Computational Physics – Lecture 13: How to solve Maxwell's equations numerically? III

Kristel Michielsen

Institute for Advanced Simulation
Jülich Supercomputing Centre
Research Centre Jülich
k.michielsen@fz-juelich.de
http://www.fz-juelich.de/ias/jsc/qip



Contents

- Yee algorithm with product formula approach (discretizing exact formal solution)
 - Conditionally stable, Courant number
- Unconditionally stable method from discretizing the exact formal solution
- Exercise: Simulation of transmission and reflection of light by a glass plate with the Yee algorithm

Yee algorithm:

Time-stepping approach: Alternatingly the \vec{E} field and \vec{H} field is updated

Discretization of space, no discretization of time

$$H_{y}\Big|_{l+1/2}^{t} \qquad E_{z}\Big|_{l+1}^{t} \qquad H_{y}\Big|_{l+3/2}^{t} \qquad E_{z}\Big|_{l+2}^{t} \qquad H_{y}\Big|_{l+5/2}^{t}$$

$$l+1/2 \qquad l+1 \qquad l+3/2 \qquad l+2 \qquad l+5/2$$

$$\wedge$$

Maxwell equations:

$$\begin{split} & \frac{\partial \left. H_{\boldsymbol{y}} \right|_{l+1/2}^{t}}{\partial t} = \frac{1}{\Delta} \left(E_{\boldsymbol{z}} \right|_{l+1}^{t} - E_{\boldsymbol{z}} \right|_{l}^{t} \right) \\ & \frac{\partial \left. E_{\boldsymbol{z}} \right|_{l}^{t}}{\partial t} = \frac{1}{\Delta} \left(H_{\boldsymbol{y}} \right|_{l+1/2}^{t} - H_{\boldsymbol{y}} \right|_{l-1/2}^{t} \right) \end{split}$$

Boundary conditions:

$$\left|E_z\right|_0^t = E_z\Big|_L^t = 0$$

No update

in matrix notation:

$$\left\| \frac{\partial \Psi(t)}{\partial t} = \mathsf{L} \Psi(t) \right\|$$

with:

$$\Psi^{T}(t) = \left(E_{z}|_{1}^{t} \cdots E_{z}|_{L-1}^{t} H_{y}|_{1/2}^{t} \cdots H_{y}|_{L-1/2}^{t}\right)$$

and:

$$\frac{\left[\frac{\partial H_{y}|_{l+1/2}^{t}}{\partial t} = \frac{1}{\Delta} \left(E_{z}|_{l+1}^{t} - E_{z}|_{l}^{t}\right)\right]}{\left[\frac{\partial E_{z}|_{l}^{t}}{\partial t} = \frac{1}{\Delta} \left(H_{y}|_{l+1/2}^{t} - H_{y}|_{l-1/2}^{t}\right)\right]}$$

$$\frac{\partial}{\partial t} \begin{pmatrix} E \\ H \end{pmatrix} = \mathbf{L} \begin{pmatrix} E \\ H \end{pmatrix}$$

$$= \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} A & B \\ A & B \end{pmatrix}$$

$$= \begin{pmatrix} AE + BH \\ CE + DH \end{pmatrix}$$

From the construction it is clearly seen that L is skew symmetric ($L^T = -L$) Choose $L = L_1 + L_2$, where

$$\mathsf{L} = \begin{pmatrix} 0 & -A^T \\ A & 0 \end{pmatrix} \mathsf{L}_1 = \begin{pmatrix} 0 & -A^T \\ 0 & 0 \end{pmatrix} \Rightarrow \mathsf{L}_1^2 = 0 \quad \mathsf{L}_2 = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix} \Rightarrow \mathsf{L}_2^2 = 0$$

and
$$A = \frac{1}{\Delta} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ -1 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 \end{pmatrix}$$
Alichielsen All Rights Reserved \cdots 0 -1

2x2 matrices with block matrices as elements

 L_1 and L_2 are not skew symmetric

Note: The decomposition $L = L_1 + L_2$ is general, that is it works also for 2D and 3D problems but the particular form of A is directly linked to the specific 1D example considered.

The decomposition should be such that we can readily calculate $e^{\tau \mathsf{L}_1} \Phi$ and $e^{\tau \mathsf{L}_2} \Phi$ for all τ and Φ

$$e^{\tau\mathsf{L}_1} = \sum_{n=0}^{\infty} \frac{\left(\tau\mathsf{L}_1\right)^n \mathsf{exact!}}{n!} = 1 + \tau\mathsf{L}_1, \ e^{\tau\mathsf{L}_2} = \sum_{n=0}^{\infty} \frac{\left(\tau\mathsf{L}_2\right)^n}{n!} = 1 + \tau\mathsf{L}_2$$

$$e^{\tau \mathsf{L}_1} \Psi(t) = (1 + \tau \mathsf{L}_1) \Psi(t)$$

$$= \begin{pmatrix} 1 & -\tau A^T \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E_z | t \\ H_y | t \end{pmatrix} = \begin{pmatrix} E_z | t - \tau A^T H_y | t \\ H_y | t \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} E_z \big|^{t+\tau} \\ H_y \big|^{t+\tau} \end{pmatrix} = \begin{pmatrix} E_z \big|^t - \tau A^T H_y \big|^t \\ H_y \big|^t \end{pmatrix}$$

 \vec{E} update

$$e^{\tau L_2} \Psi(t) = (1 + \tau L_2) \Psi(t)$$

$$= \begin{pmatrix} 1 & 0 \\ \tau A & 1 \end{pmatrix} \begin{pmatrix} E_z | t \\ H_y | t \end{pmatrix} = \begin{pmatrix} E_z | t \\ H_y | t + \tau A E_z | t \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} E_z \big|^{t+\tau} \\ H_y \big|^{t+\tau} \end{pmatrix} = \begin{pmatrix} E_z \big|^t \\ H_y \big|^t + \tau A E_z \big|^t \end{pmatrix}$$

 \dot{H} update

$$e^{\tau L} \Psi(t) = e^{\tau L_1} e^{\tau L_2} \Psi(t)$$

First \vec{H} update, then \vec{E} update

Note: Equivalent is

$$e^{\tau L} \Psi(t) = e^{\tau L_2} e^{\tau L_1} \Psi(t)$$

First \vec{E} update, then \vec{H} update

Note: Yee algorithm with leapfrog scheme

$$\begin{split} E_{z}\big|_{l}^{n+1/2} &= \left(\frac{1 - \frac{\sigma_{l}\tau}{2\varepsilon_{l}}}{1 + \frac{\sigma_{l}\tau}{2\varepsilon_{l}}}\right) E_{z}\big|_{l}^{n-1/2} + \left(\frac{\frac{\tau}{\varepsilon_{l}}}{1 + \frac{\sigma_{l}\tau}{2\varepsilon_{l}}}\right) \left[\frac{H_{y}\big|_{l+1/2}^{n} - H_{y}\big|_{l-1/2}^{n}}{\Delta} - J_{\text{source}_{z}}\big|_{l}^{n}\right] \\ H_{y}\big|_{l+1/2}^{n+1} &= \left(\frac{1 - \frac{\sigma_{t+1/2}^{*}\tau}{2\mu_{l+1/2}}}{1 + \frac{\sigma_{t+1/2}^{*}\tau}{2\mu_{l+1/2}}}\right) H_{y}\big|_{l+1/2}^{n} + \left(\frac{\frac{\tau}{\mu_{l+1/2}}}{1 + \frac{\sigma_{t+1/2}^{*}\tau}{2\mu_{l+1/2}}}\right) \left[\frac{E_{z}\big|_{l+1}^{n+1/2} - E_{z}\big|_{l}^{n+1/2}}{\Delta} - M_{\text{source}_{y}}\big|_{l+1/2}^{n+1/2}\right] \end{split}$$



 \blacktriangleright First $\stackrel{f}{E}$ update and then $\stackrel{f}{H}$ update

Note: Yee algorithm with leapfrog scheme

$$e^{\tau L} \Psi(t) = e^{\tau L_2} e^{\tau L_1} \Psi(t)$$

$$e^{\tau \mathsf{L}_1} \Psi(t)$$

$$\Rightarrow \begin{pmatrix} E_z | ^n \\ H_y | ^{n+1/2} \end{pmatrix} = \begin{pmatrix} 1 & -\tau A^T \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E_z | ^{n-1/2} \\ H_y | ^n \end{pmatrix} = \begin{pmatrix} E_z | ^{n-1/2} - \tau A^T H_y | ^n \\ H_y | ^n \end{pmatrix}$$

$$\Rightarrow E_z \Big|^n = E_z \Big|^{n-1/2} - \tau A^T H_y \Big|^n$$

$$H_{y}\Big|^{n+1/2} = H_{y}\Big|^{n}$$

Note: Yee algorithm with leapfrog scheme

$$e^{\tau L} \Psi(t) = e^{\tau L_2} e^{\tau L_1} \Psi(t)$$

$$e^{\tau L_2} e^{\tau L_1} \Psi(t)$$

$$\Rightarrow \begin{pmatrix} E_{z} \big|^{n+1/2} \\ H_{y} \big|^{n+1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \tau A & 1 \end{pmatrix} \begin{pmatrix} E_{z} \big|^{n} \\ H_{y} \big|^{n+1/2} \end{pmatrix} = \begin{pmatrix} E_{z} \big|^{n} \\ H_{y} \big|^{n+1/2} + \tau A E_{z} \big|^{n} \end{pmatrix}$$

$$\Rightarrow E_{z} \big|^{n+1/2} = E_{z} \big|^{n}$$

$$H_{y} \big|^{n+1} = H_{y} \big|^{n+1/2} + \tau A E_{z} \big|^{n}$$

Note: Yee algorithm with leapfrog scheme

$$\Rightarrow E_{z}|^{n} = E_{z}|^{n-1/2} - \tau A^{T} H_{y}|^{n}$$

$$H_{y}|^{n+1/2} = H_{y}|^{n}$$

$$E_{z}|^{n+1/2} = E_{z}|^{n}$$

$$H_{y}|^{n+1} = H_{y}|^{n+1/2} + \tau A E_{z}|^{n}$$

$$\Rightarrow E_{z}|^{n+1/2} = E_{z}|^{n-1/2} - \tau A^{T} H_{y}|^{n}$$

$$H_{y}|^{n+1} = H_{y}|^{n} + \tau A E_{z}|^{n+1/2}$$

Stability:
$$||e^{\tau L_2}e^{\tau L_1}|| \le 1$$
?

$$\begin{aligned} \left\| e^{\tau \mathsf{L}_2} e^{\tau \mathsf{L}_1} \right\| &= \left\| (1 + \tau \mathsf{L}_2) (1 + \tau \mathsf{L}_1) \right\| \\ &= \left\| 1 + \tau \mathsf{L} + \tau^2 \mathsf{L}_2 \mathsf{L}_1 \right\| \\ &= \left\| X \right\| \le 1? \end{aligned}$$

where $||X||^2 = \text{maximum eigenvalue of } X^T X$

Stability: $||e^{\tau L_2}e^{\tau L_1}|| \le 1$?

From the eigenvalue equation it follows that

$$\tau \|A\| \le 2 \text{ with } A = \frac{1}{\Delta} \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix}$$

We make use of $||A||^2 \le ||A^T||_1 ||A||_1$, where

$$||A||_1 = \max_j \left(\sum_i |A_{ij}| \right)$$

and consider a time step τ such that

$$\tau \|A\| \le \tau \sqrt{\|A^T\|_1 \|A\|_1} = \tau \sqrt{\frac{2}{\Delta} \frac{2}{\Delta}} \le 2$$

Hence

$$\left| \frac{\tau}{\Delta} \le 1 \right|$$

Courant number

Unconditionally stable method from discretizing the exact formal solution

Maxwell equation in 1D

In matrix form:

$$\frac{\partial}{\partial t} \begin{pmatrix} E_z(x,t) \\ H_y(x,t) \end{pmatrix} = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} E_z(x,t) \\ H_y(x,t) \end{pmatrix} - \begin{pmatrix} J_{\text{source}_z}(x,t) \\ 0 \end{pmatrix}$$



$$\frac{\partial}{\partial t} \Psi(t) = \mathbf{L} \Psi(t) - \mathbf{S}(t)$$

$$\frac{\partial}{\partial t} \Psi(t) = \mathsf{L} \Psi(t) :$$

How to solve numerically?

• In case of variables y and numbers k:

$$\frac{\partial y}{\partial t} = ky \Longrightarrow y(t) = e^{tk} y(0)$$

• In case of vectors Ψ and matrices L :

$$\frac{\partial}{\partial t} \Psi(t) = \mathsf{L} \Psi(t) \Rightarrow \Psi(t) = e^{\mathsf{tL}} \Psi(0)$$

How to deal with the matrix exponential?

- L is a large non-trivial matrix \rightarrow in general no practical algorithm to compute e^{tL} directly
- But for instance $L = L_1 + L_2$ and e^{tL_1} , e^{tL_2} can be calculated
 - Can we calculate e^{tL} if we know how to calculate e^{tL_1} and e^{tL_2} ?
 - Yes, as a controlled approximation
 - → defines a particular algorithm

From the definition

$$\Psi(t) = \begin{pmatrix} E_z(x,t) & H_y(x,t) \end{pmatrix}^T \text{ and } L = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix} \in \mathbf{R}$$

it follows that

$$\left\langle \Psi(t) \middle| \mathsf{L} \; \Psi(t) \right\rangle = \int \left[E_z(x,t) \frac{\partial H_y(x,t)}{\partial x} + H_y(x,t) \frac{\partial E_z(x,t)}{\partial x} \right] dx$$

$$\int_{E_z \cdot H_y \Big|_{-\infty}^{+\infty}}^{+\infty} = 0$$

$$= -\int \left[\left(\frac{\partial E_z(x,t)}{\partial x} \right) H_y(x,t) + E_z(x,t) \frac{\partial H_y(x,t)}{\partial x} \right] dx$$

$$= -\langle \mathsf{L} \Psi(t) | \Psi(t) \rangle$$

Hence,

$$\langle \Psi(t) | L \Psi(t) \rangle = -\langle L \Psi(t) | \Psi(t) \rangle$$

and

$$\langle \Psi(t) | \mathsf{L} \Psi(t) \rangle = \langle \mathsf{L}^T \Psi(t) | \Psi(t) \rangle$$

so that

$$L^T = -L$$

→ L is skew-symmetric

The time-evolution operator e^{tL} is a unitary

matrix (
$$A^{-1} = A^{T}$$
):
 $(e^{tL})^{-1} = e^{-tL} = e^{tL^{T}} = (e^{tL})^{T}$

It follows that

$$\left\langle e^{t\mathsf{L}}\Psi(0) \middle| e^{t\mathsf{L}}\Psi(0) \right\rangle = \left\langle \Psi(t) \middle| \Psi(t) \right\rangle = \left\langle \left(e^{t\mathsf{L}} \right)^T e^{t\mathsf{L}}\Psi(0) \middle| \Psi(0) \right\rangle = \left\langle \Psi(0) \middle| \Psi(0) \right\rangle$$
Hence the time-evolution operator leaves $\|\Psi\|$

Hence, the time-evolution operator leaves $\|\Psi\|$ unchanged.

The energy density of the EM fields does © Kristel Michielsen Norts Change with time

Hence,

$$\|\Psi(t)\| = \|e^{tL}\Psi(0)\| \le \|e^{tL}\| \|\Psi(0)\|$$

$$\|AX\| \le \|A\| \|X\|$$

$$\|\Psi(t)\| \le \|\Psi(0)\|$$
STABILITY (requirement: $\|e^{tL}\| \le 1$ for all t)

Note that for skew-symmetric L , e^{tL} is a unitary operator. A unitary operator rotates the vector Ψ without changing its length. Hence, $\|\Psi(t)\| = \|\Psi(0)\|$

In order to get an unconditionally stable algorithm from the product formula approach the skew symmetric matrix L should be decomposed in matrices that are skew symmetric themselves.

$$\Psi^{T}(t) = \left(H_{y}\Big|_{1/2}^{t} E_{z}\Big|_{1}^{t} \cdots E_{z}\Big|_{L-1}^{t} H_{y}\Big|_{L-1/2}^{t}\right) \begin{bmatrix} \frac{\partial H_{y}\Big|_{l+1/2}^{t}}{\partial t} = \frac{1}{\Delta}\left(E_{z}\Big|_{l+1}^{t} - E_{z}\Big|_{l}^{t}\right) \\ \frac{\partial E_{z}\Big|_{l}^{t}}{\partial t} = \frac{1}{\Delta}\left(H_{y}\Big|_{l+1/2}^{t} - H_{y}\Big|_{l-1/2}^{t}\right) \end{bmatrix}$$

and:

$$\frac{\partial E_{1}}{\partial t} = \frac{1}{\Delta} (H_{3/2} - H_{1/2})$$

$$\frac{\partial E_{2}}{\partial t} = \frac{1}{\Delta} (H_{5/2} - H_{3/2})$$

$$\frac{\partial E_{L-2}}{\partial t} = \frac{1}{\Delta} (H_{L-3/2} - H_{L-5/2})$$

$$\frac{\partial E_{L-1}}{\partial t} = \frac{1}{\Delta} (H_{L-1/2} - H_{L-3/2})$$

$$\frac{\partial H_{1/2}}{\partial t} = \frac{1}{\Delta} E_{1}$$

$$\frac{\partial H_{3/2}}{\partial t} = \frac{1}{\Delta} (E_{2} - E_{1})$$

$$\frac{\partial H_{L-3/2}}{\partial t} = \frac{1}{\Delta} (E_{L-1} - E_{L-2})$$

$$\frac{\partial H_{L-1/2}}{\partial t} = -\frac{1}{\Delta} E_{L-1}$$

From the construction it is clearly seen that L is skew-symmetric

Choose
$$L = L_1 + L_2$$
, where

$$\mathsf{L}_1 = \frac{1}{\Delta} \begin{bmatrix} 0 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 0 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 1 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 & 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 & 0 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 1 & \vdots \\ \vdots & \ddots & 1 & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \end{bmatrix}$$
 ichielsen All Rights Reserved

BLOCK MATRICES

and

BLOCK MATRICES

From the construction it is clearly seen that L_1 and L_2 are both skew-symmetric

- L₁ and L₂ display a block-matrix structure wherein each block matrix has at most dimensions 2x2
- The matrix exponential of a block diagonal matrix is also block diagonal (with the same structure as the matrix itself)
- >Finding the explicit form of the matrix exponentials of L₁ and L₂ requires, at most, the calculation of a matrix exponential of a 2x2 matrix

 \rightarrow In order to calculate $e^{\tau L_1}$ and $e^{\tau L_2}$, we first calculate $e^{\tau X}$ with

$$X = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

We use

$$e^{\tau X} = \sum_{k=0}^{\infty} \frac{\tau^k}{k!} X^k$$

$$X^0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv I$$

$$X^{1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{1} = X$$

$$X^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -I$$

$$X^3 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^3 = -X$$

$$X^4 = I$$

$$X^5 = X$$

4

$$\Rightarrow e^{\tau X} = I + \tau X - \frac{\tau^{2}}{2!} I - \frac{\tau^{3}}{3!} X + \frac{\tau^{4}}{4!} I + \frac{\tau^{5}}{5!} X - \frac{\tau^{6}}{6!} I - \dots$$

$$= \left(1 - \frac{\tau^{2}}{2!} + \frac{\tau^{4}}{4!} - \frac{\tau^{6}}{6!} + \dots\right) I + \left(\tau - \frac{\tau^{3}}{3!} + \frac{\tau^{5}}{5!} - \dots\right) X$$

$$= (\cos \tau) I + (\sin \tau) X$$

$$= \left(\frac{\cos \tau}{0} + \frac{0}{\cos \tau}\right) + \left(\frac{0}{-\sin \tau} + \frac{\sin \tau}{0}\right)$$

$$= \left(\frac{\cos \tau}{-\sin \tau} + \frac{\sin \tau}{\cos \tau}\right)$$

$$= \sin x = \sum_{k=0}^{\infty} \frac{(-1)^{k}}{(2k+1)!} x^{2k+1} = x - \frac{x^{3}}{3!} + \frac{x^{5}}{5!} - \dots$$

 $\cos x = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} x^{2k} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots$

 \rightarrow The expressions for $e^{\tau L_1}$ and $e^{\tau L_2}$ are

where $c = \cos(\tau/\Delta)$ and $s = \sin(\tau/\Delta)$

```
PROGRAM:
                            (psi(1:2*L-1))
r=tau/delta
c = cos(r)
s=sin(r)
do i=istart, 2*L-2, 2
r=psi(i)
psi(i) = c*r+s*psi(i+1)
psi(i+1) = c*psi(i+1) - s*r
enddo
e^{\tau L_1}: istart=1
e^{\tau L_2}: istart=2
```

9 operations: 4 multiplications

2 summations

3 moves

For comparison: Yee algorithm with same structure for $\Psi(t)$

$$\Psi^{T}(t) = \left(H_{y}|_{1/2}^{t} E_{z}|_{1}^{t} \cdots E_{z}|_{L-1}^{t} H_{y}|_{L-1/2}^{t}\right)$$

and:

 $L_1: \vec{E}$ update

$$\begin{split} \frac{\partial E_{1}}{\partial t} &= \frac{1}{\Delta} \left(H_{3/2} - H_{1/2} \right) \\ \frac{\partial E_{2}}{\partial t} &= \frac{1}{\Delta} \left(H_{5/2} - H_{3/2} \right) \\ \frac{\partial E_{L-2}}{\partial t} &= \frac{1}{\Delta} \left(H_{L-3/2} - H_{L-5/2} \right) \\ \frac{\partial E_{L-1}}{\partial t} &= \frac{1}{\Delta} \left(H_{L-1/2} - H_{L-3/2} \right) \end{split}$$

L₁ is not skew-symmet

For comparison: Yee algorithm with same structure for $\Psi(t)$

$$\Psi^{T}(t) = \left(H_{y}\Big|_{1/2}^{t} E_{z}\Big|_{1}^{t} \cdots E_{z}\Big|_{L-1}^{t} H_{y}\Big|_{L-1/2}^{t}\right)$$

and:

$$\mathsf{L}_2 = \frac{1}{\Delta} \begin{bmatrix} 0 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & -1 & 0 & 1 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 & 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 1 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 1 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 0 \end{bmatrix}$$

$$\mathsf{L}_2 \text{ is not skew-symm}$$

 $L_2: \vec{H}$ update

$$\begin{split} \frac{\partial H_{1/2}}{\partial t} &= \frac{1}{\Delta} E_1 \\ \frac{\partial H_{3/2}}{\partial t} &= \frac{1}{\Delta} \left(E_2 - E_1 \right) \\ \frac{\partial H_{L-3/2}}{\partial t} &= \frac{1}{\Delta} \left(E_{L-1} - E_{L-2} \right) \\ \frac{\partial H_{L-1/2}}{\partial t} &= -\frac{1}{\Delta} E_{L-1} \end{split}$$

L₂ is not skew-symmetr

For comparison: Yee algorithm with same structure for $\Psi(t)$

 \rightarrow The expression for $e^{\tau L_1} = 1 + \tau L_1$ is

$$e^{\tau \mathsf{L}_1} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -\tau/\Delta & 1 & \tau/\Delta & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 1 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -\tau/\Delta & 1 & \tau/\Delta & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 & 1 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & -\tau/\Delta & 1 & \tau/\Delta & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & -\tau/\Delta & \ddots & \tau/\Delta \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix}$$

For comparison: Yee algorithm with same structure for $\Psi(t)$

 \rightarrow The expression for $e^{\tau L_2} = 1 + \tau L_2$ is

$$e^{\tau L_2} = \begin{pmatrix} 1 & \tau/\Delta & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & 0 & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & -\tau/\Delta & 1 & \tau/\Delta & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & 1 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\tau/\Delta & 1 & \tau/\Delta & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 & 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & -\tau/\Delta & \ddots & \tau/\Delta & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\tau/\Delta & 1 \end{pmatrix}$$

For comparison: Yee algorithm with same structure for $\Psi(t)$

```
PROGRAM:
                         (psi(1:2*L-1))
r=tau/delta
if (istart ==1) then c=0 else c=psi(1)
do i=istart, 2*L-2, 2
s=psi(i+1)
                                   6 operations:
psi(i) = r*(s-c) + psi(i)
                                   1 multiplication
                                   2 summations
C=S
                                   3 moves
enddo
if (istart ==1) psi(2*L-1)=psi(2*L-1)-r*c
e^{\tau L_1}:istart=2
```

Product formula approach: general

•
$$\Psi(t+\tau) = e^{\tau L} \Psi(t)$$

First order approximation:

$$e^{\tau L} = \left(e^{\tau L/m}\right)^m \approx \left(e^{\tau L_1/m}e^{\tau L_2/m}\right)^m$$

Second order approximation:

$$e^{\tau L} = \left(e^{\tau L/m}\right)^m \approx \left(e^{\tau L_1/2m}e^{\tau L_2/m}e^{\tau L_1/2m}\right)^m$$

Note: L_1 and L_2 can be interchanged © Kristel Michielsen All Rights Reserved

Product formula approach: general

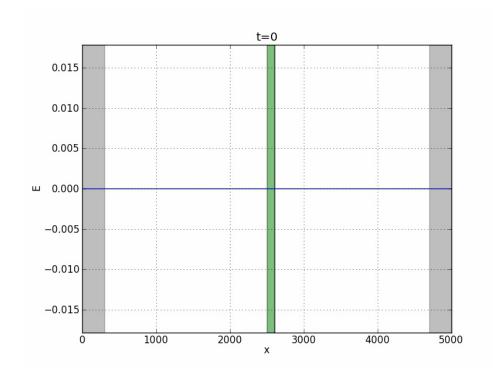
Technical note:

$$\left(e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{2}/m}e^{\tau\mathsf{L}_{1}/2m}\right)^{m} = \left(e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{2}/m}e^{\tau\mathsf{L}_{1}/2m}\right)\left(e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{2}/m}e^{\tau\mathsf{L}_{1}/2m}\right)\left(e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{1}/2m}\right)...\left(e^{\tau\mathsf{L}_{1}/2m}e^{\tau\mathsf{L}_{2}/m}e^{\tau\mathsf{L}_{1}/2m}\right)$$

$$m \quad \text{factors}$$

$$= e^{\tau \mathsf{L}_1/2m} e^{\tau \mathsf{L}_2/m} e^{\tau \mathsf{L}_1/m} e^{\tau \mathsf{L}_2/m} e^{\tau \mathsf{L}_1/m} e^{\tau \mathsf{L}_2/m} e^{\tau \mathsf{L}_1/2m} \dots e^{\tau \mathsf{L}_1/2m} e^{\tau \mathsf{L}_2/m} e^{\tau \mathsf{L}_1/2m}$$

Simulation of transmission and reflection of light by a glass plate with the Yee algorithm.



Parameters:

- Wavelength (sets the length scale): $\lambda = 1$
- Number of grid points per wavelength: 50
- Spatial resolution: $\Delta = \lambda / 50 = 0.02$
- Temporal resolution: $\tau = 0.9\Delta$, $\tau = 1.05\Delta$ (Courant condition!)
- Length of simulation box: $X = 100\lambda = L\Delta \Rightarrow L = 5000$
- Source frequency: $f = v / \lambda = 1 / \lambda = 1 \Rightarrow \omega = 2\pi f = 2\pi$
- Number of time steps: m = 10000

- Materials:
 - Matched boundary layers for reflectionless absorption of the EM waves at the boundary

$$\sigma(x) = \sigma^*(x) = \begin{cases} 1 & \text{if} \quad 0 \le x \le 6\lambda \\ 0 & \text{if} \quad 6\lambda < x < L\Delta - 6\lambda \\ 1 & \text{if} \quad L\Delta - 6\lambda \le x \le L\Delta \end{cases}$$

Gray areas in the picture

Materials:

- Glass layer of thickness 2λ placed in the middle of the system (green area in the picture)
- Index of refraction of glass: n = 1.46

$$\varepsilon(x) = \begin{cases} 1 & \text{if} \quad 0 \le x < L\Delta/2 \\ n^2 & \text{if} \quad L\Delta/2 \le x < L\Delta/2 + 2\lambda \\ 1 & \text{if} \quad L\Delta/2 + 2\lambda \le x \le L\Delta \end{cases}$$

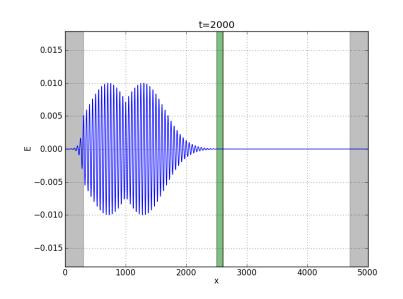
$$\mu(x) = 1$$

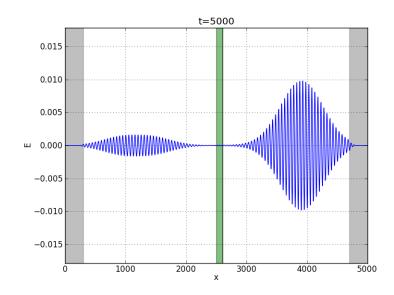
- Current source at $x_S = 20\lambda \Leftrightarrow i_S = x_S / \Delta = 1000$
- To create a nice wave packet, we turn on the source slowly and we also turn it of slowly

$$J_S(i_S, t) = \sin(2\pi t f) e^{-((t-30)/10)^2}$$

where f = 1 is the frequency of the current source

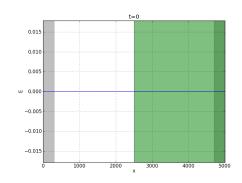
Plot the *E*-field for various numbers of time steps

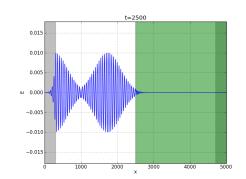


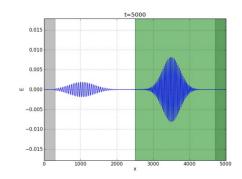


• What happens for $\tau = 1.05\Delta$?

 Make the glass plate very thick, as shown in these pictures







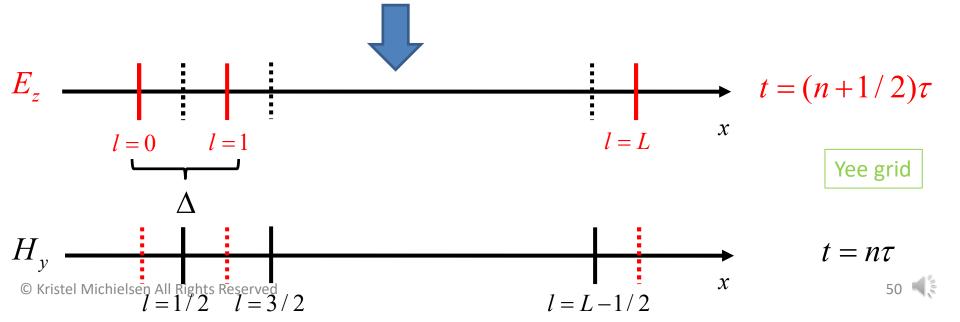
 From the maximum of the incident wave packet and the reflected wave packet, estimate the reflection coefficient of glass

Exercise: 1D Maxwell equation

Consider the Maxwell equation in 1D

$$\frac{\partial H_{y}(x,t)}{\partial t} = \frac{1}{\mu(x)} \left[\frac{\partial E_{z}(x,t)}{\partial x} - \sigma^{*}(x) H_{y}(x,t) \right]$$

$$\frac{\partial E_{z}(x,t)}{\partial t} = \frac{1}{\varepsilon(x)} \left[\frac{\partial H_{y}(x,t)}{\partial x} - J_{\text{source}_{z}}(x,t) - \sigma(x) E_{z}(x,t) \right]$$



$$\begin{split} & \frac{\left|H_{y}\right|_{l+1/2}^{n+1} - H_{y}\right|_{l+1/2}^{n}}{\tau} = \frac{1}{\mu_{l+1/2}} \left[\frac{E_{z}|_{l+1}^{n+1/2} - E_{z}|_{l}^{n+1/2}}{\Delta} - \sigma_{l+1/2}^{*} H_{y}|_{l+1/2}^{n+1/2}\right] \\ & \frac{E_{z}|_{l}^{n+1/2} - E_{z}|_{l}^{n-1/2}}{\tau} = \frac{1}{\varepsilon_{l}} \left[\frac{H_{y}|_{l+1/2}^{n} - H_{y}|_{l-1/2}^{n}}{\Delta} - J_{\text{source}_{z}}|_{l}^{n} - \sigma_{l} E_{z}|_{l}^{n}\right] \end{split}$$



$$\left| H_{y} \right|_{l+1/2}^{n+1} = H_{y} \Big|_{l+1/2}^{n} + \frac{\tau}{\mu_{l+1/2}} \left[\frac{E_{z} \Big|_{l+1}^{n+1/2} - E_{z} \Big|_{l}^{n+1/2}}{\Delta} - \sigma_{l+1/2}^{*} \left(\frac{H_{y} \Big|_{l+1/2}^{n+1} + H_{y} \Big|_{l+1/2}^{n}}{2} \right) \right] \\ E_{z} \Big|_{l}^{n+1/2} = E_{z} \Big|_{l}^{n-1/2} + \frac{\tau}{\varepsilon_{l}} \left[\frac{H_{y} \Big|_{l+1/2}^{n} - H_{y} \Big|_{l-1/2}^{n}}{\Delta} - J_{\text{source}_{z}} \Big|_{l}^{n} - \sigma_{l} \left(\frac{E_{z} \Big|_{l}^{n-1/2} + E_{z} \Big|_{l}^{n+1/2}}{2} \right) \right]$$

$$\left\| H_{y} \right\|_{l+1/2}^{n+1} = H_{y} \Big|_{l+1/2}^{n} + \frac{\tau}{\mu_{l+1/2}} \left[\frac{E_{z} \Big|_{l+1}^{n+1/2} - E_{z} \Big|_{l}^{n+1/2}}{\Delta} - \sigma_{l+1/2}^{*} \left(\frac{H_{y} \Big|_{l+1/2}^{n+1} + H_{y} \Big|_{l+1/2}^{n}}{2} \right) \right]$$

$$\left| E_z \big|_l^{n+1/2} = E_z \big|_l^{n-1/2} + \frac{\tau}{\varepsilon_l} \left[\frac{H_y \Big|_{l+1/2}^n - H_y \Big|_{l-1/2}^n}{\Delta} - J_{\text{source}_z} \Big|_l^n - \sigma_l \left(\frac{E_z \Big|_l^{n-1/2} + E_z \Big|_l^{n+1/2}}{2} \right) \right] \right|_{l=1/2}^n$$



$$\boxed{ \left(1 + \frac{\sigma_{l+1/2}^* \tau}{2\mu_{l+1/2}} \right) H_y \Big|_{l+1/2}^{n+1} = \left(1 - \frac{\sigma_{l+1/2}^* \tau}{2\mu_{l+1/2}} \right) H_y \Big|_{l+1/2}^{n} + \frac{\tau}{\mu_{l+1/2}} \boxed{ \frac{E_z \Big|_{l+1}^{n+1/2} - E_z \Big|_{l}^{n+1/2}}{\Delta} } \\ \left(1 + \frac{\sigma_l \tau}{2\varepsilon_l} \right) E_z \Big|_{l}^{n+1/2} = \left(1 - \frac{\sigma_l \tau}{2\varepsilon_l} \right) E_z \Big|_{l}^{n-1/2} + \frac{\tau}{\varepsilon_l} \boxed{ \frac{H_y \Big|_{l+1/2}^{n} - H_y \Big|_{l-1/2}^{n}}{\Delta} - J_{\text{source}_z} \Big|_{l}^{n} }$$

$$\begin{split} & \left| H_{y} \right|_{l+1/2}^{n+1} = \left(\frac{1 - \frac{\sigma_{l+1/2}^{*}\tau}{2\mu_{l+1/2}}}{1 + \frac{\sigma_{l+1/2}^{*}\tau}{2\mu_{l+1/2}}} \right) H_{y} \right|_{l+1/2}^{n} + \left(\frac{\frac{\tau}{\mu_{l+1/2}}}{1 + \frac{\sigma_{l+1/2}^{*}\tau}{2\mu_{l+1/2}}} \right) \left[\frac{E_{z} \Big|_{l+1}^{n+1/2} - E_{z} \Big|_{l}^{n+1/2}}{\Delta} \right] \\ & E_{z} \Big|_{l}^{n+1/2} = \left(\frac{1 - \frac{\sigma_{l}\tau}{2\varepsilon_{l}}}{1 + \frac{\sigma_{l}\tau}{2\varepsilon_{l}}} \right) E_{z} \Big|_{l}^{n-1/2} + \left(\frac{\frac{\tau}{\varepsilon_{l}}}{1 + \frac{\sigma_{l}\tau}{2\varepsilon_{l}}} \right) \left[\frac{H_{y} \Big|_{l+1/2}^{n} - H_{y} \Big|_{l-1/2}^{n}}{\Delta} - J_{\text{source}_{z}} \Big|_{l}^{n} \right] \end{split}$$

Update rules

$$H_{y}\Big|_{l+1/2}^{n+1} = A_{l+1/2} H_{y}\Big|_{l+1/2}^{n} + B_{l+1/2} \left[\frac{E_{z}\Big|_{l+1}^{n+1/2} - E_{z}\Big|_{l}^{n+1/2}}{\Delta} \right]$$

$$E_{z}\big|_{l}^{n+1/2} = C_{l} \left. E_{z} \right|_{l}^{n-1/2} + D_{l} \left[\left. \frac{H_{y} \right|_{l+1/2}^{n} - H_{y} \right|_{l-1/2}^{n}}{\Delta} - J_{\mathrm{source}_{z}} \right|_{l}^{n}$$

Update rules

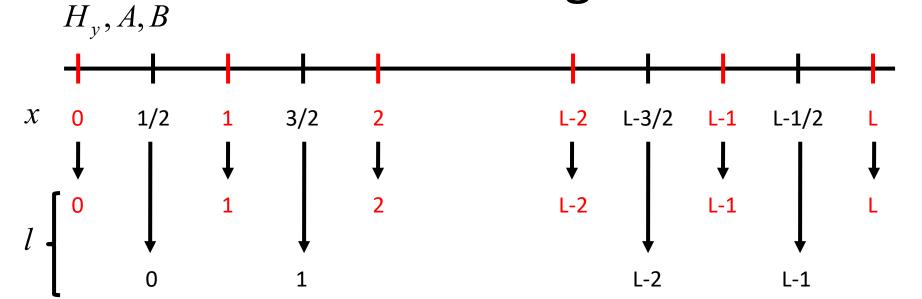
Length of the line: $L\Delta = X$

Boundary conditions: Absorbing boundaries ($\sigma = \sigma^* = 1$)

Source: Pulsed source

Boundary conditions: $E_z = E_L = 0$

Exercise: Yee algorithm E_z, C, D



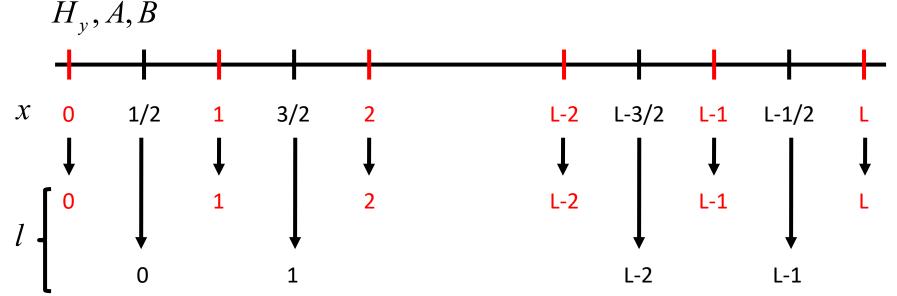
$$E_z: l = 0, \dots, L; x = l\Delta$$

$$H_y: l = 0, ..., L-1; x = (l+1/2)\Delta$$

Initialize:
$$E(0:L) = 0$$
; $C(0:L)$; $D(0:L)$

$$H(0:L-1) = 0;$$
 $A(0:L-1);$ $B(0:L-1)$

E_z , C, D Exercise: Yee algorithm



Iteration:
$$E_l^{n+1/2} = \frac{D_l}{\Delta} (H_{l+1/2}^n - H_{l-1/2}^n) + C_l E_l^{n-1/2} - \delta_{l,l_S} D_{l_S} J(l_S, n\tau)$$

$$H_{l+1/2}^{n+1} = \frac{B_{l+1/2}}{\Lambda} \left(E_{l+1}^{n+1/2} - E_{l}^{n+1/2} \right) + A_{l+1/2} H_{l+1/2}^{n}$$

$$E(1:L-1) = D(1:L-1) * [H(1:L-1) - H(0:L-2)] / \Delta + C(1:L-1) * E(1:L-1)$$

$$E(l_S) = E(l_S) - D(l_S)J(l_S, n\tau)$$

$$H(0:L-1) = B(0:L-1) * [E(1:L) - E(0:L-1)] / \Delta + A(0:L-1) * H(0:L-1)$$
© Kristel Michielsen All Rights Reserved

- Implementation of the Yee algorithm
 - Use one array for the \vec{E} field
 - Use one array for the \vec{H} field
 - Use only one vector for the \vec{E} field and for the \vec{H} field and update their elements!
 - Instead of using four separate arrays for $\varepsilon, \mu, \sigma, \sigma^*$ use four arrays for the coefficients A, B, C, D in the Maxwell equation

Report

Ms. Vrinda MehtaDr. Madita Willschv.mehta@fz-juelich.dem.willsch@fz-juelich.deDr. Fengping JinDr. Dima Nabokf.jin@fz-juelich.ded.nabok@fz-juelich.de

- <u>Filename:</u> Report_6_Surname1_Surname2.pdf, where Surname1 <
 Surname2 (alphabetical order). Example: Report_6_Jin_Willsch.pdf
 (Do not use "umlauts" or any other special characters in the names)
- Content of the report:
 - Names + matricle numbers + e-mail addresses + title
 - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
 - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
 - Simulation results: show figures (use grids, with figure captions!)
 depicting the simulation results. Give a brief description of the results (write in complete sentences)
 - Discussion: summarize your findings
 - Appendix: Include the listing of the program

Due date: 10 AM, June 19, 2023