Current Status of Time Domain Wakefield Solver for Resistive Structures

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TEMF – DESY Collaboration Meeting

15 June 2015
DESY, Hamburg

- *Achievements*
- *Ongoing activity*

General Requirements on Wakefield Solver

Solver Capabilites

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

Numerical Method

- 3D Numerical Scheme
- Dispersion Free in longitudinal direction

- Moving Window
- Parallel computing

General Requirements on Wakefield Solver

Solver Capabilites

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

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

Numerical Method

- Time Domain SIBC Model and Special Implementation to Preserve Dispersion Properties of 3D Method
- No Time & Mesh refinement

- 3D Numerical Scheme
- Dispersion Free in longitudinal direction

- Moving Window
- Parallel computing

Dispersion-Free Numerical Method

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Staggered Finite Volume Time Domain Method

Volume Integral Form of Maxwell's Equations

$$\oint_{\partial V} \vec{E} \times d\vec{A} = -\frac{d}{dt} \int_V \mu \vec{H} \, dV$$

$$\oint_{\partial V} \vec{H} \times d\vec{A} = \int_V \left[\vec{J} + \frac{d}{dt} \varepsilon \vec{E} \right] dV$$

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

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

Space Discretization

Time Continuous MGE

$$\frac{d}{dt} h = -M_{\mu^{-1}} C \cdot e$$

$$\frac{d}{dt} e = M_{\varepsilon^{-1}} C \cdot h - M_{\varepsilon^{-1}} \cdot j$$

Time Integration

No Splitting

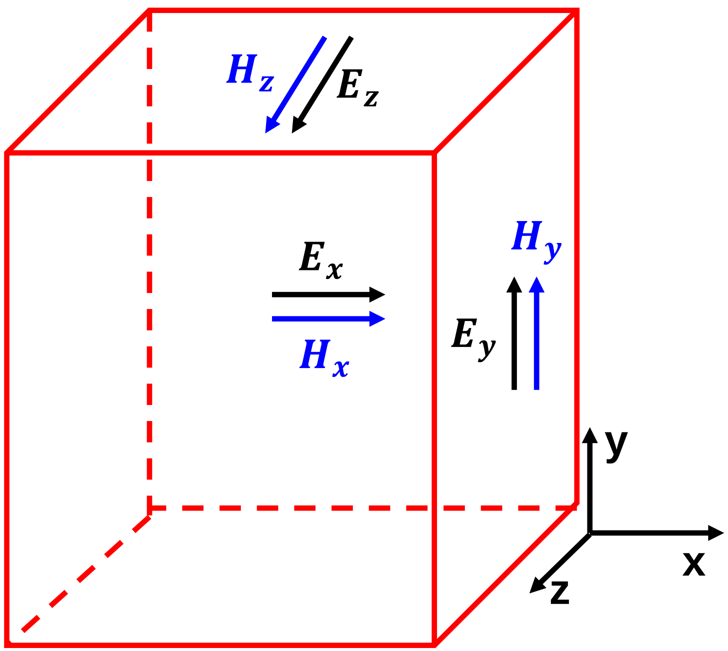
$$\begin{pmatrix} e \\ h \end{pmatrix}^{n+1} = G(\Delta t) \begin{pmatrix} e \\ h \end{pmatrix}^{n}$$

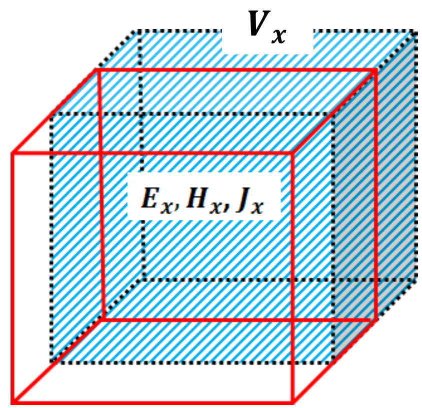
Dispersion-free in longitudinal direction

- E. Gjonaj, T. Lau, T. Weiland, Wakefield Computation with the PBCI Code using a Non-Split Finite Volume Method, Proceedings of PAC09, Vancouver, Canada, 2009, pp. 4516-4518

Finite Volume Time Domain Method

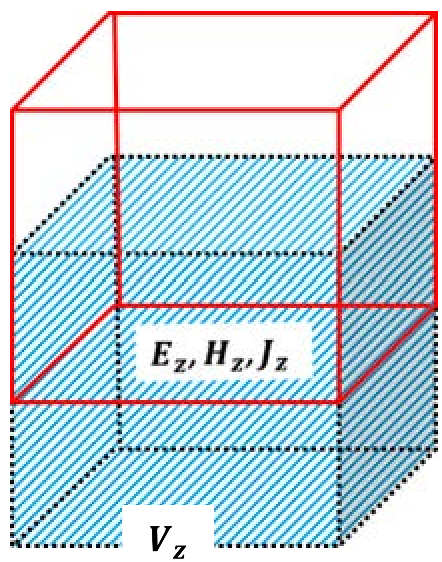
Allocations of E&M Field Components on Cartesian Grid

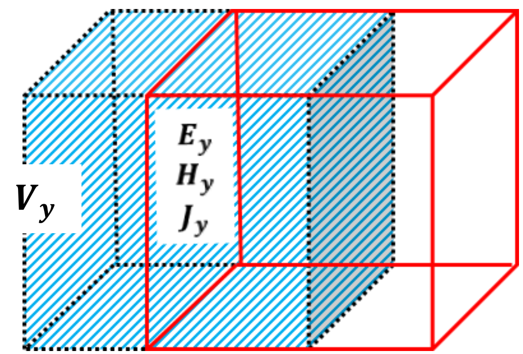




$$\frac{d}{dt}\int_V \mu\vec{H}\,dV = -\oint_{\partial V}\vec{E}\times d\vec{A}$$

$$\frac{d}{dt}\int_V \varepsilon\vec{E}\,dV = \oint_{\partial V}\vec{H}\times d\vec{A} - \int_V \vec{J}\,dV$$

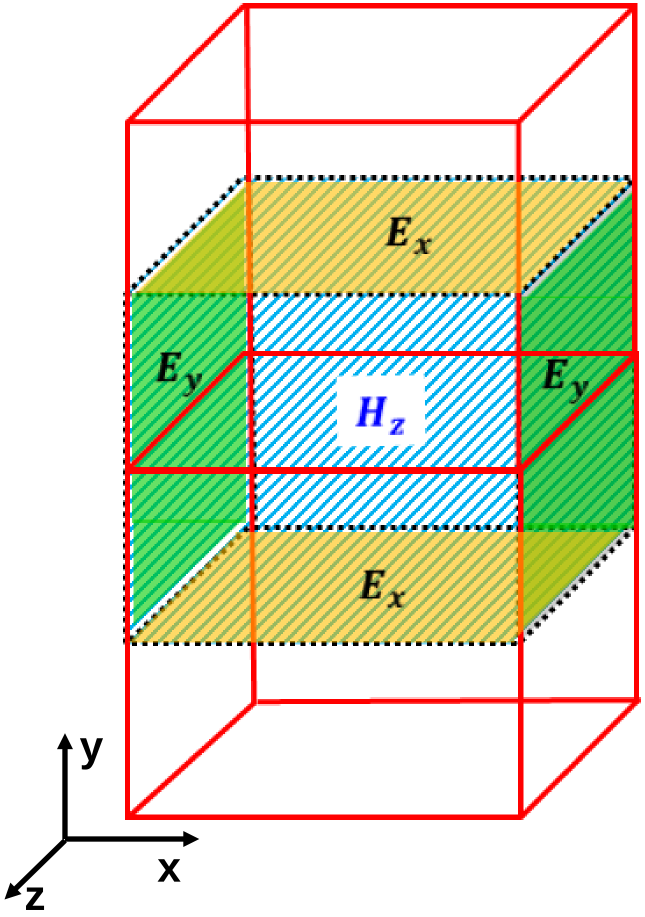




Finite Volume Time Domain Method

Faraday's Law

$$\frac{d}{dt}\int_V \mu\vec{H}\, dV = -\oint_{\partial V} \vec{E}\times d\vec{A}$$



Finite Volume Time Domain Method

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Faraday's Law

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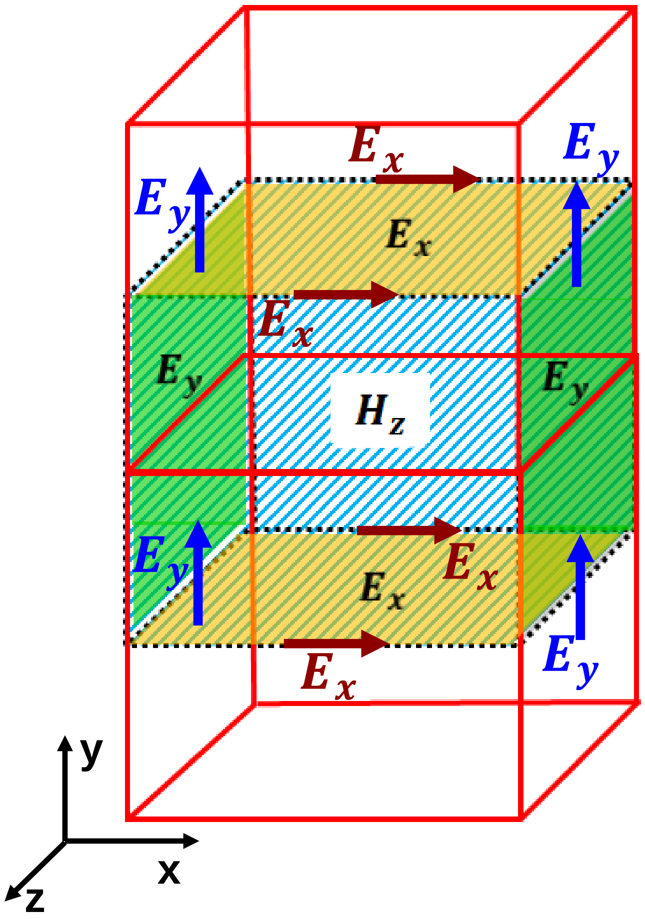


Finite Volume Time Domain Method

Faraday's Law

$$\frac{d}{dt}\int_V \mu\vec{H}\,dV = -\oint_{\partial V}\vec{E}\times d\vec{A}$$

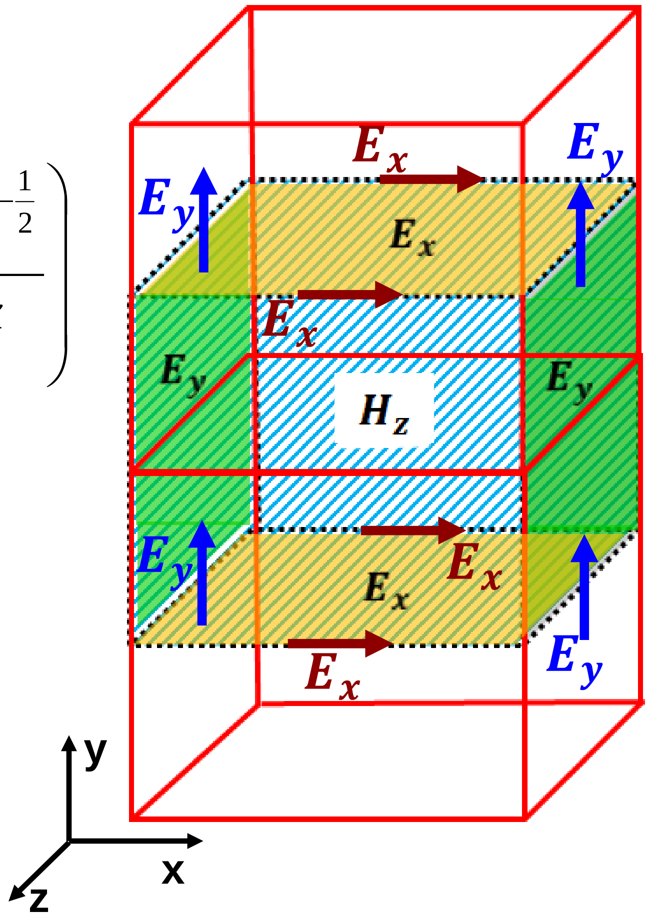
4-Point Derivative Stencil

$$\frac{d}{dt}\mu_z H_z^{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{1}{2}\left(\frac{\partial E_x^{k+1}}{\partial y}+\frac{\partial E_x^{k}}{\partial y}\right)-\frac{1}{2}\left(\frac{\partial E_y^{j+\frac{1}{2}}}{\partial x}+\frac{\partial E_y^{j-\frac{1}{2}}}{\partial x}\right)$$

$$\frac{\partial E_x^{k}}{\partial y} \equiv \frac{E_x^{i+\frac{1}{2},j+\frac{1}{2},k}-E_x^{i+\frac{1}{2},j-\frac{1}{2},k}}{\Delta_y}$$

$$\frac{\partial E_y^{j+\frac{1}{2}}}{\partial x} \equiv \frac{E_y^{i+1,j+\frac{1}{2},k+\frac{1}{2}}-E_y^{i,j+\frac{1}{2},k+\frac{1}{2}}}{\Delta_x}$$

The transverse derivative operators have averaging in longitudinal direction, while in FIT they have not.



Dispersion Properties of Numerical Methods

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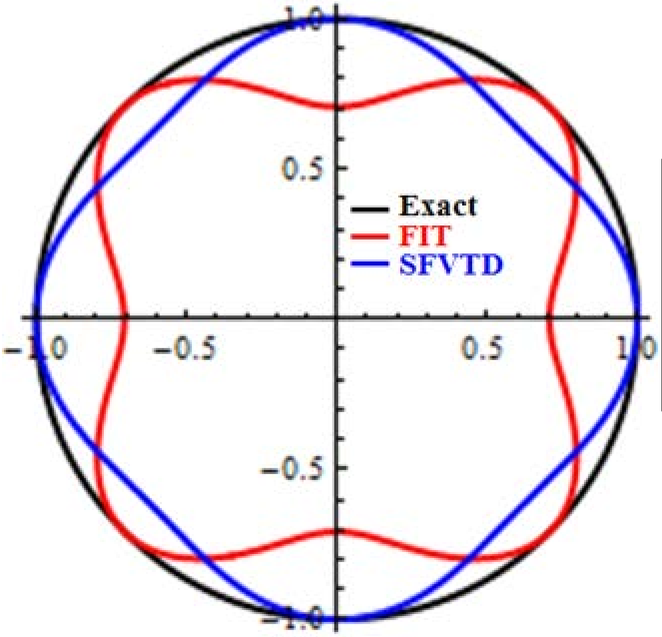
Numerical phase velocity vs propagation direction

2D – Δ=λ/2



Stability Limits

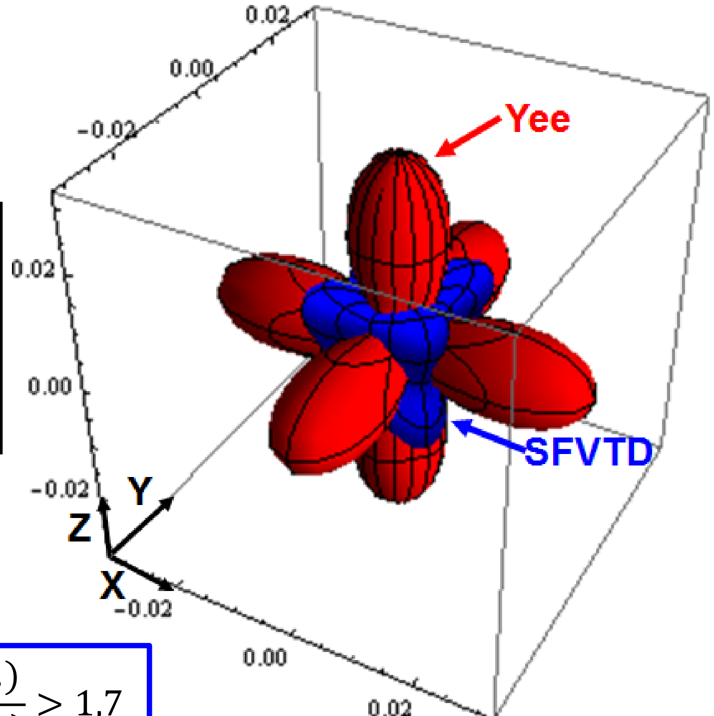
$$\Delta t^{2D}_{FIT} = \Delta / \sqrt{2}$$

$$\Delta t^{3D}_{FIT} = \Delta / \sqrt{3}$$

$$\Delta t^{2D}_{SFVM} = \Delta t^{3D}_{SFVM} = \Delta$$

Numerical phase velocity error vs propagation direction

3D – Δ=λ/5



$$\frac{\max(\Delta V_{Yee})}{\max(\Delta V_{FVM})} > 1{,}7$$

SIBC Time Domain Model

SIBC in Frequency Domain

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

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

Rational Function Approximation (RFA)

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

SIBC Time Domain Model

SIBC in Frequency Domain

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

Transformation to TD

SIBC in Time Domain

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

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

Rational Function Approximation (RFA)

Auxiliary Differential Equations (ADE)

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

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

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

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

SIBC Time Domain Model

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Surface Impedance of Good Conductors

$$Z_s(\omega) \cong \sqrt{\frac{j\omega\mu_0}{\sigma(\omega) + j\omega\varepsilon_0}}$$

$$\sigma(\omega) \approx \frac{\sigma_0}{1 - j\omega\tau}$$

Metal Type	*Conductivity [MS/m]*	*Relaxation Time [fs]*
Cu	58	24.6
Al	36.6	7.1
SS 316	1.34	2.4
Ti-6Al-4V	0.5	1.04 (?)

SIBC Time Domain Model

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Cu	58	24.6
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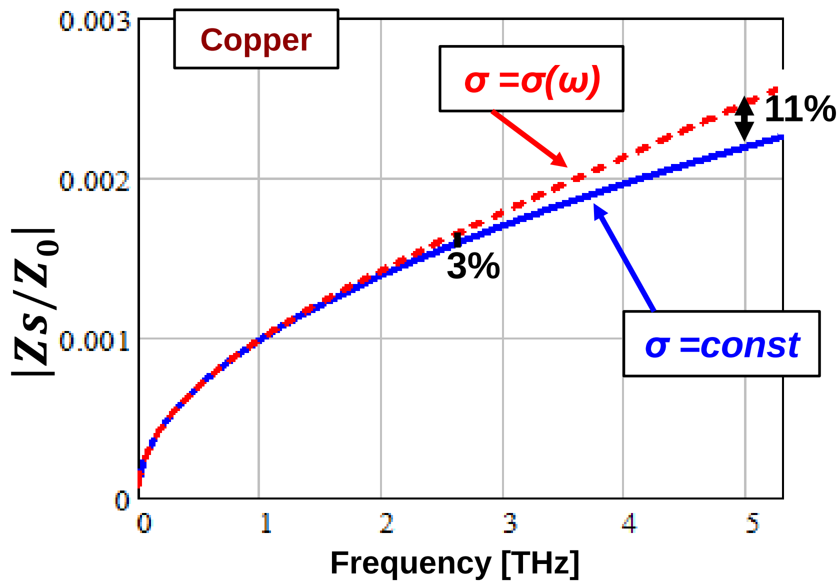
SS 316	1.34	2.4
Ti-6Al-4V	0.5	1.04 (?)

Example : Short bunch

$$\sigma_{Bunch} \approx 10\mu m$$

$$f \sim \frac{c}{\sigma_{Bunch}} \approx 5\,THz$$



SIBC Time Domain Model

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Boundary Effects

$$Z_s(\omega) = Z_s^{\sigma}(\omega) + Z_s^{L}(\omega)$$

- ***Finite Resistivity***

$$Z_s^{\sigma}(\omega) \approx \sqrt{\frac{j\omega\mu}{\sigma(\omega) + j\omega\varepsilon}}$$

$$\sigma(\omega) \approx \frac{\sigma_0}{1 - j\omega\tau}$$

- ***Surface Roughness***
- ***Metal Oxidation***

$$Z_s^{L}(\omega) \approx j\omega L$$

$$L \approx \mu_0 \left[\frac{\varepsilon_r - 1}{\varepsilon_r} \cdot \Delta_{oxide} + 0.01 \cdot \Delta_{rough} \right]$$

$$\varepsilon_r \sim 10$$
$$\Delta_{oxide} \sim 7\,nm$$

$$\Delta_{rough} \sim 500\,nm$$

- M. Dohlus. TESLA report 2001-26, 2001
- K. Bane, G. Stupakov, SLAC-PUB-10707, 2004
- A. Tsakanian, M. Dohlus, I. Zagorodnov, TESLA-FEL-2009-05, 2009

SIBC Time Domain Model

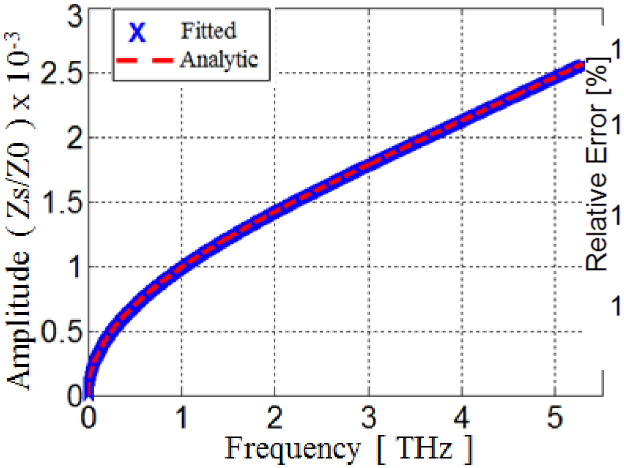
Accuracy of Vector-Fitting technique

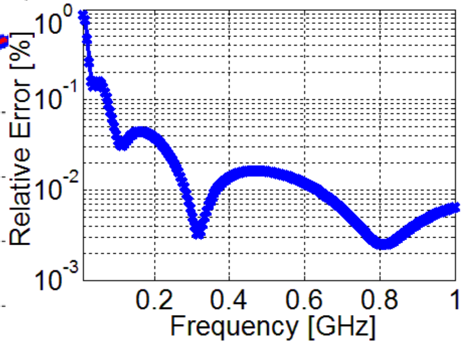
Good Conductors

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

Example : Cu – Np=21,

Frequency range ~ 10MHz-5THz, Δf~5MHz





SIBC Time Domain Model

Accuracy of Vector-Fitting technique

Good Conductors

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

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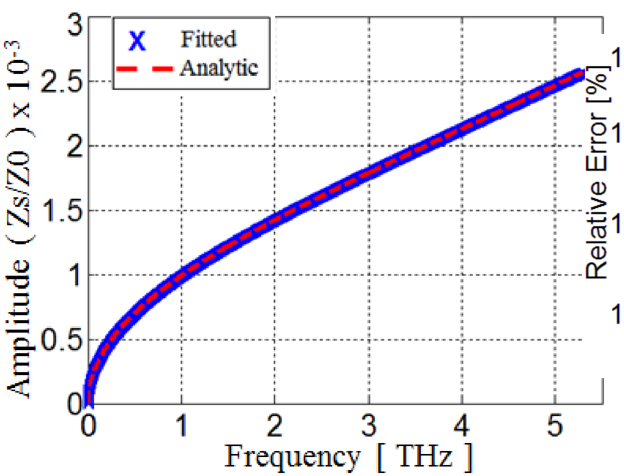
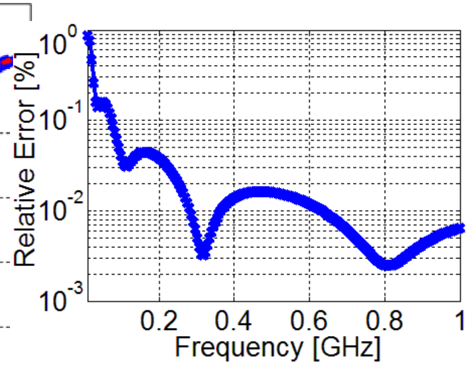
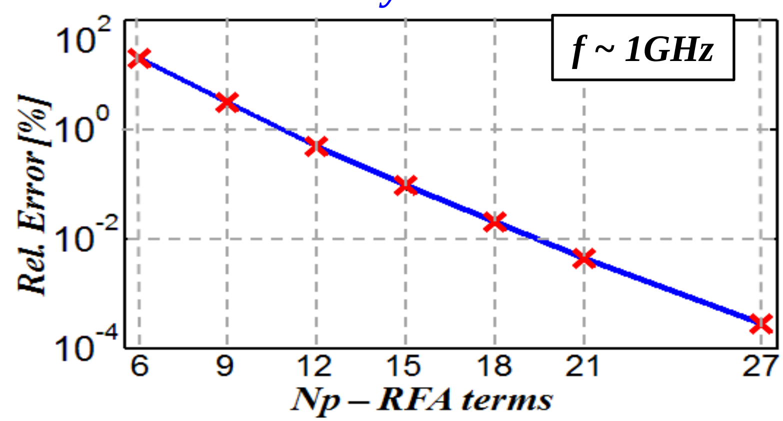




Sensitivity on RFA terms



SFVTD Method with SIBC-TD

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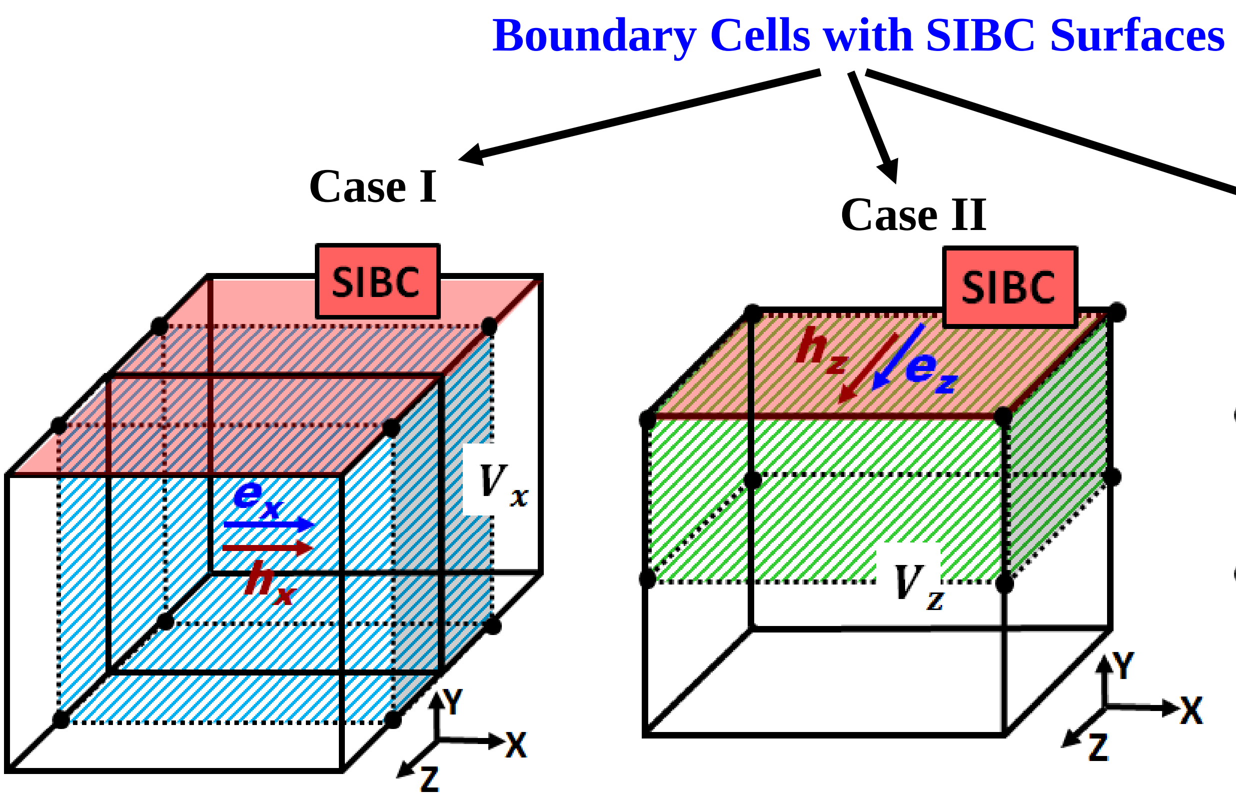

Control volumes (shaded) at SIBC boundaries (red) and associated DoFs with respect to a cell volume of primary grid (black).

SFVTD Method with SIBC-TD

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Semi-Discrete ADE Formulation in Time Continuous MGE with SIBC

Faraday's Law with SIBC - TD

$$\frac{d}{dt} G_i + \beta_i \cdot G_i = \alpha_i\, h$$

$$\left(M_\mu + L \cdot A_c\right) \frac{d}{dt} h + \alpha_0 \cdot A_c \cdot h = -C \cdot e - A_c \cdot \sum_{i=1}^{Np} G_i$$

Ampere's Law with PEC

$$M_\varepsilon \frac{\partial}{\partial t} e = C \cdot h + j_s$$

Semi-Analytic

Time Integration

$$G_i^n = G_i^{n-1} \cdot e^{-\beta_i \Delta t} + \frac{\alpha_i}{\beta_i}\left(1 - e^{-\beta_i \Delta t}\right) \cdot h^{n-0.5}$$

SFVTD Method with SIBC-TD

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Faraday's Law with SIBC - TD

$$\frac{d}{dt}G_i + \beta_i \cdot G_i = \alpha_i h$$

$$\left(M_\mu + L \cdot A_c\right)\frac{d}{dt}h + \alpha_0 \cdot A_c \cdot h = -C \cdot e - A_c \cdot \sum_{i=1}^{Np} G_i$$

Semi-Analytic

Semi-Implicit

Ampere's Law with PEC

$$M_\varepsilon \frac{\partial}{\partial t} e = C \cdot h + j_s$$

Time Integration

$$\begin{cases} G_0^n = \alpha_0 \cdot h^{n-0.5} \\ G_i^n = G_i^{n-1} \cdot e^{-\beta_i \Delta t} + \dfrac{\alpha_i}{\beta_i}\left(1 - e^{-\beta_i \Delta t}\right) \cdot h^{n-0.5} \end{cases}$$

$$h^{n+0.5} = h^{n-0.5} - \Delta t \, \tilde{M}_{\mu^{-1}} \left(C e^n + A_c \cdot \sum_{i=0}^{N} G_i^n \right)$$

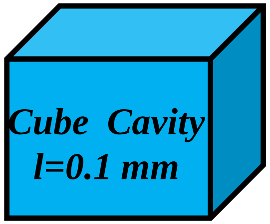
$$e^{n+1} = e^n + \Delta t \, M_{\varepsilon^{-1}} C \, h^{n+0.5} - \Delta t \, M_{\varepsilon^{-1}} \, j_s^{n+0.5}$$

Mass Matrix at the Boundary

$$\tilde{M}_{\mu^{-1}} = \frac{1}{\mu \cdot V + \alpha_0 \dfrac{\Delta t}{2} \cdot A_c + L \cdot A_c}$$

$$\tilde{M}_{\mu^{-1}}, M_{\varepsilon^{-1}}, A_c \rightarrow Diagonal$$

Numerical Example



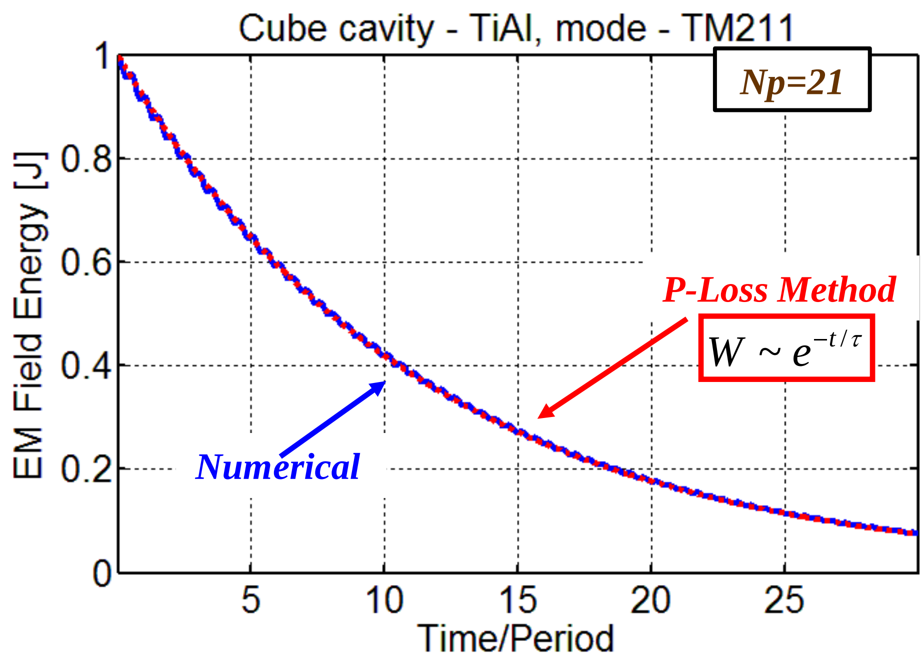
$$Mode - TM_{2,1,1}$$

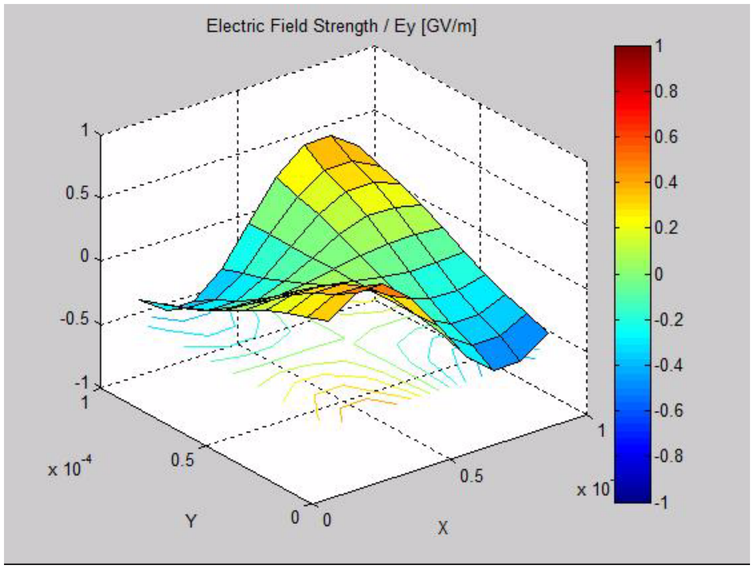
$$\lambda = 81.65\,\mu m,\ f \sim 3.5\,THz$$

$$\sigma_{TiAl} = 0.58 \cdot 10^{6}\ S/m \rightarrow c\tau \cong 0.94\,mm$$

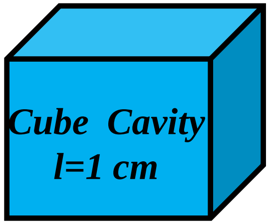
$$\sigma_{SS} = 1.34 \cdot 10^{6}\ S/m \rightarrow c\tau \cong 1.43\,mm$$

$$\sigma_{Cu} = 58 \cdot 10^{6}\ S/m \rightarrow c\tau \cong 9.42\,mm$$

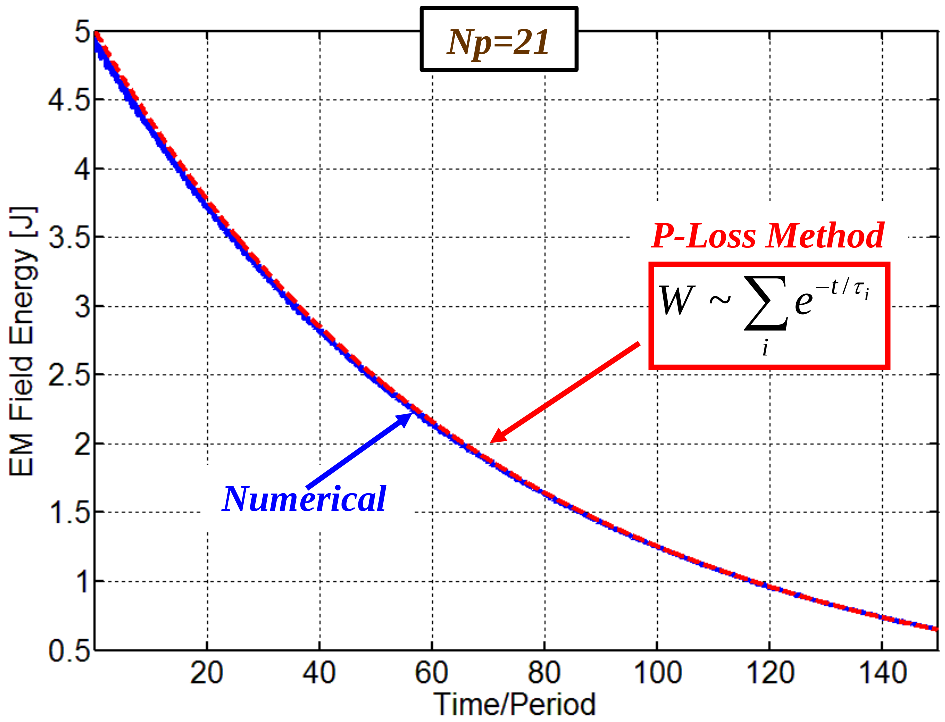




Numerical Example

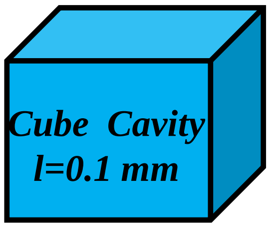


Multi-Mode Example

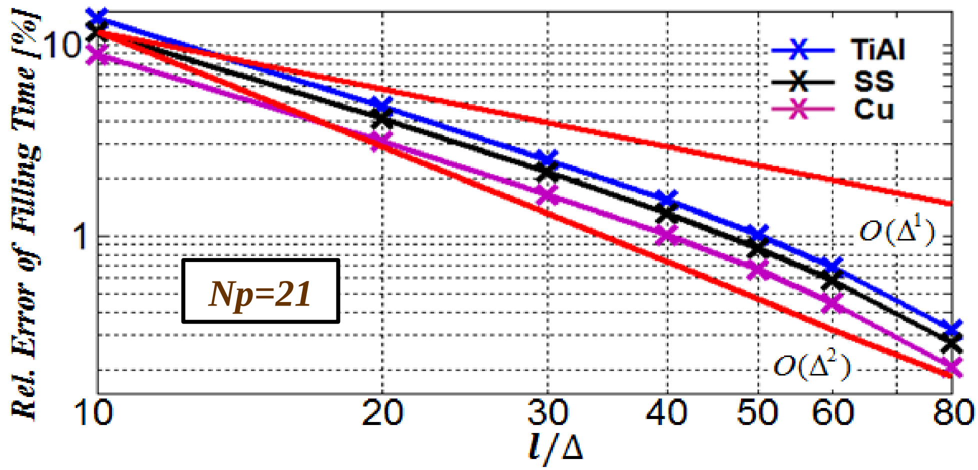


Mode	*Frequency [GHz]*	*Filling Time c τ [m]*
TM_{111}	25.9628	1.1202
TM_{211}	36.7169	0.9420
TM_{311}	49.7150	0.8095
TM_{411}	63.5956	0.7157
TM_{511}	77.8884	0.6468

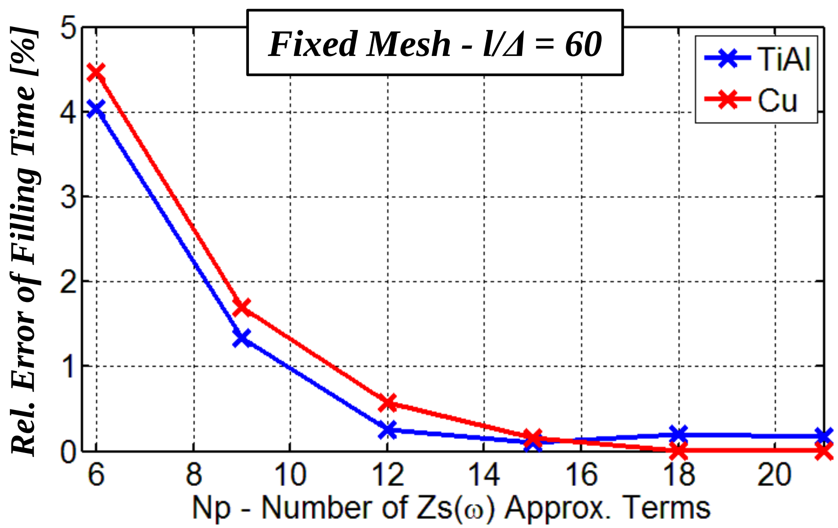
Convergence of the Scheme



$Mode - TM_{2,1,1}$



Reference Solution
Fine Mesh - l/Δ = 120



Reference Solution
Np=27

Intermediate Summary

Achievements

- Time Domain SIBC model & RFA Accuracy
- TD-SIBC Implementation in 3D SFVTD
- Stability & Convergence Analyses

- PBCI Mesher Adoption for SFVTD Method
- Implementation of SFVTD Method in PBCI
  - PEC – BC
  - TD – SIBC
  - Validation

Ongoing Activity

- Initial Fields & Current Generation – Ultra-Relativistic Bunch.

Initialization of Fields & Current

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Initial Field & Current Density Generation

Ultra-Relativistic bunch → Only transverse non-zero EM field components

Charge Density

$$\rho_{3D}(x,y,z) = \rho_{\perp}(x,y) \cdot \rho_{//}(z)$$

Initialization of Fields & Current

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$$\rho_{3D}(x,y,z) = \rho_{\perp}(x,y)\cdot\rho_{//}(z)$$

Initialization Strategy

- Create 3D Transverse Electric Field → Solve 2D E-Static Problem

2D Poisson Equation

$$\Delta_{\perp}\varphi_{2D} = \rho_{\perp}(x,y)/\varepsilon_0$$

$$BC - \varphi_{2D} = 0$$

↓

Create 3D electric potential by scaling the $\boldsymbol{\varphi_{2D}}$ with $\boldsymbol{\rho_{//}}$

↓

$$E_{\perp} = grad_{\perp}\,\varphi_{3D}$$

Initialization of Fields & Current

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2D Poisson Equation

$$\Delta_{\perp}\varphi_{2D} = \rho_{\perp}(x,y)/\varepsilon_0$$

$$BC - \varphi_{2D} = 0$$

Create 3D electric potential by scaling the $\boldsymbol{\varphi_{2D}}$ with $\boldsymbol{\rho_{//}}$

$$E_{\perp} = grad_{\perp}\,\varphi_{3D}$$

- Calculate 3D Transverse Magnetic Field from electric components.

$$H_x = -E_y \quad , \quad H_y = E_x$$

- Check Consistency of Generated Field Components with Update Equations.
- Create Current Density from Transverse Magnetic Field.

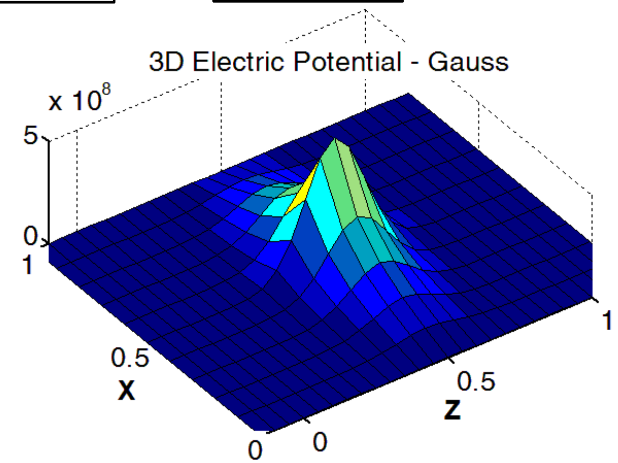
Initialization of Fields & Current

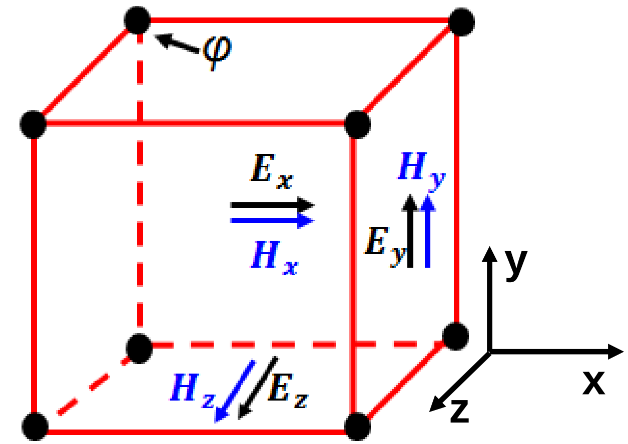
3D Transverse Electric Field

2D Potential - φ_{2D} ⇐ 2D Poisson Solver ⇒ **PBCI Solver** ⇐ Parallel

⇓

φ_{3D} = *Scale* φ_{2D} *with longitudinal charge distribution*





Initialization of Fields & Current

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3D Transverse Electric Field

2D Potential - φ_{2D} ⟸ 2D Poisson Solver ⟹ **PBCI Solver** ⟸ Parallel

⇓

φ_{3D} = *Scale* φ_{2D} *with longitudinal charge distribution*

- Construct Div & Grad FV operators

⇓

$$G = \begin{pmatrix} P_{g,x} & P_{g,y} & P_{g,y} \end{pmatrix}^T$$

$$Div = -G^T$$

⇓

Transverse E-field

$$e_{\perp}^{n} = G_{\perp} \cdot \varphi_{3D}$$

⇓

Check Field Consistency

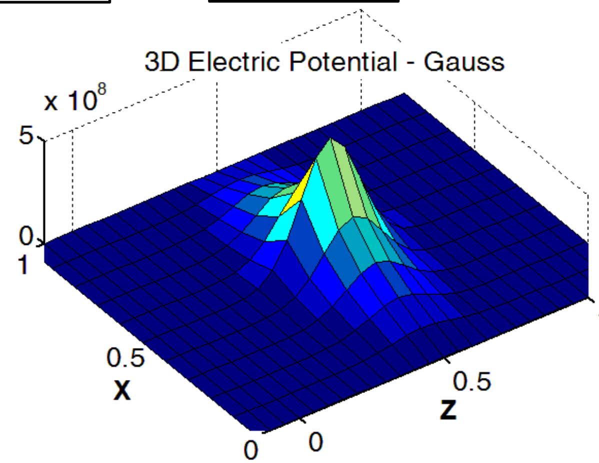
$$h_z^{n+0.5} = h_z^{n-0.5} - \Delta t \cdot M_{\mu_z}^{-1} \left(P_y^T e_x^n + P_x e_y^n \right) = 0$$

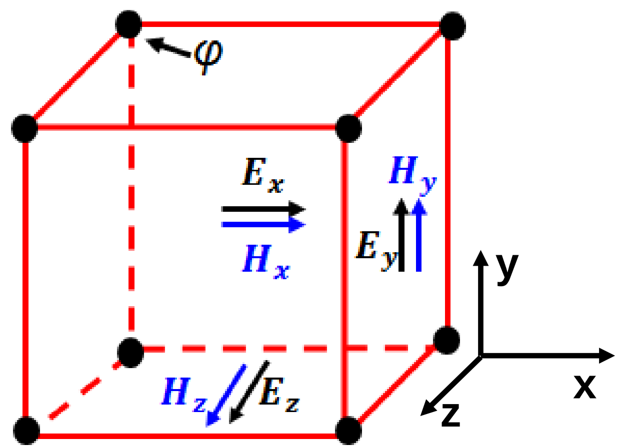
FV-Curl

$$C = \begin{pmatrix} 0 & P_z^T & P_y \\ P_z & 0 & P_x^T \\ P_y^T & P_x & 0 \end{pmatrix}$$

⇓

$$C = C^T$$



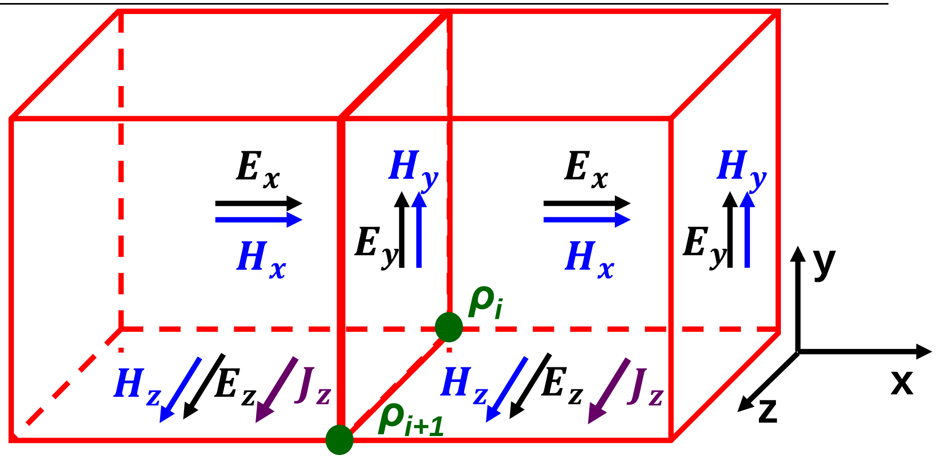


Initialization of Fields & Current

3D Transverse Magnetic Field

$$h_x^{n-0.5} \leftarrow -e_x^n$$
$$h_y^{n-0.5} \leftarrow e_y^n$$

⇒ Electric field averaging in X-direction



Check Field Consistency

$$h^{n-0.5} = \begin{pmatrix} h_x^{n-0.5} & h_y^{n-0.5} & 0 \end{pmatrix}^T$$
$$Div \cdot h^{n-0.5} = 0$$
$$Div \cdot C \cdot h^{n-0.5} = 0$$

Initialization of Fields & Current

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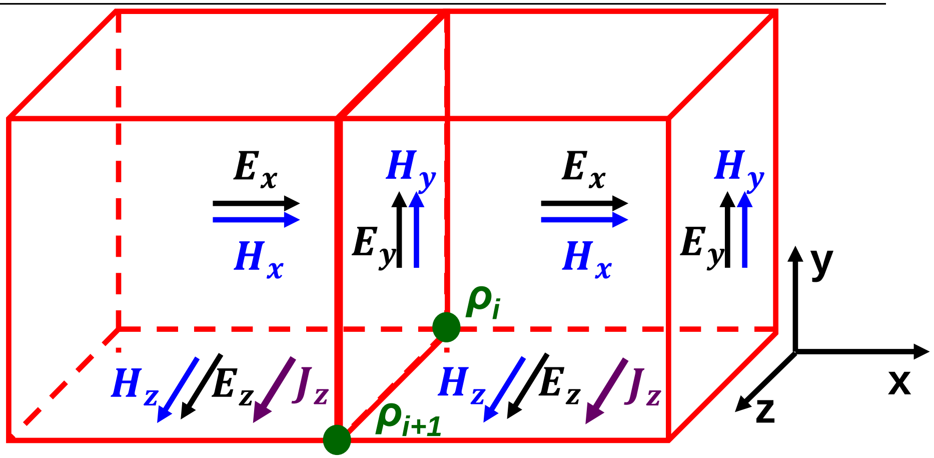
3D Transverse Magnetic Field

$$h_x^{n-0.5} \leftarrow -e_x^n \qquad h_y^{n-0.5} \leftarrow e_y^n$$

⇨ Electric field averaging in X-direction



Check Field Consistency

$$h^{n-0.5} = \begin{pmatrix} h_x^{n-0.5} & h_y^{n-0.5} & 0 \end{pmatrix}^T$$

$$Div \cdot h^{n-0.5} = 0$$

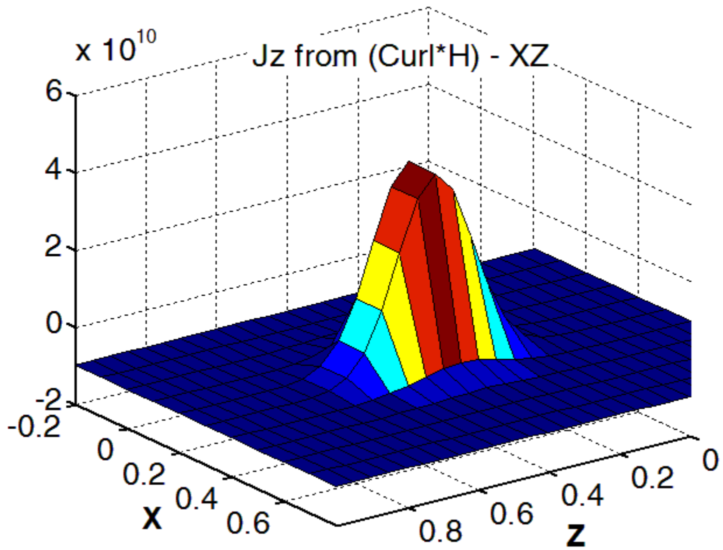
$$Div \cdot C \cdot h^{n-0.5} = 0$$

Current Density Generation

$$e_z^{n+1} = e_z^n + \Delta t \cdot M_{\varepsilon_z}^{-1}\left(P_y^T h_x^{n-0.5} + P_x h_y^{n-0.5}\right) - \Delta t \cdot M_{\varepsilon_z}^{-1} \cdot j_z^{n-0.5}$$

⇩

$$j_z^{n-0.5} = P_y^T h_x^{n-0.5} + P_x h_y^{n-0.5}$$



Initialization of Fields & Current

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Consistency of Generated Field Transverse Components with Update Equations.

Create longitudinal shift operator - **S**

H-field update

$$h_x^{n+0.5} = S \cdot h_x^{n-0.5} = I \cdot h_x^{n-0.5} - \Delta t\, M_{\mu_x}^{-1} \cdot P_z^T\, e_y^n$$

$$h_y^{n+0.5} = S \cdot h_y^{n-0.5} = I \cdot h_y^{n-0.5} - \Delta t\, M_{\mu_y}^{-1} \cdot P_z\, e_x^n$$

⇒ Fulfilled

Initialization of Fields & Current

Consistency of Generated Field Transverse Components with Update Equations.

Create longitudinal shift operator - **S**

H-field update

$$h_x^{n+0.5} = S \cdot h_x^{n-0.5} = I \cdot h_x^{n-0.5} - \Delta t\, M_{\mu_x}^{-1} \cdot P_z^T\, e_y^n$$
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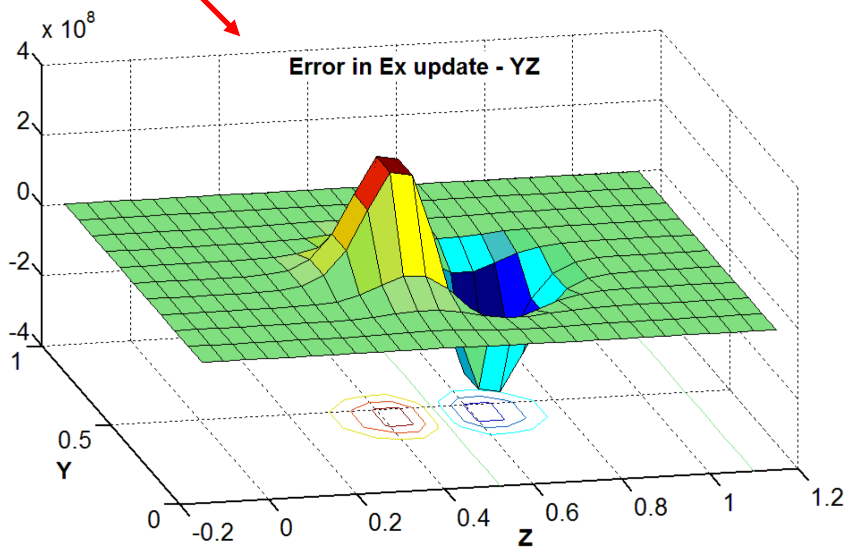
⇨ Fulfilled

E-field update

$$e_x^{n+1} = S \cdot e_x^n = I \cdot e_x^n + \Delta t\, M_{\varepsilon_x}^{-1} \cdot P_z^T \left(S\, h_y^{n-0.5}\right)$$
$$e_y^{n+1} = S \cdot e_y^n = I \cdot e_y^n + \Delta t\, M_{\varepsilon_y}^{-1} \cdot P_z \left(S\, h_x^{n-0.5}\right)$$

⇨ Failed



⇨ Is it because of longitudinal averaging in P_z & P_y ?

Initialization of Fields & Current

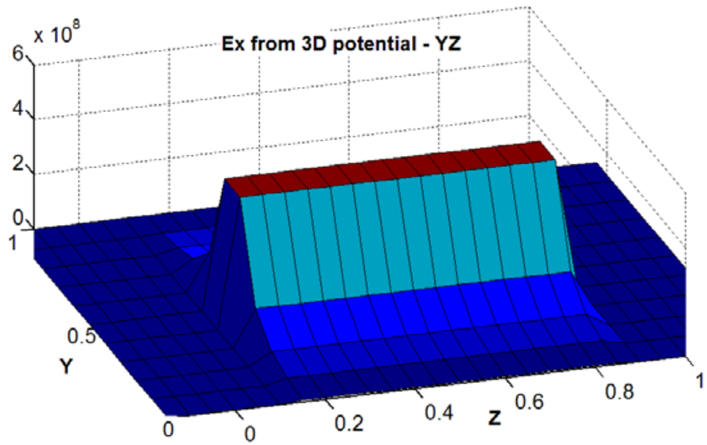
Consistency of Generated Field Transverse Components with Update Equations.

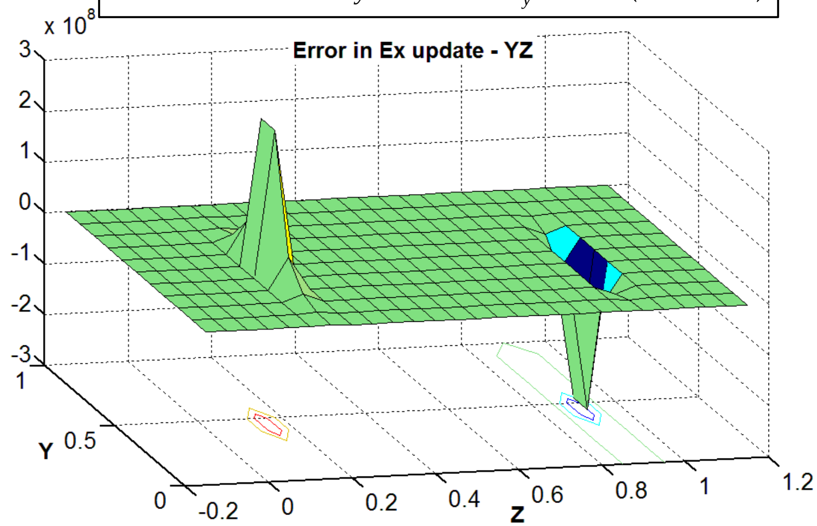
Check with charge density distribution
longitudinally uniform

E-field update

$$U = (I - S) \cdot e_x^n + \Delta t \, M_{\varepsilon_x}^{-1} \cdot P_z^T \left(S \, h_y^{n-0.5} \right)$$

$$U = (I - S) \cdot e_y^n + \Delta t \, M_{\varepsilon_y}^{-1} \cdot P_z \left(S \, h_x^{n-0.5} \right)$$





Initialization of Fields & Current

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Consistency of Generated Field Transverse Components with Update Equations.

Check with charge density distribution
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E-field update

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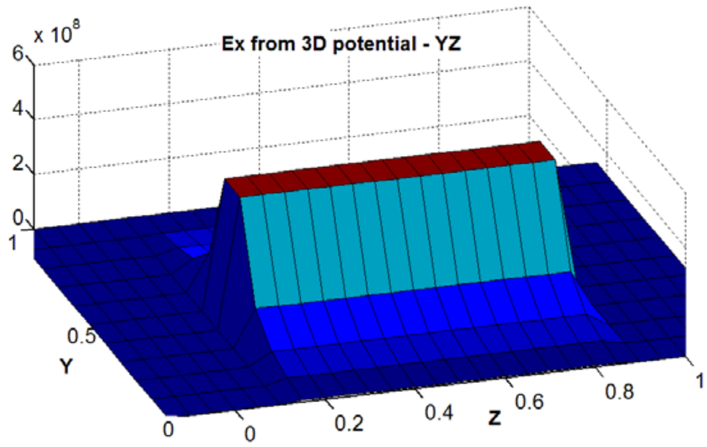

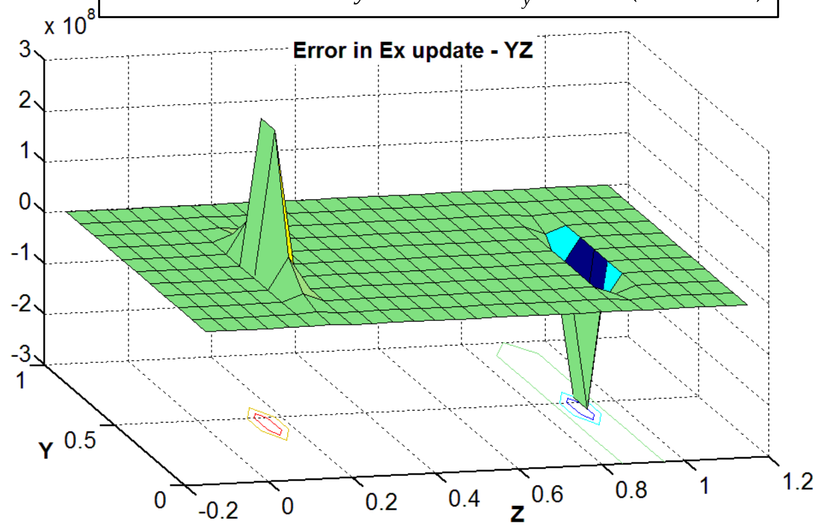

- Initial Fields & Current Generation – Ultra-Relativistic Bunch …

Initialization of Fields & Current

Consistency of Generated Field Transverse Components with Update Equations.

E-field update

$$U = (I - S) \cdot e_x^n + \Delta t\, M_{\varepsilon_x}^{-1} \cdot P_z^T \left(S\, h_y^{n-0.5}\right)$$

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Check with charge density distribution
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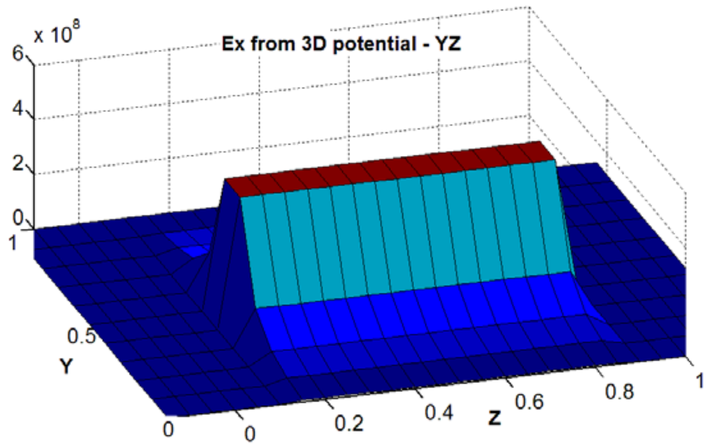

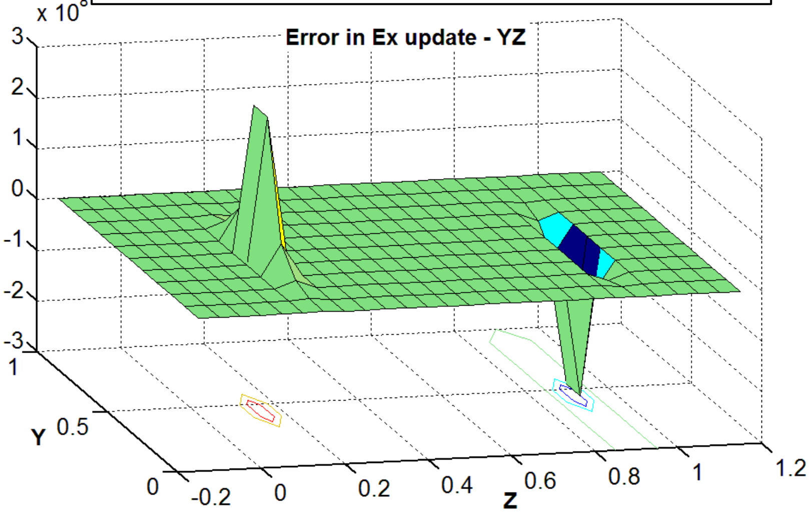

➢ Initial Fields & Current Generation – Ultra-Relativistic Bunch …

Thank You for Your Attention!

Numerical EM Field Energy

Numerical EM Field Energy

$$W = \frac{1}{2}\left(E^T \cdot M_\varepsilon \cdot E + H^T \cdot M_\mu \cdot H\right) - \frac{\Delta t}{2}\left(H^T \cdot C \cdot E\right)$$

Correction term