Computational Physics – Lecture 12:
How to solve Maxwell's equations numerically? II

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- Example: Continuum model and Yee grid in 1D
- Boundary conditions
  - Reflecting boundaries
  - Absorbing boundaries
  - Perfectly matched layer (PML) boundaries
- Maxwell equations in matrix formulation

Yee algorithm

- The Yee algorithm simultaneously simulates the point wise differential form and the macroscopic integral form
- Attributes of the lattice:
  - The finite-difference expressions for the space derivatives in the curl operators are central-difference in nature and second-order accurate
  - Continuity of tangential $\vec{E}$ and $\vec{H}$ is naturally maintained across an interface of two different materials if the interface is parallel to one of the lattice coordinate axes. For this case, there is no need to specially enforce field boundary conditions at the interface. The material permittivity and permeability are specified at each field component location (staircase approximation of the material structure with a space resolution set by the size of the lattice unit cell).
  - The Yee mesh is divergence-free with respect to its $\vec{E}$ and $\vec{H}$ fields in the absence of free electric and magnetic charge.

Yee algorithm: Divergence-free nature

- It is crucial for any grid-based solution of Maxwell’s curl equations to implicitly enforce the Gauss’ law relations for the electric and magnetic fields, which require the absence of free electric and magnetic charge in the source-free space being modeled
- Demonstration that the Yee space lattice and algorithm satisfy Gauss’ law relations for each cell in the lattice

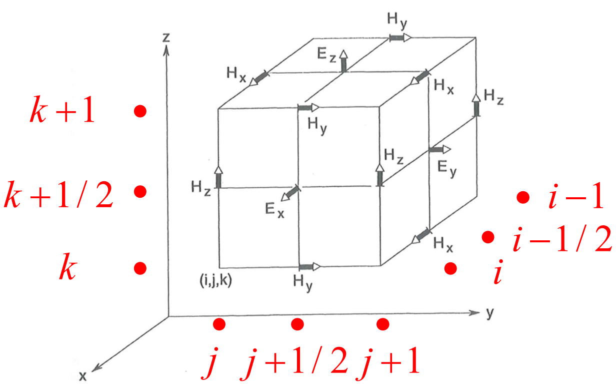
Yee algorithm: Divergence-free nature

- Assume lossless free space with no electric or magnetic current sources
- Consider the time derivative of the total electric flux over the surface of a single Yee cell

$$\frac{\partial}{\partial t}\oiint_{\text{Yee cell}} \vec{D}\cdot d\vec{s} = \underbrace{\varepsilon_0 \frac{\partial}{\partial t}\left(E_x\big|_{i,j+1/2,k+1/2} - E_x\big|_{i-1,j+1/2,k+1/2} \right)\Delta y \Delta z}_{\text{Term 1}}$$

$$+\underbrace{\varepsilon_0 \frac{\partial}{\partial t}\left(E_y\big|_{i-1/2,j+1,k+1/2} - E_y\big|_{i-1/2,j,k+1/2} \right)\Delta x \Delta z}_{\text{Term 2}}$$

$$+\underbrace{\varepsilon_0 \frac{\partial}{\partial t}\left(E_z\big|_{i-1/2,j+1/2,k+1} - E_z\big|_{i-1/2,j+1/2,k} \right)\Delta x \Delta y}_{\text{Term 3}}$$



Yee algorithm: Divergence-free nature

$$\text{Term 1} = \left(\frac{H_z\big|_{i,j+1,k+1/2} - H_z\big|_{i,j,k+1/2}}{\Delta y} - \frac{H_y\big|_{i,j+1/2,k+1} - H_y\big|_{i,j+1/2,k}}{\Delta z} \right)$$

$$- \left(\frac{H_z\big|_{i-1,j+1,k+1/2} - H_z\big|_{i-1,j,k+1/2}}{\Delta y} - \frac{H_y\big|_{i-1,j+1/2,k+1} - H_y\big|_{i-1,j+1/2,k}}{\Delta z} \right)$$

$$\times \Delta y \Delta z$$

$$\text{Term 2} = \left(\frac{H_x\big|_{i-1/2,j+1,k+1} - H_x\big|_{i-1/2,j+1,k}}{\Delta z} - \frac{H_z\big|_{i,j+1,k+1/2} - H_z\big|_{i-1,j+1,k+1/2}}{\Delta x} \right)$$

$$- \left(\frac{H_x\big|_{i-1/2,j,k+1} - H_x\big|_{i-1/2,j,k}}{\Delta z} - \frac{H_z\big|_{i,j,k+1/2} - H_z\big|_{i-1,j,k+1/2}}{\Delta x} \right)$$

$$\times \Delta x \Delta z$$

$$\text{Term 3} = \left(\frac{H_y\big|_{i,j+1/2,k+1} - H_y\big|_{i-1,j+1/2,k+1}}{\Delta x} - \frac{H_x\big|_{i-1/2,j+1,k+1} - H_x\big|_{i-1/2,j,k+1}}{\Delta y} \right)$$

$$\times \Delta x \Delta y$$

$$- \left(\frac{H_y\big|_{i,j+1/2,k} - H_y\big|_{i-1,j+1/2,k}}{\Delta x} - \frac{H_x\big|_{i-1/2,j+1,k} - H_x\big|_{i-1/2,j,k}}{\Delta y} \right)$$

Yee algorithm: Divergence-free nature

$$\text{Term 1} = \left(H_z\big|_{i,j+1,k+1/2} - H_z\big|_{i,j,k+1/2} - H_z\big|_{i-1,j+1,k+1/2} + H_z\big|_{i-1,j,k+1/2} \right) \Delta z$$

$$- \left(H_y\big|_{i,j+1/2,k+1} - H_y\big|_{i,j+1/2,k} - H_y\big|_{i-1,j+1/2,k+1} + H_y\big|_{i-1,j+1/2,k} \right) \Delta y$$

$$+ \quad \text{Term 2} = \left(H_x\big|_{i-1/2,j+1,k+1} - H_x\big|_{i-1/2,j+1,k} - H_x\big|_{i-1/2,j,k+1} + H_x\big|_{i-1/2,j,k} \right) \Delta x$$

$$- \left(H_z\big|_{i,j+1,k+1/2} - H_z\big|_{i-1,j+1,k+1/2} - H_z\big|_{i,j,k+1/2} + H_z\big|_{i-1,j,k+1/2} \right) \Delta z$$

$$+ \quad \text{Term 3} = \left(H_y\big|_{i,j+1/2,k+1} - H_y\big|_{i-1,j+1/2,k+1} - H_y\big|_{i,j+1/2,k} + H_y\big|_{i-1,j+1/2,k} \right) \Delta y$$

$$- \left(H_x\big|_{i-1/2,j+1,k+1} - H_x\big|_{i-1/2,j,k+1} - H_x\big|_{i-1/2,j+1,k} + H_x\big|_{i-1/2,j,k} \right) \Delta x$$

$= 0$ for all time-steps

Yee algorithm: Divergence-free nature

- Assuming zero-field initial conditions, the constant zero value of the time derivative of the net electric flux leaving the Yee cell means the flux never departs from zero:

$$\oiint_{\text{Yee cell}} \vec{D}(t) \cdot d\vec{s} = \frac{\partial}{\partial t} \oiint_{\text{Yee cell}} \vec{D}(t=0) \cdot d\vec{s} = 0$$

→ The Yee cell satisfies Gauss' law for the $\vec{E}$ field in charge-free space.

→ The Yee algorithm is divergence-free with respect to its $\vec{E}$ field computations

Similar proof for the $\vec{H}$ field

Yee algorithm

- Attributes of the time stepping:
  - Leapfrog time-stepping is fully explicit
    → avoids problems involved with simultaneous equations and matrix inversion
  - The finite-difference expressions for the time derivatives are central-difference in nature and second-order accurate
  - Nondissipative: Numerical wave modes propagating in the mesh do not spuriously decay due to a nonphysical artifact of the time-stepping algorithm

Yee algorithm

- Upper bound for stable operation of the algorithm (from numerical stability analysis by means of complex-frequency analysis)

$$\boxed{S \equiv \frac{c\tau}{|\Delta r|} \leq 1}$$

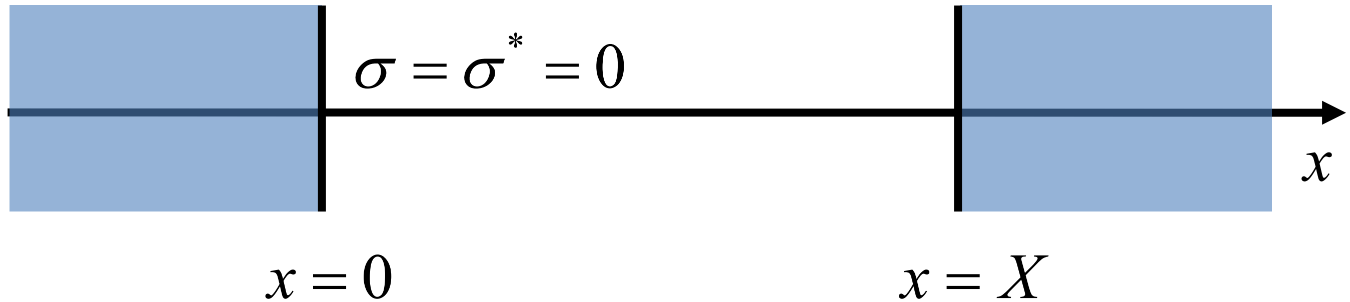
S : Numerical stability factor or Courant number

c : Velocity of light in free space

$$|\Delta r| = 1 / \sqrt{(1/\Delta x)^2 + (1/\Delta y)^2 + (1/\Delta z)^2}$$

Example: Continuum model

$$\varepsilon = \mu = 1 \Rightarrow c = 1/\sqrt{\varepsilon\mu} = 1$$



Electromagnetic standing waves in a cavity with size X at equilibrium with its surroundings must satisfy:

$$\boxed{\frac{\partial H_y(x,t)}{\partial t} = \frac{\partial E_z(x,t)}{\partial x}; \frac{\partial E_z(x,t)}{\partial t} = \frac{\partial H_y(x,t)}{\partial x}; E_z(x=0,t) = E_z(x=X,t) = 0}$$

Boundary conditions: $E_z = 0$

The boundary conditions can be met by a solution of the form:

$$E_z(x,t) = A_k \sin\omega_k t \sin\frac{\pi k x}{X}\ ; k = 1, 2, 3, \ldots$$

Make use of the Maxwell equations and prove that:

$$H_y(x,t) = -A_k \cos\omega_k t \cos\frac{\pi k x}{X}\ ; k = 1, 2, 3, \ldots$$

and

$$\omega_k^2 = \left(\frac{k\pi}{X}\right)^2 \Rightarrow \omega_k = \pm\frac{k\pi}{X}$$

We choose $\omega_k = \dfrac{\pi k}{X}$ (the minus sign can be absorbed in A_k)

The boundary conditions can also be met by a solution of the form:

$$E_z(x,t) = B_k \cos\omega_k t \sin\frac{\pi k x}{X}\;;\; k = 1, 2, 3, \ldots$$

Make use of the Maxwell equations and prove that:

$$H_y(x,t) = B_k \sin\omega_k t \cos\frac{\pi k x}{X}\;;\; k = 1, 2, 3, \ldots$$

General solution:

$$\boxed{\begin{aligned} E_z(x,t) &= \sum_{k=1}^{\infty}\left(A_k \sin\omega_k t + B_k \cos\omega_k t\right)\sin\frac{\pi k x}{X} \\ H_y(x,t) &= \sum_{k=1}^{\infty}\left(-A_k \cos\omega_k t + B_k \sin\omega_k t\right)\cos\frac{\pi k x}{X} \end{aligned}}$$

and

$$\omega_k = \frac{\pi k}{X}$$

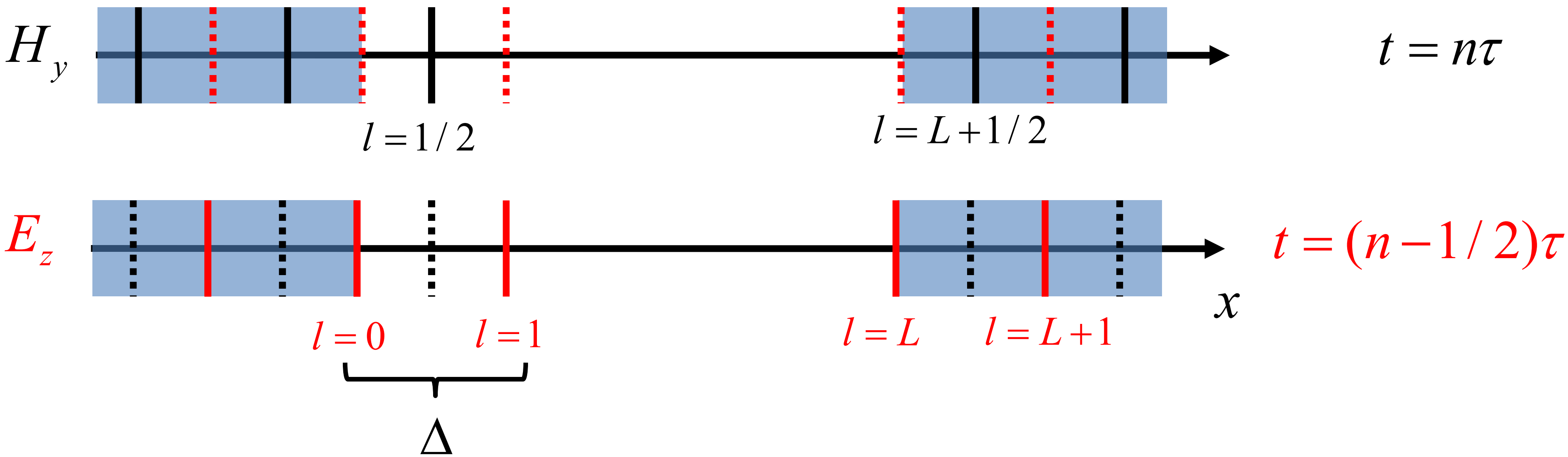
Linear dispersion, discrete modes

→ Not all frequencies are allowed in the cavity

Example: Yee grid

$$\varepsilon = \mu = 1 \Rightarrow c = 1/\sqrt{\varepsilon\mu} = 1$$

$$\sigma = \sigma^* = 0$$



Size of the cavity: $L\Delta = X$

Boundary conditions: $E_0(t) = E_L(t) = 0$ for all t

The electromagnetic standing waves in a cavity with size X at equilibrium with its surroundings must satisfy:

$$\boxed{\begin{aligned} &\frac{E_l^{n+1/2} - E_l^{n-1/2}}{\tau} = \frac{1}{\Delta}\left(H_{l+1/2}^{n} - H_{l-1/2}^{n}\right) \\ &\frac{H_{l+1/2}^{n+1} - H_{l+1/2}^{n}}{\tau} = \frac{1}{\Delta}\left(E_{l+1}^{n+1/2} - E_l^{n+1/2}\right) \\ &E_0^n = E_L^n = 0 \end{aligned}}$$

The boundary conditions can be met by a solution of the form:

$$E_l^n = A_k \sin \omega_k n\tau \sin \frac{\pi k l}{L}\,;\, k = 1, 2, 3, \ldots$$

$$H_l^n = B_k \cos \omega_k n\tau \cos \frac{\pi k l}{L}\,;\, k = 1, 2, 3, \ldots$$

Make use of the Maxwell equations and prove that:

$$B_k = -A_k$$

and

$$\boxed{\omega_k = \frac{2}{\tau}\arcsin\left(\frac{\tau}{\Delta}\sin\frac{\pi k}{2L}\right)}$$

Show that

$$E_l^n = C_k \cos\omega_k n\tau \sin\frac{\pi k l}{L}\ ;\ k = 1,2,3,\ldots$$

$$H_l^n = C_k \sin\omega_k n\tau \cos\frac{\pi k l}{L}\ ;\ k = 1,2,3,\ldots$$

are also solutions so that the general solution can be written as:

$$\boxed{\begin{aligned} E_l^n &= \sum_{k=1}^{L}\left(A_k \sin\omega_k n\tau + C_k \cos\omega_k n\tau\right)\sin\frac{\pi k l}{L} \\ H_l^n &= \sum_{k=1}^{L}\left(-A_k \cos\omega_k n\tau + C_k \sin\omega_k n\tau\right)\cos\frac{\pi k l}{L} \end{aligned}}$$

Number of solutions is finite!

Dispersion relation (numerical, on the lattice):

$$\boxed{\omega_k = \frac{2}{\tau}\arcsin\left(\frac{\tau}{\Delta}\sin\frac{\pi k}{2L}\right)}$$

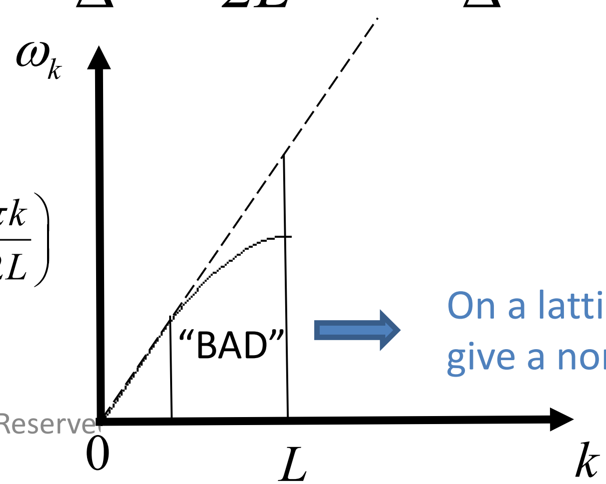
Requirement: $\frac{\tau}{\Delta} \leq 1 \Rightarrow$ Courant number $(c = 1)$

Continuum limit:

$$\lim_{\tau\to 0}\omega_k = \frac{2}{\tau}\frac{\tau}{\Delta}\sin\frac{\pi k}{2L} = \frac{2}{\Delta}\sin\frac{\pi k}{2L}$$

$$\lim_{\Delta\to 0}\lim_{\tau\to 0}\omega_k = \lim_{\Delta\to 0}\frac{2}{\Delta}\sin\frac{\pi k}{2L} = \lim_{\Delta\to 0}\frac{2}{\Delta}\sin\frac{\pi k\Delta}{2X} = \frac{2}{\Delta}\frac{\pi k\Delta}{2X} = \frac{\pi k}{X}$$

$$\omega_k = \frac{2}{\tau}\arcsin\left(\frac{\tau}{\Delta}\sin\frac{\pi k}{2L}\right)$$



Same result as in continuum model → numerical dispersion can approach ideal dispersion for sufficiently fine gridding

On a lattice with finite Δ : large k-modes give a nonlinear dispersion

Boundary conditions

- Reflecting boundaries:
  - Perfect Electrical Conductor (PEC): assume that the electric field is zero at the boundary (zero thickness wall)
    → perfect reflection for the E field
  - Perfect Magnetic Conductor (PMC): assume that the magnetic field is zero at the boundary (zero thickness wall)
    → perfect reflection for the H field

Boundary conditions

- Absorbing boundaries: A lossy medium ($\sigma \neq 0, \sigma^* \neq 0$) of finite thickness L_B physically absorbs the incident numerical wave
  - The parameters σ, σ^*, L_B are difficult to adjust for the smallest reflection
  - Optimal parameters for each problem

Boundary conditions

- Uniaxial Perfectly Matched Layer (UPML) boundaries: Artificial absorbing boundaries
  - For a PML designed to absorb waves propagating in the x direction, the derivative $\partial / \partial x$ in the wave equation is replaced by
    $\frac{\partial}{\partial x} \rightarrow \frac{1}{1+\frac{i\sigma(x)}{\omega}} \frac{\partial}{\partial x}$, where ω is the angular frequency.
    If σ is positive, then propagating waves are attenuated
    $e^{i(kx-\omega t)} \rightarrow e^{i(kx-\omega t)-\frac{k}{\omega}\int^{x} \sigma(x')dx'}$

Boundary conditions

– Perfectly matched layers are only reflectionless for the exact wave equation → discretization for simulation introduces small numerical reflections

Maxwell equations in matrix formulation

Maxwell equation in 1D

Consider

$$\boxed{\begin{aligned}\frac{\partial H_y(x,t)}{\partial t} &= \frac{1}{\mu}\left[\frac{\partial E_z(x,t)}{\partial x} - M_y(x,t)\right] \\ \frac{\partial E_z(x,t)}{\partial t} &= \frac{1}{\varepsilon}\left[\frac{\partial H_y(x,t)}{\partial x} - J_z(x,t)\right]\end{aligned}}$$

$$\Downarrow \quad \varepsilon = \mu = 1\,;\, \sigma = \sigma^* = 0\,;\, M_{\text{source}_y} = 0$$

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

Maxwell equation in 1D

In matrix form:

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

$$\Downarrow$$

$$\boxed{\frac{\partial}{\partial t}\Psi(t) = \mathsf{L}\,\Psi(t) - \cancel{S(t)}}$$

$$\boxed{\frac{\partial}{\partial t}\Psi(t) = \mathrm{L}\,\Psi(t)}$$

General structure of basic equations in physics:

- Time-dependent Maxwell equation
- Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = H\Psi(t)$$

- Diffusion equation:

$$\frac{\partial}{\partial t}\Psi(t) = D\frac{\partial^2}{\partial x^2}\Psi(t) = \mathrm{L}\,\Psi(t)$$

- Dirac equation
- Elastic wave equations, wave equation for sound, …
- Newton equation of motion: $\Psi = (x, p)$, L Liouville operator → Molecular dynamics methods

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

How to solve numerically?

- Discretize time and space $\Rightarrow$ Yee algorithm
- Discretize the exact formal solution
  Design algorithms with specific properties

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

How to solve numerically?

- In case of variables y and numbers k :

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

- In case of vectors Ψ and matrices L :

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

matrix exponential

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

How to solve numerically?

- In case of numbers k:

$$e^{tk} = \sum_{n=0}^{\infty} \frac{t^n}{n!} k^n$$

- In case of matrices L:

$$e^{t\mathsf{L}} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathsf{L}^n$$

THE SAME

n-th power of a matrix

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

How to solve numerically?

- How NOT to calculate the matrix exponential: truncated Taylor series

$$e^{tL} \approx 1 + tL + \frac{1}{2}(tL)^2 + \frac{1}{3!}(tL)^3 + \ldots + \frac{1}{n!}(tL)^n$$

  – Numerically unstable (also in the case of numbers)

- How to calculate the matrix exponential: Exploit the properties of the matrix L

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

How to solve numerically?

- Exploit the properties of the matrix L
  - The matrix is diagonal

$$\exp\begin{pmatrix} a_1 & & 0 \\ & \ddots & \\ 0 & & a_k \end{pmatrix} = \begin{pmatrix} e^{a_1} & & 0 \\ & \ddots & \\ 0 & & e^{a_k} \end{pmatrix}$$

  - The matrix is block diagonal, e.g. 2x2 blocks

$$\exp\begin{pmatrix} \mathsf{L}_1 & & 0 \\ & \ddots & \\ 0 & & \mathsf{L}_k \end{pmatrix} = \begin{pmatrix} e^{\mathsf{L}_1} & & 0 \\ & \ddots & \\ 0 & & e^{\mathsf{L}_k} \end{pmatrix}$$

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

How to solve numerically?

- Problem: L is usually a large matrix
  - 1D: L is 4000 x 4000 matrix ← NOT BIG
  - 2D: L is (4000 x 4000) x (4000 x 4000) matrix (256×10^{12} numbers) ← BIG
  - 3D ← VERY BIG

  → A clever way to handle L is needed
- Keeping L in memory → useless method for practical applications

How to compute $e^{t\mathsf{L}}$ if L is not stored in memory?

- We are only interested in $e^{t\mathsf{L}}\Phi$ for any Φ
- Can we calculate $e^{t\mathsf{L}}\Phi$ economically, i.e. # operations is of the order of the size of Φ ?

How to deal with the matrix exponential?

- L is a large non-trivial matrix → in general no practical algorithm to compute $e^{t\mathsf{L}}$ directly
- But for instance $\mathsf{L} = \mathsf{L}_1 + \mathsf{L}_2$ and $e^{t\mathsf{L}_1}, e^{t\mathsf{L}_2}$ can be calculated
  - Can we calculate $e^{t\mathsf{L}}$ if we know how to calculate $e^{t\mathsf{L}_1}$ and $e^{t\mathsf{L}_2}$?
  - Yes, as a controlled approximation → defines a particular algorithm

How to deal with the matrix exponential?

- L is a number: $e^{t\mathsf{L}} = e^{t\mathsf{L}_1} e^{t\mathsf{L}_2}$
- L is a matrix: $e^{t\mathsf{L}} \neq e^{t\mathsf{L}_1} e^{t\mathsf{L}_2}$
  because

$$e^{t\mathsf{L}} = 1 + t\mathsf{L} + \frac{t^2}{2}\mathsf{L}^2 + \frac{t^3}{3!}\mathsf{L}^3 + \ldots$$

$$= 1 + t\left(\mathsf{L}_1 + \mathsf{L}_2\right) + \frac{t^2}{2}\left(\mathsf{L}_1 + \mathsf{L}_2\right)\left(\mathsf{L}_1 + \mathsf{L}_2\right) + \ldots$$

$$= 1 + t\left(\mathsf{L}_1 + \mathsf{L}_2\right) + \frac{t^2}{2}\left(\mathsf{L}_1^2 + \mathsf{L}_2^2 + \mathsf{L}_1\mathsf{L}_2 + \mathsf{L}_2\mathsf{L}_1\right) + \ldots$$

Matrices do not commute: $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

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

How to deal with the matrix exponential?

and

$$e^{t\mathsf{L}_1}e^{t\mathsf{L}_2} = \left(1 + t\mathsf{L}_1 + \frac{t^2}{2}\mathsf{L}_1^2 + \frac{t^3}{3!}\mathsf{L}_1^3 + \ldots\right)\left(1 + t\mathsf{L}_2 + \frac{t^2}{2}\mathsf{L}_2^2 + \frac{t^3}{3!}\mathsf{L}_2^3 + \ldots\right)$$

$$= \underline{1 + t\left(\mathsf{L}_1 + \mathsf{L}_2\right) + \frac{t^2}{2}\left(\mathsf{L}_1^2 + \mathsf{L}_2^2\right.} + \underbrace{2\mathsf{L}_1\mathsf{L}_2}_{\underline{L_1L_2 + L_2L_1} - L_2L_1 + L_1L_2}\left.\vphantom{\mathsf{L}_1^2}\right) + \ldots$$

$$= \underline{e^{t\mathsf{L}}} + \frac{t^2}{2}\left[\mathsf{L}_1, \mathsf{L}_2\right] + O(t^3)$$

Hence,

$$\boxed{e^{t\mathsf{L}_1}e^{t\mathsf{L}_2} - e^{t\mathsf{L}} = \frac{t^2}{2}\left[\mathsf{L}_1, \mathsf{L}_2\right] + O(t^3)}$$

Energy

From the definition

$$\Psi(t) = \left(E_z(x,t) \quad H_y(x,t) \right)^T$$

it follows that

$$\left\langle \vec{F} \middle| \vec{G} \right\rangle = \int_V \vec{F} \cdot \vec{G}\, dr$$

$$\left\| \Psi(t) \right\|^2 = \left\langle \Psi(t) \middle| \Psi(t) \right\rangle = \int \left[E_z^2(x,t) + H_y^2(x,t) \right] dx$$

relating the length (norm) of the vector $\Psi(t)$

to the energy density

$$W(x,t) = \frac{1}{2}\varepsilon E_z^2(x,t) + \frac{1}{2}\mu H_y^2(x,t) \qquad (\varepsilon = \mu = 1)$$

of the electromagnetic fields

Stability

From the definition

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

it follows that

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

$\int u\, \mathrm{d}v = uv - \int v\, \mathrm{d}u$

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

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

$$= -\left\langle \mathsf{L}\,\Psi(t) \middle| \Psi(t) \right\rangle$$

Stability

Hence,

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

and

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

so that

$$\boxed{\mathsf{L}^T = -\mathsf{L}}$$

→ L is skew-symmetric

Stability

The time-evolution operator $e^{t\mathsf{L}}$ is a unitary matrix ($A^{-1} = A^T$):

$$\left(e^{t\mathsf{L}}\right)^{-1} = e^{-t\mathsf{L}} = e^{t\mathsf{L}^T} = \left(e^{t\mathsf{L}}\right)^T$$

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 $\|\Psi\|$ unchanged.

→ The energy density of the EM fields does not change with time

Stability

Hence,

$$\|\Psi(t)\| = \underbrace{\left\|e^{t\mathsf{L}}\Psi(0)\right\|}_{\text{norm vector}} \le \underbrace{\left\|e^{t\mathsf{L}}\right\|}_{\text{n. matrix}}\underbrace{\|\Psi(0)\|}_{\text{n. vector}} \qquad \|AX\| \le \|A\|\|X\|$$

$$\boxed{\|\Psi(t)\| \le \|\Psi(0)\|}$$ STABILITY (requirement: $\left\|e^{t\mathsf{L}}\right\| \le 1$ for all t)

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

Next lecture

- 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