Recent Developments on Beam Dynamics and Wake Field Simulations at TEMF

Wolfgang Ackermann and Erion Gjonaj

Institut für Theorie Elektromagnetischer Felder (TEMF)
Technische Universität Darmstadt

Joint DESY and University of Hamburg Accelerator Physics Seminar
December 18, 2007, DESY, Hamburg

Technische Universität Darmstadt, Fachbereich Elektrotechnik und Informationstechnik
Schlossgartenstraße 8, 64289 Darmstadt, Germany - URL: www.TEMF.de

Outline

- Wakefield Computations
  - PBCI
  - Wakefield Simulations at TEMF
- Self-Consistent PIC Simulations
  - Higher Order Finite Elements
  - Current Work
- V-Code
  - Basic principle based on the moment approach
  - Implementation using symbolic algebra transformation

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Wakefield Computations

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Motivation for improved wakefield codes

1. A new generation of LINACs with ultra-short electron bunches

- *bunch size for ILC: 300 µm*
- *bunch size for LCLS: 20 µm*

2. Geometry of tapers, collimators… far from rotational

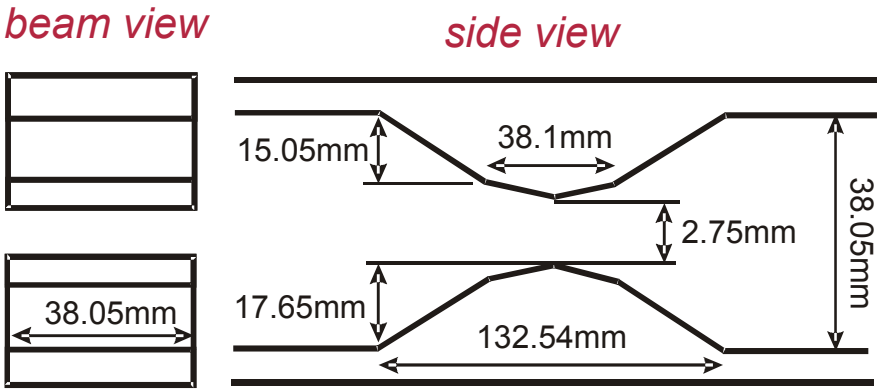
- *8 rectangular collimators at ILC-ESA in the design process*
- *30 rectangular-to-round transitions in the undulator of LCLS*

3. Many (semi-) analytical approximations become invalid

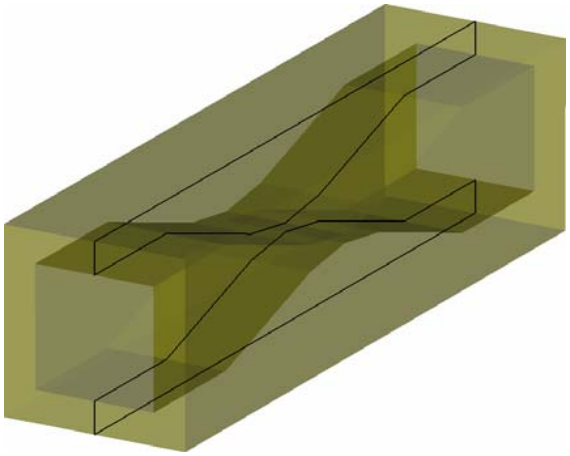
- *based on rotationally symmetric geometry*
- *low frequency assumptions (Yokoya, Stupakov)*

Wakefield Computations

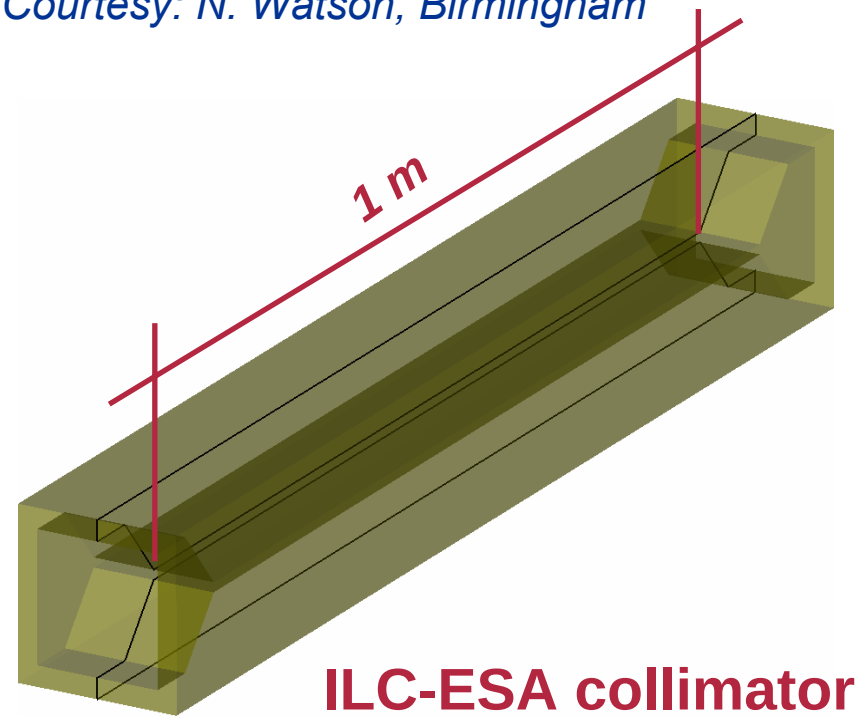
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt



Courtesy: N. Watson, Birmingham



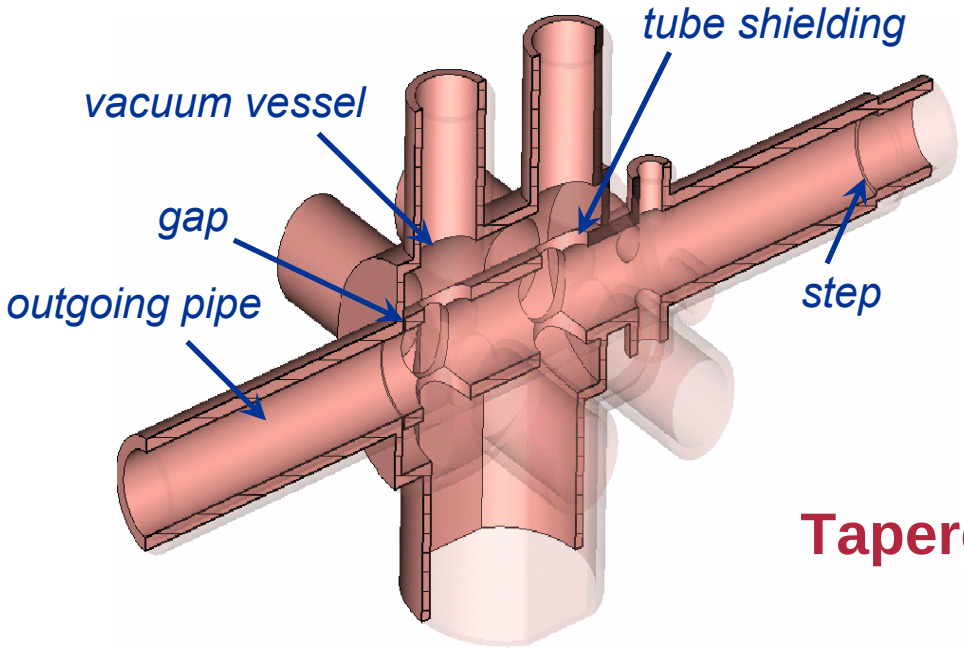
ILC-ESA collimator #8



ILC-ESA collimator #3

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

Wakefield Computations

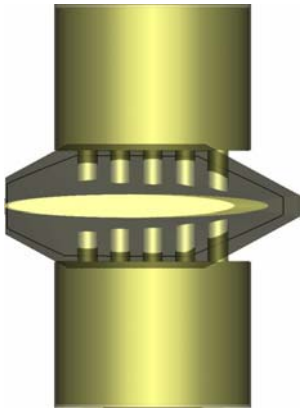


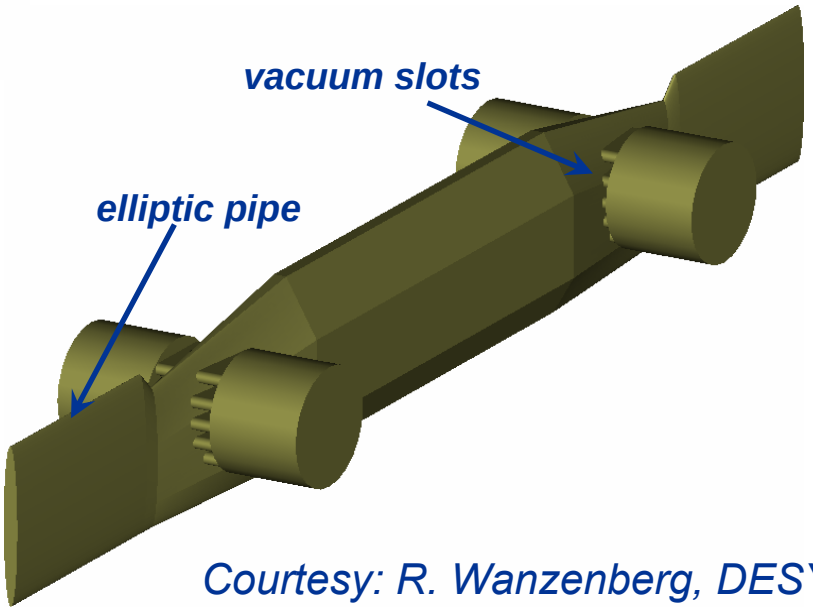
PITZ diagnostics double cross

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

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Wakefield Computations

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

There is an actual demand for:

1. Wake field simulations in arbitrary 3D-geometry

   3D-codes

2. Utilizing large computational resources

   parallelized codes

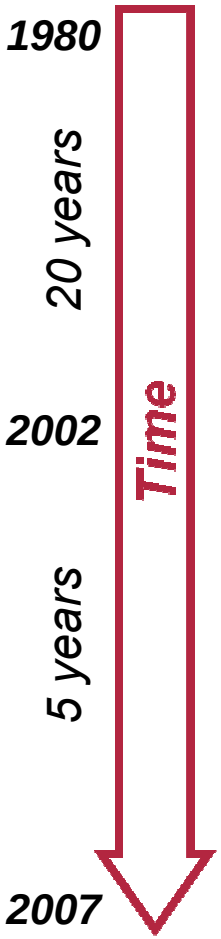
3. Specialized algorithms for long accelerator structures

   moving window – dispersion free codes

Wakefield Computations

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

An (incomplete) survey of available codes



	Dimensions	*Nondispersive*	*Parallelized*	*Moving window*
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	Yes
GdfidL	3D	No	Yes	No
Tau3P	3D	No	Yes	No
ECHO	2.5/3D	Yes	No	Yes
CST	3D	No	No	No
PBCI	3D	Yes	Yes	Yes
NEKCEM	3D	No	Yes	No

Numerical Method

Based on 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

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

$$\tilde{\mathbf{C}}\,\hat{\mathbf{h}} = \frac{d}{dt}\mathbf{M}_{\varepsilon}\hat{\mathbf{e}} + \hat{\tilde{\mathbf{j}}}$$

$$\tilde{\mathbf{S}}\,\mathbf{M}_{\varepsilon}\hat{\mathbf{e}} = \mathbf{q}$$

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

A moving window algorithm is not directly applicable:

- *Stability limit $\Delta t < \Delta x / c$*
- *Longitudinal dynamics has numerical dispersion*

Important works of I. Zagorodnov on TE/TM splitting for the ECHO code

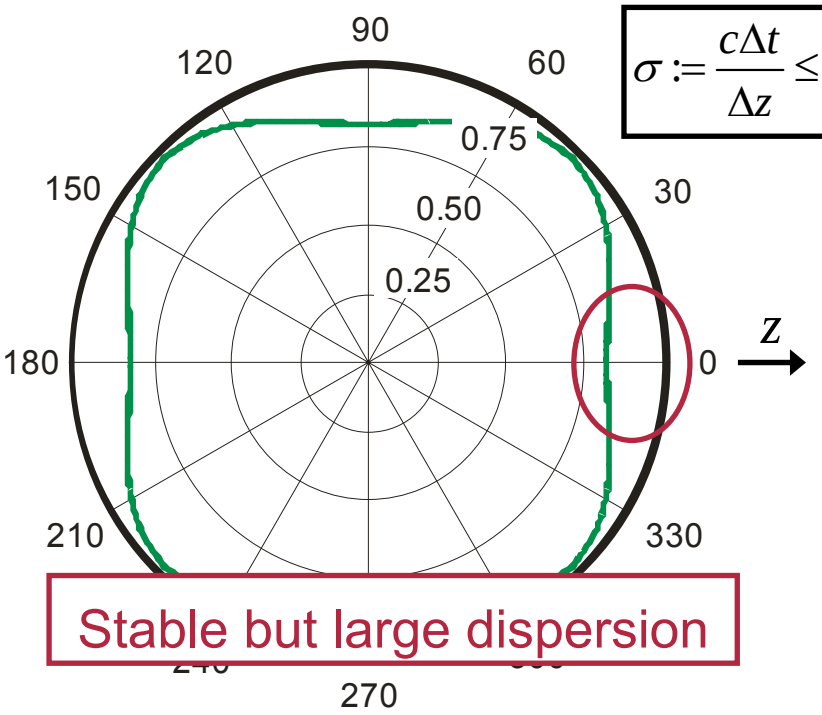
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Numerical Method

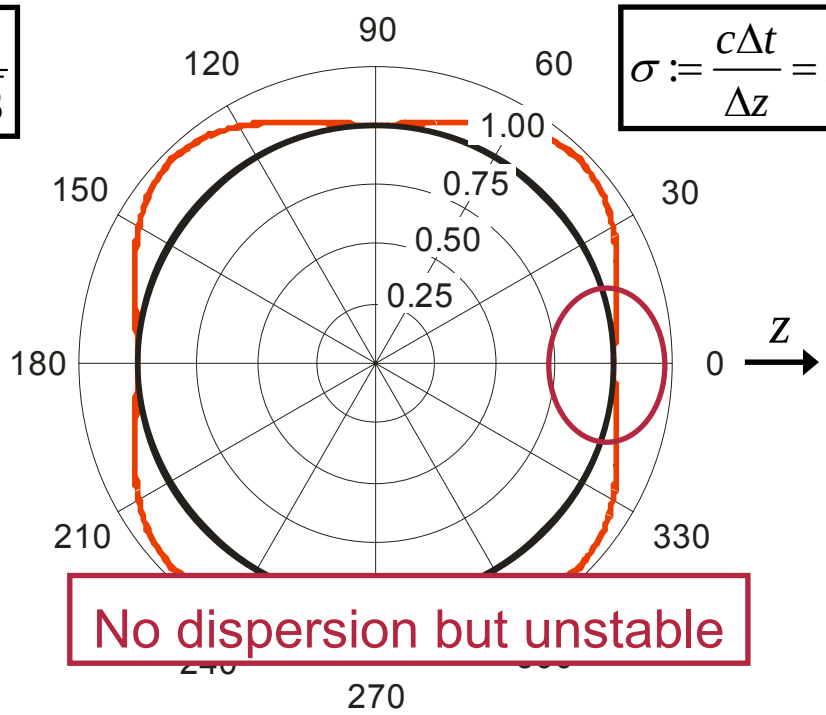
Using the conventional leapfrog time integration

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

Behavior of numerical phase velocity vs. propagation angle



Stable but large dispersion



No dispersion but unstable

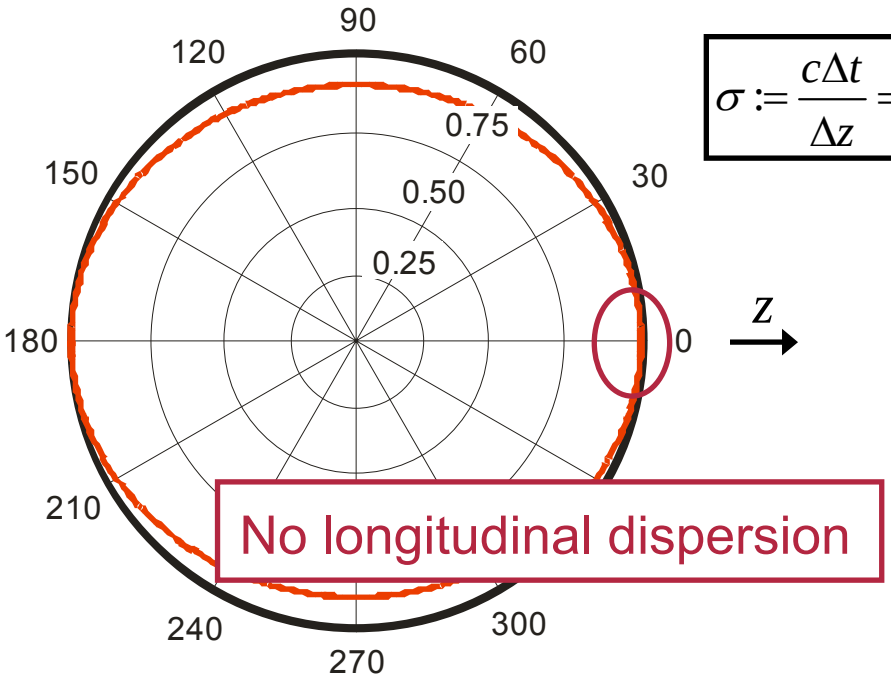
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Numerical Method

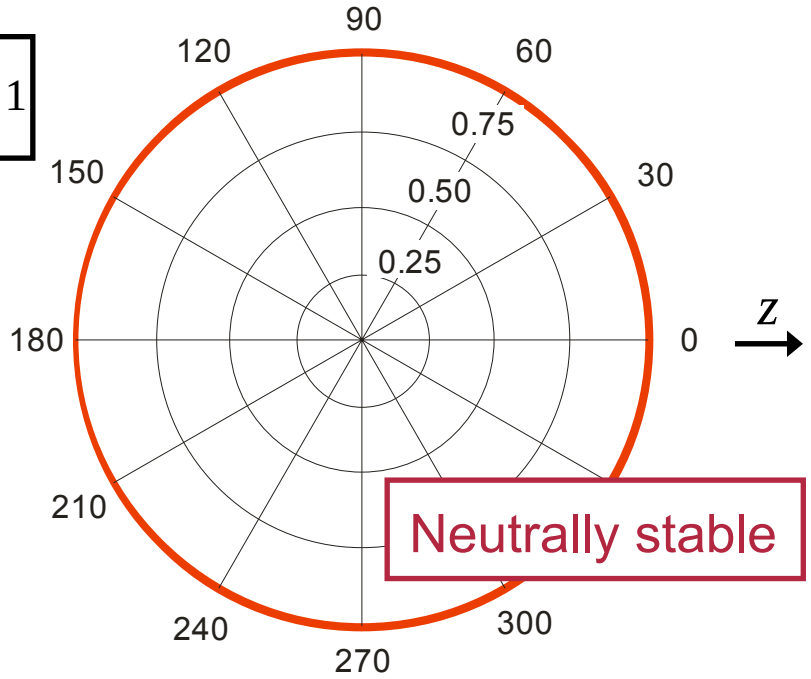
Using a split-operator method (LT)

Behavior of numerical phase velocity vs. propagation angle

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



No longitudinal dispersion



Neutrally stable

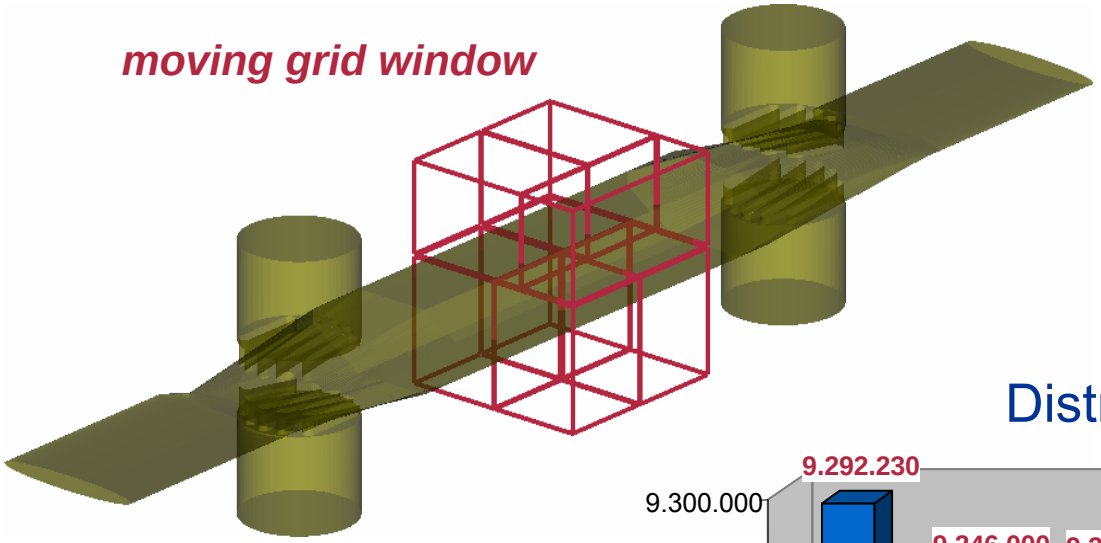
Note: The elimination of longitudinal dispersion does not necessarily improve accuracy. “Splitting error” may become important.

Non-split algorithms are currently under investigation.

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

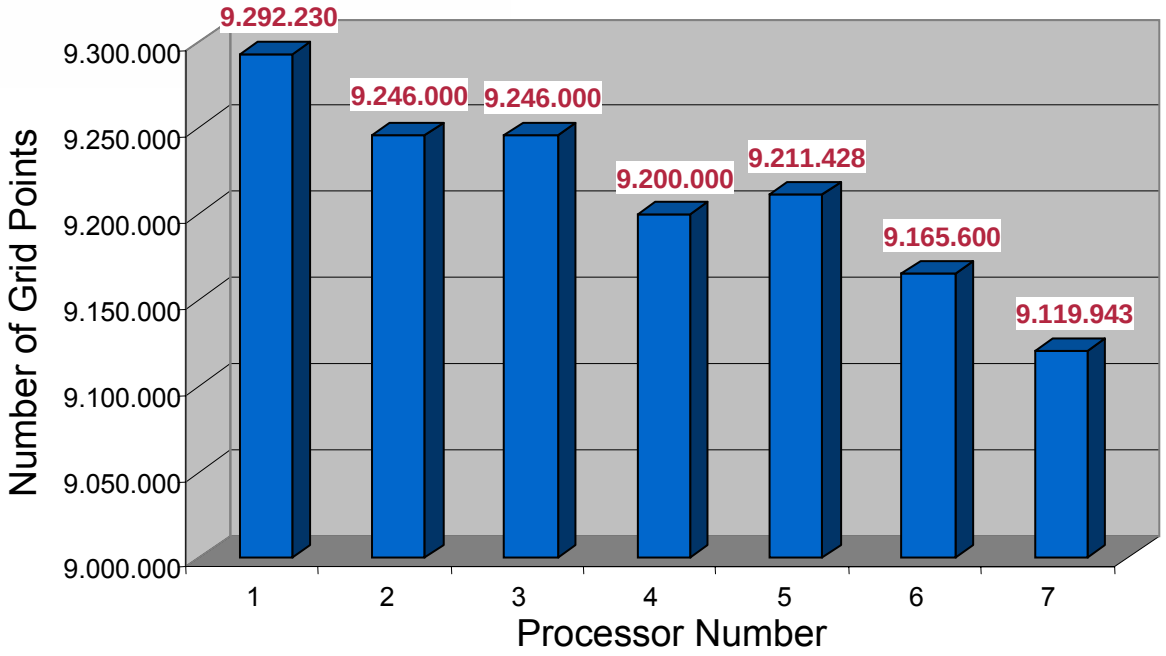
Example: Tapered transition for PETRA III



Domain partitioning pattern for 7 processors

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

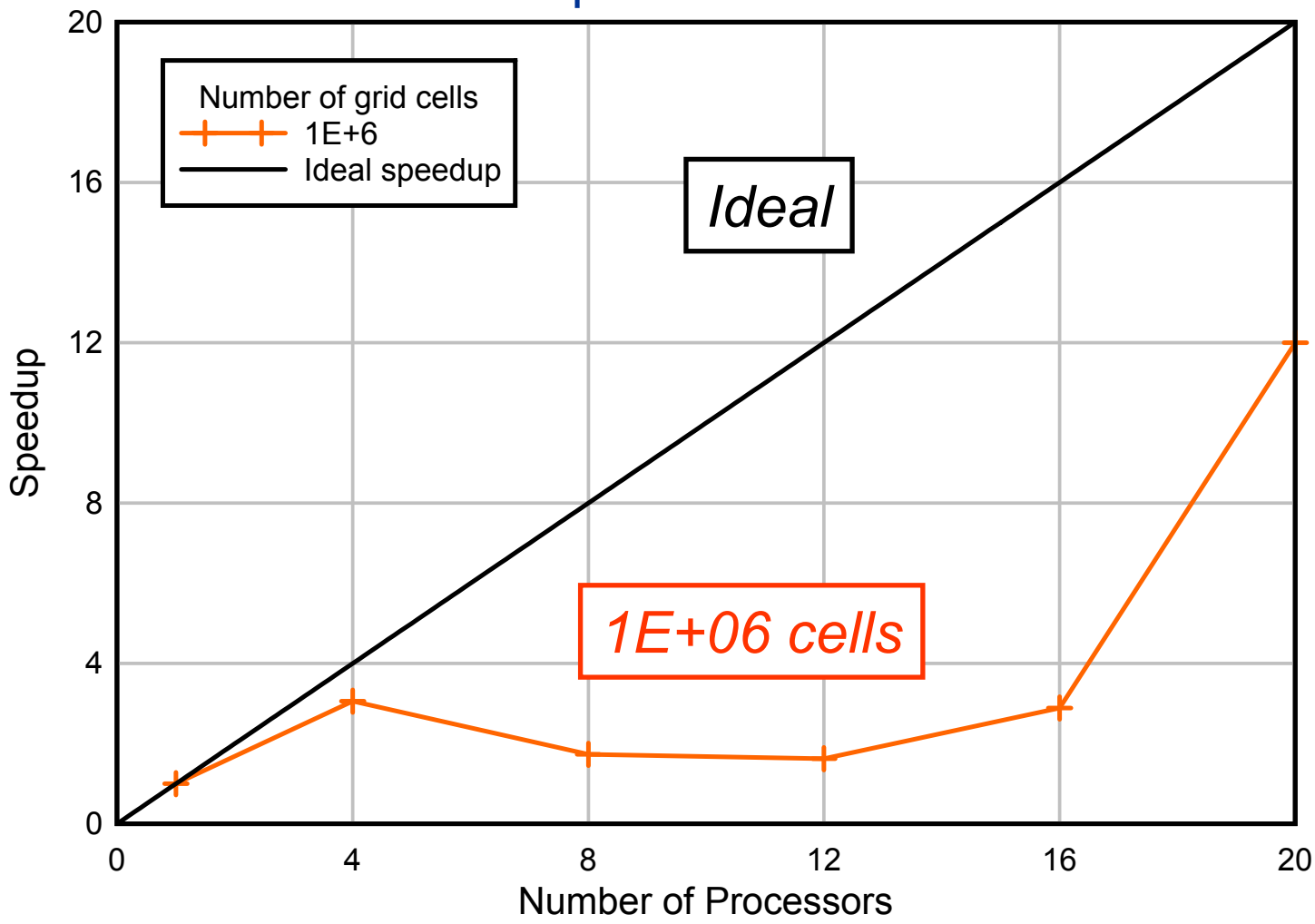
Distribution of grid points



Parallelization

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

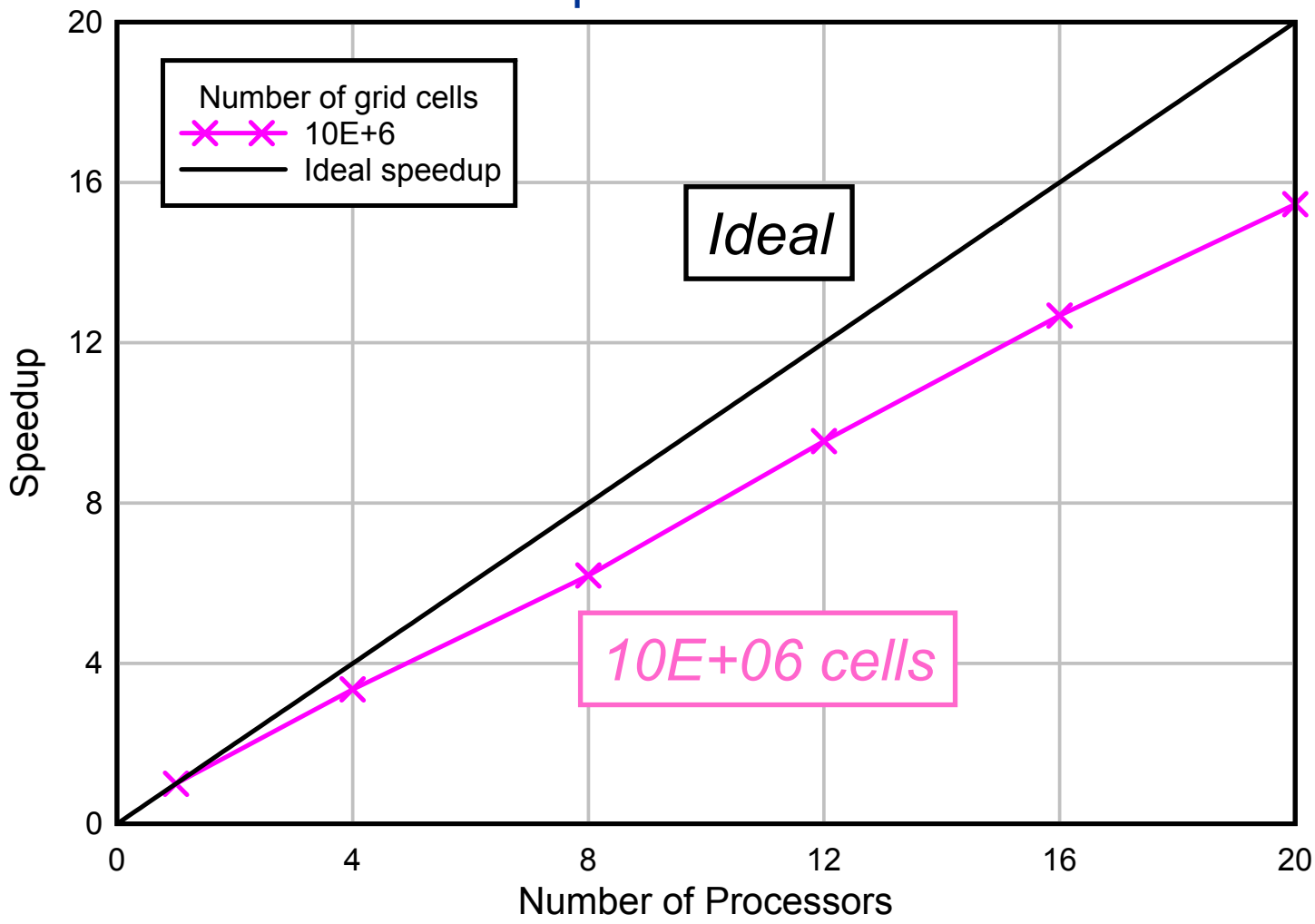
Parallel performance tests



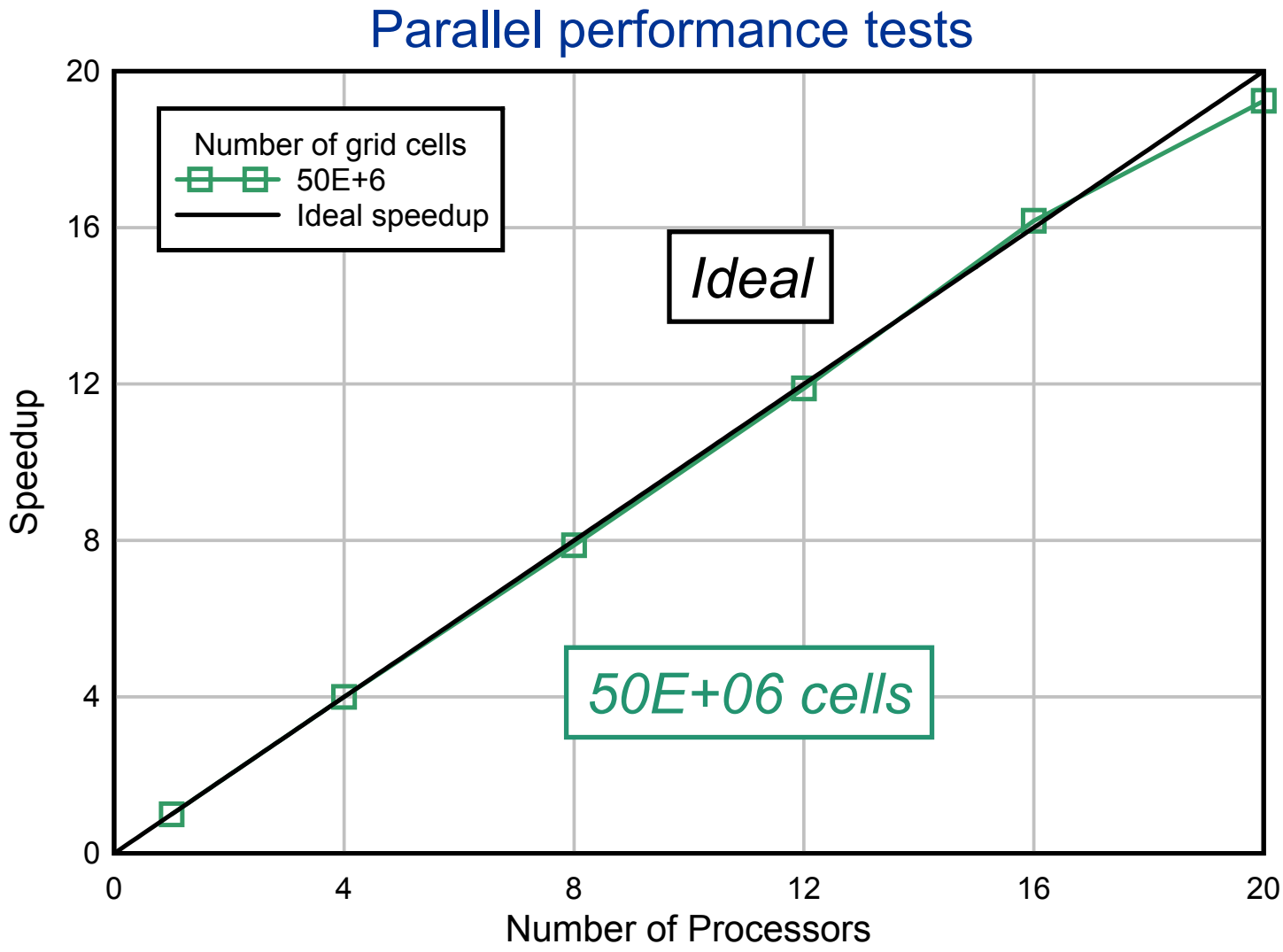
Parallelization

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Parallel performance tests

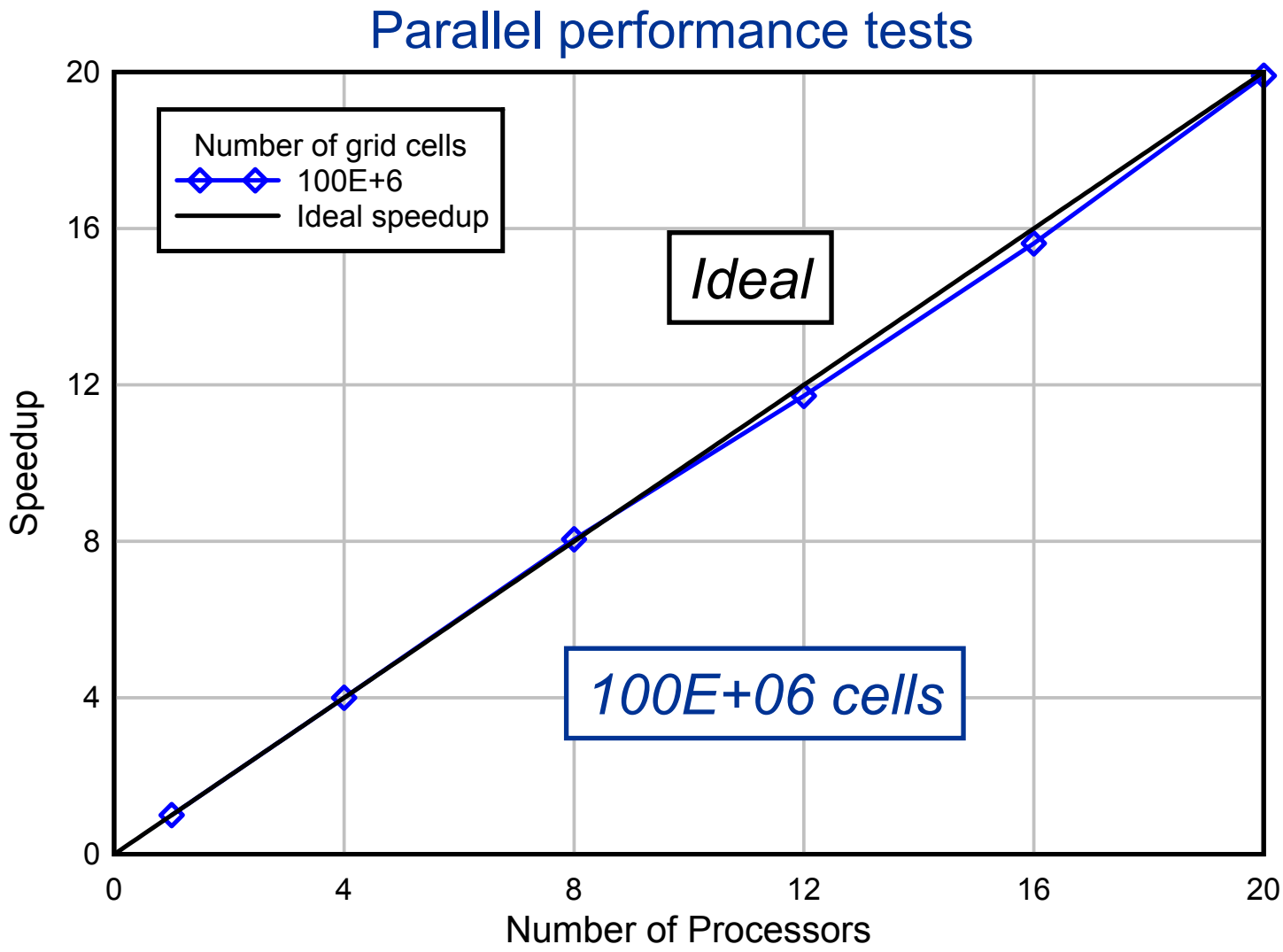


Parallelization



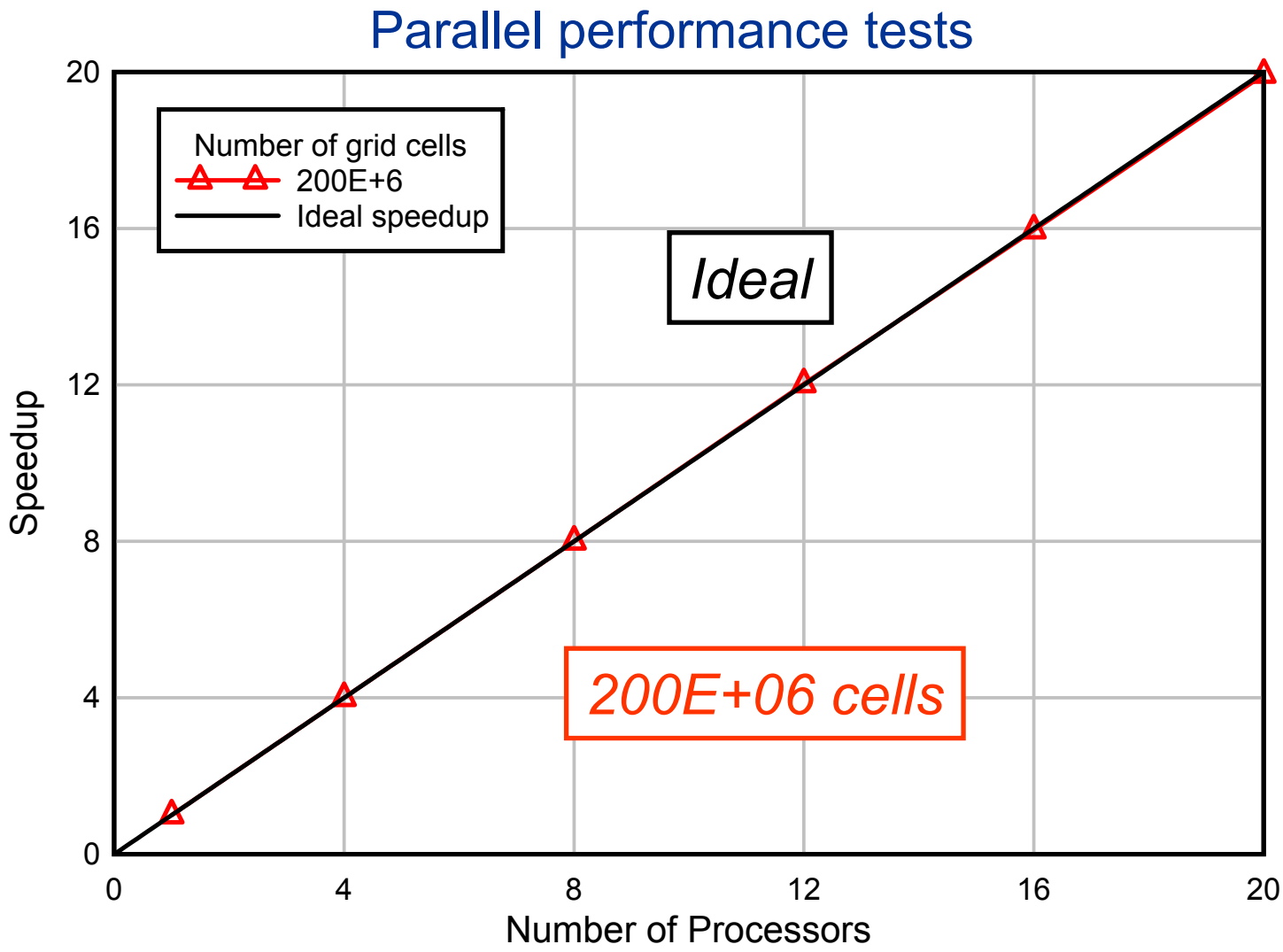
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Parallelization



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Parallelization

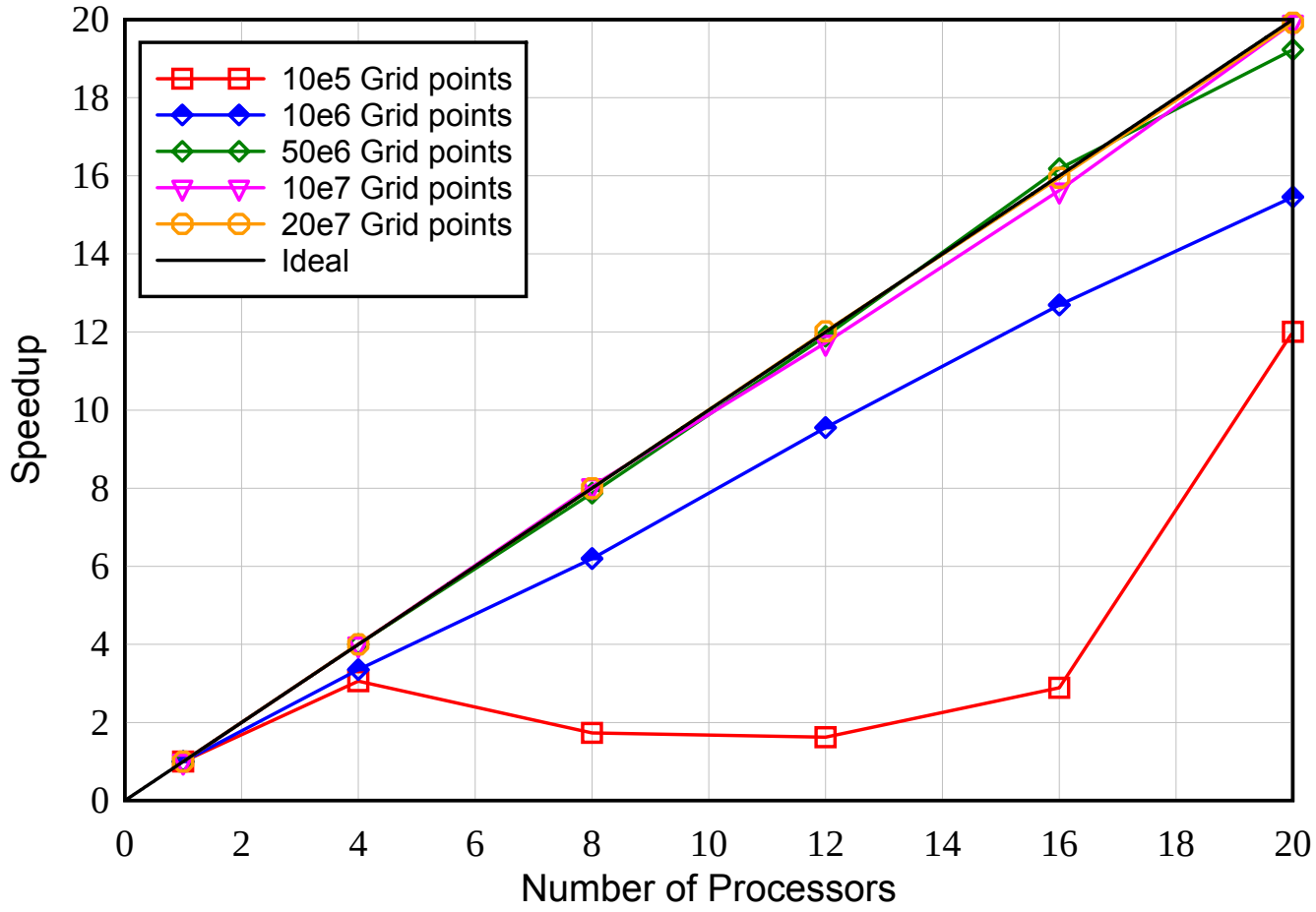


Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Parallelization

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

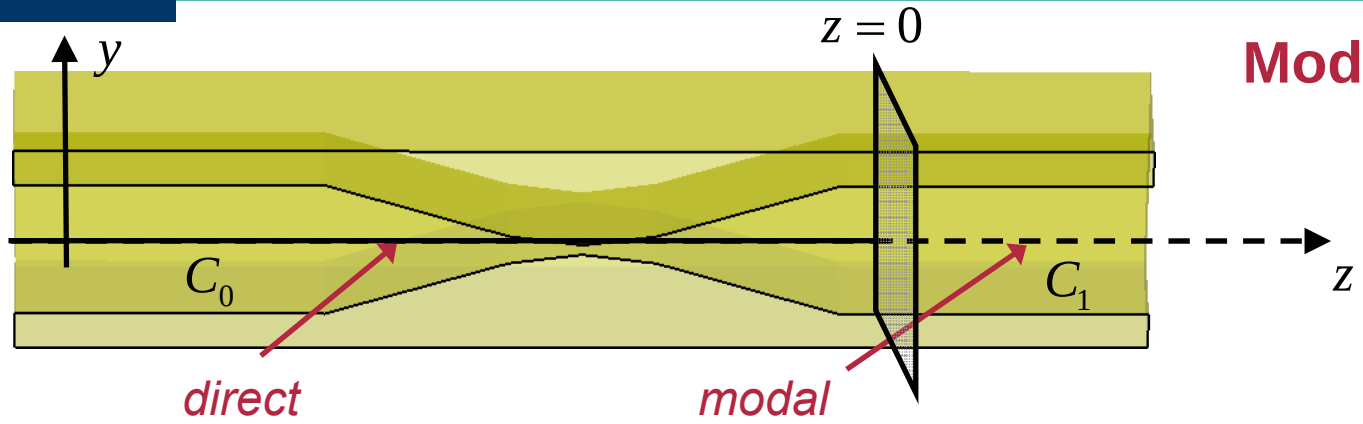
Parallel performance tests



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

Modal Termination of Pipes

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt



Modal approach

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

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

spectral coefficient of n-th (TM) mode

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

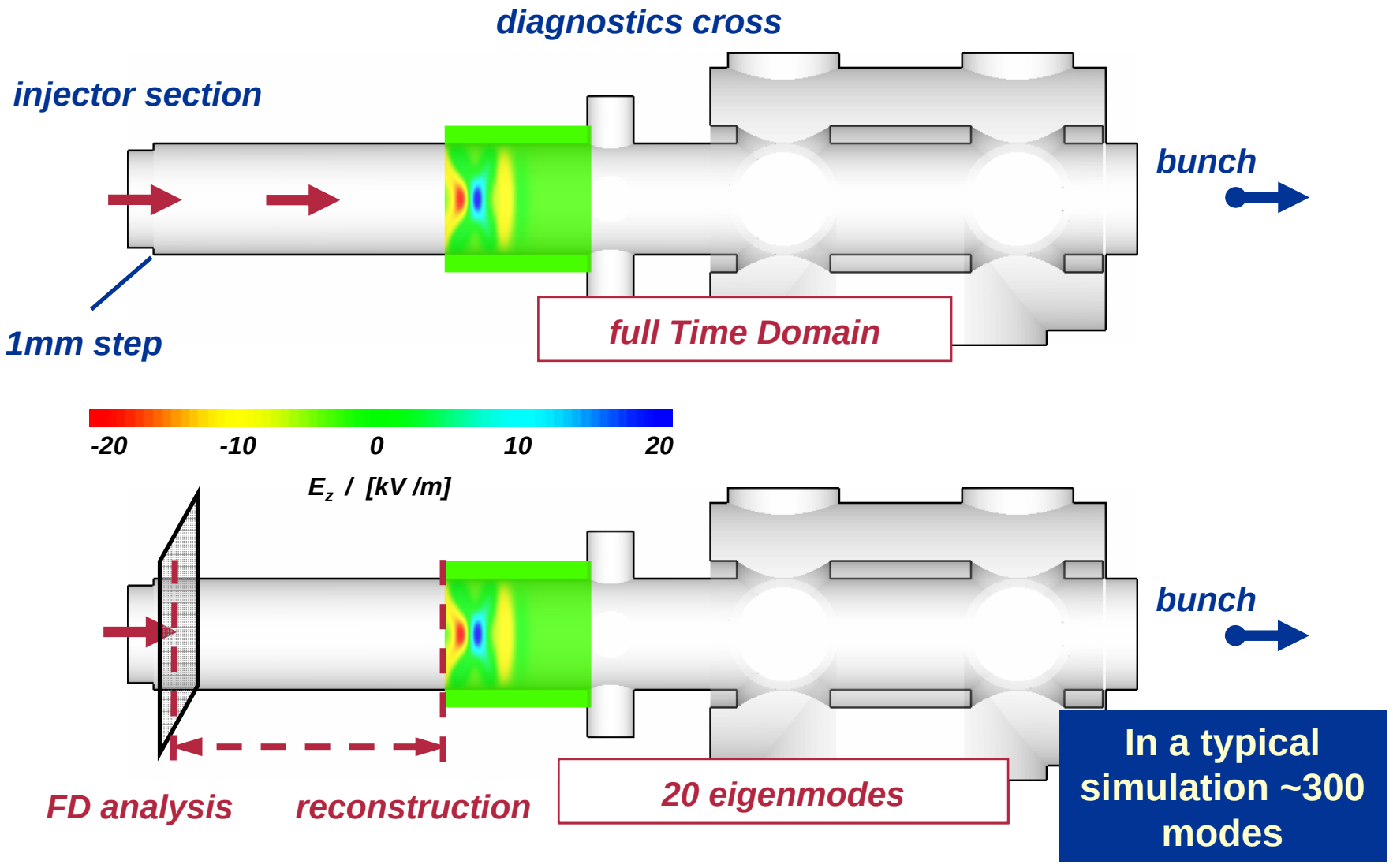
n-th (TM) mode contribution

Indirect methods for wake potential integration, I. Zagorodnov et al, PRSTAB 9, '06

Eigenmode expansion method in the indirect calculation of wake potential in 3D in structures, X. Dong et al, ICAP'06

Modal Termination of Pipes

Using modal reconstruction in long intermediate pipes



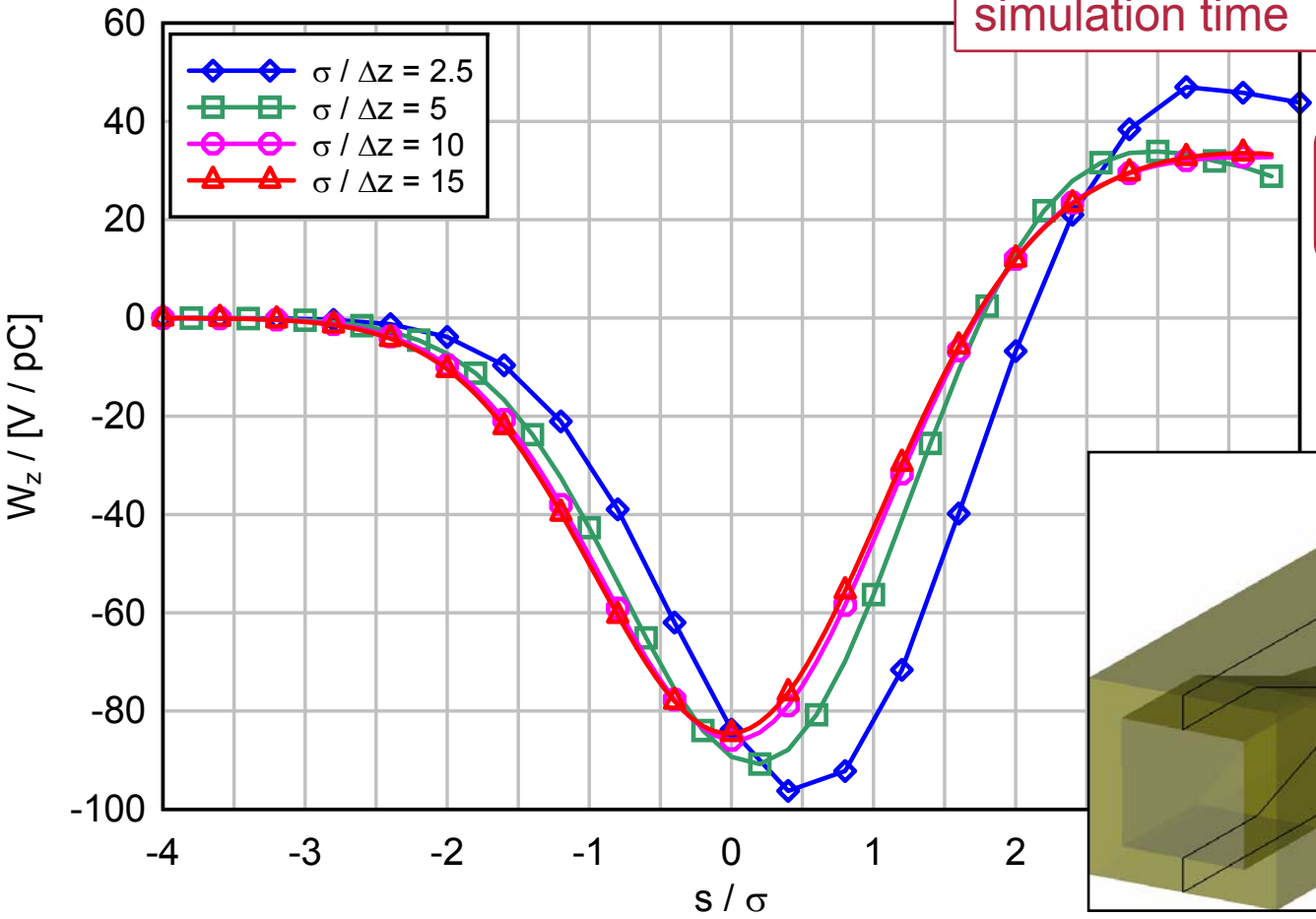
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

ILC-ESA Collimators

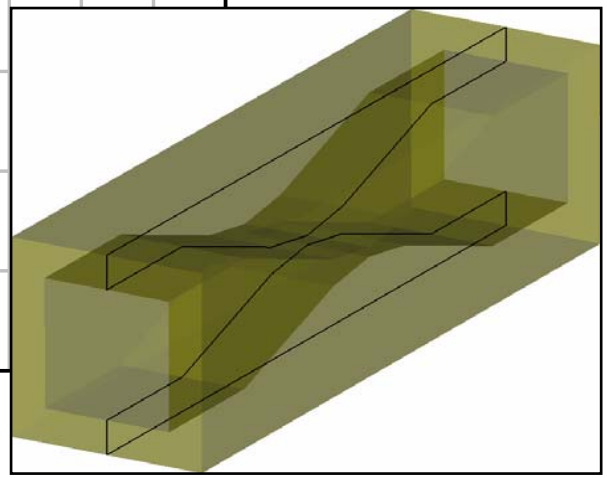
ILC-ESA collimator #8

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

Convergence vs. grid step



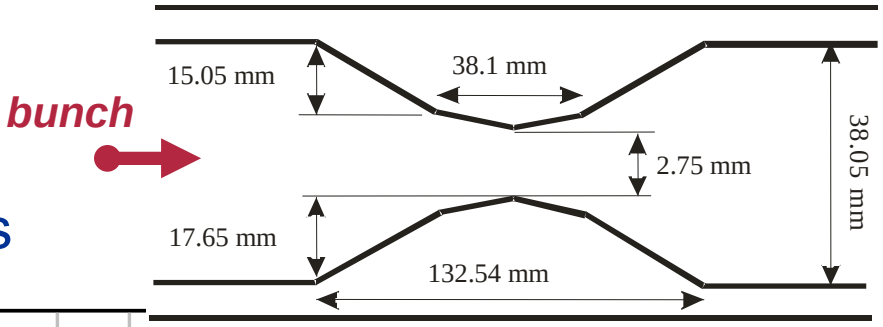
Moving window: 3 mm length



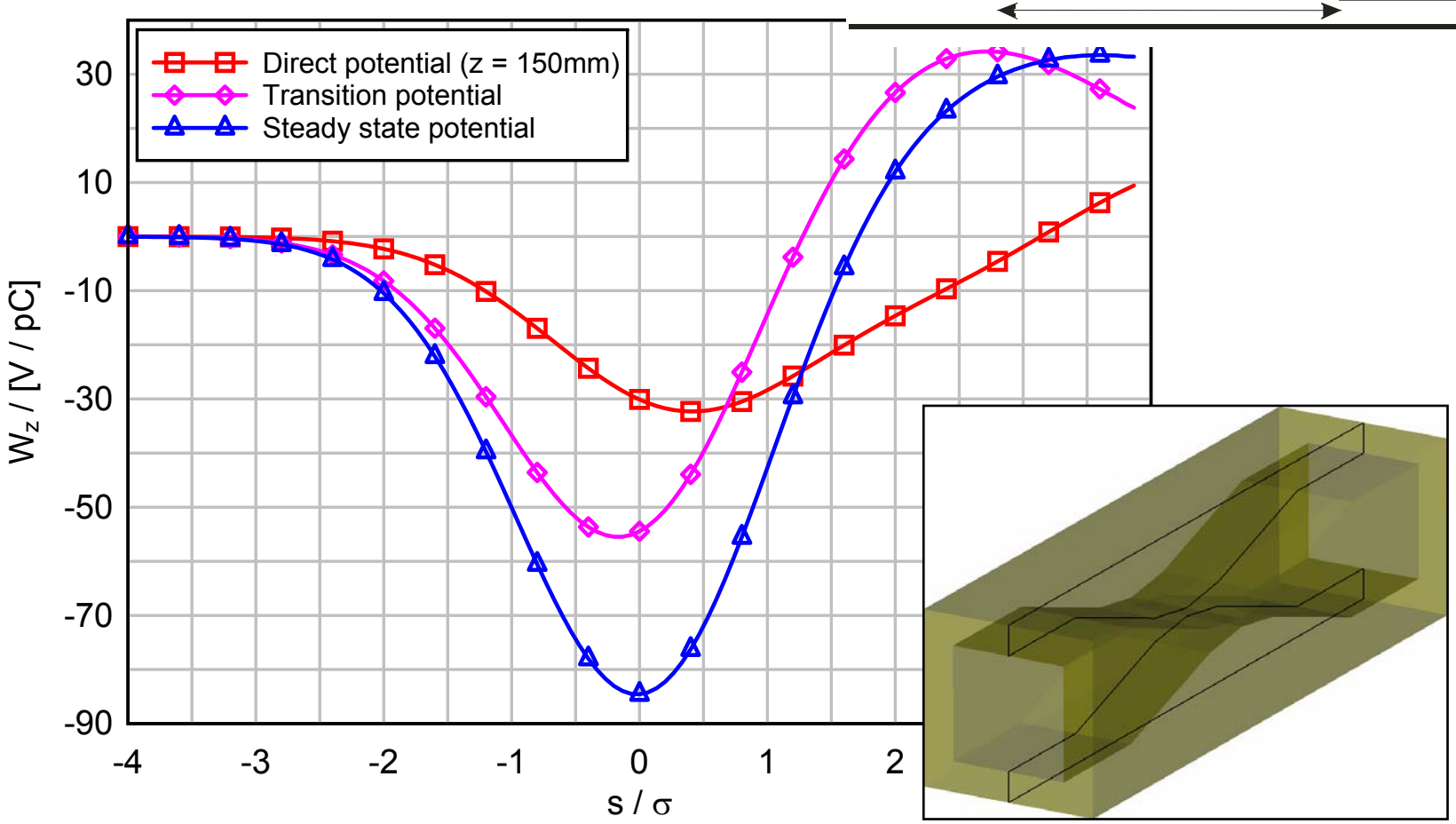
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

ILC-ESA Collimators

ILC-ESA collimator #8

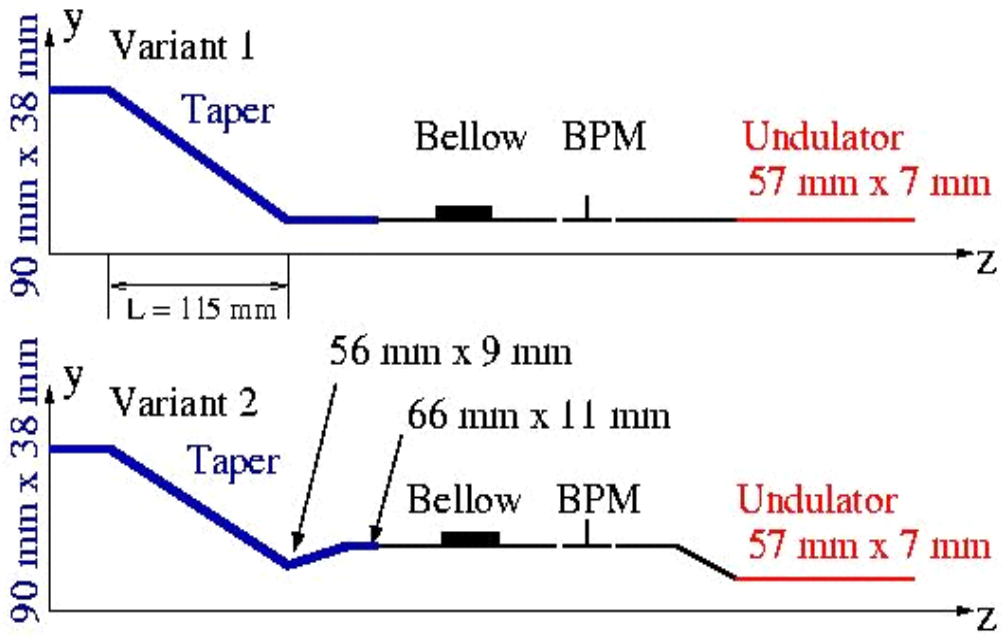


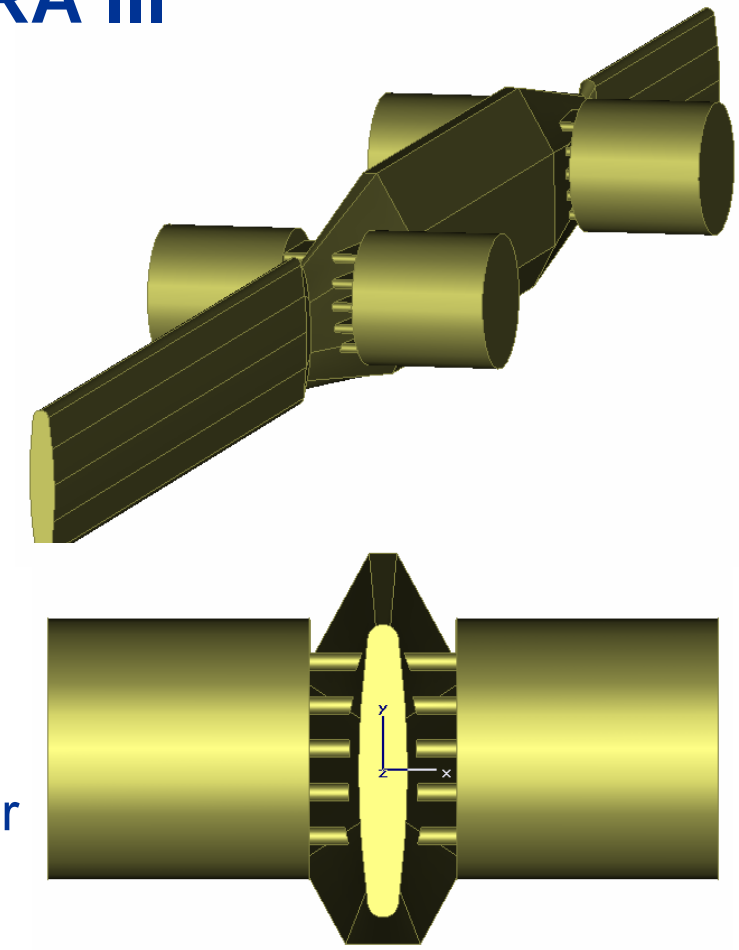
Direct vs. transition wakes



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Tapered Transitions for PETRA III



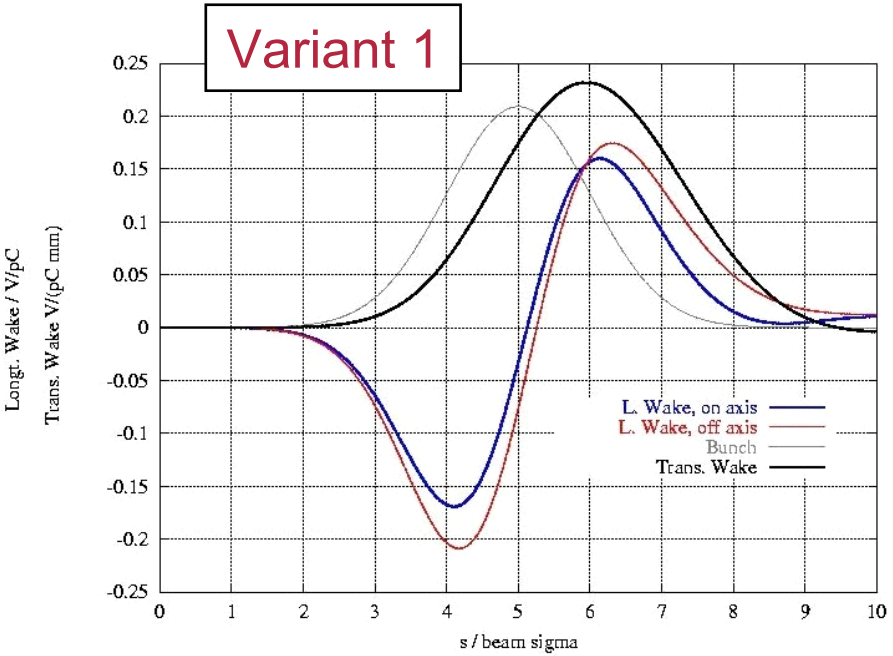


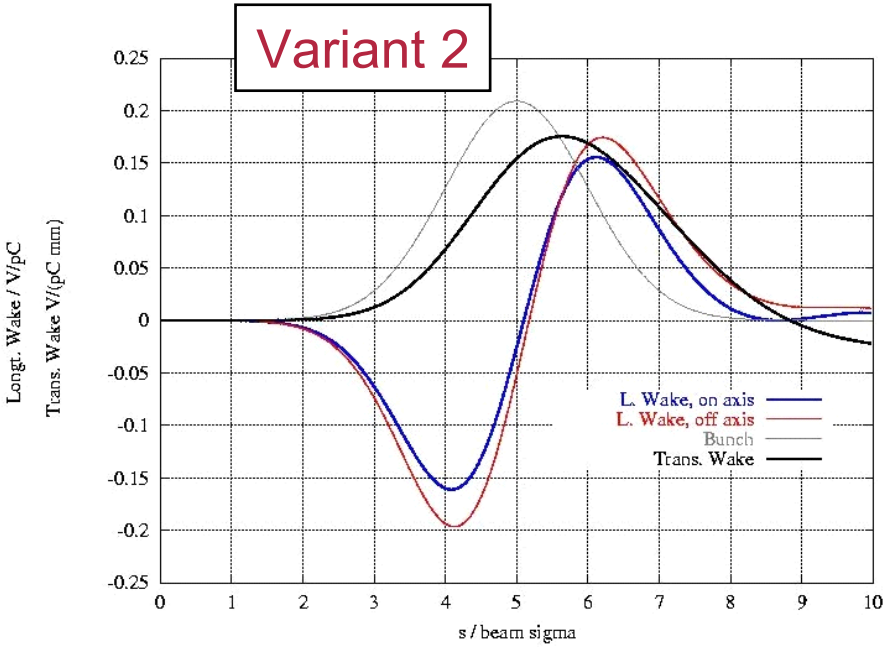
The two variants of the vacuum-to-undulator tapered transition

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

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Tapered Transition for PETRA III



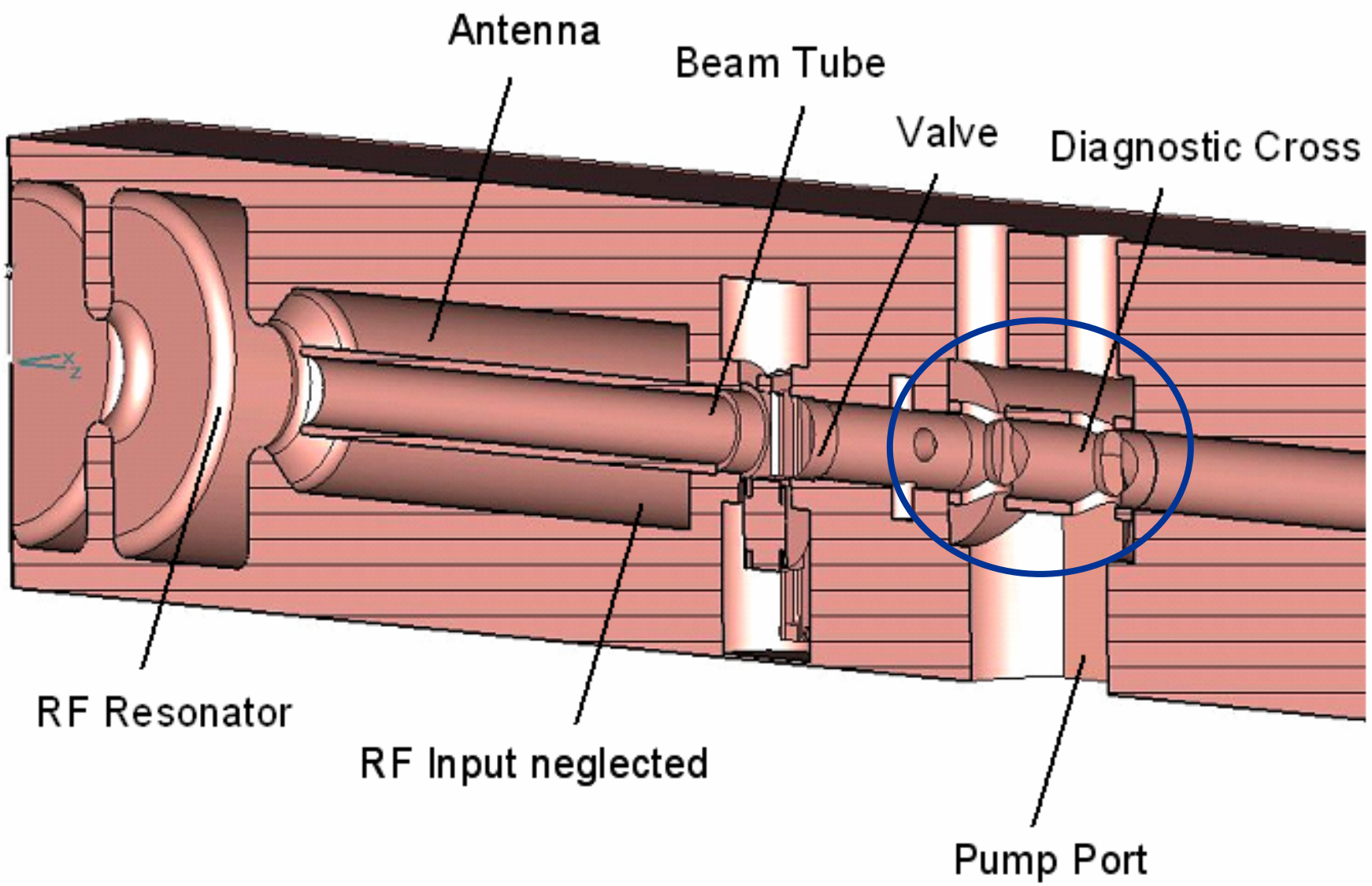


Variant / Code	$k_{\|\|}$ / (V/nC)	$k_{\|\|}(1)$ / (V/pC m)	$k_{\perp}$ / (V/pC m)
Variant1 / MAFIA	-7.4	-6.8	138.6
Variant1 / PBCI	-7.1	-4.8	75.6
Variant2 / PBCI	-5.2	-4.6	62.8

factor ~1.8 higher than PBCI due to insufficient resolution

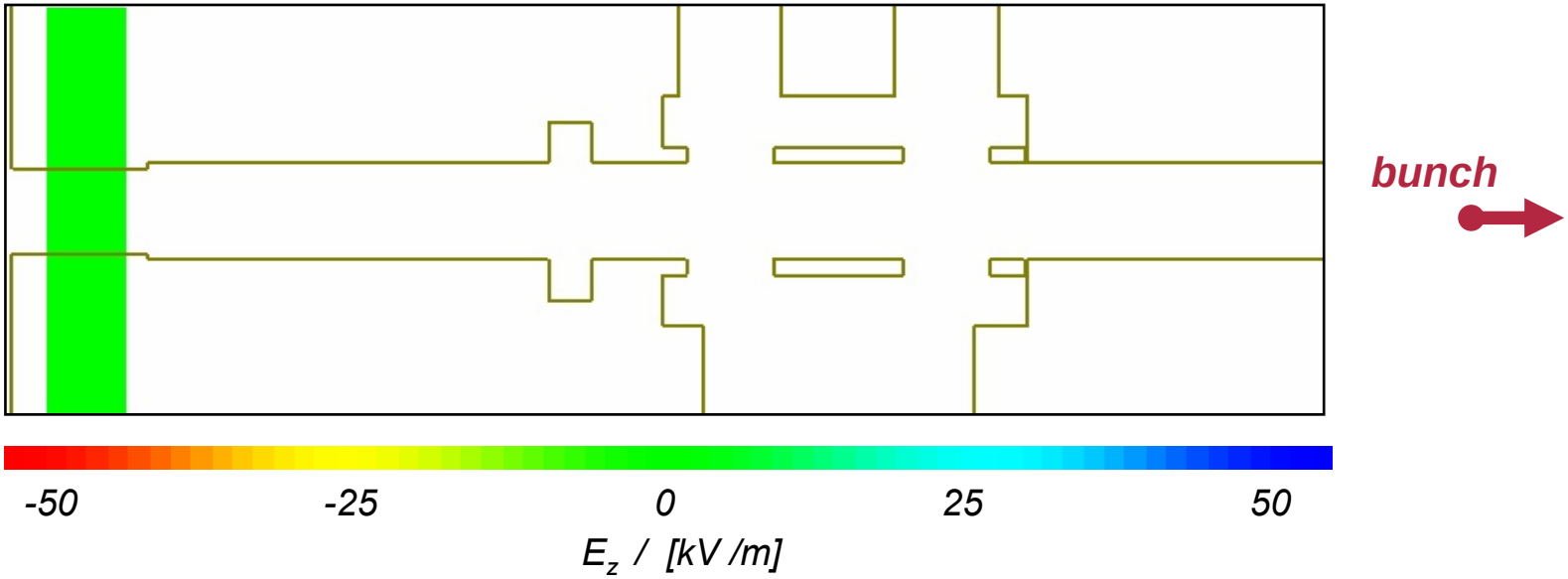
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

PITZ diagnostics double cross

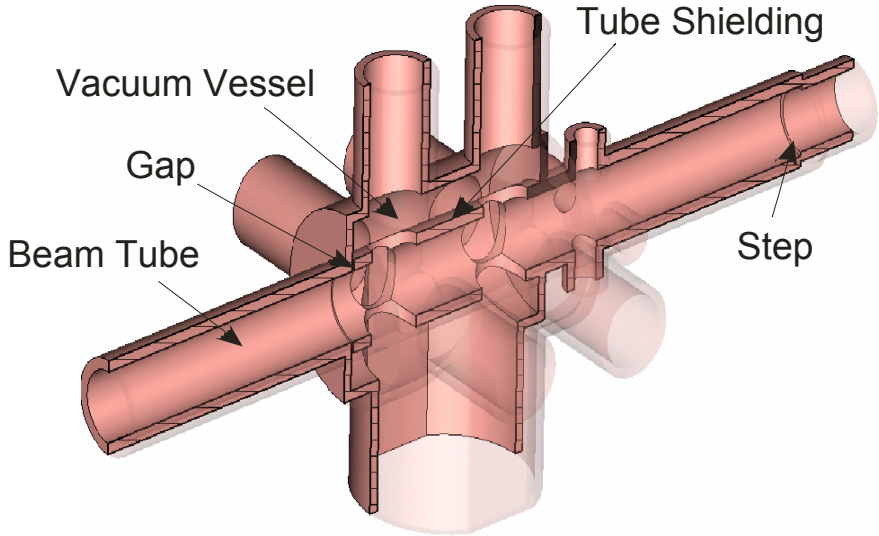


Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

PITZ diagnostics double cross



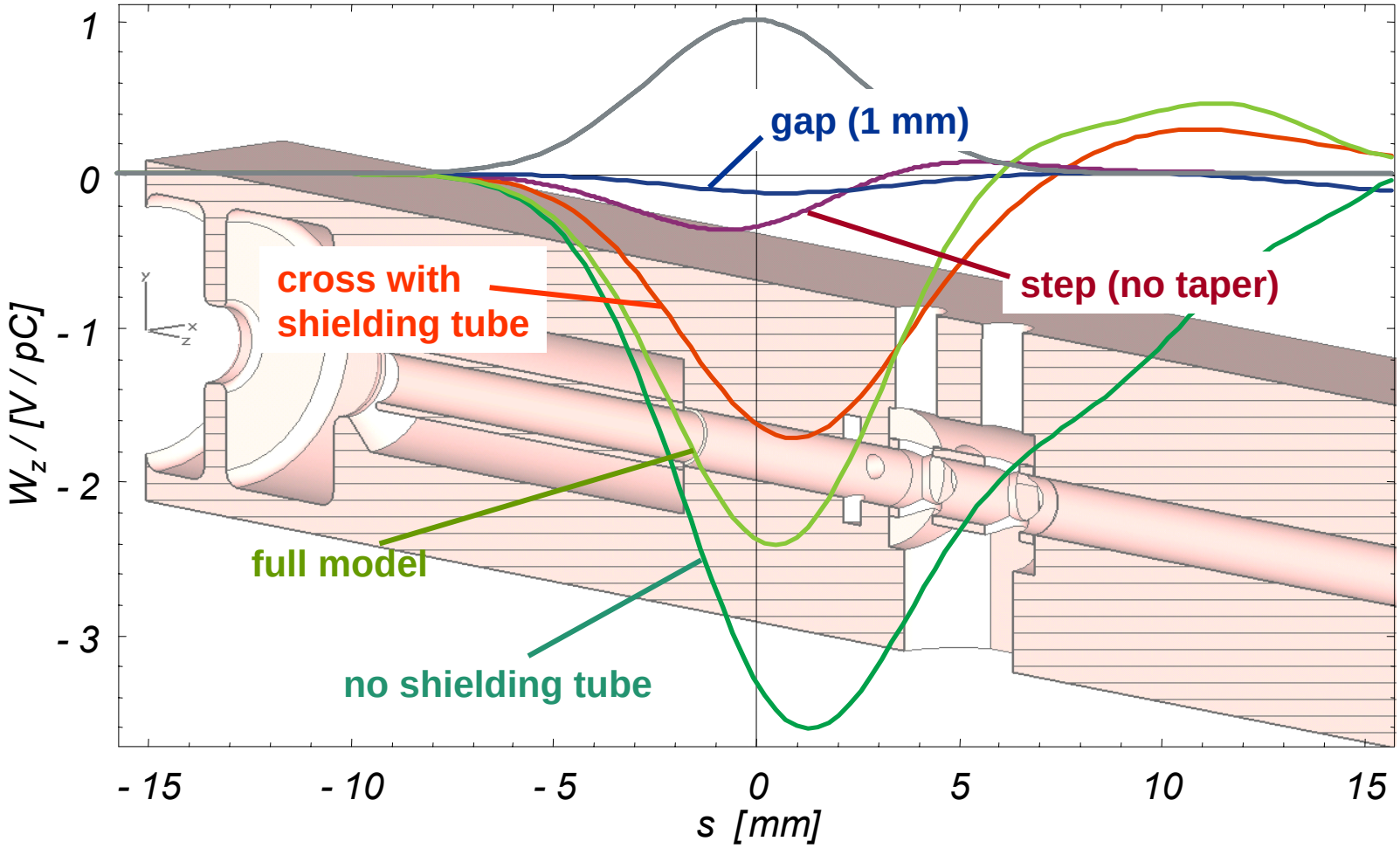
bunch size	2.5mm
σ / Δz	30
no. of grid points	~500e6
no. of processors	24
simulation time	32hrs



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

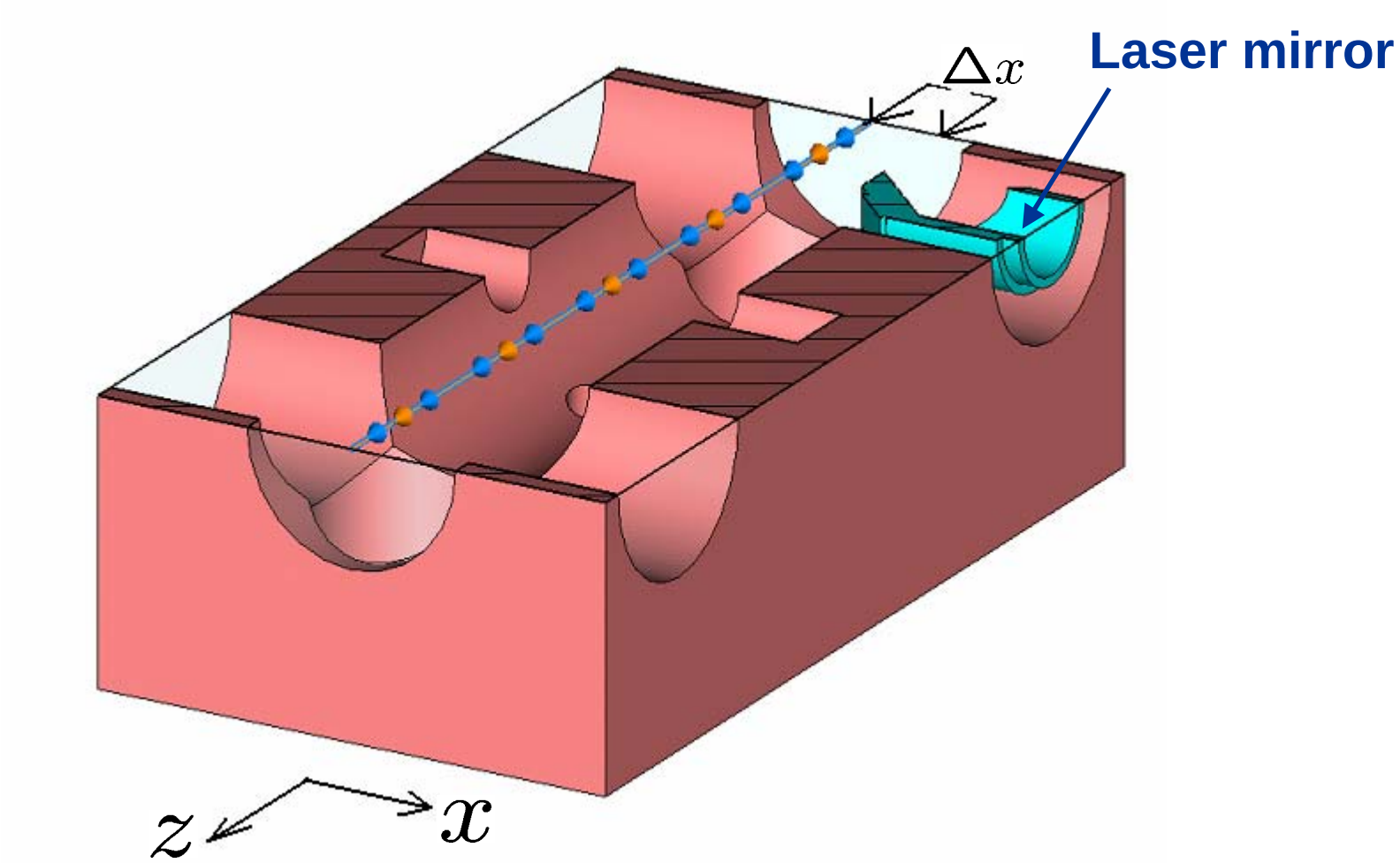
PITZ diagnostics double cross

Wake field impact of the single components



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

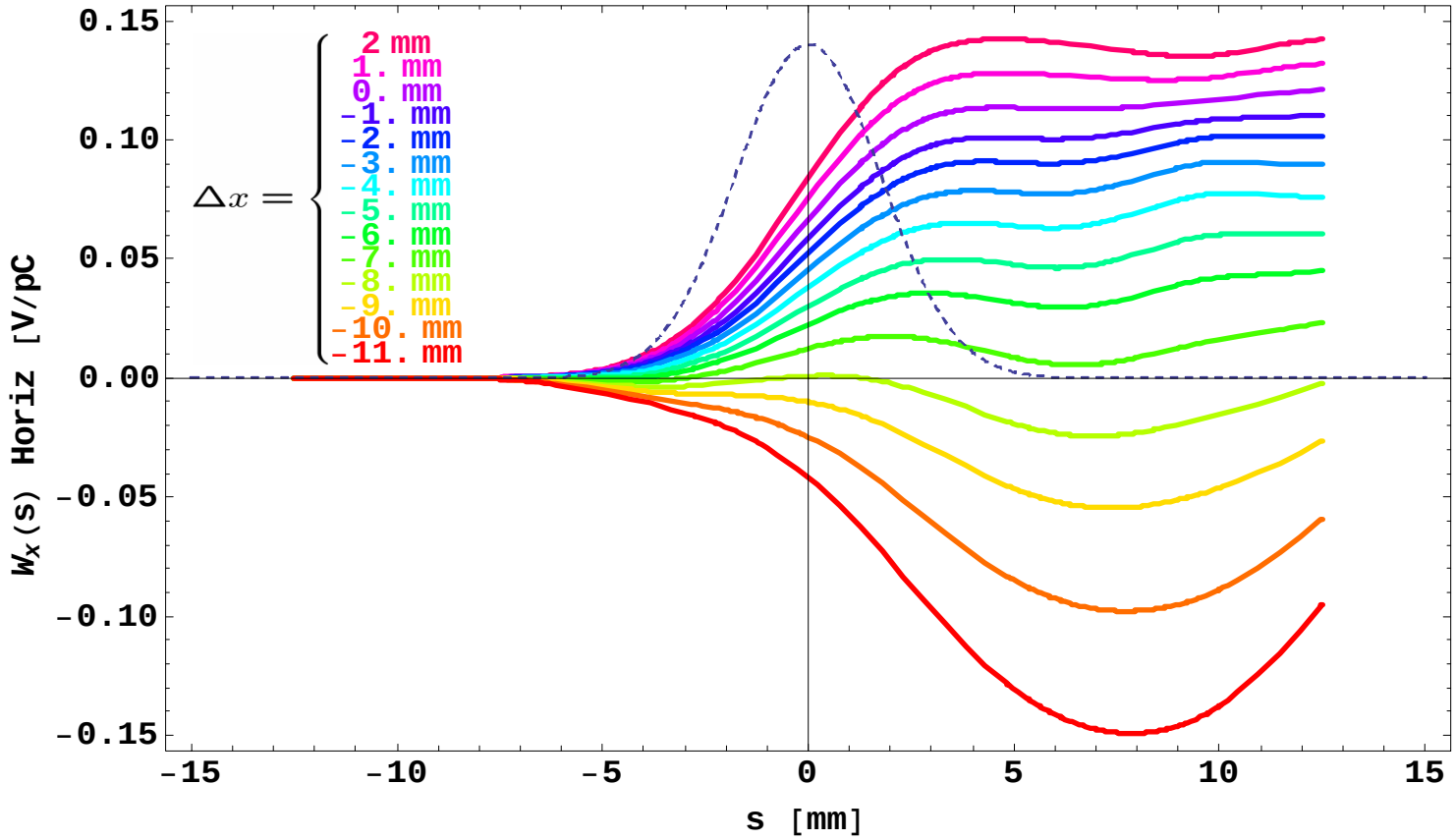
PITZ diagnostics double cross



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

PITZ diagnostics double cross

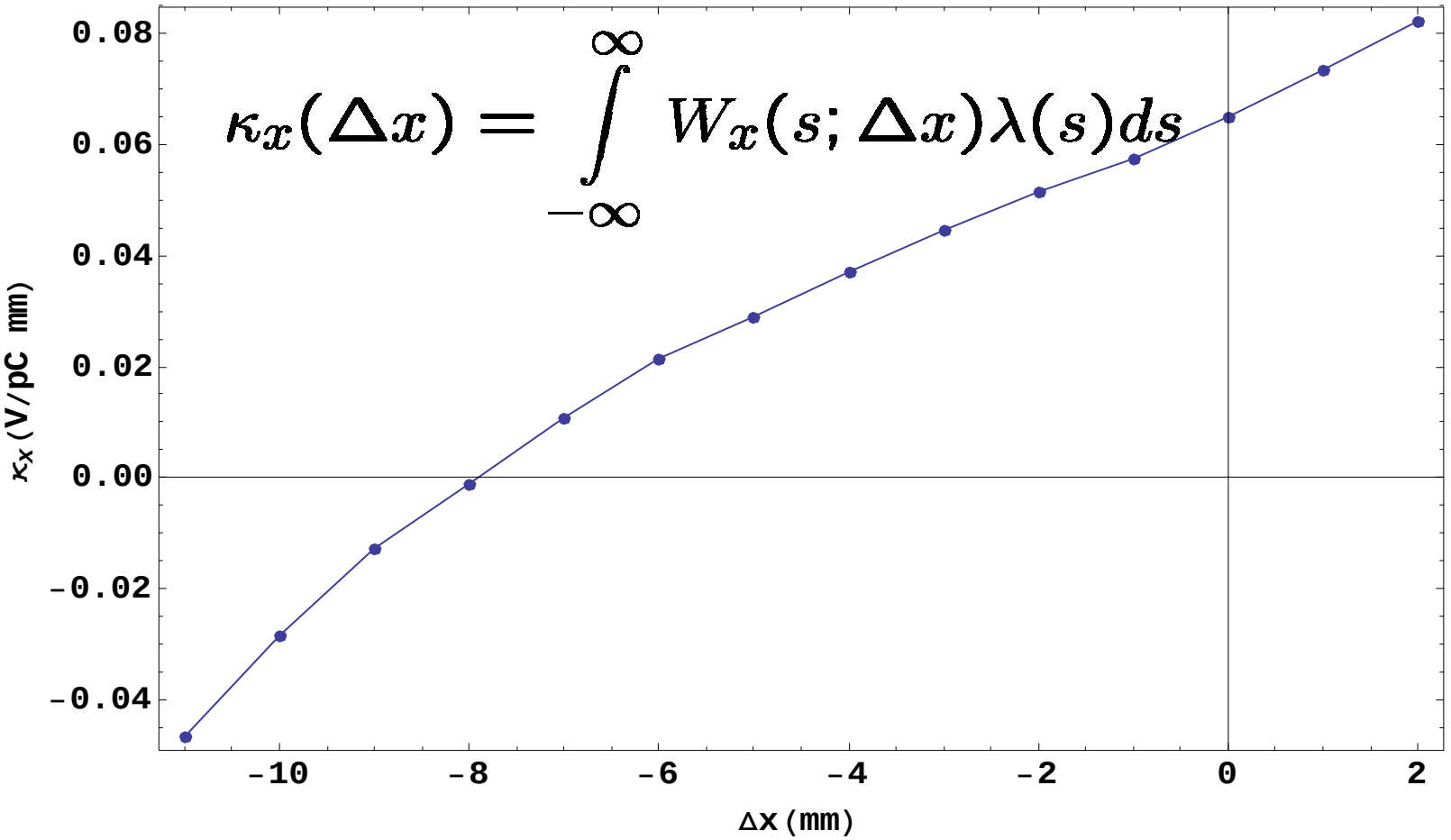
Transversal wake potentials for different beam offsets



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

PITZ Photoinjector

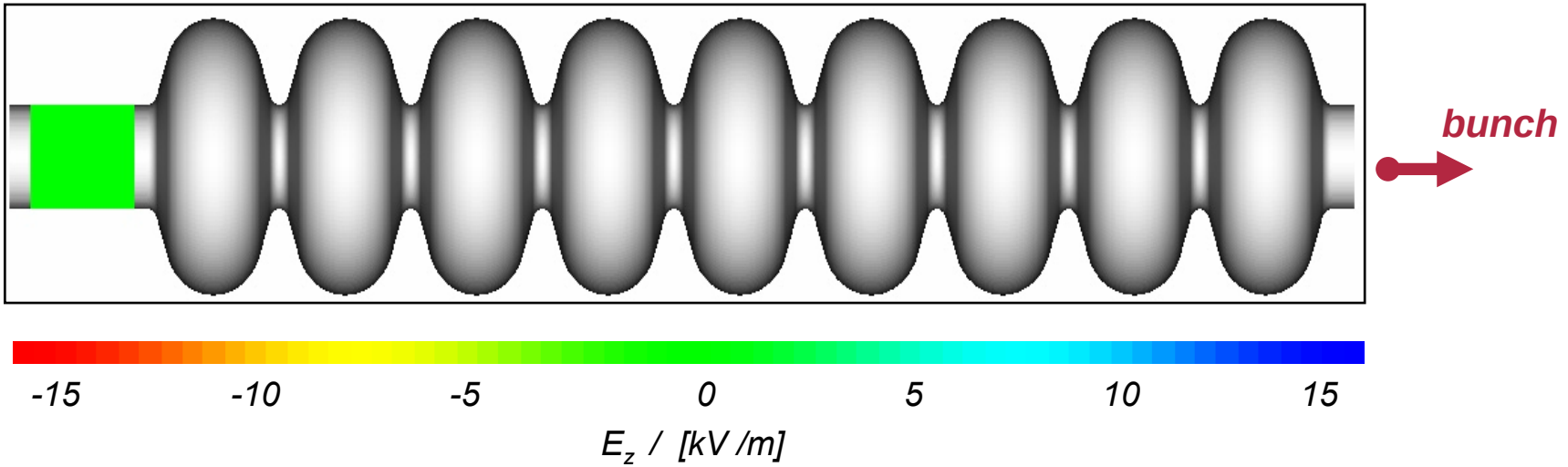
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt



„Optimal“ offset at 8mm from tube axes

TESLA / HOM coupler

TESLA 9-cell cavity

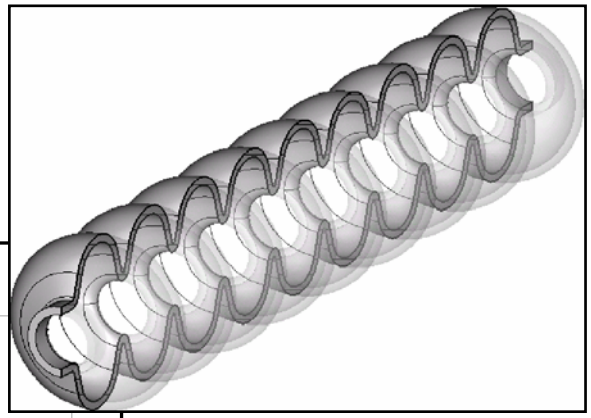


bunch length	1mm
bunch charge	1nC
cavity length	~1m
no. of grid points	~760M
no. of processor cores	408
simulation time	~40hrs

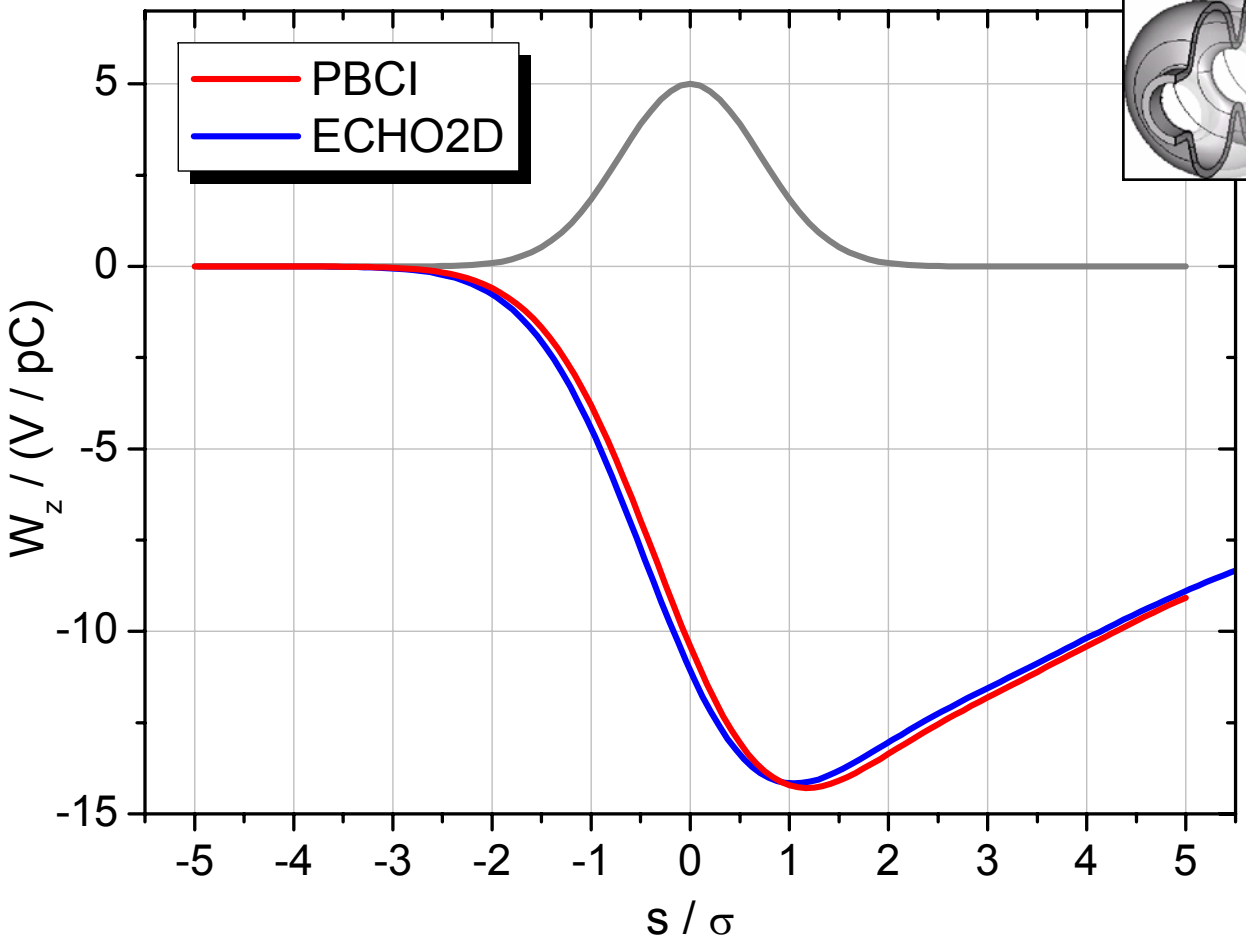
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

TESLA / HOM coupler

TESLA 9-cell cavity



Longitudinal wake potential



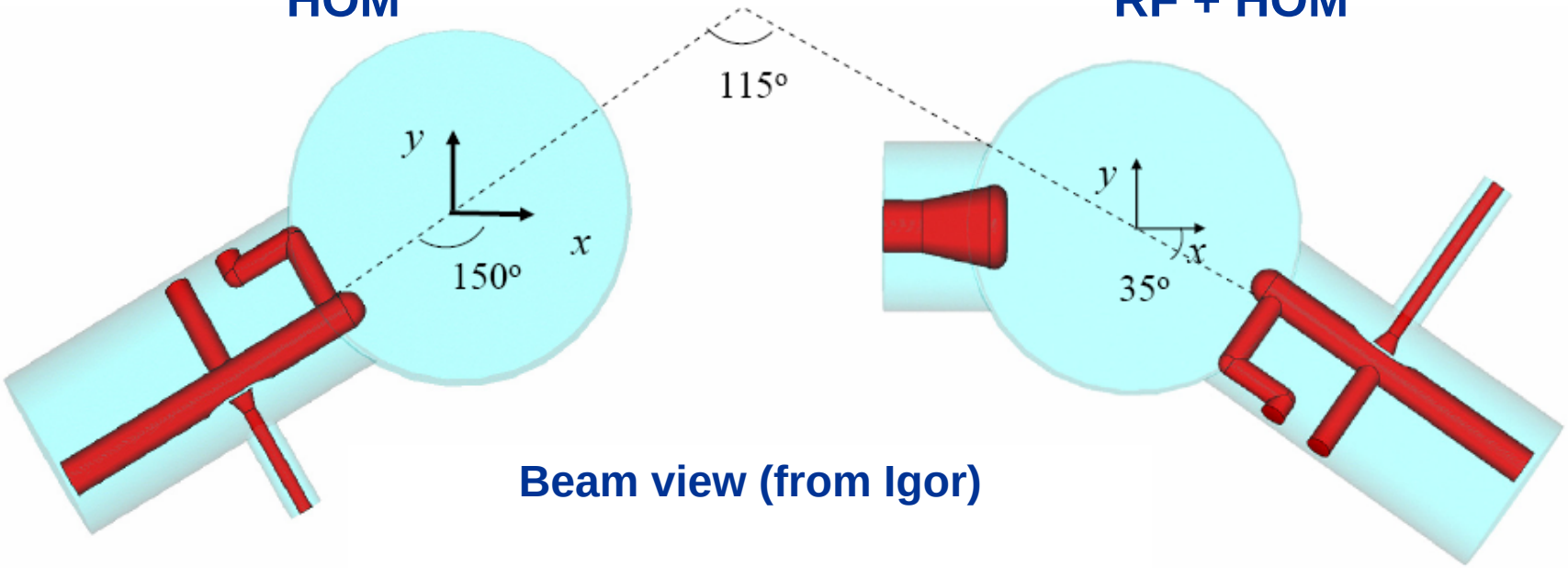
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

TESLA / HOM coupler

HOM / HOM-RF coupler (present DESY design)

Upstream coupler
HOM

Downstream coupler
RF + HOM



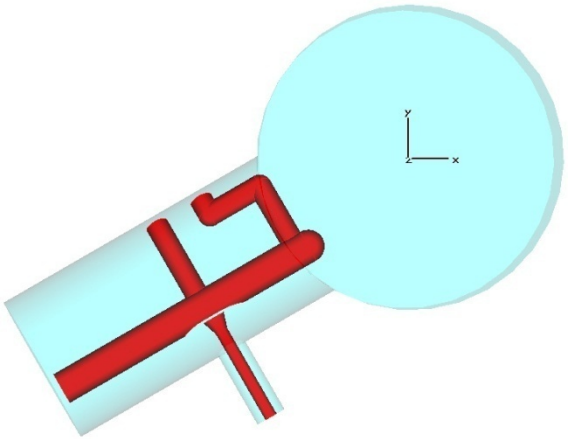
Beam view (from Igor)

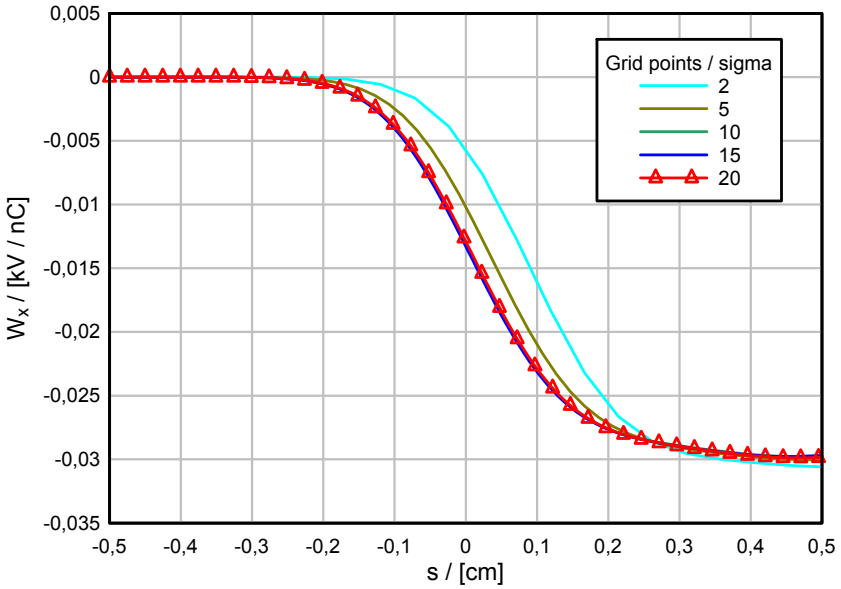
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

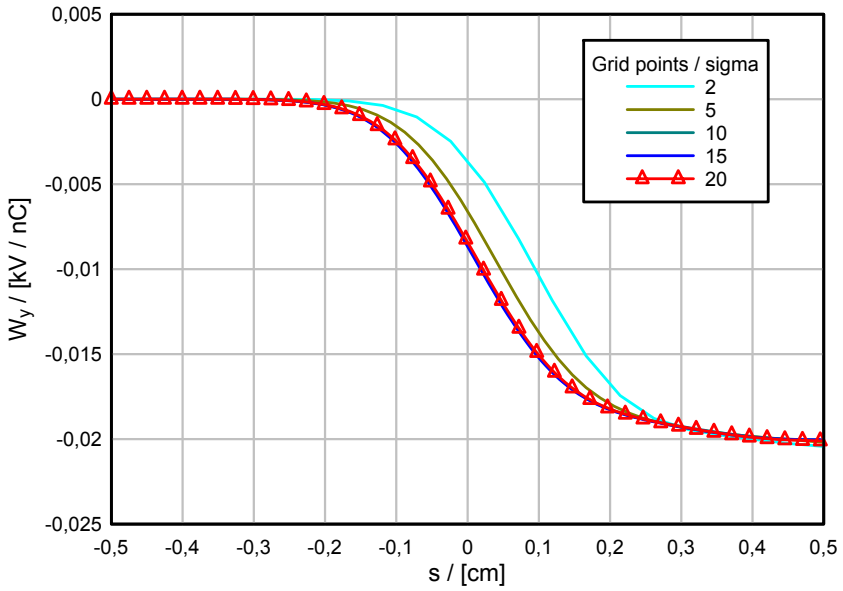
TESLA / HOM coupler

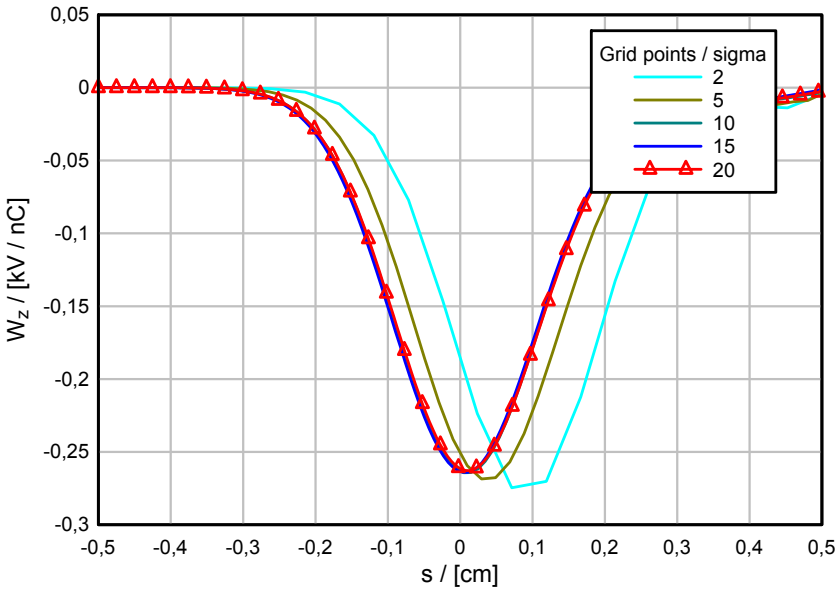
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Upstream coupler



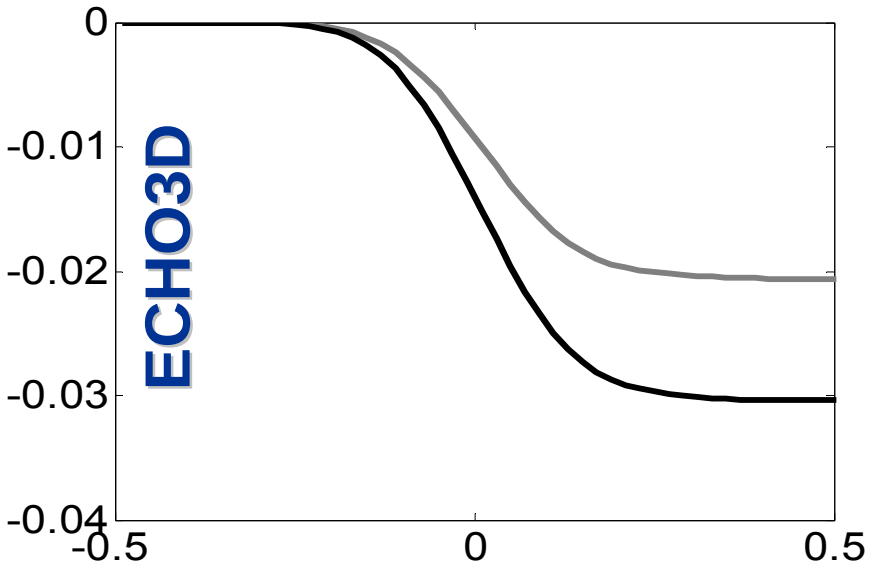


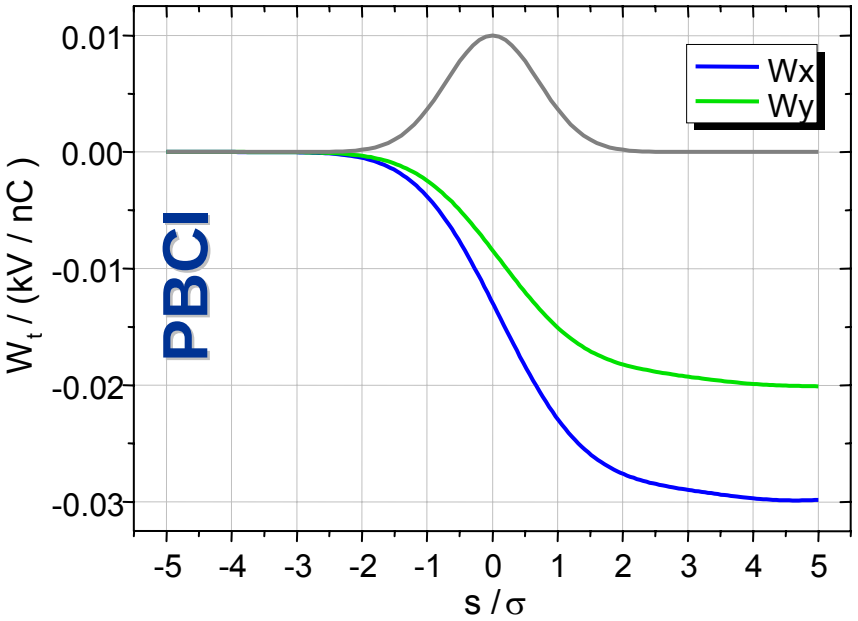




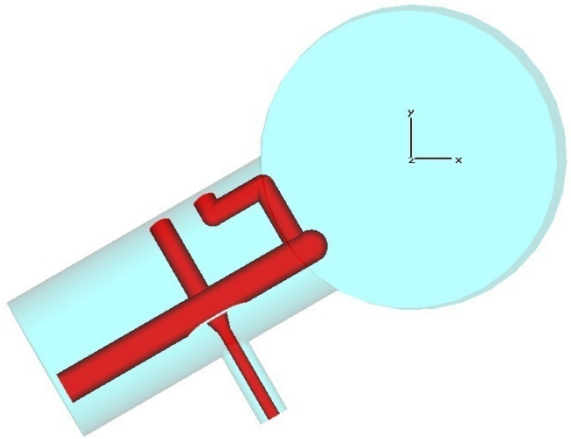
TESLA / HOM coupler

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt





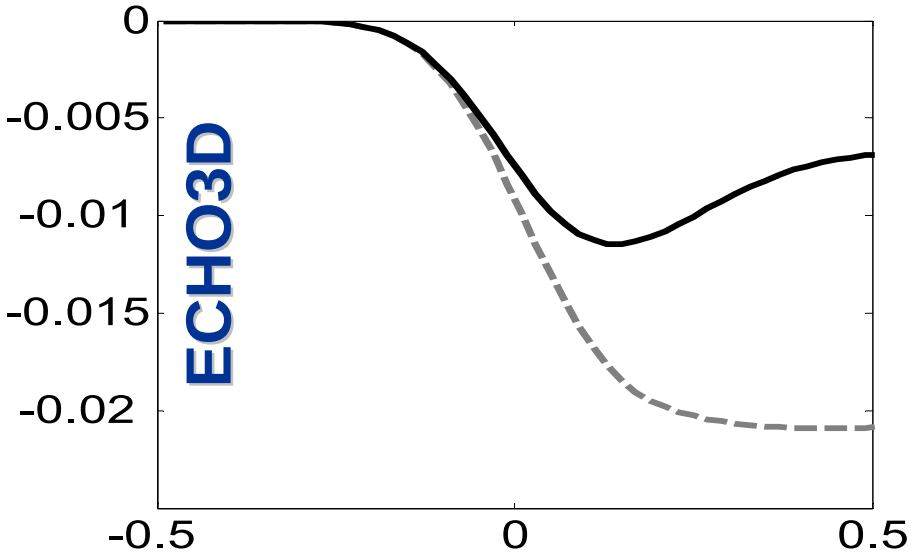
Upstream coupler



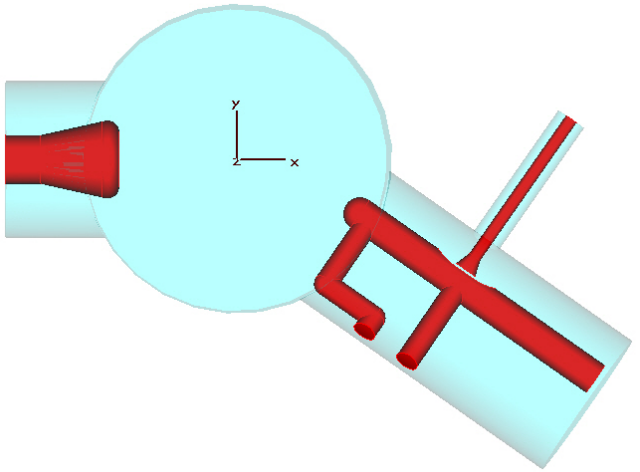
bunch length	1mm
coupler length	60mm
bunch charge	1nC
grid points (max)	~650M
processor cores	408
simulation time	~24hrs

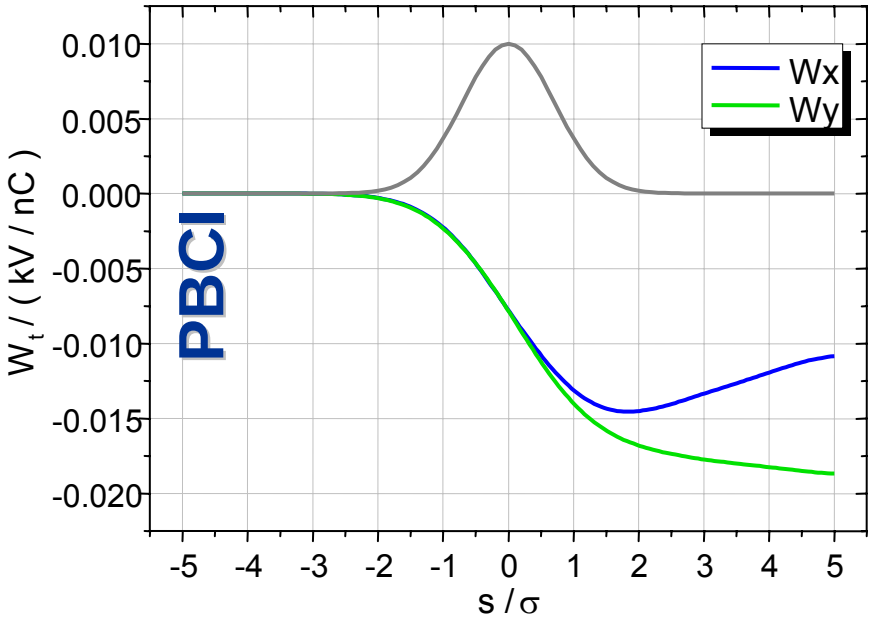
TESLA / HOM coupler

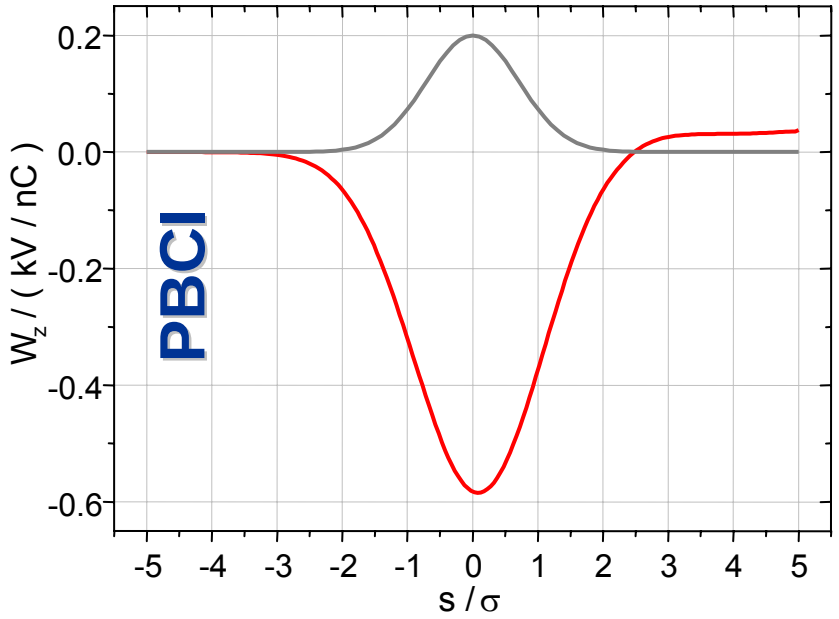
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt



Downstream coupler

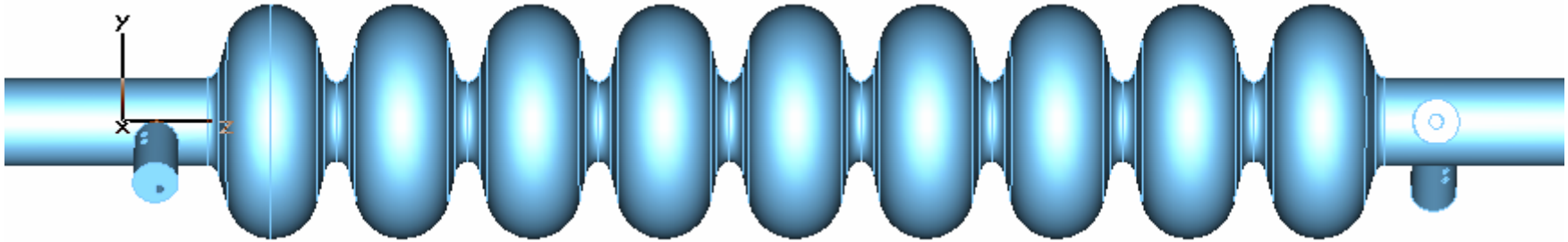




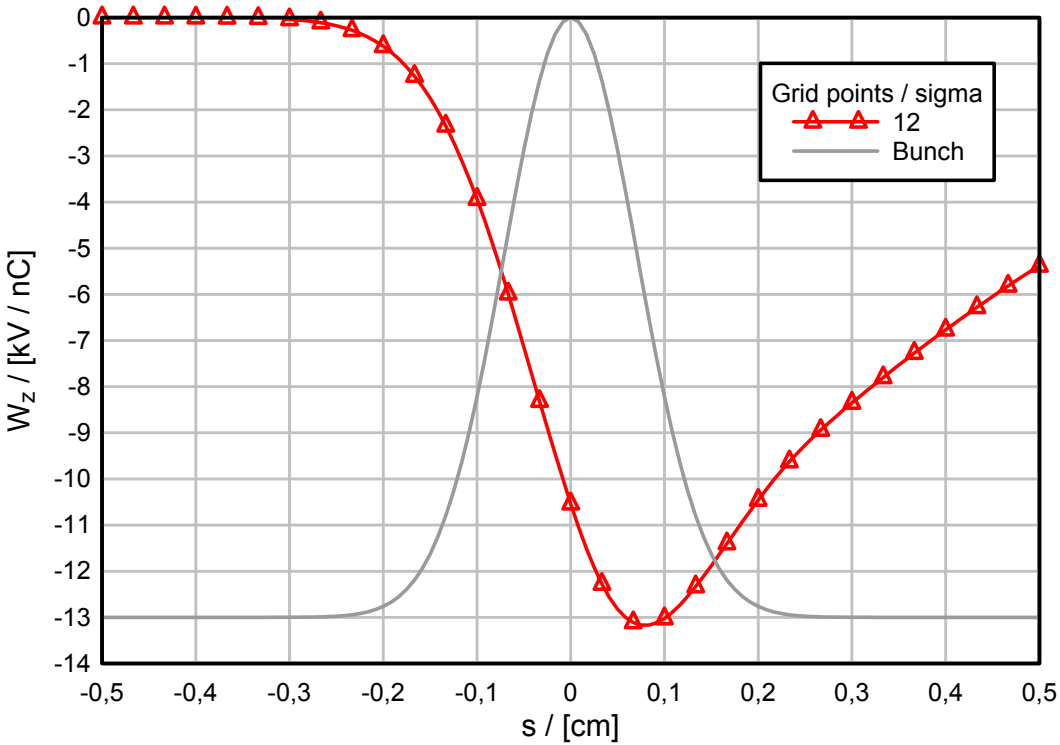


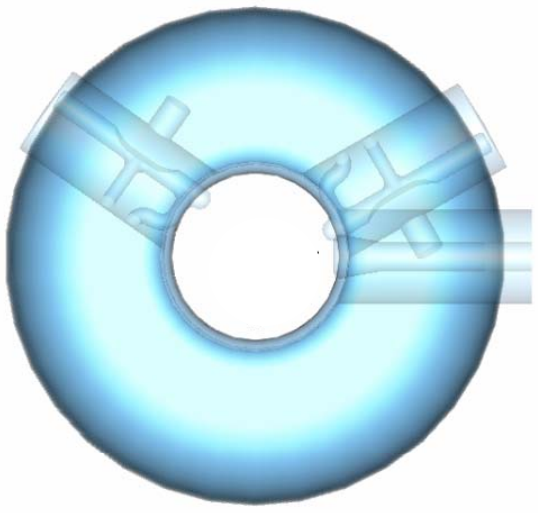
TESLA / HOM coupler

Present DESY Design



Longitudinal wake potential



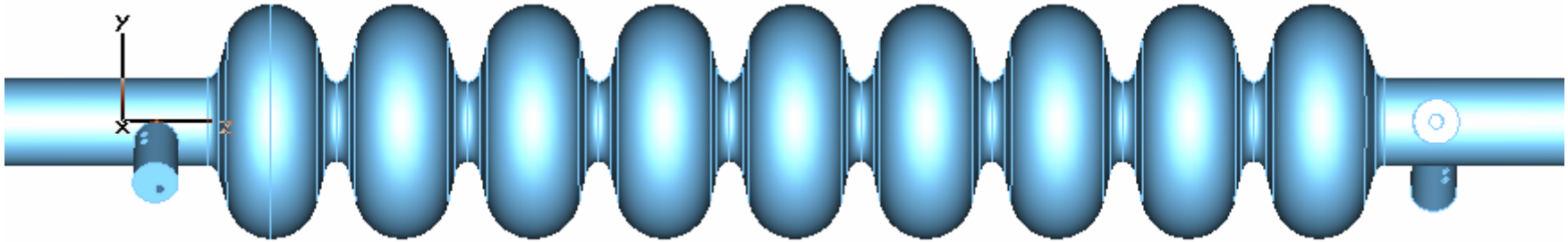


Beam view

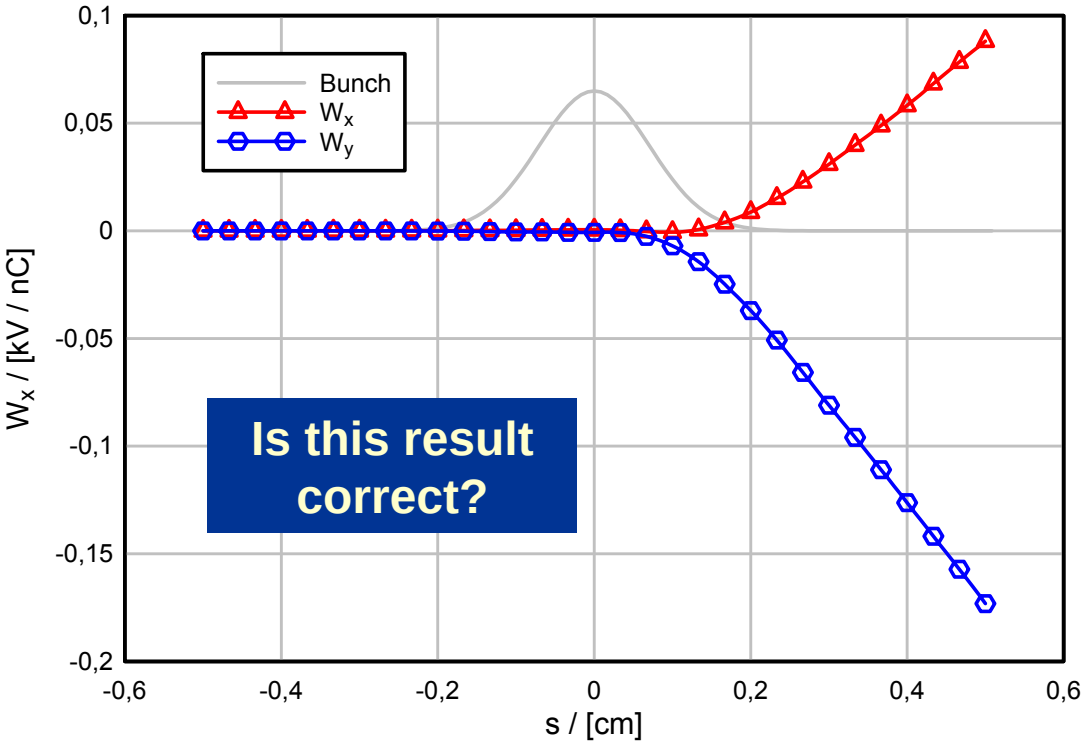
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

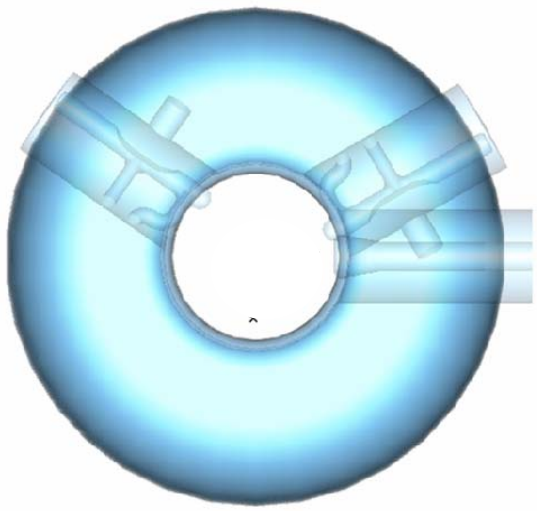
TESLA / HOM coupler

Present DESY Design



Transversal wake potentials





Beam view

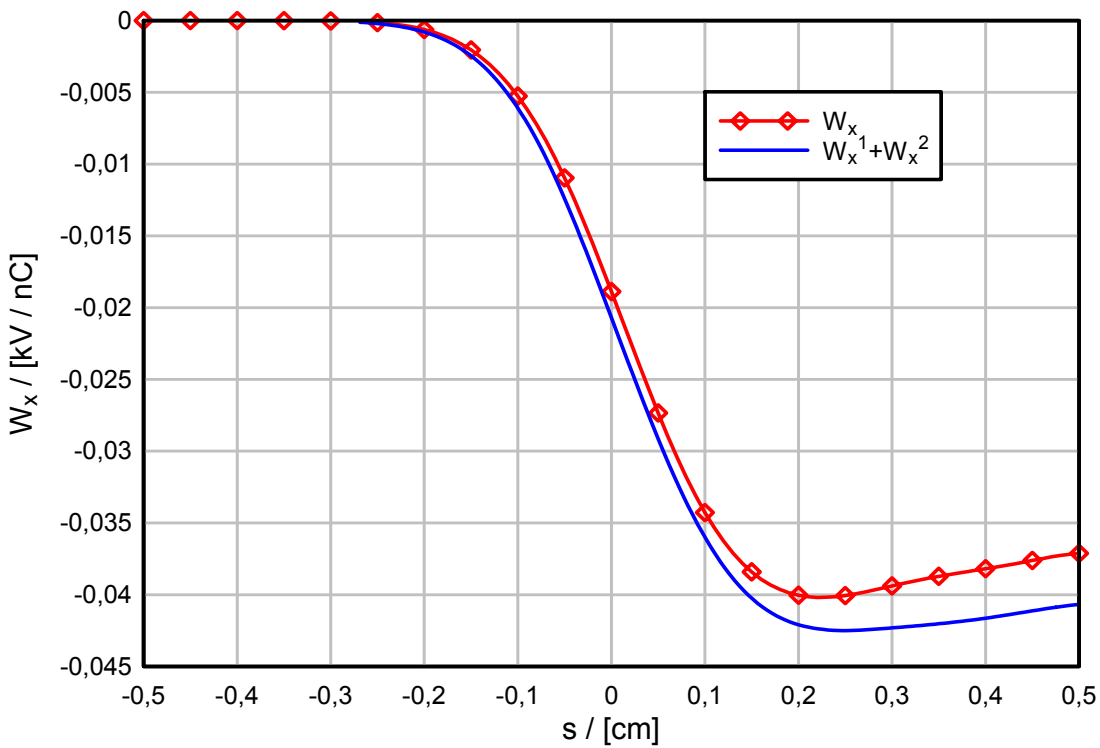
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

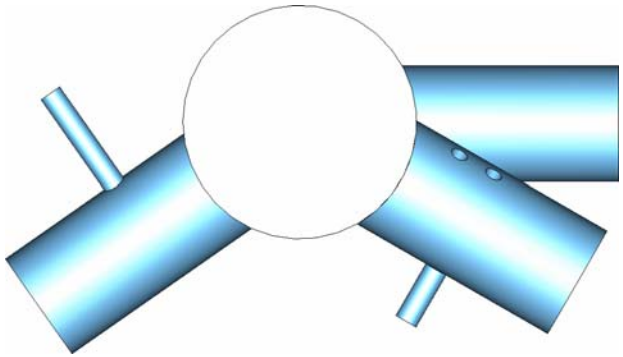
TESLA / HOM coupler

Simplified „Design“

Couplers connected by homogeneous beam tube

Transversal wake potentials





Beam view

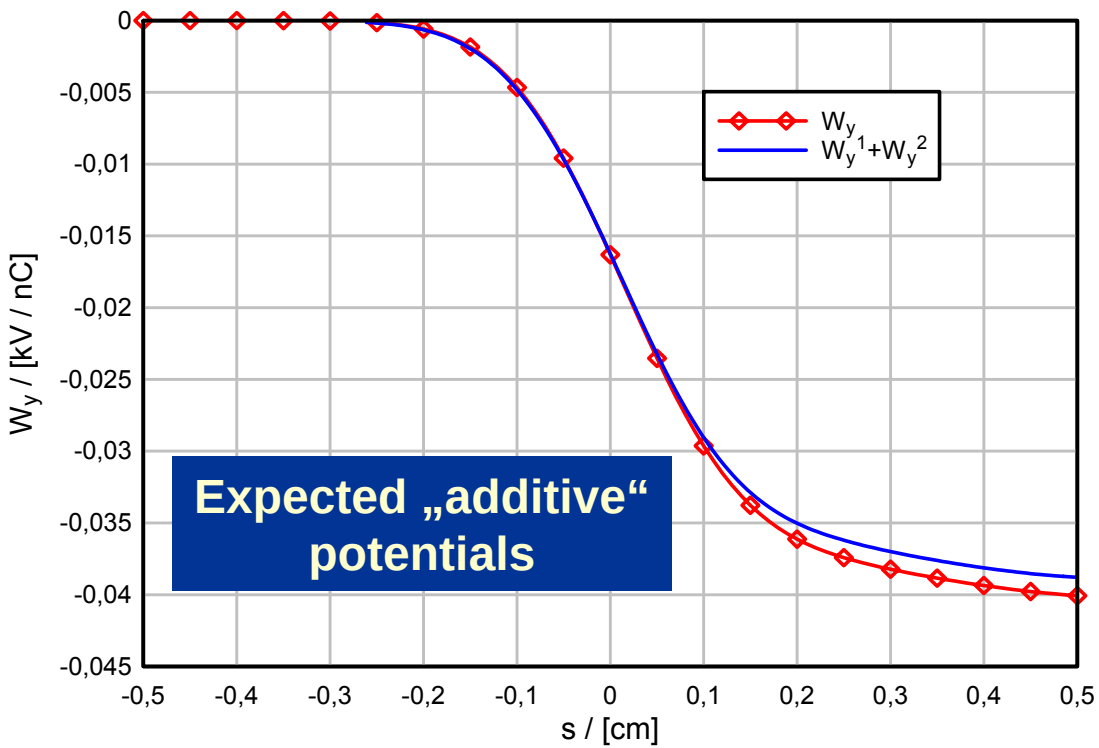
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

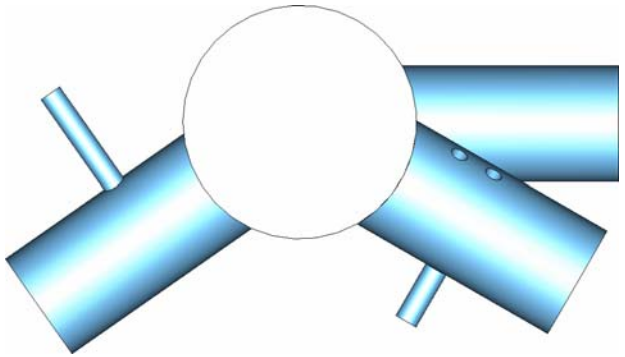
TESLA / HOM coupler

Simplified „Design“

Couplers connected by homogeneous beam tube

Transversal wake potentials

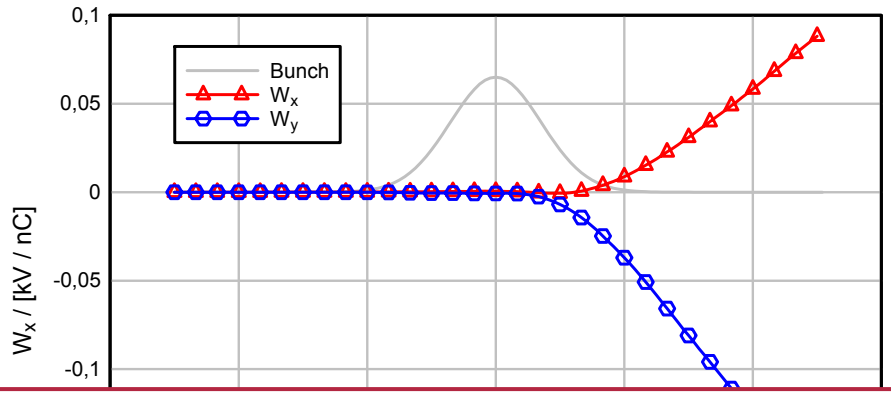


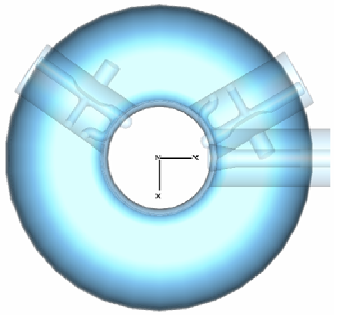


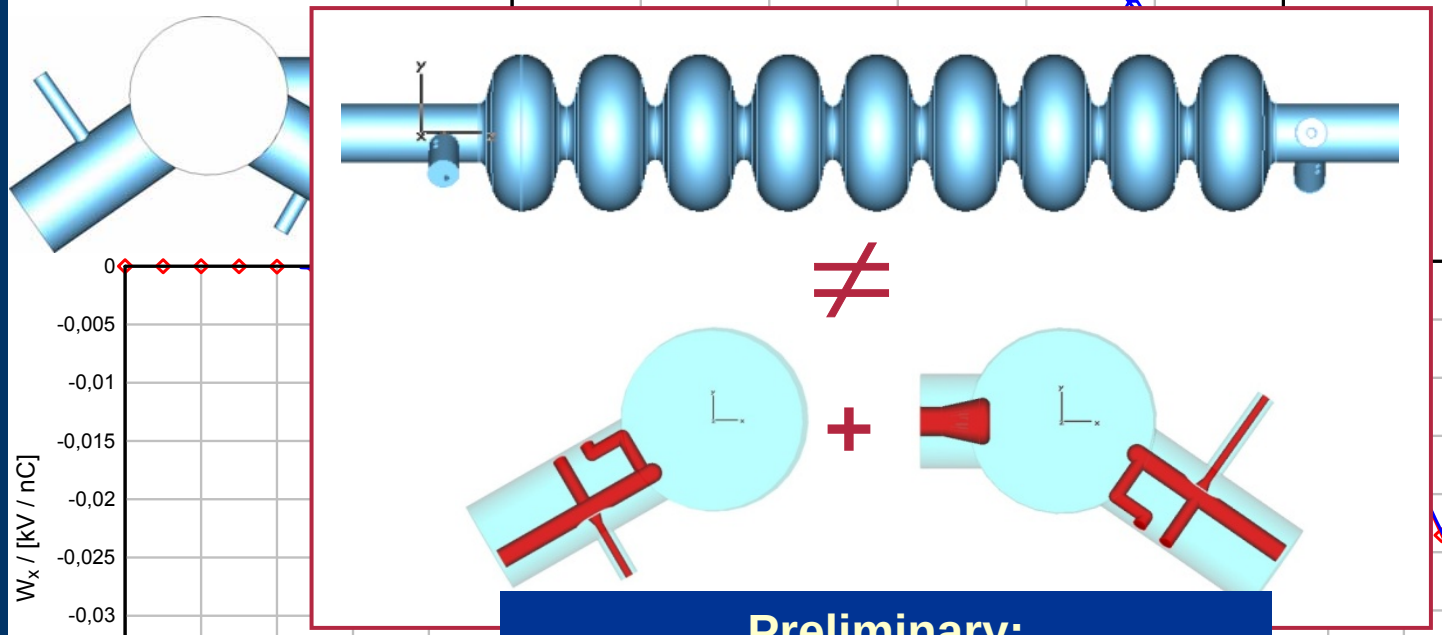
Beam view

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

TESLA / HOM coupler







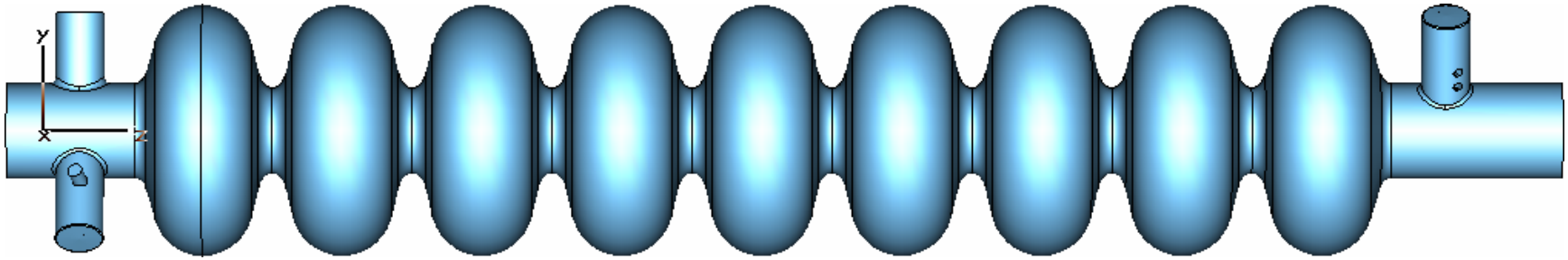
Preliminary:

Transversal wakes are affected by the crymodule?

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

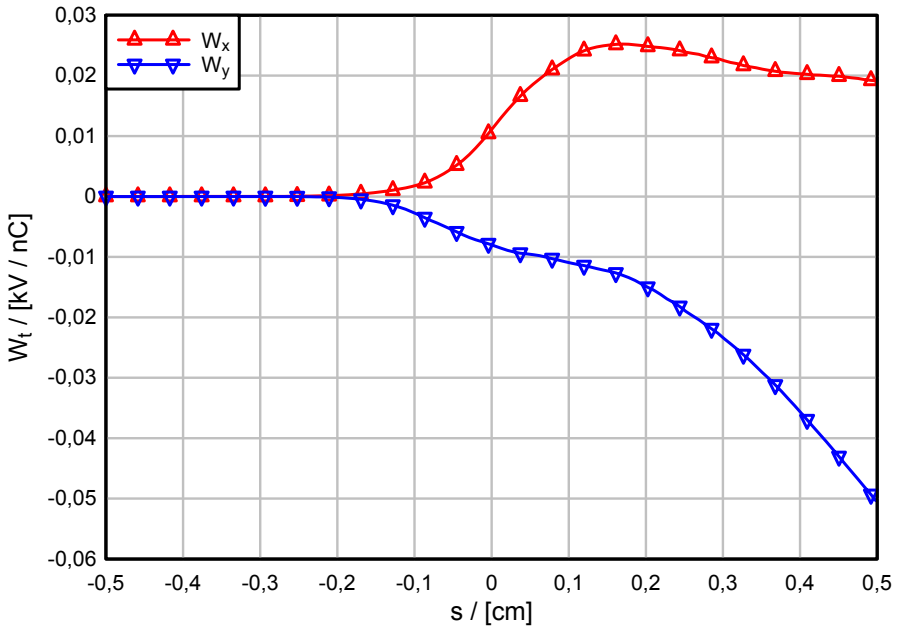
TESLA / HOM coupler

FNAL Design

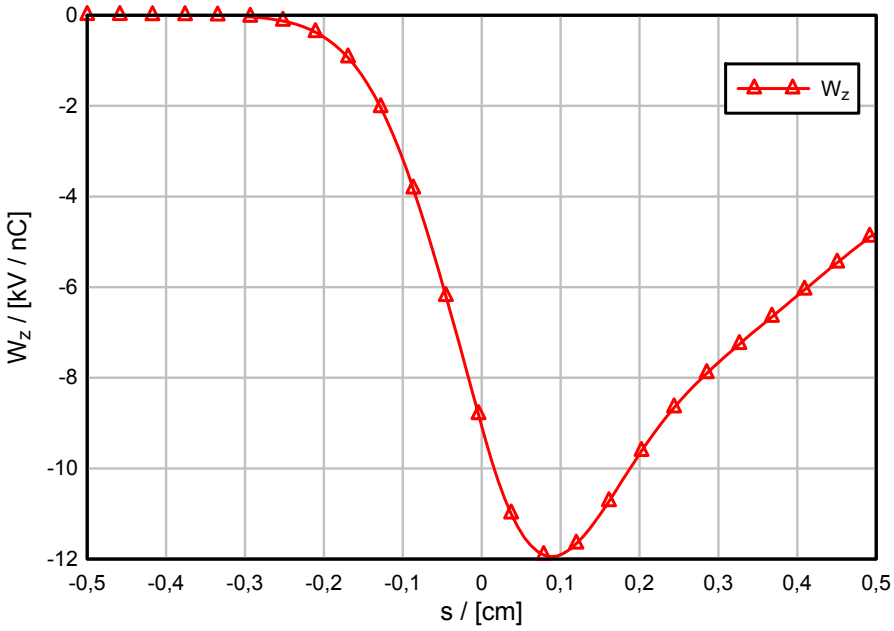


couplers are interchanged

Transversal



Longitudinal



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Wakefield Computations

Current / future work on wakefield codes at TEMF

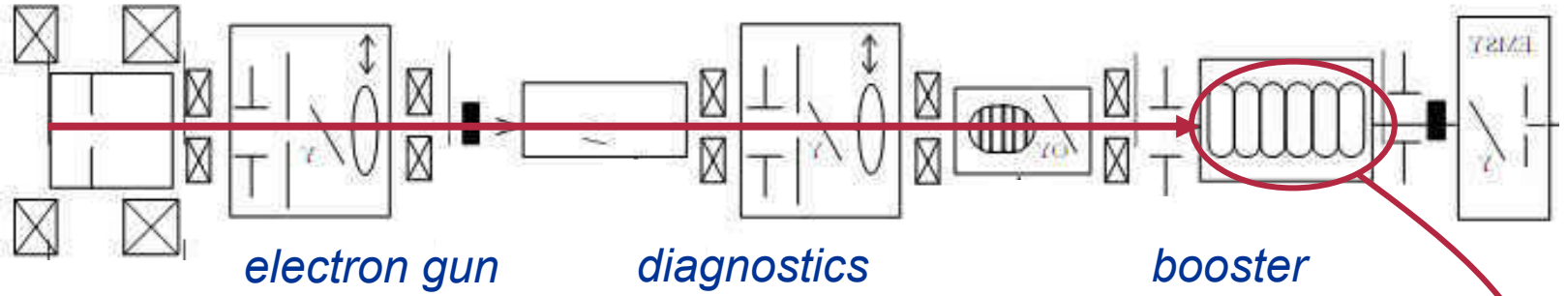
1. Non-split algorithms for moving windows: A new finite volume based algorithm is available.

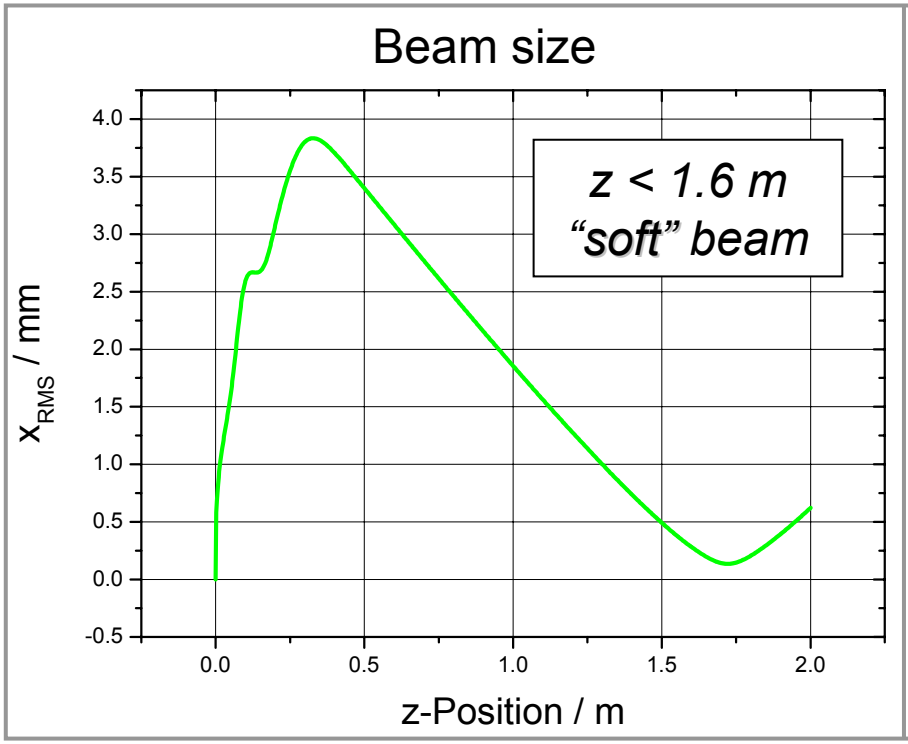
2. Implementation of impedance boundary conditions for resistivity wakes.

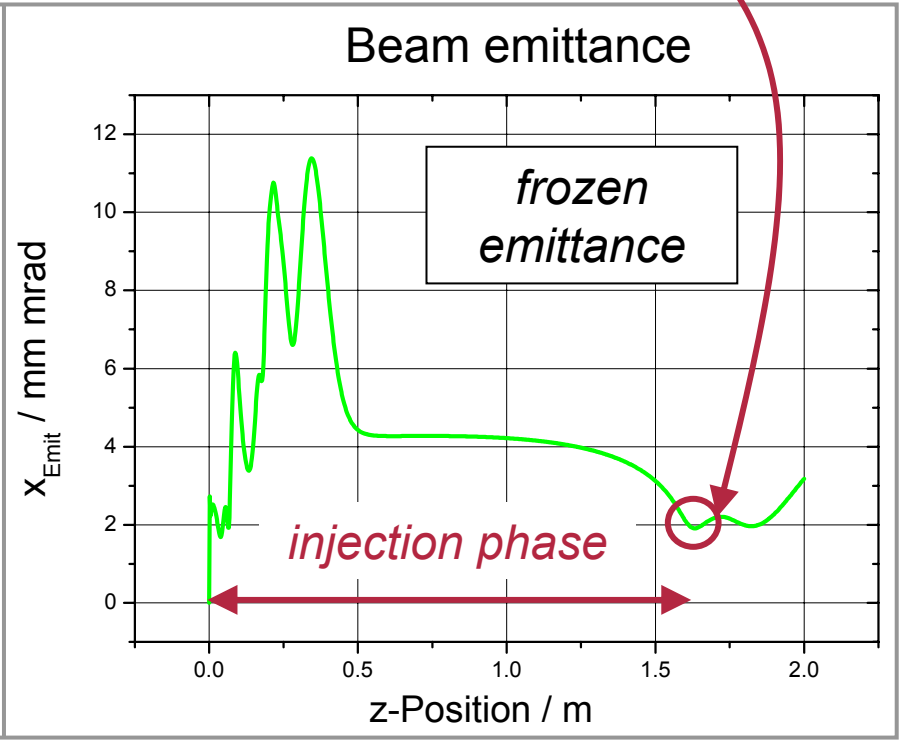
3. Handling of long (super-periodic) structures with a modal approach

Self-Consistent Simulations

The European X-Ray Laser Project XFEL at DESY, Hamburg



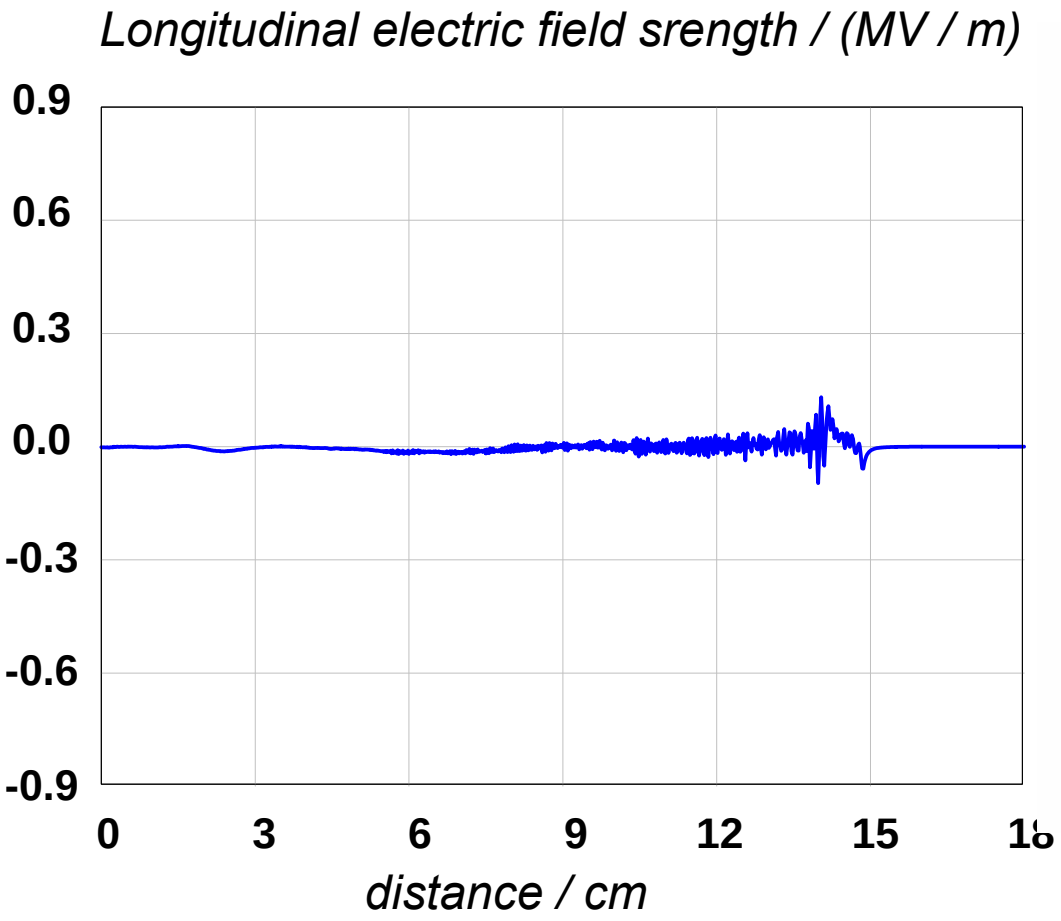


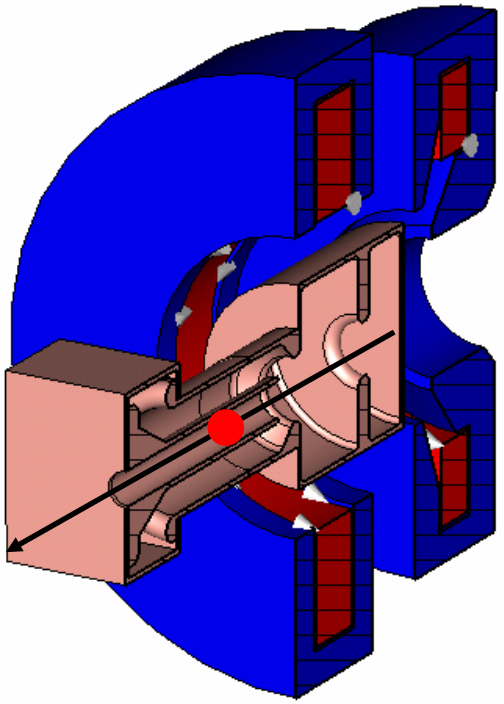


Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Self-Consistent Simulations

HF-Noise in PIC Simulations (PITZ Gun)





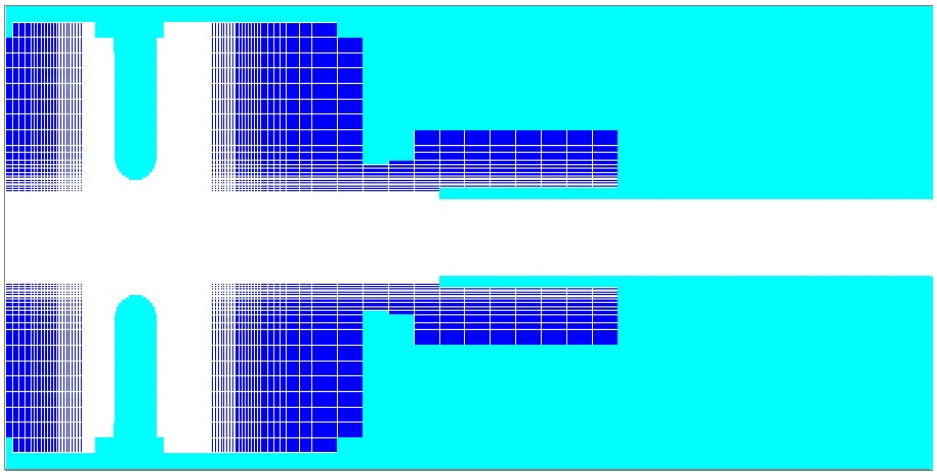
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Self-Consistent Simulations

Numerical approaches for time domain simulations

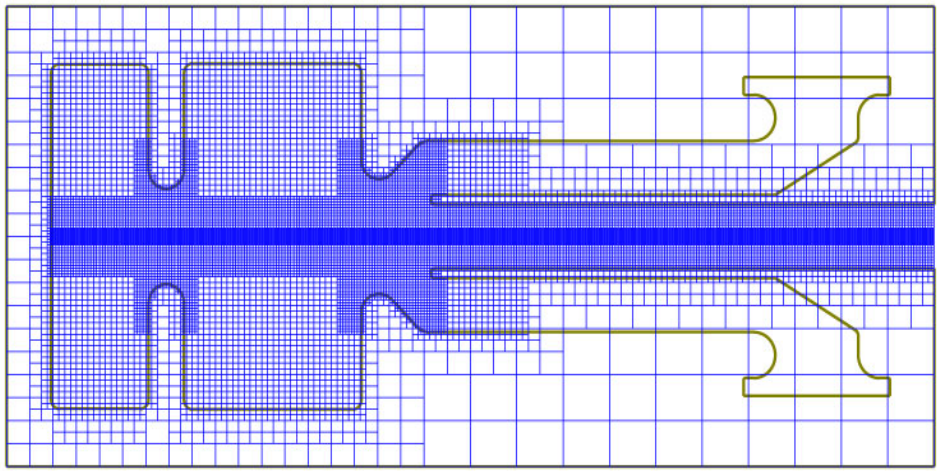
Time-adaptive mesh refinement

- *"On the fly"-discretization of bunch and structure*



Higher order FEM on unstructured grids

- *Accuracy*
- *Local mesh refinement*

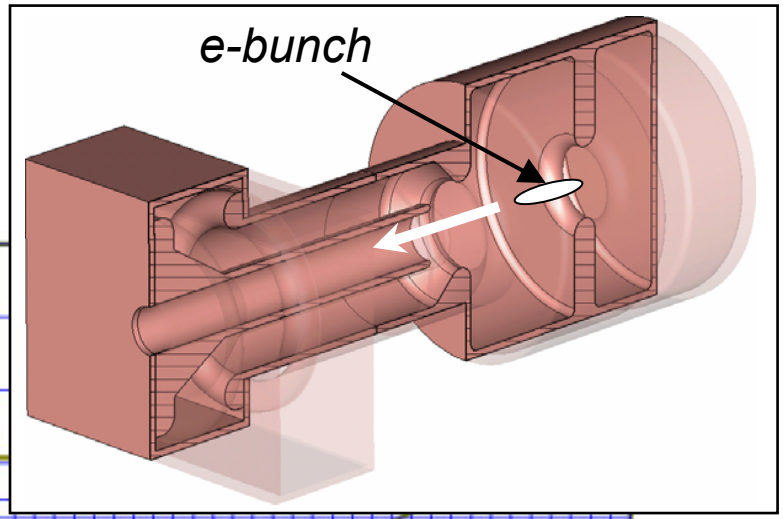


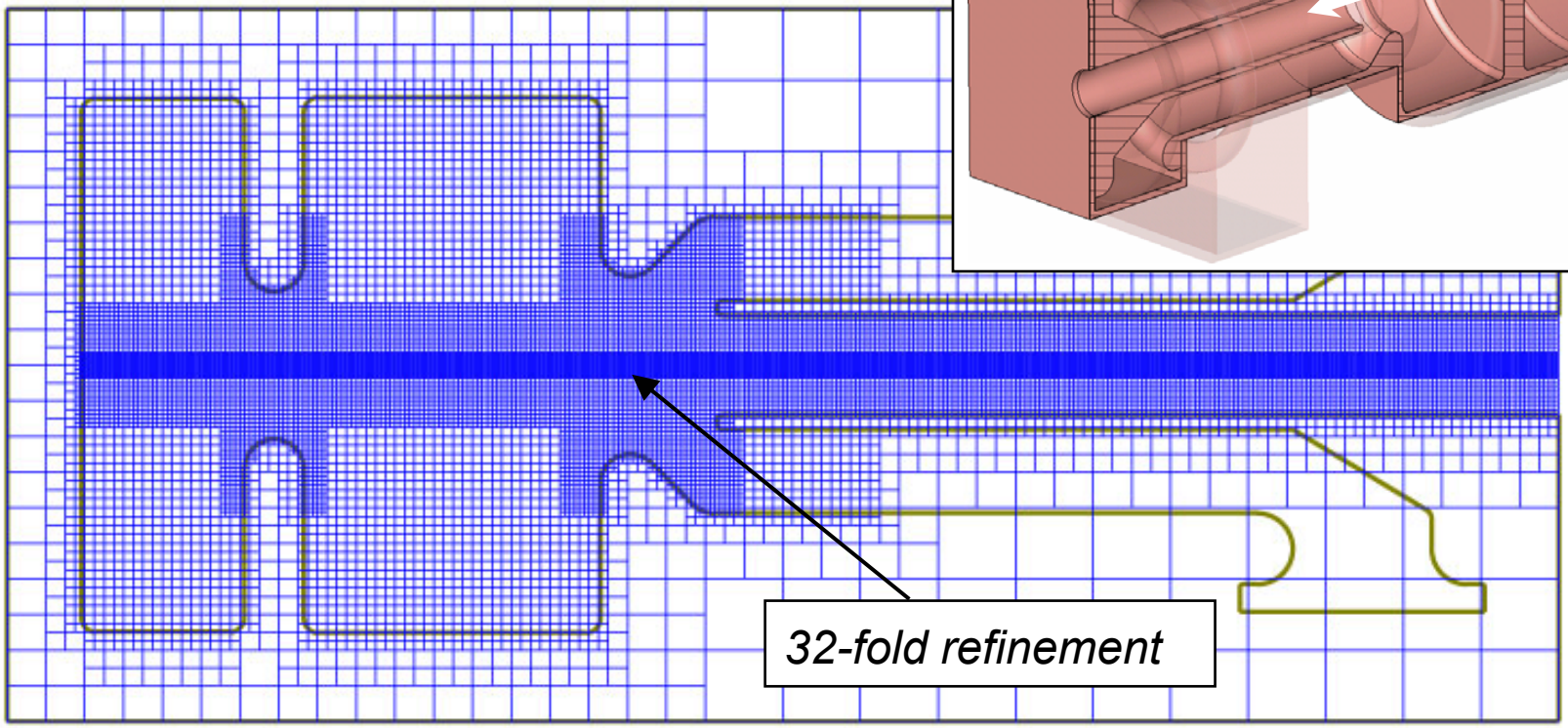
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Self-Consistent Simulations

Examples of local mesh refinement

Discretization of the RF PITZ gun





1.5 m

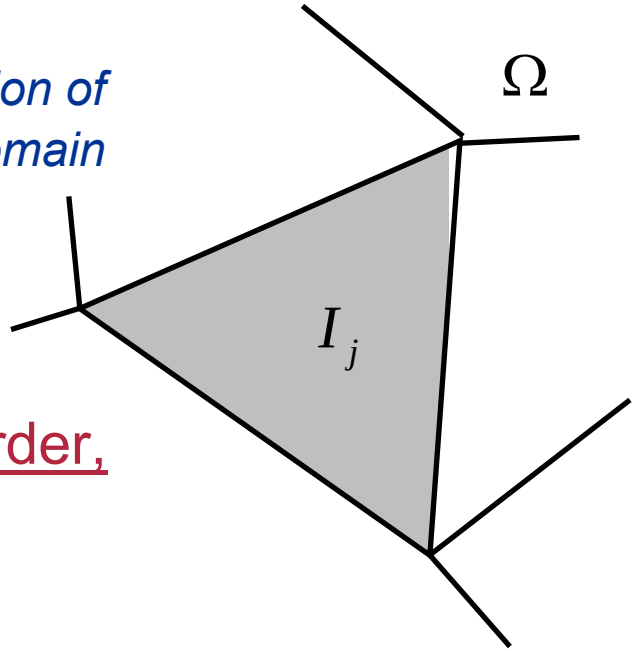
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

The DG-FEM Method

The DG-FEM formulation for Maxwell Equations

$$\begin{cases} \dfrac{\partial \varepsilon \mathbf{E}}{\partial t} - \nabla \times \mathbf{H} = 0 \\ \dfrac{\partial \mu \mathbf{H}}{\partial t} + \nabla \times \mathbf{E} = 0 \end{cases}$$

Discretization of computational domain



Approximate field components with high order, piecewise polynomial basis functions.

$$E_x(\mathbf{r},t) \approx \overline{E}_x(\mathbf{r},t) = \sum_{j,p} E^x_{j;p}(t)\varphi_{j;p}(\mathbf{r})$$

$$E_y(\mathbf{r},t) \approx \overline{E}_y(\mathbf{r},t) = \sum_{j,p} E^y_{j;p}(t)\varphi_{j;p}(\mathbf{r})$$

$$\vdots$$

$$H_z(\mathbf{r},t) \approx \overline{H}_z(\mathbf{r},t) = \sum_{j,p} H^z_{j;p}(t)\varphi_{j;p}(\mathbf{r})$$

$$\overline{\mathbf{E}}(\mathbf{r},t) = \sum_{j,p} \mathbf{E}_{j;p}(t)\varphi_{j;p}(\mathbf{r})$$

$$\overline{\mathbf{H}}(\mathbf{r},t) = \sum_{j,p} \mathbf{H}_{j;p}(t)\varphi_{j;p}(\mathbf{r})$$

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

The DG-FEM Method

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Test approximate equations (e.g., Ampere's law)

$$\int_{I_i} d^3\mathbf{r}\frac{\partial\varepsilon\overline{\mathbf{E}}}{\partial t}\varphi-\int_{I_i} d^3\mathbf{r}\nabla\times\overline{\mathbf{H}}\varphi=\int_{I_i} d^3\mathbf{r}\frac{\partial\varepsilon\overline{\mathbf{E}}}{\partial t}\varphi-\int_{I_i} d^3\mathbf{r}\nabla\times\left(\overline{\mathbf{H}}\varphi\right)+\int_{I_i} d^3\mathbf{r}\left(\nabla\varphi\right)\times\overline{\mathbf{H}}=0$$

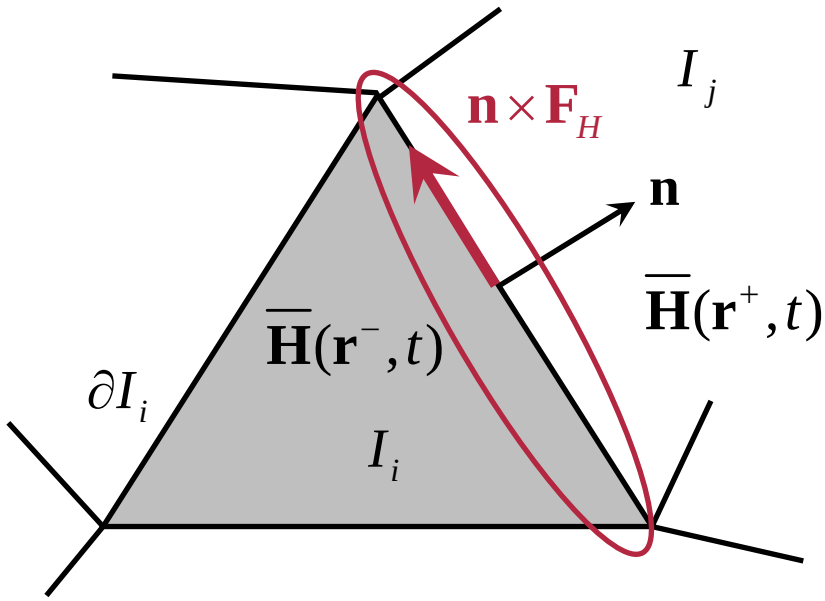
$$\Rightarrow\int_{I_i} d^3\mathbf{r}\frac{\partial\varepsilon\overline{\mathbf{E}}}{\partial t}\varphi-\int_{\partial I_i} d^2\mathbf{r}\left(\mathbf{n}\times\mathbf{F}_H\right)\varphi+\int_{I_i} d^3\mathbf{r}\left(\nabla\varphi\right)\times\overline{\mathbf{H}}=0$$

numerical flux

Ansatz: centered flux for tangential fields at element boundaries:

$$\mathbf{n}\times\mathbf{F}_E=\frac{1}{2}\mathbf{n}\times\left[\overline{\mathbf{E}}(\mathbf{r}^-,t)+\overline{\mathbf{E}}(\mathbf{r}^+,t)\right],$$

$$\mathbf{n}\times\mathbf{F}_H=\frac{1}{2}\mathbf{n}\times\left[\overline{\mathbf{H}}(\mathbf{r}^-,t)+\overline{\mathbf{H}}(\mathbf{r}^+,t)\right]$$



The DG-FEM Method

Matrix representation of semidiscrete equations

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

semidiscrete DG formulation

skew-symmetric

$$\mathbf{e}=\begin{pmatrix}\mathbf{e}_x\\ \mathbf{e}_y\\ \mathbf{e}_z\end{pmatrix},\quad \mathbf{h}=\begin{pmatrix}\mathbf{h}_x\\ \mathbf{h}_y\\ \mathbf{h}_z\end{pmatrix}$$

Recovers FDTD for piecewise constant basis functions, on Cartesian grids

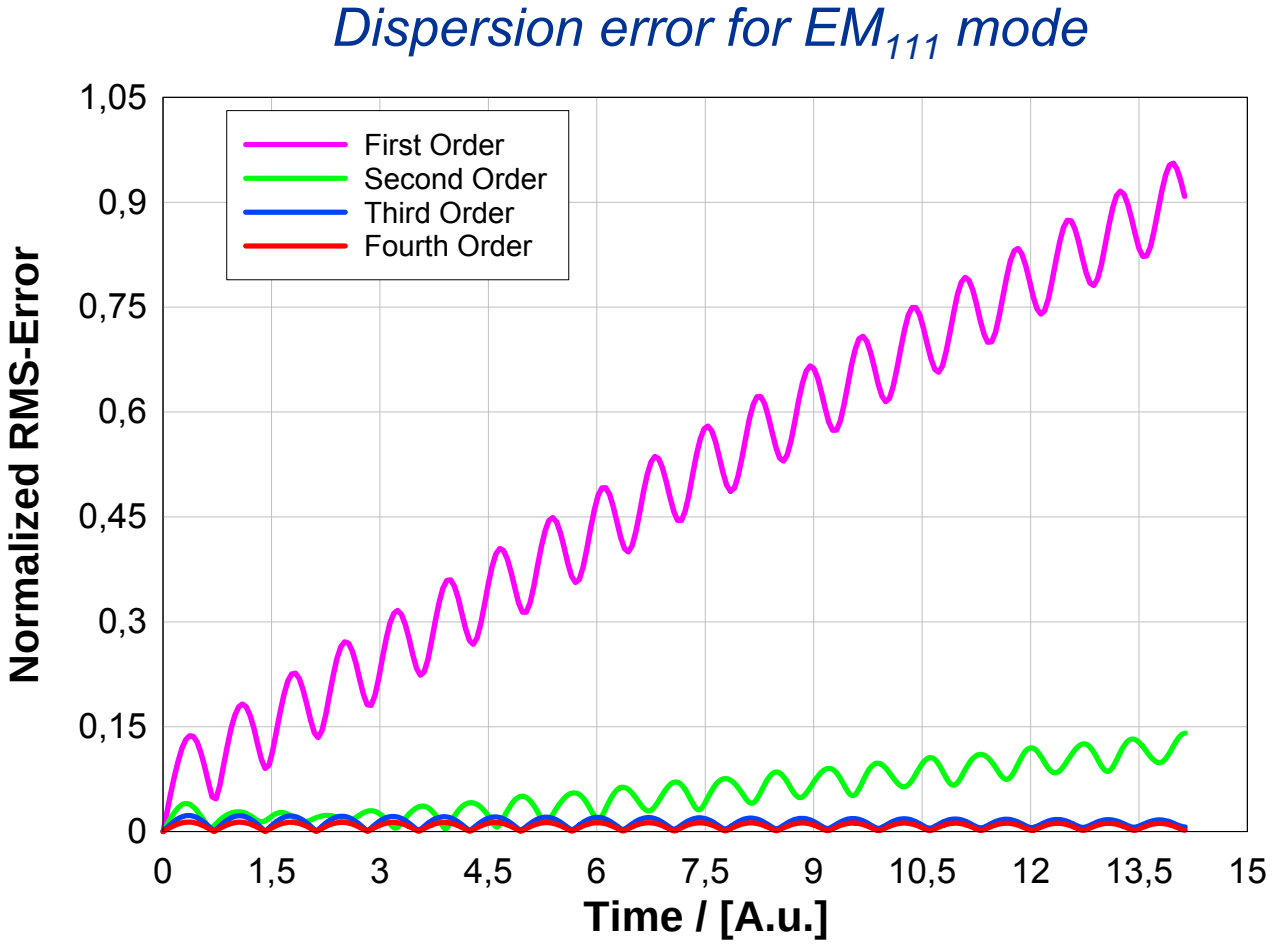
symmetric, positive, *(block-) diagonal*

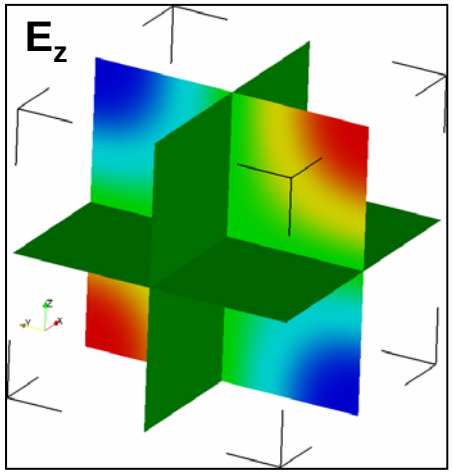
symmetric: $\mathbf{C}^T=\mathbf{C}$

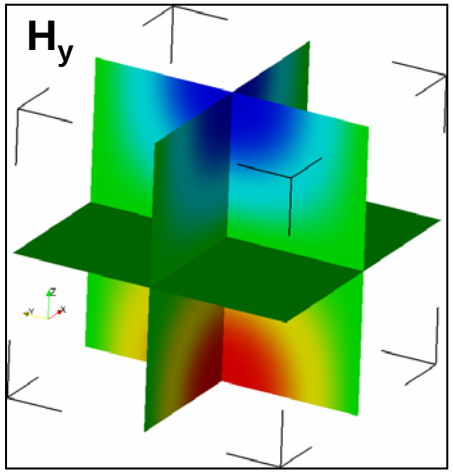
$$\mathbf{M}_\varepsilon=\begin{pmatrix}\mathbf{M}_{\varepsilon_x} & 0 & 0\\ 0 & \mathbf{M}_{\varepsilon_y} & 0\\ 0 & 0 & \mathbf{M}_{\varepsilon_z}\end{pmatrix},\quad \mathbf{M}_\mu=\begin{pmatrix}\mathbf{M}_{\mu_x} & 0 & 0\\ 0 & \mathbf{M}_{\mu_y} & 0\\ 0 & 0 & \mathbf{M}_{\mu_z}\end{pmatrix},\quad \mathbf{C}=\begin{pmatrix}0 & -\mathbf{P}_z & \mathbf{P}_y\\ \mathbf{P}_z & 0 & -\mathbf{P}_x\\ -\mathbf{P}_y & \mathbf{P}_x & 0\end{pmatrix}$$

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Periodic solution in resonator box



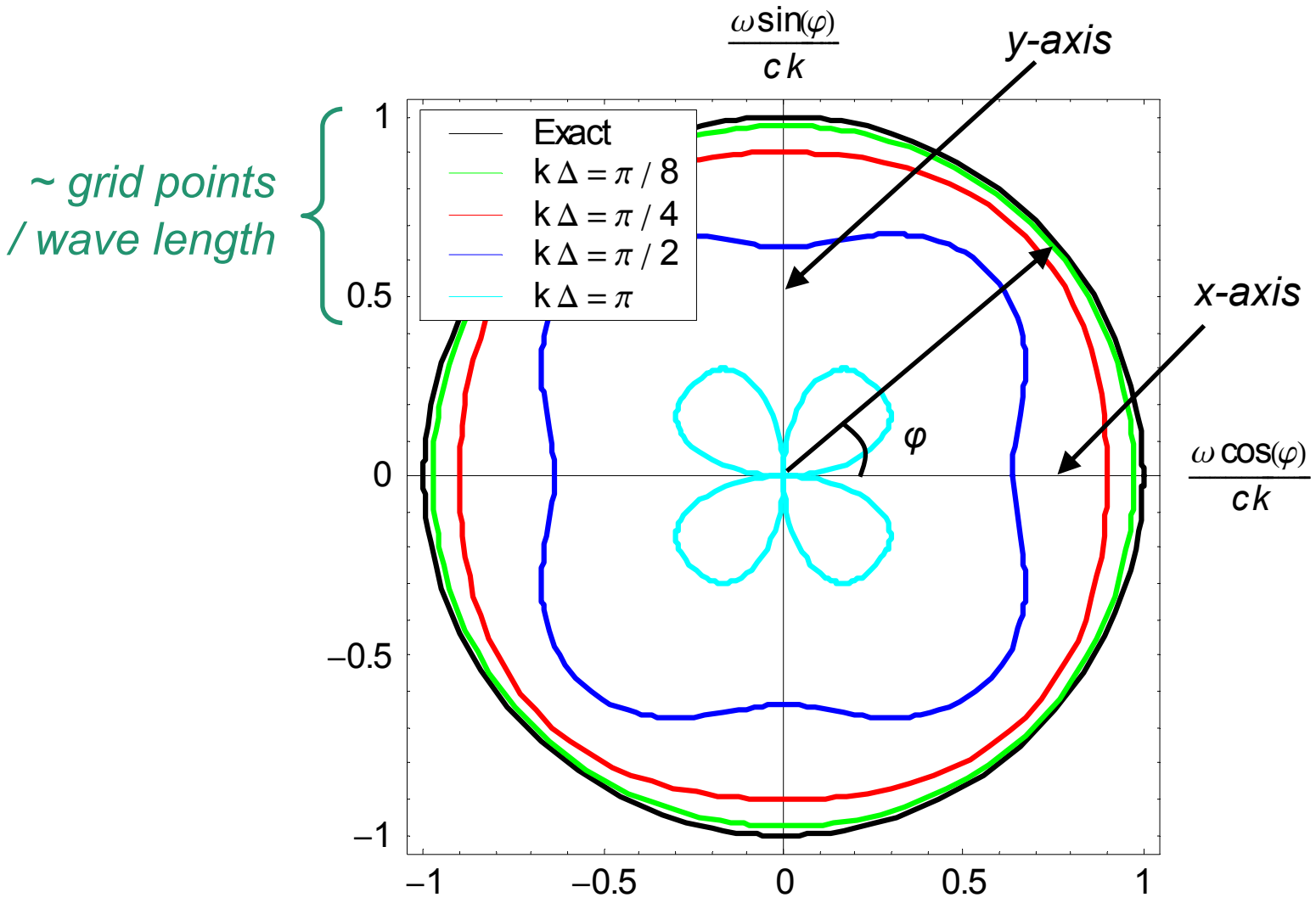




Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

The DG-FEM Method

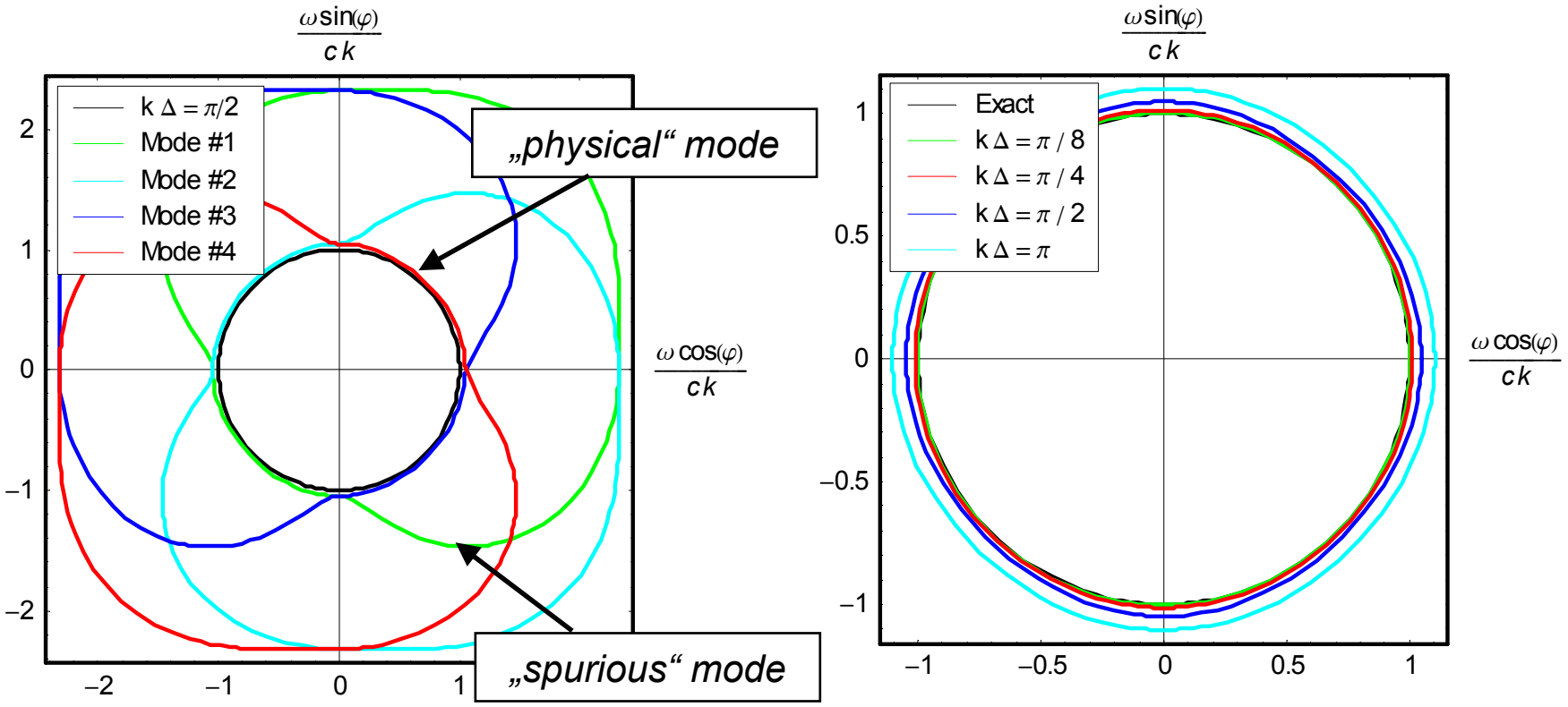
Dispersion analysis. The P^0 x P^0 x P^0 -case



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Dispersion analysis. The P^1 x P^1 x P^1 -case

Dispersion curves in the xy-plane



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

The Problem of Charge Conservation

Define a (consistent) divergence operator as: $\mathbf{S} = \begin{pmatrix} \mathbf{P}_x & \mathbf{P}_y & \mathbf{P}_z \end{pmatrix}$

Continuity equations for electric and magnetic charges:

$$\frac{d}{dt}\left(\mathbf{S}\,\mathbf{d}\right) = \frac{d}{dt}\left(\mathbf{S}\,\mathbf{M}_\varepsilon \mathbf{e}\right) = \frac{d}{dt}\left(\mathbf{S}\,\mathbf{C}\,\mathbf{h}\right) \stackrel{?}{=} 0$$

(source free case)

$$\frac{d}{dt}\left(\mathbf{S}\,\mathbf{b}\right) = \frac{d}{dt}\left(\mathbf{S}\,\mathbf{M}_\mu \mathbf{h}\right) = -\frac{d}{dt}\left(\mathbf{S}\,\mathbf{C}\,\mathbf{e}\right) \stackrel{?}{=} 0$$

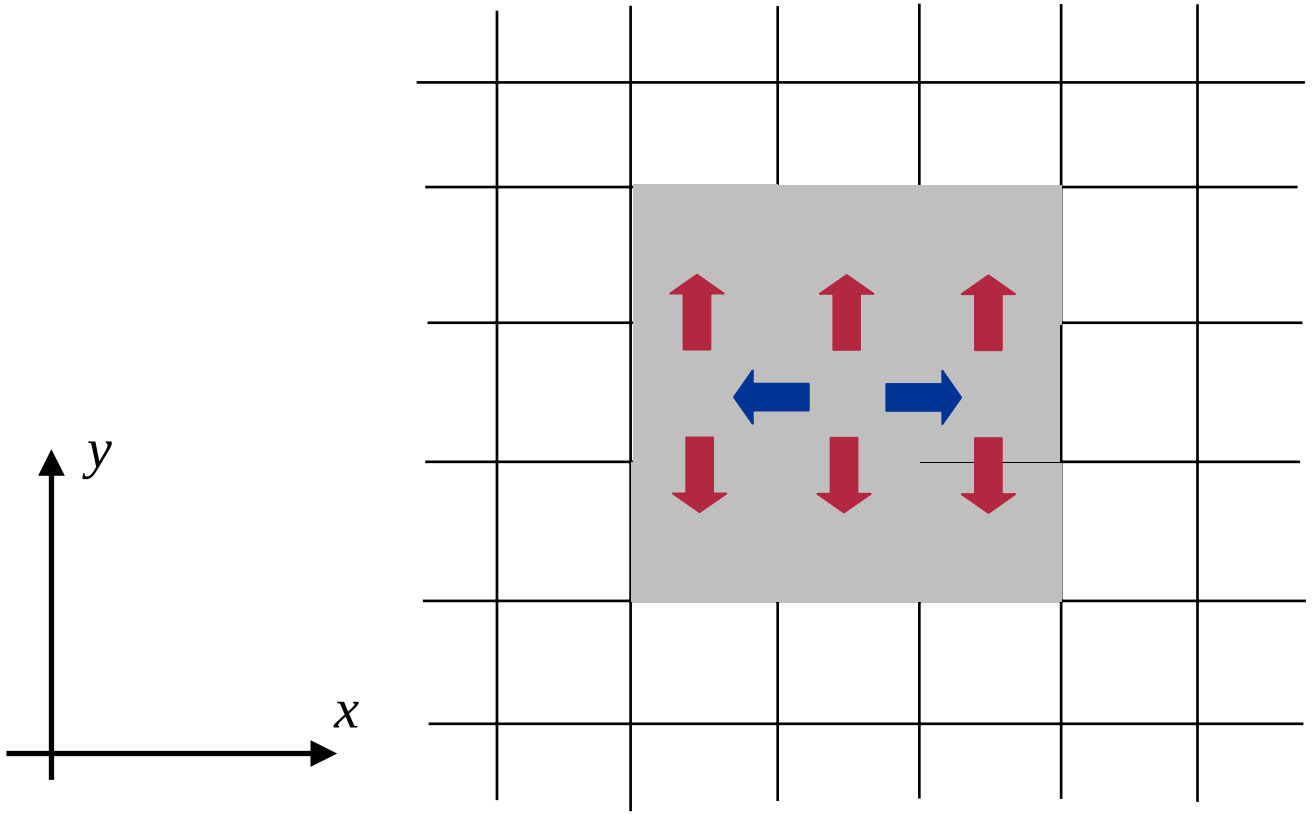
Sufficient and necessary conditions for charge conservation:

1. $\mathbf{S}\,\mathbf{C} = 0$
2. $\left[\mathbf{P}_x, \mathbf{P}_y\right] = \left[\mathbf{P}_x, \mathbf{P}_z\right] = \left[\mathbf{P}_y, \mathbf{P}_z\right] = 0$ *pairwise commuting derivatives*

Conservation of Charge

The tensor product case

Domain of influence of product derivative operators



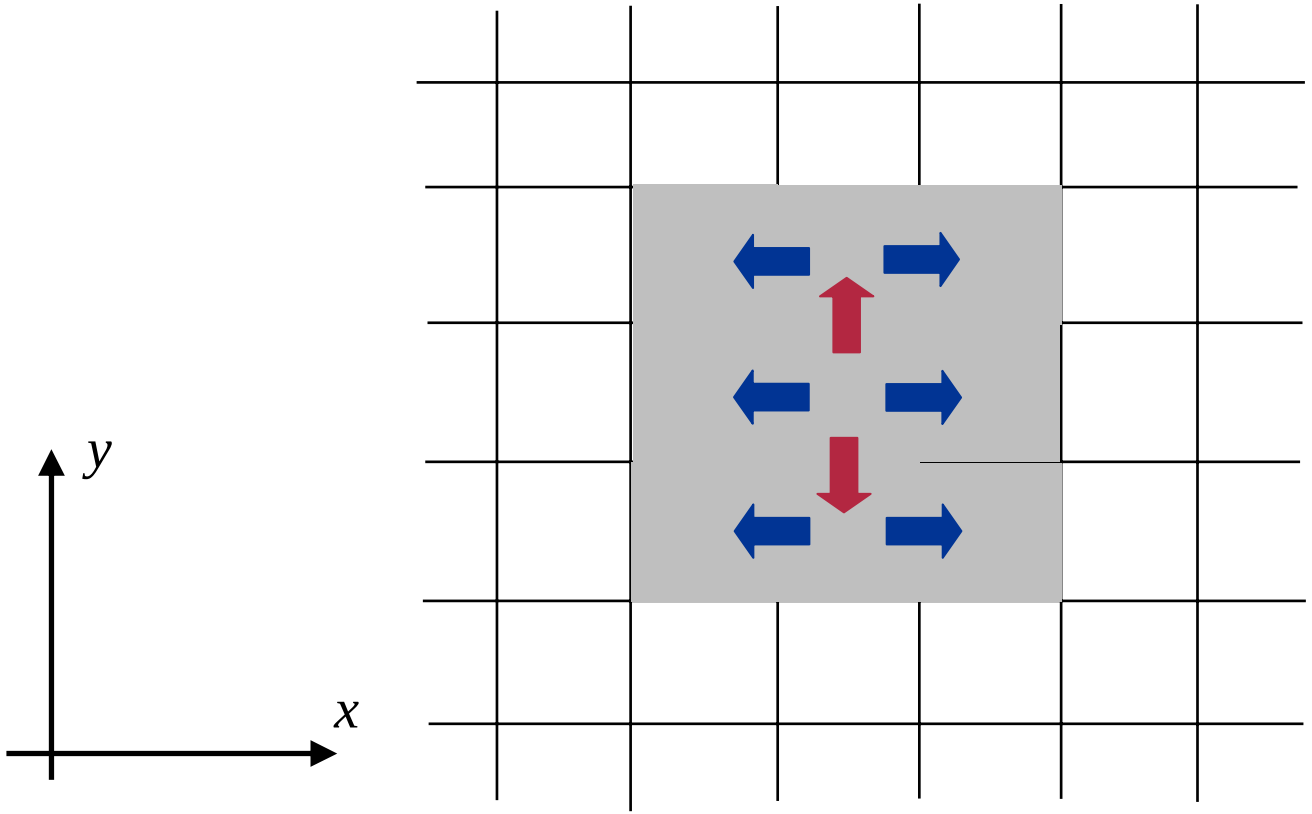
$\mathbf{P}_y \square \mathbf{P}_x$

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Conservation of Charge

The tensor product case

Domain of influence of product derivative operators



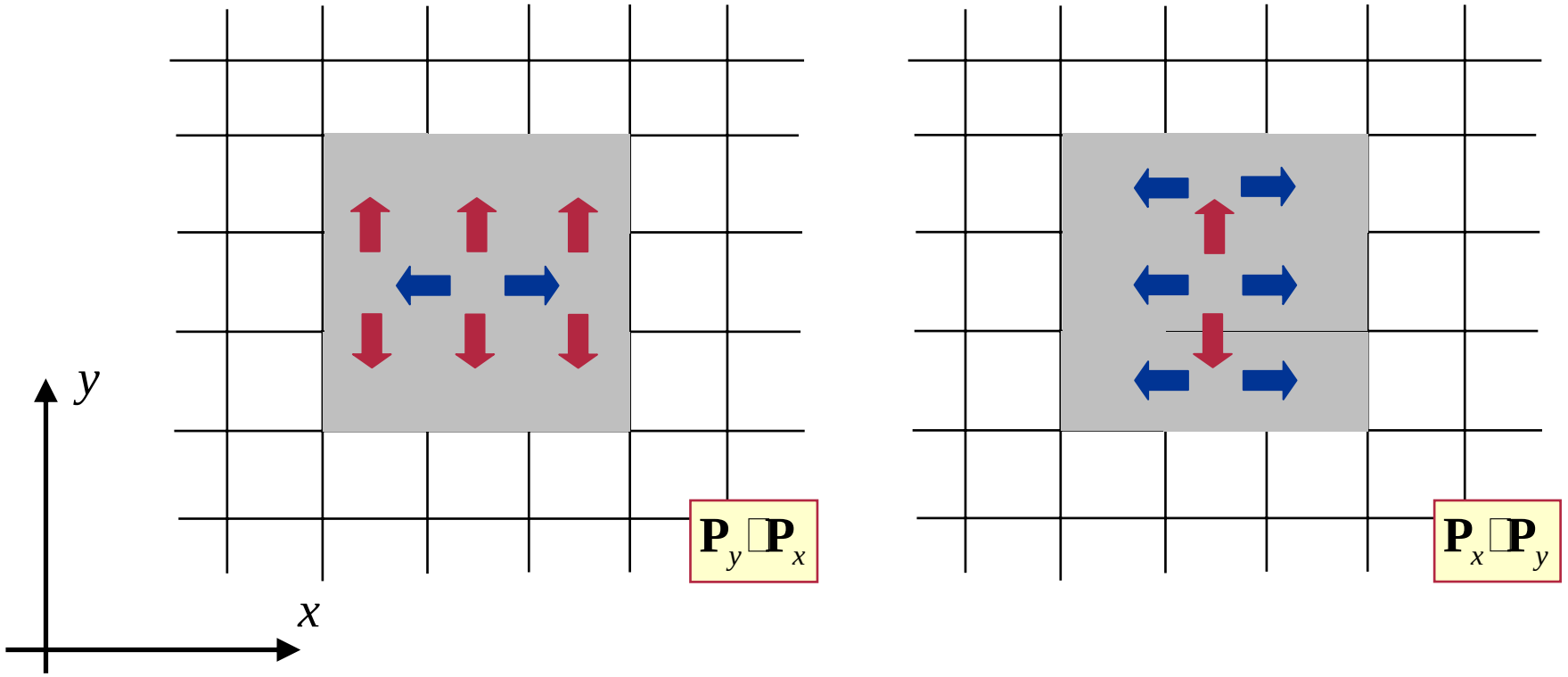
$\mathbf{P}_x \square \mathbf{P}_y$

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Conservation of Charge

The tensor product case

Domain of influence of product derivative operators



Conservation of discrete charges on regular grids (PIC).

Gjonaj, Lau, Weiland, ICEAA 2007

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Self-Consistent Simulations

Example of a long-distance PIC simulation with DG-FEM (later…)

Current work on PIC codes at TEMF

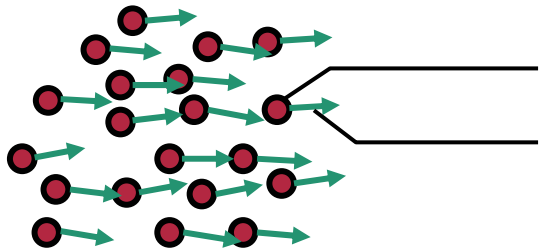
1. Application for the PITZ injector
2. Development of moving grid algorithms (S. Schnepp)
3. Combined (hp-) grid / order refinement
4. Dynamic parallel partitioning for higher order

V-Code: Motivation

- Basic principle

  Description of the particle distribution by moments

Distribution:

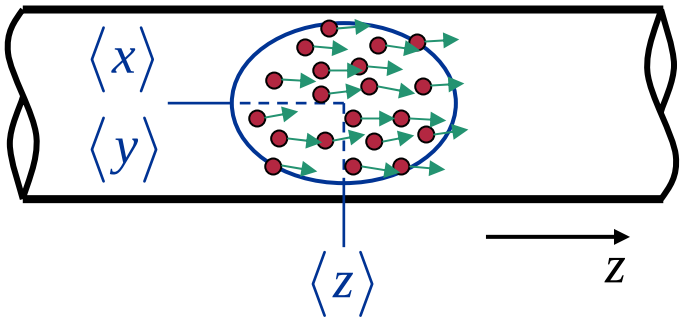


position

momentum

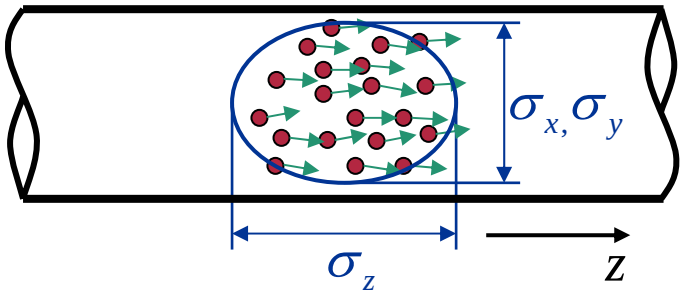
First order moments:

$$\langle x \rangle = \int x \, f \, \mathrm{d}\vec{r}\mathrm{d}\vec{p}$$



Second order moments:

$$\sigma_x^2 = \int \left(x - \langle x \rangle\right)^2 \, f \, \mathrm{d}\vec{r}\mathrm{d}\vec{p}$$

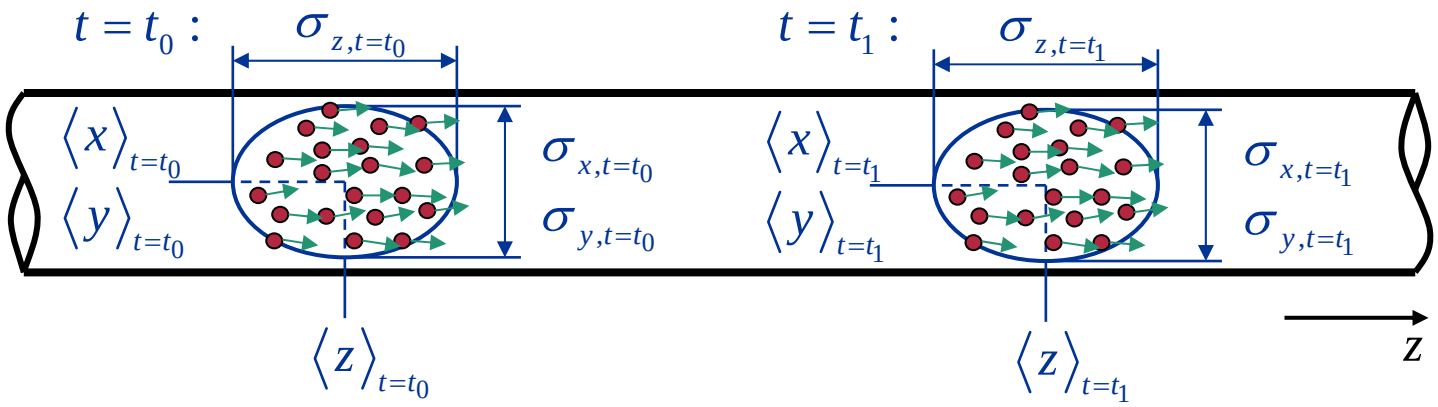


Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

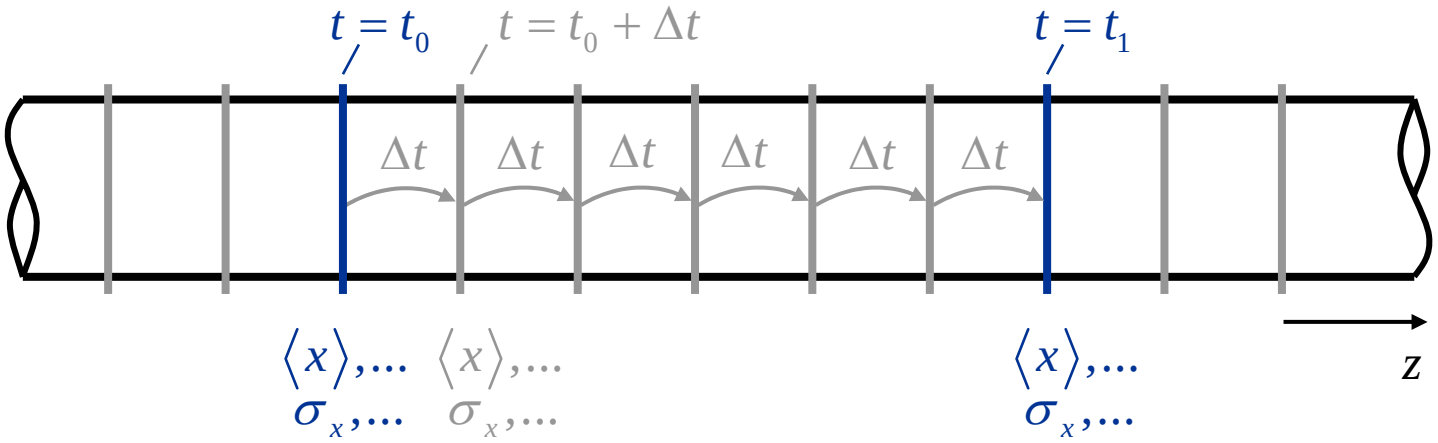
Motivation

- Evolution of the moments in time

  Bunch parameter at different time instants



  Simplified description



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Motivation

- Possible ensemble parameter (1)

Raw moments

$$\mu_{ijk}(x,y,z) = \left\langle x^i \cdot y^j \cdot z^k \right\rangle$$

$$\left\langle \mu \right\rangle = \int \mu \cdot f \; \mathrm{d}\vec{r}\,\mathrm{d}\vec{p}$$

Order 0: $\mu_{000} = 1$

Order 1: $\mu_{100} = \langle x \rangle, \quad \mu_{010} = \langle y \rangle, \quad \mu_{001} = \langle z \rangle$

Order 2: $\mu_{200} = \langle x^2 \rangle, \; \mu_{020} = \langle y^2 \rangle, \; \mu_{002} = \langle z^2 \rangle$

$\mu_{110} = \langle xy \rangle, \; \mu_{101} = \langle xz \rangle, \; \mu_{011} = \langle yz \rangle$

Order 3: …

Property

$$\mu_{ijk}(x-a, y-b, z-c) \neq \mu_{ijk}(x,y,z)$$

(not translatory invariant)

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Motivation

- Possible ensemble parameter (2)

Centralized moments

$$\sigma_{ijk}(x,y,z) = \left\langle \left(x - \langle x \rangle\right)^i \cdot \left(y - \langle y \rangle\right)^j \cdot \left(z - \langle z \rangle\right)^k \right\rangle$$

$$\langle \mu \rangle = \int \mu \cdot f \; \mathrm{d}\vec{r}\,\mathrm{d}\vec{p}$$

Order 0: $\sigma_{000} = 1$

Order 1: $\sigma_{100} = 0, \quad \sigma_{010} = 0, \quad \sigma_{001} = 0$

Order 2: $\sigma_{200} = \sigma_x^2, \; \sigma_{020} = \sigma_y^2, \; \sigma_{002} = \sigma_z^2$ (variance)

$\sigma_{110} = \sigma_{xy}, \; \sigma_{101} = \sigma_{xz}, \; \sigma_{011} = \sigma_{yz}$ (covariance)

Order 3: …

Property

$$\sigma_{ijk}(x-a, y-b, z-c) = \sigma_{ijk}(x,y,z)$$ (translatory invariant)

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Motivation

- Appropriate moments in 6-D phase space

Order 1: $M_\mu = \langle \mu \rangle \quad \mu \in \{x, y, z, p_x, p_y, p_z\}$

$$\left(M_x, M_y, M_z, M_{p_x}, M_{p_y}, M_{p_z}\right) \qquad {}^wC_6^1 = \binom{6}{1} = 6 \qquad \Sigma 6$$

Order 2: $M_{\mu\nu} = \left\langle \left(\mu - \langle \mu \rangle\right) \cdot \left(\nu - \langle \nu \rangle\right) \right\rangle \quad \mu, \nu \in \{x, y, z, p_x, p_y, p_z\}$

$$\begin{pmatrix} M_{xx} & M_{xy} & M_{xz} & M_{xp_x} & M_{xp_y} & M_{xp_z} \\ M_{yx} & M_{yy} & M_{yz} & M_{yp_x} & M_{yp_y} & M_{yp_z} \\ M_{zx} & M_{zy} & M_{zz} & M_{zp_x} & M_{zp_y} & M_{zp_z} \\ M_{p_x x} & M_{p_x y} & M_{p_x z} & M_{p_x p_x} & M_{p_x p_y} & M_{p_x p_z} \\ M_{p_y x} & M_{p_y y} & M_{p_y z} & M_{p_y p_x} & M_{p_y p_y} & M_{p_y p_z} \\ M_{p_z x} & M_{p_z y} & M_{p_z z} & M_{p_z p_x} & M_{p_z p_y} & M_{p_z p_z} \end{pmatrix} \qquad {}^wC_6^2 = \binom{7}{2} = 21 \qquad \Sigma 27$$

$$\text{Order 3: } \ldots \qquad {}^wC_6^3 = \binom{8}{3} = 56 \qquad \Sigma 83$$

$$\text{Order 4: } \ldots \qquad {}^wC_6^4 = \binom{9}{4} = 126 \qquad \Sigma 209$$

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Motivation

- Number of moments in 6-D phase space

Order	Moments per order	Total number of moments
1	6	6
2	21	27
3	56	83
4	126	209
5	252	461
6	462	923
7	792	1715
8	1287	3002
9	2002	5004
10	3003	8007

Ensemble Model

- Method to solve the VLASOV equation
  - Basic formulation

$$\frac{\partial f}{\partial \tau} + \frac{\partial f}{\partial \vec{r}} \cdot \frac{\vec{p}}{\gamma} + \frac{\partial f}{\partial \vec{p}} \cdot \frac{\vec{F}}{m_0 c^2} = 0 \qquad \vec{F} = \text{LORENTZ force}$$

  - Moment approach
    - Integration over phase space reduces PDE to ODE
    - Approximation: limited amount of moments used to describe the particle distribution function

$$\frac{\partial <\mu>}{\partial \tau} = \frac{\partial}{\partial \tau} \int_{\infty} \mu \, f(\tau, \vec{r}, \vec{p}) \, \mathrm{d}\vec{r} \, \mathrm{d}\vec{p}$$

time evolution

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Ensemble Model

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

- Evolution of raw and centralized moments in time

$$\frac{\partial\langle\mu\rangle}{\partial\tau}=\frac{\partial}{\partial\tau}\int\mu\ f\ \mathrm{d}\vec{r}\mathrm{d}\vec{p} \qquad \mu\in\left\{x,y,z,p_x,p_y,p_z,x^2,\ldots,\left(x-\langle x\rangle\right)^2,\ldots\right\}$$

$$=\int\frac{\partial\mu f}{\partial\tau}\mathrm{d}\vec{r}\mathrm{d}\vec{p} \quad = \quad \int\left(f\ \frac{\partial\mu}{\partial\tau}+\mu\ \frac{\partial f}{\partial\tau}\right)\mathrm{d}\vec{r}\mathrm{d}\vec{p}$$

$$=\int f\left(\mathrm{grad}_{\langle\vec{r}\rangle}(\mu)\cdot\frac{\partial\langle\vec{r}\rangle}{\partial\tau}+\mathrm{grad}_{\langle\vec{p}\rangle}(\mu)\cdot\frac{\partial\langle\vec{p}\rangle}{\partial\tau}\right)\mathrm{d}\vec{r}\mathrm{d}\vec{p}$$

$$-\int\mu\left(\mathrm{grad}_{\vec{r}}(f)\cdot\frac{\vec{p}}{\gamma}+\mathrm{grad}_{\vec{p}}(f)\cdot\frac{\vec{F}}{m_0c^2}+f\ \mathrm{div}_{\vec{p}}\left(\frac{\vec{F}}{m_0c^2}\right)\right)\mathrm{d}\vec{r}\mathrm{d}\vec{p}$$

$$\frac{\partial\langle\mu\rangle}{\partial\tau}=\left\langle\mathrm{grad}_{\langle\vec{r}\rangle}(\mu)\right\rangle\cdot\left\langle\frac{\vec{p}}{\gamma}\right\rangle+\left\langle\mathrm{grad}_{\langle\vec{p}\rangle}(\mu)\right\rangle\cdot\left\langle\frac{\vec{F}}{m_0c^2}\right\rangle$$
$$+\left\langle\mathrm{grad}_{\vec{r}}(\mu)\cdot\frac{\vec{p}}{\gamma}\right\rangle+\left\langle\mathrm{grad}_{\vec{p}}(\mu)\cdot\frac{\vec{F}}{m_0c^2}\right\rangle$$

$$\tau=c\cdot t$$

$$\lim_{\vec{r},\vec{p}\to\infty}(f)=0$$

Ensemble Model

Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

- Evolution of raw and centralized moments in time

General form:

$$\frac{\partial\langle\mu\rangle}{\partial\tau}=\left\langle \mathrm{grad}_{\langle\vec{r}\rangle}(\mu)\right\rangle\cdot\left\langle\frac{\vec{p}}{\gamma}\right\rangle+\left\langle \mathrm{grad}_{\langle\vec{p}\rangle}(\mu)\right\rangle\cdot\left\langle\frac{\vec{F}}{m_0c^2}\right\rangle+\left\langle \mathrm{grad}_{\vec{r}}(\mu)\cdot\frac{\vec{p}}{\gamma}\right\rangle+\left\langle \mathrm{grad}_{\vec{p}}(\mu)\cdot\frac{\vec{F}}{m_0c^2}\right\rangle$$

$$\tau=c\cdot t$$

First component, order 1:

$$\frac{\partial\langle x\rangle}{\partial\tau}=\left\langle\frac{p_x}{\gamma}\right\rangle$$

$$\frac{\partial\langle p_x\rangle}{\partial\tau}=\left\langle\frac{F_x}{m_0c^2}\right\rangle$$

Aim:

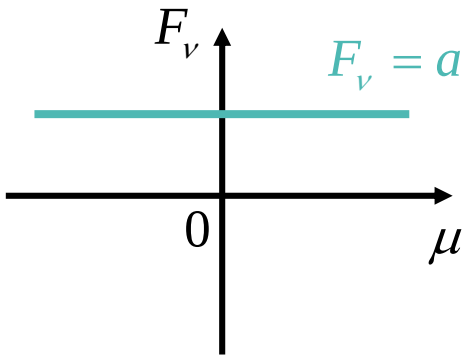
Expand all arguments of the right hand side such that the resulting expression can be interpreted as a moment description form

Ensemble Model

- Incorporation of the influencing forces

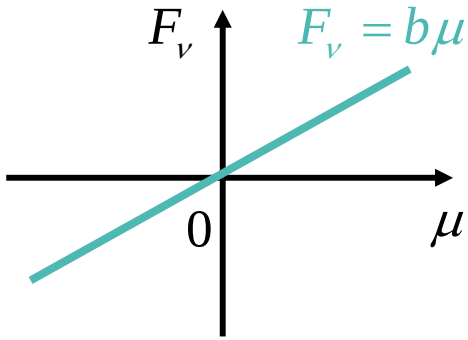
  TAYLOR series expansion

constant



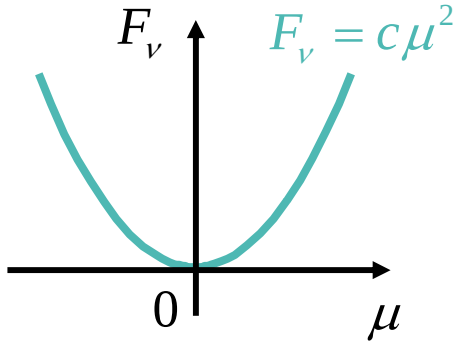
$$\langle F_\nu \rangle = a$$
$$\langle \mu F_\nu \rangle = 0$$

linear



$$\langle F_\nu \rangle = 0$$
$$\langle \mu F_\nu \rangle = b\, M_{\mu\mu}$$

quadratic



$$\langle F_\nu \rangle = c\, M_{\mu\mu}$$
$$\langle \mu F_\nu \rangle = c\, M_{\mu\mu\mu}$$

Series expansion of the forces for all beam line elements

➡ Dipole magnets, quadrupoles, solenoids, resonators, ...

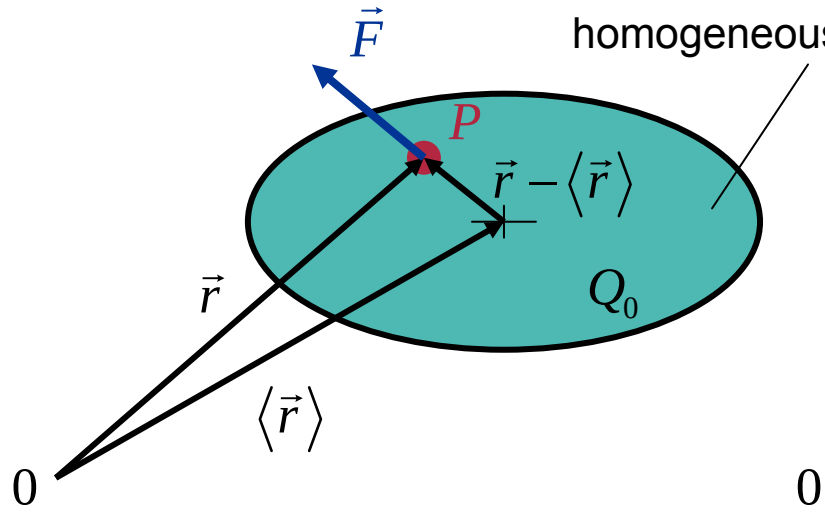
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Ensemble Model

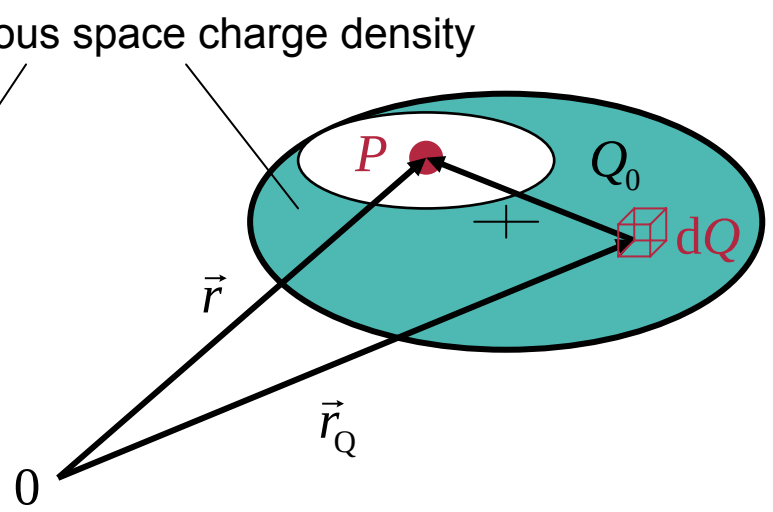
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

- Linear space charge model

Configuration



Calculation

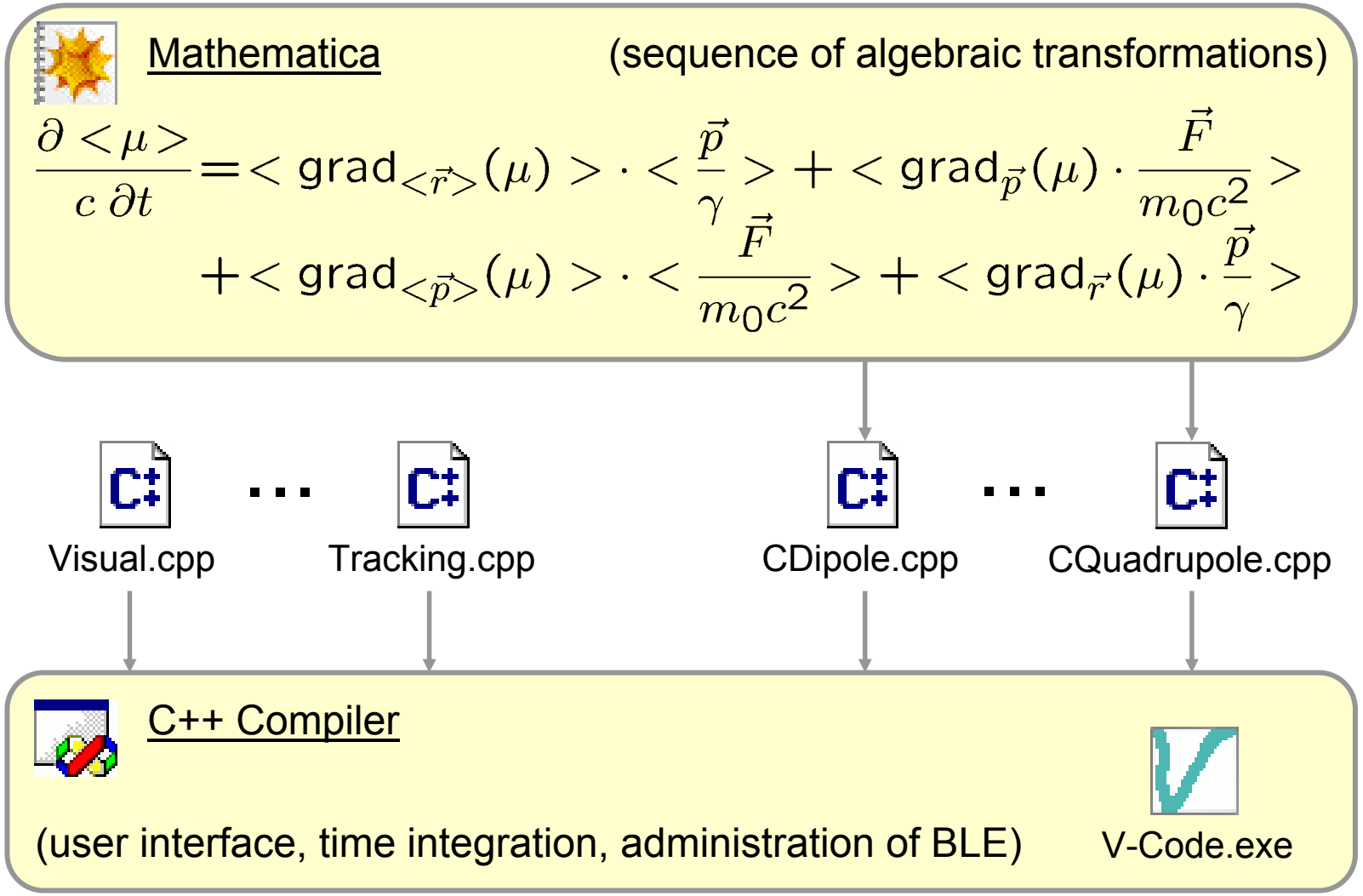


$$\vec{F}(\vec{r}) \approx G\left(\frac{2\gamma\sigma_z}{\sigma_x+\sigma_y}\right)\cdot\frac{eQ_0}{\gamma^2}\cdot\frac{\vec{r}-\langle\vec{r}\rangle}{V_G}$$

$$G(u)=\left(1-\exp(-u)\right)\cdot\begin{pmatrix}1&0&0\\0&1&0\\0&0&\gamma/u\end{pmatrix}$$

Implementation

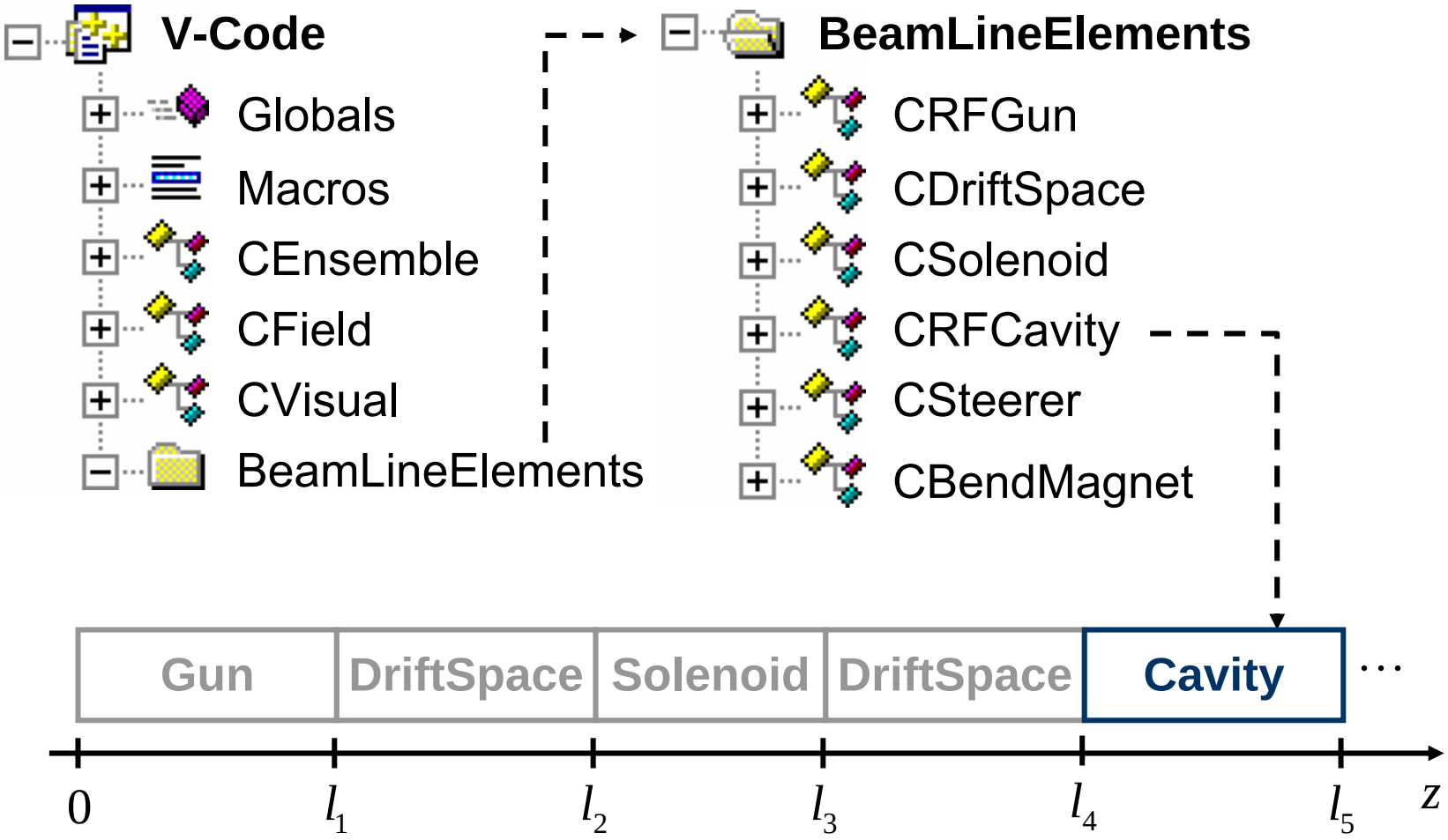
- Implementation using a symbolic algebra program



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Implementation

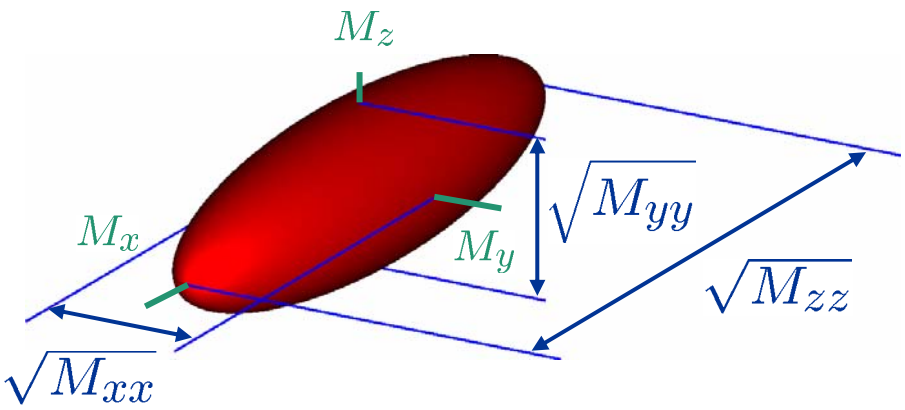
- Decomposition in individual beam line elements



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

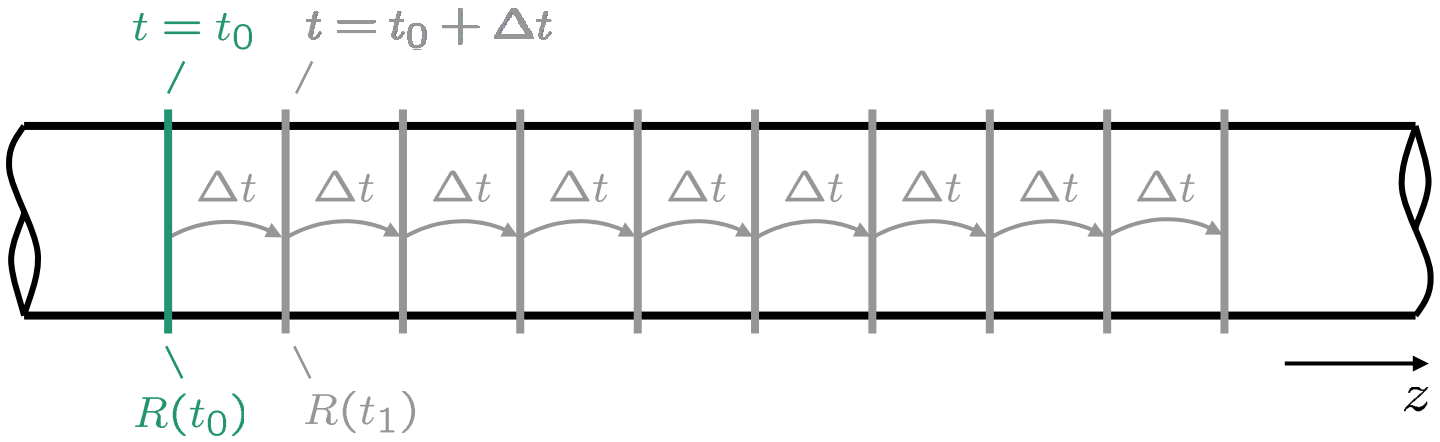
Implementation

- Solving the assembled moment equations
  - Time dependent ensemble parameter



$$R(t) = \begin{pmatrix} M_x \\ M_y \\ M_z \\ M_{p_x} \\ M_{p_y} \\ M_{p_z} \\ M_{xx} \\ M_{xy} \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ \vdots \end{pmatrix}$$

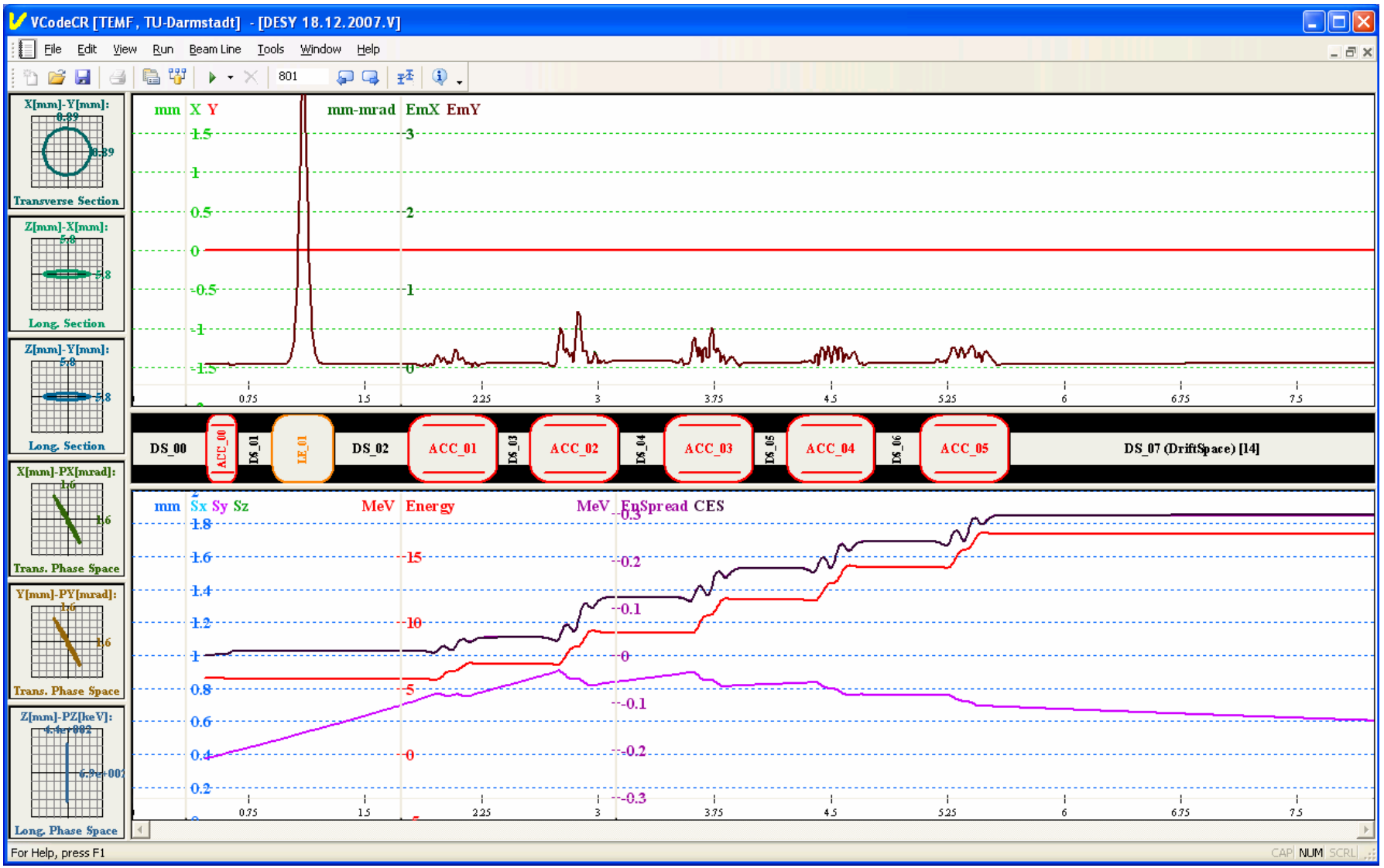
  - Initial condition and time stepping technique



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Implementation

- V-Code user interface



Application

Courtesy: Georg Hofstaetter, Cornell University

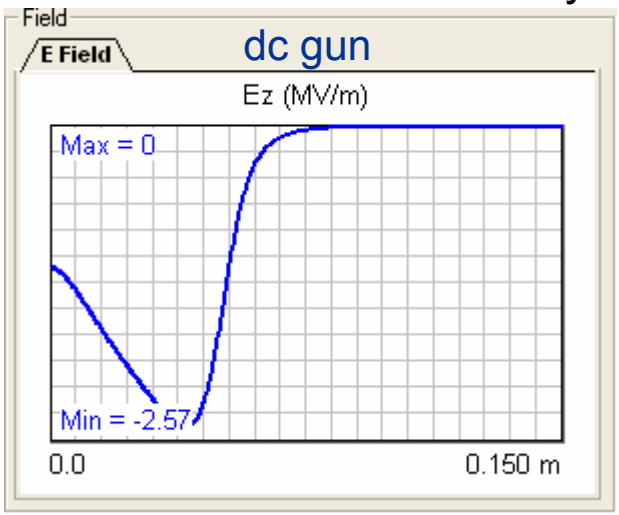
- Layout

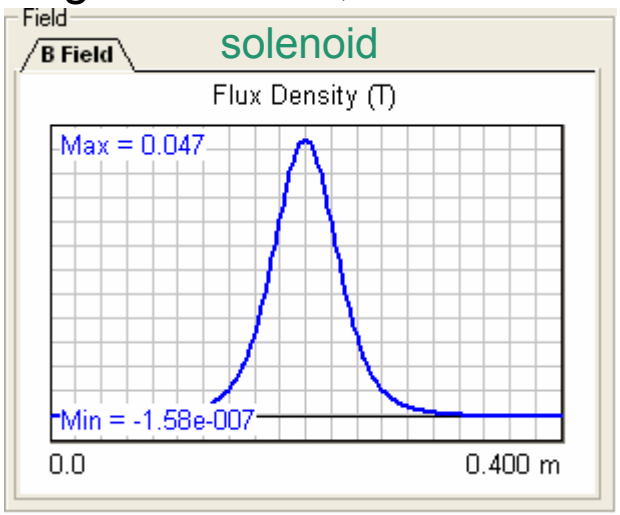
Bunch:

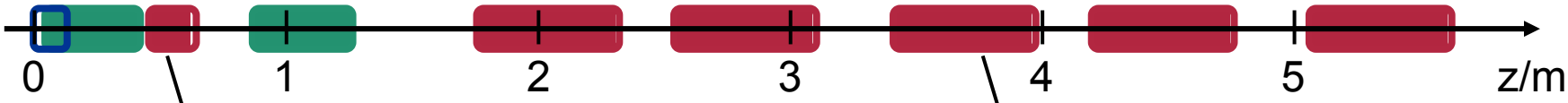
T_{rms}= 11.146 ps

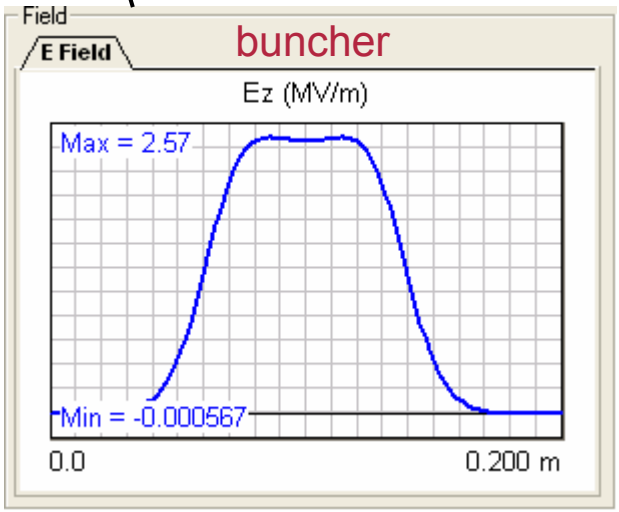
XY_{rms}= 0.294907 mm

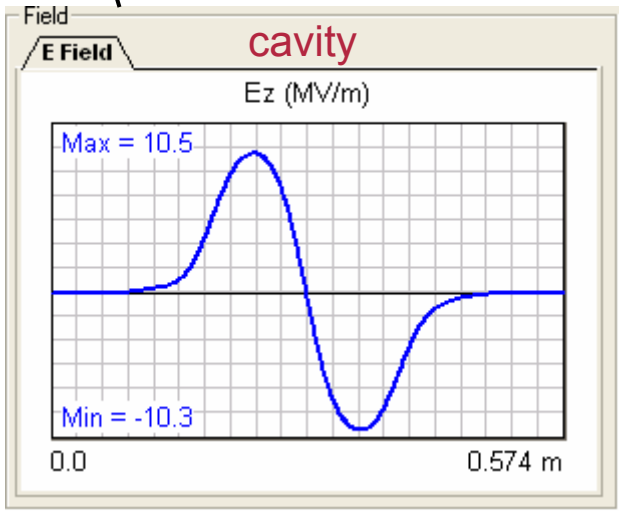
Q_{bunch}= 0.107743 nC







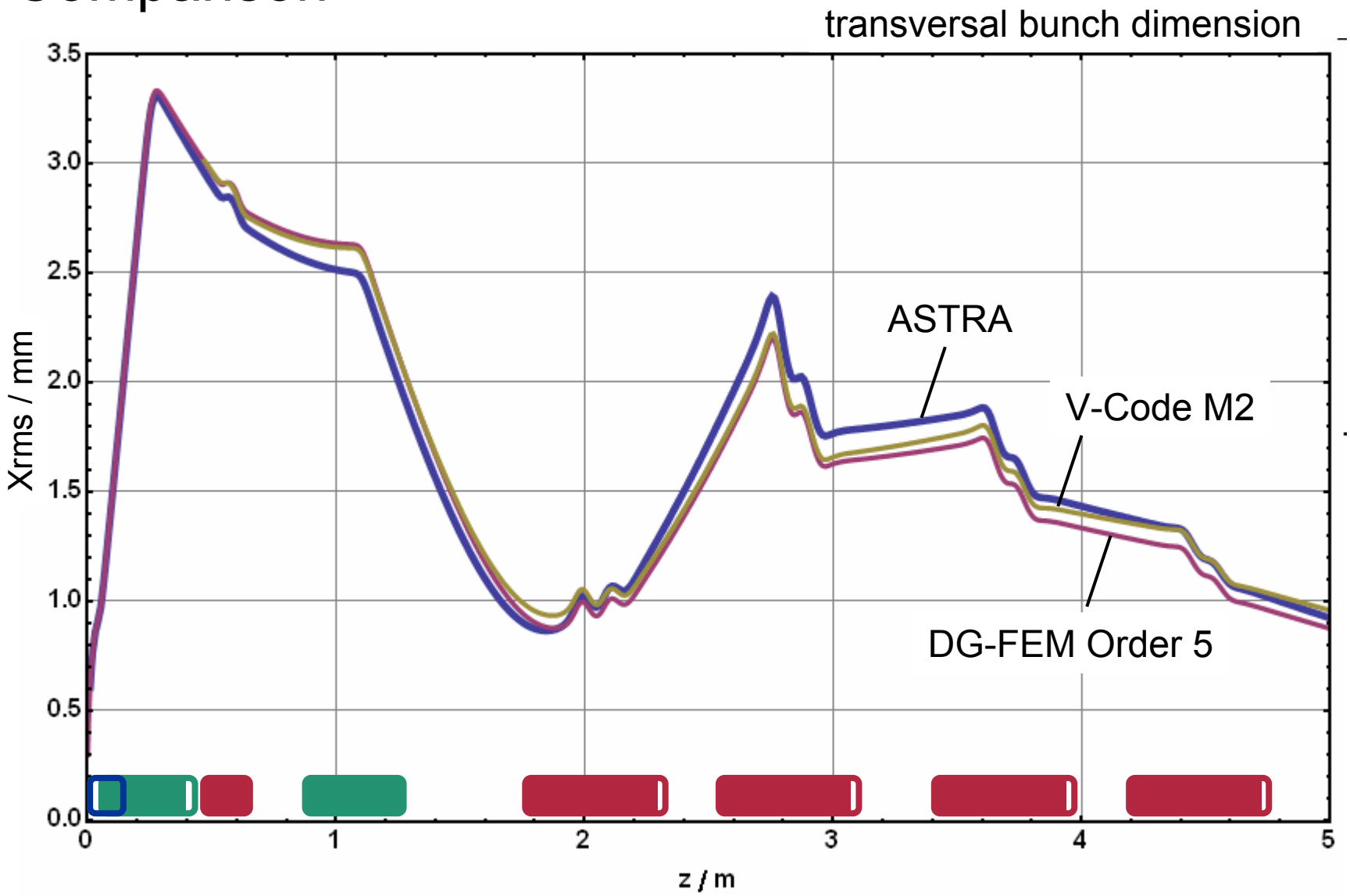




Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

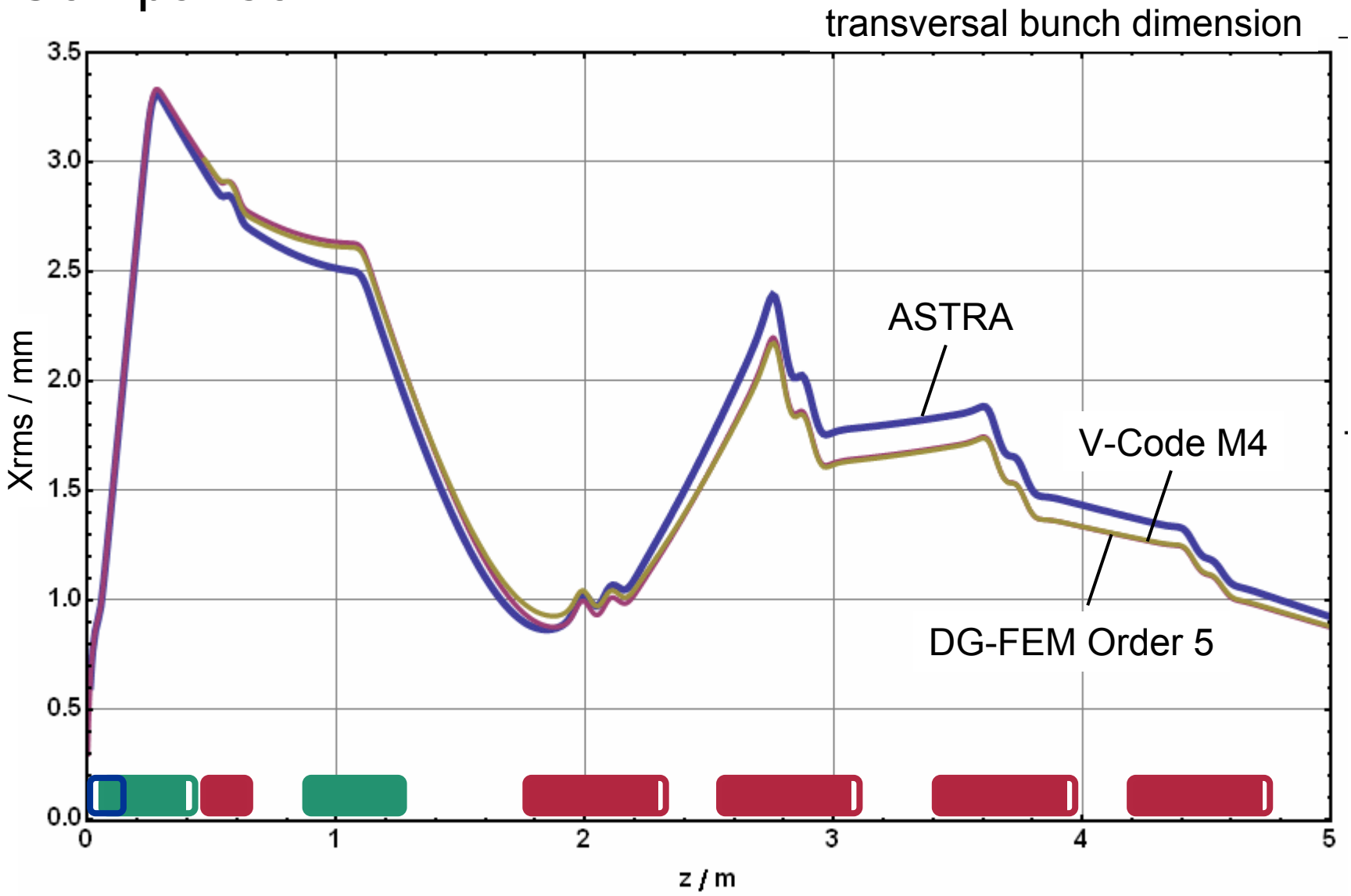
Application

- Comparison



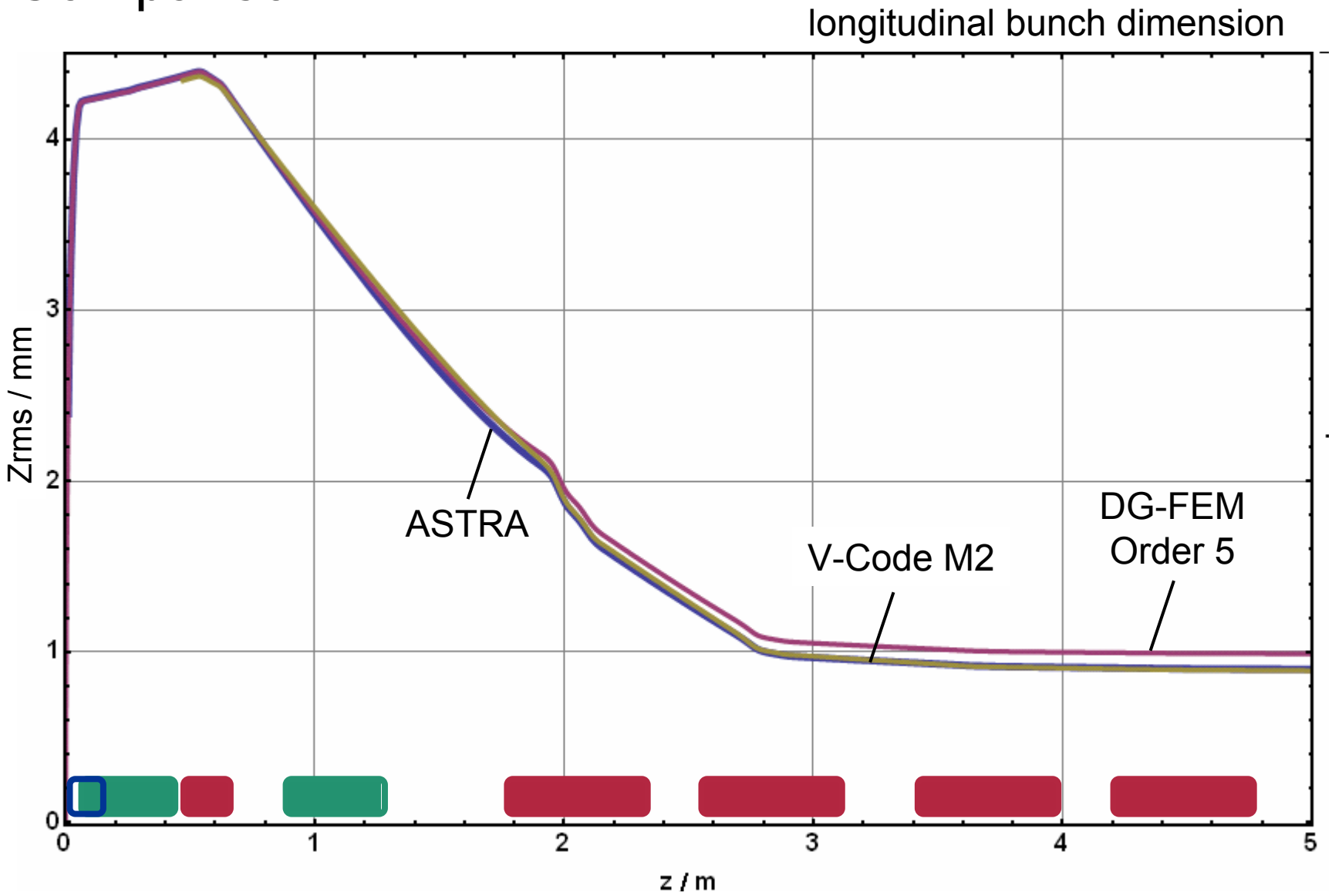
Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

- Comparison



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

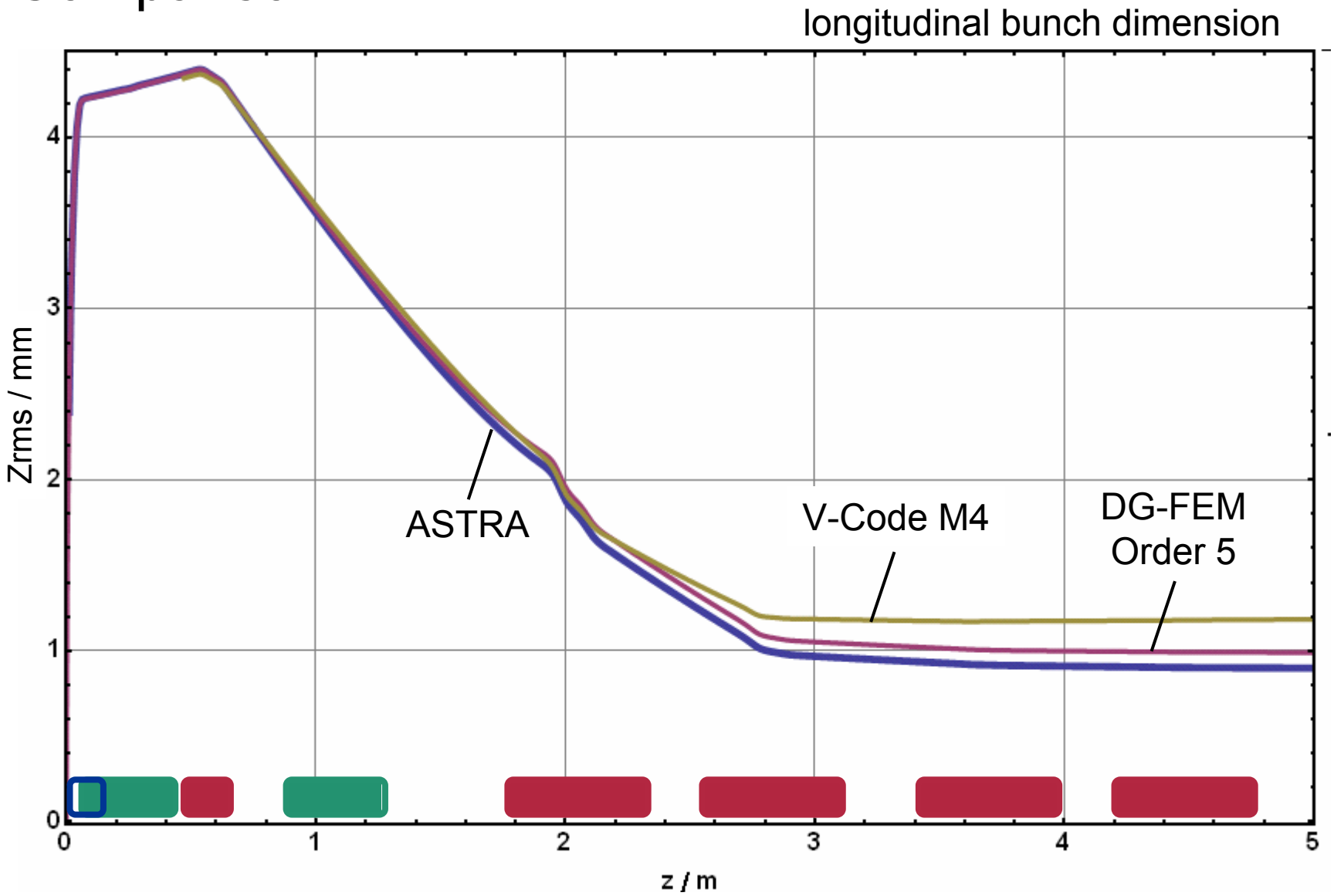
- Comparison



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Application

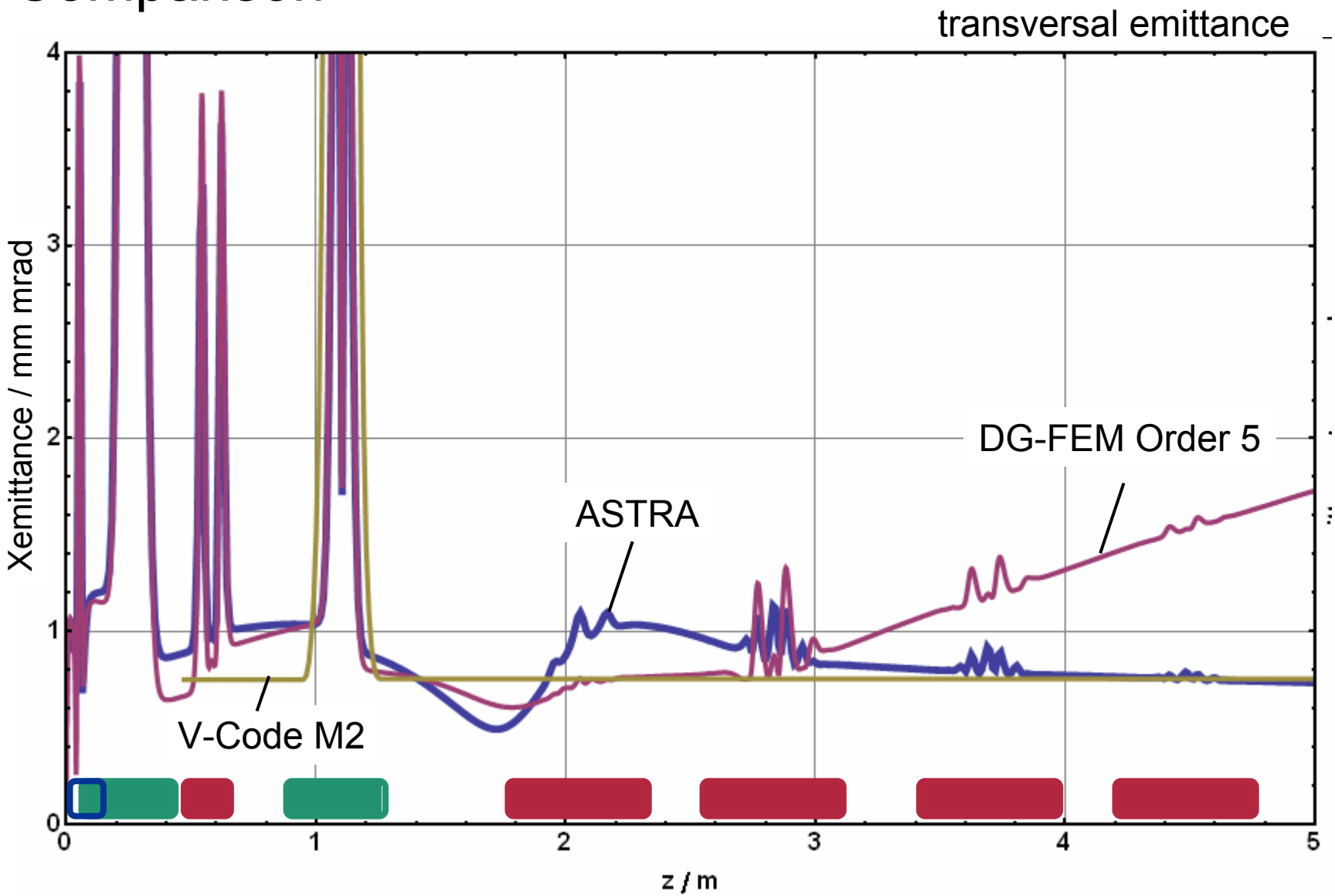
- Comparison



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Application

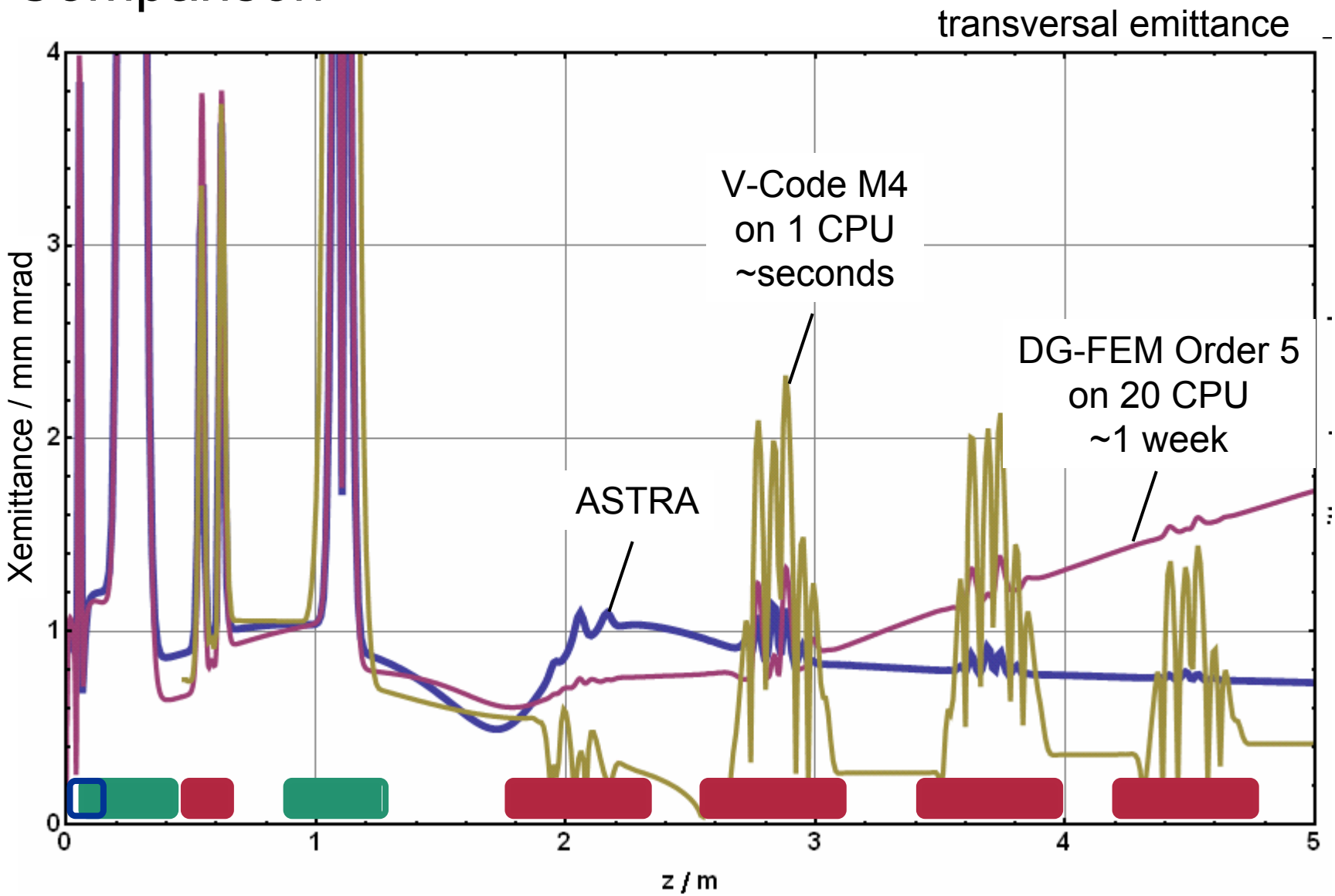
- Comparison



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Application

- Comparison



Wolfgang Ackermann and Erion Gjonaj
Institut Theorie Elektromagnetischer Felder, TU Darmstadt

Current Work and Outlook

- Current Work related to V-Code
  - Implementation of multi-ensemble formulation
  - Incorporation of VCode into the control system at the S-DALINAC to assist operation
  - Extension of the BLE library to enable alpha-magnet simulation for the new S-DALINAC injector
- Outlook
  - Improved and consistent space charge model for single and multi-ensemble formulation
  - Automatic ensemble decomposition