Geometric and resistive wake field calculations with PBCI

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TEMF – DESY Collaboration Meeting

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TEMF, Darmstadt

The PBCI Code

Parallel Beam Cavity Interaction (PBCI) - Dedicated code for short range wakefield computations in 3D geometry

- Based on FIT
- Dispersion free in longitudinal direction
- Moving window
- Parallelization
- On-the-fly (parallel) meshing for arbitrary 3D geometry
- Indirect integration

E. Gjonaj, X. Dong, R. Hampel, M. K¨arkkäinen, T. Lau, W.F.O. Müller, T. Weiland, “Large Scale, Parallel Wake Field Computations for 3D-Accelerator Structures with the PBCI Code,” ICAP 2006

Dispersion-Free Numerical Method

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Maxwell's Grid Equation written as ODE system

$$y=\begin{pmatrix} h \\ e \end{pmatrix} \qquad A=\begin{pmatrix} 0 & -C \\ C^T & 0 \end{pmatrix}$$

$$\frac{\partial}{\partial t} y = A\cdot y$$

Splitting

$$R_{L,T}(\Delta t)\equiv\left(1+\frac{\Delta t}{2}U_{L,T}\right)\left(1+\Delta t\, L_{L,T}\right)\left(1+\frac{\Delta t}{2}U_{L,T}\right)$$

$$U_{L,T}\equiv\begin{pmatrix} 0 & -C_{L,T} \\ 0 & 0 \end{pmatrix},\quad L_{L,T}\equiv\begin{pmatrix} 0 & 0 \\ C_{L,T}^T & 0 \end{pmatrix}$$

LT-1

$$e^{A\cdot\Delta t}=R_T\left(\frac{\Delta t}{2}\right)R_L(\Delta t)R_T\left(\frac{\Delta t}{2}\right)$$

LT-2

$$e^{A\cdot\Delta t}=R_L\left(\frac{\Delta t}{2}\right)R_T(\Delta t)R_L\left(\frac{\Delta t}{2}\right)$$

Updates Equations

LT-1:

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

LT-2:

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

NO=30 **Number of Operations** ***NO=24***

Dispersion Free in Longitudinal Direction

Stability

LT-1

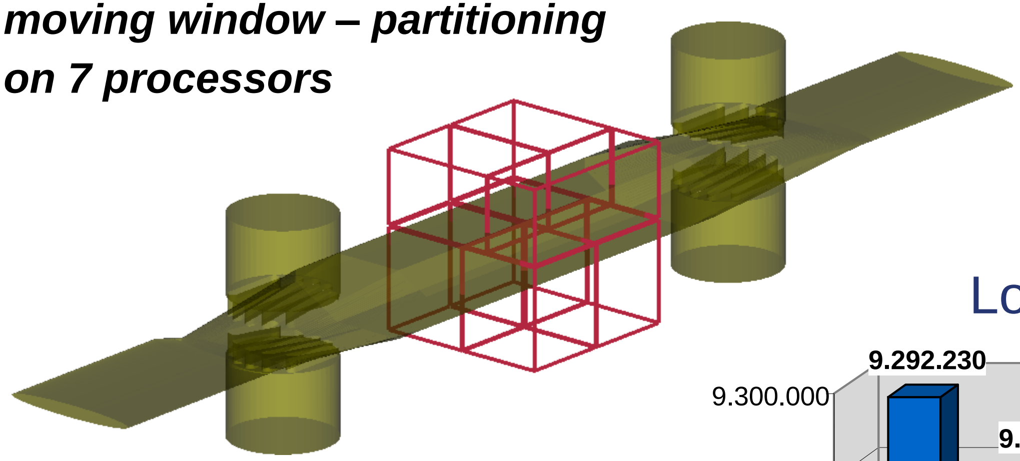
$$c\,\Delta t\le min(\Delta_x,\Delta_y,\Delta_z)$$

LT-2 = TE/TM

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

Moving window and parallelization

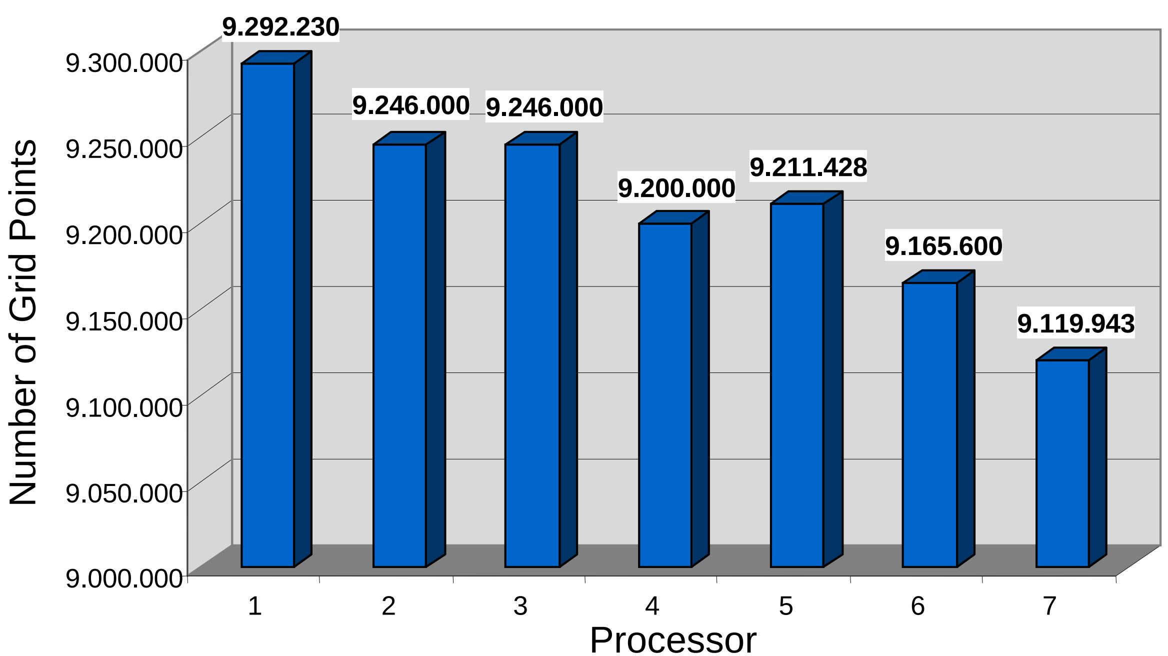
moving window – partitioning on 7 processors



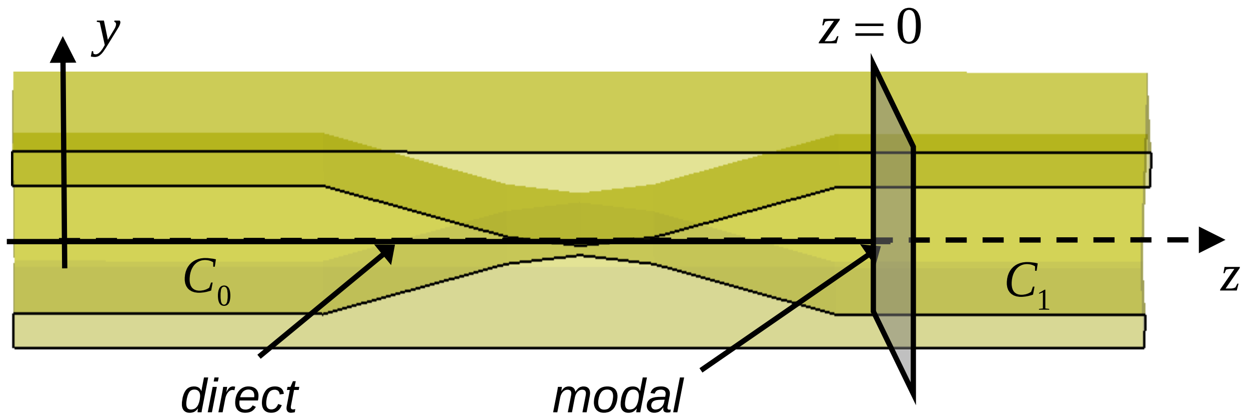
Example: tapered transition for PETRA III

	Grid points
Total	64.481.201
Min.	9.119.943
Max.	9.292.230
Dev.	**< 1.0%**

Load distribution (# of grid points)



Modal termination technique for indirect integration



Eigenmode expansion method in the indirect calculation of wake potential in 3D structures, X. Dong, E. Gjonaj, ICAP’06

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

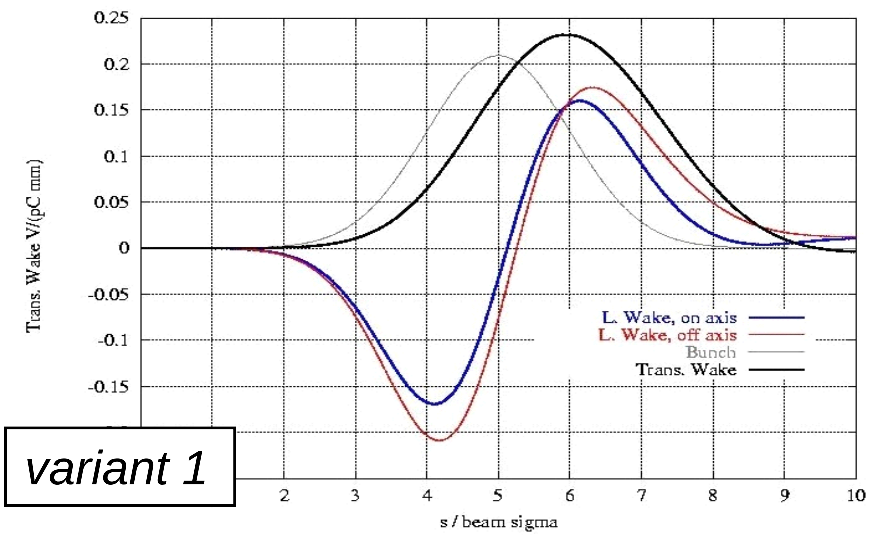
$$\int_0^{\infty} dz\, E_z(x,y,z,t=(z+s)/c) = \int_0^{\infty} dz\left[\int_{-\infty}^{\infty} d\omega \sum_n C_n(\omega)\, e_z^n(x,y)\, e^{ik_n(\omega)z}\, e^{-i\omega\frac{z+s}{c}}\right] =$$

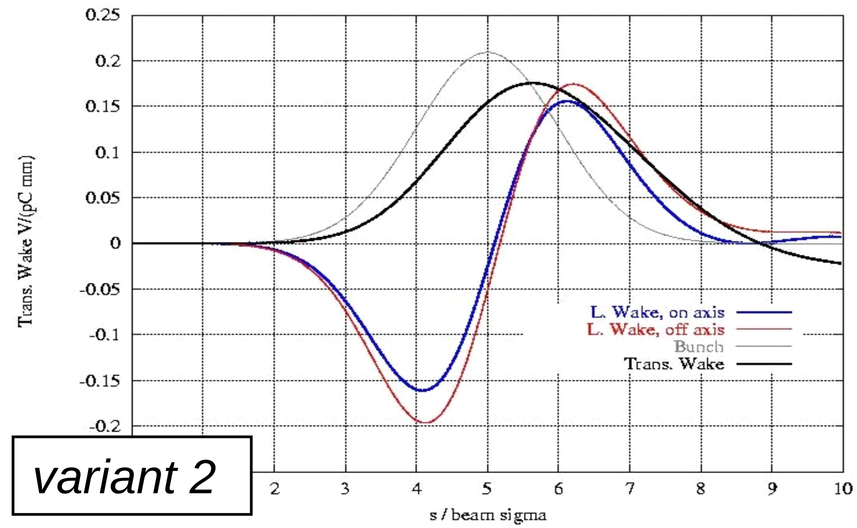
spectral coefficient of n-th (TM) mode

$$= \sum_n e_z^n(x,y) \underbrace{\int_{-\infty}^{\infty} d\omega\, C_n(\omega)\, \frac{1}{i\left(\omega/c - k_{z,n}(\omega)\right)}\, e^{-i(\omega/c)s}}_{\text{n-th (TM) mode contribution}}$$

PBCI Applications

Tapered undulator transitions for PETRA III



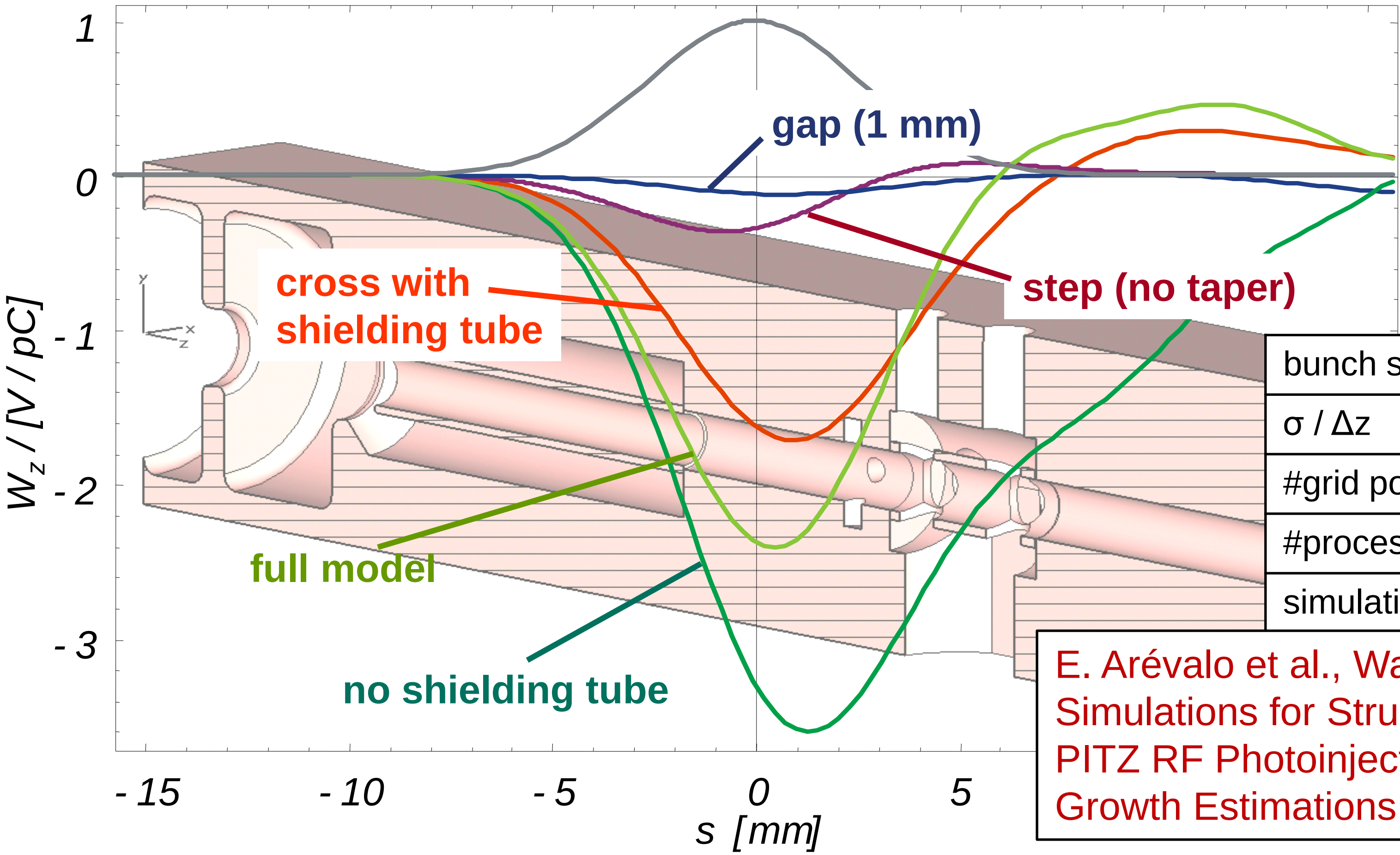


Variant / Code	$k_{\|\|}$ / (V/nC)	$k_{\|\|}(1)$ / (V/pC m)	$k_{\perp}$ / (V/pC m)
Variant 1 / MAFIA	-7.4	-6.8	138.6
Variant 1 / PBCI	-7.1	-4.8	75.6
Variant 2 / PBCI	-5.2	-4.6	62.8

"Wake Computations for Undulator Vacuum Chambers of PETRA III",
R. Wanzenberg et al, PAC'07

PBCI Applications

PITZ diagnostics double cross

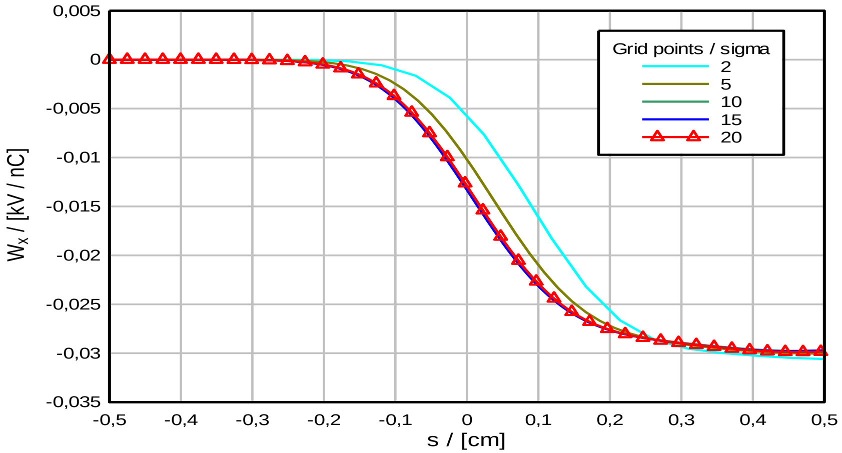


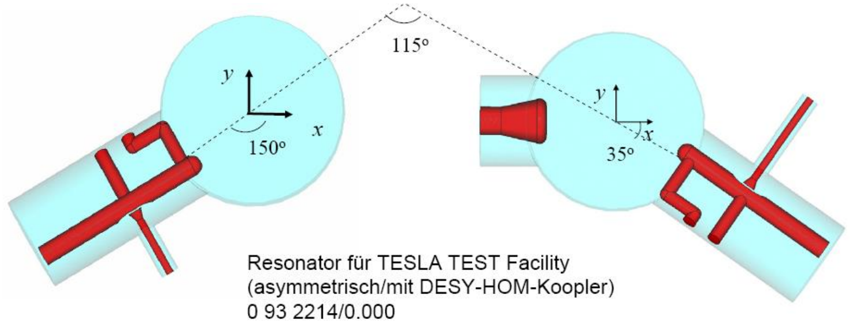
bunch size	2.5mm
σ / Δz	30
#grid points	~500e6
#processors	24
simulation time	32hrs

E. Arévalo et al., Wake Field Simulations for Structures of the PITZ RF Photoinjector: Emittance Growth Estimations, EPAC08.

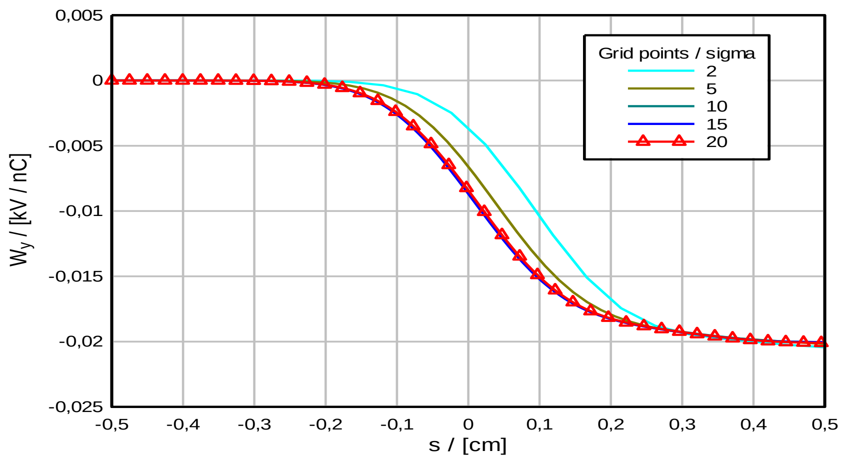
PBCI Applications

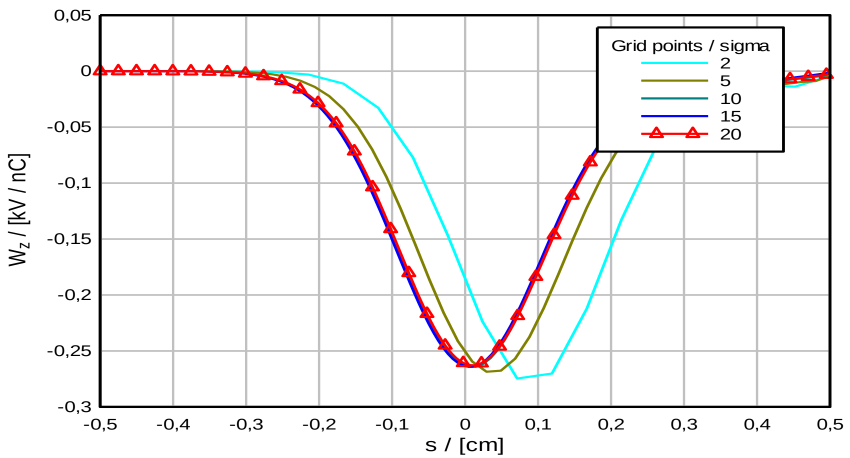
Tesla HOM-Copplers





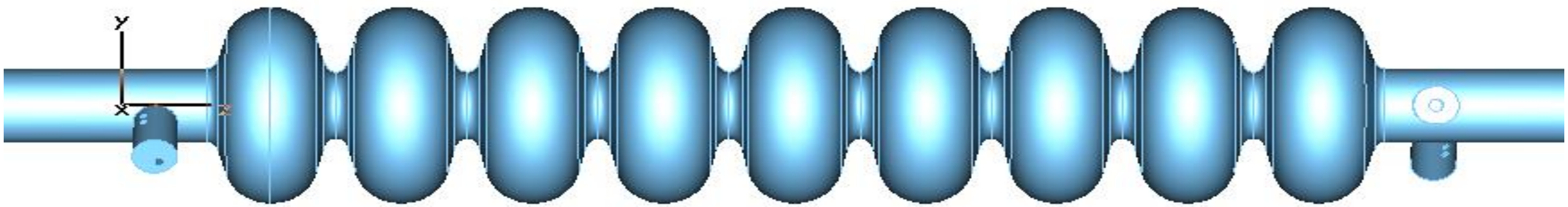
M. Dohlus et al. Coupler Kick for Very Short Bunches and its Compensation. EPAC08

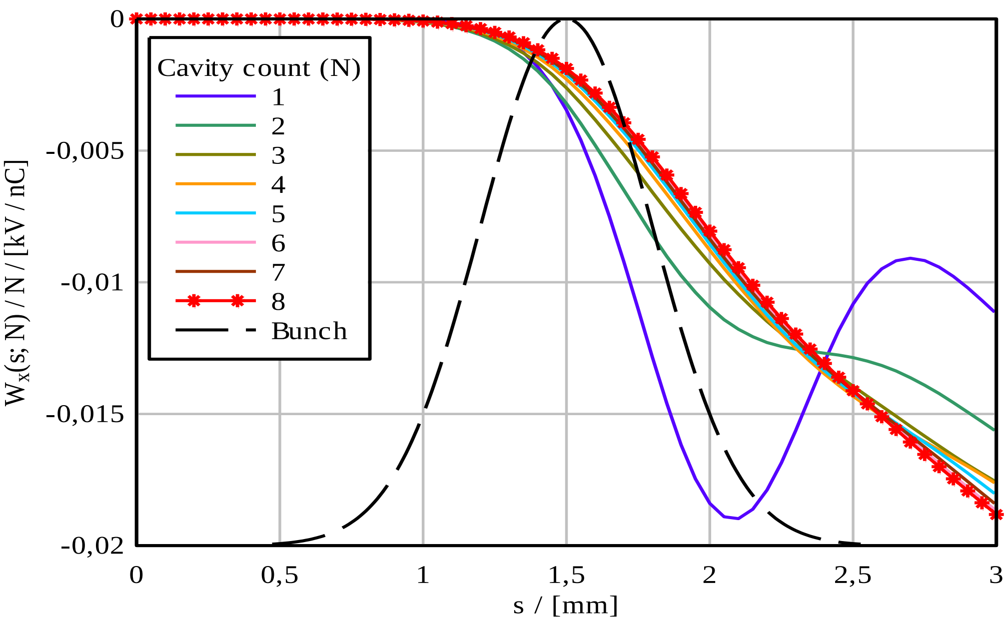




PBCI Applications

Full TESLA cavity + HOM-Coppler simulation



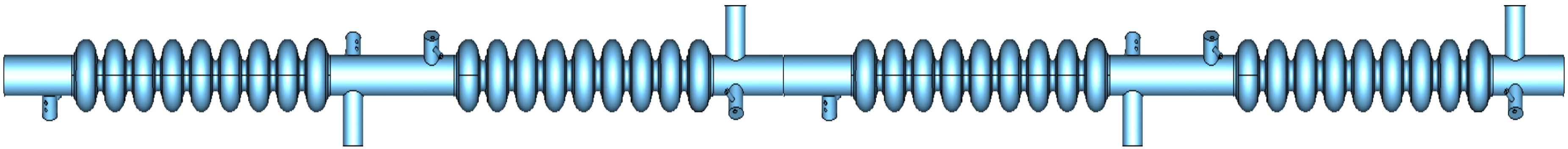


K. Bane et al, Wakefield and RF Kicks Due to Coupler Asymmetry in TESLA-Type Accelerating Cavities, SLAC-PUB-13276

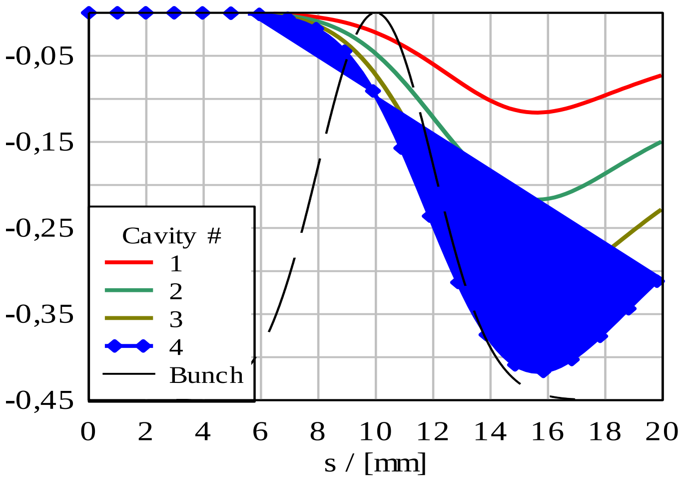
bunch length	0.3mm
bunch charge	1nC
module length	~10m
# of grid points	~250M
# of processors	408
simulation time	~7 days

PBCI Applications

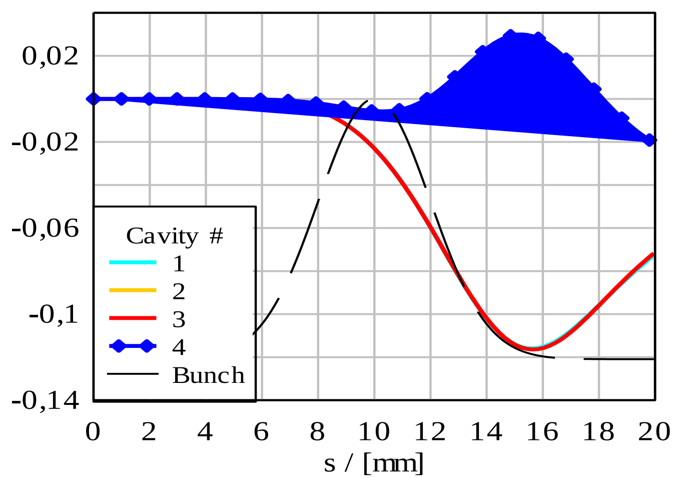
3.9GHz Module for the XFEL



Case (a): W_x / (V / pC)



Case (b): W_x / (V / pC)



E. Gjonaj et al., Coupler Kicks in the Third Harmonic Module for the XFEL, PAC09

PBCI Applications

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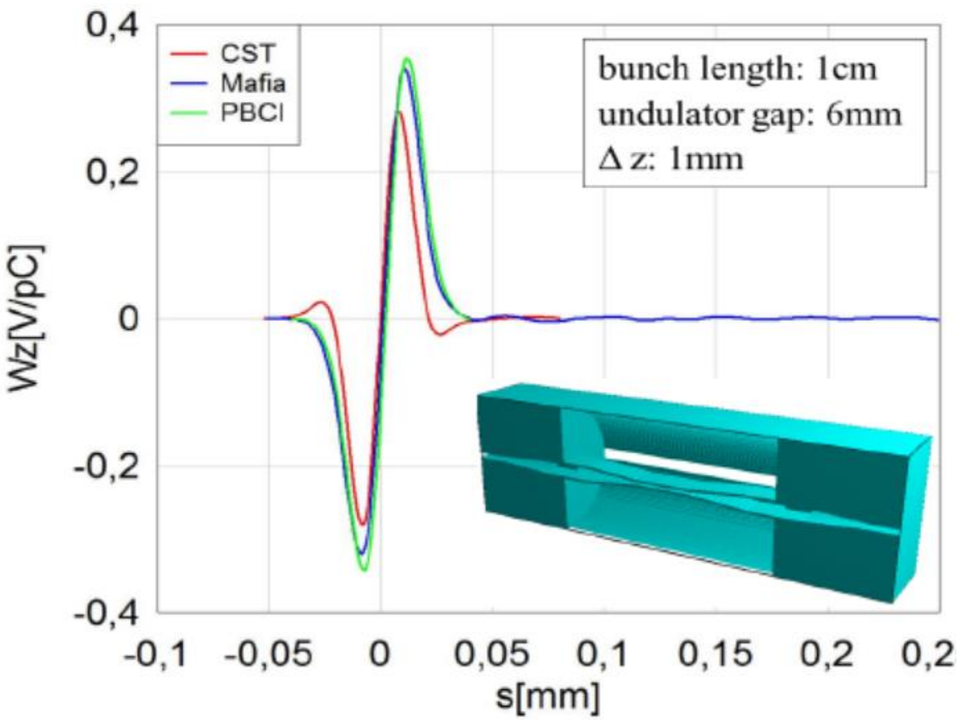
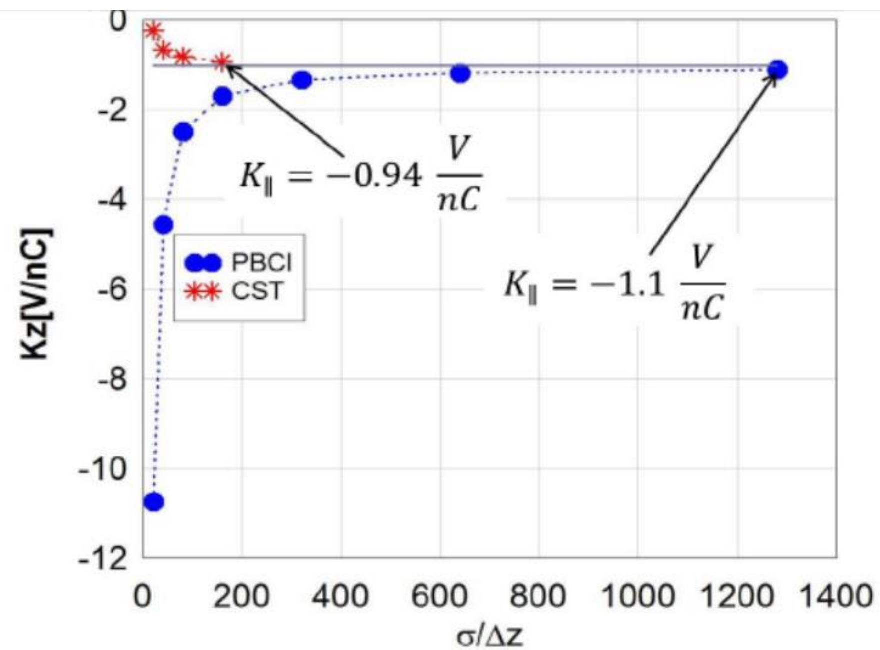
In-vacuum Undulator for PETRA III



E. Gjonaj et al., Computation of Wakefields for an In-vacuum Undulator at PETRA III, IPAC13



Resistive Wall Wakefields

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Solver Capabilites

- Fully Time Domain
- 3D Complex Structures
- Ultra-short bunches

- Resistive Walls with Freq. Dep. Conductivity
- Surface Roughness & Metal Oxidation Effects

Numerical Method

- Time Domain SIBC Model and Special Implementation to Preserve stability of 3D Method

- 3D Numerical Scheme
- Dispersion Free in longitudinal direction

- Robust and efficient implementation on a moving / parallel grid
- User friendly interface

- Moving Window
- Parallel computing

ADE Approach for SIBC-TD

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SIBC in Frequency Domain

$$\vec{E}_\tau(\omega) = Z_s(\omega)\,[\vec{n}\times\vec{H}_\tau(\omega)]$$

Transformation to TD

SIBC in Time Domain

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

$$Z_s(\omega) \cong j\omega L + \alpha_0 + \sum_{i=1}^{Np}\frac{\alpha_i}{j\omega+\beta_i}$$

Rational Function Approximation (RFA)

Auxiliary Differential Equations (ADE)

$$\vec{G}_0 = \alpha_0\,[\vec{n}\times\vec{H}_\tau]$$
$$\frac{d}{dt}\vec{G}_i + \beta_i\vec{G}_i = \alpha_i\,[\vec{n}\times\vec{H}_\tau]$$

- B. Gustavsen, Improving the pole relocating properties of vector fitting, *IEEE Trans. on Power Delivery*, vol. 21, pp. 1587–1592, 2006

- J. Woyna, E. Gjonaj, and T. Weiland, Broadband surface impedance boundary conditions for higher order time domain discontinuous galerkin method, COMPEL, vol. 33, no. 4, pp. 1082–1096, 2014.

SIBC Time Domain Model

Accuracy of Vector-Fitting technique

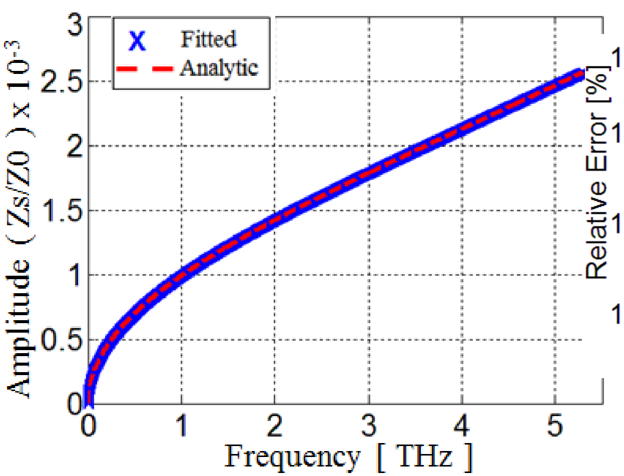
Good Conductors

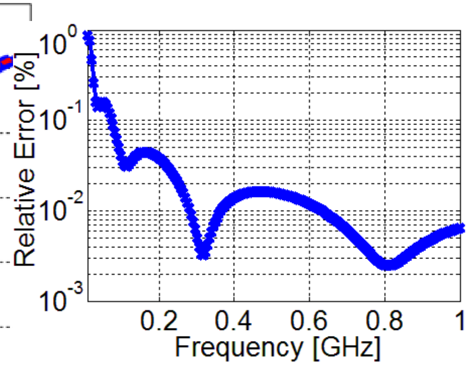
$$Z_s(\omega) \cong \sqrt{\frac{j\,\omega\,\mu}{\sigma(\omega) + j\,\omega\,\varepsilon}} \quad \xrightarrow{\text{VF}} \quad Z_s(\omega) \cong j\omega L + \alpha_0 + \sum_{i=1}^{Np} \frac{\alpha_i}{j\omega + \beta_i}$$

Pole-residue representation applies to any impedance function.

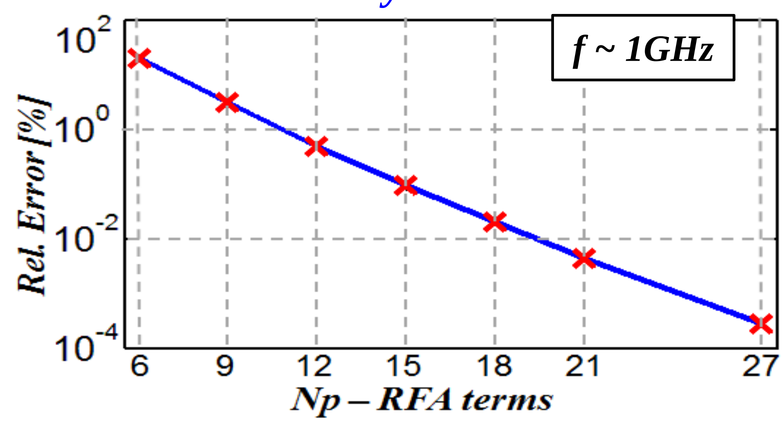
Example : Cu – Np=21,

Frequency range ~ 10MHz-5THz, Δf~5MHz





Sensitivity on RFA terms



TD-SIBC Implementation

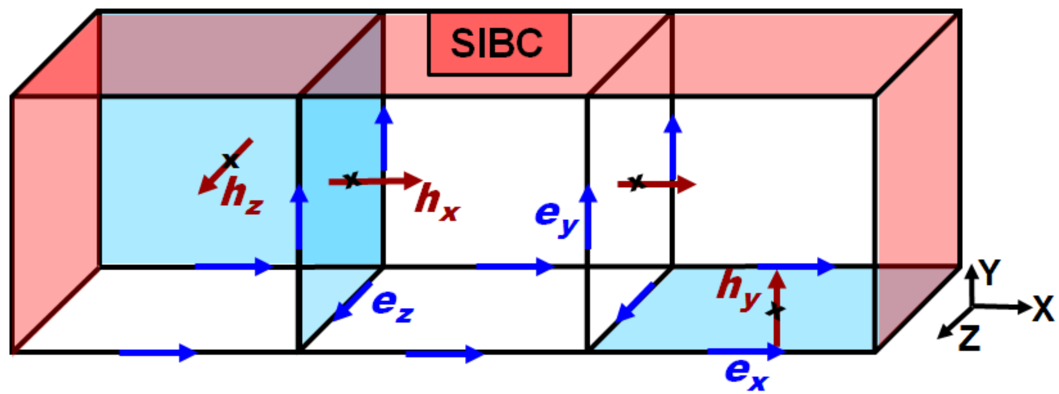
Faraday's Law with SIBC - TD

$$\left(M_\mu + L\cdot l_c\right)\frac{d}{dt}\hat{h} = -C\cdot\hat{e} - l_c\cdot\sum_{i=0}^{Np} G_i$$

Auxiliary Differential Equations (ADE)

$$\vec{G}_0 = \alpha_0\ [\,\vec{n}\times\vec{H}_\tau\,]$$
$$\frac{d}{dt}\vec{G}_i + \beta_i\vec{G}_i = \alpha_i\ [\,\vec{n}\times\vec{H}_\tau\,]$$

Boundary Cells with SIBC Surfaces



Ampere's Law with PEC

$$M_\varepsilon\frac{\partial}{\partial t}\hat{e} = C^T\cdot\hat{h} + \hat{\hat{j}}_s$$

Semi-Discrete Maxwell's Equations with TD-SIBC

$$\frac{d}{dt}\begin{pmatrix}\hat{e}\\ \hat{h}\\ 0\\ G_1\\ \vdots\\ G_N\end{pmatrix} = \begin{pmatrix} 0 & M_\varepsilon^{-1}C^T & 0 & 0 & \cdots & 0\\ -M_\mu^{-1}C & 0 & C_B & C_B & \cdots & C_B\\ 0 & \alpha_0 & 1 & 0 & \cdots & 0\\ 0 & -\alpha_1 & 0 & \beta_1 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & -\alpha_N & 0 & 0 & \cdots & \beta_N\end{pmatrix}\begin{pmatrix}\hat{e}\\ \hat{h}\\ G_0\\ G_1\\ \vdots\\ G_N\end{pmatrix}$$

TD-SIBC Implementation

Black-Box Strategy

MGE with TD-SIBC as ODE system

$$y = \begin{pmatrix} \hat{e} \\ \hat{h} \\ G_0 \\ G_1 \\ \vdots \\ G_N \end{pmatrix} \qquad \boxed{\frac{\partial}{\partial t} y = A \cdot y}$$

A_c $\quad$ A_{SIBC}

$$A = \begin{pmatrix} 0 & M_\varepsilon^{-1} C^T & 0 & 0 & \cdots & 0 \\ -M_\mu^{-1} C & 0 & C_B & C_B & \cdots & C_B \\ 0 & \alpha_0 & 1 & 0 & \cdots & 0 \\ 0 & -\alpha_1 & 0 & \beta_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -\alpha_N & 0 & 0 & \cdots & \beta_N \end{pmatrix}$$

Strang Splitting - Second Order

$$\boxed{e^{A*\Delta t} = e^{A_{SIBC}*\Delta t/2} * e^{A_c*\Delta t} * e^{A_{SIBC}*\Delta t/2}}$$

- **ADE update [Δt/2]**
- **Add Loss to each h-comp.**

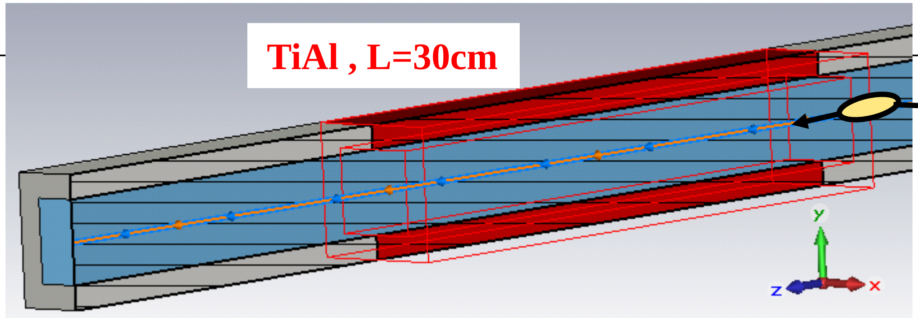
- **Main 3D Num. Scheme update (Δt)**

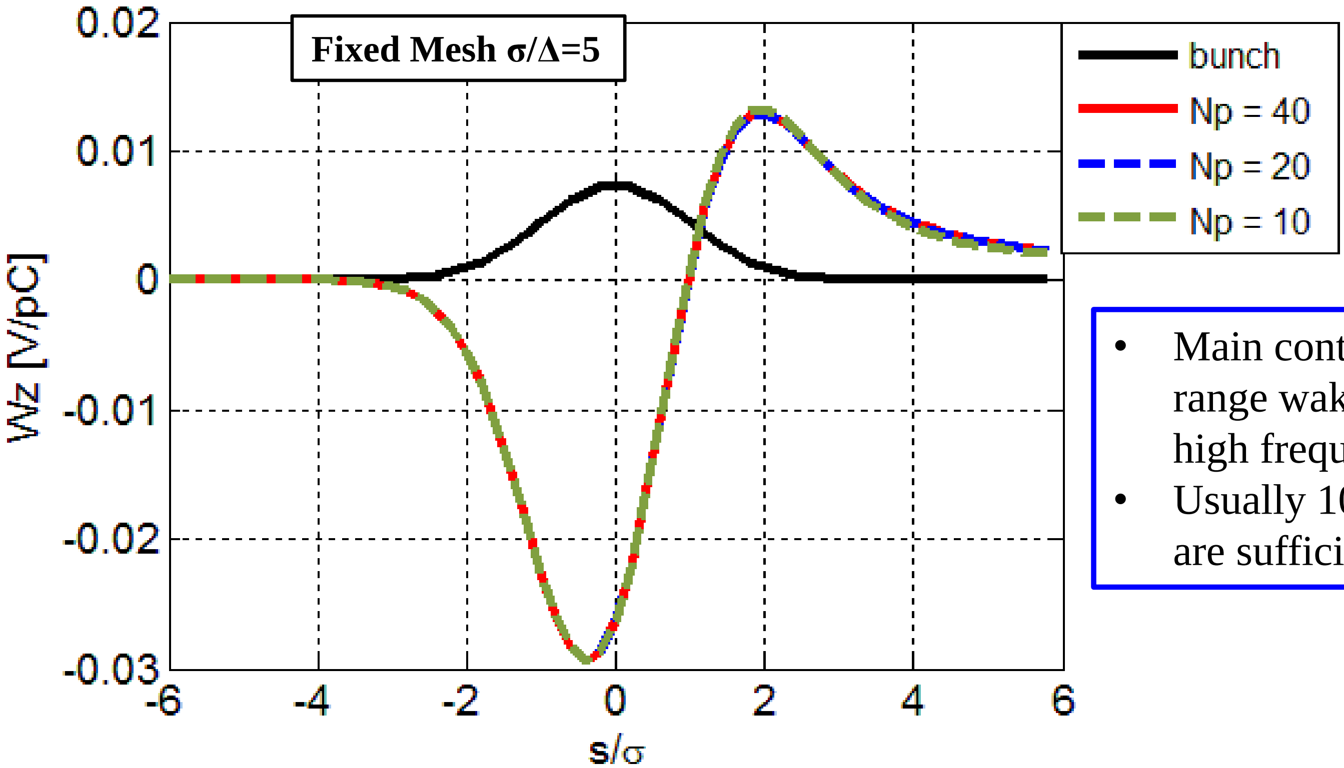
- **ADE update [Δt/2]**
- **Add Loss to each h-comp.**

Applicable for FIT based methods with different time integrations

For example: LT, TE/TM, LF

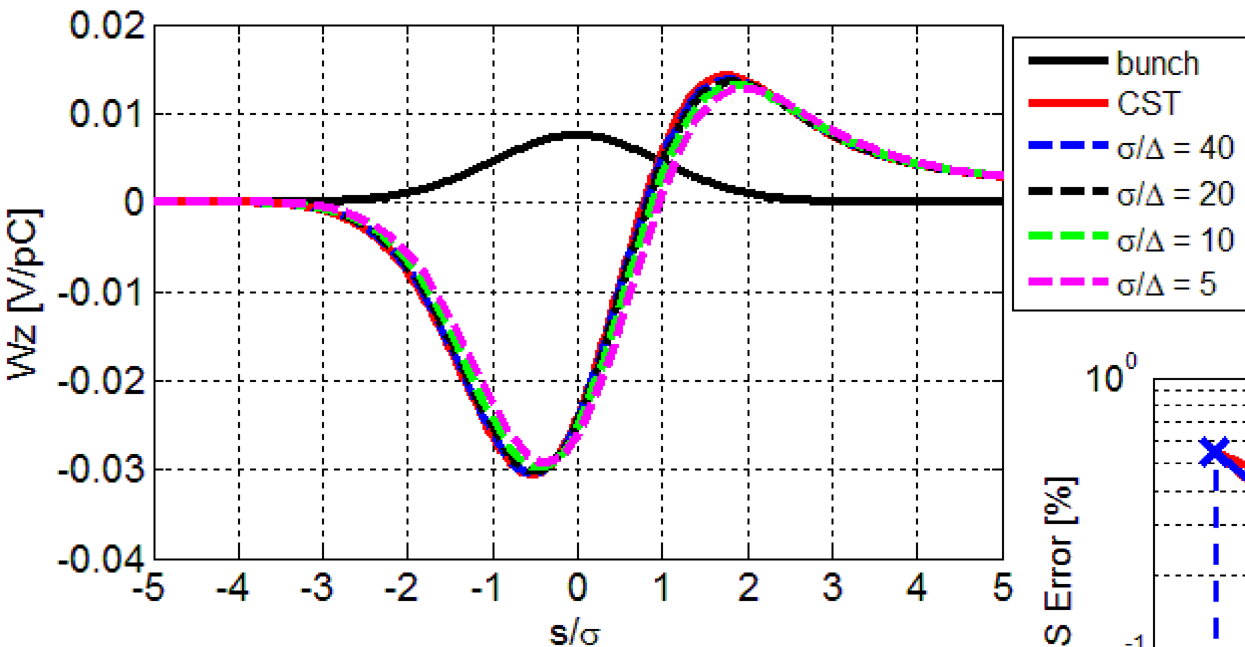
Resistive Wake Test on TD-SIBC order

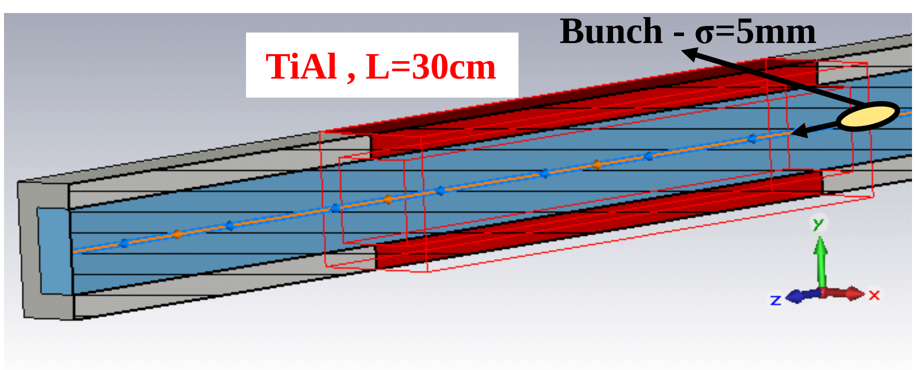


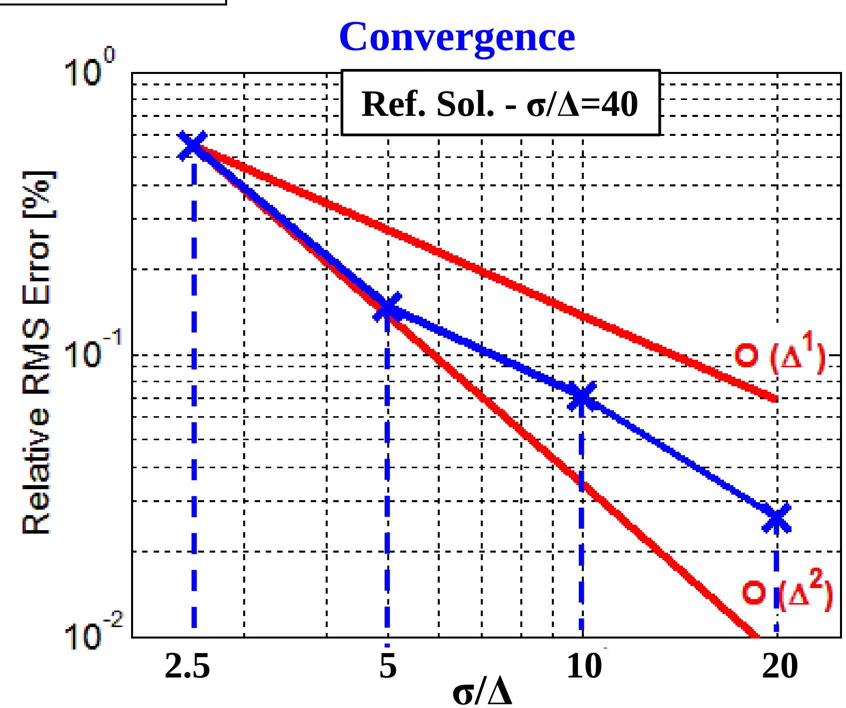


- Main contribution in short range wakes is from SIBC high frequency part.
- Usually 10-20 terms in VF are sufficient.

Comparison with CST







Summary

Achievements

- Time Domain SIBC model & RFA Accuracy
- Successful TD-SIBC Implementation (*Black-Box Strategy*) in FIT Based 3D methods.
- Stability & Convergence Analyses
- Verification for Rectangular Beampipe.
- Moving Window & Parallelized for PEC Boundaries.
- Empirical solution for staircase verified for cylindrical beampipe case.

Further Steps

- Empirical Solution for Staircase – verification is required for 3D none-symmetric geometries.
- TD-SIBC Part Parallelization & Performance Optimization.
- Application to Realistic Structures with Complex Geometries.

- Further development - application of conformal boundary approximation.

Thank You for Your Attention!