3-Weeks Presentation

FERRARI: The **F**ast**E**st **R**eta**R**get**A**ble FDTD Solve**R** **I**n the West

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Table of Contents

Maxwell's Equations

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

Where:

$\mathbf{J}$ is the current density

ρ is the charge density

Maxwell's Equations in Terms of Potentials

$$\nabla^2 \phi - \frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\varepsilon_0}$$
$$\nabla^2 \mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu_0 \mathbf{J}$$

With field definitions:

$$\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t}$$
$$\mathbf{B} = \nabla \times \mathbf{A}$$

Maxwell's Equations in Natural Units

In natural units, Maxwell's equations become:

$$\left.\begin{aligned} \nabla^2\phi - \frac{\partial^2\phi}{\partial t^2} &= -\rho \\ \nabla^2\mathbf{A} - \frac{\partial^2\mathbf{A}}{\partial t^2} &= -\mathbf{J} \end{aligned}\right\} \text{Both wave equations}$$

With field definitions:

$$\mathbf{E} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Mur's 1st Order Absorbing Boundary Conditions

Mur's 1st order absorbing boundary conditions are used to absorb outgoing waves, left-moving at $x = 0$ and right-moving at $x = N - 1$.

Mathematical formulation:

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right)\psi\bigg|_{x=0} = 0 \text{ according to [Mur, 1981]} \tag{1}$$

$$\left(\frac{\partial^2}{\partial x \partial t} - \frac{\partial^2}{\partial t^2}\right)\psi\bigg|_{x=0} = 0 \text{ according to according to [Fallahi, 2020]} \tag{2}$$

Equations of motion for particles

The relativistic equation of motion for electron particles reads as

$$\frac{\partial}{\partial t}(\gamma m \mathbf{v}) = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \text{ and } \frac{\partial \mathbf{r}}{\partial t} = \mathbf{v} \tag{3}$$

Spatial and temporal field Discretization

$$
\begin{aligned}
\frac{\partial^2 \psi(x,y,z,t)}{\partial x^2} &= \frac{\psi^n_{i+1,j,k} - 2\psi^n_{i,j,k} + \psi^n_{i-1,j,k}}{\Delta x^2} \\
\frac{\partial^2 \psi(x,y,z,t)}{\partial y^2} &= \frac{\psi^n_{i,j+1,k} - 2\psi^n_{i,j,k} + \psi^n_{i,j-1,k}}{\Delta y^2} \\
\frac{\partial^2 \psi(x,y,z,t)}{\partial z^2} &= \frac{\psi^n_{i,j,k+1} - 2\psi^n_{i,j,k} + \psi^n_{i,j,k-1}}{\Delta z^2} \\
\frac{\partial^2 \psi(x,y,z,t)}{\partial t^2} &= \frac{\psi^{n+1}_{i,j,k} - 2\psi^n_{i,j,k} + \psi^{n-1}_{i,j,k}}{\Delta t^2}
\end{aligned}
$$

where ψ represents either a component of $\mathbf{A}$ or ϕ.

Particle Discretization

Interpolation of a particle attribute to the grid: For a particle with position

$$p = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} = \begin{bmatrix} i\Delta x + \delta_x \\ j\Delta x + \delta_y \\ k\Delta x + \delta_z \end{bmatrix} \tag{4}$$

the Cloud-In-Cell interpolation is done as follows

$$\rho^p_{i+I,j+J,k+K} = \rho \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right) \tag{5}$$

with $(I, J, K) \in \{0, 1\}^3$.

Gathering field attributes

Interpolating field attributes to particles works analogously:

$$\psi^p = \sum_{I,I,K \in \{0,1\}^3} \psi \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right)$$

Current Deposition

Cloud-In-Cell deposition of current: We define the deposition point p^m as the midpoint between two adjacent timesteps:

$$p^m = \begin{bmatrix} \frac{p_x^n + p_x^{n+1}}{2} \\ \frac{p_y^n + p_y^{n+1}}{2} \\ \frac{p_z^n + p_z^{n+1}}{2} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x^m}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y^m}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z^m}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} \tag{6}$$

$$\mathbf{J}^p_{i+I,j+J,k+K} = \rho \mathbf{v} \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right) \tag{7}$$

Current Deposition

Cloud-In-Cell deposition of current: We define the deposition point p^m as the midpoint between two adjacent timesteps:

$$p^m = \begin{bmatrix} \frac{p_x^n + p_x^{n+1}}{2} \\ \frac{p_y^n + p_y^{n+1}}{2} \\ \frac{p_z^n + p_z^{n+1}}{2} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x^m}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y^m}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z^m}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} \tag{6}$$

$$\mathbf{J}^p_{i+I,j+J,k+K} = \rho \mathbf{v} \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right) \tag{7}$$

If a particle travels across a cell boundary, this scheme violates

$$\nabla \cdot \mathbf{E} = \rho \tag{8}$$

Boris Correction

To satisfy

$$\nabla \cdot \mathbf{E} = \rho$$

we simply add a correction term equivalent to the negative error [Lehe, 2016]:

$$\mathbf{E}' = \mathbf{E} - \nabla\delta\phi \text{ with } \nabla \cdot (\nabla\delta\phi) = \nabla \cdot \mathbf{E} - \rho \tag{9}$$

Zigzag Current Deposition

Alternatively change current deposition scheme: Particle motion from p_1 to p_2 is decomposed into two separate movements, p_1 to p_r and p_r to p_2 [Fallahi, 2020].

$$
\begin{aligned}
x_r &= \min\left(\min(i_1\Delta x, i_2\Delta x) + \Delta_x, \max\left(\min(i_1\Delta x, i_2\Delta x), \frac{x_1 + x_2}{2}\right)\right) \\
y_r &= \min\left(\min(j_1\Delta x, j_2\Delta y) + \Delta_y, \max\left(\min(j_1\Delta y, j_2\Delta y), \frac{y_1 + y_2}{2}\right)\right) \\
z_r &= \min\left(\min(k_1\Delta x, k_2\Delta z) + \Delta_z, \max\left(\min(k_1\Delta z, k_2\Delta z), \frac{z_1 + z_2}{2}\right)\right)
\end{aligned}
$$

Then two Cloud-In-Cell interpolations of with points $\frac{p_1+p_r}{2}$ and $\frac{p_r+p_2}{2}$ [Umeda et al., 2003] satisfy the conservation of current.

Radiation Reactions

Radiation reaction in classical electrodynamics [Di Piazza et al., 2012] in the ultra-relativistic limit of Landau & Lifshitz can be described by

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}_L - \frac{2e^4\gamma}{3m^3c^5}\mathbf{p}\left(\mathbf{E}_\perp + \frac{\mathbf{pB}}{\gamma mc}\right) \tag{10}$$

Pair Creation

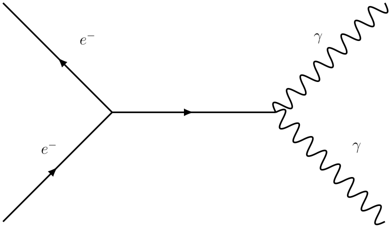


Figure: Feynman Diagram

Pair Creation

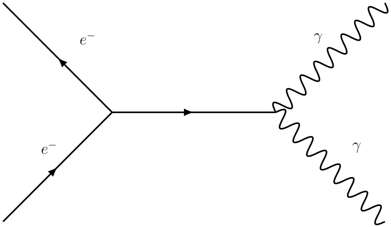


Figure: Feynman Diagram

- Accumulate cross-section $d\sigma$ of possible interaction graphs

Pair Creation

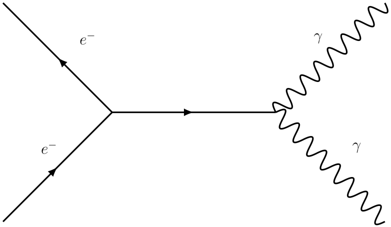


Figure: Feynman Diagram

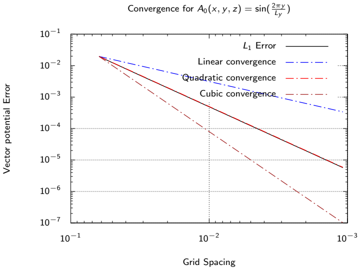
- Accumulate cross-section $d\sigma$ of possible interaction graphs
- Insert / resample particles

Results

L_1 error of numerical solution of

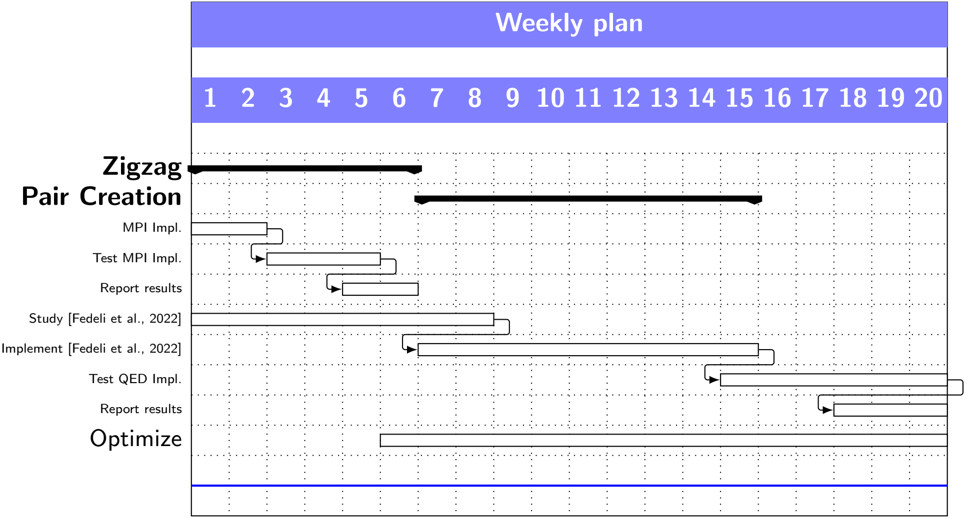
$$\nabla^2\phi - \frac{\partial^2\phi}{\partial t^2} = -\rho$$

after one timestep



Temporal evolution of **E**

Project Milestones



References

Di Piazza, A., Müller, C., Hatsagortsyan, K. Z., and Keitel, C. H. (2012).
Extremely high-intensity laser interactions with fundamental quantum systems.
Rev. Mod. Phys., 84:1177–1228.

Fallahi, A. (2020).
Mithra 2.0: A full-wave simulation tool for free electron lasers.

Fedeli, L., Zaïm, N., Sainte-Marie, A., Thé venet, M., Huebl, A., Myers, A., Vay, J.-L., and Vincenti, H. (2022).
PICSAR-QED: a monte carlo module to simulate strong-field quantum electrodynamics in particle-in-cell codes for exascale architectures.
New Journal of Physics, 24(2):025009.

Lehe, R. (2016).
Advanced electromagnetic particle-in-cell simulations.
In *USPAS Short Course Series: Computational Methods in Accelerator Physics*.

Mur, G. (1981).
Absorbing boundary conditions for the finite-difference approximation of the time-domain electromagnetic-field equations.
Transactions on Electromagnetic Compatibility, 23(4):1–6.

Umeda, T., Omura, Y., Tominaga, T., and Matsumoto, H. (2003).
A new charge conservation method in electromagnetic particle-in-cell simulations.
Computer Physics Communications, 156(1):73–85.