



## Integrating UPIC Algorithms into OSIRIS - Introduction to Spectral Methods in PIC codes OSIRIS Workshop 2017

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# Outline

## 1 Introduction to UPIC-EMMA Maxwell Solver

- UPIC framework
- UPIC-EMMA
- Units
- Spectral Method
- UPIC-EMMA Maxwell Solver

## 2 Emulation of a Finite Difference Scheme

- Yee Scheme
- Implementation in a Spectral Solver
- 2D Academic Case : Cylindrical wave

## 3 Absorbing Boundary Conditions

- Perfectly Matched Layer (PML) Technique for Finite Difference Schemes
- Implementation in a Spectral Solver
- Implicit Scheme
- 2D Academic Case : Cylindrical Waves

# UPIC framework @ <https://picksc.idre.ucla.edu/>

The screenshot shows the homepage of the UCLA Particle-in-Cell and Kinetic Simulation Software Center (PICKSC). At the top, there is a navigation bar with links for NEWS, PEOPLE, PUBLICATIONS, SOFTWARE, RESEARCH, OPPORTUNITIES, and DISCUSSION BOARD. Below the navigation bar is a large image of a plasma simulation showing a density distribution with a central bright region and surrounding filaments. To the right of the image is a text box containing information about the center's mission and activities. At the very top of the page, there are logos for UCLA, the National Science Foundation (NSF), and SciDAC, along with a search bar.

**PICKSC** Particle-in-Cell and Kinetic Simulation Software Center

UCLA

Search this website...

Funded by:

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NEWS ▾ PEOPLE PUBLICATIONS ▾ SOFTWARE ▾ RESEARCH ▾ OPPORTUNITIES DISCUSSION BOARD

The UCLA Particle-in-Cell (PIC) and Kinetic Simulation Software Center (PICKSC) was created through an NSF Software Infrastructure for Sustained Innovation (SI2) Award. It is housed within the UCLA Departments of Physics and Astronomy and of Electrical Engineering, and Institute for Digital Research and Education (IDRE).

PICKSC's mission is to support an international community of PIC and plasma kinetic software developers, users, and educators; to increase the use of this software for accelerating the rate of scientific discovery; and to be a repository of knowledge and history for PIC.

PICKSC aims to make available and document illustrative open-source software programs for different computing hardware, a flexible open-source Framework for rapid construction of parallelized PIC programs, and distinct production programs; to host activities on developing and comparing different PIC algorithms and on documenting best practices for developing and using PIC programs; to coordinate a community development of educational software for undergraduate and graduate courses in plasma physics and computer science; and to sponsor an annual workshop to help build a community of developers and users.

Please [contact us](#) if you would like your news, software, presentations, publications, or notes to be posted on this site.

# UPIC-EMMA (1)

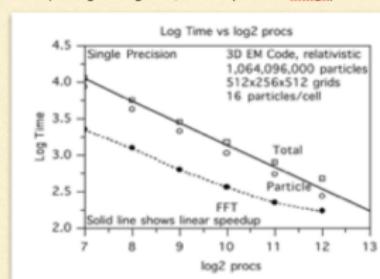
## UPIC-EMMA

**UPIC-EMMA is a fully relativistic and fully parallelized electromagnetic PIC code, inherited from the UPIC framework<sup>1</sup>**

### UPIC Features:

- Message-Passing Interface and Multi-Tasking Open-MP parallelization
- Relativistic Binary Collision Module
- Spectral (parallelized FFT algorithm) or
  - Arbitrary order Finite Difference Scheme for solving Maxwell equations
  - Customized solver to eliminate NCI
  - Charge conserving current deposition schemes
- PML absorbing Boundary Conditions + open b.c. for particles
- Parallel I/O for diagnostics (using HDF5, and leverages OSIRIS' visualization packages)
- Antenna-generated laser pulses
- High order particle shapes
- Boosted frame
- GPU & Phi-enabled versions can be adapted quickly from UPIC

Excellent parallel scalability on supercomputer :  
(Strong scaling data, courtesy of V. K. Decyk)



IDEAL for accurate and extensive Laser Plasma interaction simulations related to High Energy Density Physics or Laser-Based Particle Accelerator Physics



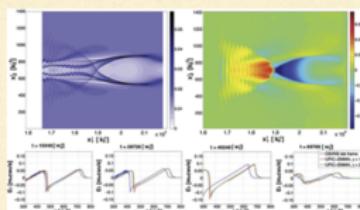
<http://picksc.idre.ucla.edu/>

<sup>1</sup>V. K. Decyk, Comp. Phys. Com., Volume 177, Issues 1–2, July 2007, Pages 95-97

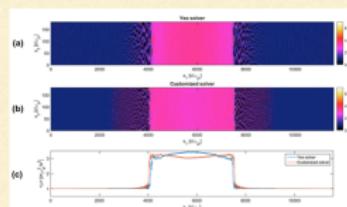
# UPIC-EMMA (2)

## UPIC-EMMA

### Some UPIC-EMMA Applications



Laser wakefield simulation in the Lorentz boosted frame<sup>2</sup>



Relativistic shock simulation<sup>3</sup>

UPIC-EMMA will soon be available on GitHub through an Open Source License:

GitHub Group ID: **UCLA-Plasma-Simulation-Group**  
Project ID: **upic-emma**



<http://picksc.idre.ucla.edu/>

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<sup>2</sup> P.Yu et al., Jour. Comp. Phys., Volume 266, 1 June 2014, Pages 124-138

<sup>3</sup> P.Yu, Yu, PhD Dissertation, UCLA: Electrical Engineering 0303 (2016)

# Units

## Units

Let's note the plasma electron frequency and the thermal electron velocity

$$\omega_p = \sqrt{\frac{4\pi n_{e,0} e^2}{m_e}} \text{ where } n_{e,0} = \frac{N_e d_e}{N_x N_y N_z \Delta^3} \frac{1}{\Delta_x \Delta_y \Delta_z} \text{ and } v_{Th} = \sqrt{\frac{k_B T_{e,0}}{m_e}}.$$

Normalized quantity	$\underline{t}$	$\underline{r}$	$\underline{k}$	$\underline{v}_{a,\ell}$	$\underline{m}_a$	$\underline{p}_{a,\ell}$	$\underline{q}_a$	$\underline{\rho}$
=	$\omega t$	$\frac{\mathbf{r}}{\Delta}$	$\mathbf{k}\Delta$	$\frac{\mathbf{v}_{a,\ell}}{\omega\Delta}$	$\frac{m_a}{m_e}$	$\frac{\mathbf{p}_{a,\ell}}{m_a\omega\Delta}$	$\frac{q_a}{e}$	$\frac{\rho}{en_0}$

Normalized quantity	$\underline{\mathbf{j}}$	$\underline{\mathbf{E}}$	$\underline{\mathbf{B}}$
=	$\frac{\mathbf{j}}{en_0\Delta\omega}$	$\frac{e\mathbf{E}}{m_e\omega^2\Delta}$	$\frac{e\mathbf{B}}{m_e\omega^2\Delta}$

$(\Delta, \omega)$  are free parameters choosen by the user :

$$\left\{ \begin{array}{lll} \text{Electrostatic units :} & (\Delta, \omega) & = \left( \frac{v_{Th}/\omega_p}{}, \frac{\omega_p}{}, \right) \\ \text{Electromagnetic units :} & (\Delta, \omega) & = \left( \frac{c/\omega_p}{}, \frac{\omega_p}{}, \right) \\ \text{LPI units :} & (\Delta, \omega) & = \left( \frac{c/\omega_L}{}, \frac{\omega_L}{}, \right) \end{array} \right.$$

# OSIRIS versus UPIC-EMMA units

## Electrical Charge and Current Deposit

$$\underline{\rho} = \sum_{a=e, i} \sum_{\ell=1}^{N_a} q_a w_f S_a^3 [\underline{r} - \underline{r}_{a,\ell}(t)] \text{ and } \underline{j} = \sum_{a=e, i} \sum_{\ell=1}^{N_a} q_a w_f v_{a,\ell}(t) S_a^3 [\underline{r} - \underline{r}_{a,\ell}(t)] \text{ where } w_f = \frac{1}{n_0 \Delta^3}$$

## Maxwell Equations

$$\text{Maxwell-Gauss : } \nabla \cdot \underline{\mathbf{E}} = a_f \underline{\rho} \quad \text{Maxwell-Faraday : } \frac{\partial \underline{\mathbf{B}}}{\partial t} = - \underline{\mathbf{c}} \nabla \times \underline{\mathbf{E}}$$

$$\text{Maxwell-Thomson : } \nabla \cdot \underline{\mathbf{B}} = 0 \quad \text{Maxwell-Ampere : } \frac{\partial \underline{\mathbf{E}}}{\partial t} = \underline{\mathbf{c}} \nabla \times \underline{\mathbf{B}} - a_f \underline{j}$$

$$\text{where } \underline{\mathbf{c}} = \frac{\underline{\mathbf{c}}}{\omega \Delta} \text{ and } a_f = \frac{\omega_0^2}{\omega^2} \text{ with } \omega_0 = \sqrt{\frac{4\pi n_0 e^2}{m_e}}$$

## Macro particle pusher

$$\frac{d\underline{r}_{a,\ell}}{dt} = \underline{v}_{a,\ell}(t) = \frac{\underline{p}_{a,\ell}(t)}{\gamma_{a,\ell}(t)} \frac{d\underline{p}_{a,\ell}}{dt} = \frac{q_a}{m_a} \left( \underline{\mathbf{E}} + \frac{\underline{v}_{a,\ell}}{\underline{\mathbf{c}}} \times \underline{\mathbf{B}} \right)$$

## OSIRIS choice

$$a_f = 1 \Leftrightarrow n_0 = \frac{m_e \omega^2}{4\pi e^2} \text{ and } w_f = \frac{1}{n_0 \Delta^3}$$

## UPIC-EMMA choice

$$w_f = 1 \Leftrightarrow n_0 = \frac{1}{\Delta^3} \text{ and } a_f = \frac{4\pi e^2}{m_e \omega^2 \Delta^3}$$

# Longitudinal and Transverse components Splitting

## Longitudinal and Transverse components Splitting

Let us note

$$\underline{\mathbf{E}} = \underline{\mathbf{E}}_L + \underline{\mathbf{E}}_T \text{ and } \underline{\mathbf{j}} = \underline{\mathbf{j}}_L + \underline{\mathbf{j}}_T$$

where  $\left\{ \begin{array}{l} \nabla \cdot \underline{\mathbf{E}}_T = 0 \\ \nabla \cdot \underline{\mathbf{E}}_L = 0 \end{array} \right.$  and  $\left\{ \begin{array}{l} \nabla \cdot \underline{\mathbf{j}}_T = 0 \\ \nabla \cdot \underline{\mathbf{j}}_L = 0 \end{array} \right.$

## Maxwell equations with UPIC-EMMA units

Maxwell-Gauss :  $\nabla \cdot \underline{\mathbf{E}}_L = a_f \rho \text{ and } \nabla \cdot \underline{\mathbf{E}}_T = 0$

Maxwell-Thomson :  $\nabla \cdot \underline{\mathbf{B}} = 0$

Maxwell-Faraday :  $\frac{\partial \underline{\mathbf{B}}}{\partial t} = -c \nabla \times \underline{\mathbf{E}}_T \text{ and } \nabla \times \underline{\mathbf{E}}_L = 0$

Maxwell-Ampere :  $\frac{\partial \underline{\mathbf{E}}_T}{\partial t} = c \nabla \times \underline{\mathbf{B}} - a_f \underline{\mathbf{j}}_T \text{ and } \frac{\partial \underline{\mathbf{E}}_L}{\partial t} = -a_f \underline{\mathbf{j}}_L$

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# Spectral Method (1)

Continuous and  $\underline{L}_x$ ,  $\underline{L}_y$  and  $\underline{L}_z$ -Periodic Solutions : Fourier series

$$\forall \underline{E} \in \{\underline{\rho}, \underline{j}, \underline{E}, \underline{B}\}$$

$$\underline{E}(\underline{r}, \underline{t}) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} \widehat{\underline{E}}^{p,q,r}(\underline{t}) \exp \left[ \iota \left( \underline{k}_x^p \underline{x} + \underline{k}_y^q \underline{y} + \underline{k}_z^r \underline{z} \right) \right]$$

where

$$\widehat{\underline{E}}^{p,q,r}(\underline{t}) = \frac{1}{\underline{L}_x} \frac{1}{\underline{L}_y} \frac{1}{\underline{L}_z} \int_0^{\underline{L}_x} d\underline{x} \int_0^{\underline{L}_y} d\underline{y} \int_0^{\underline{L}_z} d\underline{z} \underline{E}(\underline{r}, \underline{t}) \exp \left[ -\iota \left( \underline{k}_x^p \underline{x} + \underline{k}_y^q \underline{y} + \underline{k}_z^r \underline{z} \right) \right]$$

and

$$\forall (p, q, r) \in \mathbb{N}^3, \underline{k}_{p,q,r} = \begin{pmatrix} \underline{k}_x^p \\ \underline{k}_y^q \\ \underline{k}_z^r \end{pmatrix} = \begin{pmatrix} 2\pi(p-1)/\Delta_x \\ 2\pi(q-1)/\Delta_y \\ 2\pi(r-1)/\Delta_z \end{pmatrix}.$$

All Electromagnetic Modes ( $\underline{E}^{p,q,r}$ ,  $\underline{B}^{p,q,r}$ ) are given now by Maxwell Equations with...

$$\underline{\nabla} \rightarrow \iota \underline{k}_{p,q,r}$$

(ideal method for Linear Partial Differential Equations)

## Spectral Method (2)

### Discretization of space and time

Let us note  $N_x = \underline{L}_x / \Delta_x$ ,  $N_y = \underline{L}_y / \Delta_y$ ,  $N_z = \underline{L}_z / \Delta_z$ ,  $t_n = (n - 1) \Delta_t$  and

$$\forall (i, j, k) \in [1, N_x] \times [1, N_y] \times [1, N_z], \mathbf{r}_{i,j,k} = \begin{pmatrix} \underline{x}_i \\ \underline{y}_j \\ \underline{z}_k \end{pmatrix} = \begin{pmatrix} (i - 1) \Delta_x \\ (j - 1) \Delta_y \\ (r - 1) \Delta_z \end{pmatrix}.$$

### Discrete and $\underline{L}_x$ , $\underline{L}_y$ and $\underline{L}_z$ -Periodic Solutions : Discrete Fourier Transform (DFT)

$$\underline{E}^{i,j,k,n} = \underline{E}(\mathbf{r}_{i,j,k}, t_n) \stackrel{\text{DFT}}{=} \sum_{p=1}^{N_x} \sum_{q=1}^{N_y} \sum_{r=1}^{N_z} \widehat{\underline{E}}^{p,q,r,n} \exp \left[ \iota \left( \underline{k}_x^p \underline{x}_i + \underline{k}_y^q \underline{y}_j + \underline{k}_z^r \underline{z}_k \right) \right]$$

$$\text{and } \widehat{\underline{E}}^{p,q,r,n} \stackrel{\text{IDFT}}{=} \frac{1}{N_x} \frac{1}{N_y} \frac{1}{N_z} \sum_{i=1}^{N_x} \sum_{q=1}^{N_y} \sum_{r=1}^{N_z} \underline{E}^{i,j,k,n} \exp \left[ -\iota \left( \underline{k}_x^p \underline{x}_i + \underline{k}_y^q \underline{y}_j + \underline{k}_z^r \underline{z}_k \right) \right]$$

that becomes  $2\pi/\Delta_x$ ,  $2\pi/\Delta_y$  and  $2\pi/\Delta_z$ -periodic along the  $k_x$ ,  $k_y$  and  $k_z$ -direction.

$$\Rightarrow \underline{\mathbf{k}}_{\text{Nyquist}} = \left( \underline{k}_x^{1+\frac{N_x}{2}}, \underline{k}_y^{1+\frac{N_y}{2}}, \underline{k}_z^{1+\frac{N_z}{2}} \right) = \left( \frac{\pi}{\Delta_x}, \frac{\pi}{\Delta_y}, \frac{\pi}{\Delta_z} \right) = \text{highest mode.}$$

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# UPIC-EMMA Maxwell Solver (1)

## UPIC-EMMA Maxwell Solver

$$\widehat{\underline{E}}_L^{p,q,r,n+1} = -\frac{\iota \underline{k}_{p,q,r}}{\underline{k}_{p,q,r}^2} \textcolor{red}{a_f} \widehat{\underline{\rho}}^{p,q,r,n+1}$$

$$\widehat{\underline{j}}_T^{p,q,r,n+1/2} = \widehat{\underline{j}}^{p,q,r,n+1/2} - \widehat{\underline{j}}_L^{p,q,r,n+1/2} \quad \text{with} \quad \widehat{\underline{j}}_L^{p,q,r,n+1/2} = \frac{\underline{k}_{p,q,r}}{\underline{k}_{p,q,r}^2} \underline{k}_{p,q,r} \cdot \widehat{\underline{j}}^{p,q,r,n+1/2}$$

$$\left\{ \begin{array}{lcl} \widehat{\underline{B}}^{p,q,r,n+1/2} & = & \widehat{\underline{B}}^{p,q,r,n} - \frac{\Delta_t}{2} \textcolor{red}{c} (\iota \underline{k}_{p,q,r}) \times \widehat{\underline{E}}_T^{p,q,r,n} \\ \widehat{\underline{E}}_T^{p,q,r,n+1} & = & \widehat{\underline{E}}_T^{p,q,r,n} + \Delta_t \textcolor{red}{c} (\iota \underline{k}_{p,q,r}) \times \widehat{\underline{B}}^{p,q,r,n+1/2} \\ \widehat{\underline{B}}^{p,q,r,n+1} & = & \widehat{\underline{B}}^{p,q,r,n+1/2} - \frac{\Delta_t}{2} \textcolor{red}{a_f} \widehat{\underline{j}}_T^{p,q,r,n+1/2} \end{array} \right.$$

without forgetting

$$\left\{ \begin{array}{lcl} \iota \underline{k}_{p,q,r} \cdot \underline{E}_T^{p,q,r,n} & = & 0 \\ \iota \underline{k}_{p,q,r} \cdot \underline{j}_T^{p,q,r,n+\frac{1}{2}} & = & 0 \\ \iota \underline{k}_{p,q,r} \cdot \underline{B}^{p,q,r,n+\frac{1}{2}} & = & 0 \end{array} \right.$$

$$\Rightarrow \forall (p, q, r) \neq 1, \left\{ \begin{array}{lcl} \underline{E}_{T,x}^{p,1,1,n} & = & \underline{E}_{T,y}^{1,q,1,n} = \underline{E}_{T,z}^{1,1,r,n} = 0 \\ \underline{j}_{T,x}^{p,1,1,n+\frac{1}{2}} & = & \underline{j}_{T,y}^{1,q,1,n+\frac{1}{2}} = \underline{j}_{T,z}^{1,1,r,n+\frac{1}{2}} = 0 \\ \underline{B}_x^{p,1,1,n+\frac{1}{2}} & = & \underline{B}_y^{1,q,1,n+\frac{1}{2}} = \underline{B}_z^{1,1,r,n+\frac{1}{2}} = 0 \end{array} \right. .$$

## UPIC-EMMA Maxwell Solver (2)

### Deduced Numerical Helmholtz Equations

$$\begin{aligned} \frac{\hat{\mathbf{E}}_T^{p,q,r,n+1} - 2\hat{\mathbf{E}}_T^{p,q,r,n} + \hat{\mathbf{E}}_T^{p,q,r,n-1}}{\Delta t^2} + \underline{k}_{p,q,r}^2 \underline{c}^2 \hat{\mathbf{E}}_T^{p,q,r,n} &= -\underline{a}_f \frac{\hat{\mathbf{j}}_T^{p,q,r,n+\frac{1}{2}} - \hat{\mathbf{j}}_T^{p,q,r,n-\frac{1}{2}}}{\Delta t} \\ \frac{\hat{\mathbf{B}}^{p,q,r,n+\frac{3}{2}} - 2\hat{\mathbf{B}}^{p,q,r,n+\frac{1}{2}} + \hat{\mathbf{B}}^{p,q,r,n-\frac{1}{2}}}{\Delta t^2} + \underline{k}_{p,q,r}^2 \underline{c}^2 \hat{\mathbf{B}}_T^{p,q,r,n+\frac{1}{2}} &= \underline{a}_f \underline{c} (\underline{\epsilon} \underline{k}_{p,q,r}) \times \hat{\mathbf{j}}_T^{p,q,r,n+\frac{1}{2}} \end{aligned}$$

### Deduced Stability Condition

$$\Delta t \leq \sqrt{2} / |\underline{k}_{\text{Nyquist}}| \underline{c}.$$

SLIGHTLY MORE RESTRICTIVE THAN THE YEE SCHEME CFL CONDITION!

## UPIC-EMMA Maxwell Solver (3)

### Electromagnetic Fields Initialization : Darwin Fields

$$\underline{\widehat{\mathbf{E}}}_L^{p,q,r,0} = -\frac{i\underline{\mathbf{k}}_{p,q,r}}{\underline{\mathbf{k}}_{p,q,r}^2} \textcolor{red}{a_f} \underline{\widehat{\rho}}^{p,q,r,0},$$

$$\underline{\widehat{\mathbf{j}}}_T^{p,q,r,0} = \underline{\widehat{\mathbf{j}}}^{p,q,r,0} - \underline{\widehat{\mathbf{j}}}_L^{p,q,r,0} \text{ with } \underline{\widehat{\mathbf{j}}}_L^{p,q,r,0} = \frac{\underline{\mathbf{k}}_{p,q,r}}{\underline{\mathbf{k}}_{p,q,r}^2} \underline{\mathbf{k}}_{p,q,r} \cdot \underline{\widehat{\mathbf{j}}}^{p,q,r,0},$$

$$\frac{\partial \underline{\widehat{\mathbf{j}}}_T}{\partial t} \Big|^{p,q,r,0} = \frac{\partial \underline{\widehat{\mathbf{j}}}}{\partial t} \Big|^{p,q,r,0} - \frac{\partial \underline{\widehat{\mathbf{j}}}_L}{\partial t} \Big|^{p,q,r,0} \text{ with } \frac{\partial \underline{\widehat{\mathbf{j}}}_L}{\partial t} \Big|^{p,q,r,0} = \frac{\underline{\mathbf{k}}_{p,q,r}}{\underline{\mathbf{k}}_{p,q,r}^2} \underline{\mathbf{k}}_{p,q,r} \cdot \frac{\partial \underline{\widehat{\mathbf{j}}}}{\partial t} \Big|^{p,q,r,0}$$

and

$$\left\{ \begin{array}{l} \underline{\widehat{\mathbf{B}}}^{p,q,r,0} = \frac{\textcolor{red}{a_f}}{c} \frac{1}{\underline{\mathbf{k}}_{p,q,r}^2} (\iota \underline{\mathbf{k}}_{p,q,r}) \times \underline{\widehat{\mathbf{j}}}_T^{p,q,r,0} \\ \underline{\widehat{\mathbf{E}}}_T^{p,q,r,0} = -\frac{\textcolor{red}{a_f}}{c^2} \frac{1}{\underline{\mathbf{k}}_{p,q,r}^2} \frac{\partial \underline{\widehat{\mathbf{j}}}_T}{\partial t} \Big|^{p,q,r,0} \end{array} \right. \ll \left\{ \begin{array}{l} \nabla \times \underline{\widehat{\mathbf{B}}} = \frac{\textcolor{red}{a_f}}{c} \underline{\widehat{\mathbf{j}}} + \frac{1}{c} \frac{\partial \underline{\widehat{\mathbf{E}}}_L}{\partial t} \\ \nabla \times \underline{\widehat{\mathbf{E}}}_T = -\frac{1}{c} \frac{\partial \underline{\widehat{\mathbf{B}}}}{\partial t} \end{array} \right.$$

without forgetting

$$\forall (p, q, r) \neq 1, \left\{ \begin{array}{l} \underline{\mathbf{E}}_T^{p,1,1,0} = \underline{\mathbf{E}}_T^{1,q,1,0} = \underline{\mathbf{E}}_T^{1,1,r,0} = 0 \\ \underline{\mathbf{B}}_x^{p,1,1,0} = \underline{\mathbf{B}}_y^{1,q,1,0} = \underline{\mathbf{B}}_z^{1,1,r,0} = 0 \end{array} \right..$$

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Yee Scheme with an order of accuracy  $N = 2s$  - Magnetic Field UpdateYee Scheme with an order of accuracy  $N = 2s$  - Magnetic Field Update

$$\left\{ \begin{array}{l} \frac{\underline{B}_x^{i,j-\frac{1}{2},k-\frac{1}{2},n+\frac{1}{2}} - \underline{B}_x^{i,j-\frac{1}{2},k-\frac{1}{2},n-\frac{1}{2}}}{\Delta_t} = \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,y}^{i,j-\frac{1}{2},k+m-1,n} - \underline{E}_{T,y}^{i,j-\frac{1}{2},k-m,n}}{\Delta_z} \\ \quad - \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,z}^{i,j+m-1,k-\frac{1}{2},n} - \underline{E}_{T,z}^{i,j-m,k-\frac{1}{2},n}}{\Delta_y} \\ \frac{\underline{B}_y^{i-\frac{1}{2},j,k-\frac{1}{2},n+\frac{1}{2}} - \underline{B}_y^{i-\frac{1}{2},j,k-\frac{1}{2},n-\frac{1}{2}}}{\Delta_t} = \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,z}^{i+m-1,j,k-\frac{1}{2},n} - \underline{E}_{T,z}^{i-m,j,k-\frac{1}{2},n}}{\Delta_x} \\ \quad - \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,x}^{i-\frac{1}{2},j,k+m-1,n} - \underline{E}_{T,x}^{i-\frac{1}{2},j,k-m,n}}{\Delta_z} \\ \frac{\underline{B}_z^{i-\frac{1}{2},j-\frac{1}{2},k,n+\frac{1}{2}} - \underline{B}_z^{i-\frac{1}{2},j-\frac{1}{2},k,n-\frac{1}{2}}}{\Delta_t} = \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,x}^{i-\frac{1}{2},j+m-1,k,n} - \underline{E}_{T,x}^{i-\frac{1}{2},j-m,k,n}}{\Delta_y} \\ \quad - \underline{c} \sum_{m=1}^s C_m \frac{\underline{E}_{T,y}^{i+m-1,j-\frac{1}{2},k,n} - \underline{E}_{T,y}^{i-m,j-\frac{1}{2},k,n}}{\Delta_x} \end{array} \right.$$

with

$$C_m = \frac{1}{2m-1} \prod_{\substack{l=1 \\ l \neq m}}^s \frac{(2l-1)^2}{(2l-1)^2 - (2m-1)^2}.$$

# Yee Scheme with an order of accuracy $N = 2s$ - Electric Field Update

Yee Scheme with an order of accuracy  $N = 2s$  - Electric Field Update

$$\left\{ \begin{array}{lcl}
 \frac{\underline{E}_{T,x}^{i-\frac{1}{2},j,k,n+1} - \underline{E}_{T,x}^{i-\frac{1}{2},j,k,n}}{\Delta t} & = & -a_f \underline{j}_{T,x}^{i-\frac{1}{2},j,k,n+\frac{1}{2}} \\
 & + & \sum_{m=1}^s c_m \frac{\underline{B}_z^{i-\frac{1}{2},j-\frac{1}{2}+m,k,n+\frac{1}{2}} - \underline{B}_z^{i-\frac{1}{2},j-\frac{1}{2}-m+1,k,n+\frac{1}{2}}}{\Delta y} \\
 & - & \sum_{m=1}^s c_m \frac{\underline{B}_y^{i-\frac{1}{2},j,k-\frac{1}{2}+m,n+\frac{1}{2}} - \underline{B}_y^{i-\frac{1}{2},j,k-\frac{1}{2}-m+1,n+\frac{1}{2}}}{\Delta z} \\
 \\ 
 \frac{\underline{E}_{T,y}^{i,j-\frac{1}{2},k,n+1} - \underline{E}_{T,y}^{i,j-\frac{1}{2},k,n}}{\Delta t} & = & -a_f \underline{j}_{T,y}^{i,j-\frac{1}{2},k,n+\frac{1}{2}} \\
 & = & \sum_{m=1}^s c_m \frac{\underline{B}_x^{i,j-\frac{1}{2},k-\frac{1}{2}+m,n+\frac{1}{2}} - \underline{B}_x^{i,j-\frac{1}{2},k-\frac{1}{2}-m+1,n+\frac{1}{2}}}{\Delta z} \\
 & - & \sum_{m=1}^s c_m \frac{\underline{B}_z^{i-\frac{1}{2}+m,j-\frac{1}{2},k,n-\frac{1}{2}} - \underline{B}_z^{i-\frac{1}{2}-m+1,j-\frac{1}{2},k,n+\frac{1}{2}}}{\Delta x} \\
 \\ 
 \frac{\underline{E}_{T,z}^{i,j,k-\frac{1}{2},n+1} - \underline{E}_{T,z}^{i,j,k-\frac{1}{2},n}}{\Delta t} & = & -a_f \underline{j}_{T,z}^{i,j,k-\frac{1}{2},n+\frac{1}{2}} \\
 & = & \sum_{m=1}^s c_m \frac{\underline{B}_y^{i-\frac{1}{2}+m,j,k-\frac{1}{2},n+\frac{1}{2}} - \underline{B}_y^{i-\frac{1}{2}-m+1,j,k-\frac{1}{2},n+\frac{1}{2}}}{\Delta x} \\
 & - & \sum_{m=1}^s c_m \frac{\underline{B}_x^{i,j-\frac{1}{2}+m,k-\frac{1}{2},n+\frac{1}{2}} - \underline{B}_x^{i,j-\frac{1}{2}-m+1,k-\frac{1}{2},n+\frac{1}{2}}}{\Delta y}
 \end{array} \right.$$

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- Implementation in a Spectral Solver
- 2D Academic Case : Cylindrical wave

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# Implementation in a Spectral Solver (1)

Inverse Discrete Fourier Transform (IDFT) of B field equations

$$\left\{ \begin{array}{l} \frac{\left[ \hat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-\iota(\theta_y^q + \theta_z^r)} \right] - \left[ \hat{B}_x^{p,q,r,n-\frac{1}{2}} e^{-\iota(\theta_y^q + \theta_z^r)} \right]}{\Delta t} \\ \quad = \iota \left\{ k_z^r \right\} \subseteq e^{-\iota \theta_z^r} \left[ \hat{E}_{T,y}^{p,q,r,n} e^{-\iota \theta_y^q} \right] \\ \quad - \iota \left\{ k_y^q \right\} \subseteq e^{-\iota \theta_y^q} \left[ \hat{E}_{T,z}^{p,q,r,n} e^{-\iota \theta_z^r} \right] \\ \\ \frac{\left[ \hat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-\iota(\theta_x^p + \theta_z^r)} \right] - \left[ \hat{B}_y^{p,q,r,n-\frac{1}{2}} e^{-\iota(\theta_x^p + \theta_z^r)} \right]}{\Delta t} \\ \quad = \iota \left\{ k_x^p \right\} \subseteq e^{-\iota \theta_x^p} \left[ \hat{E}_{T,z}^{p,q,r,n} e^{-\iota \theta_z^r} \right] \\ \quad - \iota \left\{ k_z^r \right\} \subseteq e^{-\iota \theta_z^r} \left[ \hat{E}_{T,x}^{p,q,r,n} e^{-\iota \theta_x^p} \right] \\ \\ \frac{\left[ \hat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-\iota(\theta_x^p + \theta_y^q)} \right] - \left[ \hat{B}_z^{p,q,r,n-\frac{1}{2}} e^{-\iota(\theta_x^p + \theta_y^q)} \right]}{\Delta t} \\ \quad = \iota \left\{ k_y^q \right\} \subseteq e^{-\iota \theta_y^q} \left[ \hat{E}_{T,x}^{p,q,r,n} e^{-\iota \theta_x^p} \right] \\ \quad - \iota \left\{ k_x^p \right\} \subseteq e^{-\iota \theta_x^p} \left[ \hat{E}_{T,y}^{p,q,r,n} e^{-\iota \theta_y^q} \right] \end{array} \right.$$

$$\text{with } \left\{ \begin{array}{l} \left\{ k_x^p \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)k_x^p \Delta_x / 2]}{\Delta_x / 2} \\ \left\{ k_y^q \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)k_y^q \Delta_y / 2]}{\Delta_y / 2} \\ \left\{ k_z^r \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)k_z^r \Delta_z / 2]}{\Delta_z / 2} \end{array} \right.$$

$$\text{and } \left\{ \begin{array}{l} \theta_x^p = \frac{k_x^p \Delta_x}{2} \\ \theta_y^q = \frac{k_y^q \Delta_y}{2} \\ \theta_z^r = \frac{k_z^r \Delta_z}{2} \end{array} \right.$$

# Implementation in a Spectral Solver (1)

Inverse Discrete Fourier Transform (IDFT) of B field equations

$$\left\{ \begin{array}{l}
 \frac{\left[ \hat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_y + \theta_z)} \right] - \left[ \hat{B}_x^{p,q,r,n-\frac{1}{2}} e^{-i(\theta_y + \theta_z)} \right]}{\Delta t} \\
 \\ 
 \frac{\left[ \hat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x + \theta_z)} \right] - \left[ \hat{B}_y^{p,q,r,n-\frac{1}{2}} e^{-i(\theta_x + \theta_z)} \right]}{\Delta t} \\
 \\ 
 \frac{\left[ \hat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x + \theta_y)} \right] - \left[ \hat{B}_z^{p,q,r,n-\frac{1}{2}} e^{-i(\theta_x + \theta_y)} \right]}{\Delta t}
 \end{array} \right. = \begin{array}{l}
 i \left\{ k_z^r \right\} \subseteq e^{-i\theta_z} \left[ \hat{E}_{T,y}^{p,q,r,n} e^{-i\theta_y} \right] \\
 - i \left\{ k_y^q \right\} \subseteq e^{-i\theta_y} \left[ \hat{E}_{T,z}^{p,q,r,n} e^{-i\theta_z} \right] \\
 \\ 
 i \left\{ k_x^p \right\} \subseteq e^{-i\theta_x} \left[ \hat{E}_{T,z}^{p,q,r,n} e^{-i\theta_z} \right] \\
 - i \left\{ k_z^r \right\} \subseteq e^{-i\theta_z} \left[ \hat{E}_{T,x}^{p,q,r,n} e^{-i\theta_x} \right] \\
 \\ 
 i \left\{ k_y^q \right\} \subseteq e^{-i\theta_y} \left[ \hat{E}_{T,x}^{p,q,r,n} e^{-i\theta_x} \right] \\
 - i \left\{ k_x^p \right\} \subseteq e^{-i\theta_x} \left[ \hat{E}_{T,y}^{p,q,r,n} e^{-i\theta_y} \right]
 \end{array}$$

where  $\left\{ \begin{array}{l} \left\{ k_x^p \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)\underline{k}_x^p \Delta_x / 2]}{\Delta_x / 2} \\ \left\{ k_y^q \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)\underline{k}_y^q \Delta_y / 2]}{\Delta_y / 2} \\ \left\{ k_z^r \right\} = \sum_{m=1}^s c_m \frac{\sin[(2m-1)\underline{k}_z^r \Delta_z / 2]}{\Delta_z / 2} \end{array} \right.$

and  $\left\{ \begin{array}{l} \theta_x^p = \underline{k}_x^p \Delta_x / 2 \\ \theta_y^q = \underline{k}_y^q \Delta_y / 2 \\ \theta_z^r = \underline{k}_z^r \Delta_z / 2 \end{array} \right.$

# Implementation in a Spectral Solver (2)

Inverse Discrete Fourier Transform (IDFT) of E field equations

$$\left\{ \begin{array}{l}
 \frac{\left[ \widehat{E}_{T,x}^{p,q,r,n+1} e^{-\iota \theta_x^p} \right] - \left[ \widehat{E}_{T,x}^{p,q,r,n} e^{-\iota \theta_x^p} \right]}{\Delta_t} = -a_f \left[ \widehat{j}_{T,x}^{p,q,r,n+\frac{1}{2}} e^{-\iota \theta_x^p} \right] \\
 - \iota \left\{ k_z^r \right\} \subseteq e^{\iota \theta_z^r} \left[ \widehat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_x^p + \theta_z^r)} \right] \\
 + \iota \left\{ k_y^q \right\} \subseteq e^{\iota \theta_y^q} \left[ \widehat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_x^p + \theta_y^q)} \right] \\
 \\ 
 \frac{\left[ \widehat{E}_{T,y}^{p,q,r,n+1} e^{-\iota \theta_y^q} \right] - \left[ \widehat{E}_{T,y}^{p,q,r,n} e^{-\iota \theta_y^q} \right]}{\Delta_t} = -a_f \left[ \widehat{j}_{T,y}^{p,q,r,n+\frac{1}{2}} e^{-\iota \theta_y^q} \right] \\
 - \iota \left\{ k_x^p \right\} \subseteq e^{\iota \theta_x^p} \left[ \widehat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_x^p + \theta_y^q)} \right] \\
 + \iota \left\{ k_z^r \right\} \subseteq e^{\iota \theta_z^r} \left[ \widehat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_y^q + \theta_z^r)} \right] \\
 \\ 
 \frac{\left[ \widehat{E}_{T,z}^{p,q,r,n+1} e^{-\iota \theta_z^r} \right] - \left[ \widehat{E}_{T,z}^{p,q,r,n} e^{-\iota \theta_z^r} \right]}{\Delta_t} = -a_f \left[ \widehat{j}_{T,z}^{p,q,r,n+\frac{1}{2}} e^{-\iota \theta_z^r} \right] \\
 - \iota \left\{ k_y^q \right\} \subseteq e^{\iota \theta_y^q} \left[ \widehat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_y^q + \theta_z^r)} \right] \\
 + \iota \left\{ k_x^p \right\} e^{\iota \theta_x^p} \subseteq \left[ \widehat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-\iota (\theta_x^p + \theta_z^r)} \right]
 \end{array} \right. .$$

# Implementation in a Spectral Solver (2)

Inverse Discrete Fourier Transform (IDFT) of E field equations

$$\left\{ \begin{array}{l}
 \frac{\left[ \widehat{E}_{T,x}^{p,q,r,n+1} e^{-i\theta_x^p} \right] - \left[ \widehat{E}_{T,x}^{p,q,r,n} e^{-i\theta_x^p} \right]}{\Delta t} = -a_f \left[ \widehat{j}_{T,x}^{p,q,r,n+\frac{1}{2}} e^{-i\theta_x^p} \right] \\
 \quad - \iota \left\{ k_z^r \right\} \underline{c} e^{i\theta_z^r} \left[ \widehat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x^p + \theta_z^r)} \right] \\
 \quad + \iota \left\{ k_y^q \right\} \underline{c} e^{i\theta_y^q} \left[ \widehat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x^p + \theta_y^q)} \right] \\
 \\ 
 \frac{\left[ \widehat{E}_{T,y}^{p,q,r,n+1} e^{-i\theta_y^q} \right] - \left[ \widehat{E}_{T,y}^{p,q,r,n} e^{-i\theta_y^q} \right]}{\Delta t} = -a_f \left[ \widehat{j}_{T,y}^{p,q,r,n+\frac{1}{2}} e^{-i\theta_y^q} \right] \\
 \quad - \iota \left\{ k_x^p \right\} \underline{c} e^{i\theta_x^p} \left[ \widehat{B}_z^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x^p + \theta_y^q)} \right] \\
 \quad + \iota \left\{ k_z^r \right\} \underline{c} e^{i\theta_z^r} \left[ \widehat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_y^q + \theta_z^r)} \right] \\
 \\ 
 \frac{\left[ \widehat{E}_{T,z}^{p,q,r,n+1} e^{-i\theta_z^r} \right] - \left[ \widehat{E}_{T,z}^{p,q,r,n} e^{-i\theta_z^r} \right]}{\Delta t} = -a_f \left[ \widehat{j}_{T,z}^{p,q,r,n+\frac{1}{2}} e^{-i\theta_z^r} \right] \\
 \quad - \iota \left\{ k_y^q \right\} \underline{c} e^{i\theta_y^q} \left[ \widehat{B}_x^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_y^q + \theta_z^r)} \right] \\
 \quad + \iota \left\{ k_x^p \right\} \underline{c} e^{i\theta_x^p} \left[ \widehat{B}_y^{p,q,r,n+\frac{1}{2}} e^{-i(\theta_x^p + \theta_z^r)} \right]
 \end{array} \right. .$$

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# Initialization

## Nominal Simulation Parameters

- 2D
- Periodic boundary conditions
- Electromagnetic units ( $\epsilon = 1$ )
- 4 MPI nodes and 2 OpenMP threads per node
- $L_x = L_y = 128$
- $L_{PML} = 30$
- $\Delta_x = \Delta_y = 1$
- $L_t = 128$
- $a_f = 1$

## Electrical Current Density Initialization and Expected Solutions

$$j_T^{i,j,k,n} = \begin{cases} j_0 \sin(\omega_0 t_n) \mathbf{e}_z & \text{if } \begin{cases} 63 \leq x_i \leq 65 \\ 63 \leq y_j \leq 65 \end{cases} \\ 0 & \text{else} \end{cases} \quad \text{with } \omega_0 = 1 \text{ and } j_0 = -10.$$

$$\Rightarrow \begin{cases} E_{T,r}^{i,j,k,n} &= 0 \\ E_{T,z}^{i,j,k,n} &\approx \frac{E_0}{\sqrt{|r_{i,j,k} - r_0|}} \cos(\omega_0 t_n - k_0 |r_{i,j,k} - r_0|) \\ B_r^{i,j,k,n} &\approx \frac{E_0}{\sqrt{|r_{i,j,k} - r_0|}} \sin(\omega_0 t_n - k_0 |r_{i,j,k} - r_0|) \\ B_z^{i,j,k,n} &= 0 \end{cases}$$

with  $E_0 = a_f j_0 / \omega_0 = 10$ ,  $r_0 = (64, 64)$  and  $k_0 = \omega_0 / \epsilon = 1$ .

## FTFD order 2 - Yee versus Spectrally Emulated

Figure 1:  $E_z$  (left),  $B_x$  (middle) and  $B_y$  (right) in log scale (top) and emulated (bottom)

## Emulated FTFD order $N = 128$ versus Spectral

Figure 2: FTFD-128  $E_z$  (left),  $B_x$  (middle) and  $B_y$  (right) in log scale (top) and spectral (bottom)

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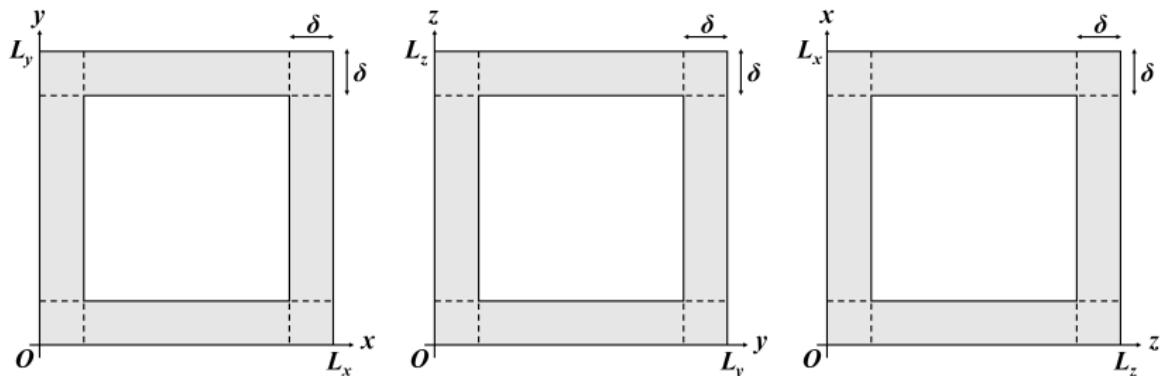
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# Absorbing boundary conditions (1)



## Michael D. Meyers Idea

The spectral solver remains exact if we dump the electromagnetic fields in the grey regions of thickness  $\delta$  according to the Perfectly Matched Layers (PML) method developed for Finite Difference schemes such that the electromagnetic fields vanishes at the simulation box boundaries.

$$\begin{aligned} \forall j &\in [1, N_y], \quad \forall k &\in [1, N_z], \quad \underline{\mathbf{E}}^{1,j,k,n} = \underline{\mathbf{E}}^{N_x,j,k,n} = \mathbf{0}, \\ \forall i &\in [1, N_x], \quad \forall j &\in [1, N_y], \quad \underline{\mathbf{E}}^{i,j,1,n} = \underline{\mathbf{E}}^{i,j,N_z,n} = \mathbf{0} \text{ and} \\ \forall k &\in [1, N_z], \quad \forall i &\in [1, N_x], \quad \underline{\mathbf{E}}^{i,1,k,n} = \underline{\mathbf{E}}^{i,N_y,k,n} = \mathbf{0}. \end{aligned}$$

## Absorbing boundary conditions (2)

### PML method

- ➊ Dumping terms are added into Maxwell-Ampere and Maxwell-Faraday :

$$\frac{\partial \underline{\mathbf{E}}_T}{\partial \underline{t}} + \underline{\sigma} \cdot \underline{\mathbf{E}}_T = \underline{c} \nabla \times \underline{\mathbf{B}} - a_f \underline{\mathbf{j}}_T \text{ and } \frac{\partial \underline{\mathbf{B}}}{\partial \underline{t}} + \underline{\sigma}^* \cdot \underline{\mathbf{B}} = -\underline{c} \nabla \times \underline{\mathbf{E}}_T$$

- ➋ Each component of the electromagnetic field is split into two parts :

$$\begin{cases} E_{T,x} = E_{xy} + E_{xz} \\ E_{T,y} = E_{yz} + E_{yx} \\ E_{T,z} = E_{zx} + E_{zy} \end{cases} \quad \text{and} \quad \begin{cases} B_x = B_{xy} + B_{xz} \\ B_y = B_{yz} + B_{yx} \\ B_z = B_{zx} + B_{zy} \end{cases}$$

and we have to solve the PML equations

$$\begin{cases} \partial_{\underline{t}} \underline{E}_{xy} + \underline{\sigma}_y(y) \underline{E}_{xy} = +\partial_y \underline{B}_z^{\text{PML}} \\ \partial_{\underline{t}} \underline{E}_{xz} + \underline{\sigma}_z(z) \underline{E}_{xz} = -\partial_z \underline{B}_y^{\text{PML}} \\ \partial_{\underline{t}} \underline{E}_{yz} + \underline{\sigma}_z(z) \underline{E}_{yz} = +\partial_z \underline{B}_x^{\text{PML}} \\ \partial_{\underline{t}} \underline{E}_{yx} + \underline{\sigma}_x(x) \underline{E}_{yx} = -\partial_x \underline{B}_z^{\text{PML}} \\ \partial_{\underline{t}} \underline{E}_{zx} + \underline{\sigma}_x(x) \underline{E}_{zx} = +\partial_x \underline{B}_y^{\text{PML}} \\ \partial_{\underline{t}} \underline{E}_{zy} + \underline{\sigma}_y(y) \underline{E}_{zy} = -\partial_y \underline{B}_x^{\text{PML}} \end{cases}$$

and

$$\begin{cases} \partial_{\underline{t}} \underline{B}_{xy} + \underline{\sigma}_y^*(y) \underline{B}_{xy} = -\partial_y \underline{E}_z^{\text{PML}} \\ \partial_{\underline{t}} \underline{B}_{xz} + \underline{\sigma}_z^*(z) \underline{B}_{xz} = +\partial_z \underline{E}_y^{\text{PML}} \\ \partial_{\underline{t}} \underline{B}_{yz} + \underline{\sigma}_z^*(z) \underline{B}_{yz} = -\partial_z \underline{E}_x^{\text{PML}} \\ \partial_{\underline{t}} \underline{B}_{yx} + \underline{\sigma}_x^*(x) \underline{B}_{yx} = +\partial_x \underline{E}_z^{\text{PML}} \\ \partial_{\underline{t}} \underline{B}_{zx} + \underline{\sigma}_x^*(x) \underline{B}_{zx} = -\partial_x \underline{E}_y^{\text{PML}} \\ \partial_{\underline{t}} \underline{B}_{zy} + \underline{\sigma}_y^*(y) \underline{B}_{zy} = +\partial_y \underline{E}_x^{\text{PML}} \end{cases}$$

with  $\sigma_\xi^*(\xi) = \sigma_\xi(\xi) = \sigma_m(|\xi - \xi_I|/\delta)^n$  ( $\xi = \xi_I \equiv \text{PML medium / simulation box interface}$ )

Remark :  $\sigma_\xi$  and  $\sigma_\xi^*$  depends on  $\xi \Rightarrow$  The PML Equations are not linear!

## Absorbing Boundary Conditions

Perfectly Matched Layer (PML) Technique for Finite Difference Schemes

## Absorbing boundary conditions (3)

PML Equations - Yee scheme - Electric field update

$$\left\{
 \begin{array}{lcl}
 E_{xy}^{i-1/2,j,k,n+1} & = & \alpha_y^j E_{xy}^{i-1/2,j,k,n} - \gamma_y^{i,j,k} j_{T,x}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_y^j \sum_{m=1}^s c_m \left( \underline{B}_z^{i-1/2,j-1/2+m,k,n+1/2} - \underline{B}_z^{i-1/2,j-1/2-m+1,k,n+1/2} \right) \\
 E_{xz}^{i-1/2,j,k,n+1} & = & \alpha_z^k E_{xz}^{i-1/2,j,k,n} - \gamma_z^{i,j,k} j_{T,x}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_z^k \sum_{m=1}^s c_m \left( \underline{B}_y^{i-1/2,j,k-1/2+m,n+1/2} - \underline{B}_y^{i-1/2,j,k-1/2-m+1,n+1/2} \right) \\
 E_{yz}^{i,j-1/2,k,n+1} & = & \alpha_z^k E_{yz}^{i,j-1/2,k,n} - \gamma_z^{i,j,k} j_{T,y}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_z^k \sum_{m=1}^s c_m \left( \underline{B}_x^{i,j-1/2,k-1/2+m,n+1/2} - \underline{B}_x^{i,j-1/2,k-1/2-m+1,n+1/2} \right) \\
 E_{yx}^{i,j-1/2,k,n+1} & = & \alpha_x^i E_{yx}^{i,j-1/2,k,n} - \gamma_x^{i,j,k} j_{T,y}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_x^i \sum_{m=1}^s c_m \left( \underline{B}_z^{i-1/2+m,j-1/2,k,n+1/2} - \underline{B}_z^{i-1/2-m+1,j-1/2,k,n+1/2} \right) \\
 E_{zx}^{i,j,k-1/2,n+1} & = & \alpha_x^i E_{zx}^{i,j,k-1/2,n} - \gamma_x^{i,j,k} j_{T,z}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_x^i \sum_{m=1}^s c_m \left( \underline{B}_y^{i-1/2+m,j,k-1/2,n+1/2} - \underline{B}_y^{i-1/2-m+1,j,k-1/2,n+1/2} \right) \\
 E_{zy}^{i,j,k-1/2,n+1} & = & \alpha_y^j E_{zy}^{i,j,k-1/2,n} - \gamma_y^{i,j,k} j_{T,z}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_y^j \sum_{m=1}^s c_m \left( \underline{B}_x^{i,j-1/2+m,k-1/2,n+1/2} - \underline{B}_x^{i,j-1/2-m+1,k-1/2,n+1/2} \right)
 \end{array}
 \right.$$

with  $\forall \xi \in \{x, y, z\}$ ,  $\alpha_\xi^{i,j,k} = \frac{1 - \sigma_\xi^{i,j,k} \Delta t / 2}{1 + \sigma_\xi^{i,j,k} \Delta t / 2}$ ,  $\beta_\xi^{i,j,k} = \frac{\epsilon \Delta t / \Delta \xi}{1 + \sigma_\xi^{i,j,k} / 2}$  and  $\gamma_\xi^{i,j,k} = \frac{\epsilon \Delta t}{1 + \sigma_\xi^{i,j,k} / 2}$

# Absorbing boundary conditions (4)

PML Equations - Yee scheme - Magnetic field update

$$\left\{ \begin{array}{lcl} \underline{B}_{xy}^{i,j-1/2,k-1/2,n+1/2} & = & \alpha_y^{*j-1/2} \underline{B}_{xy}^{i,j-1/2,k-1/2,n-1/2} \\ & - & \beta_y^{*j+1} \sum_{m=1}^s c_m \left( \underline{E}_z^{i,j+m-1,k-1/2,n} - \underline{E}_z^{i,j-m,k-1/2,n} \right) \\ \underline{B}_{xz}^{i,j-1/2,k-1/2,n+1/2} & = & \alpha_z^{*k-1/2} \underline{B}_{xz}^{i,j-1/2,k-1/2,n-1/2} \\ & + & \beta_z^{*k-1/2} \sum_{m=1}^s c_m \left( \underline{E}_y^{i,j-1/2,k+m-1,n} - \underline{E}_y^{i,j-1/2,k-m,n} \right) \\ \underline{B}_{yz}^{i-1/2,j,k-1/2,n+1/2} & = & \alpha_z^{*k-1/2} \underline{B}_{yz}^{i-1/2,j,k-1/2,n-1/2} \\ & - & \beta_z^{*k-1/2} \sum_{m=1}^s c_m \left( \underline{E}_x^{i-1/2,j,k+m-1,n} - \underline{E}_x^{i-1/2,j,k-m,n} \right) \\ \underline{B}_{yx}^{i-1/2,j,k-1/2,n+1/2} & = & \alpha_x^{*i-1/2} \underline{B}_{yx}^{i-1/2,j,k-1/2,n-1/2} \\ & + & \beta_x^{*i-1/2} \sum_{m=1}^s c_m \left( \underline{E}_z^{i+m-1,j,k-1/2,n} - \underline{E}_z^{i-m,j,k-1/2,n} \right) \\ \underline{B}_{zx}^{i-1/2,j-1/2,k,n+1/2} & = & \alpha_x^{*i-1/2} \underline{B}_{zx}^{i-1/2,j-1/2,k,n-1/2} \\ & - & \beta_x^{*i-1/2} \sum_{m=1}^s c_m \left( \underline{E}_y^{i+m-1,j-1/2,k,n} - \underline{E}_y^{i-m,j-1/2,k,n} \right) \\ \underline{B}_{zy}^{i-1/2,j-1/2,k,n+1/2} & = & \alpha_y^{*j-1/2} \underline{B}_{zy}^{i-1/2,j-1/2,k,n-1/2} \\ & + & \beta_y^{*j-1/2} \sum_{m=1}^s c_m \left( \underline{E}_x^{i-1/2,j+m-1,k,n} - \underline{E}_x^{i-1/2,j-m,k,n} \right) \end{array} \right.$$

$$\text{with } \forall \xi \in \{x, y, z\}, \quad \alpha_\xi^{*i,j,k} = \frac{1 - \sigma_\xi^{*i,j,k} \Delta t / 2}{1 + \sigma_\xi^{*i,j,k} \Delta t / 2}, \quad \beta_\xi^{*i,j,k} = \frac{\epsilon \Delta t / \Delta \xi}{1 + \sigma_\xi^{*i,j,k} \Delta t / 2}.$$

# Outline

## 1 Introduction to UPIC-EMMA Maxwell Solver

- UPIC framework
- UPIC-EMMA
- Units
- Spectral Method
- UPIC-EMMA Maxwell Solver

## 2 Emulation of a Finite Difference Scheme

- Yee Scheme
- Implementation in a Spectral Solver
- 2D Academic Case : Cylindrical wave

## 3 Absorbing Boundary Conditions

- Perfectly Matched Layer (PML) Technique for Finite Difference Schemes
- Implementation in a Spectral Solver
- Implicit Scheme
- 2D Academic Case : Cylindrical Waves

# Implementation in a Spectral Solver

## Implementation in a Spectral Solver

$$① \quad \hat{E}_{xy}^{p,q,r,0} = \hat{E}_{xz}^{p,q,r,0} = \hat{E}_x^{p,q,r,0}/2, \quad \hat{E}_{yx}^{p,q,r,0} = \hat{E}_{yz}^{p,q,r,0} = \hat{E}_y^{p,q,r,0}/2 \text{ etc...}$$

$$② \quad \underline{\hat{B}}^{p,q,r,n+1/2,*} = \underline{\hat{B}}^{p,q,r,n,*} - \frac{\Delta t}{2} \underline{\epsilon} (\underline{\imath k}_{p,q,r}) \times \underline{\hat{E}}_T^{p,q,r,n}$$

$$③ \quad \begin{cases} \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n+1/2} &= \text{IDFT} \left\{ \frac{1}{1 + \sigma_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n+1/2,*} \right\}^{i,j,k} \right\}^{p,q,r} \\ \underline{\hat{E}}_{\xi\zeta}^{p,q,r,n,*} &= \text{IDFT} \left\{ \left( 1 - \sigma_{\zeta}^{i,j,k} \frac{\Delta t}{2} \right) \text{DFT} \left\{ \underline{\hat{E}}_{\xi\zeta}^{p,q,r,n} \right\}^{i,j,k} \right\}^{p,q,r} \end{cases}$$

$$④ \quad \underline{\hat{E}}_T^{p,q,r,n+1/2,*} = \underline{\hat{E}}_T^{p,q,r,n,*} + \Delta t \underline{\epsilon} (\underline{\imath k}_{p,q,r}) \times \underline{\hat{B}}^{p,q,r,n+1/2} - \Delta t \underline{\alpha f} \underline{\hat{I}}_T^{p,q,r,n+1/2}$$

$$⑤ \quad \begin{cases} \underline{\hat{E}}_{\xi\zeta}^{p,q,r,n+1} &= \text{IDFT} \left\{ \frac{1}{1 + \sigma_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \underline{\hat{E}}_{\xi\zeta}^{p,q,r,n+1,*} \right\}^{i,j,k} \right\}^{p,q,r} \\ \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n+1/2,*} &= \text{IDFT} \left\{ \left( 1 - \sigma_{\zeta}^{i,j,k} \frac{\Delta t}{2} \right) \text{DFT} \left\{ \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n-1/2} \right\}^{i,j,k} \right\}^{p,q,r} \end{cases}$$

$$⑥ \quad \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n+1} = \text{IDFT} \left\{ \frac{1}{1 + \sigma_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \underline{\hat{B}}_{\xi\zeta}^{p,q,r,n+1,*} \right\}^{i,j,k} \right\}^{p,q,r}$$

$$⑦ \quad \hat{E}_x^{p,q,r,n+1} = \hat{E}_{xz}^{p,q,r,n+1} + \hat{E}_{xy}^{p,q,r,n+1}, \quad \hat{E}_y^{p,q,r,n+1} = \hat{E}_{yx}^{p,q,r,n+1} + \hat{E}_{yz}^{p,q,r,n+1} \text{ etc...}$$

Steps 1, 3 and 5 actually concerns the splitted PML components  $\hat{E}_{xy}^{p,q,r,n}$ ,  $\hat{E}_{xz}^{p,q,r,n}$  etc... and NOT the common fields!

It has been written like this just for illustrating the scheme more efficiently.

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# Fully Implicit Scheme for the Dumping Terms (1)

PML Equations - Yee scheme except for the dumping term taken fully implicitly - Electric field update

$$\left\{
 \begin{array}{lcl}
 E_{xy}^{i-1/2,j,k,n+1} & = & \alpha_y^j E_{xy}^{i-1/2,j,k,n} - \gamma_y^{i,j,k} j_{T,x}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_y^j \sum_{m=1}^s c_m \left( \underline{B}_z^{i-1/2,j-1/2+m,k,n+1/2} - \underline{B}_z^{i-1/2,j-1/2-m+1,k,n+1/2} \right) \\
 E_{xz}^{i-1/2,j,k,n+1} & = & \alpha_z^k E_{xz}^{i-1/2,j,k,n} - \gamma_z^{i,j,k} j_{T,x}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_z^k \sum_{m=1}^s c_m \left( \underline{B}_y^{i-1/2,j,k-1/2+m,n+1/2} - \underline{B}_y^{i-1/2,j,k-1/2-m+1,n+1/2} \right) \\
 E_{yz}^{i,j-1/2,k,n+1} & = & \alpha_z^k E_{yz}^{i,j-1/2,k,n} - \gamma_z^{i,j,k} j_{T,y}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_z^k \sum_{m=1}^s c_m \left( \underline{B}_x^{i,j-1/2,k-1/2+m,n+1/2} - \underline{B}_x^{i,j-1/2,k-1/2-m+1,n+1/2} \right) \\
 E_{yx}^{i,j-1/2,k,n+1} & = & \alpha_x^i E_{yx}^{i,j-1/2,k,n} - \gamma_x^{i,j,k} j_{T,y}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_x^i \sum_{m=1}^s c_m \left( \underline{B}_z^{i-1/2+m,j-1/2,k,n+1/2} - \underline{B}_z^{i-1/2-m+1,j-1/2,k,n+1/2} \right) \\
 E_{zx}^{i,j,k-1/2,n+1} & = & \alpha_x^i E_{zx}^{i,j,k-1/2,n} - \gamma_x^{i,j,k} j_{T,z}^{i-1/2,j,k,n+1/2} / 2 \\
 & + & \beta_x^i \sum_{m=1}^s c_m \left( \underline{B}_y^{i-1/2+m,j,k-1/2,n+1/2} - \underline{B}_y^{i-1/2-m+1,j,k-1/2,n+1/2} \right) \\
 E_{zy}^{i,j,k-1/2,n+1} & = & \alpha_y^j E_{zy}^{i,j,k-1/2,n} - \gamma_y^{i,j,k} j_{T,z}^{i-1/2,j,k,n+1/2} / 2 \\
 & - & \beta_y^j \sum_{m=1}^s c_m \left( \underline{B}_x^{i,j-1/2+m,k-1/2,n+1/2} - \underline{B}_x^{i,j-1/2-m+1,k-1/2,n+1/2} \right)
 \end{array}
 \right.$$

$$\text{with } \forall \xi \in \{x, y, z\}, \quad \alpha_\xi^{i,j,k} = \frac{1}{1 + \sigma_\xi^{i,j,k} \Delta t / 2}, \quad \beta_\xi^{i,j,k} = \frac{\epsilon \Delta t / \Delta \xi}{1 + \sigma_\xi^{i,j,k} / 2} \text{ and } \gamma_\xi^{i,j,k} = \frac{\epsilon \Delta t}{1 + \sigma_\xi^{i,j,k} / 2}$$

## Fully Implicit Scheme for the Dumping Terms (2)

### Implicit Scheme

$$① \quad \hat{E}_{xy}^{p,q,r,0} = \hat{E}_{xz}^{p,q,r,0} = \hat{E}_x^{p,q,r,0}/2, \quad \hat{E}_{yx}^{p,q,r,0} = \hat{E}_{yz}^{p,q,r,0} = \hat{E}_y^{p,q,r,0}/2 \text{ etc...}$$

$$② \quad \hat{B}_{\xi\zeta}^{p,q,r,n+1/2,*} = \hat{B}_{\xi\zeta}^{p,q,r,n,*} - \frac{\Delta t}{2} \underline{\epsilon}(\underline{\omega}_{p,q,r}) \times \hat{E}_T^{p,q,r,n}$$

$$③ \quad \hat{B}_{\xi\zeta}^{p,q,r,n+1/2} = \text{IDFT} \left\{ \frac{1}{1 + \underline{\sigma}_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \hat{B}_{\xi\zeta}^{p,q,r,n+1/2,*} \right\}^{i,j,k} \right\}^{p,q,r}$$

$$④ \quad \hat{E}_T^{p,q,r,n+1,*} = \hat{E}_T^{p,q,r,n,*} + \Delta t \underline{\epsilon}(\underline{\omega}_{p,q,r}) \times \hat{B}_{\xi\zeta}^{p,q,r,n+1/2} - \Delta t \underline{\alpha}_f \hat{I}_T^{p,q,r,n+1/2}$$

$$⑤ \quad \hat{E}_{\xi\zeta}^{p,q,r,n+1} = \text{IDFT} \left\{ \frac{1}{1 + \underline{\sigma}_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \hat{E}_{\xi\zeta}^{p,q,r,n+1,*} \right\}^{i,j,k} \right\}^{p,q,r}$$

$$⑥ \quad \hat{B}_{\xi\zeta}^{p,q,r,n+1} = \text{IDFT} \left\{ \frac{1}{1 + \underline{\sigma}_{\zeta}^{i,j,k} \frac{\Delta t}{2}} \text{DFT} \left\{ \hat{B}_{\xi\zeta}^{p,q,r,n+1,*} \right\}^{i,j,k} \right\}^{p,q,r}$$

$$⑦ \quad \hat{E}_x^{p,q,r,n+1} = \hat{E}_{xz}^{p,q,r,n+1} + \hat{E}_{xy}^{p,q,r,n+1}, \quad \hat{E}_y^{p,q,r,n+1} = \hat{E}_{yx}^{p,q,r,n+1} + \hat{E}_{yz}^{p,q,r,n+1} \text{ etc...}$$

Steps 1, 3 and 5 actually concerns the splitted PML components  $\hat{E}_{xy}^{p,q,r,n}$ ,  $\hat{E}_{xz}^{p,q,r,0}$  etc... and NOT the common fields!

It has been written like this just for illustrating the scheme more efficiently.

# Initialization

## Nominal Simulation Parameters

- 2D
- Filter used with  $a_x = a_y = .912871$
- Electromagnetic units ( $\epsilon = 1$ )
- 4 MPI nodes and 2 OpenMP threads per node
- $L_x = L_y = 128$
- $\delta = 30$
- $\Delta_x = \Delta_y = 1$
- $L_t = 128$
- $a_f = 1$

## Best PML conductivity expression for the FTFD Yee Scheme <sup>1</sup>

$$\begin{cases} \sigma_x(x) &= \sigma_m \left( \frac{|x - x_I|}{\delta} \right)^\beta \\ \sigma_y(y) &= \sigma_m \left( \frac{|y - y_I|}{\delta} \right)^\beta \end{cases} \text{ where}$$

$$3 \leq \beta \leq 4 \text{ and } \sigma_m = \frac{\alpha \ln 10 (\beta + 1) \epsilon}{2\delta} = 0.8(\beta + 1)\epsilon$$

<sup>1</sup> Computational electrodynamics, the FDTD method, A. Taflove and S C Hagness, Eq. (7.62) and (7.66)

## Electrical Current Density Initialization and Expected Solutions

$$j_T^{i,j,k,n} = \begin{cases} j_0 \sin(\omega_0 t_n) \mathbf{e}_z & \text{if } \begin{cases} 63 \leq x_i \leq 65 \\ 63 \leq y_j \leq 65 \end{cases} \\ 0 & \text{else} \end{cases} \quad \text{with } \omega_0 = 1 \text{ and } j_0 = -10.$$

$$\Rightarrow \begin{cases} E_{T,r}^{i,j,k,n} &= 0 \\ E_{T,z}^{i,j,k,n} &\approx \frac{E_0}{\sqrt{|r_{i,j,k} - r_0|}} \cos(\omega_0 t_n - k_0 |r_{i,j,k} - r_0|) \\ B_r^{i,j,k,n} &\approx \frac{E_0}{\sqrt{|r_{i,j,k} - r_0|}} \sin(\omega_0 t_n - k_0 |r_{i,j,k} - r_0|) \\ B_z^{i,j,k,n} &= 0 \end{cases}$$

with  $E_0 = a_f j_0 / \omega_0 = 10$ ,  $r_0 = (64, 64)$  and  $k_0 = \omega_0 / \epsilon = 1$ .

## Periodic versus Absorbing

$E_z$  (left),  $B_x$  (middle) and  $B_y$  (right) with periodic (top) and PML-Yee (bottom) boundary conditions