Manuel Winkler, S. Mayani, A. Adelmann :: AMAS Group, LSM

Performance portable FDTD Implementation

January 30, 2024

Contact: flaschenholz@protonmail.ch

Overview

Field Update

Define the four potential $A^\alpha = (\phi, \mathbf{A})$ which evolves according to a wave equation:

$$\frac{\partial^2 A^\alpha}{\partial t^2} = \Delta A^\alpha + S^\alpha$$
$$\text{where } S^\alpha = (\rho, \mathbf{J})$$

Field Update

Define the four potential $A^\alpha = (\phi, \mathbf{A})$ which evolves according to a wave equation:

$$\frac{\partial^2 A^\alpha}{\partial t^2} = \Delta A^\alpha + S^\alpha$$
$$\text{where } S^\alpha = (\rho, \mathbf{J})$$

The magnetic and electric fields can be evaluated with

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

Stencil

Use a three-point second derivative stencil:

$$\frac{\partial^2 A^\alpha}{\partial \beta^2}(\vec{x}) \approx \frac{1}{\beta^2}\left(A^\alpha(\vec{x}+\beta) - 2A^\alpha(\vec{x}) + A^\alpha(\vec{x}-\beta)\right)$$

where β is an arbitrary vector.
In a cartesian grid this simplifies to

$$\frac{\partial^2 A^\alpha}{\partial x^2}(\vec{x}) \approx \frac{1}{\Delta x^2}\left(A^\alpha_{i+1,\dots} - 2A^\alpha_{i,\dots} + A^\alpha_{i-1,\dots}\right)$$

where i is the index corresponding to the direction of x

FDTD Formulation

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

where ψ represents a component of the four-potential.

FDTD Formulation

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

where ψ represents a component of the four-potential.

Only unknown: $\psi^{n+1}_{i,j,k}$.

Accuracy Analysis

Consider the one-dimensional analytical function around $x_0 = 0$

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2}f''(0) + \frac{x^3}{6}f'''(0) + \frac{x^4}{24}f''''(0) + \mathcal{O}(\Delta x^5)$$

Accuracy Analysis

Consider the one-dimensional analytical function around $x_0 = 0$

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2}f''(0) + \frac{x^3}{6}f'''(0) + \frac{x^4}{24}f''''(0) + \mathcal{O}(\Delta x^5)$$

We can add the evaluations at $\pm\Delta x$ and subtract twice the evaluation at 0:

$$f(\Delta x) + f(-\Delta x) - 2f(0) =$$

Accuracy Analysis

Consider the one-dimensional analytical function around $x_0 = 0$

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2}f''(0) + \frac{x^3}{6}f'''(0) + \frac{x^4}{24}f''''(0) + \mathcal{O}(\Delta x^5)$$

We can add the evaluations at $\pm\Delta x$ and subtract twice the evaluation at 0:

$$f(\Delta x) + f(-\Delta x) - 2f(0) =$$

$$\begin{aligned}
&f(0) + \Delta x f'(0) + \frac{\Delta x^2}{2}f''(0) + \frac{\Delta x^3}{6}f'''(0) + \frac{\Delta x^4}{24}f''''(0) + \mathcal{O}(\Delta x^5)\\
+\ &f(0) - \Delta x f'(0) + \frac{\Delta x^2}{2}f''(0) - \frac{\Delta x^3}{6}f'''(0) + \frac{\Delta x^4}{24}f''''(0) + \mathcal{O}(\Delta x^5)\\
-&2f(0) = \Delta x^2 f''(0) + \frac{\Delta x^4}{12}f''''(0) + \mathcal{O}_E(\Delta x^6)
\end{aligned}$$

where $\mathcal{O}_E$ implies only even terms.

Accuracy Analysis

We therefore can see that

$$\frac{1}{\Delta x^2}\left(f(\Delta x) + f(-\Delta x) - 2f(0)\right) = f''(0) + \frac{\Delta x^2}{12} f''''(0) + \mathcal{O}_E(\Delta x^4)$$

approximates the second derivative of f in 0 with an error that is proportional to $f''''(0)$

First test case

Consider the 1D wave equation

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial t^2}$$
$$f(t = 0, x) = \sin(\pi x)$$

with periodic boundary conditions defined on $[-1, 1]$.

First test case

Consider the 1D wave equation

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial t^2}$$
$$f(t=0,x) = \sin(\pi x)$$

with periodic boundary conditions defined on $[-1, 1]$.
Analytical solution:

$$\begin{aligned} f(t,x) = &\quad \sin(\pi x)\cos(\pi t) \\ \text{implying } \frac{\partial^4 f}{\partial x^4}(0) = &\ \pi^4 \sin(\pi x)\cos(\pi t) \\ \text{and } f(1,x) = &-\sin(\pi x) \end{aligned}$$

Evolving this equation numerically with $\Delta x \neq \Delta t$ up to $t = 1$ yields

$$f_n(1,x) = -\sin(\pi x) + k\frac{\Delta t}{\Delta t}(\Delta x^2) + \mathcal{O}(\Delta x^4)$$

First test case

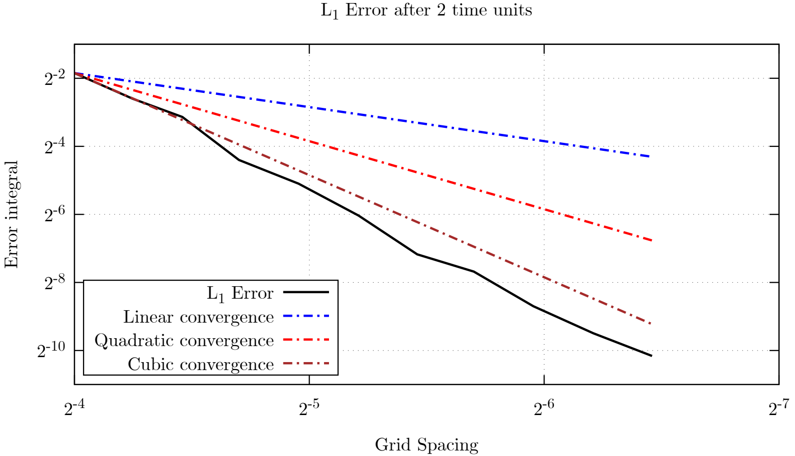
Due to linearity, we can separate the evolution of the exact solution and the error.

$$
\begin{aligned}
f_n(1, x) &= -\sin(\pi x) + k\Delta x^2 + \mathcal{O}_E(\Delta x^4) \\
\implies f_n(2, x) &= \quad \sin(\pi x) - k\Delta x^2 + k\Delta x^2 + \mathcal{O}_{12}(\Delta x^4) + \mathcal{O}_E(\Delta x^4) \\
&= \quad \sin(\pi x) + \mathcal{O}\ (\Delta x^4)
\end{aligned}
$$

First test case

Due to linearity, we can separate the evolution of the exact solution and the error.

$$\begin{aligned} f_n(1,x) &= -\sin(\pi x) + k\Delta x^2 + \mathcal{O}_E(\Delta x^4) \\ \implies f_n(2,x) &= \quad \sin(\pi x) - k\Delta x^2 + k\Delta x^2 + \mathcal{O}_{12}(\Delta x^4) + \mathcal{O}_E(\Delta x^4) \\ &= \quad \sin(\pi x) + \mathcal{O}\ (\Delta x^4) \end{aligned}$$



Additionally, in the case of $\Delta t = \Delta x$, the numerical wave operator

$$\frac{1}{\Delta x^2}\left(A^{\alpha}_{i+1,\dots} - 2A^{\alpha}_{i,\dots} + A^{\alpha}_{i-1,\dots}\right) - \frac{1}{\Delta t^2}\left(A^{\alpha}_{\dots,n+1} - 2A^{\alpha}_{\dots,n} + A^{\alpha}_{\dots,n-1}\right)$$

reduces to zero for the exact solution

$$f(t,x) = \sin(\pi x)\cos(\pi t)$$

Additionally, in the case of $\Delta t = \Delta x$, the numerical wave operator

$$\frac{1}{\Delta x^2}\left(A^\alpha_{i+1,\dots} - 2A^\alpha_{i,\dots} + A^\alpha_{i-1,\dots}\right) - \frac{1}{\Delta t^2}\left(A^\alpha_{\dots,n+1} - 2A^\alpha_{\dots,n} + A^\alpha_{\dots,n-1}\right)$$

reduces to zero for the exact solution

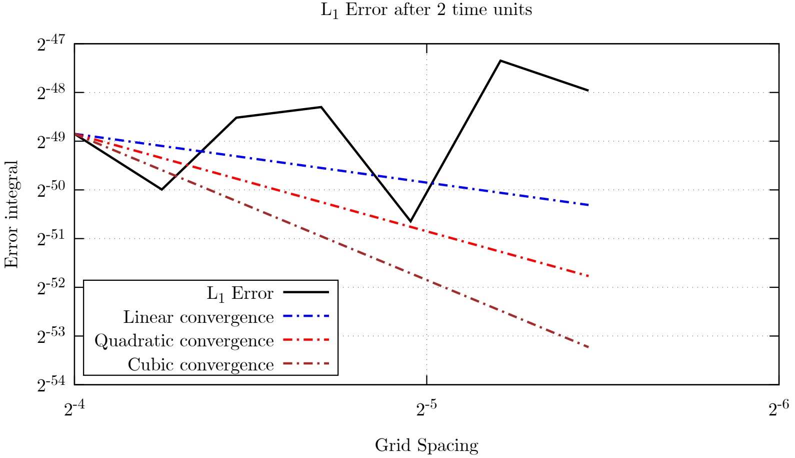
$$f(t,x) = \sin(\pi x)\cos(\pi t)$$

because the even derivatives cancel:

$$\frac{\partial^{2n} f(t,x)}{\partial t^{2n}} = \frac{\partial^{2n} f(t,x)}{\partial x^{2n}} = \pi^{2n}\sin(\pi x)\cos(\pi t)$$

Exact stepper

This results in machine precision accuracy for any grid spacing:



Boundary conditions

Absorbing boundary conditions: Custom timestep rule on the boundary.

Mathematical formulation:

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

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

Boundary conditions

Absorbing boundary conditions: Custom timestep rule on the boundary.

Mathematical formulation:

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

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

Equation 2 can be used for boundaries with $\frac{\partial \psi}{\partial x}$, i.e. external fields:

$$\mathbf{E} = \mathbf{e}_x$$
$$\phi = x$$

is a stationary solution only for 2.

Initial conditions

For an initial source term

$$S = \begin{bmatrix} \rho_0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

we solve the poisson equation

$$-\Delta\phi = \rho_0$$

Initial conditions

For an initial source term

$$S = \begin{bmatrix} \rho_0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

we solve the poisson equation

$$-\Delta\phi = \rho_0$$

For inital conditions with one moving particle:

$$\phi(\vec{r}, 0) = \frac{q}{4\pi(1 - \vec{\beta} \cdot \vec{n})||\vec{r} - \vec{R}(t_{ret})||}$$
$$\text{and } \mathbf{A}(\vec{r}, 0) = \phi(r, 0)\vec{\beta}_{ret}$$

$$\text{where } t_{ret} = -||\vec{r} - \vec{R}(t_{ret})||$$

Initial conditions

For an initial source term

$$S = \begin{bmatrix} \rho_0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

we solve the poisson equation

$$-\Delta\phi = \rho_0$$

For inital conditions with one moving particle:

$$\phi(\vec{r}, 0) = \frac{q}{4\pi(1 - \vec{\beta} \cdot \vec{n})||\vec{r} - \vec{R}(t_{ret})||}$$
$$\text{and } \mathbf{A}(\vec{r}, 0) = \phi(r, 0)\vec{\beta}_{ret}$$

$$\text{where } t_{ret} = -||\vec{r} - \vec{R}(t_{ret})||$$

For p particles and n gridpoints: $\mathcal{O}(p \cdot n)$!

1. Governing equations

2. Field Discretization

3. Particle Discretization and Interpolation

4. Outlook

Particle Update

Lorentz Force:

$$\vec{F_L} = q\mathbf{E} + q\vec{v} \times \mathbf{B}$$

Lorentz acceleration:

$$\vec{a_L} = \frac{q}{m_r}\mathbf{E} + q\vec{v} \times \mathbf{B}$$
$$\text{where } m_r = \gamma m_0$$

Particle timestep

Boris update scheme with boosted E and B: Fallahi [2020]

$$\left(r^m, \gamma\beta^{m-\frac{1}{2}}\right) \rightarrow \left(r^{m+1}, \gamma\beta^{m+\frac{1}{2}}\right)$$

$$\begin{aligned}
\mathbf{t}_1 &= \gamma\beta^{m-\frac{1}{2}} + \frac{e\Delta t_b \mathbf{E}_t^m}{2m} \\
&\vdots \\
\mathbf{r}^{m+1} &= r^m + \frac{\Delta t_b \gamma\beta^{m+\frac{1}{2}}}{\sqrt{1 + \|\gamma\beta^{m+\frac{1}{2}}\|^2}}
\end{aligned}$$

Particle timestep

Boris update scheme with boosted E and B: Fallahi [2020]

$$\left(r^m, \gamma\beta^{m-\frac{1}{2}}\right) \to \left(r^{m+1}, \gamma\beta^{m+\frac{1}{2}}\right)$$

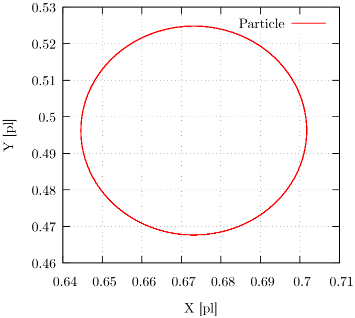
$$\begin{aligned}
\mathbf{t}_1 &= \gamma\beta^{m-\frac{1}{2}} + \frac{e\Delta t_b \mathbf{E}_t^m}{2m} \\
&\vdots \\
\mathbf{r}^{m+1} &= r^m + \frac{\Delta t_b \gamma\beta^{m+\frac{1}{2}}}{\sqrt{1 + \|\gamma\beta^{m+\frac{1}{2}}\|^2}}
\end{aligned}$$

Note that

$$\begin{aligned}
\beta &= \frac{\gamma\beta}{\sqrt{1 + \|\gamma\beta\|^2}} \\
\gamma &= \sqrt{1 + \|\gamma\beta\|^2}
\end{aligned}$$

Test of Boris Stepper

Setup: Shoot charged particle in constant z-aligned magnetic field



- Traces a perfect circle
- Conserves energy up to machine precision

Particle Discretization

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

$$p = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} = \begin{bmatrix} i\Delta x + \delta_x \\ j\Delta x + \delta_y \\ k\Delta x + \delta_z \end{bmatrix} \tag{3}$$

the Cloud-In-Cell interpolation is done as follows

$$\rho^p_{i+I,j+J,k+K} = \rho \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right) \tag{4}$$

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:

$$p^m = \begin{bmatrix} \frac{p_x^n + p_x^{n+1}}{2} \\ \frac{p_y^n + p_y^{n+1}}{2} \\ \frac{p_z^n + p_z^{n+1}}{2} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x^m}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y^m}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z^m}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} \tag{5}$$

$$\mathbf{J}^p_{i+I,j+J,k+K} = \rho \mathbf{v} \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right) \tag{6}$$

$$\text{where } \mathbf{v} = \frac{r^{m+1} - r^{m-1}}{2\Delta t} \tag{7}$$

Current Deposition

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

$$p^m = \begin{bmatrix} \frac{p_x^n + p_x^{n+1}}{2} \\ \frac{p_y^n + p_y^{n+1}}{2} \\ \frac{p_z^n + p_z^{n+1}}{2} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{p_x^m}{\Delta x} \right\rfloor \Delta x + \delta_x \\ \left\lfloor \frac{p_y^m}{\Delta y} \right\rfloor \Delta y + \delta_y \\ \left\lfloor \frac{p_z^m}{\Delta z} \right\rfloor \Delta z + \delta_z \end{bmatrix} \tag{5}$$

$$\mathbf{J}^p_{i+I,j+J,k+K} = \rho\mathbf{v}\left(\frac{1}{2} + (-1)^I \left|\frac{1}{2} - \frac{\delta x}{\Delta x}\right|\right)\left(\frac{1}{2} + (-1)^J \left|\frac{1}{2} - \frac{\delta y}{\Delta y}\right|\right)\left(\frac{1}{2} + (-1)^K \left|\frac{1}{2} - \frac{\delta z}{\Delta z}\right|\right) \tag{6}$$

$$\text{where } \mathbf{v} = \frac{r^{m+1} - r^{m-1}}{2\Delta t} \tag{7}$$

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].

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

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.

Test of current deposition and field update

Idea: Compare simulated radiation to Larmor:

$$P = \frac{q^2}{6\pi}\gamma^6(||\dot{\vec{\beta}}||^2 - ||\vec{\beta} \times \dot{\vec{\beta}}||^2)$$

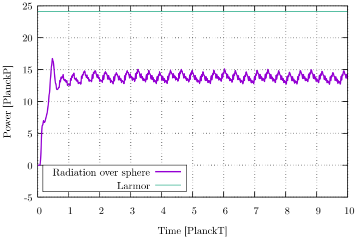


Figure: $\sigma_{init} = 0.02$

Setup:

- Initialize particles with gaussian distribution
- Rotate particles around center with fixed speed.

Test of current deposition and field update

Idea: Compare simulated radiation to Larmor:

$$P = \frac{q^2}{6\pi}\gamma^6(||\dot{\vec{\beta}}||^2 - ||\vec{\beta} \times \dot{\vec{\beta}}||^2)$$

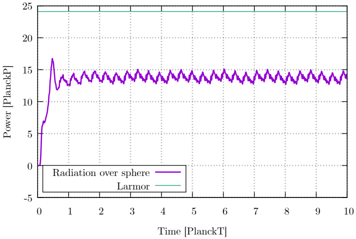


Figure: $\sigma_{init} = 0.02$

Setup:

- Initialize particles with gaussian distribution
- Rotate particles around center with fixed speed.

Observations:

- Constant outward radiation
- Different particle trajectories interfere destructively

Test of current deposition and field update

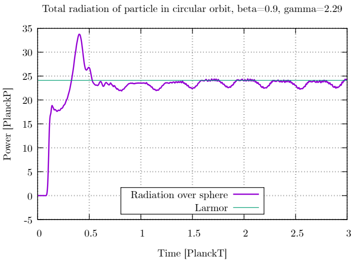


Figure: $\sigma_{init} = 0.005$

Setup:

- Initialize particles with gaussian distribution
- Rotate particles around center with fixed speed.

Observations:

- Constant outward radiation
- Different particle trajectories interfere destructively

Test of coupled field and particle update

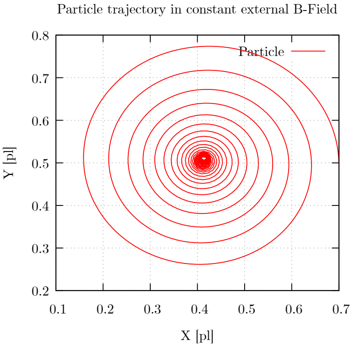


Figure: $\sigma_{init} = 0.0$

Setup:

- Initialize particles with gaussian distribution
- Let particles be guided by Lorentz force

Observations:

- Particle progressively loses energy and spirals inward

Test of coupled field and particle update

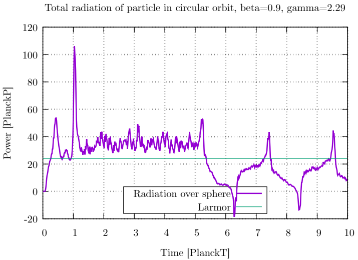


Figure: $\sigma_{init} = 0.0$

Setup:

- Initialize particles with gaussian distribution
- Let particles be guided by Lorentz force

Observations:

- Constant outward radiation up until all energy is lost

Undulators and Lorentz boosts

Transformation of undulator fields:

$$\mathbf{B}_{lab}(\mathbf{r}) = \begin{bmatrix} 0 \\ B_0 \cosh\left(k \cdot y_{lab}\right) \sin\left(k \cdot z_{lab}\right) \\ B_0 \sinh\left(k \cdot y_{lab}\right) \cos\left(k \cdot z_{lab}\right) \end{bmatrix}$$

Undulators and Lorentz boosts

Transformation of undulator fields:

$$\mathbf{B}_{lab}(\mathbf{r}) = \begin{bmatrix} 0 \\ B_0 \cosh(k \cdot y_{lab}) \sin(k \cdot z_{lab}) \\ B_0 \sinh(k \cdot y_{lab}) \cos(k \cdot z_{lab}) \end{bmatrix}$$

$$r_{lab} = \mathbf{\Lambda}^{-1}(r_{bunch})$$

$$\mathbf{E}_{bunch} = \gamma(\mathbf{E}_{lab} + \mathbf{v} \times \mathbf{B}_{lab}) - (\gamma - 1)\left(\mathbf{E}_{lab} \cdot \frac{\mathbf{v}}{||\mathbf{v}||}\right)$$

$$\mathbf{B}_{bunch} = \gamma(\mathbf{B}_{lab} - \mathbf{v} \times \mathbf{E}_{lab}) - (\gamma - 1)\left(\mathbf{B}_{lab} \cdot \frac{\mathbf{v}}{||\mathbf{v}||}\right)$$

or equivalently $\mathbf{F}^{\alpha\beta}_{bunch} = \mathbf{\Lambda}^{\beta}_{\alpha}\mathbf{F}^{\alpha\beta}_{lab}\mathbf{\Lambda}^{\alpha}_{\beta}$

In code:

```
{
  lorentzBoost<double> boost({0.0, 0.0, 0.99});
                                        //Lab to bunch frame
  ippl::Matrix<double, 4, 4> mat = boost.unprimedToPrimed();
}
```

Resampling

Assign weight w_i to each particle p_i.

Resampling

Assign weight w_i to each particle p_i. Resampling must conserve:

$$\sum_{i=1}^{N_b} w_i^b = \sum_{j=1}^{N_a} w_j^a$$

The "true" quantity q of particle p_i is given by $\rho_i \cdot w_i$.

Resampling

Assign weight w_i to each particle p_i. Resampling must conserve:

$$\sum_{i=1}^{N_b} w_i^b = \sum_{j=1}^{N_a} w_j^a$$

The "true" quantity q of particle p_i is given by $\rho_i \cdot w_i$.

Preferrably also conserve

$$\bar{\mathbf{r}} = \sum_{i=1}^{N} \frac{\mathbf{r_i}}{N} \quad \text{(Center of mass)}$$

$$\sigma = \sum_{i=1}^{N} \frac{(\mathbf{r_i} - \bar{\mathbf{r}})}{N} \quad \text{(Variance)}$$

Bibliography

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

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

Remi Lehe. Advanced electromagnetic particle-in-cell simulations. In *USPAS Short Course Series: Computational Methods in Accelerator Physics*, 2016. URL `https://people.nscl.msu.edu/~lund/uspas/scs_2016/lec_adv/A1a_EM_PIC.pdf`.

T Umeda, Y Omura, T Tominaga, and H Matsumoto. A new charge conservation method in electromagnetic particle-in-cell simulations. *Computer Physics Communications*, 156(1):73–85, 2003. ISSN 0010-4655. doi: https://doi.org/10.1016/S0010-4655(03)00437-5. URL `https://www.sciencedirect.com/science/article/pii/S0010465503004375`.