

PAUL SCHERRER INSTITUT



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# A performance portable FDTD implementation

## Final Presentation

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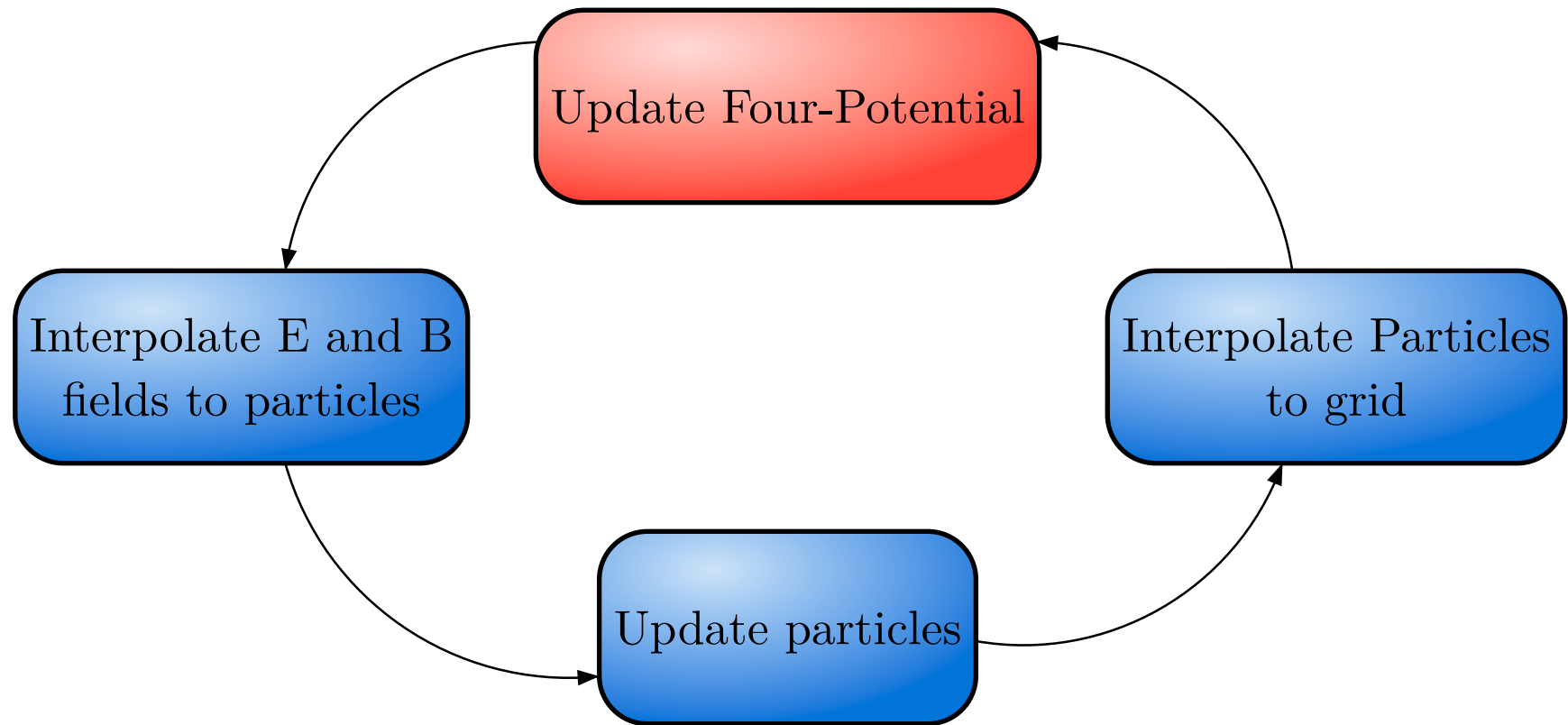
# Outline

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

# Methodology

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

# The PIC Loop



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

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

$\mathbf{A}$  is stored and updated on a grid.

$\mathbf{J}$  is obtained from particles.

# Discretization

For  $\mathbf{A}$ :

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

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



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

# Standard Finite Differences

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

where

$$\alpha_1 = 2 \left( 1 - \left( \frac{c\Delta t}{\Delta x} \right)^2 - \left( \frac{c\Delta t}{\Delta y} \right)^2 - \left( \frac{c\Delta t}{\Delta z} \right)^2 \right)$$

$$\alpha_2 = \left( \frac{c\Delta t}{\Delta x} \right)^2, \alpha_4 = \left( \frac{c\Delta t}{\Delta y} \right)^2, \alpha_6 = \left( \frac{c\Delta t}{\Delta z} \right)^2$$

$$\alpha_8 = (c\Delta t)^2$$

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

# Nonstandard Finite Differences

$$\begin{aligned}\mathbf{A}_{i,j,k}^{n+1} = & -\mathbf{A}_{i,j,k}^{n-1} + \alpha'_1 \mathbf{A}_{i,j,k}^n \\ & + \alpha'_2 \left( \mathcal{A} \mathbf{A}_{i+1,j,k-1}^n + (1 - 2\mathcal{A}) \mathbf{A}_{i+1,j,k}^n + \mathcal{A} \mathbf{A}_{i+1,j,k+1}^n \right) \\ & + \alpha'_3 \left( \mathcal{A} \mathbf{A}_{i-1,j,k-1}^n + (1 - 2\mathcal{A}) \mathbf{A}_{i-1,j,k}^n + \mathcal{A} \mathbf{A}_{i-1,j,k+1}^n \right) \\ & + \alpha'_4 \left( \mathcal{A} \mathbf{A}_{i,j+1,k-1}^n + (1 - 2\mathcal{A}) \mathbf{A}_{i,j+1,k}^n + \mathcal{A} \mathbf{A}_{i,j+1,k+1}^n \right) \\ & + \alpha'_5 \left( \mathcal{A} \mathbf{A}_{i,j-1,k-1}^n + (1 - 2\mathcal{A}) \mathbf{A}_{i,j-1,k}^n + \mathcal{A} \mathbf{A}_{i,j-1,k+1}^n \right) \\ & + \alpha'_6 \mathbf{A}_{i,j,k+1}^n + \alpha'_7 \mathbf{A}_{i,j,k-1}^n + \alpha'_8 \mathbf{J}_{i,j,k}^n\end{aligned}$$

# 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

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

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Discretize:

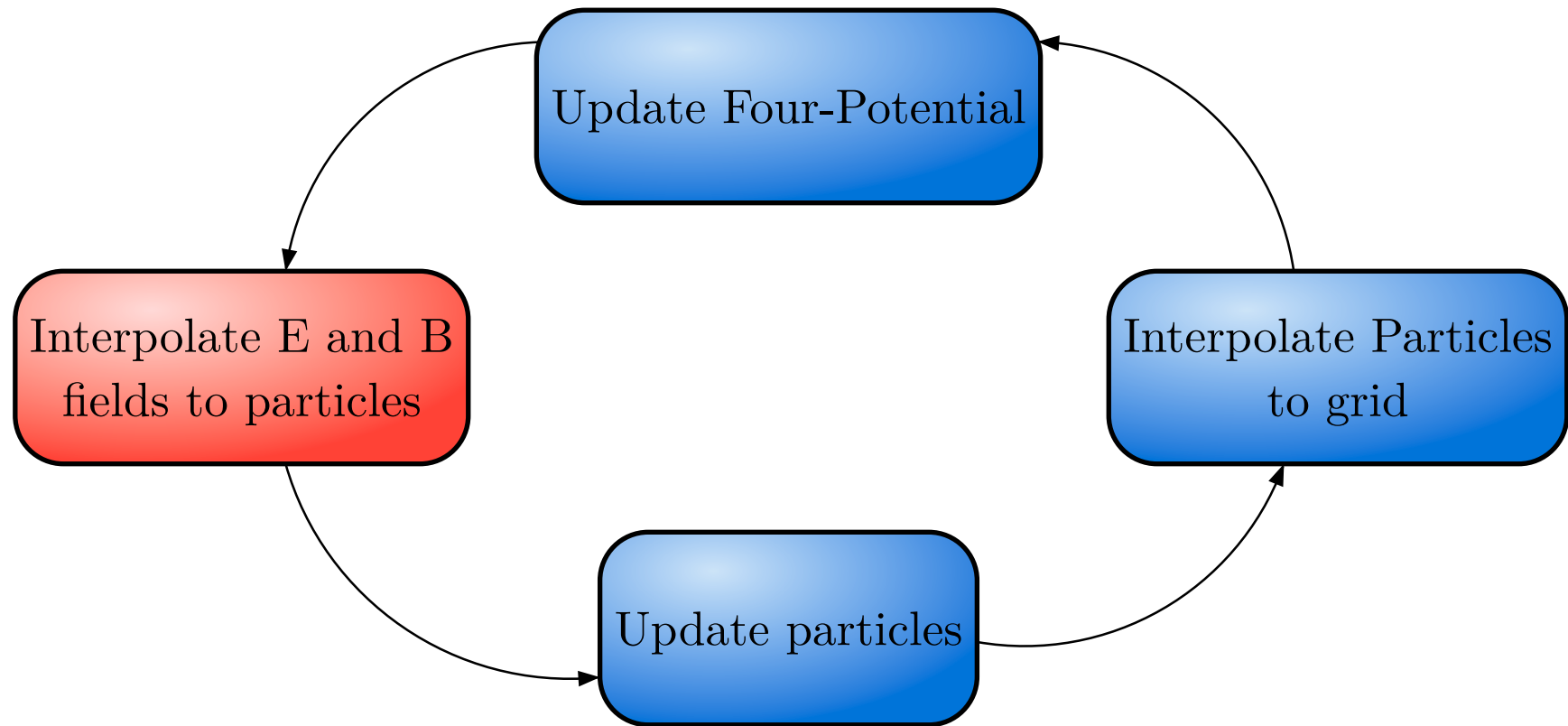
$$\pm \frac{\partial u}{\partial x} - \frac{1}{c} \frac{\partial u}{\partial t} = 0 \quad (\text{first order}),$$

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

# Initial Conditions

$$\left\{ \begin{array}{l} \text{MITHRA: } \mathbf{A} = 0 \\ \text{Electrostatic: } \Delta\varphi = \rho \mid_{t=0}, \quad \mathbf{A} = 0 \\ \text{Liénard-Wiechert: } \left\{ \begin{array}{l} \Phi(\mathbf{r}, t) = \frac{q}{4\pi\epsilon_0(1 - \boldsymbol{\beta}(t_{\text{ret}}) \cdot \mathbf{n})|\mathbf{r} - \mathbf{R}(t_{\text{ret}})|} \\ \mathbf{A}(\mathbf{r}, t) = \frac{\boldsymbol{\beta}(t_{\text{ret}})}{c} \Phi(\mathbf{r}, t) \end{array} \right. \end{array} \right.$$

# The PIC Loop





# Field Evaluation

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

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

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

# Particles

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

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

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

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(Our case:  $\gamma \approx 100$ , SwissFEL:  $\gamma \approx 11350$ )

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- $\gamma = 2048 \longrightarrow \beta > 1 - \varepsilon_{\text{fp}32}$   
(Our case:  $\gamma \approx 100$ , SwissFEL:  $\gamma \approx 11350$ )
- Guided by Lorentz force:  $\frac{d\mathbf{p}}{dt} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}$

# Grid to particle interpolation

Define interpolation indices [2]

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

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

# Grid to particle interpolation

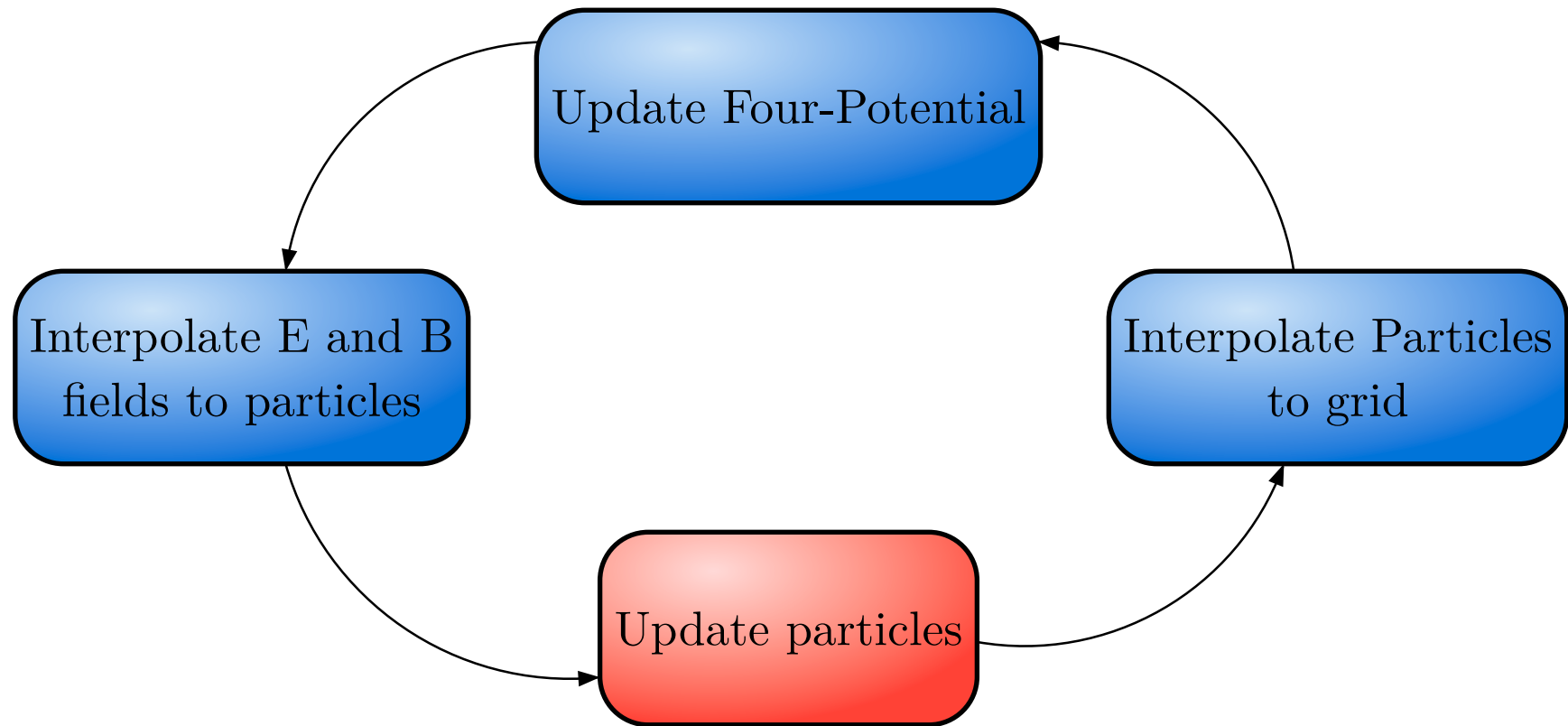
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$$\begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = \begin{bmatrix} \frac{r_x}{\Delta x} - i_{\text{int}} \\ \frac{r_y}{\Delta y} - j_{\text{int}} \\ \frac{r_z}{\Delta z} - k_{\text{int}} \end{bmatrix}$$

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

# The PIC Loop





# Updating the particles

Governing equation:

$$\frac{d\mathbf{p}}{dt} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}$$

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

$$t_1 = \gamma\beta^{n-\frac{1}{2}} + \frac{q\Delta t \mathbf{E}_t^n}{2mc}$$

$$\alpha = \frac{q\Delta t}{2m\sqrt{1 + \|t_1\|^2}}$$

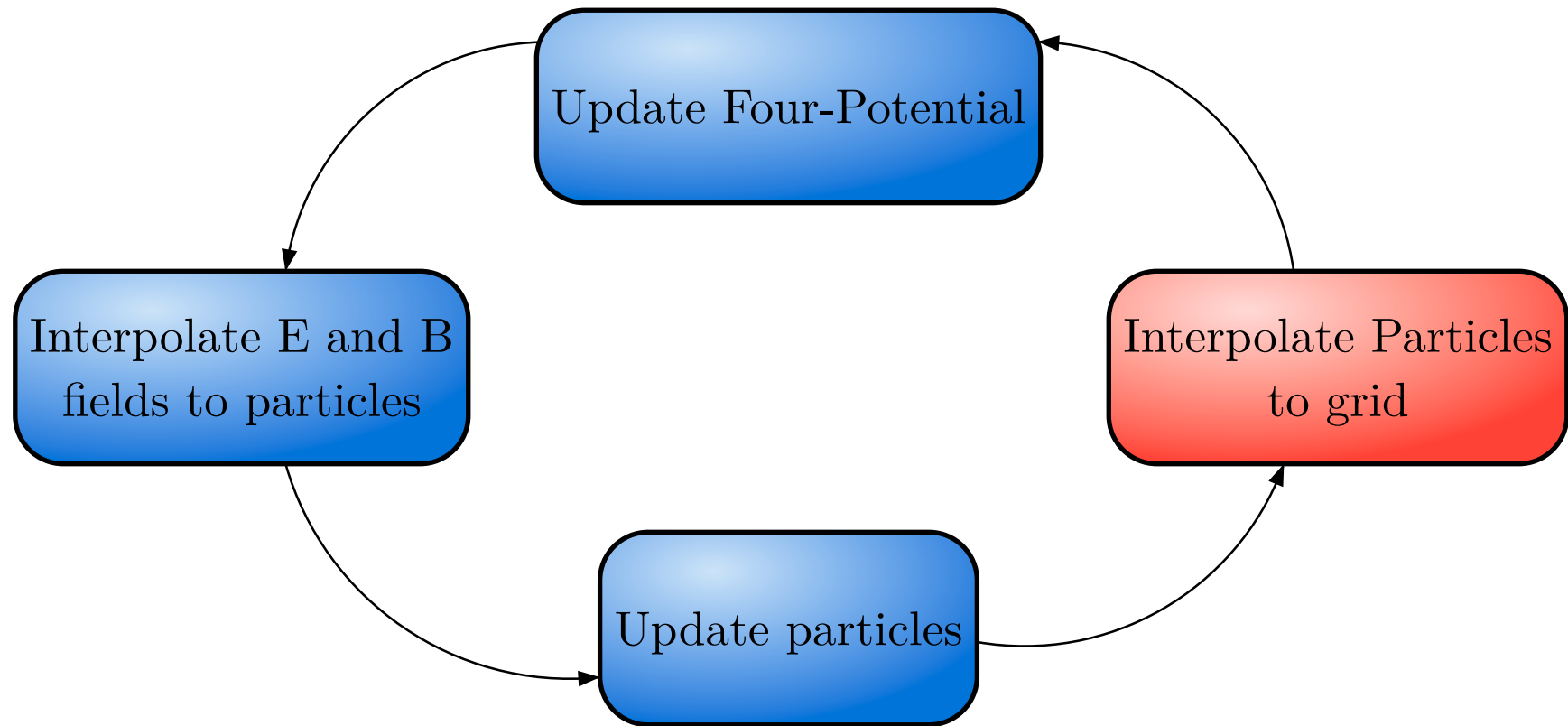
$$t_2 = t_1 + \alpha t_1 \times \mathbf{B}_t^n$$

$$t_3 = t_1 + t_2 \times \frac{2\alpha \mathbf{B}_t^n}{1 + \alpha^2 \|\mathbf{B}_t^n\|^2}$$

$$\gamma\beta^{n+\frac{1}{2}} = t_3 + \frac{q\Delta t \mathbf{E}_t^n}{2mc}$$

$$\mathbf{r}^{n+1} = \mathbf{r}^n + c\Delta t \frac{\gamma\beta^{n+\frac{1}{2}}}{\sqrt{1 + \|\gamma\beta^{n+\frac{1}{2}}\|^2}}$$

# The PIC Loop



# Charge deposition

Recall

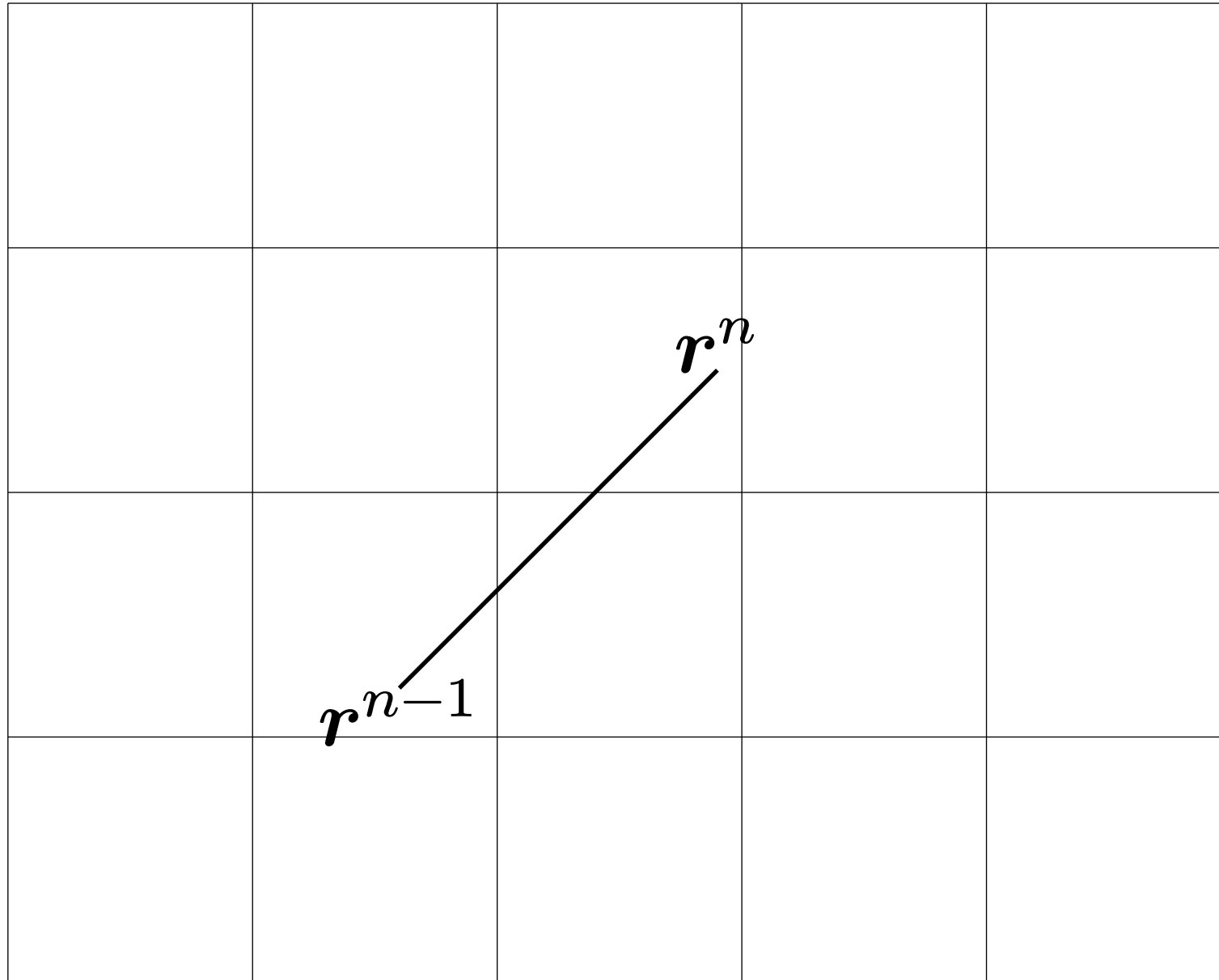
$$\Delta \mathbf{A} = \frac{\partial^2 \mathbf{A}}{\partial t^2} + \mathbf{J}, \mathbf{J} = \begin{bmatrix} \rho \\ J_x \\ J_y \\ J_z \end{bmatrix}$$

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

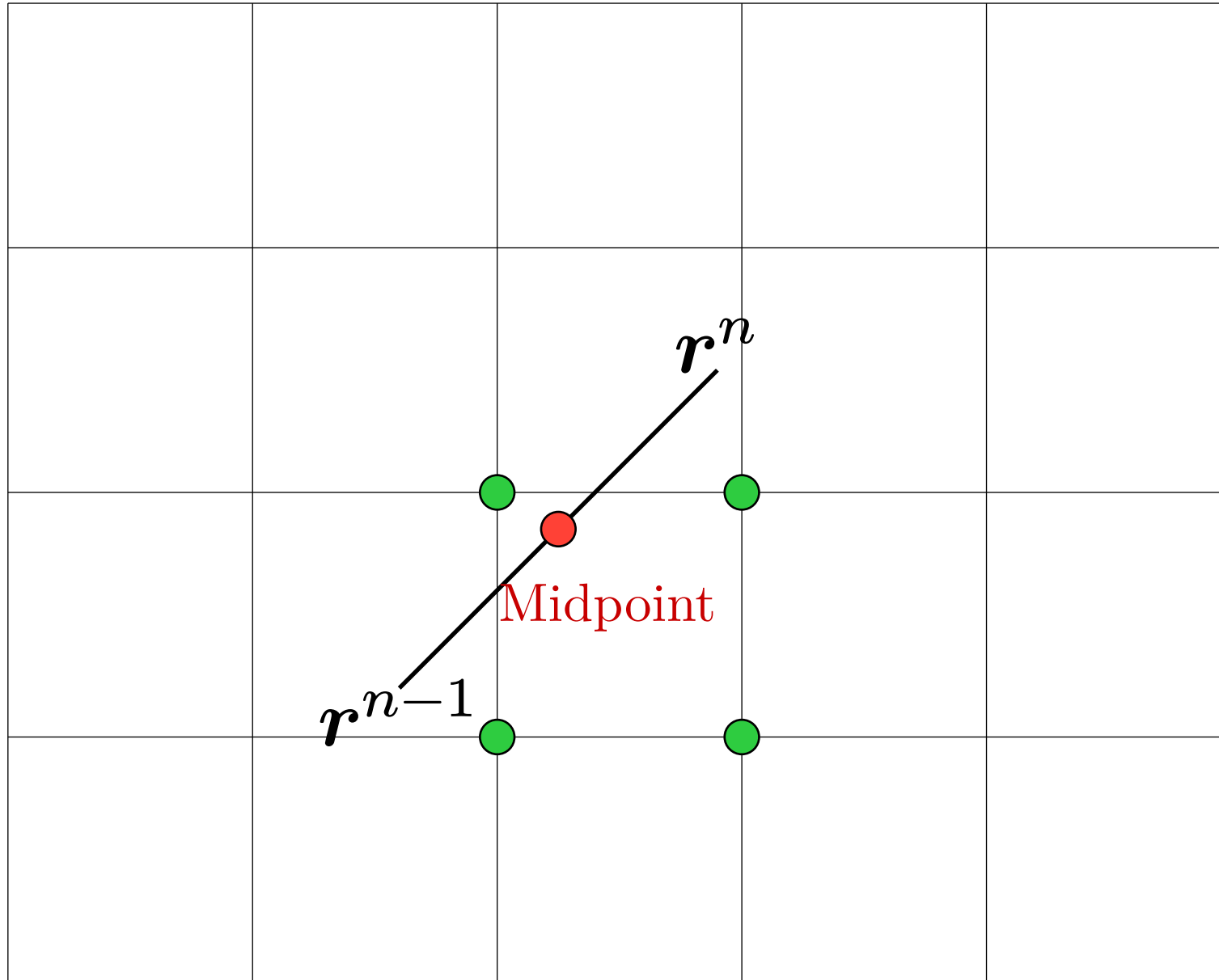
$$\Delta \rho_{i+I, j+J, k+K} = \frac{q}{\Delta x \Delta y \Delta z} \left( \frac{1}{2} + (-1)^I \left| \frac{1}{2} - \frac{\delta x}{\Delta x} \right| \right) \left( \frac{1}{2} + (-1)^J \left| \frac{1}{2} - \frac{\delta y}{\Delta y} \right| \right) \left( \frac{1}{2} + (-1)^K \left| \frac{1}{2} - \frac{\delta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

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

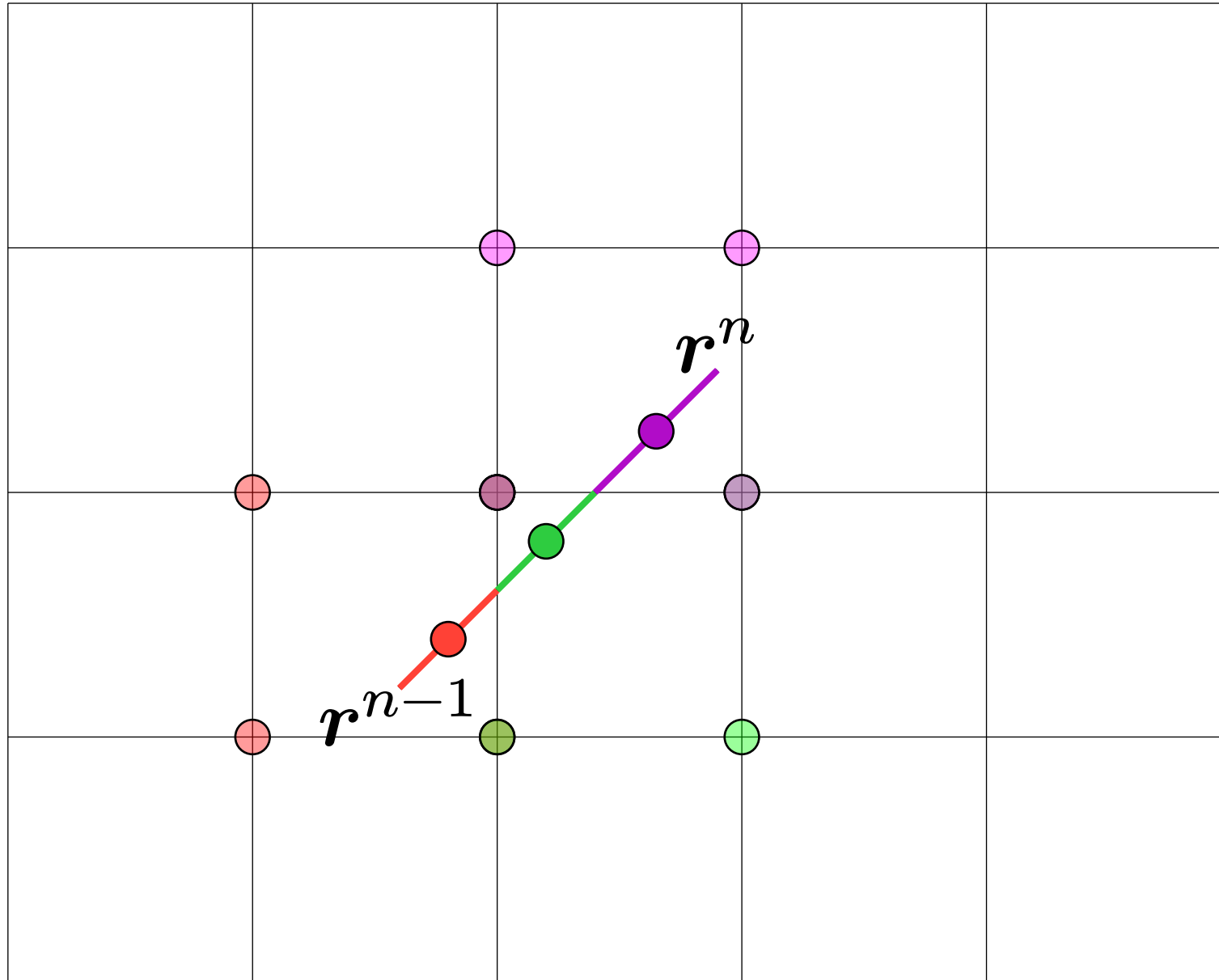
# ZigZag



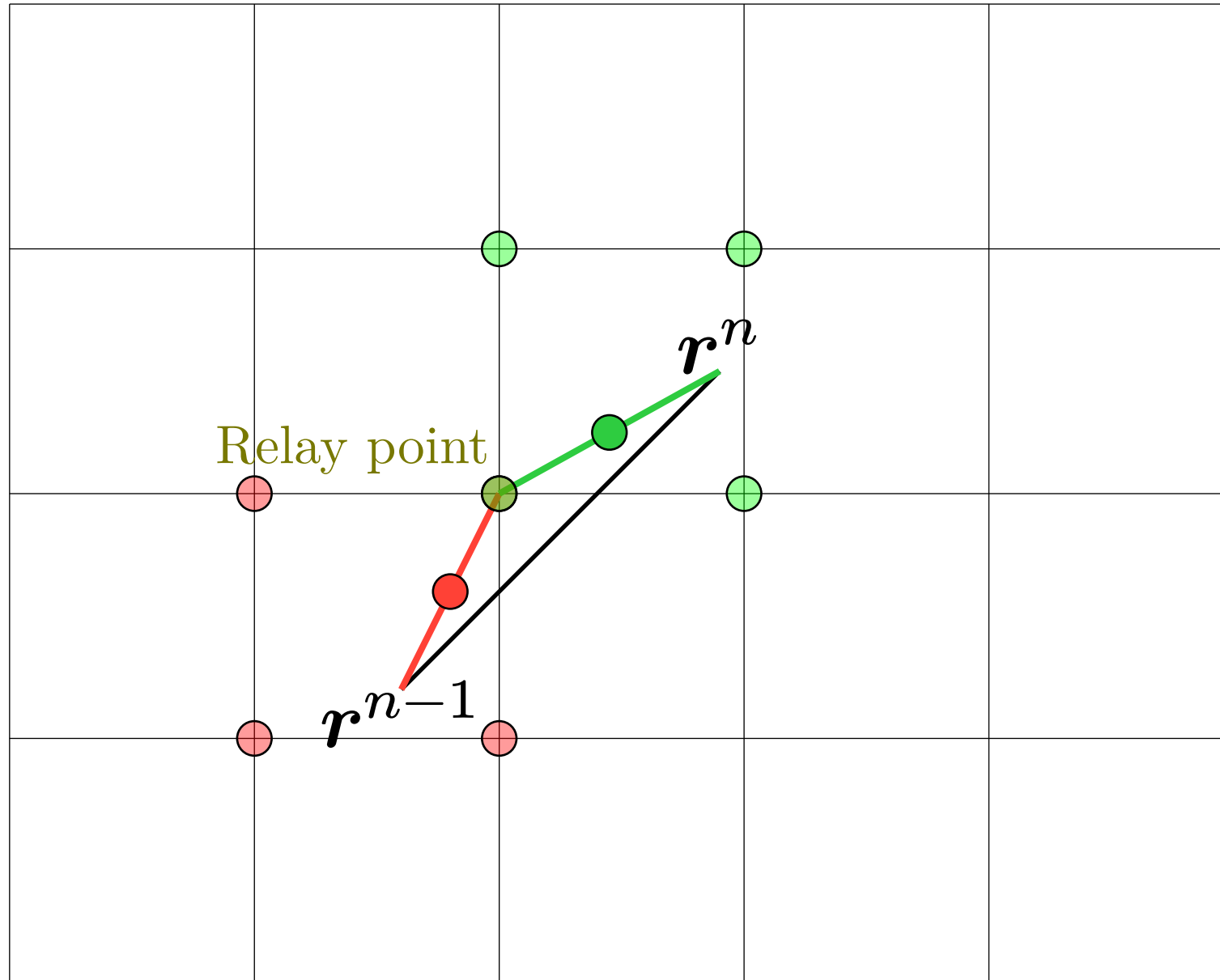
# ZigZag



# ZigZag



# ZigZag





# Current deposition

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

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

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

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

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

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

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

# The Poynting Vector

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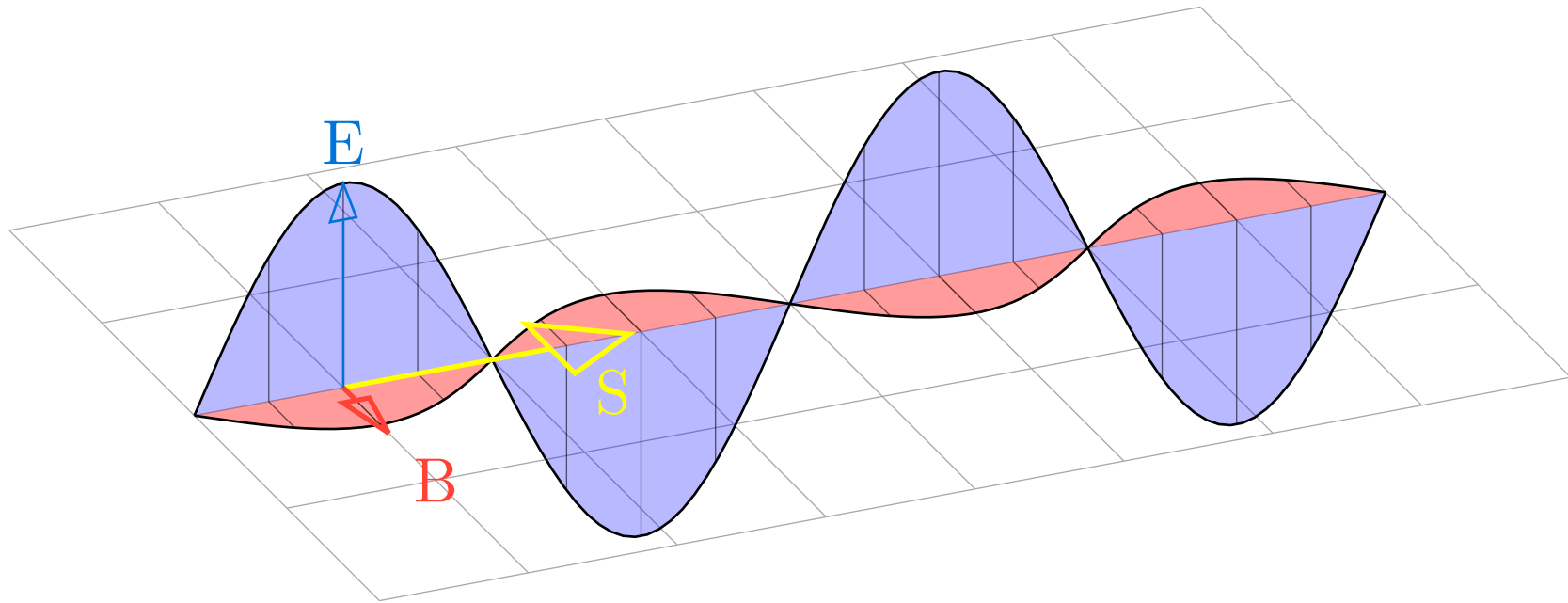
# Definition

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

→ Describes flow of energy

→ Is in unit  $\frac{\text{W}}{\text{m}^2}$

# Plane wave case



# Stationary electron

$$\mathbf{E} = \frac{q\mathbf{r}}{4\pi\epsilon_0 \|\mathbf{r}\|^3}$$

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

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

# Inertially moving electron

Liénard - Wiechert Electric Field:

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0} \left[ \frac{q(\mathbf{n} - \boldsymbol{\beta})}{\gamma^2(1 - \mathbf{n} \cdot \boldsymbol{\beta})^3 |\mathbf{r} - \mathbf{r}_s|^2} + \frac{q\mathbf{n} \times ((\mathbf{n} - \boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}})}{c(1 - \mathbf{n} \cdot \boldsymbol{\beta})^3 |\mathbf{r} - \mathbf{r}_s|} \right]_{t_r}$$

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

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

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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:

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

→ Integrating over a sphere yields

$$\frac{q^2}{6\pi\epsilon_0 c} \gamma^6 (\|\dot{\boldsymbol{\beta}}\|^2 - \|\boldsymbol{\beta} \times \dot{\boldsymbol{\beta}}\|^2)$$

# Accelerated electron

Liénard - Wiechert Electric Field:

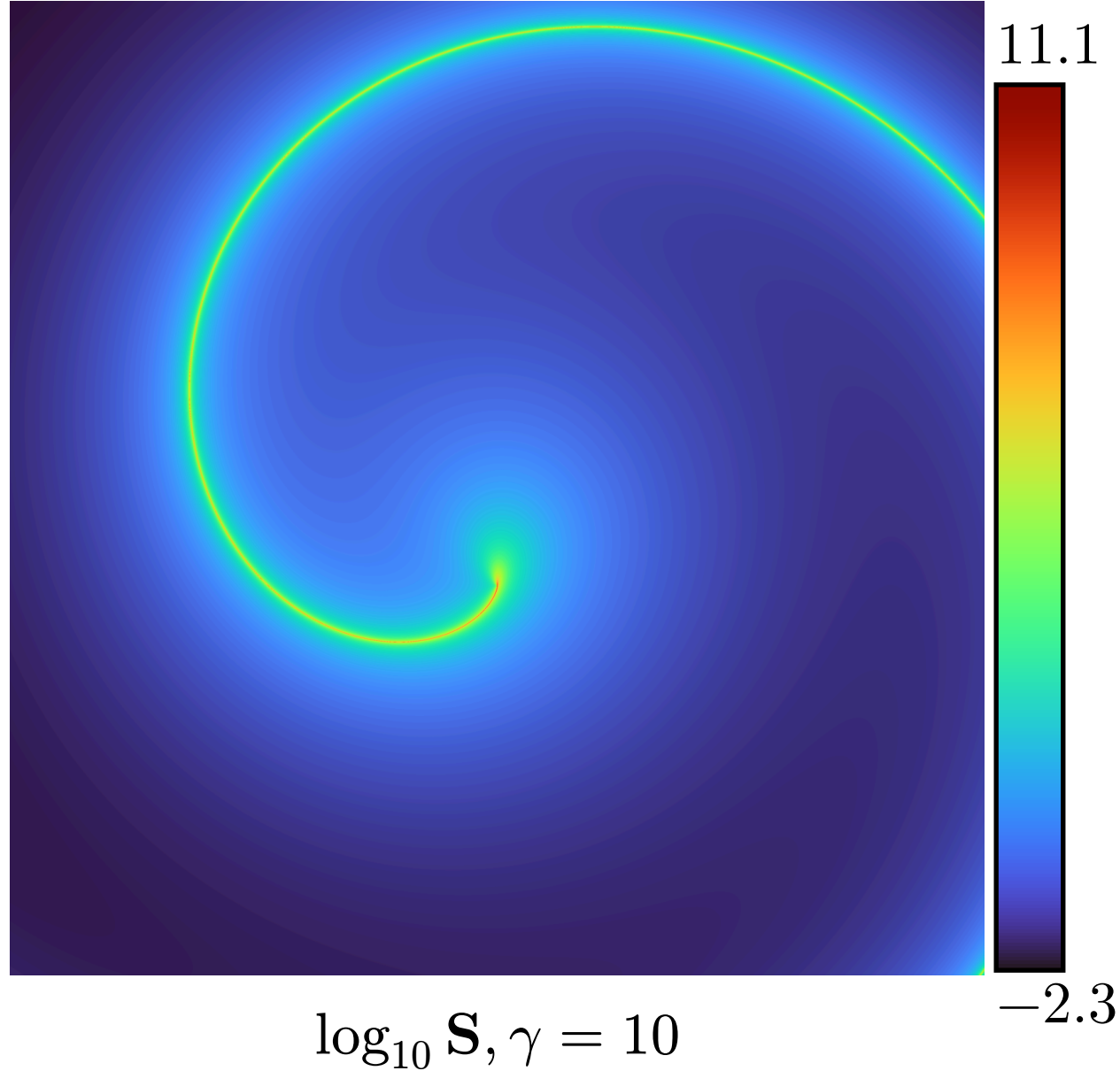
$$\mathbf{E} = \frac{1}{4\pi\epsilon_0} \left[ \frac{q(\mathbf{n} - \boldsymbol{\beta})}{\gamma^2(1 - \mathbf{n} \cdot \boldsymbol{\beta})^3 |\mathbf{r} - \mathbf{r}_s|^2} + \frac{q\mathbf{n} \times ((\mathbf{n} - \boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}})}{c(1 - \mathbf{n} \cdot \boldsymbol{\beta})^3 |\mathbf{r} - \mathbf{r}_s|} \right]_{t_r}$$

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

→ Integrating over a sphere yields

$$\frac{q^2}{6\pi\epsilon_0 c} \gamma^6 (\|\dot{\boldsymbol{\beta}}\|^2 - \|\boldsymbol{\beta} \times \dot{\boldsymbol{\beta}}\|^2)$$

# Accelerated electron



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

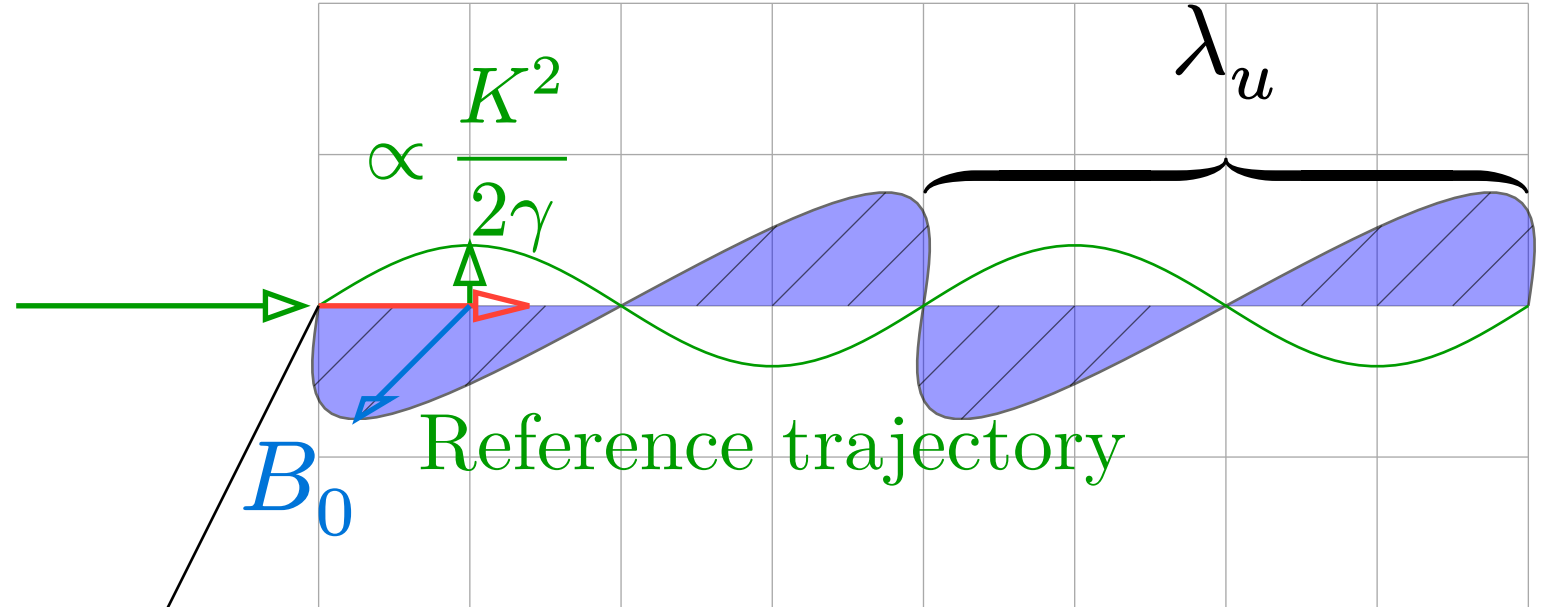
-2.3

11.1

# Free Electron Laser

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

# Undulator



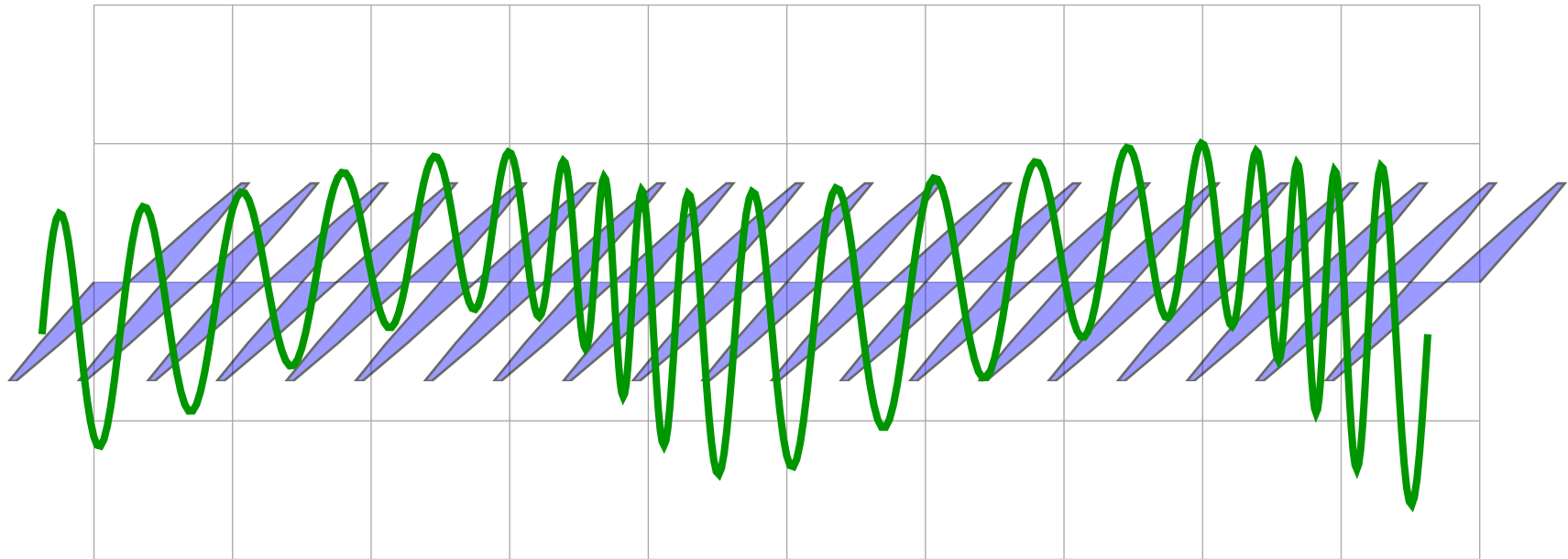
Bunch enters with  $\gamma$ ,

slowed down to  $\gamma_0 = \frac{\gamma}{\sqrt{1 + \frac{K^2}{2}}}$

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



# Ponderomotive Forces



# Moving frame

Entire simulation takes place in boosted frame:

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

# Lorentz Transforms

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

# Lorentz Transform

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

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

# Lorentz Transform

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

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

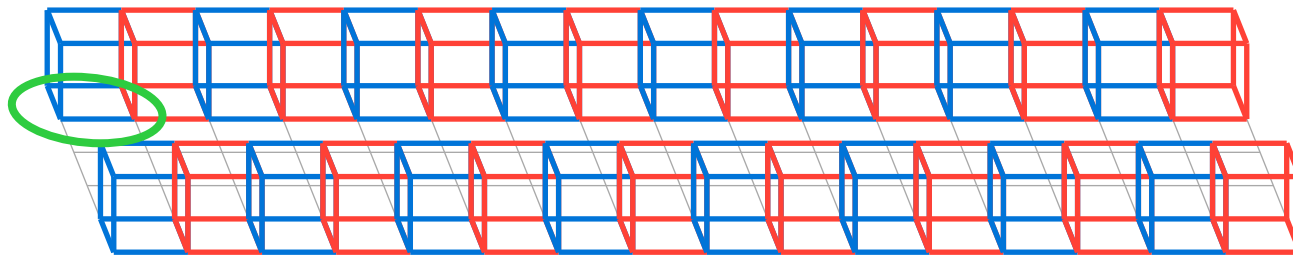
Particles end up with nonzero time  $\mathbf{r}^0$

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

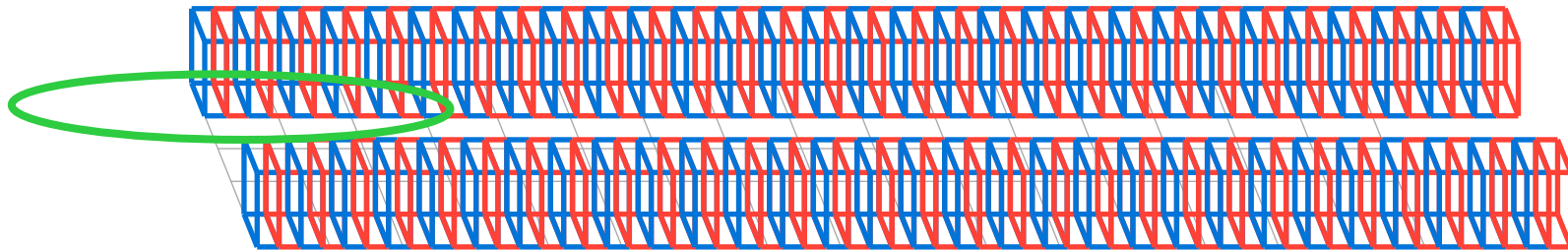
# Setup

1. Initialize particles  $\sim$  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



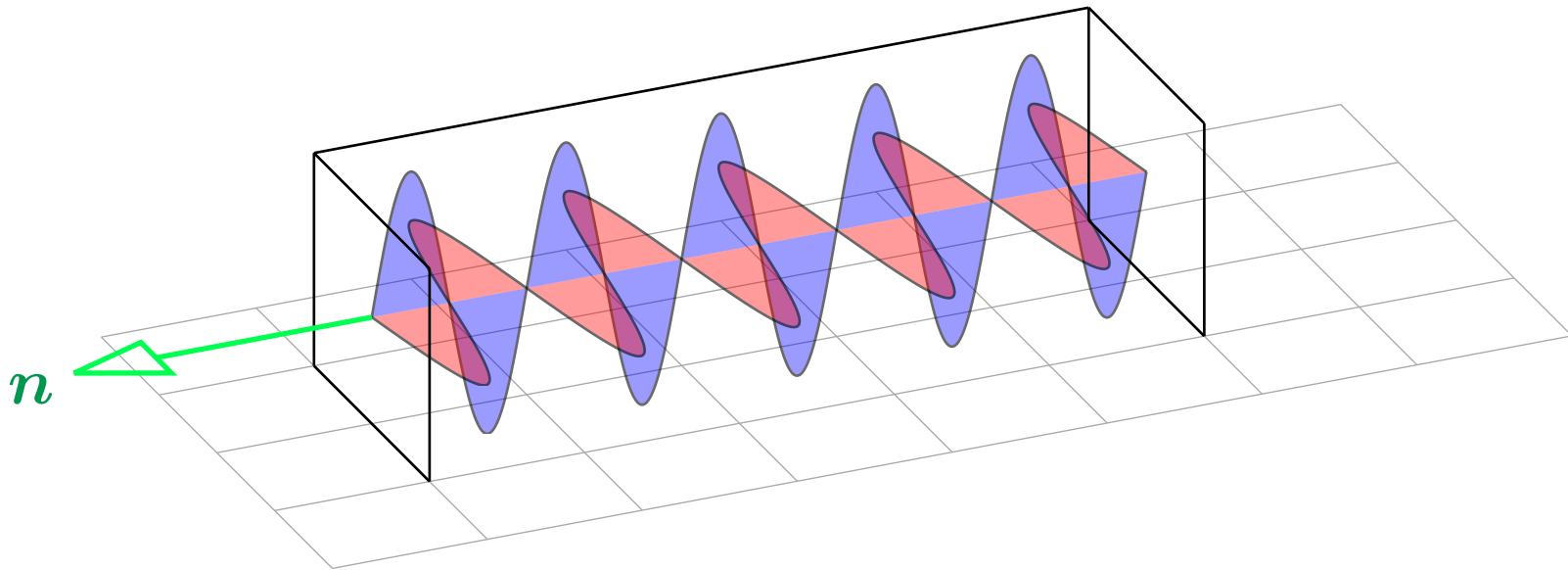
becomes



# Forward Radiation

Evaluate

$$\oint_{z^+ \text{ plane}} \mathbf{S}_{\text{lab}} d\mathbf{n}$$



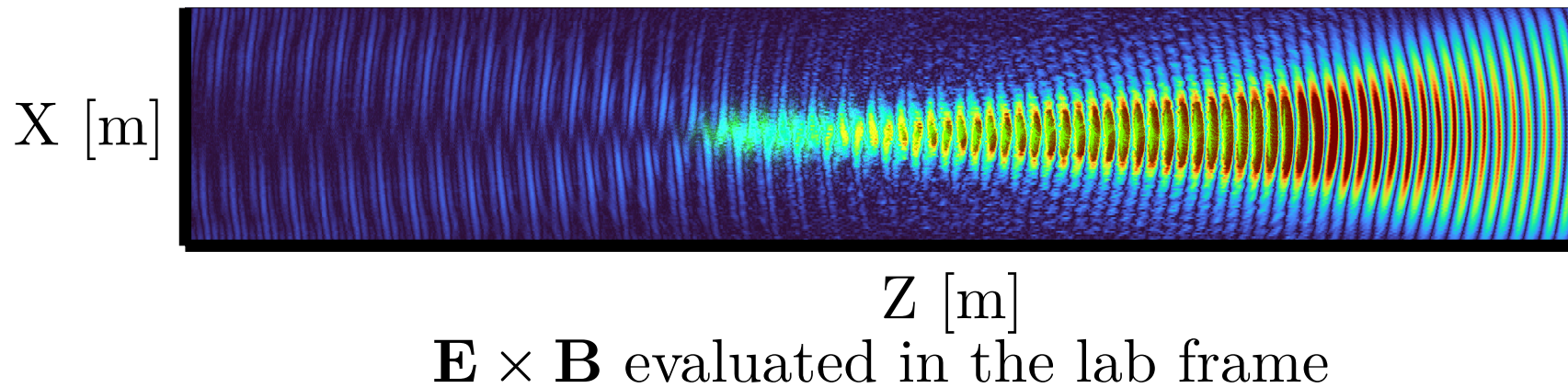
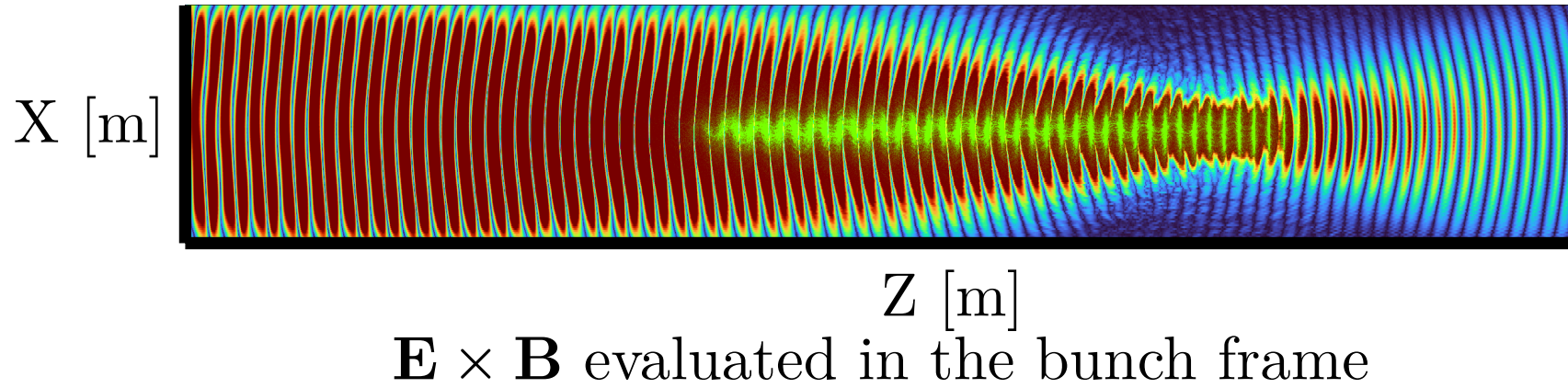


# Electromagnetic Transform

$$\mathbf{E}_{\text{lab}} = \gamma(\mathbf{E} - \mathbf{v} \times \mathbf{B}) - (\gamma - 1)(\mathbf{E} \cdot \hat{\mathbf{v}})\hat{\mathbf{v}}$$

$$\mathbf{B}_{\text{lab}} = \gamma\left(\mathbf{B} + \frac{\mathbf{v} \times \mathbf{E}}{c^2}\right) - (\gamma - 1)(\mathbf{B} \cdot \hat{\mathbf{v}})\hat{\mathbf{v}}$$

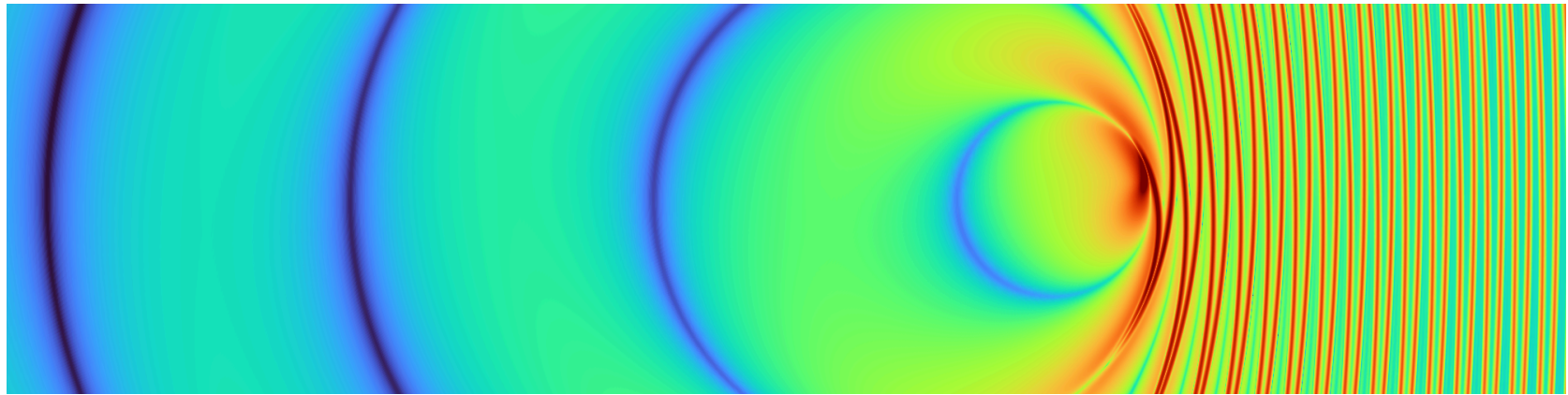
# Boost correction



# Laboratory frame

Observed wavelength:

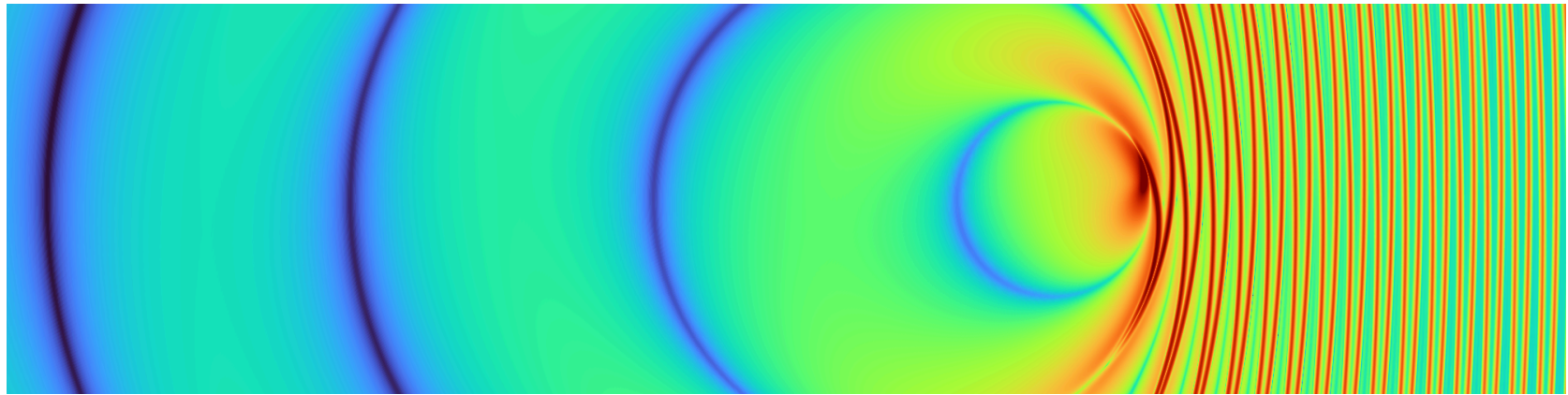
$$\lambda_u(1 - \beta_0)$$



# Laboratory frame

Observed wavelength:

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

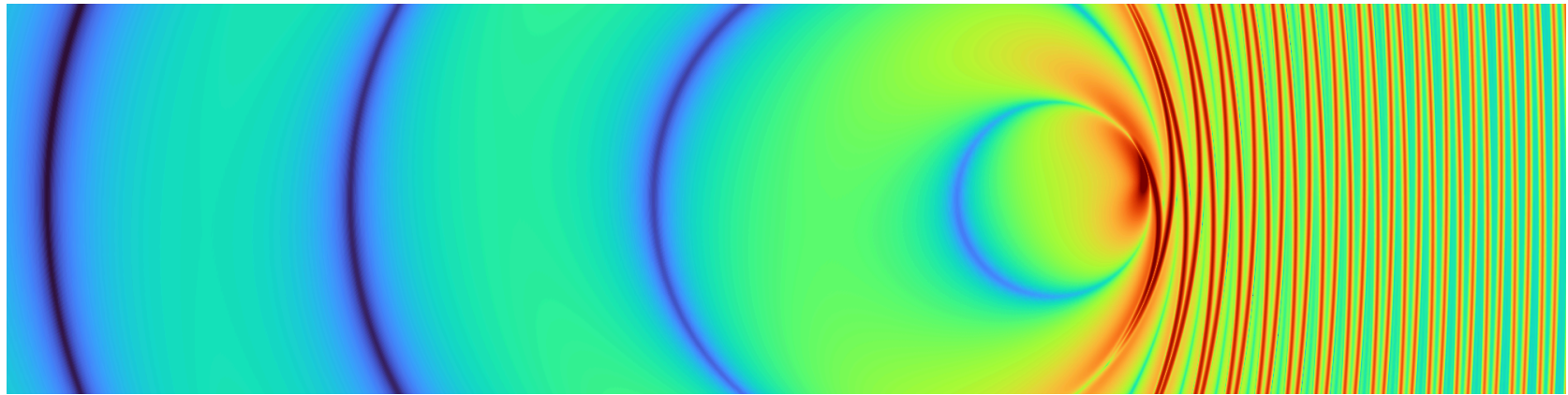


$$1 - \beta_0 = 1 - \sqrt{1 - \frac{1}{\gamma_0^2}} = \frac{1}{2\gamma_0^2} + \frac{1}{8\gamma_0^4} + \dots$$

# Laboratory frame

Observed wavelength:

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



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

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

# Implementation and Results

1. Methodology
2. The Poynting Vector
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4. **Implementation and Results**

# Memory Savings

- $\text{anmlview} = \mathbf{A}^{n-1}$
- $\text{aview} = \mathbf{A}^n$

```
1 Kokkos::parallel_for(  
    "Four potential update",  
2 ippl::getRangePolicy(aview,nghost),  
3 KOKKOS_LAMBDA(unsigned i, unsigned j, unsigned k) {  
4     FourVector_t interior =  
5     -anmlview(i, j, k) + a1 * aview(i, j, k)  
6     + a2 * (aview(i + 1, j, k) + aview(i - 1, j, k))  
7     + a4 * (aview(i, j + 1, k) + aview(i, j - 1, k))  
8     + a6 * (aview(i, j, k + 1) + aview(i, j, k - 1))  
9     + a8 * (-source_view(i, j, k));  
10    anmlview(i, j, k) = interior;  
11    }  
12 });  
13 swap(aview, anmlview);
```

# Memory Savings

- $\text{anmlview} = \mathbf{A}^{n-1}$
- $\text{aview} = \mathbf{A}^n$

```
1 Kokkos::parallel_for(  
    "Four potential update",  
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6     + a2 * (aview(i + 1, j, k) + aview(i - 1, j, k))  
7     + a4 * (aview(i, j + 1, k) + aview(i, j - 1, k))  
8     + a6 * (aview(i, j, k + 1) + aview(i, j, k - 1))  
9     + a8 * (-source_view(i, j, k));  
10    anmlview(i, j, k) = interior;  
11    }  
12 });  
13 swap(aview, anmlview);
```

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



# Memory Locality

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

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

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

# Memory Locality

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

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

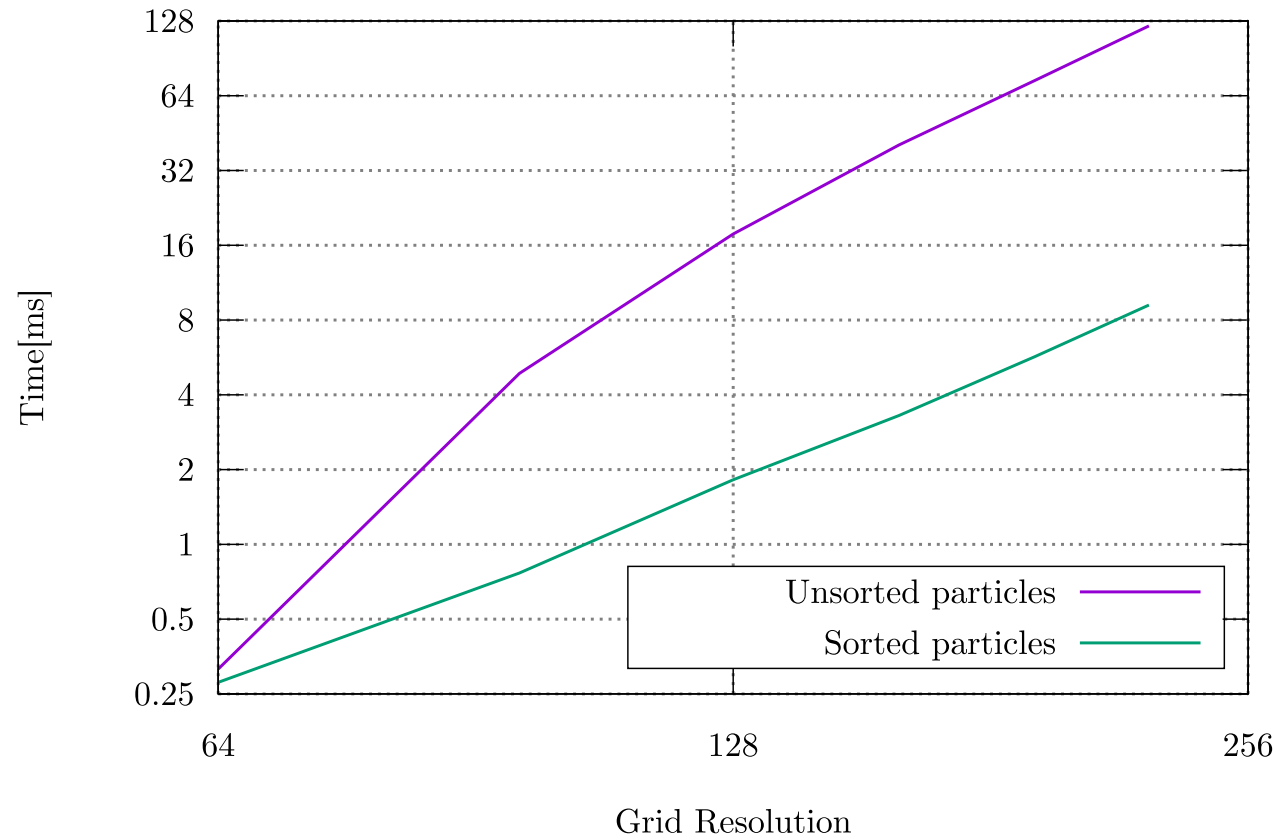
```
1 atomicAdd(&rhoview(ipos[0], ipos[1], ipos[2]), ...)  
2 //Is equivalent to  
3 atomicAdd(&rhoview[ipos[0] + ipos[1] * m + ipos[2] * m * n], ...)
```

→ Sort particles by memory index

$$i_{\text{int}} + mj_{\text{int}} + mnk_{\text{int}}$$

# Memory Locality

This yields a massive speedup

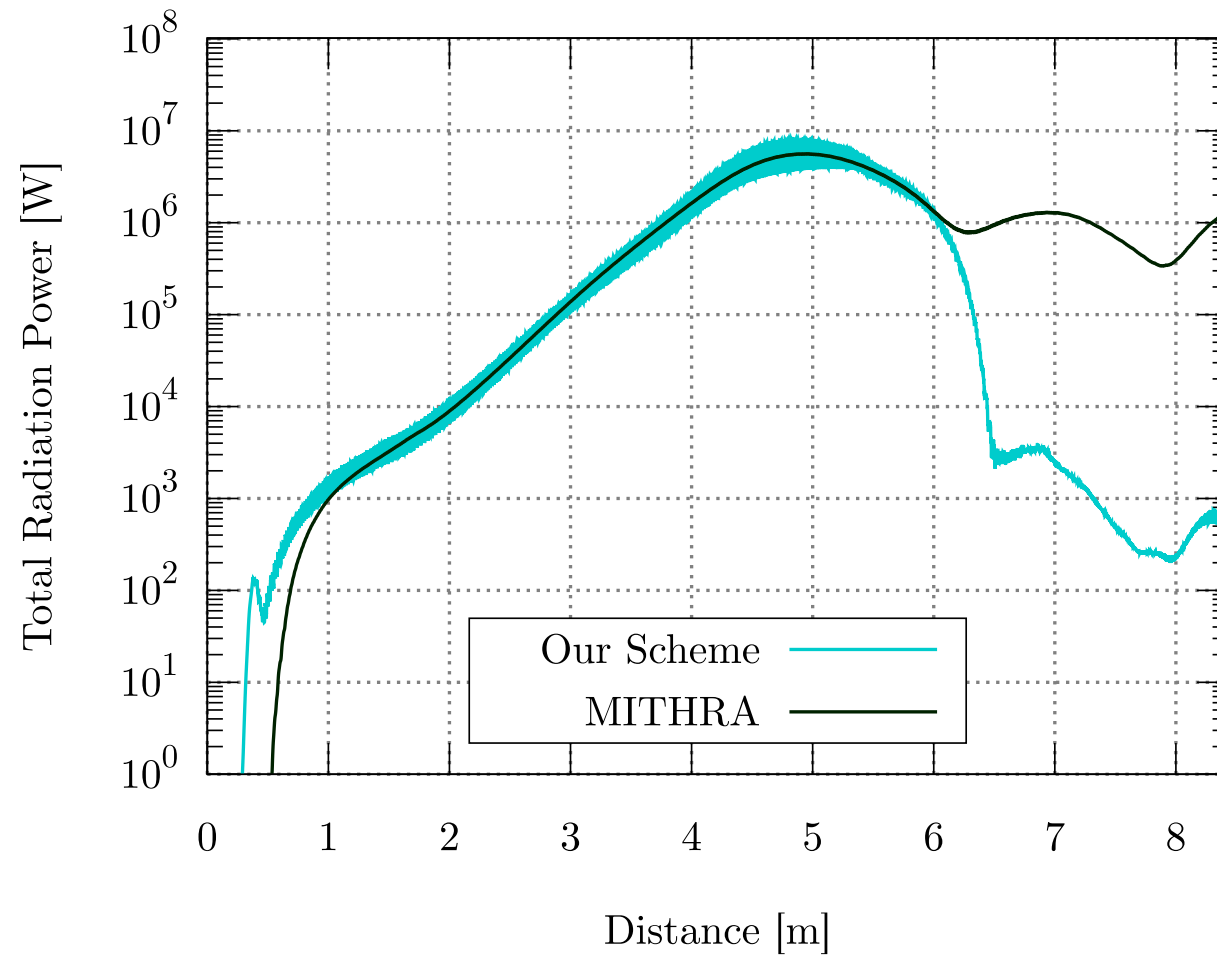


Correlated particle motion

→ sort only every 100th timestep.

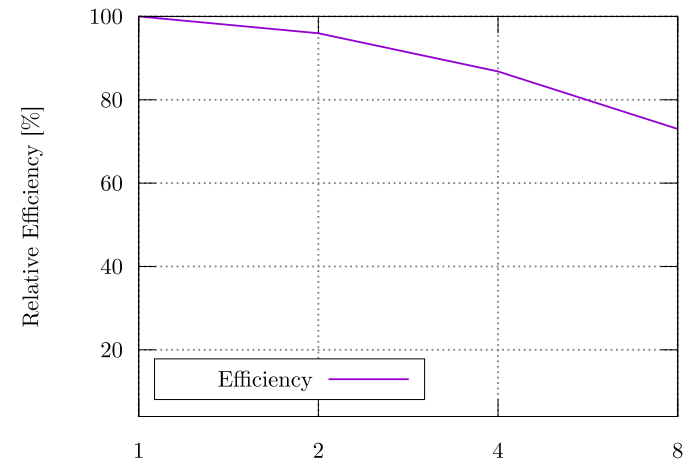
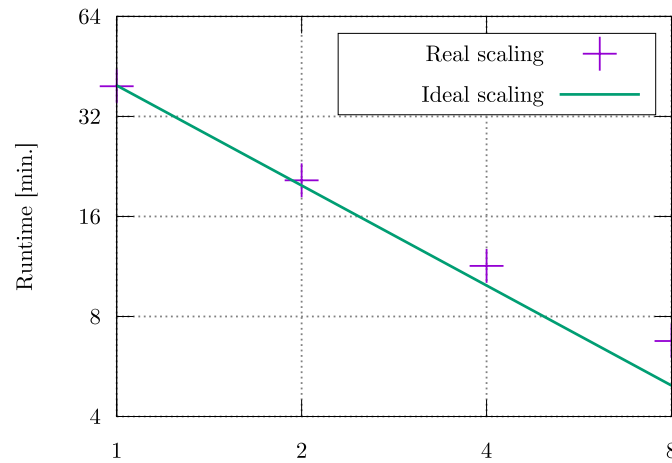
# Final result

More noise since MITHRA filters frequencies.

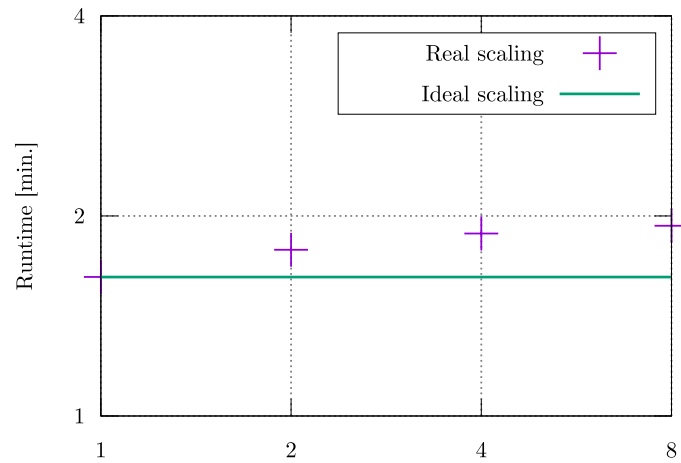


# Scaling

## Strong Scaling



## Weak Scaling



Number of GPU Ranks

## Bibliography

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- [6] T. Umeda, Y. Omura, T. Tominaga, and H. Matsumoto, “A new charge conservation method in electromagnetic particle-in-cell simulations,” *Computer Physics Communications*, vol. 156, no. 1, pp. 73–85, 2003, doi: [https://doi.org/10.1016/S0010-4655\(03\)00437-5](https://doi.org/10.1016/S0010-4655(03)00437-5).