

# Electromagnetic wave propagation in Particle-In-Cell codes

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*Self-Consistent Simulations of Beam and Plasma Systems*

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- 1 Numerical dispersion and Courant limit
  - Dispersion and Courant limit in 1D
  - Dispersion and Courant limit in 3D
  - Spectral solvers and numerical dispersion
  
- 2 Open boundaries conditions
  - Silver-Müller boundary conditions
  - Perfectly Matched Layers

# 1D discrete propagation equation in vacuum

Reminder: 1D discrete Maxwell equations in vacuum

$$\frac{B_{y\ell+1/2}^{n+1/2} - B_{y\ell+1/2}^{n-1/2}}{\Delta t} = - \left( \frac{E_{x\ell+1}^n - E_{x\ell}^n}{\Delta z} \right)$$

$$\frac{E_{x\ell}^{n+1} - E_{x\ell}^n}{\Delta t} = -c^2 \left( \frac{B_{y\ell+1/2}^{n+1/2} - B_{y\ell-1/2}^{n+1/2}}{\Delta z} \right)$$

These equations can be combined (derivation on white board) into:

1D discrete propagation equation in vacuum

$$\frac{1}{c^2} \frac{E_{x\ell}^{n+1} - 2E_{x\ell}^n + E_{x\ell}^{n-1}}{\Delta t^2} = \frac{E_{x\ell+1}^n - 2E_{x\ell}^n + E_{x\ell-1}^n}{\Delta z^2}$$

(i.e.  $\frac{1}{c^2} \partial_t^2 E_x|_\ell^n = \partial_z^2 E_x|_\ell^n$ )

# 1D dispersion relation

## 1D discrete propagation equation in vacuum

$$\frac{1}{c^2} \frac{E_{x\ell}^{n+1} - 2E_{x\ell}^n + E_{x\ell}^{n-1}}{\Delta t^2} = \frac{E_{x\ell+1}^n - 2E_{x\ell}^n + E_{x\ell-1}^n}{\Delta z^2}$$

→ **Von Neumann analysis:** assume the solutions of this equation are of the form  $E_0 e^{ikz - i\omega t}$  (propagating wave), i.e.

$$E_{x\ell'}^n = E_0 e^{ik \ell' \Delta z - i\omega n \Delta t}$$

Replacing this ansatz into the discrete propagation equation yields (demonstration on white board):

## 1D dispersion relation

$$\frac{1}{c^2 \Delta t^2} \sin^2 \left( \frac{\omega \Delta t}{2} \right) = \frac{1}{\Delta z^2} \sin^2 \left( \frac{k \Delta z}{2} \right)$$

NB: When  $\Delta t \rightarrow 0$  and  $\Delta z \rightarrow 0$ , this becomes  $\omega^2 = c^2 k^2$ .

## $c\Delta t \leq \Delta z \rightarrow$ Numerical dispersion

For  $c\Delta t \leq \Delta z$ , the discrete dispersion relation

$$\frac{1}{c^2\Delta t^2} \sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z^2} \sin^2\left(\frac{k\Delta z}{2}\right)$$

has real solutions  $\omega$ , for any  $k$ :

$$\omega = \pm \frac{2}{\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)\right)$$

Thus, the phase velocity  $v_\phi = \omega/k$  is:

$$v_\phi = \pm \frac{2}{k\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)\right)$$

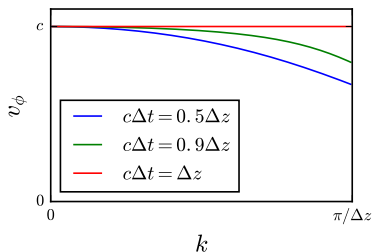
### Numerical dispersion

In a PIC code, the **electromagnetic waves** propagate (in vacuum) at a **velocity which depends on  $k$**  (and on  $\Delta t$ ,  $\Delta z$ ),

instead of propagating at the speed of light:  $v_\phi = \pm c$

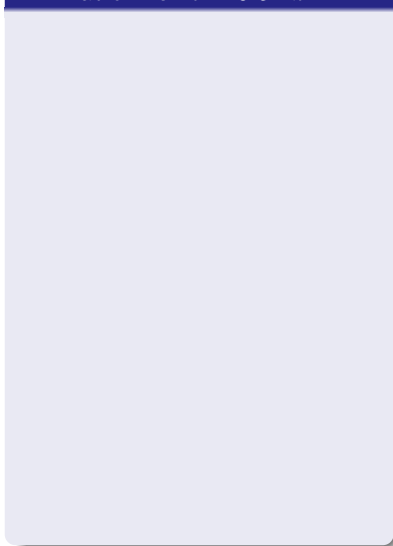
# $c\Delta t \leq \Delta z \rightarrow$ Numerical dispersion

$$v_\phi = \frac{2}{k\Delta t} \arcsin \left( \frac{c\Delta t}{\Delta z} \sin \left( \frac{k\Delta z}{2} \right) \right)$$



NB:  $k = \pi/\Delta z$ ,  $\lambda = 2\Delta z$ : shortest wavelength supported by the grid.

Animation:  $c\Delta t = 0.5\Delta z$



**The shorter the wavelength,  
the slower the propagation.**

## $c\Delta t > \Delta z \rightarrow$ Courant limit

For  $c\Delta t > \Delta z$ , the discrete dispersion relation

$$\frac{1}{c^2\Delta t^2} \sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z^2} \sin^2\left(\frac{k\Delta z}{2}\right)$$

has **no real solutions**  $\omega$ , for  $k$  close to  $\pi/\Delta z$ . The solution  $\omega$  is **imaginary** and the corresponding mode is **unstable**.

### Courant limit (a.k.a. CFL limit)

Standard EM-PIC codes are **unstable** for  $c\Delta t > \Delta z$  (in 1D).

- Thus, practical use of **electromagnetic PIC** codes is restricted to  $\Delta t \leq \Delta z/c$ .
- For a given spatial resolution  $\Delta z$ , this limits **how fast** a simulation can advance in time.
- **Electrostatic PIC codes** do not have this limitation  
→ Can be much faster than EM-PIC codes to simulate a system over a given period of time, by taking **large timesteps**  $\Delta t$ .

# Electromagnetic Waves: Outline

- 1 Numerical dispersion and Courant limit
  - Dispersion and Courant limit in 1D
  - Dispersion and Courant limit in 3D
  - Spectral solvers and numerical dispersion
  
- 2 Open boundaries conditions
  - Silver-Müller boundary conditions
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# Dispersion and Courant limit in 3D

## Derivation of dispersion relation

Combine discrete Maxwell equation  $\rightarrow$  Discrete propagation equation  
 $\rightarrow$  Von Neumann analysis  $\rightarrow$  Discrete dispersion relation

Same process in 3D. The Von Neumann analysis assumes:

$$E = E_0 e^{ik_x x + ik_y y + ik_z z - i\omega t}$$

## 3D Discrete dispersion relation

$$\frac{\sin^2\left(\frac{\omega\Delta t}{2}\right)}{c^2\Delta t^2} = \frac{\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} + \frac{\sin^2\left(\frac{k_y\Delta y}{2}\right)}{\Delta y^2} + \frac{\sin^2\left(\frac{k_z\Delta z}{2}\right)}{\Delta z^2}$$

For  $\Delta t, \Delta x, \Delta y, \Delta z \rightarrow 0$ : this becomes  $\omega^2 = c^2(k_x^2 + k_y^2 + k_z^2)$

## Courant limit (a.k.a CFL limit) in 3D

$$c\Delta t \leq \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

# Numerical dispersion in 3D

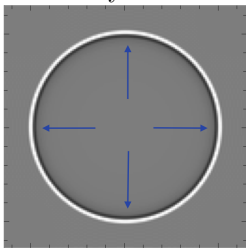
## 3D Discrete dispersion relation

$$\frac{\sin^2\left(\frac{\omega\Delta t}{2}\right)}{c^2\Delta t^2} = \frac{\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} + \frac{\sin^2\left(\frac{k_y\Delta y}{2}\right)}{\Delta y^2} + \frac{\sin^2\left(\frac{k_z\Delta z}{2}\right)}{\Delta z^2}$$

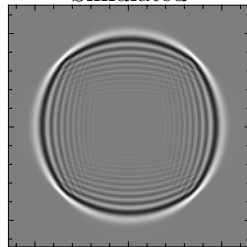
Velocity depends on the **wavelength and propagation direction**.

Example: expanding electromagnetic wave

Physical



Simulated



Even for  $\Delta t = \Delta t_{CFL}$ : waves are **slower than  $c$**  along the main axes.

# Impact of numerical dispersion

## Animation: laser-wakefield acceleration

- A short and intense **laser pulse**, followed by a relativistic **electron bunch**, enters a **plasma** (generated from a gas jet).
- The laser pulse generates a **wake** in the plasma, with **electric fields** that can **accelerate** the electron bunch.
- Simulation with the Yee scheme (and low resolution):
  - The laser is **artificially slow** (numerical dispersion)
  - Thus the electron bunch **catches up** with the laser very soon!

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# Yee scheme

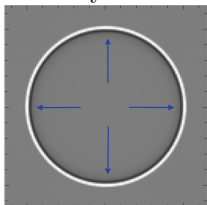
## Finite-difference in space and time

e.g. continuous equation : 
$$\frac{\partial B_z}{\partial t} = - \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right)$$

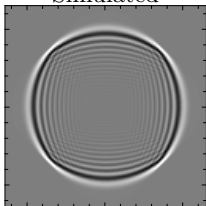
→ discrete equation : 
$$B_z^{n+1/2} = B_z^{n-1/2} - \Delta t (\hat{\partial}_x E_y|^n - \hat{\partial}_y E_x|^n)$$

with 
$$\hat{\partial}_x F|_{i,j,\ell}^n = \frac{F_{i+\frac{1}{2},j,\ell}^n - F_{i-\frac{1}{2},j,\ell}^n}{\Delta x}$$

Physical



Simulated



- Anisotropic
- Waves propagate **slower** than  $c$ .

# Pseudo-spectral solver

Fourier transform in space, finite-difference in time

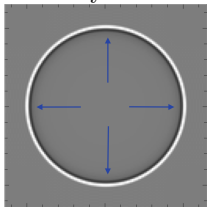
e.g. continuous equation : 
$$\frac{\partial B_z}{\partial t} = - \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right)$$

→ Fourier space : 
$$\frac{\partial \hat{B}_z}{\partial t} = - \left( k_x \hat{\mathcal{E}}_y - k_y \hat{\mathcal{E}}_x \right)$$

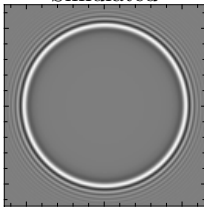
→ Finite difference in time : 
$$\hat{B}_z^{n+1/2} = \hat{B}_z^{n-1/2} - \Delta t \left( k_x \hat{\mathcal{E}}_y^n - k_y \hat{\mathcal{E}}_x^n \right)$$

→ Use backwards FFT to obtain  $B_z^{n+1/2}$  from  $\hat{B}_z^{n+1/2}$

Physical



Simulated



- Isotropic
- Waves propagate **faster** than  $c$ .

## Analytical pseudo-spectral solver (Haber et al., 1973)

Fourier transform in space, finite-difference in time

e.g. continuous equation : 
$$\frac{\partial B_z}{\partial t} = - \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right)$$

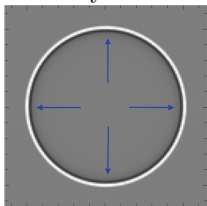
→ Fourier space : 
$$\frac{\partial \hat{B}_z}{\partial t} = - \left( k_x \hat{E}_y - k_y \hat{E}_x \right)$$

→ Analytical integration of the coupled Maxwell equations in time:

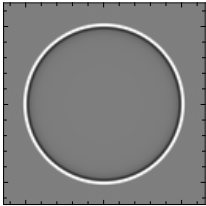
$$\hat{B}_z^{n+1} = \cos(kc\Delta t) \hat{B}_z^n - \frac{\sin(kc\Delta t)}{kc} \left( k_x \hat{E}_y^n - k_y \hat{E}_x^n \right) \quad k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

→ Use backwards FFT to obtain  $B_z^{n+1}$  from  $\hat{B}_z^{n+1}$

Physical



Simulated



- Isotropic
- Waves propagate **exactly** at  $c$ .

# Dispersion and Courant limit: conclusions

- Electromagnetic solvers have a **maximum value** for the timestep  $\Delta t$  (Courant limit), which depends on the dimension (and the method of discretization)
- Below the Courant limit, waves may propagate at speeds that **artificially differ** from  $c$  (numerical dispersion). This can have a strong impact in some physical situations.
- Spectral solvers can mitigate (or even eliminate) numerical dispersion.



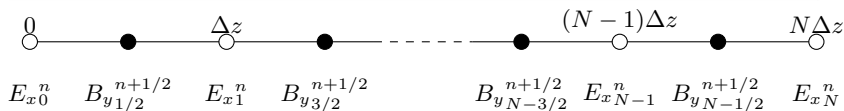
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## Boundary conditions and EM-PIC

Reminder: 1D discrete Maxwell equations in vacuum

$$\frac{B_{y_{\ell+1/2}}^{n+1/2} - B_{y_{\ell+1/2}}^{n-1/2}}{\Delta t} = -\frac{E_{x_{\ell+1}}^n - E_{x_{\ell}}^n}{\Delta z}$$

$$\frac{E_{x_{\ell}}^{n+1} - E_{x_{\ell}}^n}{\Delta t} = -c^2 \frac{B_{y_{\ell+1/2}}^{n+1/2} - B_{y_{\ell-1/2}}^{n+1/2}}{\Delta z}$$

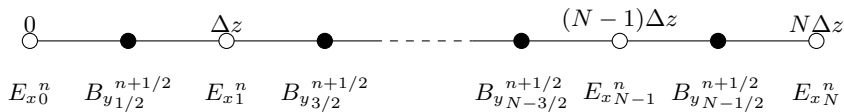


The grid is finite:

- For  $\ell = 0$ :  $B_{y_{\ell-1/2}}^{n+1/2}$  is undefined.
- For  $\ell = N$ :  $B_{y_{\ell+1/2}}^{n+1/2}$  is undefined.

→ **Assumptions** are needed, for the value of  $B_{y_{-1/2}}^{n+1/2}$  and  $B_{y_{N+1/2}}^{n+1/2}$ .

# Boundary conditions and EM-PIC



## Typical assumptions

- Periodic:  $B_{y-1/2}^{n+1/2} = B_{yN-1/2}^{n+1/2}$  and  $B_{yN+1/2}^{n+1/2} = B_{y1/2}^{n+1/2}$
- Dirichlet:  $B_{y-1/2}^{n+1/2} = 0$  and  $B_{yN+1/2}^{n+1/2} = 0$
- Neumann:  $B_{y-1/2}^{n+1/2} = B_{y1/2}^{n+1/2}$  and  $B_{yN+1/2}^{n+1/2} = B_{yN-1/2}^{n+1/2}$   
(i.e.  $\partial_z B_y|_0^{n+1/2} = 0$  and  $\partial_z B_y|_N^{n+1/2} = 0$ )

# Boundary conditions and EM-PIC

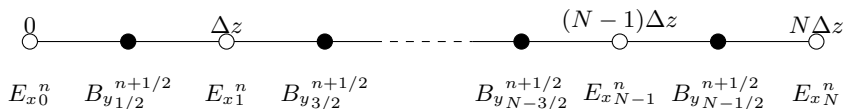
## Problem:

Dirichlet and Neumann boundary conditions **reflect** the EM waves.  
For many physical problems, we need the boundaries to **absorb** the waves.

## Animation: Neumann boundary conditions

This is because, physically, an **outgoing wave** does not satisfy  $B_y(n\Delta z) = 0$  (Dirichlet) or  $\partial_z B_y(n\Delta z) = 0$  (Neumann)

# Silver-Müller absorbing boundary (right-hand side)



The value of  $B_{yN+1/2}^{n+1/2}$  should be chosen so as to be **consistent with an outgoing wave.**

**Physically**, for an outgoing wave propagating to the right (from Maxwell's equation):

$$B_y(z, t) = \frac{1}{c} E_x(z, t)$$

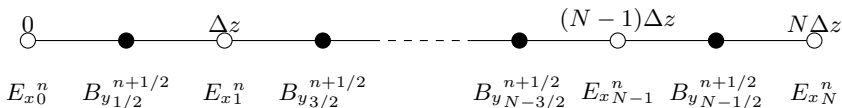
**Numerically**, we can express it as:

$$B_y|_N^{n+1/2} = \frac{1}{c} E_x|_N^{n+1/2}$$

Because of **staggering**:

$$\frac{B_{yN+1/2}^{n+1/2} + B_{yN-1/2}^{n+1/2}}{2} = \frac{1}{c} \frac{E_{xN}^{n+1} + E_{xN}^n}{2}$$

# Silver-Müller absorbing boundary (right-hand side)



By combining the equations:

$$\frac{B_{y_{N+1/2}}^{n+1/2} + B_{y_{N-1/2}}^{n+1/2}}{2} = \frac{1}{c} \frac{E_{xN}^{n+1} + E_{xN}^n}{2} \quad (\text{right-propagating wave})$$

$$\frac{E_{xN}^{n+1} - E_{xN}^n}{\Delta t} = -c^2 \frac{B_{y_{N+1/2}}^{n+1/2} - B_{y_{N-1/2}}^{n+1/2}}{\Delta z} \quad (\text{Maxwell equation})$$

we obtain

Silver-Müller boundary condition (right-hand side)

$$E_{xN}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{xN}^n + \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{y_{N-1/2}}^{n+1/2}$$

See e.g. Bjorn Engquist (1977)

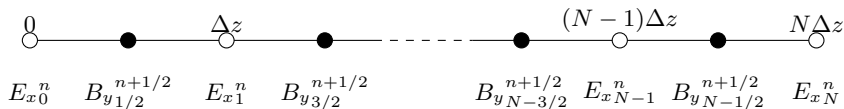
# Silver-Müller absorbing boundary (right-hand side)

Silver-Müller boundary condition (right-hand side)

$$E_{x_N}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{x_N}^n + \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{y_{N-1/2}}^{n+1/2}$$

**Animation: Silver-Müller boundary conditions**

## Silver-Müller absorbing boundary (left-hand side)



By combining the equations:

$$\frac{B_{y1/2}^{n+1/2} + B_{y-1/2}^{n+1/2}}{2} = -\frac{1}{c} \frac{E_{x0}^{n+1} + E_{x0}^n}{2} \quad (\text{left-propagating wave})$$

$$\frac{E_{x0}^{n+1} - E_{x0}^n}{\Delta t} = -c^2 \frac{B_{y1/2}^{n+1/2} - B_{y-1/2}^{n+1/2}}{\Delta z} \quad (\text{Maxwell equation})$$

we obtain

Silver-Müller boundary condition (left-hand side)

$$E_{x0}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{x0}^n - \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{y1/2}^{n+1/2}$$



# Silver-Müller absorbing boundary in 3D

Maxwell equation:

$$\frac{E_{x_{i+\frac{1}{2},j,\ell}}^{n+1} - E_{x_{i+\frac{1}{2},j,\ell}}^n}{c^2 \Delta t} = \frac{B_{z_{i+\frac{1}{2},j+\frac{1}{2},0}}^{n+\frac{1}{2}} - B_{z_{i+\frac{1}{2},j-\frac{1}{2},0}}^{n+\frac{1}{2}}}{\Delta y} - \frac{B_{y_{i+\frac{1}{2},j,\ell+\frac{1}{2}}}^{n+\frac{1}{2}} - B_{y_{i+\frac{1}{2},j,\ell-\frac{1}{2}}}^{n+\frac{1}{2}}}{\Delta z}$$

Silver-Müller boundary condition (left-hand side)

$$E_{x_{i+\frac{1}{2},j,0}}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{x_{i+\frac{1}{2},j,0}}^n - \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{y_{i+\frac{1}{2},j,\frac{1}{2}}}^{n+\frac{1}{2}} + c^2\Delta t \frac{B_{z_{i+\frac{1}{2},j+\frac{1}{2},0}}^{n+\frac{1}{2}} - B_{z_{i+\frac{1}{2},j-\frac{1}{2},0}}^{n+\frac{1}{2}}}{\Delta y}$$

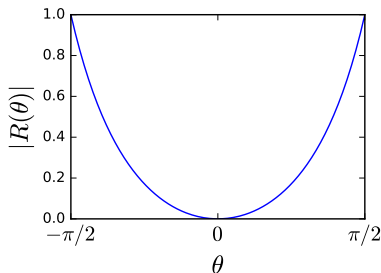
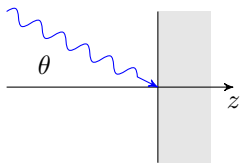
- + Similar equations for the right-hand side
- + Similar equations for  $B_x$  and  $E_y$

# Silver-Müller absorbing boundary in 3D

## Limitation

In 3D, the Silver-Müller boundary conditions are only well-adapted for waves in **normal incidence**.

The reflection coefficient  $R(\theta)$  quickly increases with the angle of incidence  $\theta$ .



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# Perfectly Matched Layers (in 2D)

## Perfectly Matched Layers (Berenger, 1994)

Surround the simulation box by **additional layers of cells**, where the Maxwell equations are **modified** so as to **progressively damp** the waves.

In the bulk:

$$\partial_t E_x = c^2 \partial_y B_z$$

$$\partial_t E_y = -c^2 \partial_x B_z$$

$$\partial_t B_z = -\partial_x E_y + \partial_y E_x$$

In e.g. the **right-hand layer**:

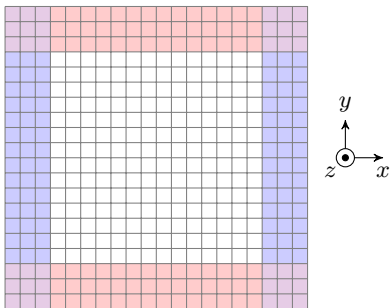
$$\partial_t E_x = c^2 \partial_y B_z$$

$$\partial_t E_y = -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y$$

$$B_z = B_{zx} + B_{zy}$$

$$\partial_t B_{zx} = -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx}$$

$$\partial_t B_{zy} = \partial_y E_x$$



Modified Maxwell equations:

- Artificial (unphysical) conductivity  $\sigma$
- The  $B_z$  field is (artificially) split in two

# Perfectly Matched Layers (in 2D)

Animation with  
propagating waves:

- Waves in normal incidence are **absorbed**.
- Waves in grazing incidence **propagate** as if they did not “feel” the boundary.

# Perfectly Matched Layers: normal incidence

Explanation based on **continuous equations**

Transverse EM wave propagating along x

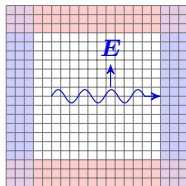
$$E_x = 0 \quad E_y \neq 0 \quad \rightarrow \quad B_{zy} = 0 \quad B_z = B_{zx}$$

In the bulk:

$$\begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y + \partial_y E_x \end{aligned} \quad \rightarrow \quad \begin{aligned} \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y \end{aligned}$$

In the **right-hand layer**:

$$\begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ B_z &= B_{zx} + B_{zy} \\ \partial_t B_{zx} &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx} \\ \partial_t B_{zy} &= \partial_y E_x \end{aligned} \quad \rightarrow \quad \begin{aligned} \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ \partial_t B_z &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_z \end{aligned}$$



# Perfectly Matched Layers: normal incidence

There is a solution (continuous in  $E_y$  and  $B_z$ ) with **no reflected wave**.

In the bulk ( $x < 0$ ):

$$\begin{aligned}\partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y\end{aligned}$$

Solution:

$$E_y = E_0 \cos(k(x - ct))$$

$$B_z = \frac{E_0}{c} \cos(k(x - ct))$$

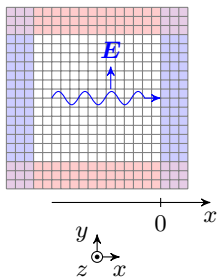
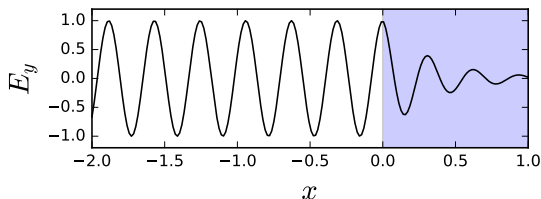
In the **right-hand layer** ( $x > 0$ ):

$$\begin{aligned}\partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ \partial_t B_z &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_z\end{aligned}$$

Solution:

$$E_y = E_0 \cos(k(x - ct)) e^{-\frac{\sigma}{\epsilon_0 c} x}$$

$$B_z = \frac{E_0}{c} \cos(k(x - ct)) e^{-\frac{\sigma}{\epsilon_0 c} x}$$



The wave is damped before reaching the end of the outer layer.

# Perfectly Matched Layers: grazing incidence

Transverse EM wave propagating along y

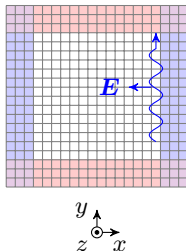
$$E_x \neq 0 \quad E_y = 0 \quad \rightarrow \quad B_{zx} = 0 \quad B_z = B_{zy}$$

In the bulk:

$$\begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y + \partial_y E_x \end{aligned} \quad \rightarrow \quad \begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t B_z &= \partial_y E_x \end{aligned}$$

In the right-hand layer:

$$\begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ B_z &= B_{zx} + B_{zy} \\ \partial_t B_{zx} &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx} \\ \partial_t B_{zy} &= \partial_y E_x \end{aligned} \quad \rightarrow \quad \begin{aligned} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t B_z &= \partial_y E_x \end{aligned}$$



The propagation equations are **identical** in the bulk and the outer layer. A wave in **grazing incidence** does not “feel” the boundary.



# Open boundary conditions: conclusion

- If no **special care** is taken at the boundary, it will **by default** produce a reflected wave.
- **Silver-Müller boundary conditions:**
  - Easy to implement
  - But only cancels reflection for waves at normal incidence
- **Perfectly Matched Layers**
  - Need extra layers of cells, where the Maxwell equations are artificially modified.
  - The anisotropic Maxwell equations lead to proper behavior for waves with any incidence angle.

# References

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- Haber, I., Lee, R., Klein, H., and Boris, J. (1973).