Computation of Electromagnetic Fields Generated by Relativistic Beams in Complicated Structures

Algorithms and Applications



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Overview

Motivation

- Numerical Methods
 - > low-dispersive schemes
 - boundary approximation
 - indirect integration algorithm
 - > modelling of conductive walls
- Code Status and Applications
 - geometries of revolution (ECHOz1, ECHOz2)
 - rectangular structures (ECHO2D)
 - > fully 3D geometries (ECHO3D)
 - Particle-In-Cell code



Motivation

Wake field calculation – estimation of the effect of the geometry variations on the bunch



First codes in **time domain** ~ 1980 A. Novokhatski (BINP), T. Weiland (CERN)

$$W_{\parallel}(\mathbf{r}_{0},\mathbf{r},s) = \frac{1}{Q} \int_{-\infty}^{\infty} E_{z}\left(\mathbf{r}_{0},\mathbf{r},z,\frac{z-s}{c}\right) dz$$

$$\frac{\partial}{\partial s} \mathbf{W}_{\perp}(\mathbf{r}_0, \mathbf{r}, s) = \nabla_{\perp} W_{\parallel}(\mathbf{r}_0, \mathbf{r}, s)$$



Motivation

MAFIA* (the Year 2000)

- rotationally symmetric and 3D
- Iongitudinal and transverse wakes
- triangular geometry approximation;
- arbitrary materials
- moving window
- dispersion error
- * MAFIA Collaboration, *MAFIA Manual*, CST GmbH, Darmstadt, 1997.

NOVO** (the Year 2000)

- rotationally symmetric
- only longitudinal wake (scalar wave equation)
- "staircase" geometry approximation;
- only PEC
- moving mesh
- Iow dispersion error

** A. Novokhatski, M. Timm, T.Weiland, *Transition Dynamics of the Wake Fields of Ultra Short Bunches*, Proc.ICAP1998, Monterey, USA.



Motivation

New projects with

- short bunches;
- Iong structures;
- tapered collimators

Solutions

- zero dispersion in longitudinal direction;
- "conformal" meshing;
 - moving mesh and "explicit" or "split" methods

Cryomodule housing: 8 cavities, quadrupole and BPM





Maxwell Grid Equations*

$$\mathbf{C}\widehat{\mathbf{e}} = -\frac{d}{dt}\widehat{\widehat{\mathbf{b}}} , \quad \widetilde{\mathbf{C}}\widehat{\mathbf{h}} = \frac{d}{dt}\widehat{\widehat{\mathbf{d}}} + \widehat{\widehat{\mathbf{j}}},$$
$$\mathbf{S}\widehat{\widehat{\mathbf{b}}} = \mathbf{0}, \quad \widetilde{\mathbf{S}}\widehat{\widehat{\mathbf{d}}} = \mathbf{q},$$
$$\widehat{\mathbf{e}} = \mathbf{M}_{\varepsilon^{-1}}\widehat{\widehat{\mathbf{d}}} , \qquad \widehat{\mathbf{h}} = \mathbf{M}_{\mu^{-1}}\widehat{\widehat{\mathbf{b}}}$$

$$curl \Box \mathbf{C} = \begin{pmatrix} \mathbf{0} & -\mathbf{P}_z & \mathbf{P}_y \\ \mathbf{P}_z & \mathbf{0} & -\mathbf{P}_x \\ -\mathbf{P}_y & \mathbf{P}_x & \mathbf{0} \end{pmatrix}$$

* T. Weiland, *A discretization method for the solution of Maxwell's equations for six-component fields*, Electronics and Communication (AEÜ) **31**, p. 116 (1977)

$$div \Box \mathbf{S} = \begin{pmatrix} \mathbf{P}_x^* & \mathbf{P}_y^* & \mathbf{P}_z^* \end{pmatrix}$$







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FDTD (1966)

$$\frac{\mathbf{e}^{n+1/2} - \mathbf{e}^{n-1/2}}{\Delta t} = \mathbf{M}_{\varepsilon^{-1}} (\mathbf{C}^* \mathbf{h}^n - \mathbf{j}^n) \qquad \mathbf{h}^n = \begin{pmatrix} \mathbf{h}_x^n \\ \mathbf{h}_y^n \\ \mathbf{h}_z^n \end{pmatrix} \qquad \mathbf{e}^{n+0.5} = \begin{pmatrix} \mathbf{e}_x^{n+0.5} \\ \mathbf{e}_y^{n+0.5} \\ \mathbf{e}_z^{n+0.5} \\ \mathbf{e}_z^{n+0.5} \end{pmatrix}$$

Implicit Scheme* (2002) C = T + L

$$\frac{\mathbf{e}^{n+1/2} - \mathbf{e}^{n-1/2}}{\Delta t} = \mathbf{M}_{\varepsilon^{-1}} (\mathbf{T}^* \overline{\mathbf{h}}^n + \mathbf{L}^* \mathbf{h}^n - \mathbf{j}^n)$$

$$\frac{\mathbf{h}^{n+1} - \mathbf{h}^n}{\Delta t} \mathbf{h}^n = \mathbf{M}_{\mu^{-1}} \mathbf{C} \mathbf{e}^{n+1/2} \qquad \overline{\mathbf{h}}^n \equiv \theta \mathbf{h}^{n+1} + (1 - 2\theta) \mathbf{h}^n + \theta \mathbf{h}^{n-1}$$

I. Zagorodnov, R. Schuhmann, T. Weiland, Long-Time Numerical Computation of Electromagnetic Fields in the Vicinity of a Relativistic Source, Journal of Computational Physics **191**, No.2, pp. 525-541 (2003)



Implicit Scheme (2002)

$$\mathbf{a}^n = \int_{-\infty}^{t_n} \widehat{\mathbf{h}}_s d\tau$$

$$(\mathbf{I} + \boldsymbol{\theta} \mathbf{T}_{1}) \mathbf{a}^{n+1} = 2\mathbf{a}^{n} - \mathbf{a}^{n-1} - \mathbf{T}_{1} ((1 - 2\boldsymbol{\theta})\mathbf{a}^{n} + \boldsymbol{\theta}\mathbf{a}^{n-1}) - \mathbf{L}_{1}\mathbf{a}^{n} + \mathbf{F}^{n}$$
$$\mathbf{T}_{1} = \Delta t^{2} \mathbf{M}_{\mu^{-1}} \mathbf{C} \mathbf{M}_{\varepsilon^{-1}} \mathbf{T}^{*}, \quad \mathbf{L}_{1} = \Delta t^{2} \mathbf{M}_{\mu^{-1}} \mathbf{C} \mathbf{M}_{\varepsilon^{-1}} \mathbf{L}^{*}$$

For fully rotationally symmetric problems (**monopole** mode m=0) our scheme in staircase approximation with θ =0.5 coincides with the equation realized in code NOVO^{**}.

$$\mathbf{M}_{\mu_{\varphi}^{-1}}^{-1} \Delta t^{-2} \left(\mathbf{a}_{\varphi}^{n+1} - 2\mathbf{a}_{\varphi}^{n} + \mathbf{a}_{\varphi}^{n-1} \right) = \mathbf{P}_{z} \mathbf{M}_{\varepsilon_{r}^{-1}} \mathbf{P}_{z}^{T} \mathbf{a}_{\varphi}^{n} + \mathbf{P}_{r} \mathbf{M}_{\varepsilon_{z}^{-1}} \mathbf{P}_{r}^{T} \frac{\mathbf{a}_{\varphi}^{n+1} + \mathbf{a}_{\varphi}^{n-1}}{2} + \mathbf{F}_{\varphi}^{n},$$

** A. Novokhatski, M. Timm, T. Weiland, *Transition Dynamics of the Wake Fields of Ultra Short Bunches,* Proc. ICAP 1998, Monterey, California, USA.



E/M and TE/TM* splitting (2004)



Subdue the updating procedure to the bunch motion

* Zagorodnov I.A, Weiland T., *TE/TM Field Solver for Particle Beam Simulations without Numerical Cherenkov Radiation*, Phys. Rev. ST Accel. Beams **8**, 042001 (2005)

E/M splitting (Yee's Scheme)

$$\mathbf{h}^{n} = \begin{pmatrix} \mathbf{h}_{x}^{n} \\ \mathbf{h}_{y}^{n} \\ \mathbf{h}_{z}^{n} \end{pmatrix} \quad \mathbf{e}^{n+0.5} = \begin{pmatrix} \mathbf{e}_{x}^{n+0.5} \\ \mathbf{e}_{y}^{n+0.5} \\ \mathbf{e}_{z}^{n+0.5} \end{pmatrix}$$

TE/TM splitting





Curl operator splitting

$$\mathbf{C}_{0} = c^{-1} \mathbf{M}_{\mu^{-1}}^{1/2} \mathbf{C} \mathbf{M}_{\varepsilon^{-1}}^{1/2} = \begin{pmatrix} \mathbf{0} & -\mathbf{P}_{z}^{0} & \mathbf{P}_{y}^{0} \\ \mathbf{P}_{z}^{1} & \mathbf{0} & -\mathbf{P}_{x}^{0} \\ -\mathbf{P}_{y}^{1} & \mathbf{P}_{x}^{1} & \mathbf{0} \end{pmatrix}$$

transversal plane longitudinal direction
$$\mathbf{T}_{i} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & -\mathbf{P}_{y}^{i} \\ \mathbf{0} & \mathbf{0} & \mathbf{P}_{x}^{i} \\ (\mathbf{P}_{y}^{i})^{*} & -(\mathbf{P}_{x}^{i})^{*} & \mathbf{0} \end{pmatrix}, i = 0, 1 \qquad \mathbf{L} = \begin{pmatrix} \mathbf{0} & \mathbf{P}_{z}^{0} & \mathbf{0} \\ -\mathbf{P}_{z}^{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}$$



E/M splitting (1966)

TE/TM splitting (2004)





dispersion error $\Delta \tau < \Delta z$

 $\Delta \tau = \Delta z$



Implicit TE/TM formulation





ADI and Explicit TE/TM formulations (2009)



 $\mathbf{W}^{e}_{CN} = \mathbf{W}^{e}_{ADI2} + O(\Delta \tau^{4})$ - splitting error

Explicit TE/TM scheme*

X

$$\mathbf{W}^e = \mathbf{W}^h = \mathbf{I}$$

**

 $\mathbf{W}_{CN}^{e} = \mathbf{I} + O(\Delta \tau^{2})$ - splitting error

* Dohlus M., Zagorodnov I., *Explicit TE/TM Scheme for Particle Beam Simulations*, Journal of Computational Physics **225**, No. 8, pp. 2822-2833 (2009)



Stability, energy and charge conservation

$$\mathbf{B}\frac{\mathbf{y}^{n+1}-\mathbf{y}^n}{\Delta\tau}+\mathbf{A}\mathbf{y}^n=\mathbf{f}^n$$

The stability condition $\mathbf{Q} \equiv \mathbf{B} - 0.5 \Delta \tau \mathbf{A} \ge 0$



$$\Delta \tau \le \min\left(\frac{1}{\sqrt{\Delta x^{-2} + \Delta y^{-2}}}, \Delta z\right)$$

dispersion error suppressed for $\Delta \tau = \Delta z$



Dispersion relation in the transverse plane

$$\frac{\sin^2 \Omega}{\Delta \tau^2} = \frac{\sin^2 K_z}{\Delta z^2} + \left(\frac{\sin^2 K_x}{\Delta x^2} + \frac{\sin^2 K_y}{\Delta y^2}\right) \cos^2 \Omega$$

Implicit TE/TM scheme

$$\frac{\sin^2 \Omega}{\Delta \tau^2} = \frac{\sin^2 K_z}{\Delta z^2} + \left(\frac{\sin^2 K_x}{\Delta x^2} + \frac{\sin^2 K_y}{\Delta y^2}\right) \left(1 - \frac{\Delta \tau^2}{\Delta z^2} \sin^2 K_z\right)$$

Explicit TE/TM scheme



No dispersion in z-direction + no dispersion along XY diagonals



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Standard Conformal Scheme (1997)



Dey S, Mittra R. *A locally conformal finite-difference time-domain (FDTD) algorithm for modeling threedimensional perfectly conducting objects*, IEEE Microwave and Guided Wave Letters 7(9):273–275 (1997)

Thoma P. *Zur numerischen Lösung der Maxwellschen Gleichungen im Zeitbereich*, Dissertation DI7: TH Darmstadt, 1997.





Time step is not reduced!

* Zagorodnov I., Schuhmann R., Weiland T., *A Uniformly Stable Conformal FDTD-Method on Cartesian Grids*, International Journal on Numerical Modeling, vol. 16, No.2, pp. 127-141 (2003)





Square rotate by angle $\pi/8$.

$$\delta = \frac{\left\| H_z - \tilde{H}_z \right\|_{L_2^h}}{\left\| H_z \right\|_{L_2^h}}$$

PFC (Partially Filled Cells) ~ Dey-Mittra USC (Uniformly Stable Conformal)





Error in loss factor for a taper $\delta = |L_{calc} - L|L^{-1}$

The error δ relative to the extrapolated loss factor *L*=-7.63777 V/pC for bunch with σ =1 mm is shown.



Indirect Integration Algorithm



$$\int_{C_0} e_z^s dz = -\frac{1}{2} \left(\int_{C_1} \left(r_0^m \omega_D + r_0^{-m} \omega_S - \frac{\beta}{a^m} \omega_S \right) - \frac{\beta}{a^m} \int_{C_2} \omega_S \right)$$

I. Zagorodnov, R. Schuhmann, T. Weiland, Journal of Computational Physics **191**, No.2 , pp. 525-541 (2003)

O. Napoly, Y. Chin, and B. Zotter, Nucl. Instrum. Methods Phys. Res. Sect. A **334**, 255 (1993)



Indirect Integration Algorithm



$$QW_{\parallel}(\vec{r}_{0},s) = -\int_{C_{-1}(\vec{r}_{0},z_{0}-s)} E_{z}^{\text{sc}}[\vec{r}_{0},z,t(z,s)]dz - u(\vec{r}_{0},s), \qquad t(z,s) = \frac{z+s}{c}$$

$$\Delta u(\vec{r},s) = -\left[\frac{\partial}{\partial s} + \frac{\partial}{c\partial t}\right] E_{z}^{\text{sc}}(\vec{r},z_{0}-s,t_{0}), \qquad \vec{r} \in \Omega_{\text{out}}^{\perp}, \qquad u(\vec{r},s) = 0, \qquad \vec{r} \in \partial \Omega_{\text{out}}^{\perp}.$$

Zagorodnov I., *Indirect Methods for Wake Potential Integration*, Phys. Rev. STAB **9**, 102002 (2006)

H. Henke and W. Bruns, in Proceedings of EPAC 2006, Edinburgh, Scotland (WEPCH110, 2006)



Indirect Integration Algorithm



a = 8 mm, b = 5 mm, and c = 20 mm

Gaussian bunch with rms length 25 μm





Modelling of Conductive Walls



FIG. 6. A boundary cell in the vacuum and 1D conductive line in the metal.

Tsakanian A., Dohlus M., Zagorodnov I., *Hybrid TE-TM scheme for time domain numerical calculations of wakefields in structures with walls of finite conductivity*, Phys. Rev. STAB **15**, 054401 (2012)

Zagorodnov I., Bane K., Stupakov G., **Calculations of wakefields in 2D rectangular structures**, Phys. Rev. STAB **18**, 104401 (2015)



Modelling of Conductive Walls



Longitudinal wake potential of tapered collimator



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ECHOz1, ECHOz2 (rotationally symmetric)

- ECHO2D (rectangular and rotationally symmetric)
- ECHO3D (fully 3D)
- ECHO-PIC (Particle-In-Cell for rotationally symmetric and rectangular)

https://www.desy.de/~zagor/WakefieldCode_ECHOz/





Rotationally Symmetric Geometries

$$\begin{pmatrix} E_r \\ H_{\theta} \\ E_z \end{pmatrix} = \sum_{m=0}^{\infty} \begin{pmatrix} E_{r,m} \\ H_{\theta,m} \\ E_{z,m} \end{pmatrix} \cos(m\theta) \qquad \qquad \begin{pmatrix} H_r \\ E_{\theta} \\ H_z \end{pmatrix} = \sum_{m=0}^{\infty} \begin{pmatrix} H_{r,m} \\ E_{\theta,m} \\ H_{z,m} \end{pmatrix} \sin(m\theta)$$

$$W_{\parallel}(r_0,\theta_0,r,\theta,s) = \sum_{m=0}^{\infty} W_m(s) r_0^m r^m \cos\left(m(\theta-\theta_0)\right)$$







Only fully rotationally symmetric problems (m=0 mode)

- vector potential wave equation (slide 9)
- only PEC
- stand-alone Windows GUI application





Rotationally symmetric geometries (all modes)

- > TE/TM implicit (slide 10)
- surface conductivity
- stand-alone Windows GUI application





ECHO₂2

Short-Range Wake Functions for TESLA Cryomodule



Longitudinal wake functions was found earlier with code NOVO Novokhatski A., Timm M., Weiland T., *Single Bunch Enetgy Spread in the TESLA Cryomodule*, DESY TESLA-99-16, 1999 Transverse wake functions is found with code ECHO T. Weiland, I. Zagorodnov, *The short-range transverse wake function for TESLA accelerating structure*, TESLA Report 2003-19, 2003

ECHO₂2



Rectangular Geometries with Constant Width



$$\begin{pmatrix} E_x \\ H_y \\ H_z \end{pmatrix} = \frac{1}{w} \sum_{m=1}^{\infty} \begin{pmatrix} E_{x,m} \\ H_{y,m} \\ E_{z,m} \end{pmatrix} \cos\left(\frac{\pi}{2w}mx\right)$$
$$\begin{pmatrix} H_x \\ E_y \\ E_z \end{pmatrix} = \frac{1}{w} \sum_{m=1}^{\infty} \begin{pmatrix} H_{x,m} \\ E_{y,m} \\ E_{z,m} \end{pmatrix} \sin\left(\frac{\pi}{2w}mx\right)$$

Zagorodnov I., Bane K., Stupakov G. *Calculations of wakefields in 2D rectangular structures*, Phys. Rev. STAB **18**, 104401 (2015)

Novokhatski A., *Wakefield potentials of corrugated structures*, Phys. Rev. STAB **18**, 104402 (2015)





Wake field expansion is new (to our knowledge)

$$W_{\parallel}(x_0, y_0, x, y, s) = \frac{1}{w} \sum_{m=0}^{\infty} W_m(y_0, y, s) \sin(k_{x,m} x_0) \sin(k_{x,m} x)$$

General case

$$W_m(y_0, y, s) = \left(\cosh(k_{x,m}y_0) \quad \sinh(k_{x,m}y_0)\right) \quad \begin{pmatrix} W_m^{cc}(s) & W_m^{cs}(s) \\ W_m^{sc}(s) & W_m^{ss}(s) \end{pmatrix} \quad \begin{pmatrix} \cosh(k_{x,m}y) \\ \sinh(k_{x,m}y) \end{pmatrix}$$

With symmetry in y

$$W_m(y_0, y, s) = W_m^{cc}(s) \cosh(k_{x,m}y_0) \cosh(k_{x,m}y) + W_m^{ss}(s) \sinh(k_{x,m}y_0) \sinh(k_{x,m}y)$$





$$W_m(y_0, y, s) = W_m^H(y_0, y, s) + W_m^E(y_0, y, s)$$

$$W_m^{cc}(s) = \frac{W_m^H(y_0, y_0, s)}{\cosh(k_{x,m}y_0)^2} \qquad \qquad W_m^{ss}(s) = \frac{W_m^E(y_0, y_0, s)}{\sinh(k_{x,m}y_0)^2}$$

 $W_m(y_0, y, s) = W_m^{cc}(s) \cosh(k_{x,m}y_0) \cosh(k_{x,m}y) + W_m^{ss}(s) \sinh(k_{x,m}y_0) \sinh(k_{x,m}y)$



Rectangular and rotationally symmetric problems (all modes)

- TE/TM implicit (slide 10)
- surface conductivity
- stand-alone console application (Windows, Mac OS, Linux)
- Parallelized (MPI and threads)





Zagorodnov I., Bane K., Stupakov G., Calculations of wakefields in 2D rectangular structures, Phys. Rev. STAB 18, 104401 (2015)



Pohang Dechirper Experiment





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*P. Emma et al., Phys. Rev. Lett. **112**, 034801 (2014)



ECHO3D



3D simulation. Cavity

Moving mesh

20 TESLA cells structure



3 geometry elements

The geometric elements are loaded when the moving mesh reaches them. During the calculation only 2 geometric elements are in memory.



ECHO3D



Comparison of the wake potentials obtained by different methods for structure consisting of 20 TESLA cells excited by Gaussian bunch $\sigma = 1mm$

Г

E/M splitting
$$\Delta z \sim \sqrt{\frac{\sigma^3}{L}}$$

TE/TM splitting $\Delta z \sim \sigma$



ECHO3D

Coupler Kick (One cryomodule ~ 12 meters)



Stupakov G., *Using pipe with corrugated walls for a subterahertz free electron laser*, PR-STAB **18**, 030709 (2015)



TABLE I. Corrugation and beam parameters.

Pipe radius (mm)	2
Depth $h (\mu m)$	50
Period $p(\mu m)$	40
Gap $g(\mu m)$	10
Bunch charge (nC)	1
Energy (MeV)	5
Bunch length (ps)	10





Wakefield code ECHO (with resistivity)

Particle-in-Cell code ECHO-PIC (only longitudinal dynamics)



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Parameter	Value
Pipe length L, m	1-2
Bunch enegry E_0 , MeV	5-20
Gausian bunch rms σ , mm	0.3*8
Charge Q , nC	0.96

I [A]







DESY







