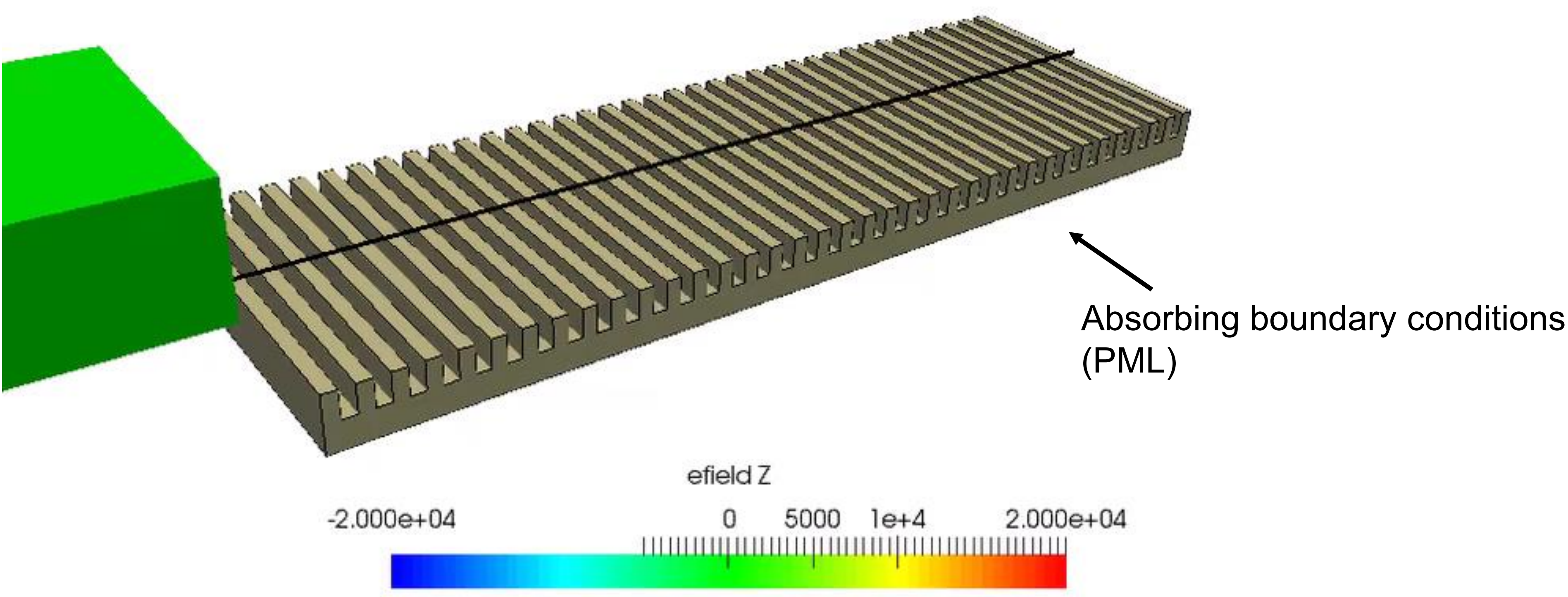




Pure space-charge vs. space-charge + wakefield simulation

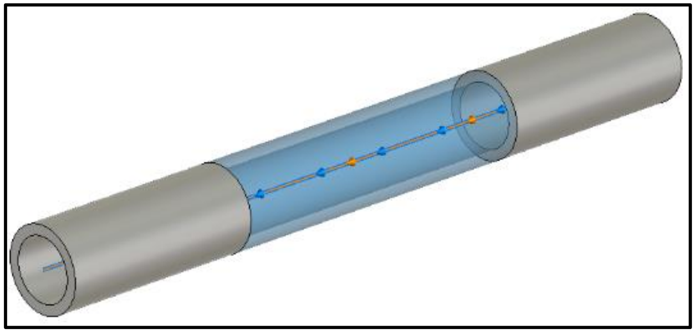
Open structures

- Single plate dechirper (with Bane, Stupakov)



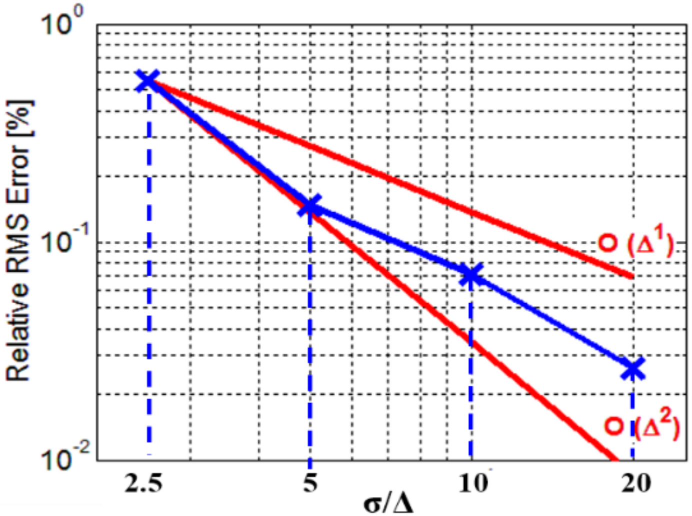
Resistive wall wakefields

- Approximation of curved PEC boundaries

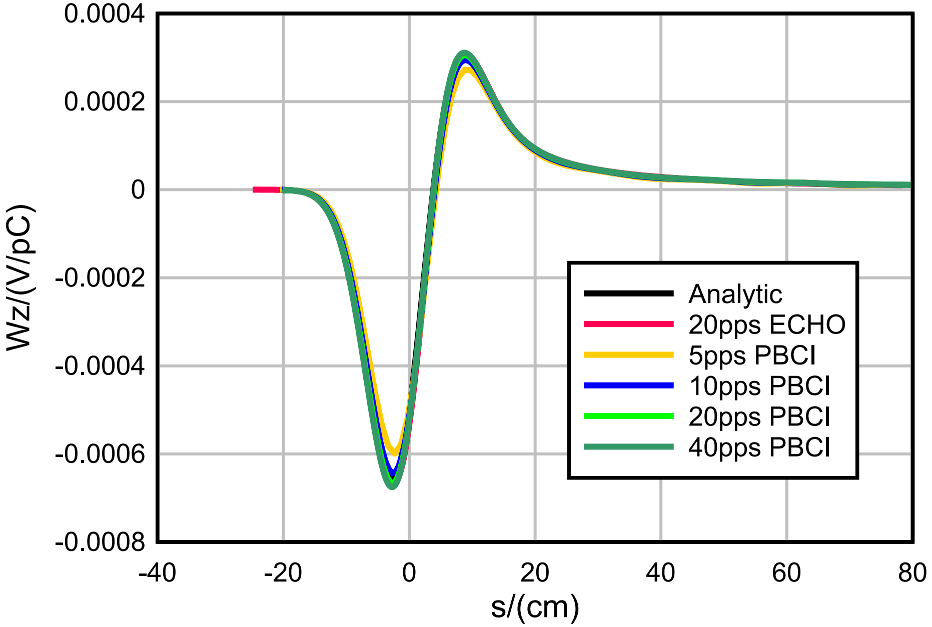


TiAl round pipe, L=60cm, R=6cm

Bunch: σ=5cm

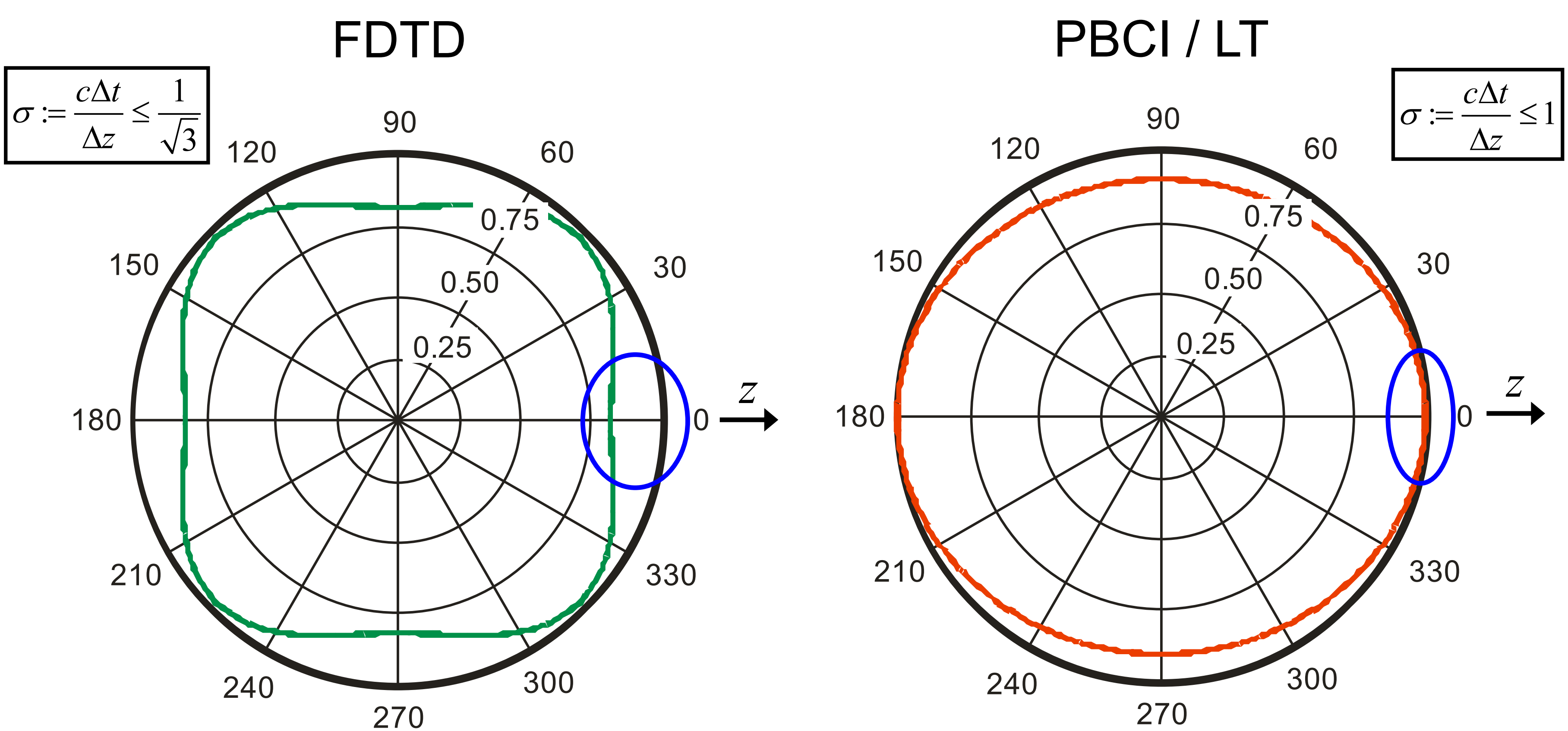


Comparison with ECHO2D and analytical solution



Dispersion-free methods

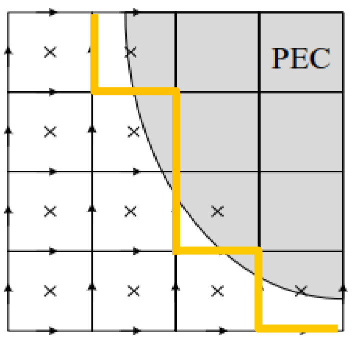
- Exact propagation in z-direction by splitting of the FDTD operators

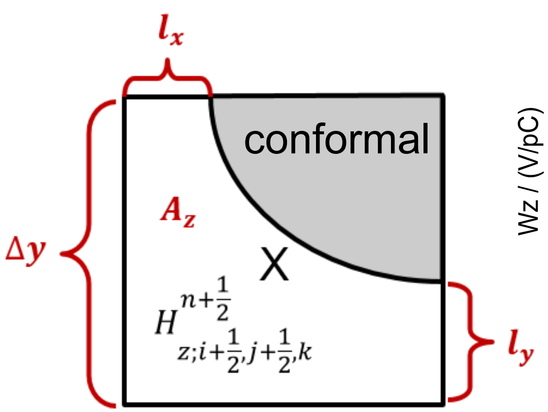


Geometry approximation

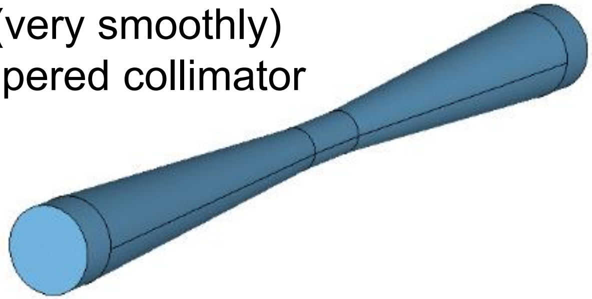
- Conformal approximation of curved boundaries
  - Local modification of discrete Faraday's law (Day&Mittra, Thoma)

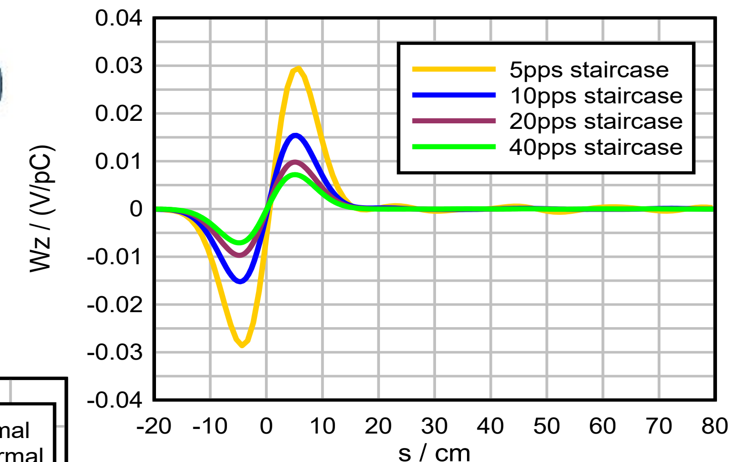
staircase

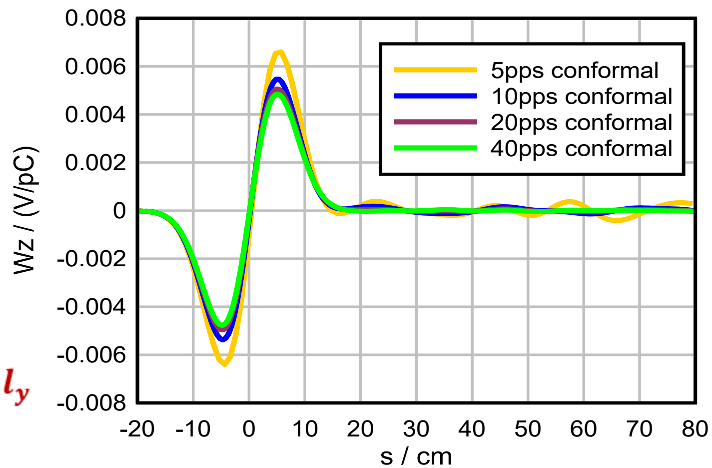




(very smoothly) tapered collimator







Up to 40 grid points per bunch length needed for good accuracy