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A performance portable FDTD implementation
Final Presentation

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May 16, 2024

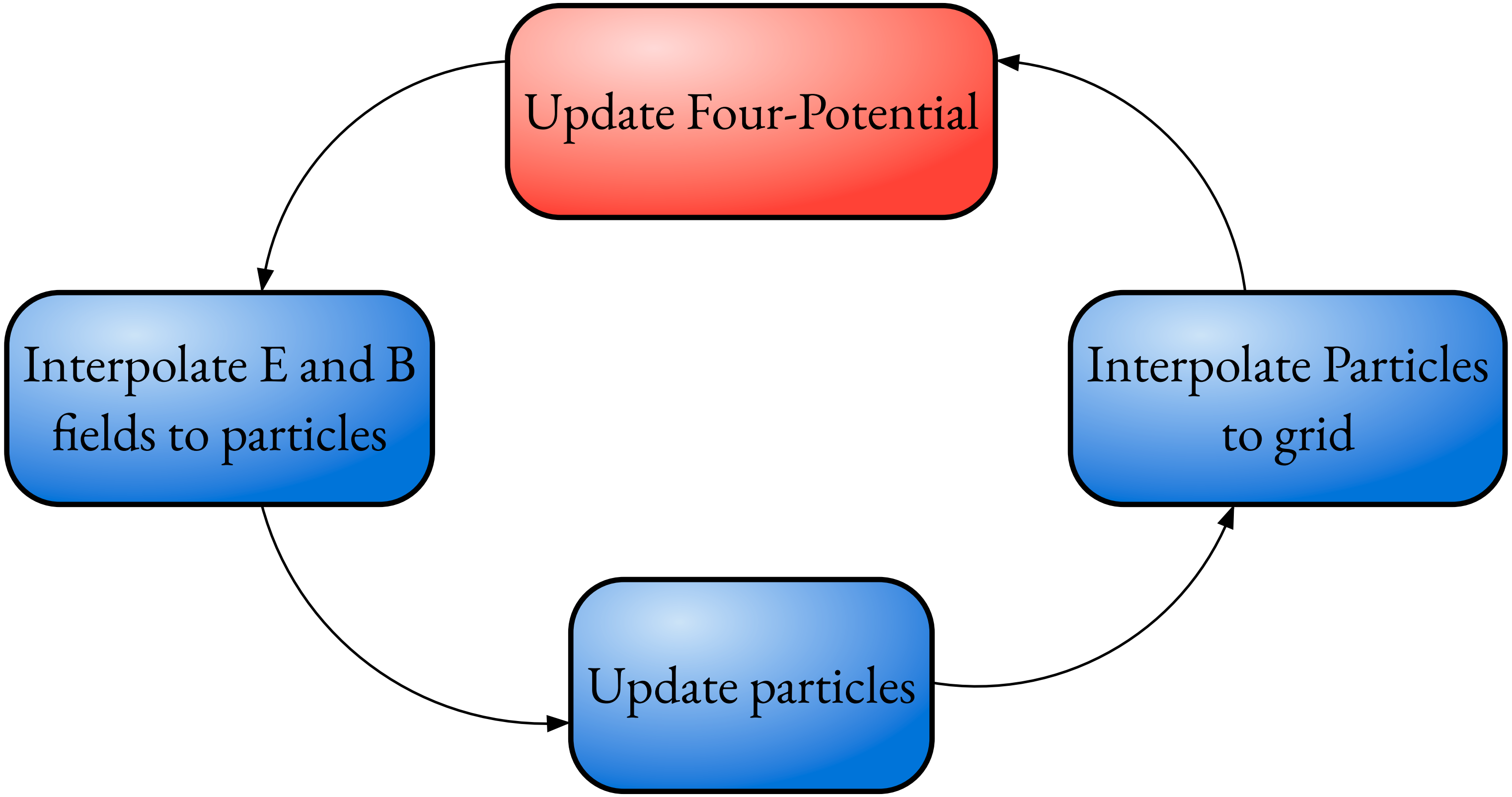
Outline

1. Methodology
2. The Poynting Vector
3. Free Electron Laser
4. Implementation and Results

Methodology

1. **Methodology**
2. The Poynting Vector
3. Free Electron Laser
4. Implementation and Results

The PIC Loop


Update Four-Potential
Interpolate E and B fields to particles
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Wave Equation

We solve the vector wave equation

$$\Delta \mathbf{A} = \frac{\partial^2 \mathbf{A}}{\partial t^2} + \mathbf{J}$$

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$$\mathbf{J} = \left[\rho, J_x, J_y, J_z\right]^T$$

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$$\mathbf{J} = \left[\rho, J_x, J_y, J_z\right]^T$$

$\mathbf{A}$ is stored and updated on a grid.
$\mathbf{J}$ is obtained from particles.

Discretization

For $\mathbf{A}$:

$$\frac{\partial^2 \mathbf{A}^n_{i,j,k}}{\partial x^2} = \frac{\mathbf{A}^n_{i+1,j,k} - 2\mathbf{A}^n_{i,j,k} + \mathbf{A}^n_{i-1,j,k}}{\Delta x^2}$$

$$\frac{\partial^2 \mathbf{A}^n_{i,j,k}}{\partial t^2} = \frac{\mathbf{A}^{n+1}_{i,j,k} - 2\mathbf{A}^n_{i,j,k} + \mathbf{A}^{n-1}_{i,j,k}}{\Delta t^2}$$

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$$\frac{\partial^2 \mathbf{A}^n_{i,j,k}}{\partial t^2} = \frac{\mathbf{A}^{n+1}_{i,j,k} - 2\mathbf{A}^n_{i,j,k} + \mathbf{A}^{n-1}_{i,j,k}}{\Delta t^2}$$

And we solve for $\mathbf{A}^{n+1}_{i,j,k}$.[1]

Standard Finite Differences

$$
\begin{aligned}
\mathbf{A}^{n+1}_{i,j,k} = -\mathbf{A}^{n-1}_{i,j,k} + \alpha_1 \mathbf{A}^{n}_{i,j,k} + \alpha_2 \mathbf{A}^{n}_{i+1,j,k} + \alpha_2 \mathbf{A}^{n}_{i-1,j,k} \\
+\alpha_4 \mathbf{A}^{n}_{i,j+,k} + \alpha_4 \mathbf{A}^{n}_{i,j-1,k} + \alpha_6 \mathbf{A}^{n}_{i,j,k+1} + \alpha_6 \mathbf{A}^{n}_{i,j,k-1} \\
+\alpha_8 \mathbf{J}^{n}_{i,j,k}
\end{aligned}
$$

where

$$
\begin{aligned}
\alpha_1 &= 2\left(1 - \left(\frac{c\Delta t}{\Delta x}\right)^2 - \left(\frac{c\Delta t}{\Delta y}\right)^2 - \left(\frac{c\Delta t}{\Delta z}\right)^2\right) \\
\alpha_2 &= \left(\frac{c\Delta t}{\Delta x}\right)^2, \alpha_4 = \left(\frac{c\Delta t}{\Delta y}\right)^2, \alpha_6 = \left(\frac{c\Delta t}{\Delta z}\right)^2 \\
\alpha_8 &= (c\Delta t)^2
\end{aligned}
$$

$$
\Delta t \leq \frac{\min(\Delta x, ...)}{\sqrt{3}}
$$

Nonstandard Finite Differences

$$
\begin{aligned}
\mathbf{A}_{i,j,k}^{n+1} = {} & -\mathbf{A}_{i,j,k}^{n-1} + \alpha_1' \mathbf{A}_{i,j,k}^{n} \\
& + \alpha_2' \Big(\mathcal{A} \mathbf{A}_{i+1,j,k-1}^{n} + (1 - 2\mathcal{A}) \mathbf{A}_{i+1,j,k}^{n} + \mathcal{A} \mathbf{A}_{i+1,j,k+1}^{n} \Big) \\
& + \alpha_3' \Big(\mathcal{A} \mathbf{A}_{i-1,j,k-1}^{n} + (1 - 2\mathcal{A}) \mathbf{A}_{i-1,j,k}^{n} + \mathcal{A} \mathbf{A}_{i-1,j,k+1}^{n} \Big) \\
& + \alpha_4' \Big(\mathcal{A} \mathbf{A}_{i,j+1,k-1}^{n} + (1 - 2\mathcal{A}) \mathbf{A}_{i,j+1,k}^{n} + \mathcal{A} \mathbf{A}_{i,j+1,k+1}^{n} \Big) \\
& + \alpha_5' \Big(\mathcal{A} \mathbf{A}_{i,j-1,k-1}^{n} + (1 - 2\mathcal{A}) \mathbf{A}_{i,j-1,k}^{n} + \mathcal{A} \mathbf{A}_{i,j-1,k+1}^{n} \Big) \\
& + \alpha_6' \mathbf{A}_{i,j,k+1}^{n} + \alpha_7' \mathbf{A}_{i,j,k-1}^{n} + \alpha_8' \mathbf{J}_{i,j,k}^{n}
\end{aligned}
$$

Nonstandard Finite Differences

$$\alpha_1' = 2\left(1 - (1-2\mathcal{A})\left(\frac{c\Delta t}{\Delta x}\right)^2 - (1-2\mathcal{A})\left(\frac{c\Delta t}{\Delta y}\right)^2 - \left(\frac{c\Delta t}{\Delta z}\right)^2\right)$$

$$\alpha_2' = \alpha_3' = \left(\frac{c\Delta t}{\Delta x}\right)^2, \alpha_4' = \alpha_5' = \left(\frac{c\Delta t}{\Delta y}\right)^2$$

$$\alpha_6' = \alpha_7' = \left(\frac{c\Delta t}{\Delta z}\right)^2 - 2\mathcal{A}\left(\frac{c\Delta t}{\Delta x}\right)^2 - 2\mathcal{A}\left(\frac{c\Delta t}{\Delta y}\right)^2$$

$$\alpha_8' = (c\Delta t)^2$$

For

$$\mathcal{A} > \frac{1}{4}, \Delta t = \Delta z$$

Absorbing Boundary Conditions

$$\left(\frac{\partial}{\partial x} - \sqrt{\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}}\right)\mathbf{A} = 0 \,\Bigg|_{x=0}$$

Absorbing Boundary Conditions

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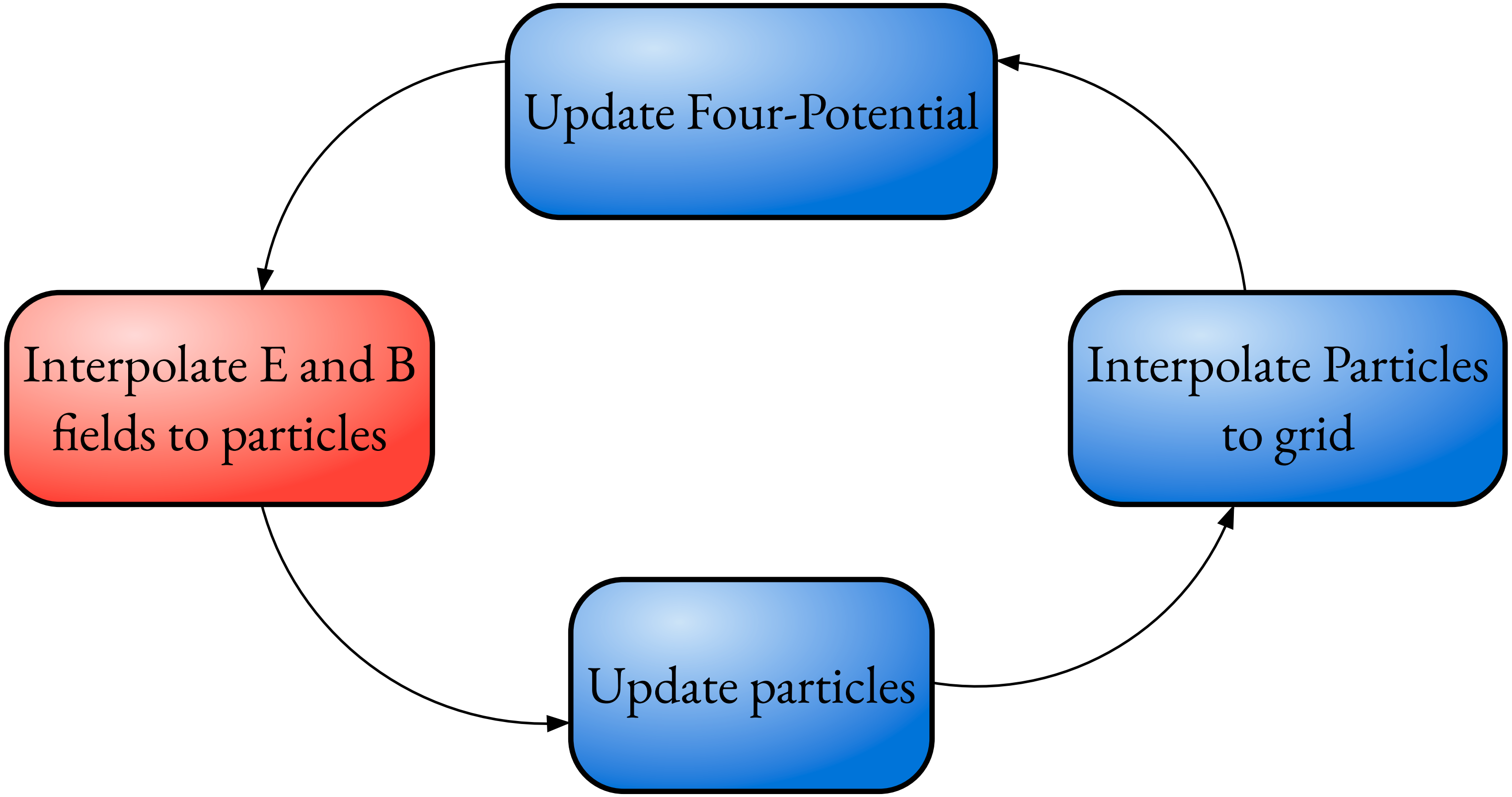
Discretize:

$$\begin{aligned} \pm\frac{\partial u}{\partial x} - \frac{1}{c}\frac{\partial u}{\partial t} &= 0 \quad \text{(first order)}, \\ \pm\frac{\partial^2 u}{\partial x \partial t} - \frac{1}{c}\frac{\partial^2 u}{\partial t^2} - \frac{c}{2}\frac{\partial^2 u}{\partial y^2} - \frac{c}{2}\frac{\partial^2 u}{\partial z^2} &= 0 \quad \text{(second order)} \end{aligned}$$

Initial Conditions

$$
\begin{cases}
\text{MITHRA: } \mathbf{A} = 0 \\[1em]
\text{Electrostatic: } \Delta\varphi = \rho \mid_{t=0}, \quad \mathrm{A} = 0 \\[1em]
\text{Liénard-Wiechert: } \begin{cases}
\Phi(\boldsymbol{r}, t) = \dfrac{q}{4\pi\varepsilon_0(1 - \boldsymbol{\beta}(t_{\text{ret}}) \cdot \boldsymbol{n})|r - \boldsymbol{R}(t_{\text{ret}})|} \\[2em]
\mathrm{A}(\boldsymbol{r}, t) = \dfrac{\boldsymbol{\beta}(t_{\text{ret}})}{\boldsymbol{c}} \Phi(\boldsymbol{r}, t)
\end{cases}
\end{cases}
$$

The PIC Loop



Update Four-Potential
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Field Evaluation

$$\mathbf{A} = \begin{bmatrix} \varphi \\ \mathrm{A} \end{bmatrix}$$

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

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

Particles

$$\mathbf{E}^n_{i,j,k} = \begin{bmatrix} -\frac{\varphi_{i+1,j,k}-\varphi_{i-1,j,k}}{2\Delta x} - \frac{\mathrm{A}^{n+1}_{x,i,j,k}-\mathrm{A}^{n}_{x,i,j,k}}{\Delta t} \\ -\frac{\varphi_{i,j+1,k}-\varphi_{i,j-1,k}}{2\Delta y} - \frac{\mathrm{A}^{n+1}_{y,i,j,k}-\mathrm{A}^{n}_{y,i,j,k}}{\Delta t} \\ -\frac{\varphi_{i,j,k+1}-\varphi_{i,j,k-1}}{2\Delta z} - \frac{\mathrm{A}^{n+1}_{z,i,j,k}-\mathrm{A}^{n}_{z,i,j,k}}{\Delta t} \end{bmatrix}$$

$$\mathbf{B}^n_{i,j,k} = \begin{bmatrix} \frac{\mathrm{A}_{z,i,j+1,k}-\mathrm{A}_{z,i,j-1,k}}{\Delta y} - \frac{\mathrm{A}_{z,i,j,k+1}-\mathrm{A}_{z,i,j,k-1}}{\Delta z} \\ \frac{\mathrm{A}_{z,i,j,k+1}-\mathrm{A}_{z,i,j,k-1}}{\Delta z} - \frac{\mathrm{A}_{z,i+1,j,k}-\mathrm{A}_{z,i-1,j,k}}{\Delta x} \\ \frac{\mathrm{A}_{z,i+1,j,k}-\mathrm{A}_{z,i-1,j,k}}{\Delta x} - \frac{\mathrm{A}_{z,i,j+1,k}-\mathrm{A}_{z,i,j-1,k}}{\Delta y} \end{bmatrix}$$

Particles

- Particles as discrete points with $m, q, \boldsymbol{r}, \dfrac{\boldsymbol{p}}{cm} = \gamma\boldsymbol{\beta}$

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- $\gamma = 2048 \longrightarrow \beta > 1 - \varepsilon_{\text{fp32}}$
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- $\gamma = 2048 \longrightarrow \beta > 1 - \varepsilon_{\mathrm{fp32}}$
  (Our case: $\gamma \approx 100$, SwissFEL: $\gamma \approx 11350$)

- Guided by Lorentz force: $\dfrac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = q\mathbf{E} + q\boldsymbol{v} \times \mathbf{B}$

Grid to particle interpolation

Define interpolation indices [2]

$$\begin{bmatrix} i_{\text{int}} \\ j_{\text{int}} \\ k_{\text{int}} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{r_x}{\Delta x} \right\rfloor \\ \left\lfloor \frac{r_y}{\Delta y} \right\rfloor \\ \left\lfloor \frac{r_z}{\Delta z} \right\rfloor \end{bmatrix}$$

$$\begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = \begin{bmatrix} \frac{r_x}{\Delta x} - i_{\text{int}} \\ \frac{r_y}{\Delta y} - j_{\text{int}} \\ \frac{r_z}{\Delta z} - k_{\text{int}} \end{bmatrix}$$

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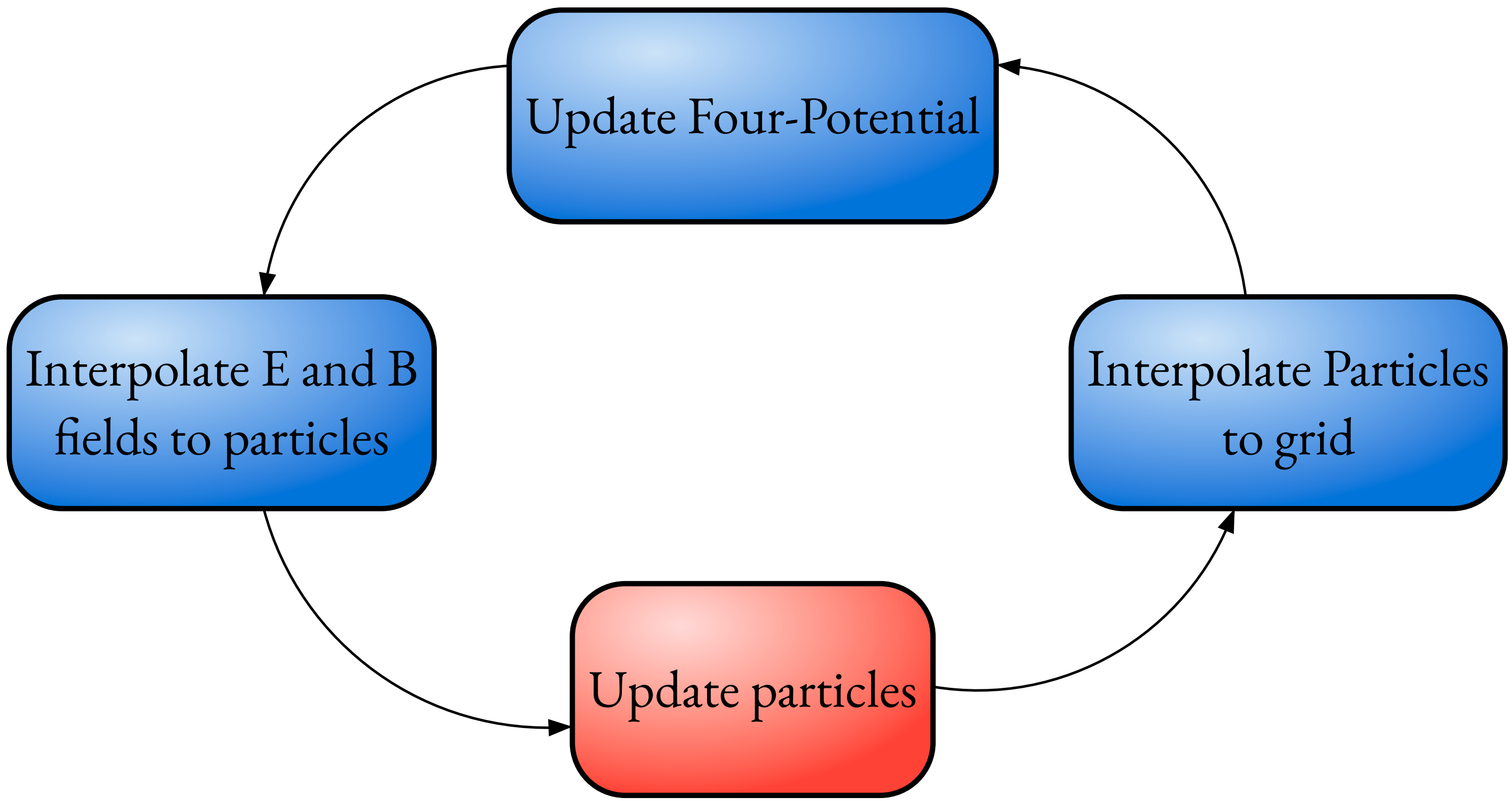
$$\mathbf{F}_p = \sum_{I,J,K \in (0,1)^3} \mathbf{F}_{i+I,j+J,k+K} \left(\frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left(\frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left(\frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta z}{\Delta z} \right| \right)$$

The PIC Loop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Updating the particles

Governing equation:

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = q\mathbf{E} + q\boldsymbol{v} \times \mathbf{B}$$

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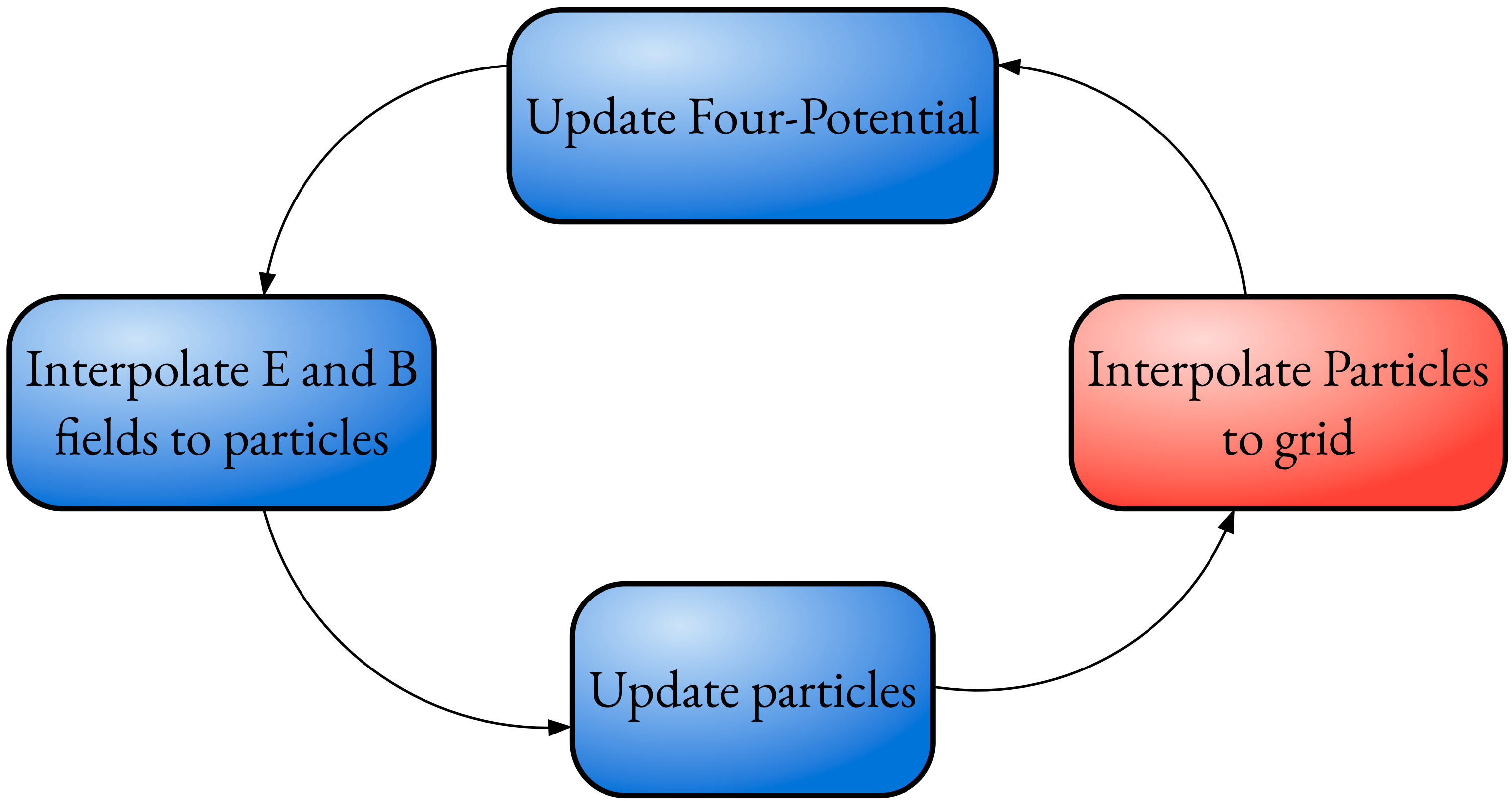
Update algorithm [3, 4]: $\left(\gamma\boldsymbol{\beta}^{n-\frac{1}{2}}, \boldsymbol{r}^n\right) \longrightarrow \left(\gamma\boldsymbol{\beta}^{n+\frac{1}{2}}, \boldsymbol{r}^{n+1}\right)$

$$\begin{aligned}
t_1 &= \gamma\beta^{n-\frac{1}{2}} + \frac{q\Delta t\mathbf{E}_t^n}{2mc} \\
\alpha &= \frac{q\Delta t}{2m\sqrt{1 + \|t_1\|^2}} \\
t_2 &= t_1 + \alpha t_1 \times \mathbf{B}_t^n \\
t_3 &= t_1 + t_2 \times \frac{2\alpha\mathbf{B}_t^n}{1 + \alpha^2\ \|\mathbf{B}_t^n\|^2} \\
\gamma\beta^{n+\frac{1}{2}} &= t_3 + \frac{q\Delta t\mathbf{E}_t^n}{2mc} \\
r^{m+1} &= r^n + c\Delta t\frac{\gamma\beta^{m+\frac{1}{2}}}{\sqrt{1 + \|\gamma\beta^{n+\frac{1}{2}}\|^2}}
\end{aligned}$$

The PIC Loop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Charge deposition

Recall

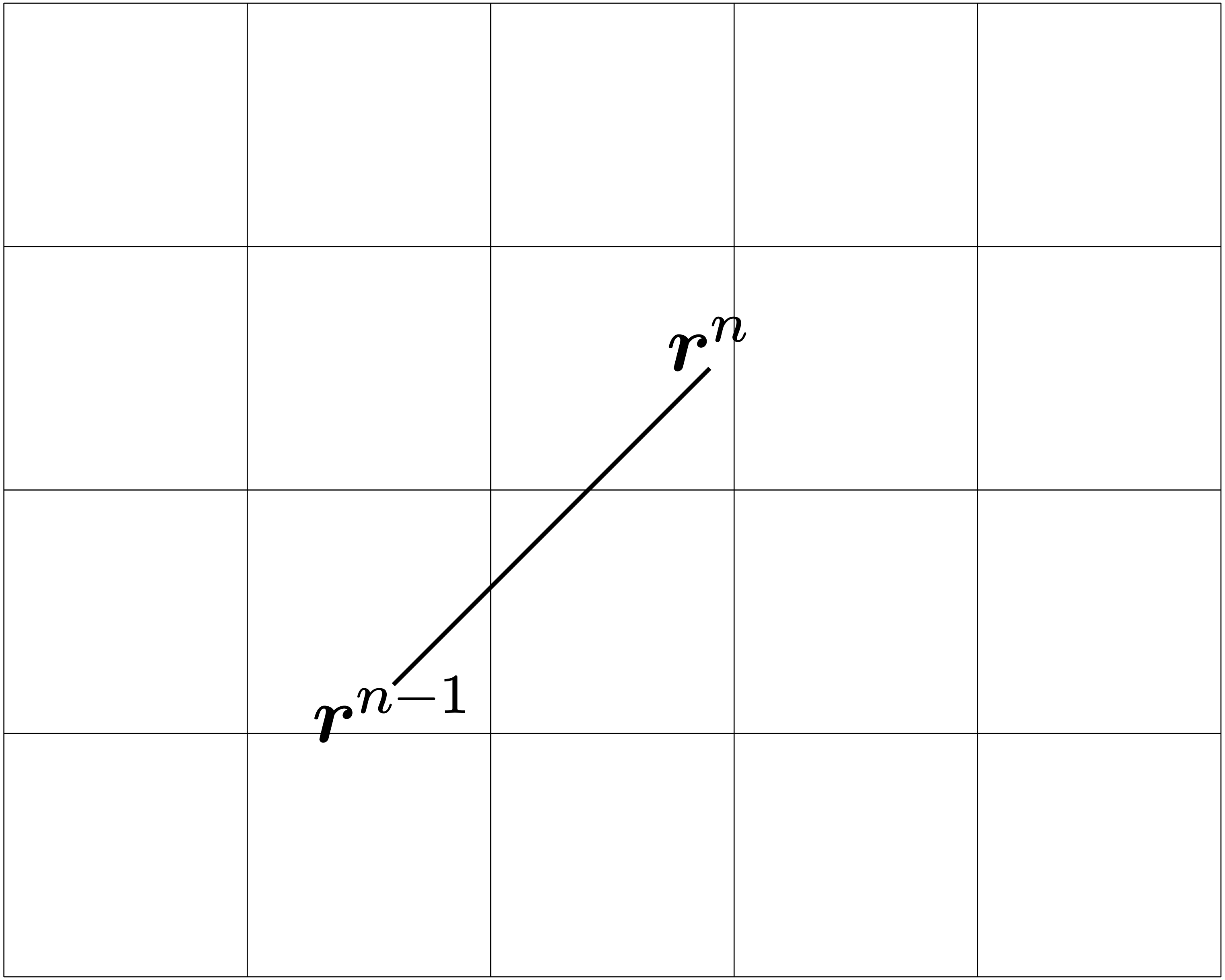
$$\Delta \mathbf{A} = \frac{\partial^2 \mathbf{A}}{\partial t^2} + \mathbf{J}, \mathbf{J} = \begin{bmatrix} \rho \\ J_x \\ J_y \\ J_z \end{bmatrix}$$

Interpolating ρ, we scatter contributions $\Delta\rho$

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

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

ZigZag



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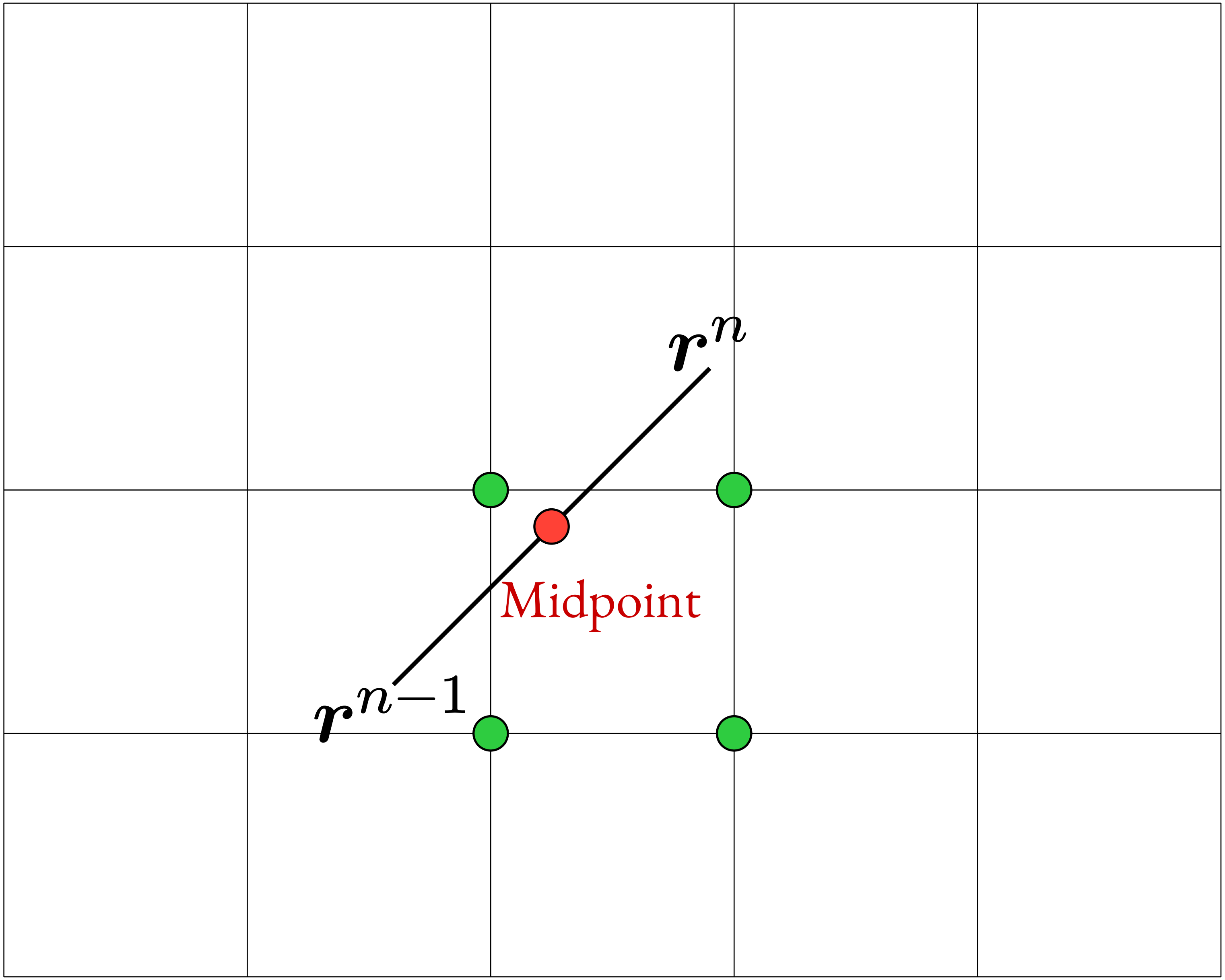

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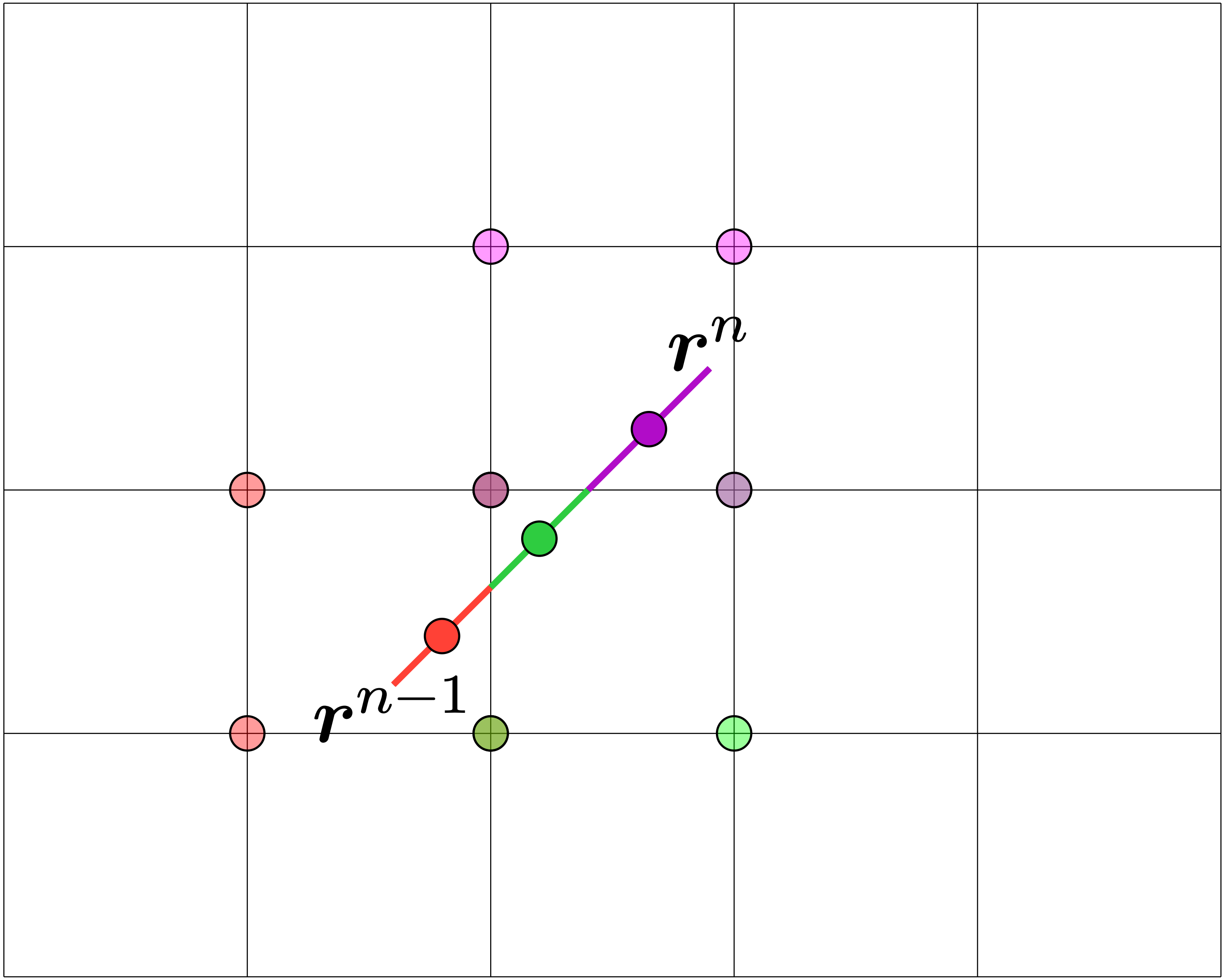

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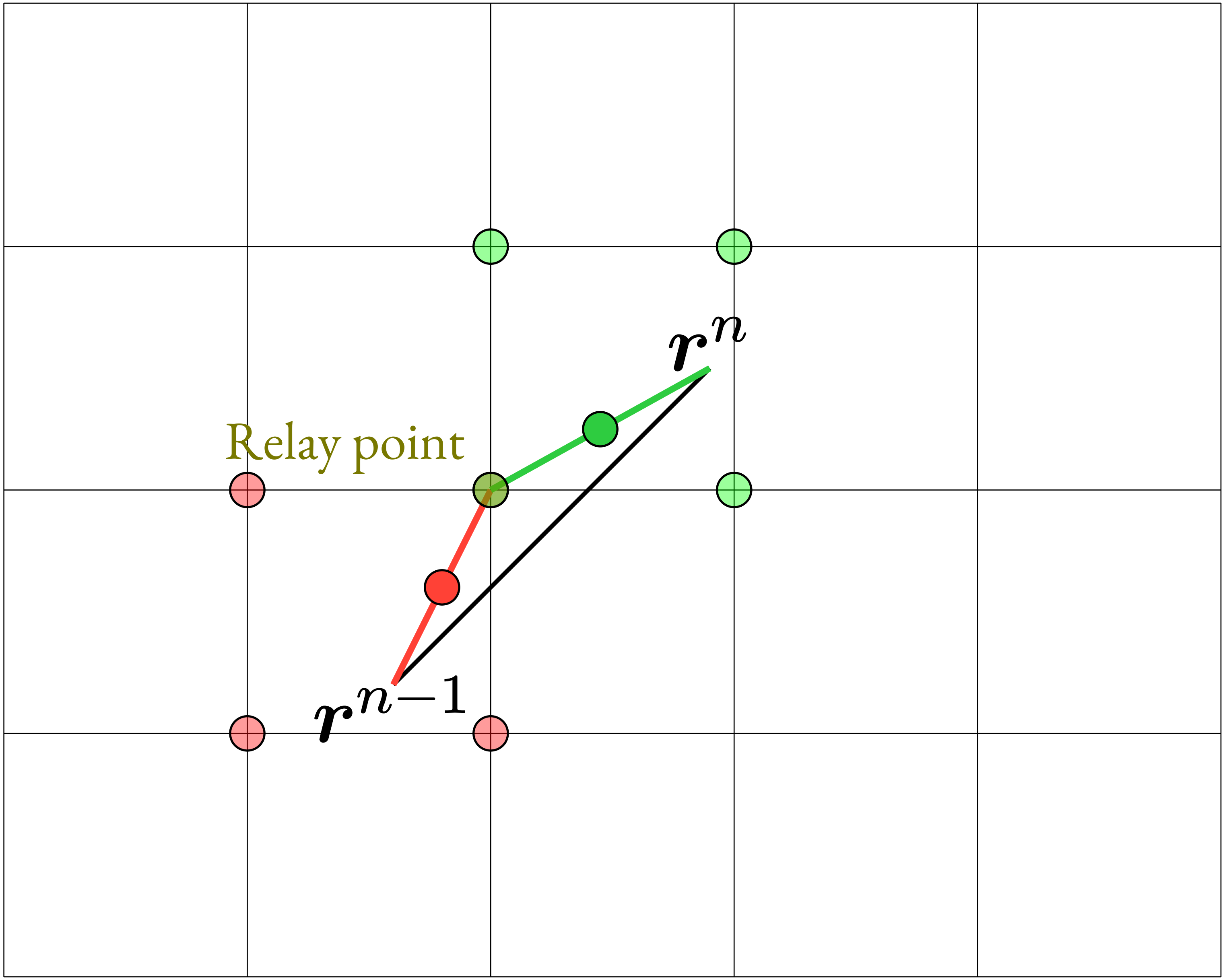

Current deposition

We want to interpolate $\frac{q(\boldsymbol{r}_n - \boldsymbol{r}_{n-1})}{\Delta t}$

Define $\{\boldsymbol{r}_{n-1}, \boldsymbol{r}_n\}$ as a *line*.

$$\boldsymbol{r}_{\text{relay}} = \begin{bmatrix} x_{\text{relay}} \\ y_{\text{relay}} \\ z_{\text{relay}} \end{bmatrix} = \begin{bmatrix} \min\left(\min(i_{n-1}\Delta x, i_n\Delta x) + \Delta x, \max\left(\max(i_{n-1}\Delta x, i_n\Delta x), \frac{r_{n-1,x}+r_{n,x}}{2}\right)\right) \\ \min\left(\min(j_{n-1}\Delta y, j_n\Delta y) + \Delta y, \max\left(\max(j_{n-1}\Delta y, j_n\Delta y), \frac{r_{n-1,y}+r_{n,y}}{2}\right)\right) \\ \min\left(\min(k_{n-1}\Delta z, k_n\Delta z) + \Delta z, \max\left(\max(k_{n-1}\Delta z, k_n\Delta z), \frac{r_{n-1,z}+r_{n,z}}{2}\right)\right) \end{bmatrix}$$

defines a split of $\{\boldsymbol{r}_{n-1}, \boldsymbol{r}_n\}$ into $\left\{\boldsymbol{r}_{n-1}, \boldsymbol{r}_{\text{relay}}\right\} + \left\{\boldsymbol{r}_{\text{relay}}, \boldsymbol{r}_n\right\}$ [5, 6, 1]

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$$\Delta \mathrm{J}_{i+I,j+J,k+K} = \frac{q(\boldsymbol{r}_n - \boldsymbol{r}_{n-1})}{\Delta x \Delta y \Delta z \Delta t}\left(\frac{1}{2} + (-1)^I\left|\frac{1}{2} - \frac{\delta x}{\Delta x}\right|\right)\left(\frac{1}{2} + (-1)^J\left|\frac{1}{2} - \frac{\delta y}{\Delta y}\right|\right)\left(\frac{1}{2} + (-1)^K\left|\frac{1}{2} - \frac{\delta z}{\Delta z}\right|\right)$$

J has units $\frac{\mathrm{A}}{\mathrm{m}^2} = \mathrm{C}\frac{\mathrm{m}}{\mathrm{s}}\frac{1}{\mathrm{m}^3}$

The Poynting Vector

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2. **The Poynting Vector**
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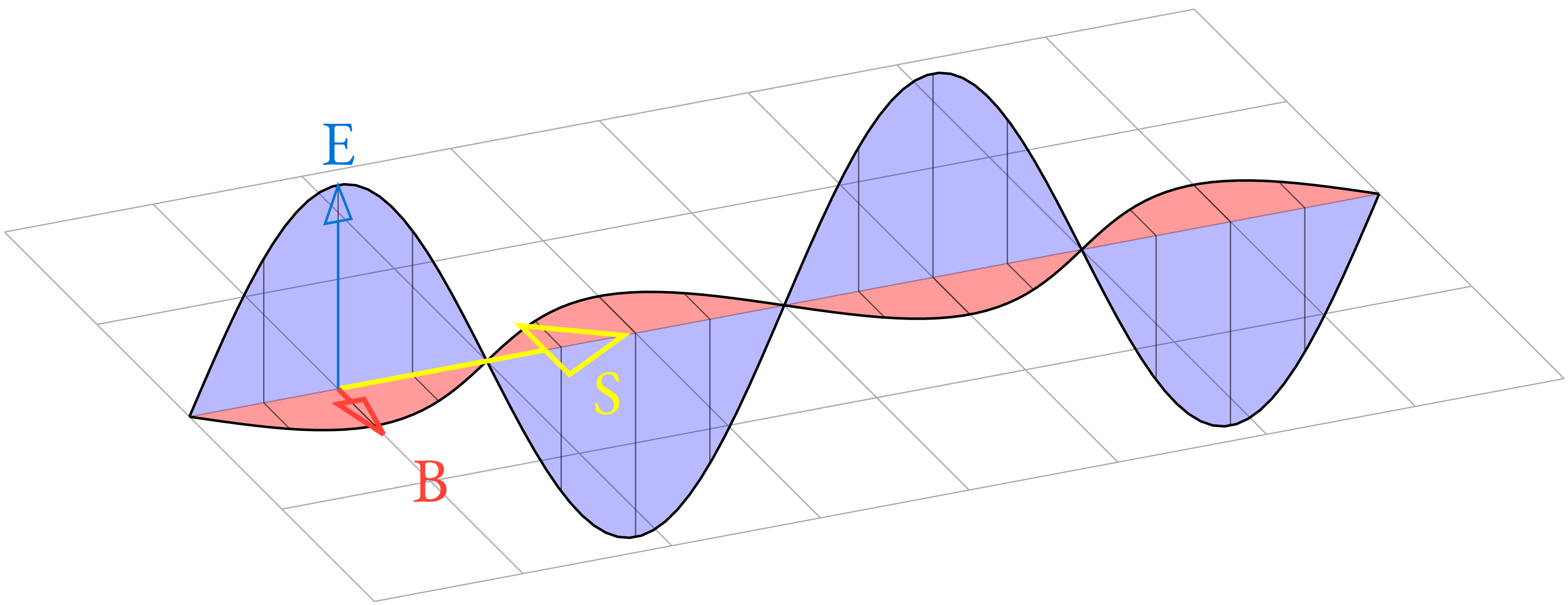
Definition

$$\mathbf{S} = \frac{1}{\mu_0}\mathbf{E} \times \mathbf{B}$$

$\longrightarrow$ Describes flow of energy

$\longrightarrow$ Is in unit $\frac{\mathrm{W}}{\mathrm{m}^2}$

Plane wave case



Stationary electron

$$\mathbf{E} = \frac{q\boldsymbol{r}}{4\pi\varepsilon_0 \left\|\boldsymbol{r}\right\|^3}$$

$$\mathbf{B} = \mathbf{0}$$

$$\implies \frac{1}{\mu_0}\mathbf{E} \times \mathbf{B} = 0$$

Inertially moving electron

Liénard - Wiechert Electric Field:

$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0}\left[\frac{q(\boldsymbol{n}-\boldsymbol{\beta})}{\gamma^2(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|^2} + \frac{q\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}\right)}{c(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|}\right]_{t_r}$$

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$$\mathbf{B} = \frac{\boldsymbol{n}\times\mathbf{E}}{c} = \frac{-q(\boldsymbol{n}\times\boldsymbol{\beta})}{c\gamma^2(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|^2}$$

$$\mathbf{S} = \text{some constant}\cdot\frac{\boldsymbol{\beta}}{|\mathbf{r}-\mathbf{r}_s|^4}$$

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$$\mathbf{S} = \text{some constant}\cdot\frac{\boldsymbol{\beta}}{|\mathbf{r}-\mathbf{r}_s|^4}$$

This means no energy is radiated away

Accelerated electron

Liénard - Wiechert Electric Field:

$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0}\left[\frac{q(\boldsymbol{n}-\boldsymbol{\beta})}{\gamma^2(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|^2} + \frac{q\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}\right)}{c(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|}\right]_{t_r}$$

$$\mathbf{B} = \frac{\boldsymbol{n}\times\mathbf{E}}{c}$$

Accelerated electron

Liénard - Wiechert Electric Field:

$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0}\left[\cancel{\frac{q(\boldsymbol{n}-\boldsymbol{\beta})}{\gamma^2(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|^2}} + \frac{q\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}\right)}{c(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|}\right]_{t_r}$$

$$\mathbf{B} = \frac{\boldsymbol{n}\times\mathbf{E}}{c}$$

$\longrightarrow$ Integrating over a sphere yields

$$\frac{q^2}{6\pi\varepsilon_0 c}\gamma^6\left(\|\dot{\boldsymbol{\beta}}\|^2 - \|\boldsymbol{\beta}\times\dot{\boldsymbol{\beta}}\|^2\right)$$

Accelerated electron

Liénard - Wiechert Electric Field:

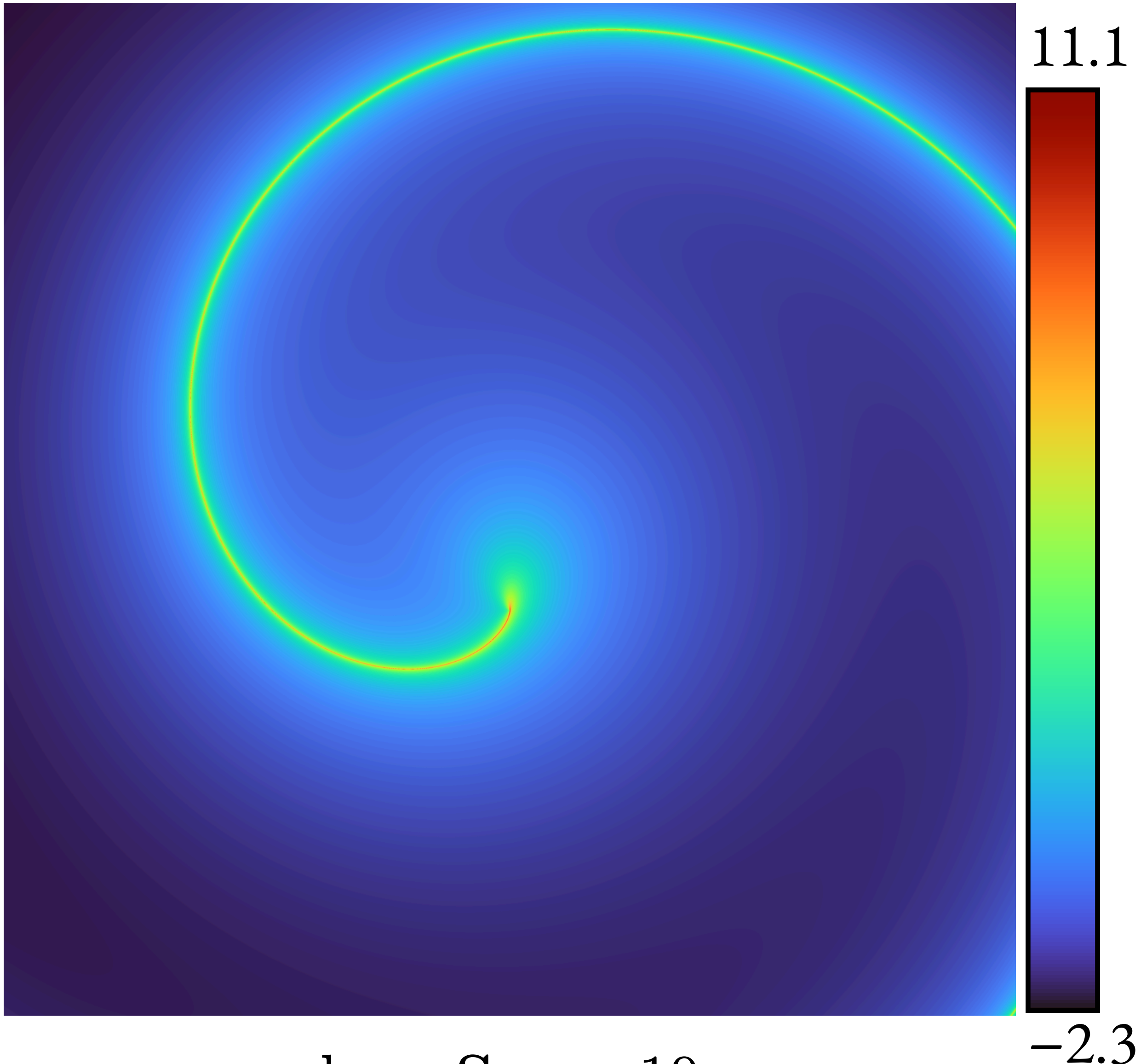
$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0}\left[\cancel{\frac{q(\boldsymbol{n}-\boldsymbol{\beta})}{\gamma^2(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|^2}} + \frac{q\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}\right)}{c(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^3|\mathbf{r}-\mathbf{r}_s|}\right]_{t_r}$$

$$\mathbf{B} = \frac{\boldsymbol{n}\times\mathbf{E}}{c}$$

$\longrightarrow$ Integrating over a sphere yields

$$\frac{q^2}{6\pi\varepsilon_0 c}\gamma^6\left(\|\dot{\boldsymbol{\beta}}\|^2 - \|\boldsymbol{\beta}\times\dot{\boldsymbol{\beta}}\|^2\right)$$

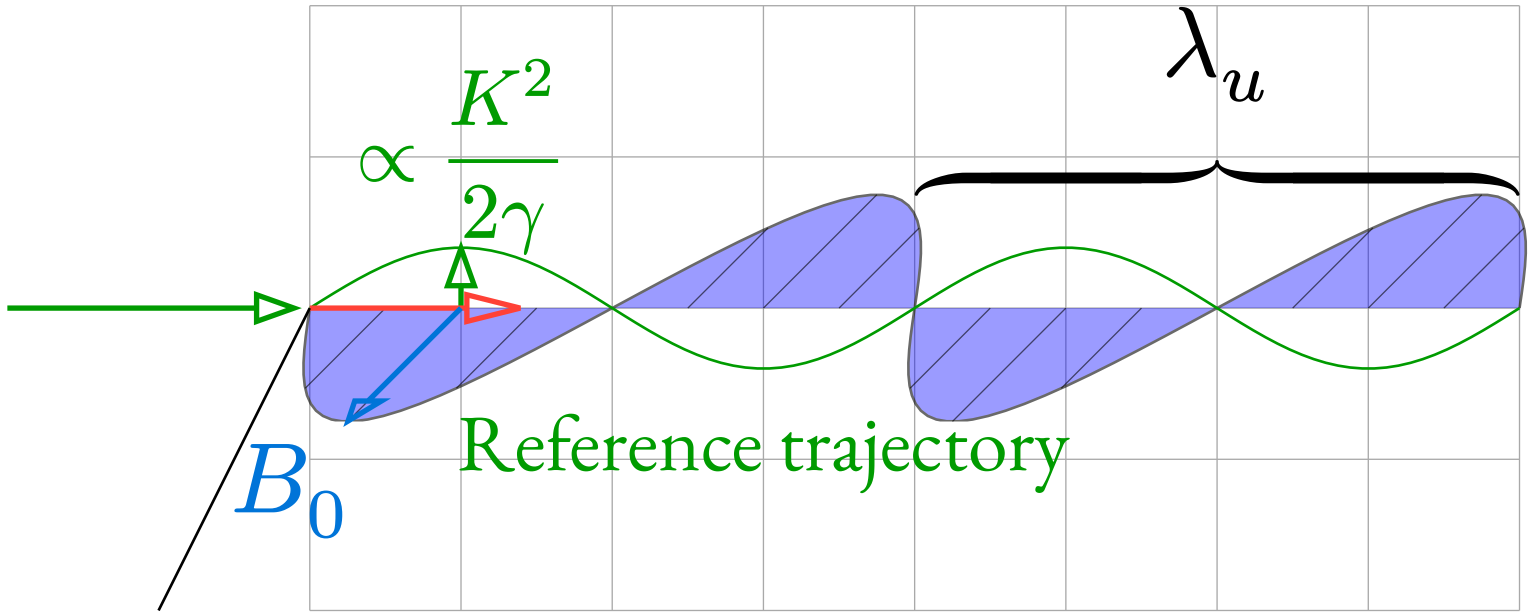
Accelerated electron



$\log_{10} \mathbf{S}, \gamma = 10$

Free Electron Laser

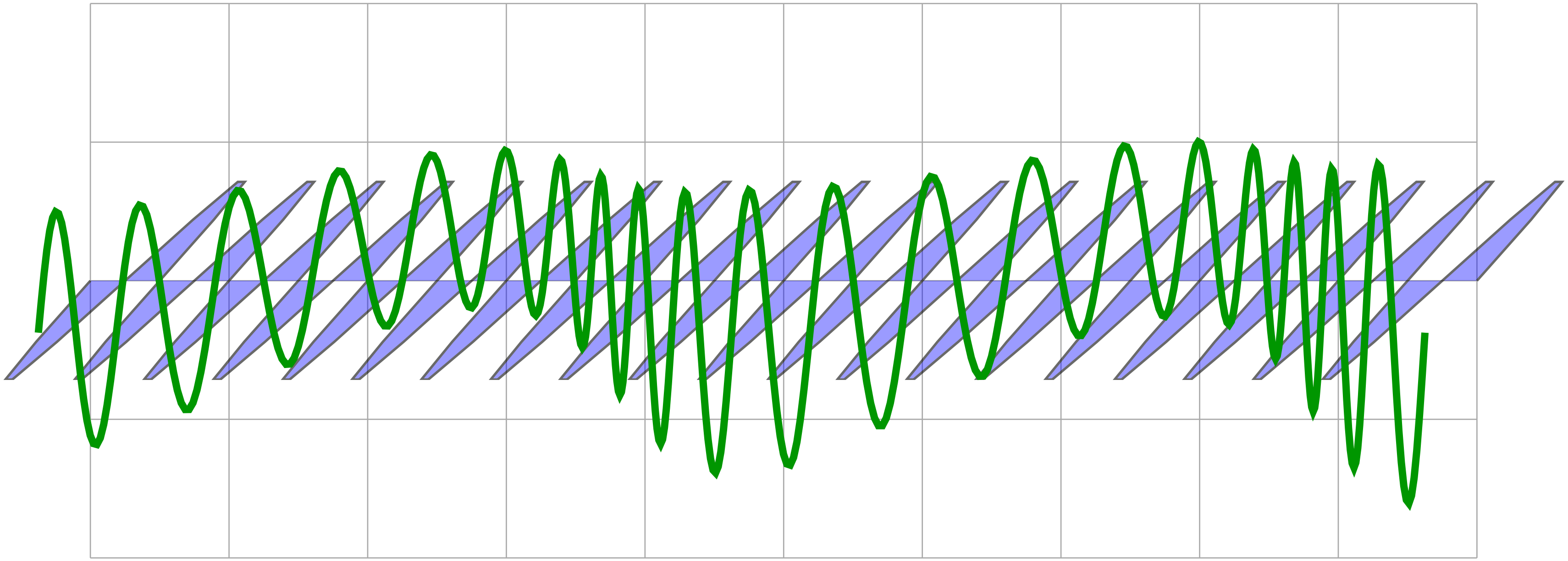
Undulator



Bunch enters with γ,
slowed down to $\gamma_0 = \frac{\gamma}{\sqrt{1+\frac{K^2}{2}}}$

$$\mathrm{K} = \frac{e}{2\pi m_e c} B_0 \lambda_u$$

Ponderomotive Forces



Moving frame

Entire simulation takes place in boosted frame:

$$\gamma_0 = \frac{\gamma}{\sqrt{1 + \frac{\mathrm{K}^2}{2}}}, \quad \mathrm{K} = \frac{e}{2\pi m_e c} B_0 \lambda_u$$

Lorentz Transforms

$$
\mathbb{L} = \begin{bmatrix}
\gamma & -\gamma\beta_x & -\gamma\beta_y & -\gamma\beta_x \\
-\gamma\beta_x & 1 + \frac{(\gamma-1)\beta_x^2}{\|\beta\|^2} & \frac{(\gamma-1)\beta_x\beta_y}{\|\beta\|^2} & \frac{(\gamma-1)\beta_x\beta_z}{\|\beta\|^2} \\
-\gamma\beta_y & \frac{(\gamma-1)\beta_x\beta_y}{\|\beta\|^2} & 1 + \frac{(\gamma-1)\beta_y^2}{\|\beta\|^2} & \frac{(\gamma-1)\beta_y\beta_z}{\|\beta\|^2} \\
-\gamma\beta_z & \frac{(\gamma-1)\beta_x\beta_z}{\|\beta\|^2} & \frac{(\gamma-1)\beta_y\beta_z}{\|\beta\|^2} & 1 + \frac{(\gamma-1)\beta_z^2}{\|\beta\|^2}
\end{bmatrix}
$$

Lorentz Transform

$$\mathbf{r}^{\alpha}_{\text{bunch}} = \mathbb{L}^{\alpha}_{\beta}\mathbf{r}^{\beta}_{\text{lab}}$$

$$\boldsymbol{\beta}_{\text{bunch}} = \frac{1}{1-(\boldsymbol{\beta}\cdot\boldsymbol{\beta}_{\text{lab}})}\left[\frac{\boldsymbol{\beta}_{\text{lab}}}{\gamma} - \boldsymbol{\beta} + \frac{\gamma}{1+\gamma}(\boldsymbol{\beta}_{\text{lab}}\cdot\boldsymbol{\beta})\boldsymbol{\beta}\right]$$

Lorentz Transform

$$\mathbf{r}^{\alpha}_{\text{bunch}} = \mathbb{L}^{\alpha}_{\beta} \mathbf{r}^{\beta}_{\text{lab}}$$

$$\boldsymbol{\beta}_{\text{bunch}} = \frac{1}{1 - (\boldsymbol{\beta} \cdot \boldsymbol{\beta}_{\text{lab}})} \left[\frac{\boldsymbol{\beta}_{\text{lab}}}{\gamma} - \boldsymbol{\beta} + \frac{\gamma}{1+\gamma} (\boldsymbol{\beta}_{\text{lab}} \cdot \boldsymbol{\beta}) \boldsymbol{\beta} \right]$$

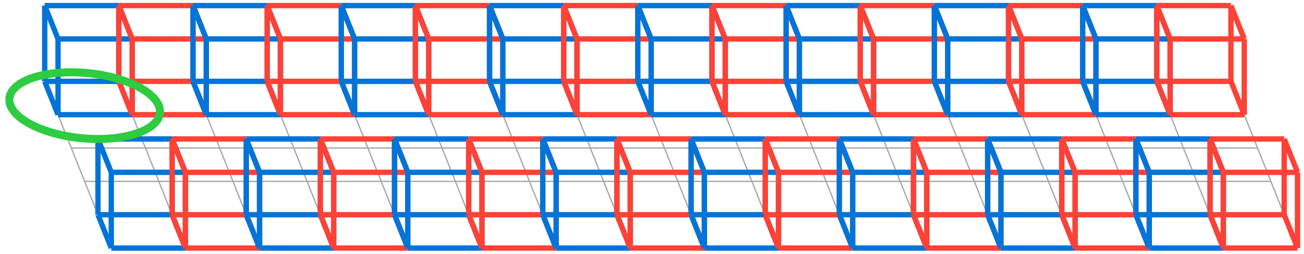
Particles end up with nonzero time $\mathbf{r}^0$

$\longrightarrow$ Correction of $\mathbf{r}^{1..3} := \mathbf{r}^{1..3} - c\boldsymbol{\beta}\mathbf{r}^0$

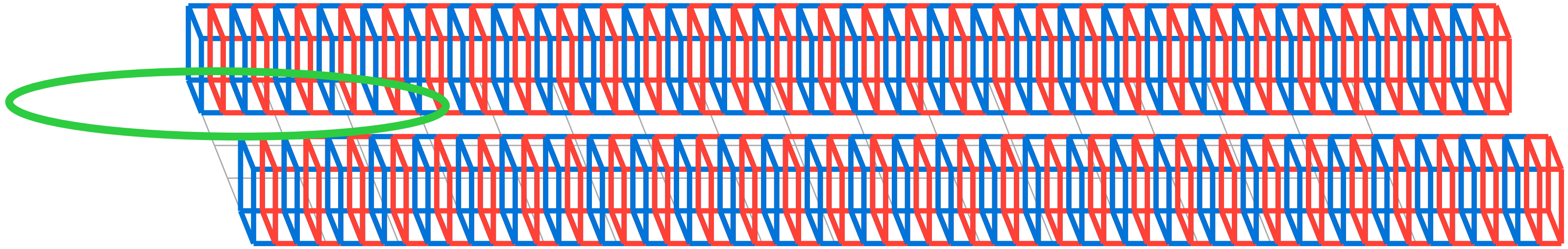
Setup

1. Initialize particles ~ gaussian distribution
2. Transform positions and velocities to a co-moving frame
3. Apply the PIC Loop
   - After every timestep, sample the forward radiation

Boost



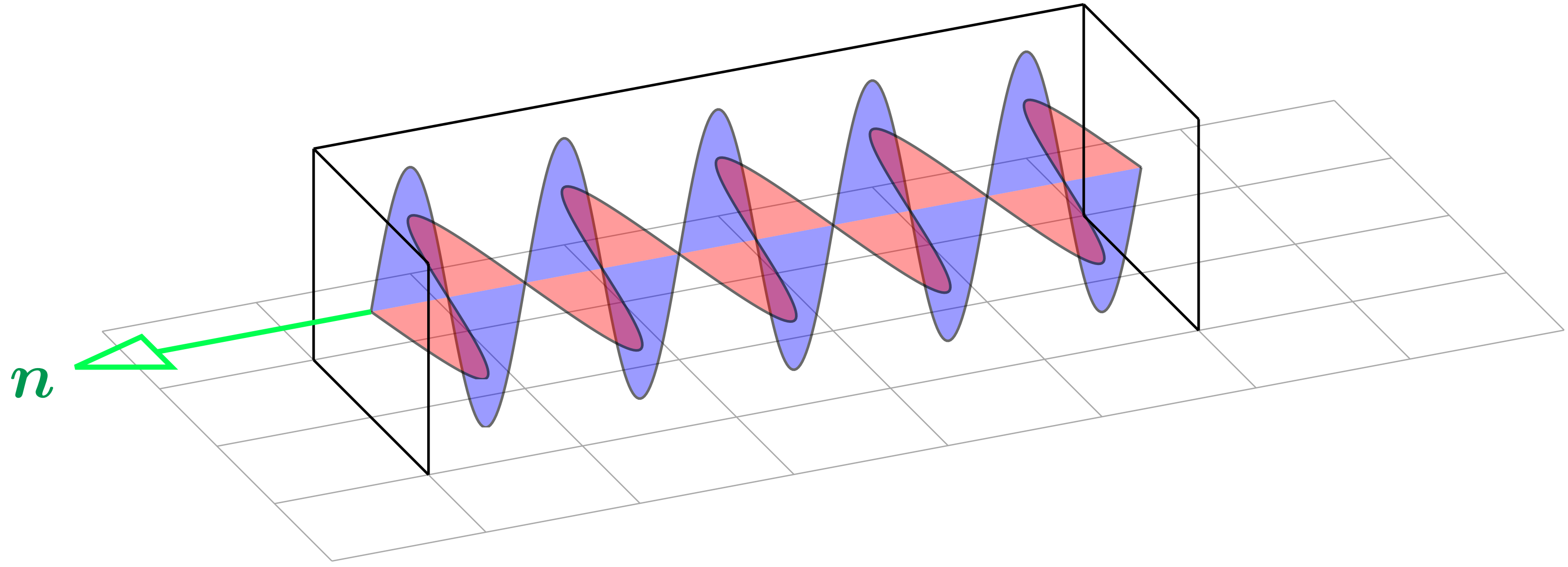
becomes



Forward Radiation

Evaluate

$$\oiint_{z^+ \text{ plane}} \mathbf{S}_{\text{lab}} \, \mathrm{d}\boldsymbol{n}$$

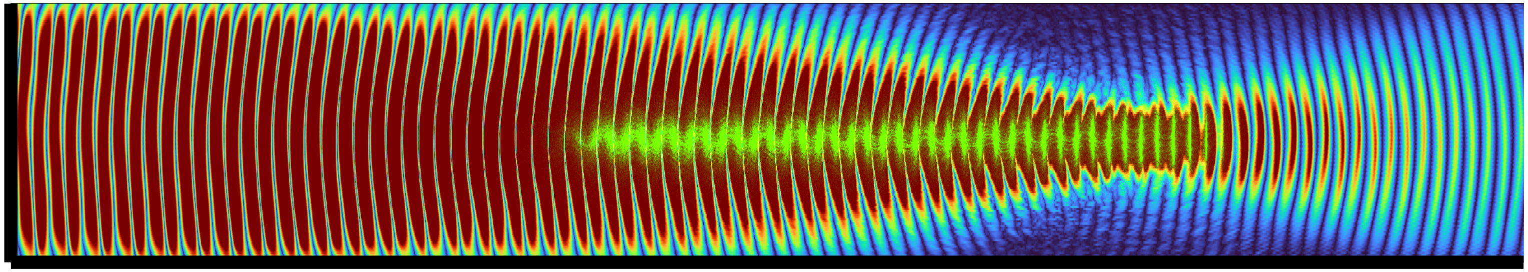


Electromagnetic Transform

$$
\begin{aligned}
\boldsymbol{E}_{\text{lab}} &= \gamma(\boldsymbol{E} - \boldsymbol{v} \times \boldsymbol{B}) \quad - (\gamma - 1)(\boldsymbol{E} \cdot \hat{\boldsymbol{v}})\hat{\boldsymbol{v}} \\
\boldsymbol{B}_{\text{lab}} &= \gamma\left(\boldsymbol{B} + \frac{\boldsymbol{v} \times \boldsymbol{E}}{c^2}\right) - (\gamma - 1)(\boldsymbol{B} \cdot \hat{\boldsymbol{v}})\hat{\boldsymbol{v}}
\end{aligned}
$$

Boost correction

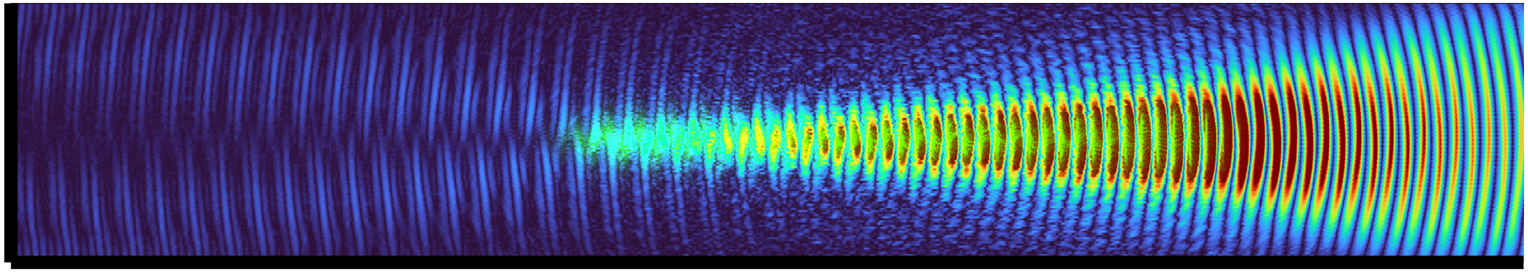
X [m]



Z [m]

$\mathbf{E} \times \mathbf{B}$ evaluated in the bunch frame

X [m]



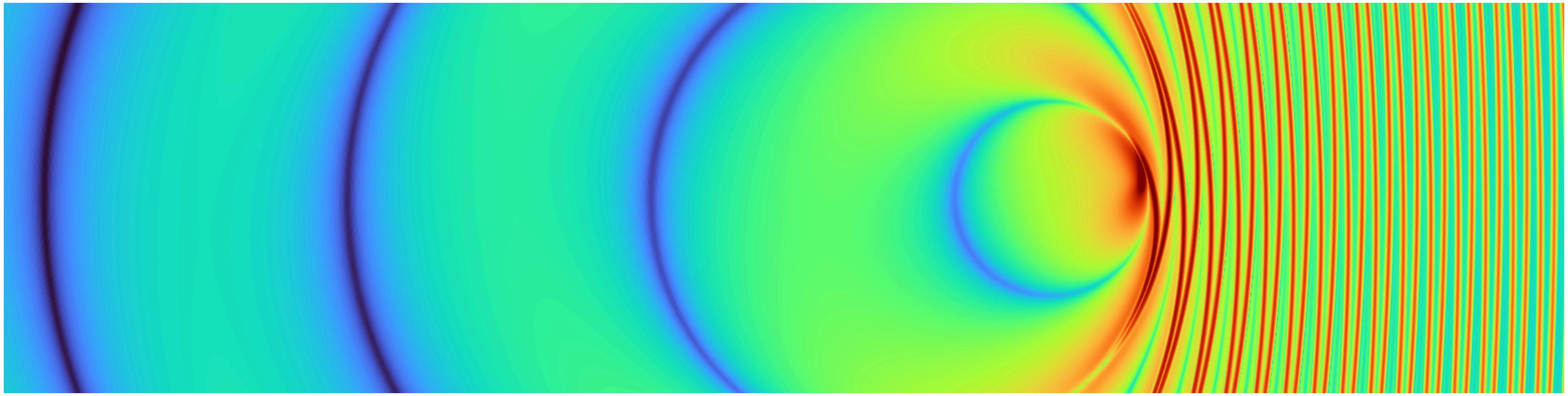
Z [m]

$\mathbf{E} \times \mathbf{B}$ evaluated in the lab frame

Laboratory frame

Observed wavelength:

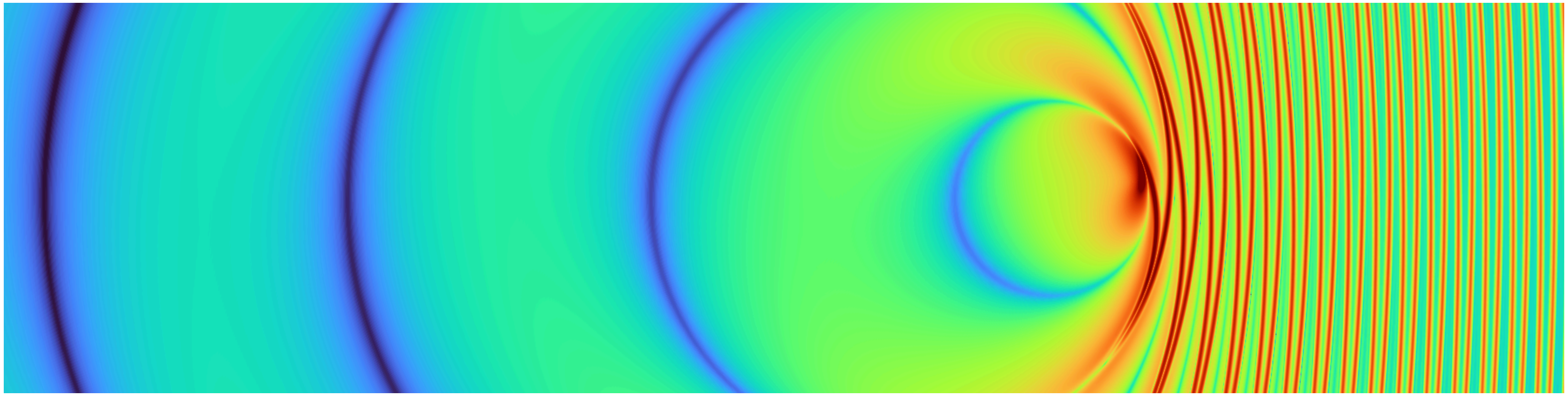
$$\lambda_u(1 - \beta_0)$$



Laboratory frame

Observed wavelength:

$$\lambda_u(1-\beta_0)$$

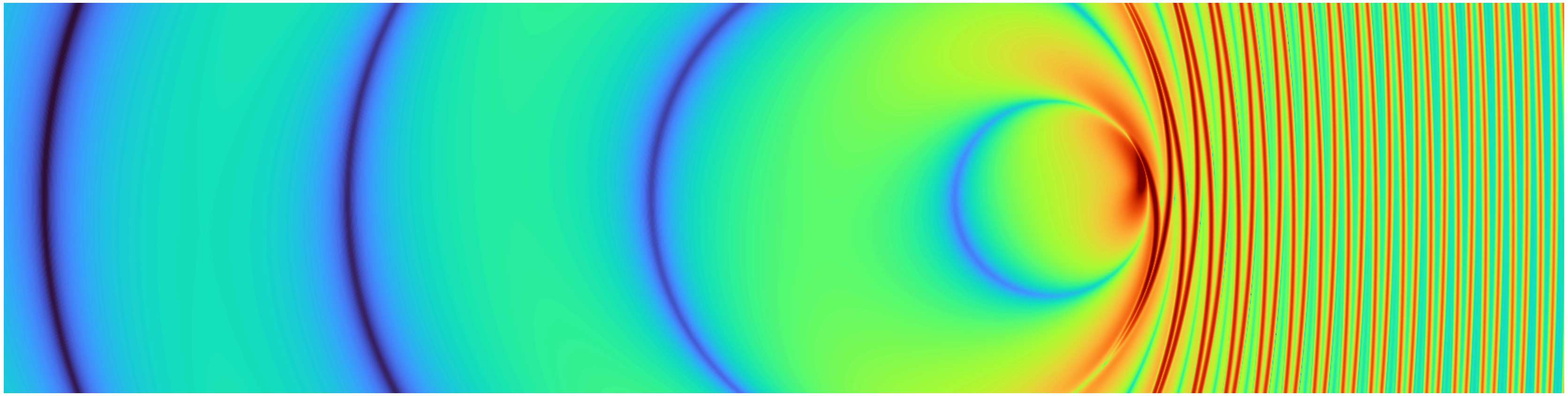


$$1-\beta_0 = 1-\sqrt{1-\frac{1}{\gamma_0^2}} = \frac{1}{2\gamma_0^2}+\frac{1}{8\gamma_0^4}+...$$

Laboratory frame

Observed wavelength:

$$\lambda_u(1-\beta_0)$$



$$1-\beta_0 = 1-\sqrt{1-\frac{1}{\gamma_0^2}} = \frac{1}{2\gamma_0^2} + \frac{1}{8\gamma_0^4} + \ldots$$

$$\lambda_u(1-\beta_0) \approx \frac{\lambda_u}{2\gamma_0^2}$$

Memory Savings

- `anm1view` $= \mathbf{A}^{n-1}$
- `aview` $= \mathbf{A}^{n}$

```
Kokkos::parallel_for(
"Four potential update",
ippl::getRangePolicy(aview,nghost),
KOKKOS_LAMBDA(unsigned i, unsigned j, unsigned k) {
      FourVector_t interior =
      -anm1view(i, j, k) + a1 * aview(i, j, k)
      + a2 * (aview(i + 1, j, k) + aview(i - 1,j, k))
      + a4 * (aview(i, j + 1, k) + aview(i, j - 1, k))
      + a6 * (aview(i, j, k + 1) + aview(i, j, k - 1))
      + a8 * (-source_view(i, j, k));
      anm1view(i, j, k) = interior;
    }
});
swap(aview, anm1view);
```

Memory Savings

- `anm1view` $= \mathbf{A}^{n-1}$
- `aview` $= \mathbf{A}^{n}$

```
Kokkos::parallel_for(
"Four potential update",
ippl::getRangePolicy(aview,nghost),
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      + a2 * (aview(i + 1, j, k) + aview(i - 1,j, k))
      + a4 * (aview(i, j + 1, k) + aview(i, j - 1, k))
      + a6 * (aview(i, j, k + 1) + aview(i, j, k - 1))
      + a8 * (-source_view(i, j, k));
      anm1view(i, j, k) = interior;
    }
});
swap(aview, anm1view);
```

Only possible if boundary conditions don't depend on $\mathbf{A}^{n+1}$

Memory Locality

$$\begin{bmatrix} i_{\text{int}} \\ j_{\text{int}} \\ k_{\text{int}} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{r_x}{\Delta x} \right\rfloor \\ \left\lfloor \frac{r_y}{\Delta y} \right\rfloor \\ \left\lfloor \frac{r_z}{\Delta z} \right\rfloor \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = \begin{bmatrix} \frac{r_x}{\Delta x} - i_{\text{int}} \\ \frac{r_y}{\Delta y} - j_{\text{int}} \\ \frac{r_z}{\Delta z} - k_{\text{int}} \end{bmatrix}$$

```
auto [ipos, fracpos] = gridCoordinatesOf(hr, orig, pos);
```

```
atomicAdd(&rhoview(ipos[0], ipos[1], ipos[2]), ...)
//Is equivalent to
atomicAdd(&rhoview[ipos[0] + ipos[1] * m + ipos[2] * m * n],  ...)
```

Memory Locality

$$\begin{bmatrix} i_{\text{int}} \\ j_{\text{int}} \\ k_{\text{int}} \end{bmatrix} = \begin{bmatrix} \left\lfloor \frac{r_x}{\Delta x} \right\rfloor \\ \left\lfloor \frac{r_y}{\Delta y} \right\rfloor \\ \left\lfloor \frac{r_z}{\Delta z} \right\rfloor \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = \begin{bmatrix} \frac{r_x}{\Delta x} - i_{\text{int}} \\ \frac{r_y}{\Delta y} - j_{\text{int}} \\ \frac{r_z}{\Delta z} - k_{\text{int}} \end{bmatrix}$$

```
auto [ipos, fracpos] = gridCoordinatesOf(hr, orig, pos);
```

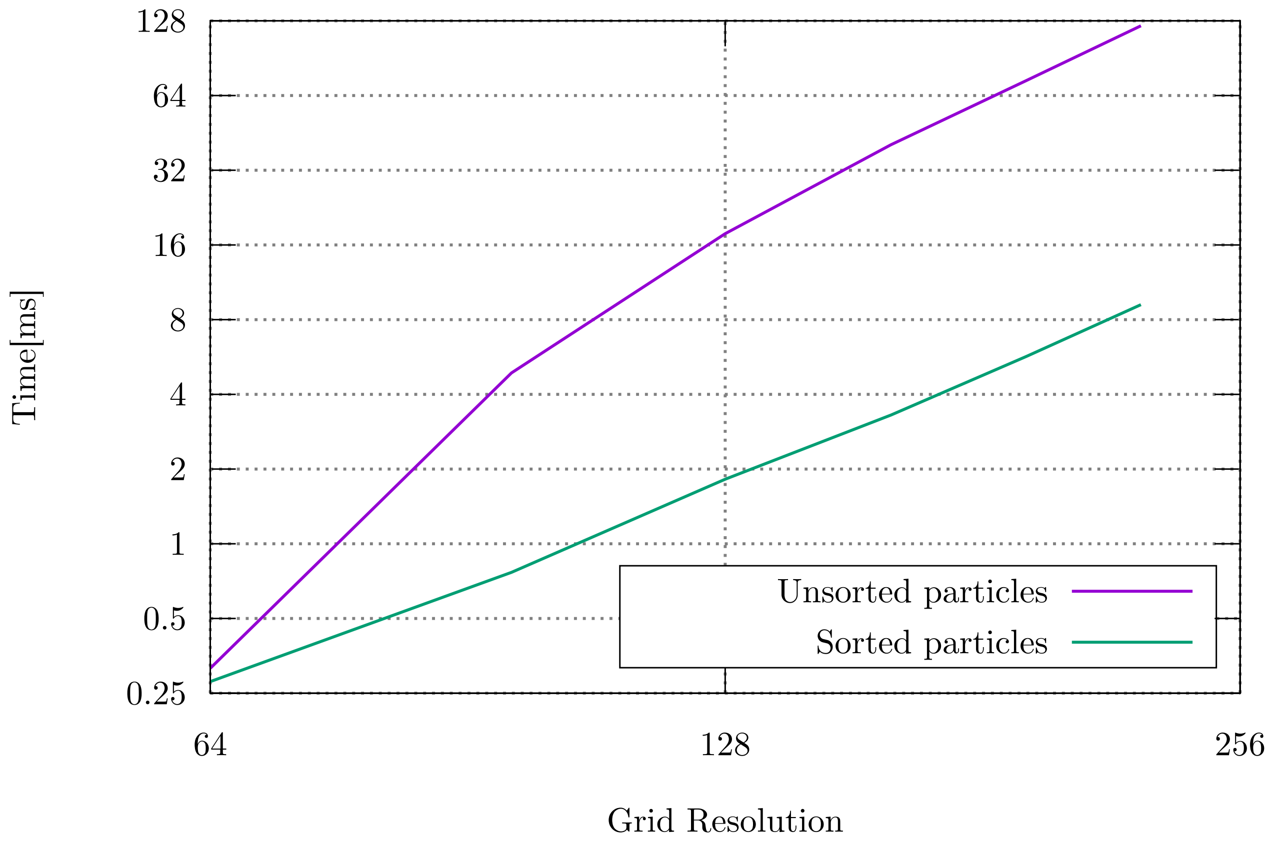
```
atomicAdd(&rhoview(ipos[0], ipos[1], ipos[2]), ...)
//Is equivalent to
atomicAdd(&rhoview[ipos[0] + ipos[1] * m + ipos[2] * m * n],  ...)
```

$\longrightarrow$ Sort particles by memory index

$$i_{\text{int}} + m j_{\text{int}} + m n k_{\text{int}}$$

Memory Locality

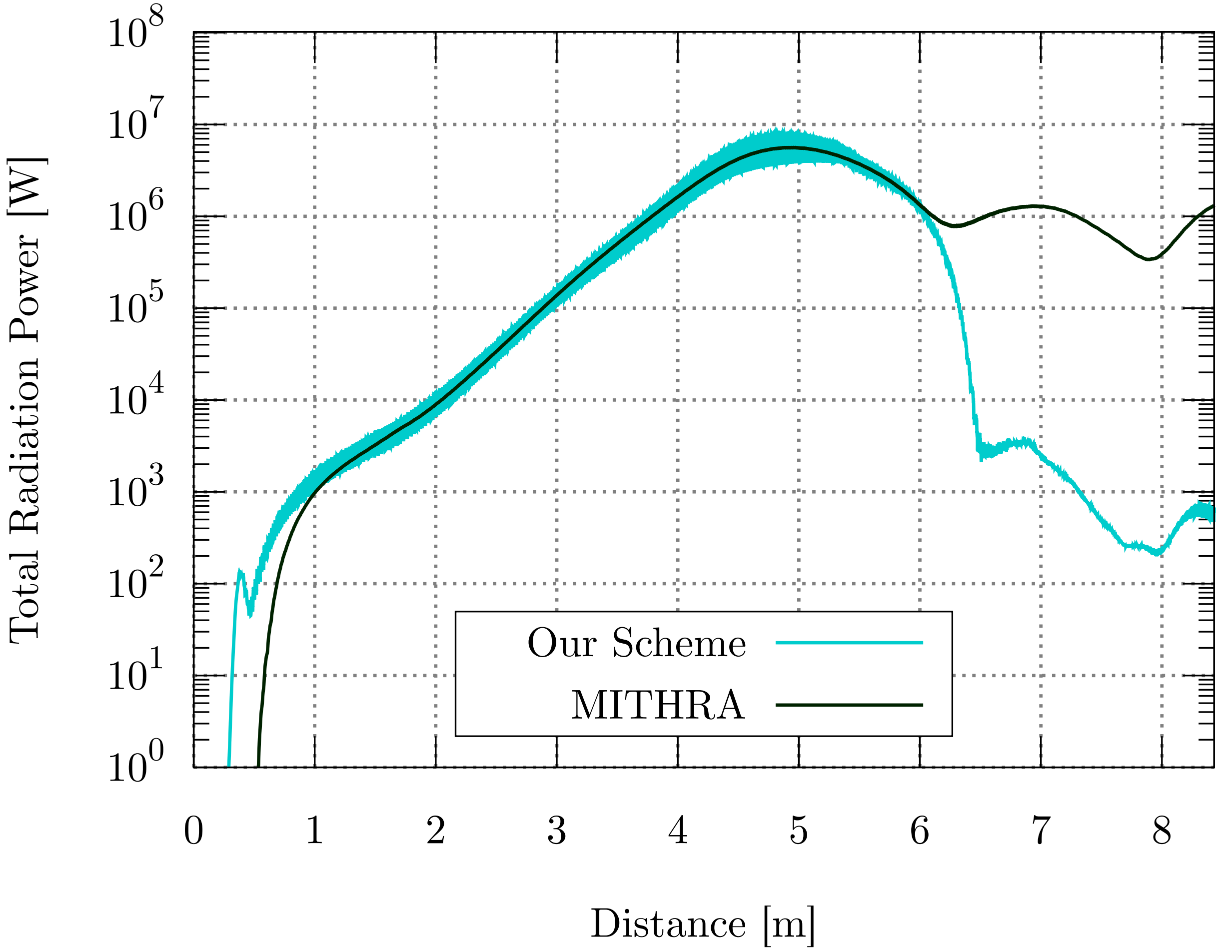
This yields a massive speedup



Correlated particle motion
$\longrightarrow$ sort only every 100th timestep.

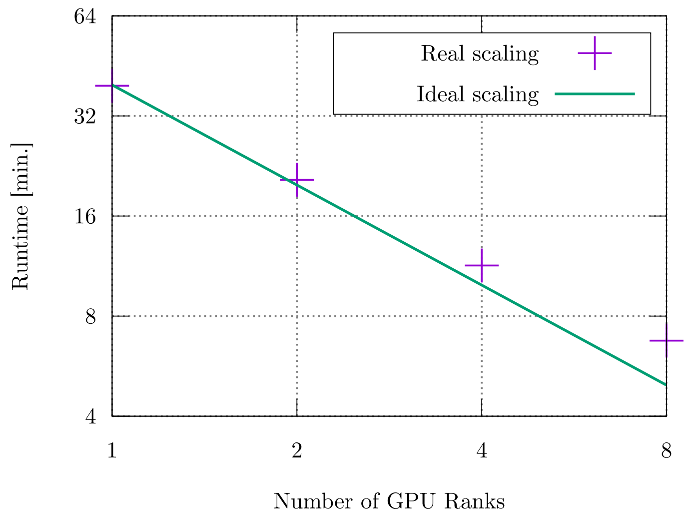
Final result

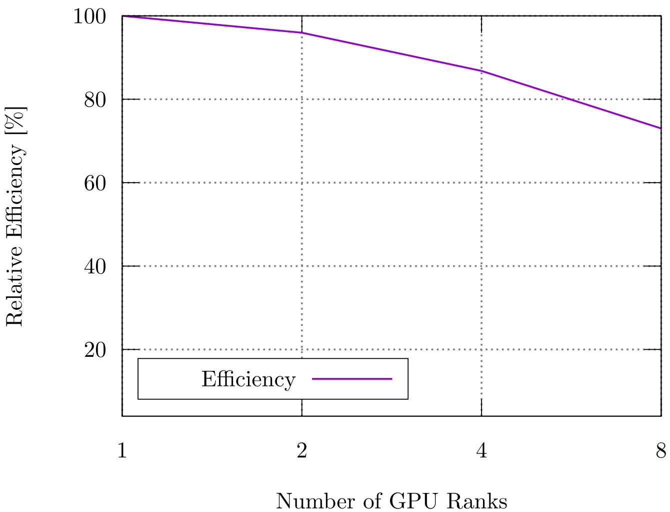
More noise since MITHRA filters frequencies.



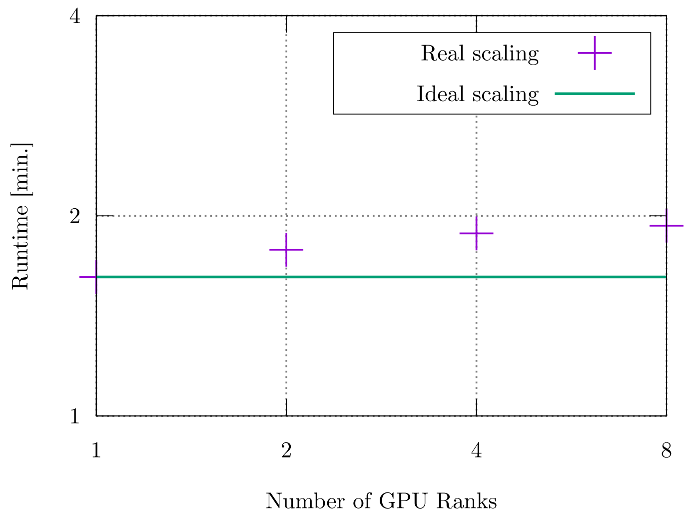
Scaling

Strong Scaling





Weak Scaling



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