Large Scale Parallel Wake Field Computations with PBCI

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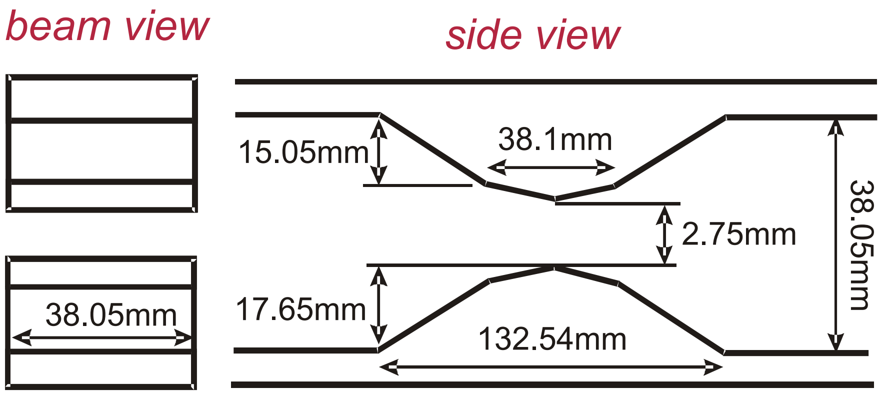
Outline

- Introduction
- Numerical Method
- Parallelization Strategy
- Modal Termination of Beam Pipes
- PBCI Simulation Examples
- Conclusions

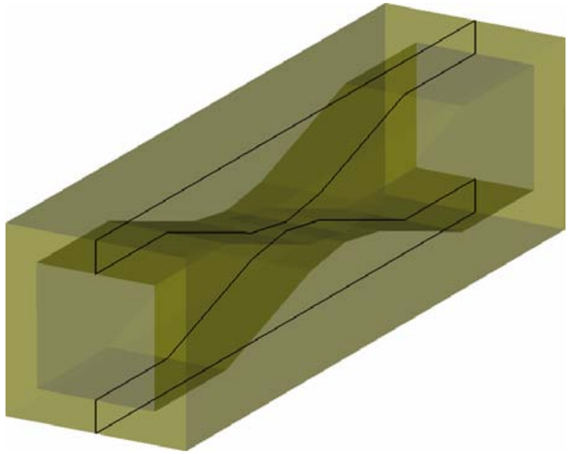
Motivation for PBCI:

1. A new generation of LINACs with ultra-short electron bunches
   a. *bunch size for ILC: 300 µm*
   b. *bunch size for LCLS: 20 µm*
2. Geometry of tapers, collimators… far from rotational
   a. *8 rectangular collimators at ILC-ESA in the design process*
   b. *30 rectangular-to-round transitions in the undulator of LCLS*
3. Many (semi-) analytical approximations become invalid
   a. *based on rotationally symmetric geometry*
   b. *low frequency assumptions (Yokoya, Stupakov)*
   c. *detailed physics needed for high frequency wakes (Bane)*

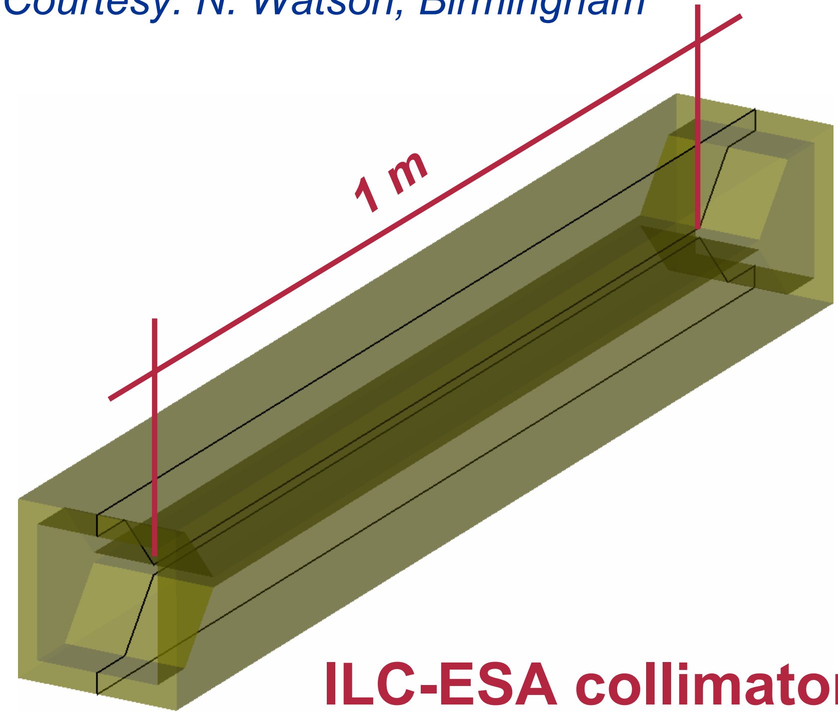
Introduction



Courtesy: N. Watson, Birmingham



ILC-ESA collimator #8



ILC-ESA collimator #3

bunch length	*300μm*
collimator length	*~1.2m*
catch-up distance	*~2.4m*

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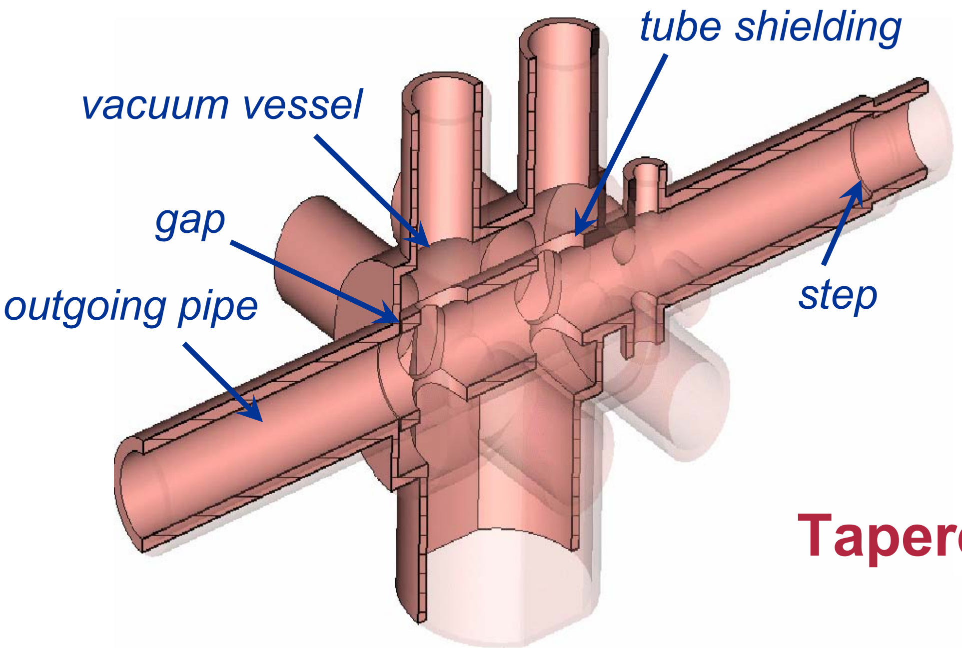
Introduction

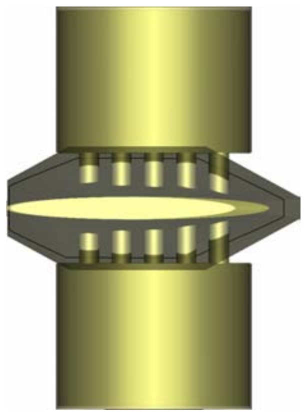


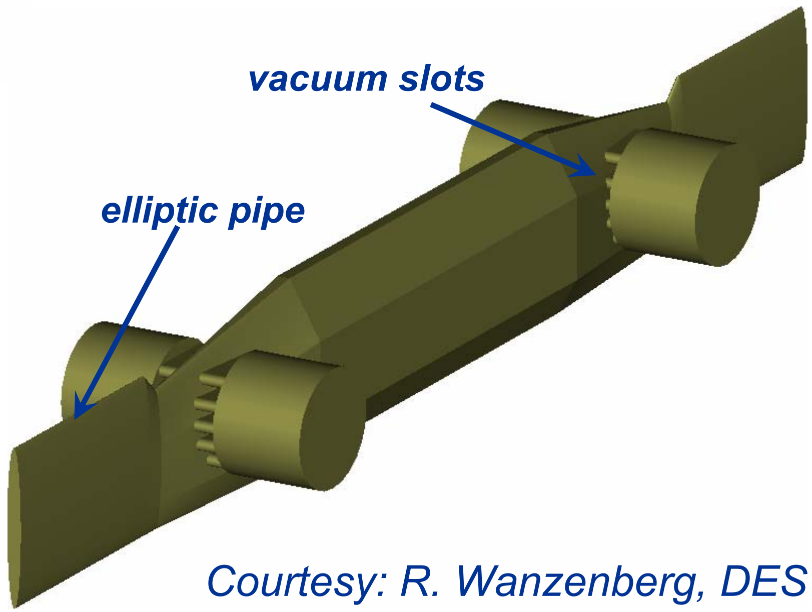
PITZ diagnostics double cross

bunch length	*2.5mm*
bunch width	*2.5mm*
structure length	*325mm*

Tapered transition @PETRA III

bunch length	*1cm*
taper length	*50cm*





Courtesy: R. Wanzenberg, DESY

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Introduction

There is an actual demand for:

1. Wake field simulations in arbitrary 3D-geometry

   3D-codes

2. Accurate numerical solutions for high frequency fields

   (quasi-) dispersionless codes

3. Utilizing large computational resources for ultra-short bunches

   parallelized codes

4. Specialized algorithms for long accelerator structures

   moving window codes

An (incomplete) survey of available codes

Time		Dimensions	Nondispersive	Parallelized	Moving window
1982	**BCI / TBCI**	2.5D	No	No	Yes
	NOVO	2.5D	Yes	No	No
	ABCI	2.5D	No	No	Yes
	MAFIA	2.5/3D	No	No	No
2002	**GdfidL**	3D	No	Yes	No
	ECHO	2.5/3D	Yes	No	Yes
2006	**PBCI**	3D	Yes	Yes	Yes

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The FIT discretization

$$\oint_{\partial A} \vec{E} \cdot d\vec{s} = -\frac{\partial}{\partial t} \iint_{A} \mu \vec{H} \cdot d\vec{A}$$

$$\oint_{\partial A} \vec{H} \cdot d\vec{s} = \iint_{A} \left(\frac{\partial}{\partial t} \varepsilon \vec{E} + \vec{J} \right) \cdot d\vec{A}$$

$$\oiint_{\partial V} \mu \vec{H} \cdot d\vec{A} = 0$$

$$\oiint_{\partial V} \varepsilon \vec{E} \cdot d\vec{A} = \iiint_{V} \rho \, dV$$

FIT $\Rightarrow$

$$\mathbf{C}\,\widehat{\mathbf{e}} = -\frac{d}{dt} \mathbf{M}_{\mu} \overset{\frown}{\mathbf{h}}$$

$$\widetilde{\mathbf{C}}\,\overset{\frown}{\mathbf{h}} = \frac{d}{dt} \mathbf{M}_{\varepsilon} \widehat{\mathbf{e}} + \overset{\frown}{\overset{\frown}{\mathbf{j}}}$$

$$\widetilde{\mathbf{S}}\,\mathbf{M}_{\varepsilon} \widehat{\mathbf{e}} = \mathbf{q}$$

$$\mathbf{S}\,\mathbf{M}_{\mu} \overset{\frown}{\mathbf{h}} = 0$$

Topology of FIT:

$\mathbf{C}^{T} = \widetilde{\mathbf{C}}$ $\Rightarrow$ *semidiscrete energy conservation*

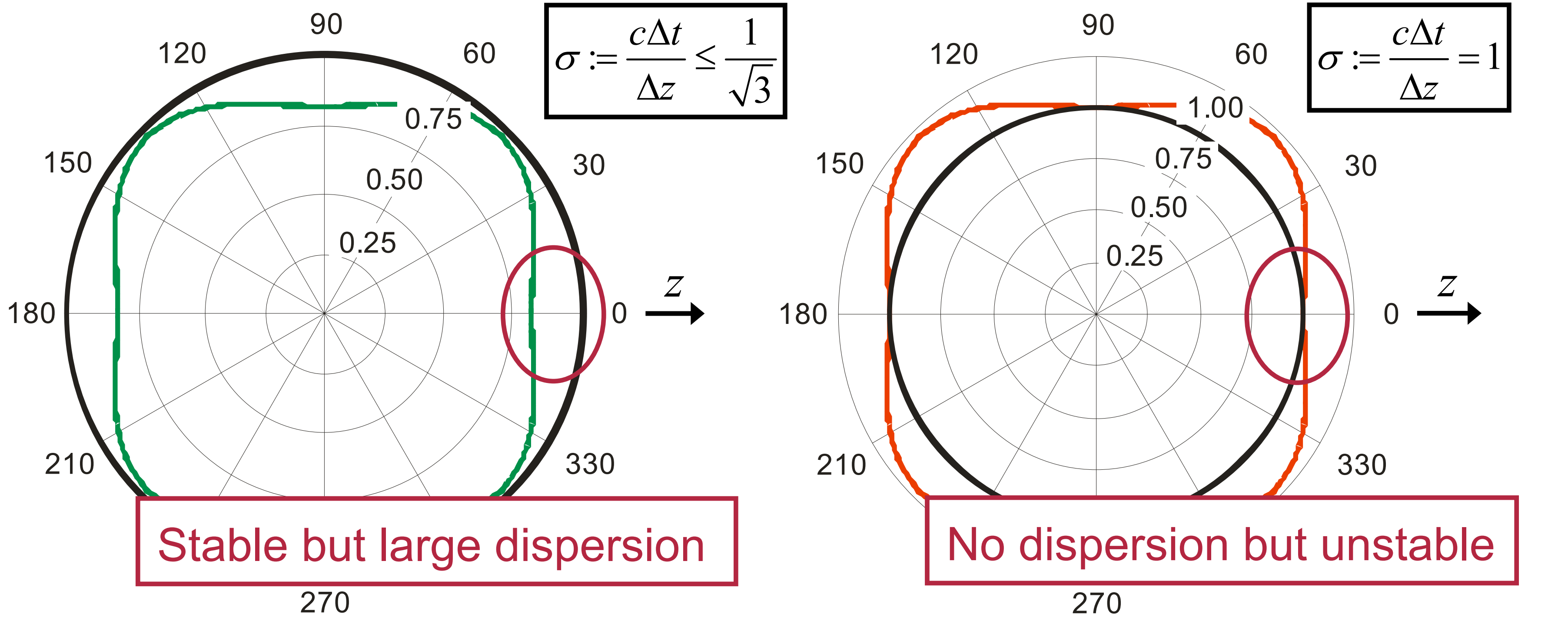
$\widetilde{\mathbf{S}}\mathbf{C} = \mathbf{S}\widetilde{\mathbf{C}} = 0$ $\Rightarrow$ *semidiscrete charge conservation*

Numerical Method

Using the conventional leapfrog time integration

$$\begin{pmatrix} \widehat{\mathbf{e}}^{n+1/2} \\ \widehat{\mathbf{h}}^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \Delta t \mathbf{M}_\varepsilon^{-1} \mathbf{C}^T \\ -\Delta t \mathbf{M}_\mu^{-1} \mathbf{C} & \mathbf{1} - \Delta t^2 \mathbf{M}_\mu^{-1} \mathbf{C} \mathbf{M}_\varepsilon^{-1} \mathbf{C}^T \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{e}}^{n-1/2} \\ \widehat{\mathbf{h}}^{n} \end{pmatrix} - \begin{pmatrix} \Delta t \mathbf{M}_\varepsilon^{-1} \widehat{\mathbf{j}}^{n} \\ \mathbf{0} \end{pmatrix}$$

Behavior of numerical phase velocity vs. propagation angle



$\sigma := \frac{c\Delta t}{\Delta z} \le \frac{1}{\sqrt{3}}$

Stable but large dispersion

$\sigma := \frac{c\Delta t}{\Delta z} = 1$

No dispersion but unstable

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Numerical Method

Idea: Reduce the integration of 3D equations to a sequence of 1D / 2D integrations along the coordinate axes

Longitudinal-Transversal (LT) splitting:

$$\mathbf{H}_t = \begin{pmatrix} \mathbf{0} & \mathbf{M}_\varepsilon^{-1}\mathbf{C}_t^T \\ -\mathbf{M}_\mu^{-1}\mathbf{C}_t & \mathbf{0} \end{pmatrix}$$

does not affect longitudinal waves

$$\mathbf{H}_l = \begin{pmatrix} \mathbf{0} & \mathbf{M}_\varepsilon^{-1}\mathbf{C}_l^T \\ -\mathbf{M}_\mu^{-1}\mathbf{C}_l & \mathbf{0} \end{pmatrix}$$

integrable in 1D without numerical dispersion

$$\boxed{\begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n+1} = e^{-\mathbf{H}\Delta t} \begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n} = e^{-\mathbf{H}_t \frac{\Delta t}{2}} e^{-\mathbf{H}_l \Delta t} e^{-\mathbf{H}_t \frac{\Delta t}{2}} \begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n} + O(\Delta t^3)}$$

modified time evolution

Second order *Strang splitting*

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Numerical Method

Idea: Reduce the integration of 3D equations to a sequence of 1D / 2D integrations along the coordinate axes

Replace each evolution operator with Verlet-leapfrog propagators:

$$\mathbf{G}_{l;t}(\Delta t) = \begin{pmatrix} \mathbf{1} - \frac{\Delta t^2}{2}\mathbf{M}_\varepsilon^{-1}\mathbf{C}_{l;t}^T\mathbf{M}_\mu^{-1}\mathbf{C}_{l;t} & \Delta t\mathbf{M}_\varepsilon^{-1}\mathbf{C}_{l;t}^T - \frac{\Delta t^3}{4}\mathbf{M}_\varepsilon^{-1}\mathbf{C}_{l;t}^T\mathbf{M}_\mu^{-1}\mathbf{C}_{l;t}\mathbf{M}_\varepsilon^{-1}\mathbf{C}_{l;t}^T \\ -\Delta t\mathbf{M}_\mu^{-1}\mathbf{C}_{l;t} & \mathbf{1} - \frac{\Delta t^2}{2}\mathbf{M}_\mu^{-1}\mathbf{C}_{l;t}\mathbf{M}_\varepsilon^{-1}\mathbf{C}_{l;t}^T \end{pmatrix}$$

Time discrete update:

$$\boxed{\begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n+1} = \mathbf{G}_t\left(\frac{\Delta t}{2}\right)\bullet\mathbf{G}_l(\Delta t)\bullet\mathbf{G}_t\left(\frac{\Delta t}{2}\right)\bullet\begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^n}$$

stable for: $\boxed{\sigma := \frac{c\Delta t}{\Delta z} = 1}$

T. Lau, E. Gjonaj and T. Weiland, Time Integration Methods for Particle Beam Simulations with the Finite Integration Theory, FREQUENZ, Vol. 59 (2005), pp. 210

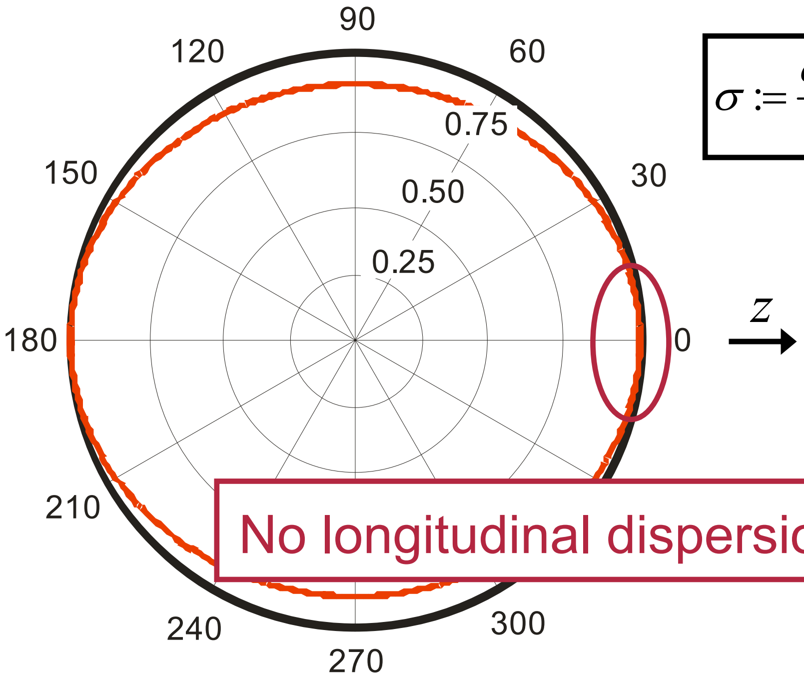
Numerical Method

Implementing the LT splitting scheme

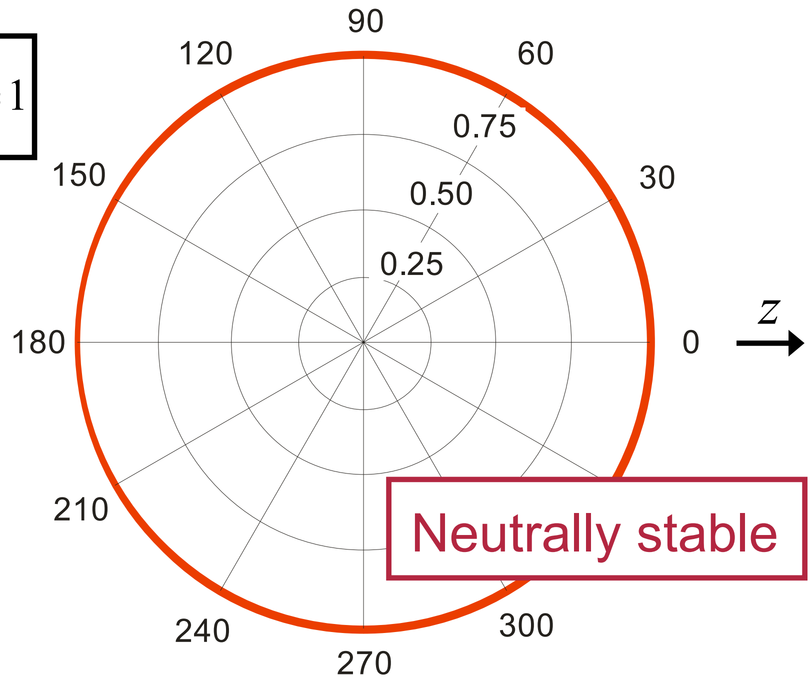
$$\begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n+1} = \mathbf{G}_t\left(\frac{\Delta t}{2}\right)\cdot\mathbf{G}_l\left(\Delta t\right)\cdot\mathbf{G}_t\left(\frac{\Delta t}{2}\right)\cdot\begin{pmatrix} \widehat{\mathbf{e}} \\ \widehat{\mathbf{h}} \end{pmatrix}^{n}$$

Numerical phase velocity and amplification vs. propagation angle

$$\sigma := \frac{c\Delta t}{\Delta z} = 1$$



No longitudinal dispersion



Neutrally stable

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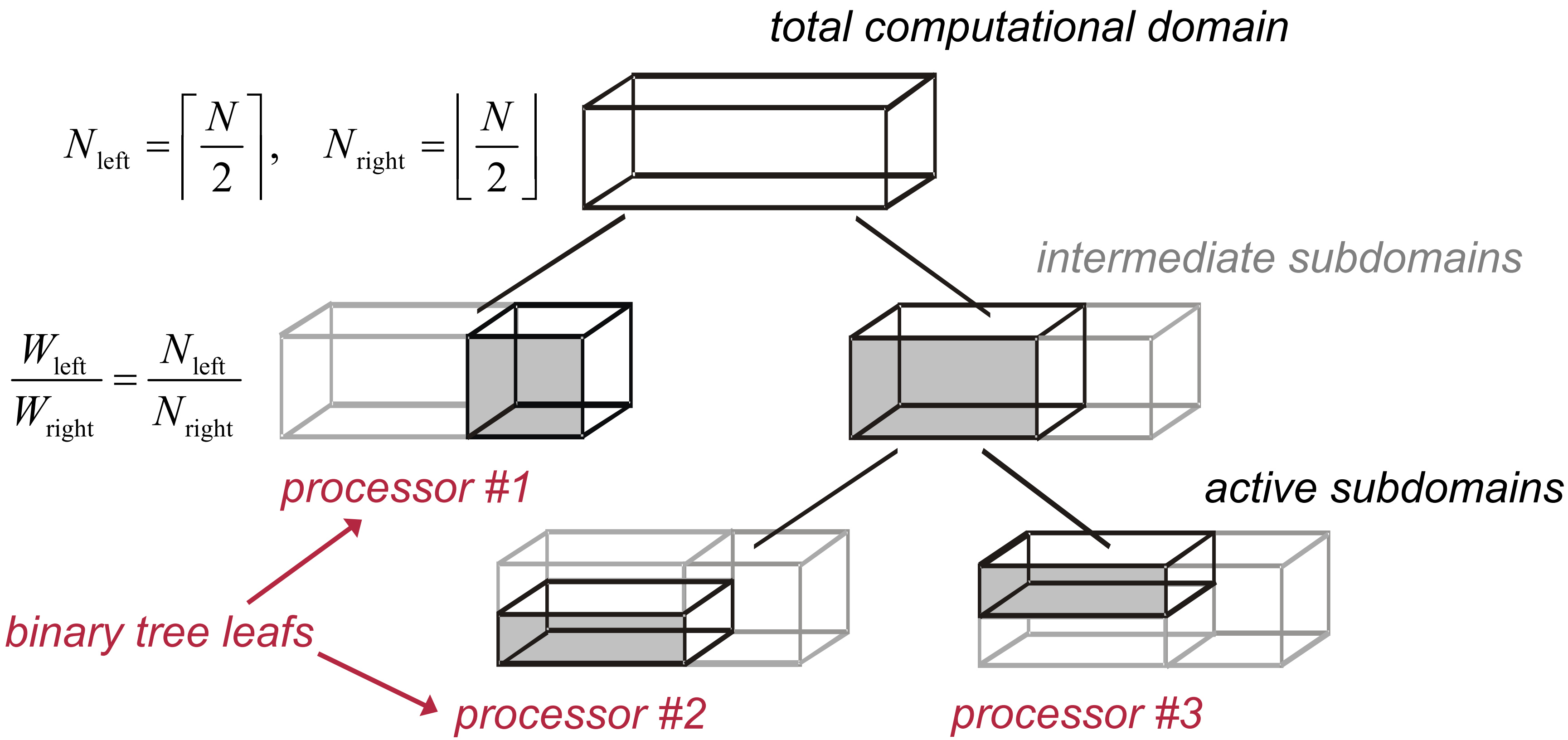
Parallelization Strategy

A balanced domain partitioning approach

$$N_{\text{left}} = \left\lceil \frac{N}{2} \right\rceil, \quad N_{\text{right}} = \left\lfloor \frac{N}{2} \right\rfloor$$

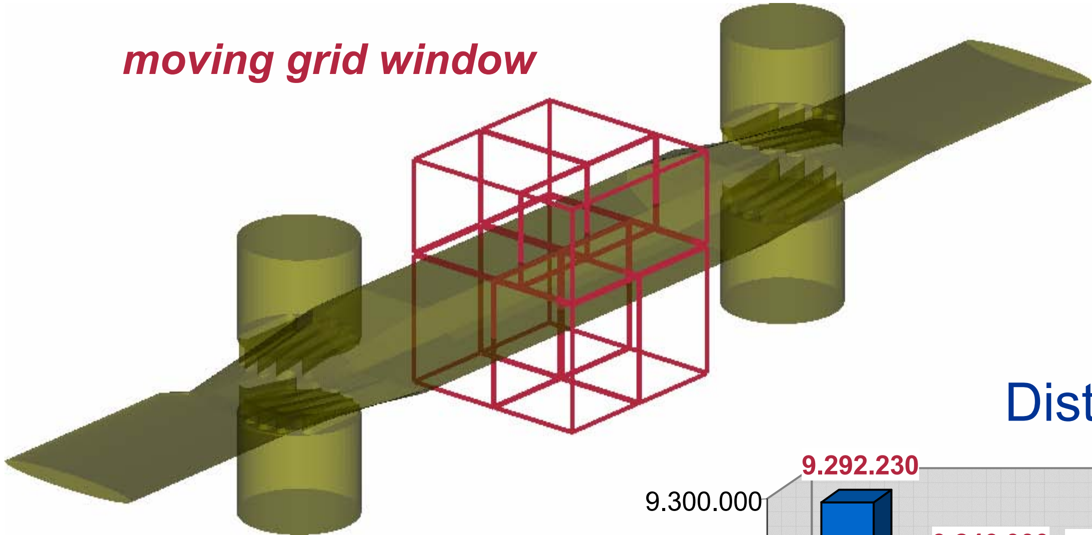
$$\frac{W_{\text{left}}}{W_{\text{right}}} = \frac{N_{\text{left}}}{N_{\text{right}}}$$



Equal loads assigned to each node: $W_{\text{Node}} = \alpha_{\text{Node}} \bullet \sum_{\text{Grid Points}} w_i$

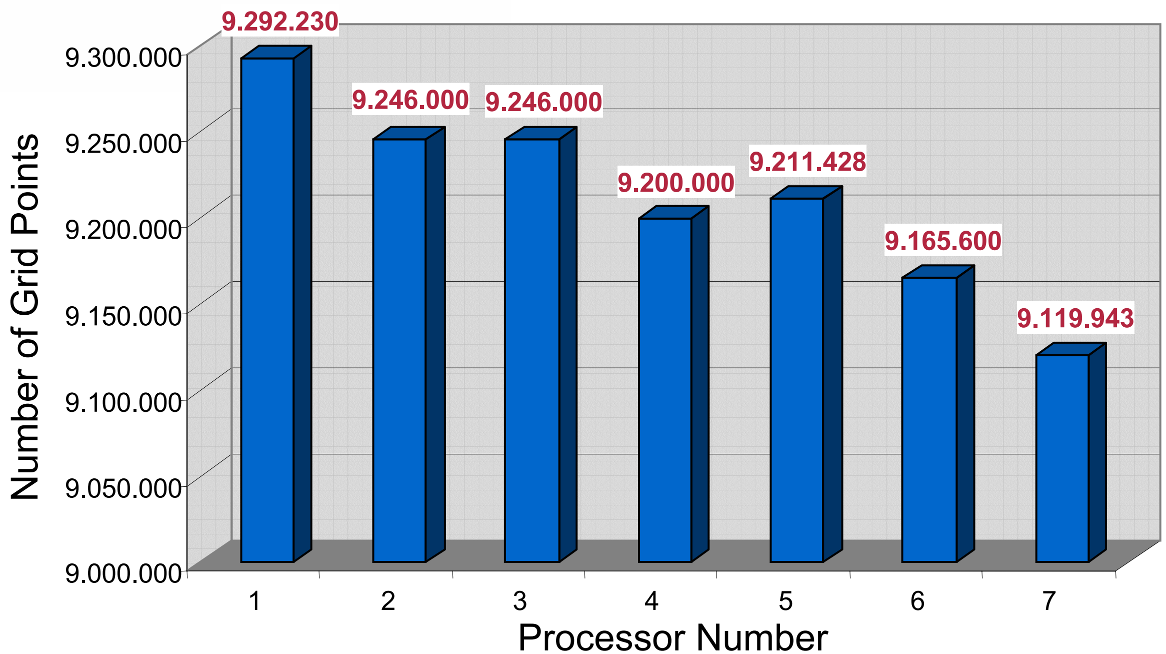
Parallelization Strategy

Example: Tapered transition for PETRA III



Domain partitioning pattern for 7 processors

Distribution of grid points



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

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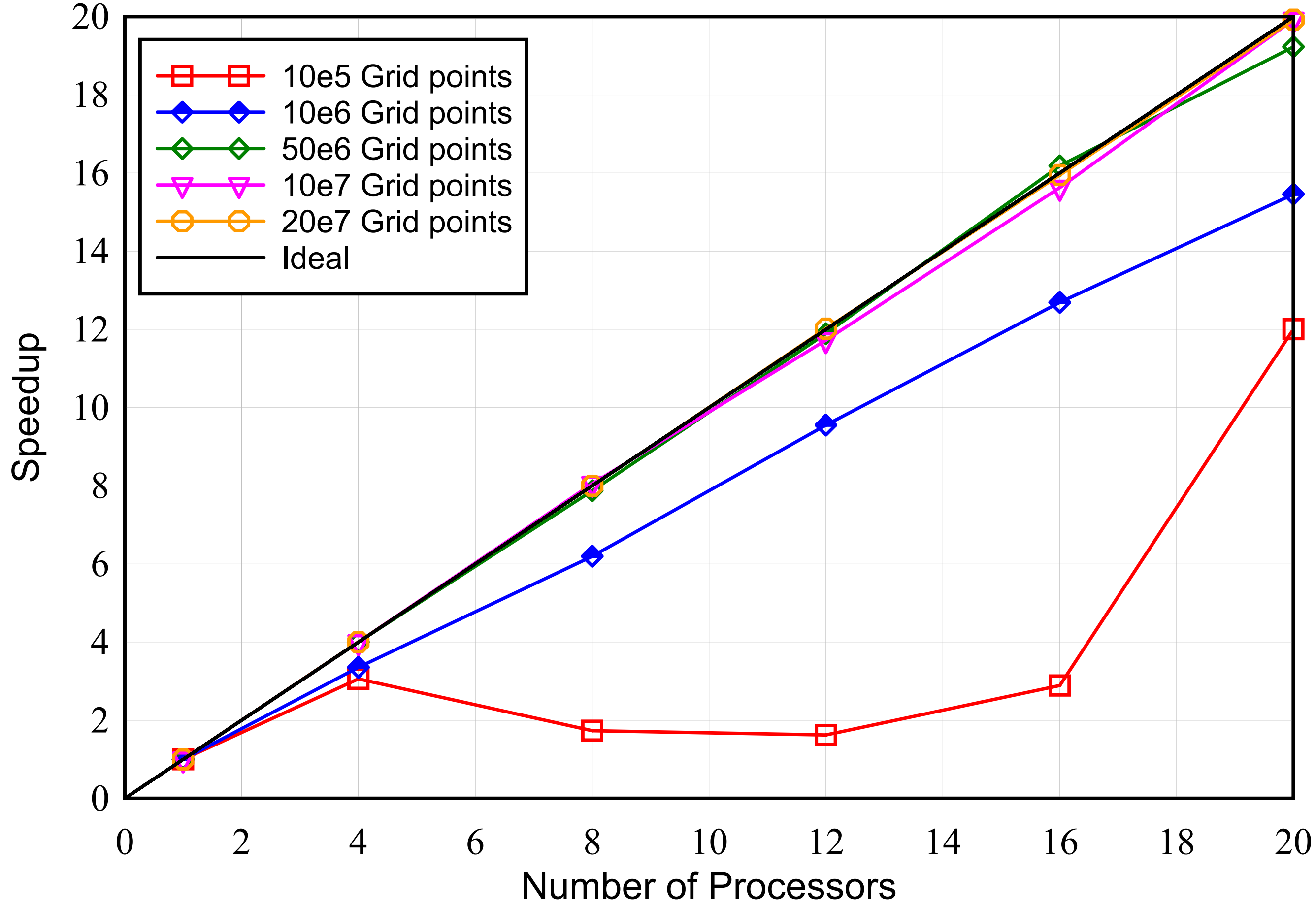
Parallelization Strategy

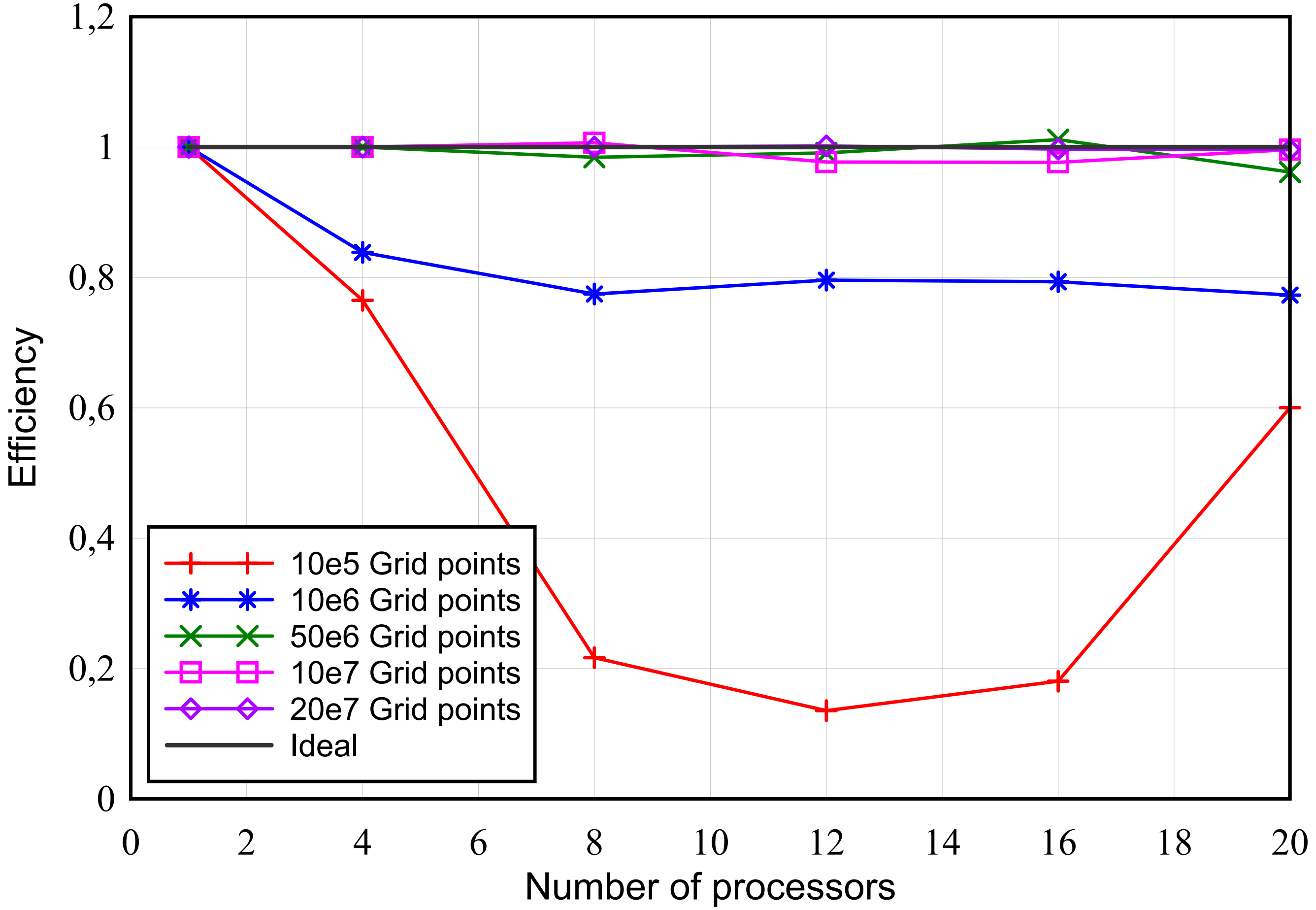
Parallel performance tests



*TEMF Cluster: **20** INTEL CPUs @ **3.4**GHz, **8**GB RAM, **1**Gbit/s Ethernet Network*

Parallelization Strategy

Parallel performance tests



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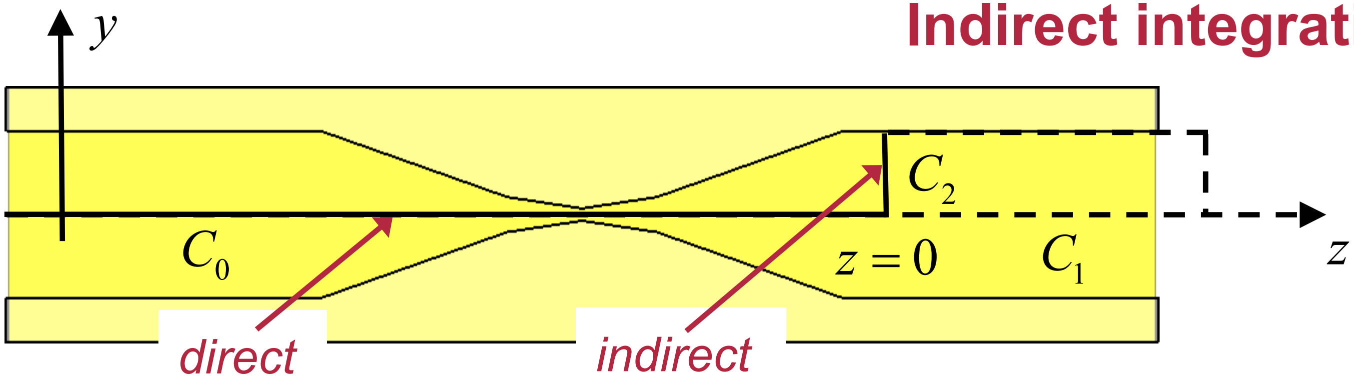
Modal Termination of Pipes

Indirect integration schemes



$$\boxed{W_z(s) = -\frac{1}{Q}\int_{-\infty}^{\infty} dz\, E_z\left(z, t = \frac{z+s}{c}\right)} = -\frac{1}{Q}\int_{C_0} dz\, E_z\left(z, t = \frac{z+s}{c}\right) - \frac{1}{Q}\int_{C_2} dy\, G_y^{TM}\left(0, t = \frac{s}{c}\right)$$

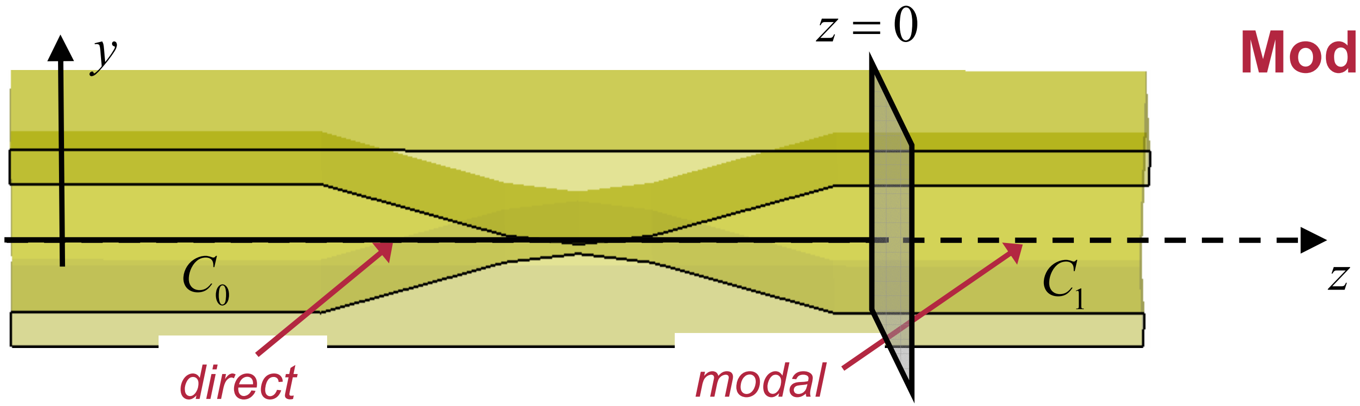
1. Indirect integration of potential for 2D-structures *(Weiland 1983, Napoly 1993)*
2. Generalization for 3D-structures *(A. Henke and W. Bruns, EPAC'06, July 2006, Edinburgh, UK)*

$$\boxed{\vec{G}^{TM} = \vec{e}_x\left(E_x^{TM} + cB_y^{TM}\right) + \vec{e}_y\left(E_y^{TM} - cB_x^{TM}\right) + \vec{e}_z E_z}$$

irrotational

Modal Termination of Pipes

Modal approach



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

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

spectral coefficient of n-th (TM) mode

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

$W_n(s)$ **n-th (TM) mode contribution**

Modal Termination of Pipes

1. Time domain integration in the inhomogeneous sections:

$$-\frac{1}{Q}\int_{-\infty}^{0} dz\, E_z(z, t = \frac{z+s}{c})$$

2. Modal analysis at z = 0: $E_z(x,y,0,t) \quad \Rightarrow \quad E_z^n(0,t),\; e_z^n(x,y)$

3. Compute spectral coefficients (FFT): $E_z^n(0,t) \quad \Rightarrow \quad C_n(\omega)$

4. Compute wake potential contribution per mode (IFFT):

$$\frac{C_n(\omega)}{i\left(\omega / c - k_{z,n}(\omega)\right)} \quad \Rightarrow \quad W_n(s)$$

5. Compute wake potential transition in the outgoing pipe:

$$-\frac{1}{Q}\int_{0}^{\infty} dz\, E_z(z, t = \frac{z+s}{c}) = -\frac{1}{Q}\sum_n e_z^n(x,y) W_n(s)$$

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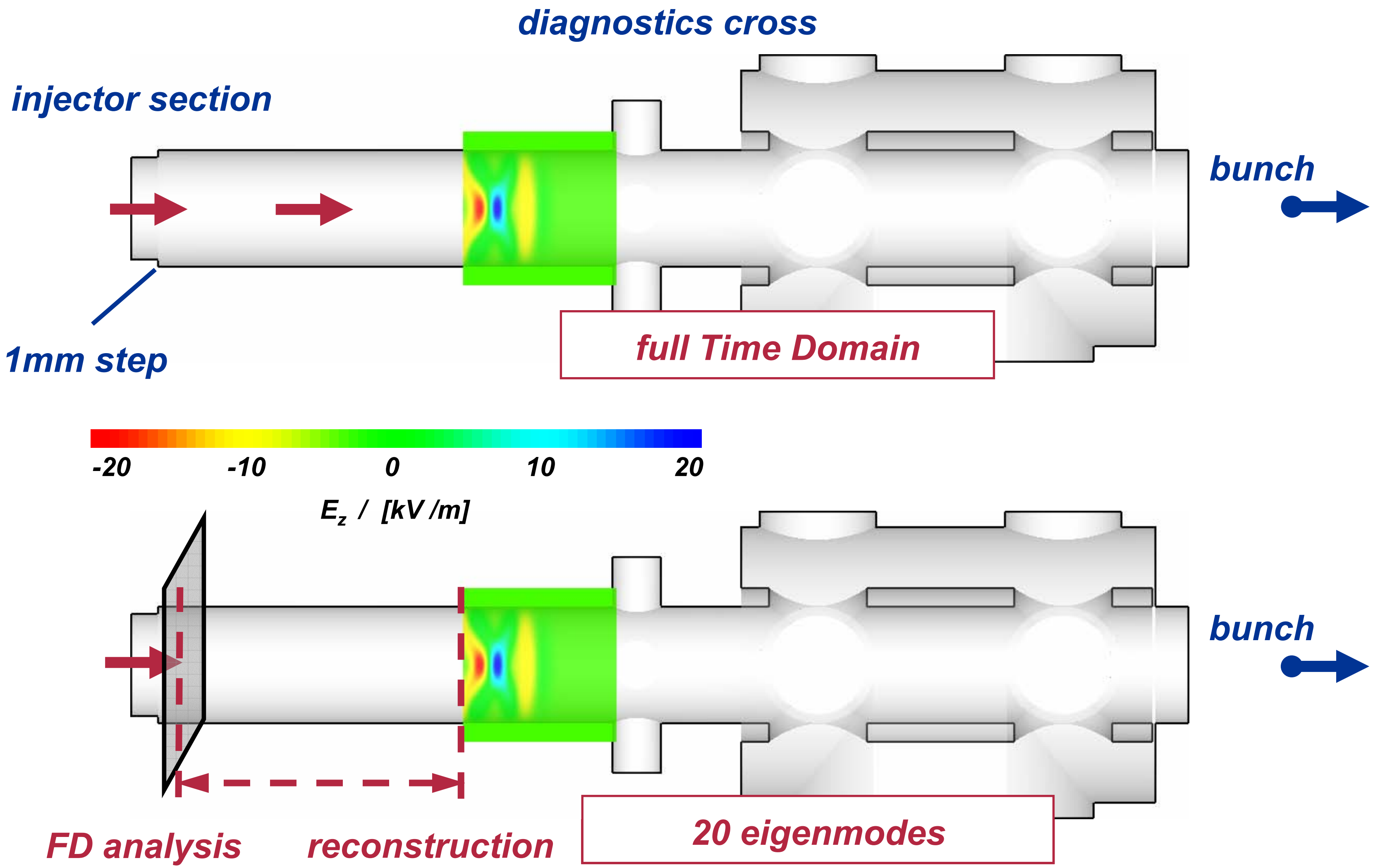
Modal Termination of Pipes

Using FD reconstruction in long intermediate pipes



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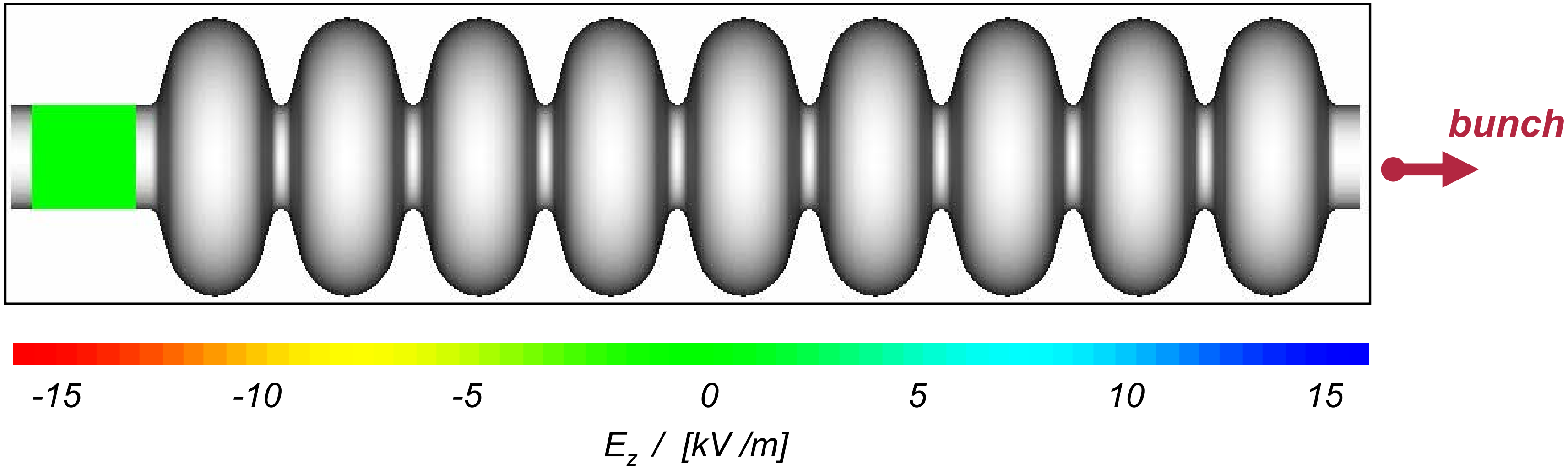
Simulation Examples

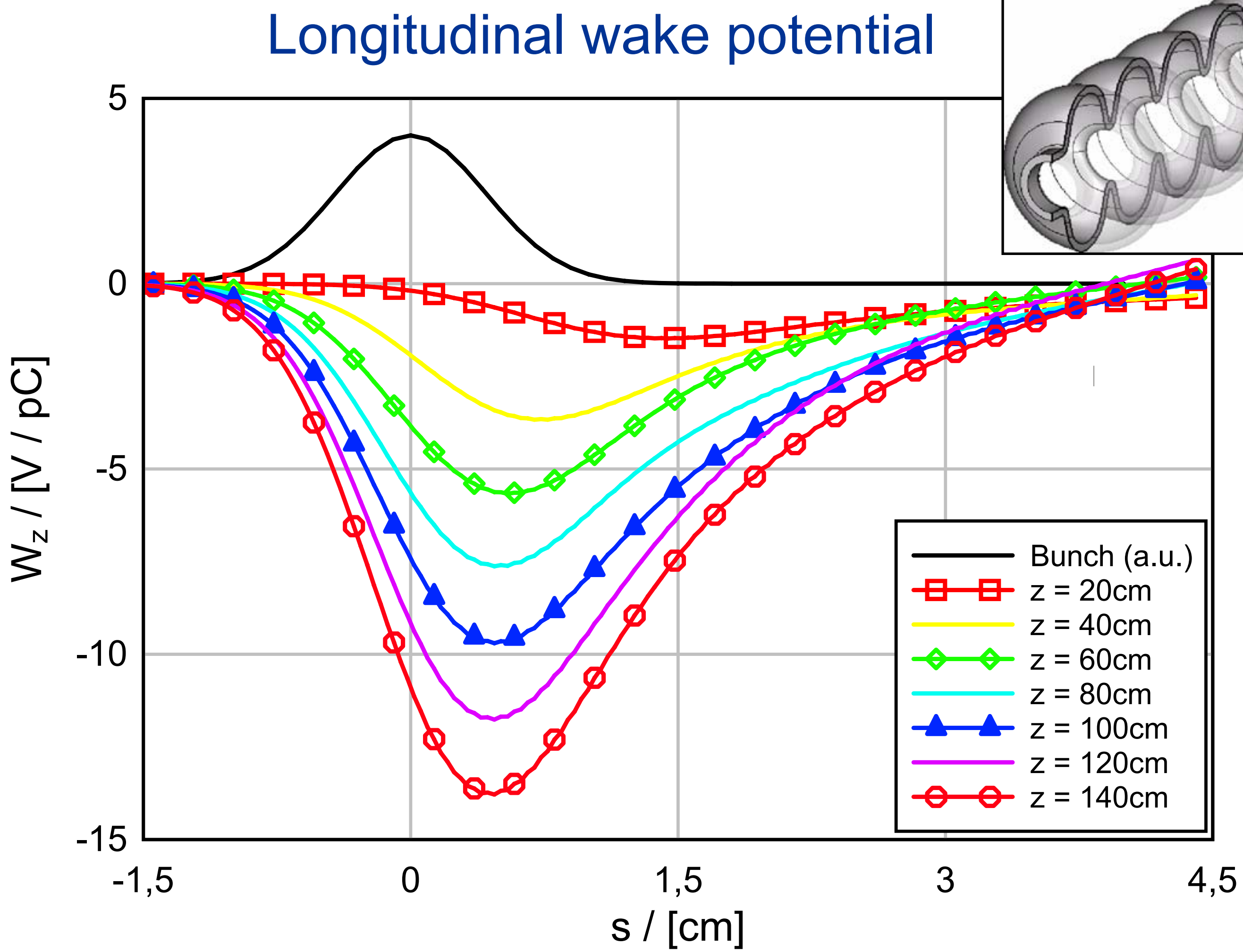
TESLA 9-cell cavity

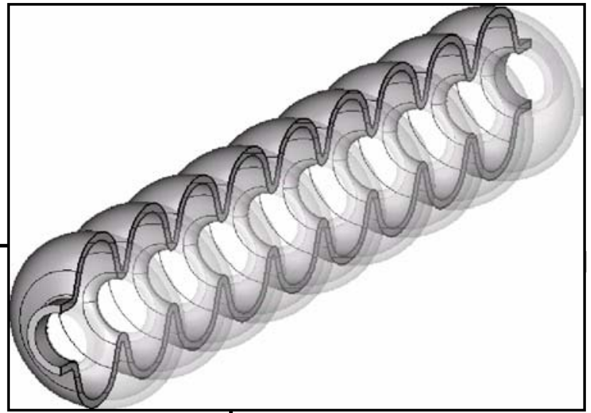


bunch length	5mm
bunch charge	1nC
cavity length	1.5m
no. of grid points	~80e6
no. of processors	24
simulation time	3hrs

Simulation Examples

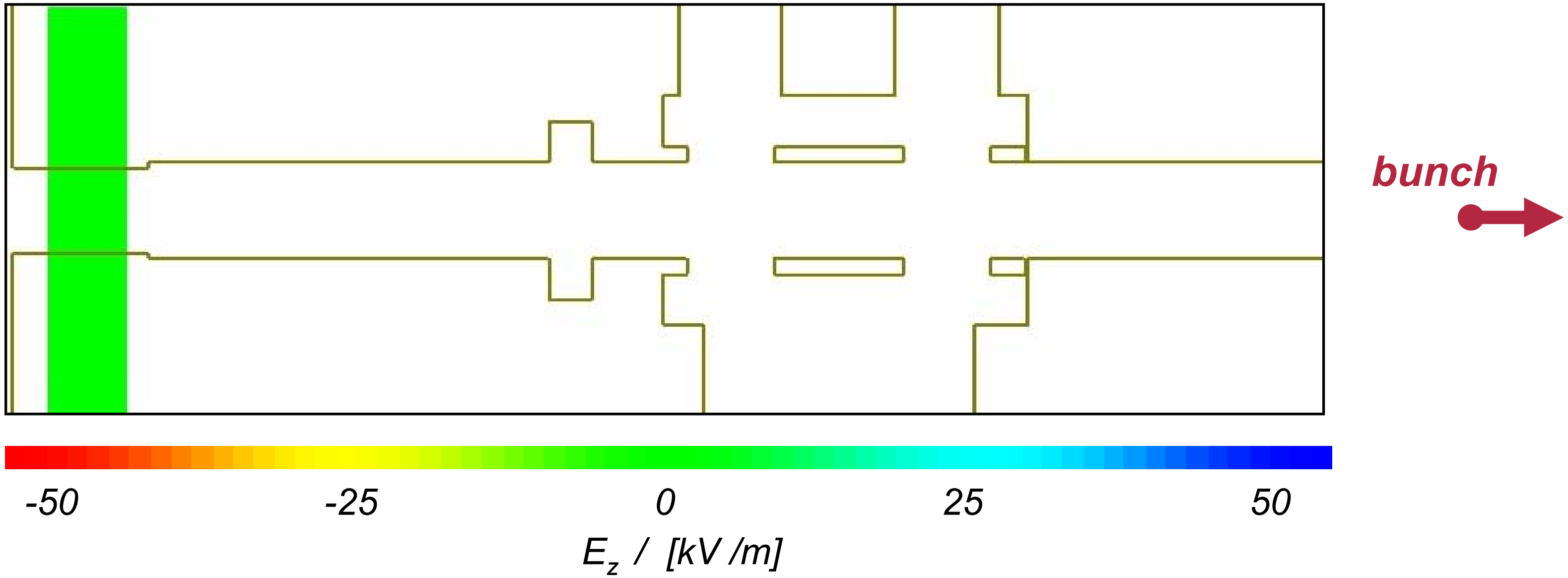
TESLA 9-cell cavity



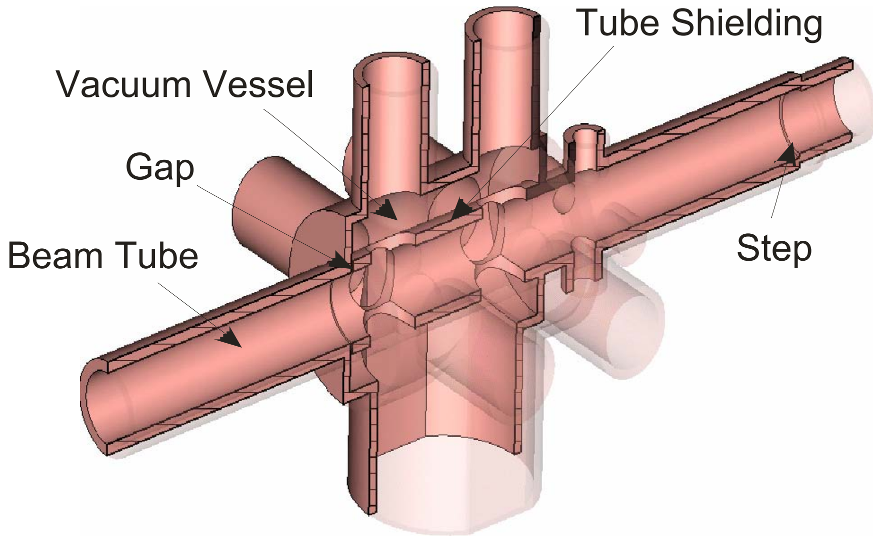


Simulation Examples

PITZ diagnostics double cross



bunch size	2.5mm
σ / Δz	30
no. of grid points	~500e6
no. of processors	24
simulation time	32hrs

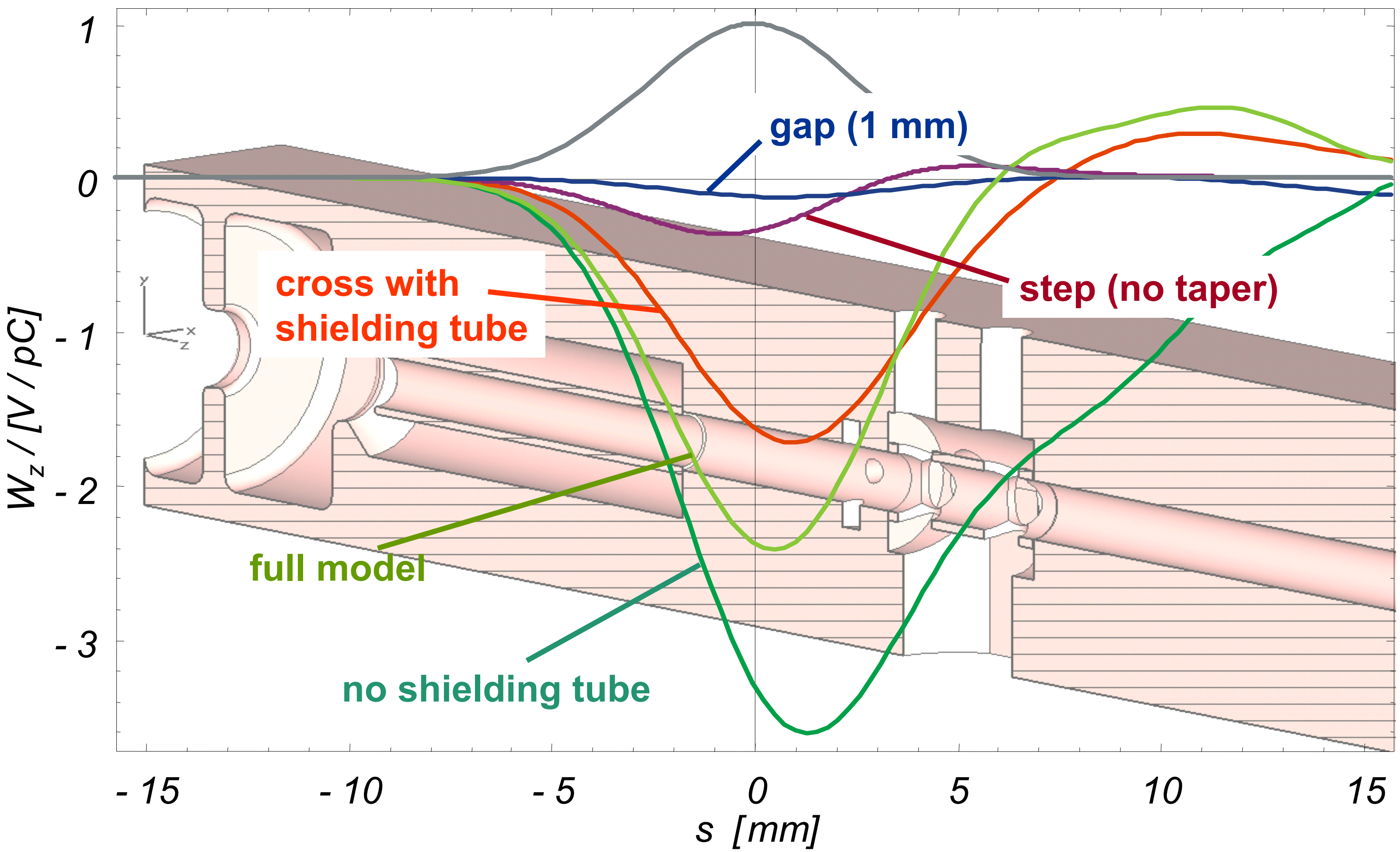


Simulation Examples

PITZ diagnostics double cross

(Ackermann, Hampel, Schnepp)

Wake field impact of the single components

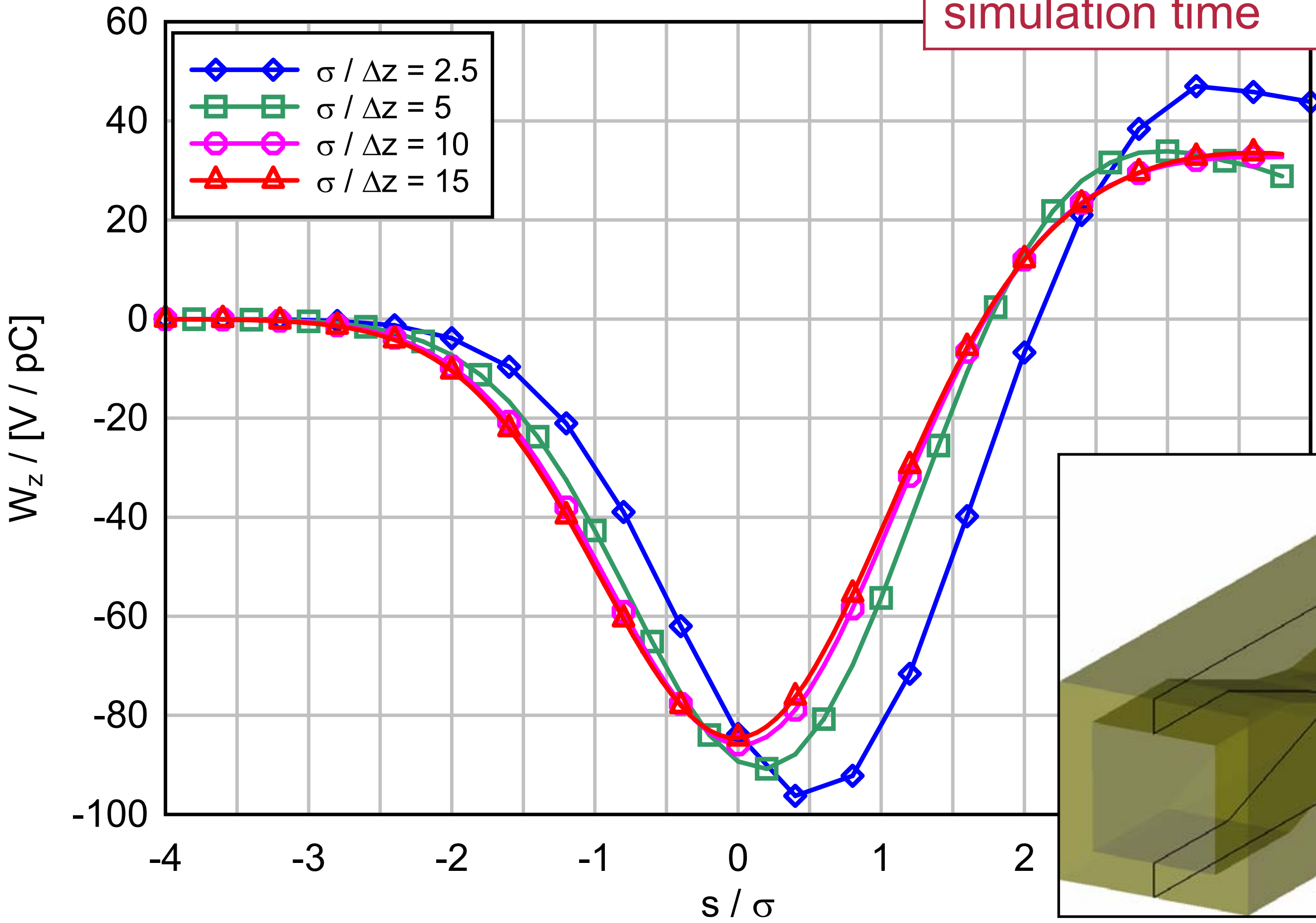


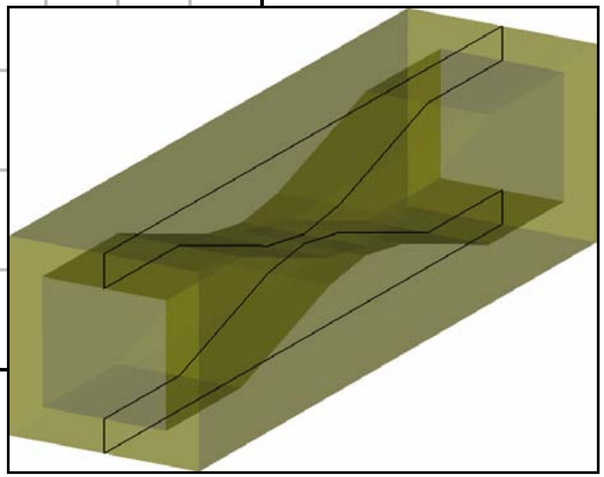
Simulation Examples

ILC-ESA collimator #8

bunch size	*300µm*
no. of grid points	~450e6
no. of processors	24
simulation time	85hrs

Convergence vs. grid step





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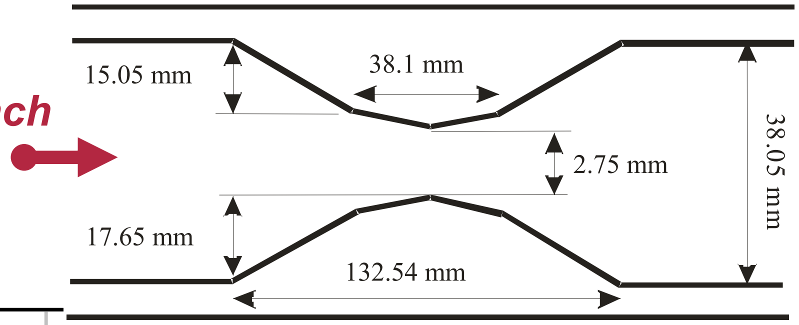
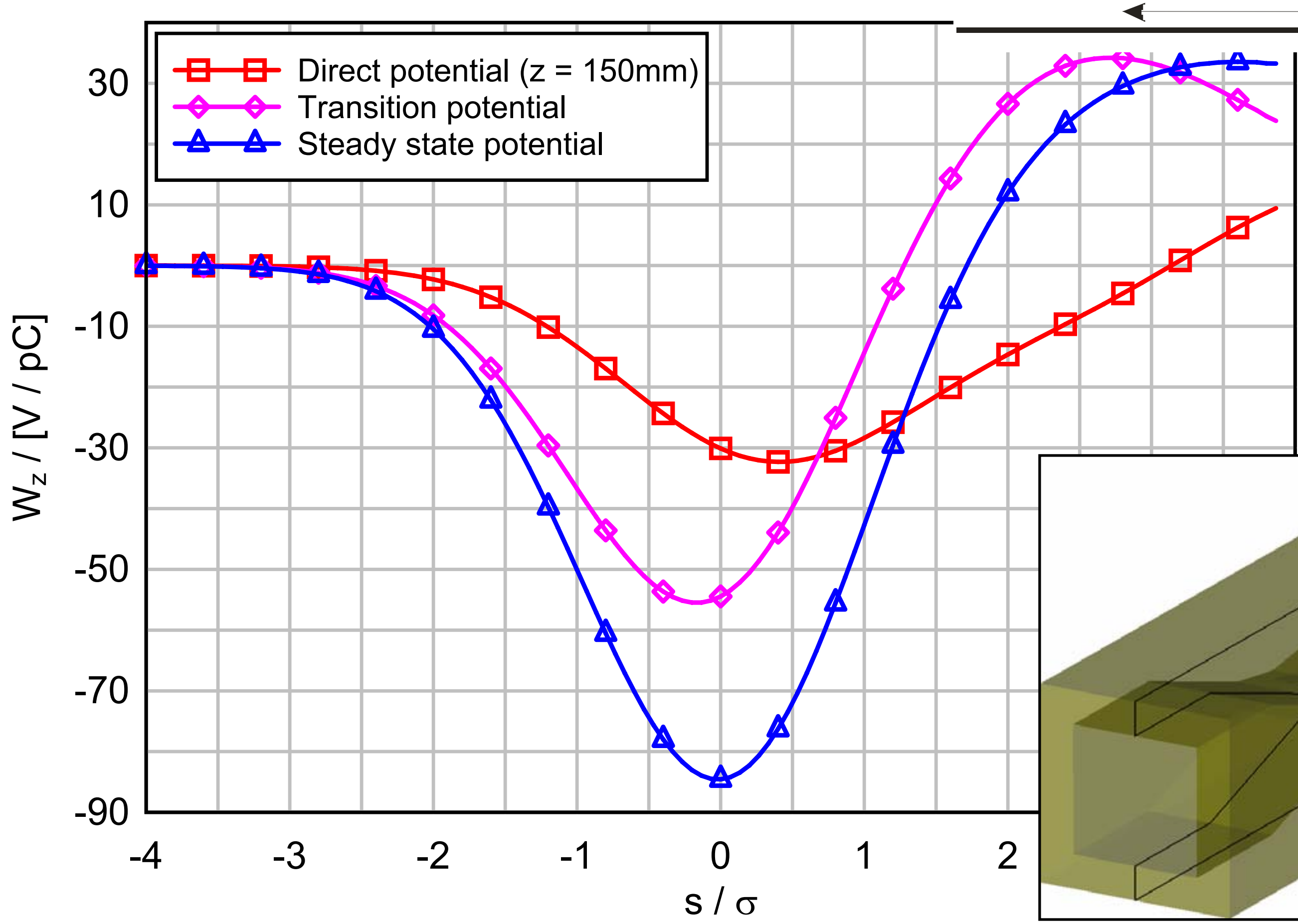
Simulation Examples

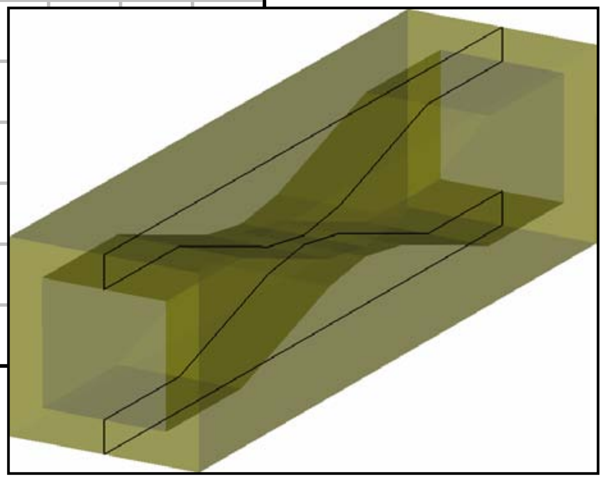
ILC-ESA collimator #8

bunch



Direct and transition wakes





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Conclusions

1. PBCI: A fully 3D- code for wake field simulations
   a. *using the moving window approach*
   b. *dispersionless in the bunch propagation direction*
   c. *massively parallelized*
   d. *using modal approach for “indirect” integration*
   e. *using modal approach for pipe termination*
2. Work still in progress for
   a. *including resistive wall wakes*
   b. *developing an appropriate boundary conformal discretization*
   c. *considering periodic structures of finite length*

Numerical Method

General split-operator schemes

$$\frac{d}{dt}\begin{pmatrix}\widehat{\mathbf{e}}\\ \widehat{\mathbf{h}}\end{pmatrix}=\begin{pmatrix}\mathbf{0} & \mathbf{M}_{\varepsilon}^{-1}\mathbf{C}^{T}\\ -\mathbf{M}_{\mu}^{-1}\mathbf{C} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\widehat{\mathbf{e}}\\ \widehat{\mathbf{h}}\end{pmatrix}$$

(homogeneous) FIT equations

Denote:

$$\boxed{\mathbf{y}=\begin{pmatrix}\widehat{\mathbf{e}}\\ \widehat{\mathbf{h}}\end{pmatrix},\qquad \mathbf{H}=\begin{pmatrix}\mathbf{0} & \mathbf{M}_{\varepsilon}^{-1}\mathbf{C}^{T}\\ -\mathbf{M}_{\mu}^{-1}\mathbf{C} & \mathbf{0}\end{pmatrix},\qquad \mathbf{H}=\mathbf{H}_1+\mathbf{H}_2}$$

Solution after one time step:

exact time evolution operator

$$\boxed{\frac{d\mathbf{y}}{dt}=\mathbf{H}\bullet\mathbf{y}\quad\Rightarrow\quad \mathbf{y}^{n+1}=e^{-\mathbf{H}\Delta t}\bullet\mathbf{y}^{n}=e^{-(\mathbf{H}_1+\mathbf{H}_2)\Delta t}\bullet\mathbf{y}^{n}}$$

approximate time evolution operator

A second order *Strang scheme*: $\boxed{\mathbf{y}^{n+1}=e^{-\mathbf{H}_1\frac{\Delta t}{2}}e^{-\mathbf{H}_2\Delta t}e^{-\mathbf{H}_1\frac{\Delta t}{2}}\bullet\mathbf{y}^{n}+O(\Delta t^{3})}$