Finite-Difference Time-Domain and Beam Propagation Methods for Maxwell's Equations

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What´s The Good Of This Course?

Numerical analysis has become easy, however:

- Blind trust in numerical data is dangerous.
- Some basic understanding of the algorithm is necessary.
- Often one operates at the limits of resources.
- So when are data reliable?

A Selection of topics is discussed:

- Basics of the FDTD algorithm
- Some properties of the BPM
- The hands-on exercises demonstrate practical issues.
- Not all material from this course will be orally presented.

In the context of photonic crystals, FDTD is of most interest, but the beam propagation method plays an important role in designing feeder waveguides, and in computing modes and propagation constants in such waveguides.

Outline

- Finite-difference time-domain (FDTD) method

  Maxwell's equations, PDE classes, plane waves, sampling
  Yee's leapfrog algorithm
  Numerical dispersion, stability, accuracy and examples
  Boundary conditions: PML, symmetries, periodicity
  Dispersive and nonlinear media

- Beam propagation method (BPM)

  Scalar Helmholtz equation
  Split-step algorithm
  Boundary conditions: Dirichlet, TBC, ABC, PML
  BPM mode solving: Imaginary distance, correlation
  Full-vectorial and semi-vectorial BPM
  Wide-angle and bi-directional BPM

- Further reading

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Maxwell´s Fundamental Equations

Ampere's law: $\text{curl}\,\vec{H} = \frac{\partial \vec{D}}{\partial t}$, Faraday's law: $\text{curl}\,\vec{E} = -\frac{\partial \vec{B}}{\partial t}$

Gauss' law: $\text{div}\,\vec{D} = 0$, $\text{div}\,\vec{B} = 0$

Constitutive: $\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$, $\vec{B} = \mu_0 \vec{H} + \vec{M}$

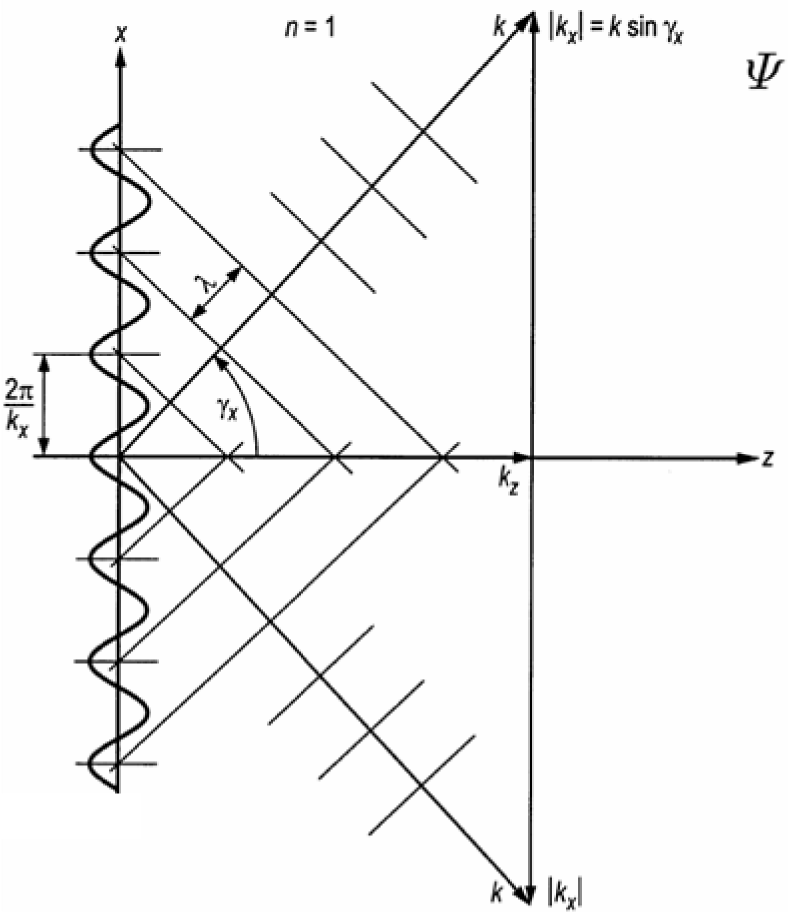
Electromagnetic waves are described by:

- magnetic and electric field vectors $\vec{H}$ and $\vec{E}$,
- electric displacement $\vec{D}$, electric material polarization $\vec{P}$,
- magnetic induction $\vec{B}$, magnetic material polarization $\vec{M}$

At operating frequencies f, the medium has

- no space charges/currents, is isotropic, linear,
- has a dielectric constant $\varepsilon = \varepsilon_0 \varepsilon_r$, polarisation $\vec{P} = \varepsilon_0(\varepsilon_r - 1)\vec{E}$,
- and a magnetic permeability $\mu = \mu_0 \mu_r$, pol. $\vec{M} = \mu_0(\mu_r - 1)\vec{H}$.
- The vacuum speed of light is $c = 1/\sqrt{\varepsilon_0 \mu_0}$, and the
- medium phase velocity is $v = c/n$ (refractive index $n = \pm\sqrt{\mu_r \epsilon_r}$).

Elementary Solution: Plane Waves and Spatial Frequencies



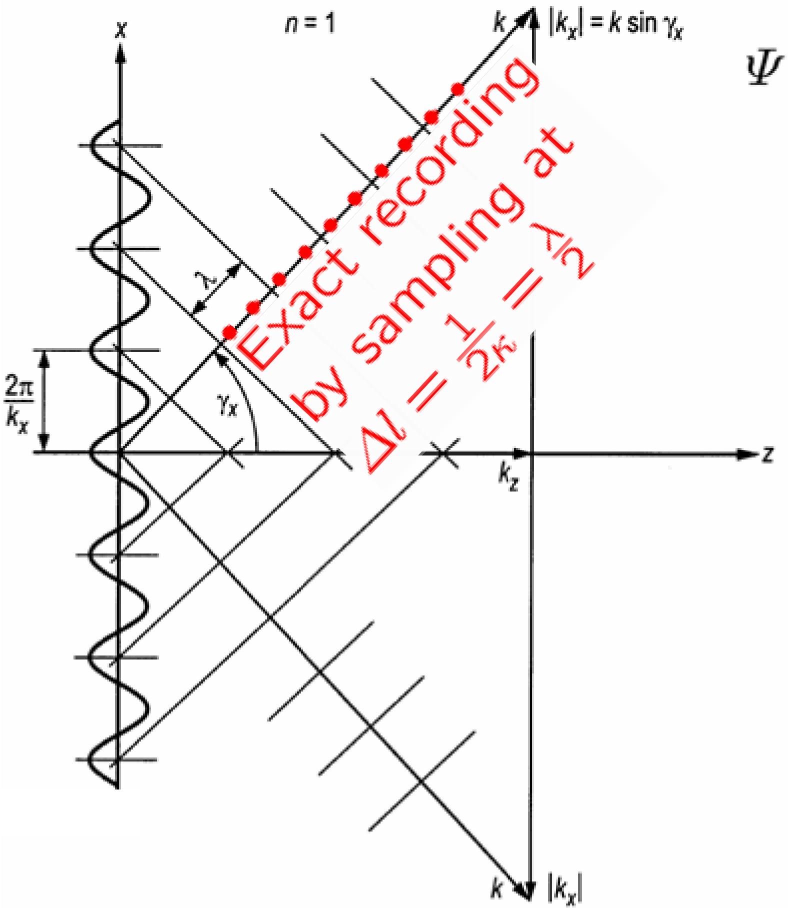
$$\Psi(x,z) = \mathrm{e}^{-\mathrm{j}(|k_x|x + k_z z)} + \mathrm{e}^{-\mathrm{j}(-|k_x|x + k_z z)}$$
$$= 2\cos(k_x x)\,\mathrm{e}^{-\mathrm{j}\,k_z z}$$
$$= 2\cos(2\pi\xi x)\,\mathrm{e}^{-\mathrm{j}\,k_z z}$$

If $k_z = 0$, the maximum spatial frequency for homogeneous plane waves is $\xi = \kappa = \frac{1}{\lambda}$. Can we go farther? Yes, if $\kappa \leq |\xi| < \infty$. But then, no propagation along $z \rightarrow \exp(-|k_z|z)$:

$$\zeta = \pm\sqrt{\kappa^2 - \xi^2} = \pm\mathrm{j}\sqrt{\xi^2 - \kappa^2} \text{ imag.!}$$

$$\Psi(t,\vec{r}) = \tilde{\Psi}(\xi,\eta)\,\mathrm{e}^{\mathrm{j}(\omega t - \vec{k}\cdot\vec{r})}, \qquad k_x = 2\pi\xi = k\sin\gamma_x,$$
$$k = |\vec{k}| = nk_0 = n\frac{\omega}{c} = 2\pi\frac{n}{\lambda} = 2\pi\kappa, \quad k_y = 2\pi\eta = k\sin\gamma_y,$$
$$\vec{k} = 2\pi\vec{\kappa} = k_x\vec{e}_x + k_y\vec{e}_y + k_z\vec{e}_z, \qquad k_z = 2\pi\zeta = \pm 2\pi\sqrt{\kappa^2 - (\xi^2 + \eta^2)}$$

Elementary Solution: Plane Waves and Spatial Sampling



$$\Psi(x,z) = e^{-j(|k_x|x + k_z z)} + e^{-j(-|k_x|x + k_z z)}$$
$$= 2\cos(k_x x)\, e^{-j\, k_z z}$$
$$= 2\cos(2\pi\xi x)\, e^{-j\, k_z z}$$

If $k_z = 0$, the maximum spatial frequency for homogeneous plane waves is $\xi = \kappa = \frac{1}{\lambda}$. Can we go farther? Yes, if $\kappa \le |\xi| < \infty$. But then, no propagation along $z \to \exp(-|k_z|z)$:

$$\zeta = \pm\sqrt{\kappa^2 - \xi^2} = \pm j\sqrt{\xi^2 - \kappa^2} \text{ imag.!}$$

$$\Psi(t, \vec{r}) = \widetilde{\Psi}(\xi, \eta)\, e^{j(\omega t - \vec{k}\cdot\vec{r})}, \qquad k_x = 2\pi\xi = k \sin\gamma_x\,,$$
$$k = |\vec{k}| = n k_0 = n\frac{\omega}{c} = 2\pi\frac{n}{\lambda} = 2\pi\kappa\,, \quad k_y = 2\pi\eta = k\sin\gamma_y\,,$$
$$\vec{k} = 2\pi\vec{\kappa} = k_x\vec{e}_x + k_y\vec{e}_y + k_z\vec{e}_z\,, \qquad k_z = 2\pi\zeta = \pm 2\pi\sqrt{\kappa^2 - (\xi^2 + \eta^2)}$$

Sampling, Nyquist Frequency and Interpolation

Sampling function $a(x)$ is self-reciprocal in Fourier space $\tilde{a}(\xi)$:

$$a(x) = X_a \sum_{n=-\infty}^{+\infty} \delta(x - nX_a) = \sum_{n=-\infty}^{+\infty} \exp\left(-\mathrm{j}\, 2\pi\, n \frac{x}{X_a}\right),$$

$$\tilde{a}(\xi) = \sum_{n=-\infty}^{+\infty} \delta(\xi - n\Xi_a), \qquad \Xi_a = 1/X_a$$

Function $\Psi(x)$ assumed to have bandlimited spatial spectrum:

$$\tilde{\Psi}(\xi) = \int_{-\infty}^{+\infty} \Psi(x) \exp(\mathrm{j}\, 2\pi\, \xi x)\, \mathrm{d}x\,, \qquad \tilde{\Psi}(|\xi| > B_x) = 0$$

$\Psi(x)$ sampled with Nyquist frequency B_x at intervals $X_a = 1/B_x$, discrete *complex* $\Psi_a(x) = \Psi(x)\, a(x)$ at positions $x_n = n/B_x$ result.

Reconstruction of $\Psi(x)$ from complex sampled data $\Psi(n/B_x)$ by filtering with ideal lowpass (transm. 1 in band $|\xi| < B_x/2$, 0 outside), i. e., with interpolation recipe (no *linear* interpolation):

$$\Psi(x) = \sum_{n=-\infty}^{+\infty} \Psi(nX_a) \frac{\sin((x - nX_a)\pi B_x)}{(x - nX_a)\pi B_x}\,, \quad X_a = \frac{1}{B_x}\,, \quad X_{a1} = \frac{1}{2B_x}$$

Oversampling needed for linear interpolation!

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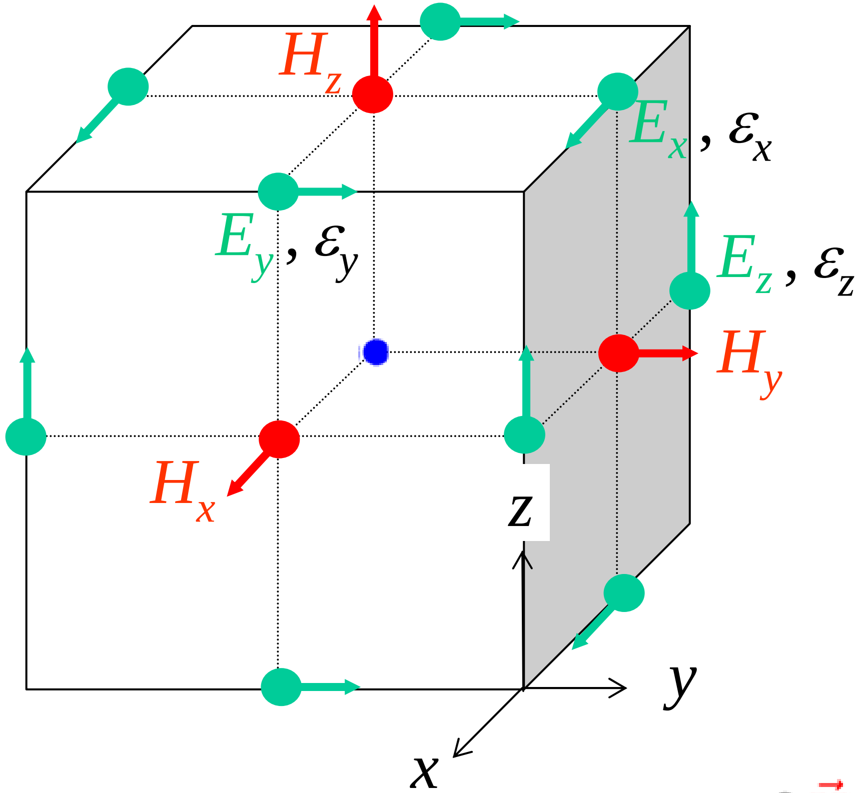
Yee´s Lattice with Cubic Unit Cells of Size $\Delta x \times \Delta y \times \Delta z$

Advantages of Yee algorithm:

- 1st-order DE for $\vec{E}$ *and* $\vec{H}$,
- more robust than 2nd-order wave equation for $\vec{E}$ *or* $\vec{H}$.
- $\vec{E}$ and $\vec{H}$ singularities naturally implemented.



cell centre:
$(i, j, k) \mathrel{\widehat{=}} (i\Delta x, j\Delta y, k\Delta z)$

- Each $\vec{E}$ component surrounded by 4 circulating $\vec{H}$ components
- each $\vec{H}$ component surrounded by 4 circulating $\vec{E}$ components

Faraday: $\text{curl}\,\vec{E} = -\mu \dfrac{\partial \vec{H}}{\partial t}$

Ampere: $\text{curl}\,\vec{H} = \varepsilon \dfrac{\partial \vec{E}}{\partial t}$

Yee, K. S.: Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media. IEEE Trans. Antennas Propag. AP-14 (1966) 302–307

FDTD Names: Kane S. Yee and Allen Taflove

Kane S. Yee received the B.S.E.E., M.S.E.E., and Ph.D. degrees in applied mathematics from the University of California, Berkeley, in 1957, 1958, and 1963, respectively.

From 1959 to 1961, he was employed at Lockheed Missiles and Space Company doing research on high-frequency asymptotic electromagnetic diffractions. From 1964 to 1966, he was employed at Lawrence Livermore National Laboratory to do work on water waves. From 1966 to 1984 he was a Professor of Mathematics and Electrical Engineering at the University of Florida and later at the Kansas State University. He has been a consultant to LLNL since 1966. He rejoined the Lawrence Livermore National Laboratory in 1984. His research areas include electromagnetics, hydrodynamics, and numerical solutions to partial differential equations.

Dr. Yee is the author of the 1966 finite difference time domain electromagnetic numerical algorithm.

IEEE AP February 1988

Allen Taflove (F'90) has been a Professor with the Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL, since 1984. Since 1972, he has pioneered basic theoretical approaches and engineering applications of FDTD computational electrodynamics. In a 1980 IEEE paper, he coined the FDTD acronym. He has authored or coauthored five books, 20 book chapters and papers, over 100 refereed journal papers, and 300 conference papers. He holds 14 U.S. patents. His research interests span much of the electromagnetic spectrum. He and his students model electrodynamic phenomena ranging from geophysically induced ultralow-frequency wave propagation about the entire Earth to the light-scattering behavior of early-stage colon cancer cells. The principle that "Maxwell's equations work from dc to light" and especially for the benefit of human society is demonstrated in his laboratory every day. His publications have resulted in his being included on ISIHighlyCited.com, the Institute of Scientific Information's list of the most-cited researchers worldwide. He has been the adviser or co-advisor of 20 Ph.D. recipients and one post-doctoral fellow, five of whom are now tenured or tenure-track university professors.

Prof. Taflove is currently an elected member of Northwestern's General Faculty Committee. He is also the faculty advisor to the Undergraduate Design Competition, the Honors Program in Undergraduate Research, and the student chapters of Eta Kappa Nu and Tau Beta Pi. His efforts on behalf of students at all levels were recognized by Northwestern in 2000, when he was named a Charles Deering McCormick Professor of Teaching Excellence.

IEEE MTT May 2006

Yee, K. S.: Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media. IEEE Trans. Antennas Propag. AP-14 (1966) 302–307

Taflove, A.; Brodwin, M. E.: Numerical solution of steady-stae electromagnetic scattering problems using the time-dependent Maxwell's equations. IEEE Trans. MTT-23 (1975) 623–620

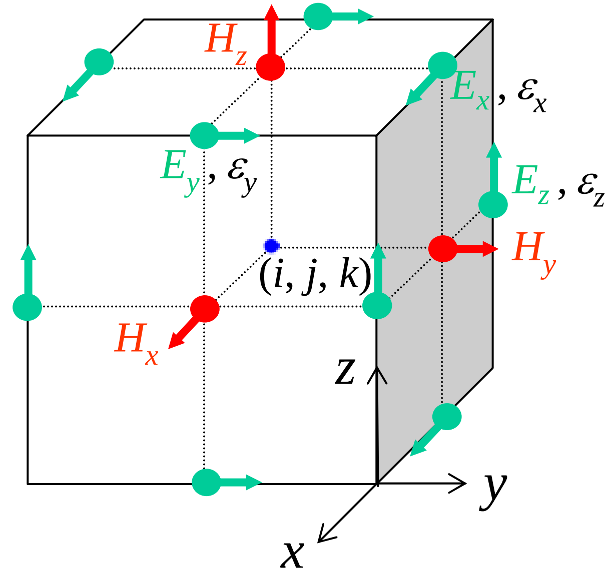
Tafove, A.: Application of the finite-difference time-domain method to sinusoidal steady-stae electromagnetic penetration problems. IEEE Trans. Electromagn. Compatibility 22 (1980) 191–202

Finite Differences in Cartesian Coordinates

Centered finite-differences over $\pm\frac{1}{2}\Delta x$, $\pm\frac{1}{2}\Delta t$

at $t = n\Delta t$, $\vec{r} = i\Delta x\,\vec{e}_x + j\Delta y\,\vec{e}_x + k\Delta z\,\vec{e}_z$

for $u(n\Delta t, i\Delta x, j\Delta y, k\Delta z) = u^n_{i,j,k}$:



$$\frac{\partial u^n_{i,j,k}}{\partial x} = \frac{u^n_{i+1/2,j,k} - u^n_{i-1/2,j,k}}{\Delta x} + \mathcal{O}(\Delta x^2)$$

$$\frac{\partial u^n_{i,j,k}}{\partial t} = \frac{u^{n+1/2}_{i,j,k} - u^{n-1/2}_{i,j,k}}{\Delta t} + \mathcal{O}(\Delta t^2)$$

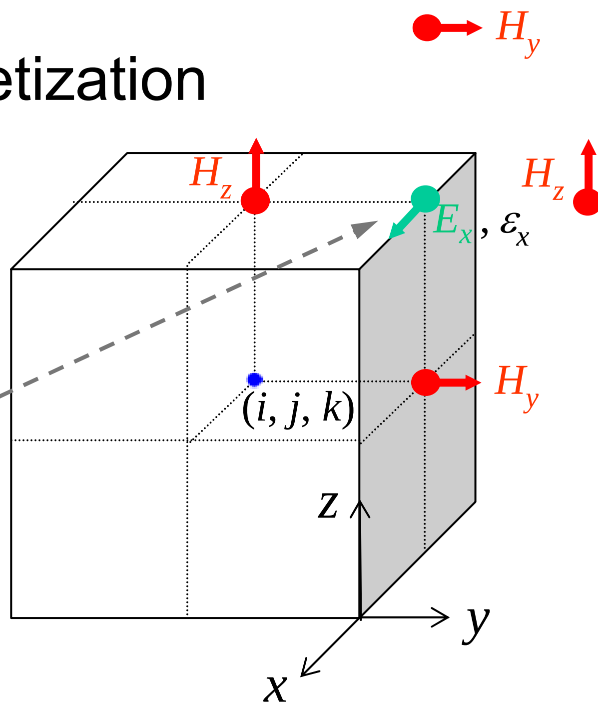
- Second-order accurate central differencing to the right and left of observation point (i, j, k) by $\frac{1}{2}\Delta x$.
- Interleaved $\vec{E}$ and $\vec{H}$ components at intervals $\frac{1}{2}\Delta x$.
- Second-order accurate central differencing to the past and future of observation point n by $\frac{1}{2}\Delta t$.
- Interleaved $\vec{E}$ and $\vec{H}$ components at intervals $\frac{1}{2}\Delta t$.
- This leads to a so-called "leapfrog" algorithm.

Central Differences and Discretization

$$\frac{\partial u^n_{i,j,k}}{\partial x} = \frac{u^n_{i+1/2,j,k} - u^n_{i-1/2,j,k}}{\Delta x} + \mathcal{O}(\Delta x^2)$$

$$\frac{\partial u^n_{i,j,k}}{\partial t} = \frac{u^{n+1/2}_{i,j,k} - u^{n-1/2}_{i,j,k}}{\Delta t} + \mathcal{O}(\Delta t^2)$$

Time-space pt: $(n, i, j+1/2, k+1/2)$



curl $\vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t}$ $\rightarrow$ only x-component:

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon_x}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right)$$

Discretization:

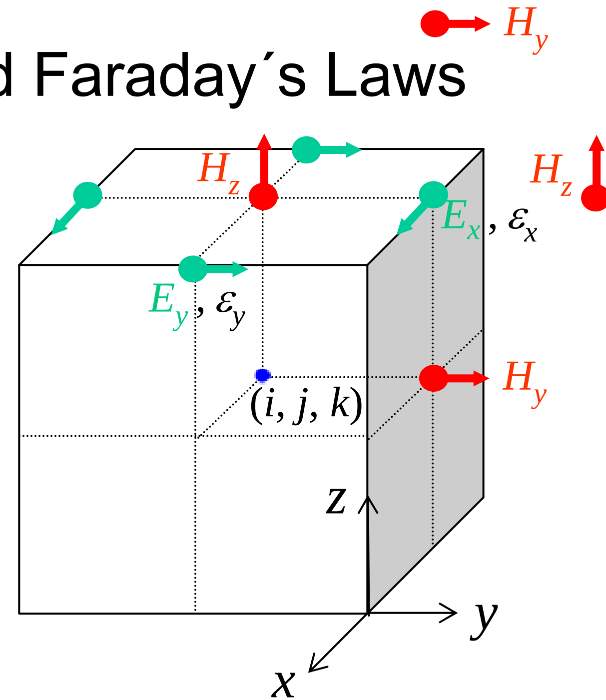
$$\frac{\partial H_y}{\partial z} \approx \frac{H_y|^n_{i,j+1/2,k+1} - H_y|^n_{i,j+1/2,k}}{\Delta z}$$

$$\frac{\partial H_z}{\partial y} \approx \frac{H_z|^n_{i,j,k+1/2} - H_z|^n_{i,j+1,k+1/2}}{\Delta y}$$

$$\frac{\partial E_x}{\partial t} \approx \frac{E_x|^{n+1/2}_{i,j+1/2,k+1/2} - E_x|^{n-1/2}_{i,j+1/2,k+1/2}}{\Delta t}$$

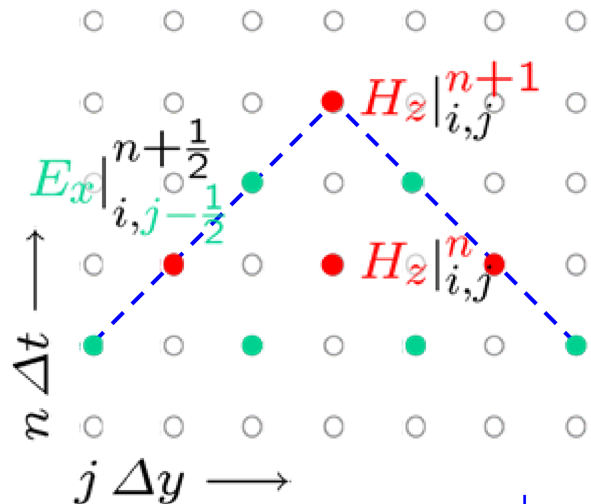
Six Update Equations for Ampere´s and Faraday´s Laws

$$E_x\Big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} = E_x\Big|^{n-\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_{i,j+\frac{1}{2},k+\frac{1}{2}}}\left(\frac{H_z\Big|^{n}_{i,j,k+\frac{1}{2}} - H_z\Big|^{n}_{i,j+1,k+\frac{1}{2}}}{\Delta y} - \frac{H_y\Big|^{n}_{i,j+\frac{1}{2},k+1} - H_y\Big|^{n}_{i,j+\frac{1}{2},k}}{\Delta z}\right)$$



$$\frac{\partial H_z}{\partial t} = -\frac{1}{\mu_z}\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)$$

$$H_z\Big|^{n+1}_{i,j,k+\frac{1}{2}} = H_z\Big|^{n}_{i,j,k+\frac{1}{2}} - \frac{\Delta t}{\mu_{i,j,k+\frac{1}{2}}}\left(\frac{E_y\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k+\frac{1}{2}} - E_y\Big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j,k+\frac{1}{2}}}{\Delta x} - \frac{E_x\Big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} - E_x\Big|^{n+\frac{1}{2}}_{i,j-\frac{1}{2},k+\frac{1}{2}}}{\Delta y}\right)$$



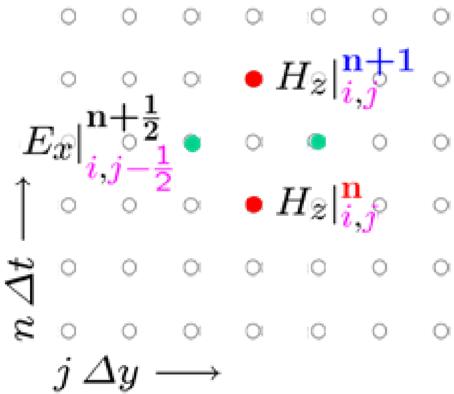
Why Leapfrog?

Leapfrog A game in which players in turn vault with parted legs over others who are bending down.

(New Oxford Dictionary of English. Oxford Univ. Press, New York 1998)

$$H_z\big|_{i,j,k+1/2}^{\mathbf{n+1}} = H_z\big|_{i,j,k+1/2}^{\mathbf{n}} - \frac{\Delta t}{\mu_{i,j,k+1/2}}\left(\frac{E_y\big|_{i+1/2,j,k+1/2}^{\mathbf{n+1/2}} - E_y\big|_{i-1/2,j,k+1/2}^{\mathbf{n+1/2}}}{\Delta x} - \frac{E_x\big|_{i,j+1/2,k+1/2}^{\mathbf{n+1/2}} - E_x\big|_{i,j-1/2,k+1/2}^{\mathbf{n+1/2}}}{\Delta y}\right)$$

Arrive at time $\mathbf{n}+1$



Start at time $\mathbf{n}$

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Numerical Dispersion

Maxwell's equations, homogeneous lossless space, parameters $\epsilon = \epsilon_0 \epsilon_r$, $\mu = \mu_0 \mu_r$, $n^2 = \epsilon_r \mu_r$, $c^2 = 1/(\epsilon_0 \mu_0)$, $Z = \sqrt{\mu/\epsilon}$:

$$\mathrm{j}\,\mathrm{curl}\left(\sqrt{\frac{\mu}{\epsilon}}\,\vec{H}\right) = \mathrm{j}\sqrt{\epsilon\mu}\,\frac{\partial}{\partial t}\left(\vec{E}\right), \qquad -\mathrm{curl}\left(\vec{E}\right) = \sqrt{\epsilon\mu}\,\frac{\partial}{\partial t}\left(\sqrt{\frac{\mu}{\epsilon}}\,\vec{H}\right)$$

In compact form, and with $\vec{V} = Z\,\vec{H} + \mathrm{j}\,\vec{E}$:

$$\mathrm{j}\,\mathrm{curl}\left(Z\,\vec{H} + \mathrm{j}\,\vec{E}\right) = \frac{n}{c}\frac{\partial}{\partial t}\left(Z\,\vec{H} + \mathrm{j}\,\vec{E}\right), \qquad \mathrm{j}\,\mathrm{curl}\,\vec{V} = \frac{n}{c}\frac{\partial \vec{V}}{\partial t}$$

Plane wave $\vec{V}(t, \vec{r}\,) = \vec{V}_0 \exp\left[\mathrm{j}\left(\omega_0 t - \vec{k}\cdot\vec{r}\,\right)\right]$ with $|\vec{k}|^2 = (n\omega_0/c)^2$, sampled in time $t = n\Delta t$ and space $\vec{r} = i\,\Delta x\,\vec{e}_x + j\,\Delta y\,\vec{e}_y + k\,\Delta z\,\vec{e}_z$. Differential operator scheme:

$$\frac{\partial \vec{V}^{n}_{i,j,k}}{\partial t} = \frac{\vec{V}^{n+\frac{1}{2}}_{i,j,k} - \vec{V}^{n-\frac{1}{2}}_{i,j,k}}{\Delta t} = \frac{\mathrm{e}^{\mathrm{j}\,\omega_0 \frac{\Delta t}{2}} - \mathrm{e}^{-\mathrm{j}\,\omega_0 \frac{\Delta t}{2}}}{\Delta t}\vec{V}^{n}_{i,j,k} = \mathrm{j}\,\omega_0 \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}}\vec{V}^{n}_{i,j,k}$$

Numerical Dispersion

Plane wave $\vec{V}(t,\vec{r}) = \vec{V}_0 \exp\left[\mathrm{j}\left(\omega_0 t - \vec{k}\cdot\vec{r}\right)\right]$ with $|\vec{k}|^2 = (n\omega_0/c)^2$.

Numerical differential operators $(q = x, y, z)$:

$$\partial_t \vec{V}^n_{i,j,k} = \mathrm{j}\,\omega_0 \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}} \vec{V}^n_{i,j,k}\,, \qquad \partial_q \vec{V}^n_{i,j,k} = -\mathrm{j}\,k_q \frac{\sin\left(k_q \frac{\Delta q}{2}\right)}{k_q \frac{\Delta q}{2}} \vec{V}^n_{i,j,k}$$

For a plane wave to fulfill the wave equation $\nabla^2 \vec{V} = \frac{n^2}{c^2}\partial_t^2 \vec{V}$:

$$\left(-k_x^2 - k_y^2 - k_z^2\right)\vec{V} = -\frac{n^2}{c^2}\omega_0^2 \vec{V}\,, \qquad |\vec{k}|^2 = \left(n\frac{\omega_0}{c}\right)^2 = n^2 k_0^2$$

For the numerical wave an equivalent condition must hold:

$$\left(-\mathrm{j}\,k_x \frac{\sin\left(k_x \frac{\Delta x}{2}\right)}{k_x \frac{\Delta x}{2}}\right)^2 + \left(-\mathrm{j}\,k_y \frac{\sin\left(k_y \frac{\Delta y}{2}\right)}{k_y \frac{\Delta y}{2}}\right)^2 + \left(-\mathrm{j}\,k_z \frac{\sin\left(k_z \frac{\Delta z}{2}\right)}{k_z \frac{\Delta z}{2}}\right)^2$$

$$= \frac{n^2}{c^2}\left(-\mathrm{j}\,\omega_0 \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}}\right)^2$$

Numerical Dispersion — Differential Operators

Plane wave $\vec{V}(t,\vec{r}) = \vec{V}_0 \exp\left[\mathrm{j}\left(\omega_0 t - \vec{k}\cdot\vec{r}\right)\right]$ with $|\vec{k}|^2 = (n\omega_0/c)^2$.

Numerical differential operators $(q = x, y, z)$:

$$\partial_t = \mathrm{j}\,\omega_0 \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}}\,, \qquad \partial_q = -\mathrm{j}\,k_q \frac{\sin\left(k_q \frac{\Delta q}{2}\right)}{k_q \frac{\Delta q}{2}}$$

For a plane wave to fulfill the wave equation $\nabla^2\vec{V} = \frac{n^2}{c^2}\,\partial_t^2\vec{V}$:

$$\left(-k_x^2 - k_y^2 - k_z^2\right)\vec{V} = -\frac{n^2}{c^2}\,\omega_0^2\,\vec{V}\,, \qquad |\vec{k}|^2 = \left(n\,\frac{\omega_0}{c}\right)^2 = n^2 k_0^2$$

For the numerical wave the above is true for $\Delta t, \Delta q \to 0$:

$$\lim_{\Delta t\to 0} \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}} = 1\,, \qquad \lim_{\Delta q\to 0} \frac{\sin\left(k_q \frac{\Delta q}{2}\right)}{k_q \frac{\Delta q}{2}} = 1$$

1D Numerical Dispersion Artefact

Numerical wave solves Maxwell's equations if (refractive index n):

$$\left(-\mathrm{j}\,k_x \frac{\sin\left(k_x \frac{\Delta x}{2}\right)}{k_x \frac{\Delta x}{2}}\right)^2 + \left(-\mathrm{j}\,k_y \frac{\sin\left(k_y \frac{\Delta y}{2}\right)}{k_y \frac{\Delta y}{2}}\right)^2 + \left(-\mathrm{j}\,k_z \frac{\sin\left(k_z \frac{\Delta z}{2}\right)}{k_z \frac{\Delta z}{2}}\right)^2$$

1D case, $k_x = k_y = 0$:

$$= \frac{n^2}{c^2}\left(-\mathrm{j}\,\omega_0 \frac{\sin\left(\omega_0 \frac{\Delta t}{2}\right)}{\omega_0 \frac{\Delta t}{2}}\right)^2$$

$$\left(\frac{\sin\left(k_z\,\Delta z/2\right)}{\Delta z/2}\right)^2 = \frac{n^2}{c^2}\left(\frac{\sin\left(\omega_0\,\Delta t/2\right)}{\Delta t/2}\right)^2,$$

$$\sin^2\left(k_z \frac{\Delta z}{2}\right) = \left(\frac{n\Delta z}{c\Delta t}\right)^2 \sin^2\left(\omega_0 \frac{\Delta t}{2}\right),$$

$$\sin\left(\omega_0 \frac{\Delta t}{2}\right) = +\frac{c\Delta t}{n\Delta z} \sin\left(k_z \frac{\Delta z}{2}\right) \quad \text{(stability factor } S = \frac{c\Delta t}{n\Delta z}\text{)},$$

$$\omega_0\,\Delta t = +2 \arcsin\left[S \sin\left(k_z \frac{\Delta z}{2}\right)\right],$$

$$n\frac{\omega_0}{c} = \left\{n\Delta z = c\Delta t\right\} = k_z$$

1D Stability and Numerical Dispersion Artefact

1D case, $k_x = k_y = 0$, stability factor (Courant number) $S = \dfrac{c\Delta t}{n\Delta z}$:

$$\sin\left(\omega_0 \frac{\Delta t}{2}\right) = S \sin\left(k_z \frac{\Delta z}{2}\right) \le S \quad (0 \le k_z \Delta z \le \pi), \qquad \omega_0 = \underbrace{\omega_r}_{\ge 0} + \mathrm{j}\underbrace{\omega_i}_{\le 0}$$

Numerical 1D wave (increasing!):

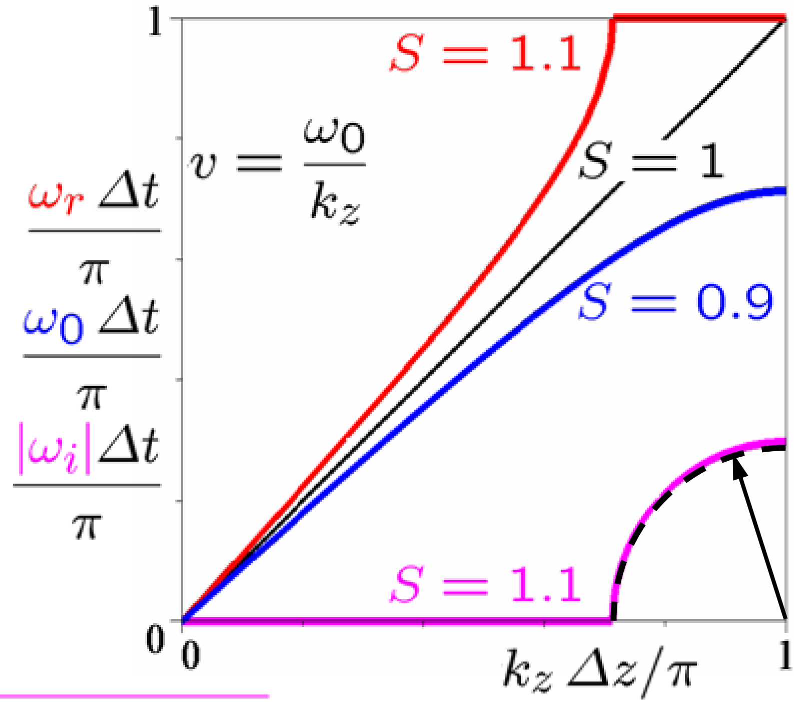
$$\vec{V}_0 \exp\left[+|\omega_i| t\right] \exp\left[\mathrm{j}\left(\omega_r t - k_z z\right)\right]$$

Growth factor p ($V^n_{i,j,k} = \left|\vec{V}^n_{i,j,k}\right|$):

$$p = V^{n+\frac{1}{2}}_{i,j,k} \Big/ V^{n-\frac{1}{2}}_{i,j,k} = \exp\left[+|\omega_i| \Delta t\right],$$

$$\omega_r \Delta t = \pi \quad \text{or} \quad 2\arcsin\left[S \sin\left(k_z \frac{\Delta z}{2}\right)\right]$$

$$|\omega_i| \Delta t = 2 \ln\left[S \sin\left(k_z \frac{\Delta z}{2}\right) + \sqrt{S^2 \sin^2\left(k_z \frac{\Delta z}{2}\right) - 1}\,\right] \quad \text{or} \quad 0$$



1D Stability and Numerical Dispersion $v = \frac{1}{S}\,\frac{c}{n}\,\frac{\arcsin\left[S\,\sin\left(k_z\,\frac{\Delta z}{2}\right)\right]}{k_z\,\frac{\Delta z}{2}}$

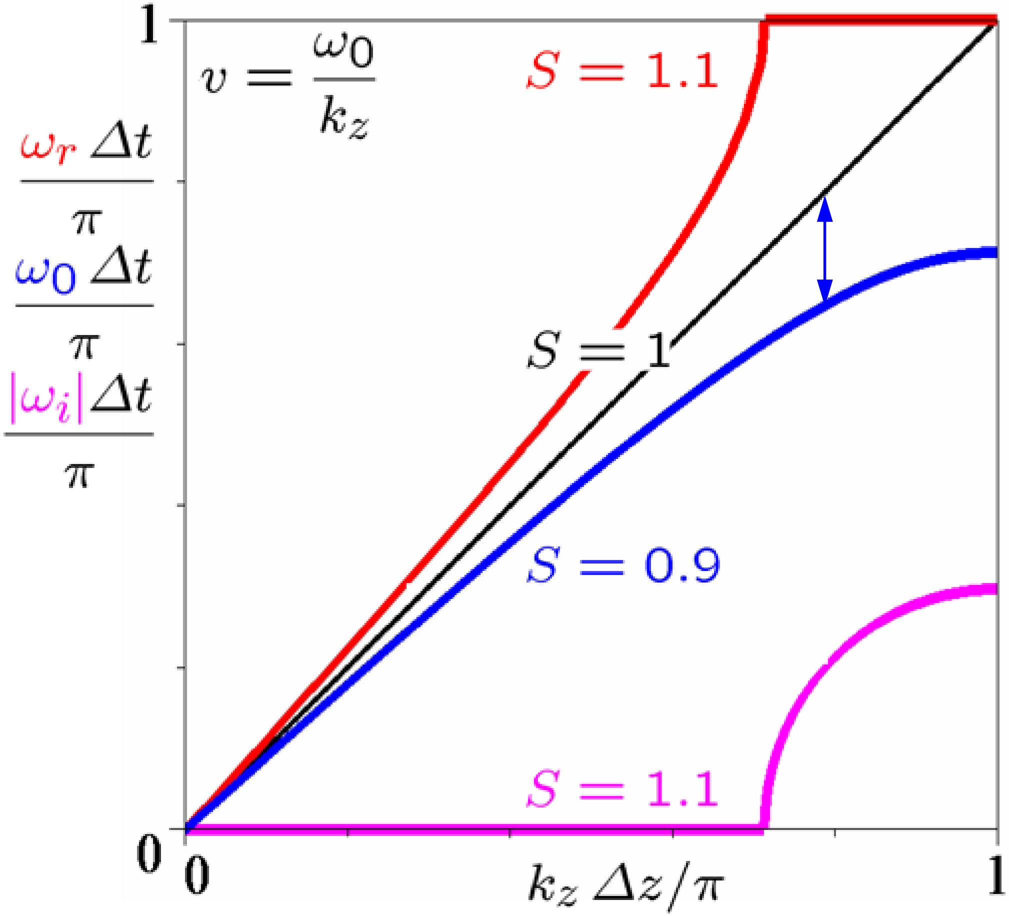
num. disp. error:

$\frac{c}{n} \le v \le \frac{1}{S}\,\frac{c}{n}\,\frac{\pi/2}{\arcsin(\frac{1}{S})}$

high-freq. oscill.

$f_r = \frac{1}{2\Delta t}$

Courant: $S = v_{\text{wrld}}\,\frac{1}{\tilde{v}} = \frac{c}{n}\,\frac{\Delta t}{\Delta z}$



light line, slope

$v = \frac{\omega_0}{k_z} = \frac{c}{n} = \frac{\Delta z}{\Delta t} = \tilde{v}$

stable, num. disp. error:

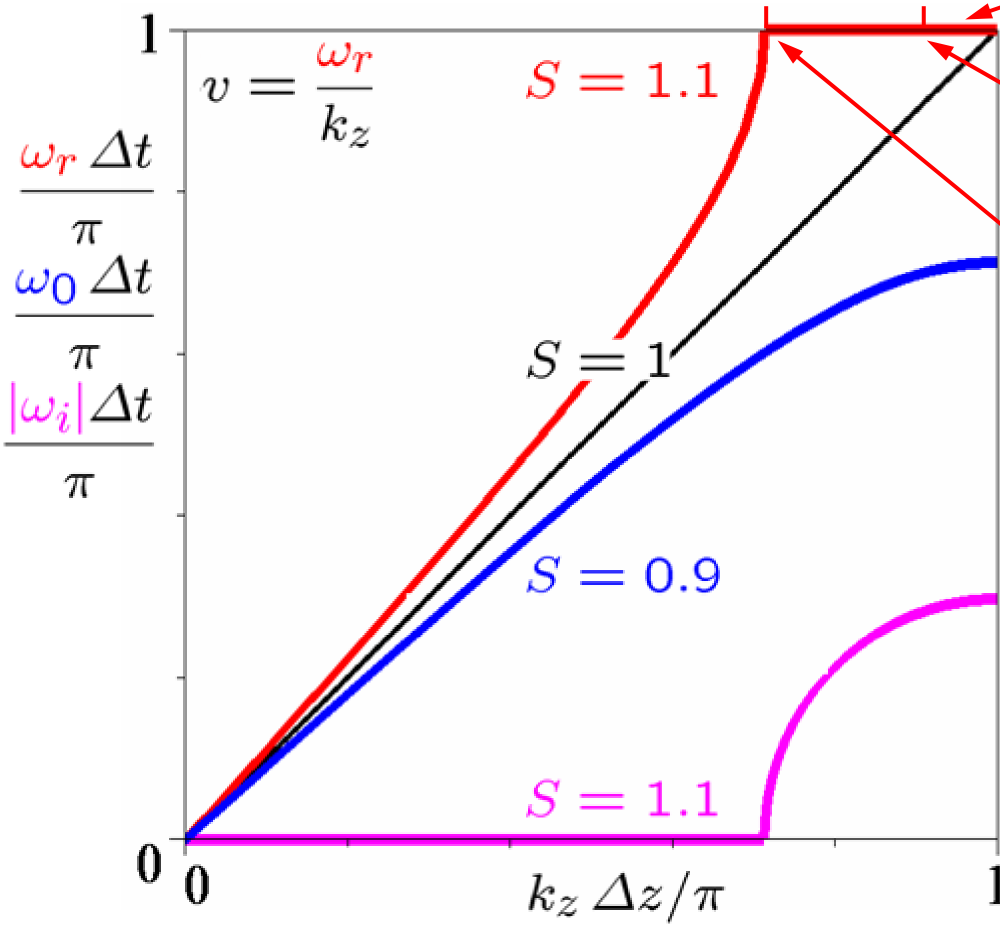
$\frac{\arcsin(S)}{\pi/2}\,\frac{1}{S}\,\frac{c}{n} \le v \le \frac{c}{n}$

Numerical wave slower than information transfer in grid.

t-instable, growth factor

$p \le \left(S + \sqrt{S^2 - 1}\right)^2$ per Δt

Numerical Dispersion — Instable Range



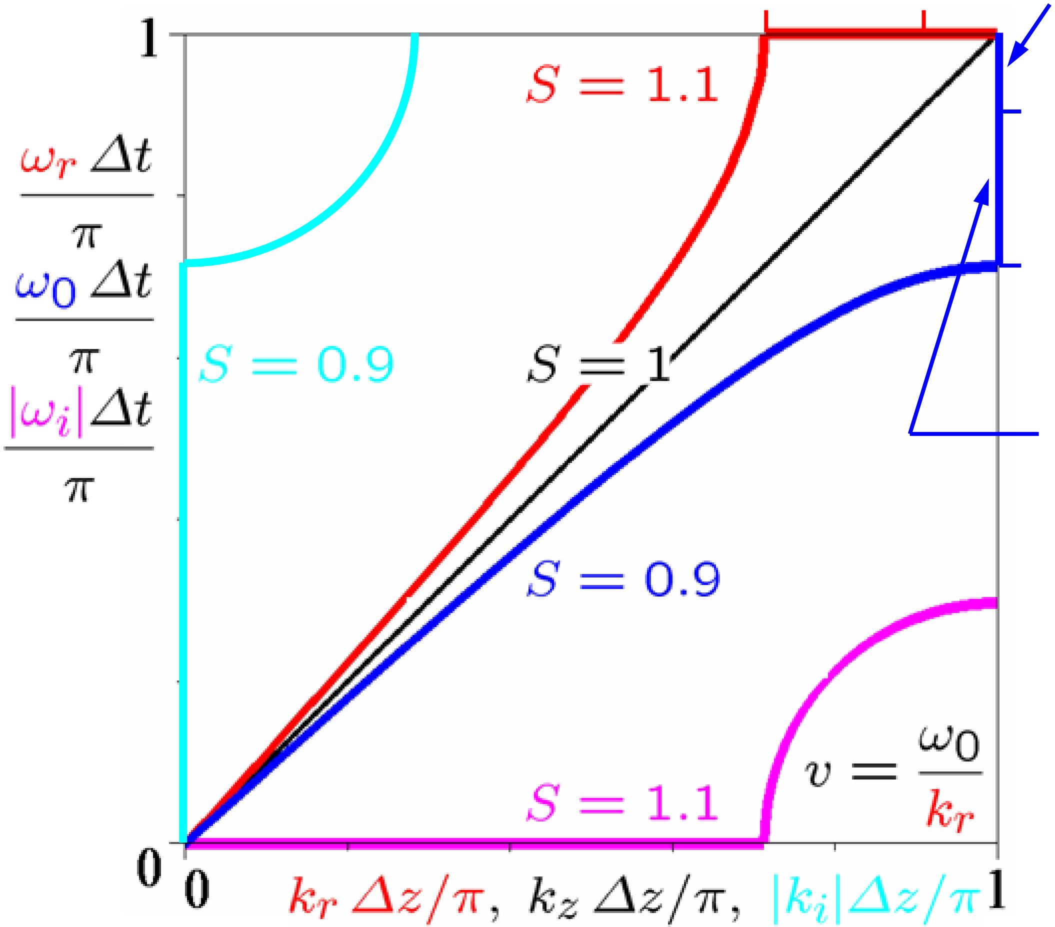
Possibly luminal propagation, temporally increasing field:

- $v = \frac{1}{S}\,\frac{c}{n}\,\frac{\pi}{k_z\,\Delta z} \geq \frac{1}{S}\,\frac{c}{n} = 0.9\,\frac{c}{n}$
- $v = \frac{c}{n} \qquad (\frac{k_z \Delta z}{\pi} = \frac{1}{S} = 0.9)$
- $v = \frac{1}{S}\,\frac{c}{n}\,\frac{\pi}{2\,\mathrm{arcsin}(\frac{1}{S})} = 1.26\,\frac{c}{n}$

Increasing with t, $\omega_i \leq 0$:
$\exp\left[+|\omega_i|t\right]\,\exp\left[\mathrm{j}\,(\omega_r t - k_z z\,)\right]$

Numerical Dispersion — Stable Range

Decreasing with z, $k_i \leq 0$:
$\exp\left[-|k_i| z\right] \exp\left[\mathrm{j}\,(\omega_0 t - k_r z)\right]$



Superluminal propagation, spatially decreasing field:

- $v = \frac{1}{S} \frac{c}{n} \frac{\omega_0 \Delta t}{\pi} \leq \frac{1}{S} \frac{c}{n} = 1.1 \frac{c}{n}$
- $v = \frac{c}{n} \quad (\frac{\omega_0 \Delta t}{\pi} = S = 0.9)$
- $v = \frac{1}{S} \frac{c}{n} \frac{2 \arcsin(S)}{\pi} = 0.79 \frac{c}{n}$

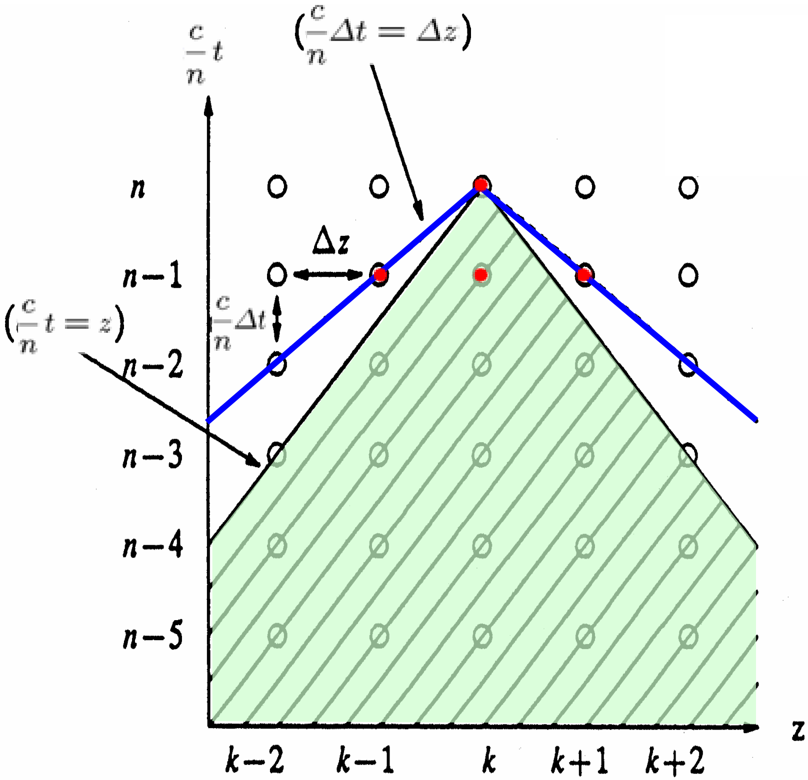
high-freq. spatial oscill.
$\zeta_r = \frac{1}{2 \Delta z}$

1D Stability — Intuitive Explanation

- A numerical value can propagate one Δz per Δt, given the local nature of the spatial difference used in the Yee algorithm, i. e., at a speed $\tilde{v} = \frac{\Delta z}{\Delta t}$.

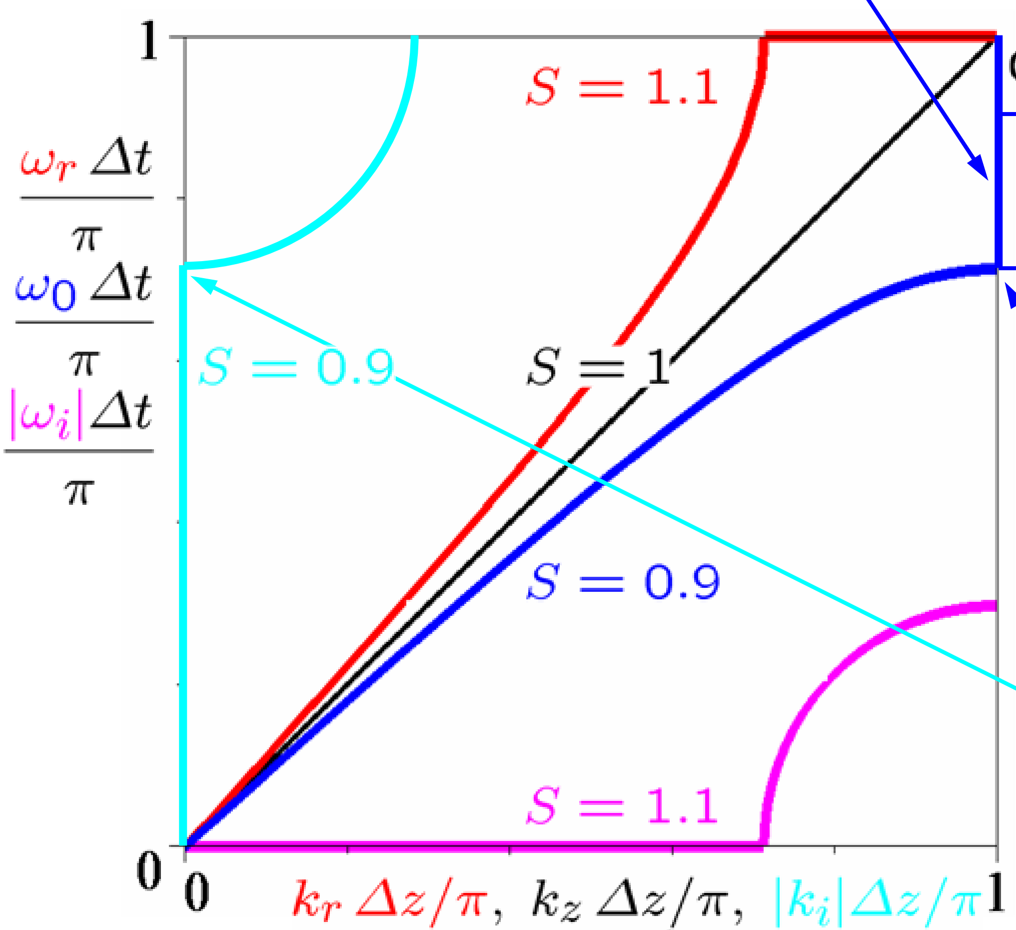
Courant: $S = \frac{c}{n} \frac{\Delta t}{\Delta z}$

$S = \frac{v_{\text{wrld}}}{\tilde{v}}$



- If the dispersion of the numerical wave is chosen such that its phase velocity $v > \tilde{v}$ exceeds the maximum speed $\tilde{v}$ provided by the algorithm, instability occurs.
- If the dispersion of the numerical wave leads to a phase velocity $v < \tilde{v}$, which is smaller than the maximum algorithm speed $\tilde{v}$, the computation is stable.

1D Stability and Numerical Dispersion



Choice of step sizes Δt, Δz:

- Signal with max. (spatial) frequency (ζ) f_0
- z-stable propagation if $k_z \Delta z/\pi \leq 1$, i. e., if
- $\Delta z \leq \frac{1}{2\zeta}$

  and if
- $\Delta t \leq \frac{\frac{2}{\pi}\arcsin(S)}{2 f_0}$

  (sampling theorem).

1D Plane Wave Dispersion and Accuracy — Choice of Step Sizes

Stability $S = \dfrac{c}{n}\dfrac{\Delta t}{\Delta z}$. Keep clear from dangerous $S = 1$, i. e., from

$$\Delta t = \frac{\Delta z}{c/n} = \frac{1}{2f_0}\frac{2\Delta z}{\lambda/n} = \frac{1}{2f_0} \quad \text{for} \quad \Delta z = \frac{\lambda/n}{2} = \frac{1}{2\zeta}.$$

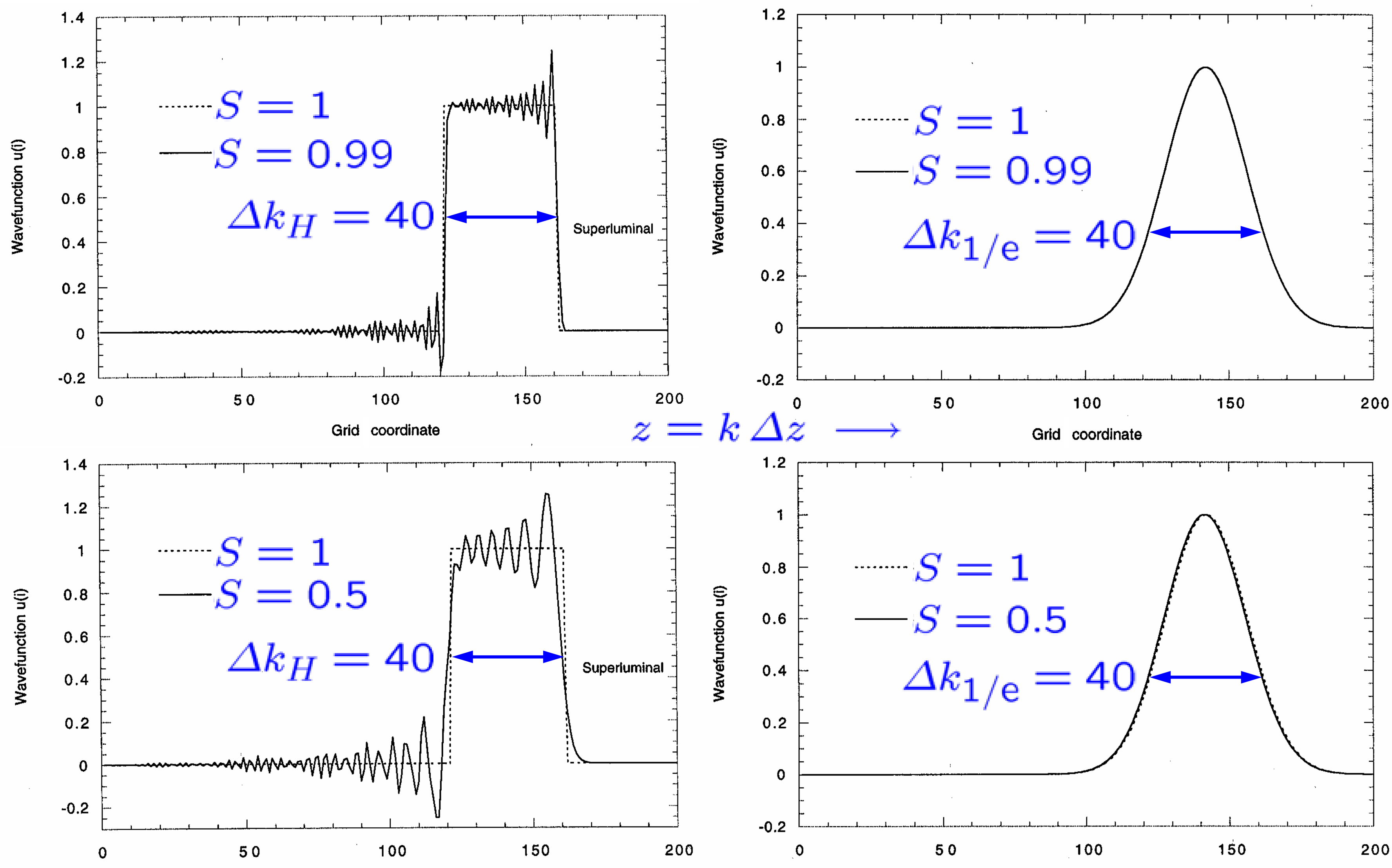
Signal frequency $f_0 = 1/T$ associated with spatial frequency $\zeta = 1/(\lambda/n)$. No temporal detail smaller than period T, no spatial detail smaller than medium wavelength λ/n may be resolved with this specific plane wave. The sampling recipe above yields an exact representation (only with sinc interpolation!): No dispersion, but risk of global or local instability.

Accuracy Choose a safe $S < 1$. For low dispersion error $< 1\,\%$ ($\arcsin(x) \leq 1.01\,x$) choose $k_z \frac{\Delta z}{2} \leq 0.16\,\frac{\pi}{2} \ll \frac{\pi}{2}$, i. e.,

$$\omega_0 \Delta t = 2\arcsin\left[S\sin\left(k_z\frac{\Delta z}{2}\right)\right] \approx S\,k_z \Delta z \leq S \times 0.16\,\pi\,,$$

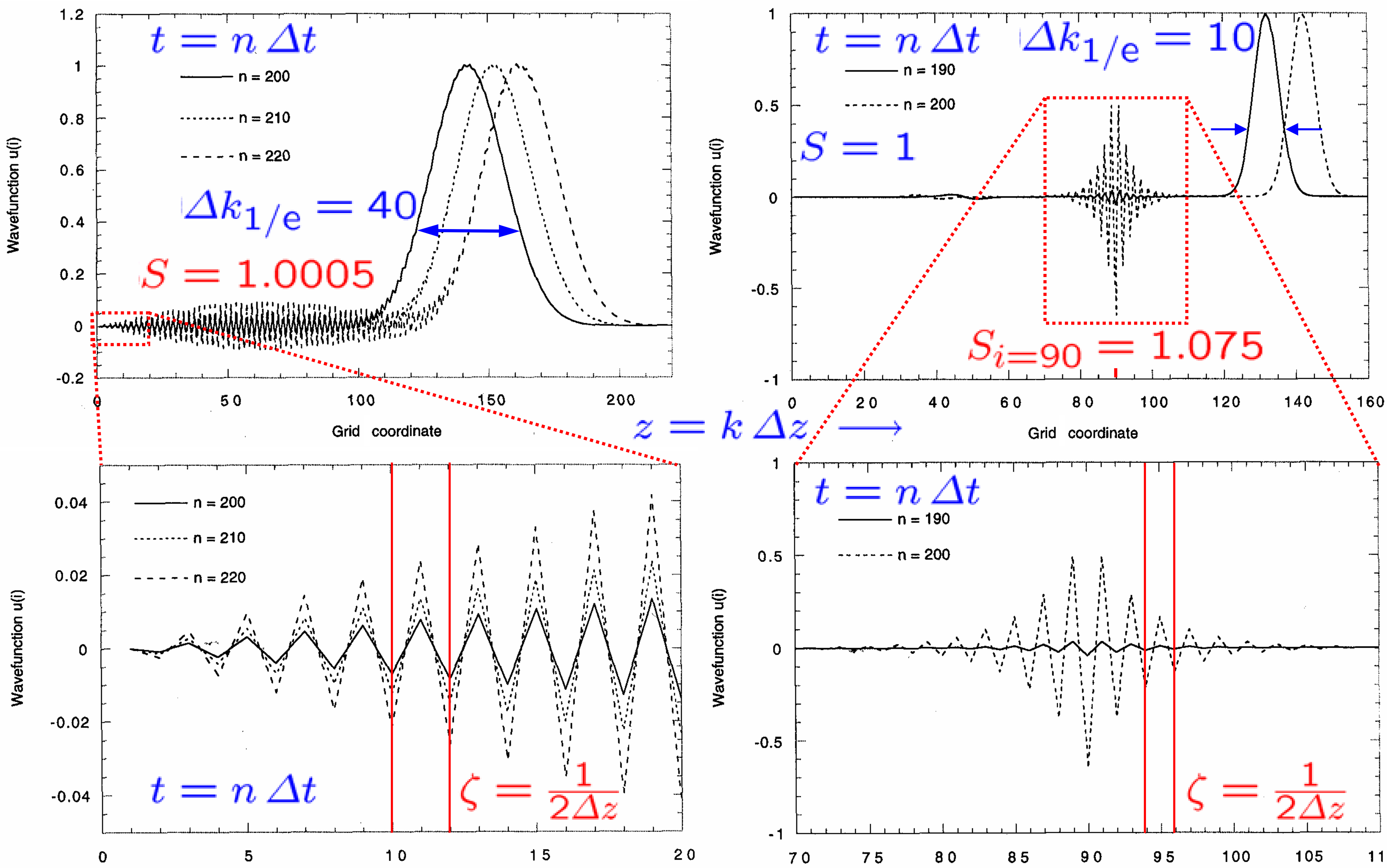
$$\omega_0 \approx \frac{c}{n}k_z \quad \text{for } S < 1 \text{ and } \Delta t \leq S\,\frac{0.16}{2f_0} \text{ or } \Delta z \leq \frac{0.16}{2\zeta}$$

Numerical Dispersion Examples



Taflove, A.; Hagness, S. C.: Computational electrodynamics: The finite-difference time-domain method, 2. Ed. Boston: Artech House 2000. Figs. 2.3,4

Global — Instability Examples — Local



Taflove, A.; Hagness, S. C.: Computational electrodynamics: The finite-difference time-domain method, 2. Ed. Boston: Artech House 2000. Figs. 2.6,7

3D Stability and Numerical Dispersion

Numerical wave *is* solution of Maxwell's equations if

$$\sin\left(\omega_0 \frac{\Delta t}{2}\right) = \frac{c\Delta t}{n}\sqrt{\left(\frac{\sin\left(k_x \frac{\Delta x}{2}\right)}{\Delta x}\right)^2 + \left(\frac{\sin\left(k_y \frac{\Delta y}{2}\right)}{\Delta y}\right)^2 + \left(\frac{\sin\left(k_z \frac{\Delta z}{2}\right)}{\Delta z}\right)^2} \leq 1$$

or if :

$$S = \frac{c}{n}\frac{\Delta t}{\Delta l} = \frac{c\Delta t}{n}\sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2 + \left(\frac{1}{\Delta z}\right)^2} \leq 1$$

Δl is maximum allowable spatial sampling interval for real propagation constant $\vec{k} = 2\pi\vec{\kappa}$ (spatial frequency $\kappa = n/\lambda$, $k_s \frac{\Delta s}{2} = \frac{\pi}{2}$):

$$\kappa = \frac{n}{\lambda} = \sqrt{\xi^2 + \eta^2 + \zeta^2} = \sqrt{\left(\frac{1}{2\Delta x}\right)^2 + \left(\frac{1}{2\Delta y}\right)^2 + \left(\frac{1}{2\Delta z}\right)^2} = \frac{1}{2\Delta l}$$

Stability limit:

$$\Delta t = \frac{\Delta l}{c/n} = \frac{1}{2f_0}\frac{2\Delta l}{\lambda/n} = \frac{1}{2f_0} \quad \text{for} \quad \Delta l = \frac{\lambda/n}{2} = \frac{1}{2\kappa}$$

3D Plane Wave Dispersion and Accuracy — Choice of Step Sizes

Stability $S = \frac{c}{n}\frac{\Delta t}{\Delta l}$. Keep clear from dangerous $S = 1$, i. e., from

$$\Delta t = \frac{\Delta l}{c/n} = \frac{1}{2f_0}\frac{2\Delta l}{\lambda/n} = \frac{1}{2f_0} \quad \text{for} \quad \Delta l = \frac{\lambda/n}{2} = \frac{1}{2\kappa}.$$

Signal frequency $f_0 = 1/T$ associated with spatial frequency $\kappa = 1/(\lambda/n)$. No temporal detail smaller than period T, no spatial detail smaller than medium wavelength λ/n may be resolved with this specific plane wave. The sampling recipe above yields an exact representation: No dispersion, but risk of global or local instability.

Accuracy Choose a safe $S < 1$. For low dispersion error $< 1\,\%$ ($\arcsin(x) \le 1.01\,x$) choose $k_s\frac{\Delta s}{2} \le 0.16\,\frac{\pi}{2} \ll \frac{\pi}{2}$ $(s = x, y, z)$, i. e.,

$$\omega_0 \Delta t = 2\arcsin\left(S\,\tfrac{1}{2}k\Delta l\right) \approx S\,k\Delta l \le S \times 0.16\,\pi \quad (|\vec{k}| = k = 2\pi\kappa),$$

$$\omega_0 \approx \frac{c}{n}k \quad \text{for } S < 1 \text{ and } \Delta t \le S\,\frac{0.16}{2f_0} \text{ or } \Delta l \le \frac{0.16}{2\kappa}$$

3D Stability — Intuitive Explanation for $\Delta = \Delta x = \Delta y = \Delta z$

- A numerical value propagates $\sqrt{3}\,\Delta \ldots 3\Delta$ per $3\Delta t$, given the local nature of the spatial difference used in the Yee algorithm, i. e., at a speed $\tilde{v} \geq \tilde{v}_\Delta = \frac{\sqrt{3}\,\Delta}{3\Delta t} = \frac{1}{\sqrt{3}} \frac{\Delta}{\Delta t}$.

Courant: $S = \frac{c}{n} \frac{\Delta t}{\Delta l}$

$S = \frac{v_{\text{wrld}}}{\tilde{v}}$

- If the dispersion of the numerical wave is chosen such that its phase velocity $v > \tilde{v}$ exceeds the slowest speed $\tilde{v}_\Delta$ provided by the algorithm, instability occurs.

- If the dispersion of the numerical wave leads to a phase velocity $v < \tilde{v}$, which is smaller than the slowest algorithm speed $\tilde{v}_\Delta$, the computation is stable.

- For a good accuracy $v \approx v_{\text{wrld}}$ the step sizes

$$\Delta t \leq \frac{1}{2f_0}\,, \quad \Delta l = \left[\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2 + \left(\frac{1}{\Delta z}\right)^2\right]^{-\frac{1}{2}} \leq \frac{1}{2\kappa} = \frac{\lambda/n}{2} = \frac{c/n}{2f_0}$$

must be significantly smaller than the Nyquist limit.

Outline

- Finite-difference time-domain (FDTD) method
  - Maxwell's equations, PDE classes, plane waves, sampling
  - Yee's leapfrog algorithm
  - Numerical dispersion, stability, accuracy and examples
  - Boundary conditions: PML, symmetries, periodicity
  - Dispersive and nonlinear media
- Beam propagation method (BPM)
  - Scalar Helmholtz equation
  - Split-step algorithm
  - Boundary conditions: Dirichlet, TBC, ABC, PML
  - BPM mode solving: Imaginary distance, correlation
  - Full-vectorial and semi-vectorial BPM
  - Wide-angle and bi-directional BPM
- Further reading

Perfectly Matched Layer (PML) Absorbing Boundary Cond. (ABC)

Computational domains are always finite, but practical problems have to be solved in unbounded regions, where the complications of reflections and losses from physical boundaries may be disregarded ("anechoic chamber").

- Plane wave incident perpendicularly on lossy isotropic half space without reflections, independent of frequency, for proper choice of parameters: $\epsilon_1 = \epsilon_2$, $\mu_1 = \mu_2$, $\sigma/\epsilon_2 = \bar{\sigma}/\mu_2$ (conductivity σ, magnetic loss $\bar{\sigma}$). Corresponds to physical absorber (anechoic chamber). — Disadvantage: Angle dependency
- Plane wave incident on lossy anisotropic (Berenger) medium. Non-physical absorber. Matched independently of frequency *and* angle of incidence. Parameters: $k_{1x} = k_{2x}$, $\epsilon_1 = \epsilon_2$, $\mu_1 = \mu_2$, $\sigma/\epsilon_2 = \bar{\sigma}/\mu_2$. Backreflection 70 dB down. — Absorptive action of PML robust relative to numerical dispersion artefacts.

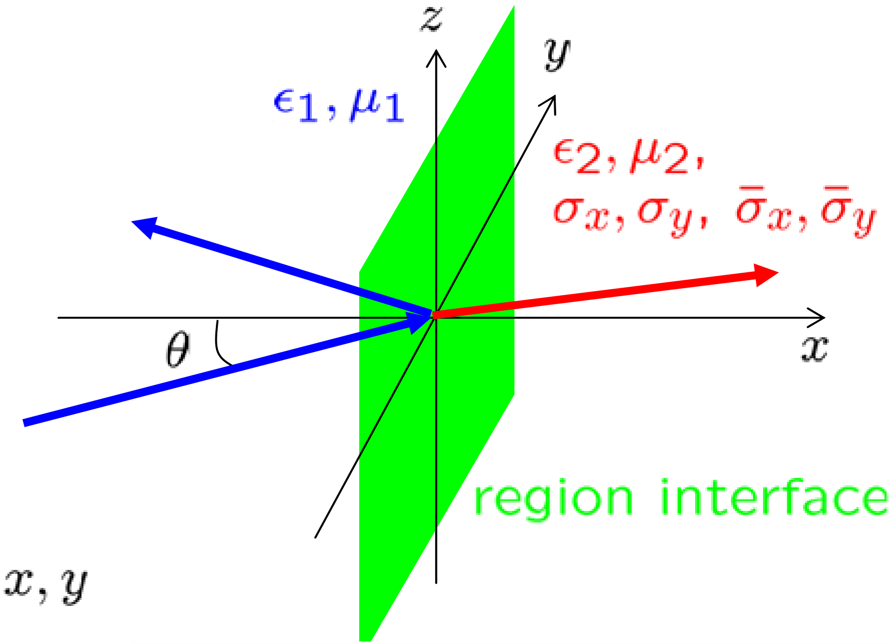
Berenger, J. P.: A perfectly matched layer for the absorption of electromagnetic waves. J. Comp. Phys. 114 (1994) 185–200
Taflove, A.; Hagness, S. C.: Computational electrodynamics: The finite-difference time-domain method, 2. Ed. Boston: Artech House 2000. Chapter 7

2D Plane Waves in Berenger´s PML Medium

Maxwell's equations:

$$\mathrm{curl}\,\vec{H} = (\mathrm{j}\omega\epsilon + \sigma)\vec{E}$$
$$= \partial_y H_z\,\vec{e}_x - \partial_x H_z\,\vec{e}_y\,,$$

$$\mathrm{curl}\,\vec{E} = -(\mathrm{j}\omega\mu + \bar{\sigma})\vec{H}$$
$$= \partial_y E_x\,\vec{e}_z - \partial_x E_y\,\vec{e}_z$$

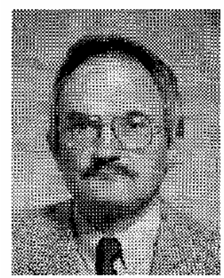


Auxiliary quantities:

$$s_q = 1 + \frac{\sigma_q}{\mathrm{j}\omega\epsilon_2}\,,\quad \bar{s}_q = 1 + \frac{\bar{\sigma}_q}{\mathrm{j}\omega\mu_2}\,,\quad q = x, y$$

Split-field $H_z = H_{zx} + H_{zy}$:

$$\mathrm{j}\omega\epsilon_2\, s_y E_x = \partial_y (H_{zx} + H_{zy}),$$
$$\mathrm{j}\omega\epsilon_2\, s_x E_y = -\partial_x (H_{zx} + H_{zy}),$$
$$\mathrm{j}\omega\mu_2 \bar{s}_x H_{zx} = -\partial_x E_y\,,$$
$$\mathrm{j}\omega\mu_2 \bar{s}_y H_{zy} = \partial_y E_x$$



J.-P. Bérenger received the Maîtrise de Physique from Université de Grenoble, in 1973, and the Diplôme d'Ingénieur from École Supérieure d'Optique de Paris, in 1975.

With the Département Études Théoriques of the Centre d'Analyse de Défense, from 1975–1984, his areas of interest were the propagation of waves and the coupling problems related to the nuclear electromagnetic pulse. During this period, he contributed to popularizing the finite-difference time-domain method in France. In 1984, he moved to the Département Nucléaire where he was involved in the development of simulation software. Since 1989, he has held a position as expert on the electromagnetic effects of nuclear events while pursuing works to improve the methods and codes used to predict the propagation of waves in such disturbed conditions.

IEEE AP January 1996

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Taflove, A.; Hagness, S. C.: Computational electrodynamics: The finite-difference time-domain method, 2. Ed. Boston: Artech House 2000. Chapter 7

2D Plane Waves and Berenger´s PML Medium

Split-field $H_z = H_{zx} + H_{zy}$:

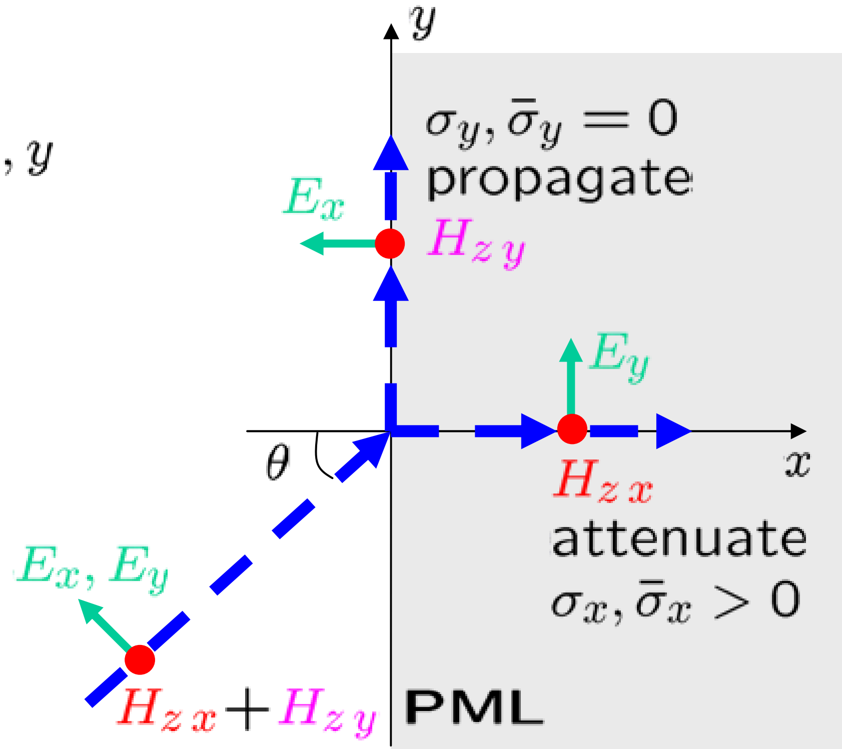
$$s_q = 1 + \frac{\sigma_q}{\mathrm{j}\omega\epsilon_2}\,, \quad \bar{s}_q = 1 + \frac{\bar{\sigma}_q}{\mathrm{j}\omega\mu_2}\,, \quad q = x, y$$

Propagate ($\sigma_y, \bar{\sigma}_y = 0,\ s_y, \bar{s}_y = 1$):

$$\begin{aligned}(\mathrm{j}\omega\epsilon_2\, s_y) E_x &= \partial_y (H_{zx} + H_{zy}),\\ (\mathrm{j}\omega\mu_2 \bar{s}_y) H_{zy} &= \partial_y E_x\end{aligned}$$

Attenuate ($\sigma_x, \bar{\sigma}_x > 0$):

$$\begin{aligned}(\mathrm{j}\omega\epsilon_2\, s_x) E_y &= -\partial_x (H_{zx} + H_{zy}),\\ (\mathrm{j}\omega\mu_2 \bar{s}_x) H_{zx} &= -\partial_x E_y\end{aligned}$$



Solution in PML medium ($k_q = \omega\sqrt{\epsilon_q \mu_q}$):

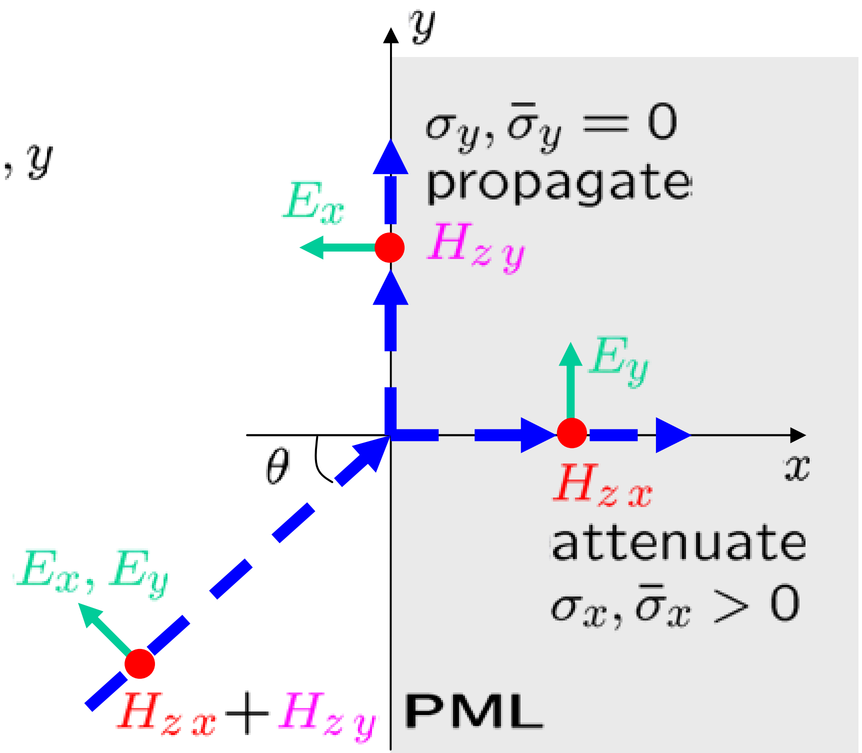
$$\begin{aligned}(\mathrm{j}\omega\epsilon_2 s_y)\partial_y E_x &= \partial_y^2 (H_{zx} + H_{zy}) = (\mathrm{j}\omega\epsilon_2 s_y)(\mathrm{j}\omega\mu_2 \bar{s}_y) H_{zy}\\ (\mathrm{j}\omega\epsilon_2 s_x)\partial_x E_y &= -\partial_x^2 (H_{zx} + H_{zy}) = -(\mathrm{j}\omega\epsilon_2 s_x)(\mathrm{j}\omega\mu_2 \bar{s}_x) H_{zx}\end{aligned}$$

$$H_z = H_{zx} + H_{zy} \;\Rightarrow\; \frac{1}{s_x \bar{s}_x}\,\partial_x^2 H_z + \frac{1}{s_y \bar{s}_y}\,\partial_y^2 H_z + k_2^2 H_z = 0$$

2D Plane Waves and Berenger´s PML Medium

Split-field $H_z = H_{z\,x} + H_{z\,y}$:

$$s_q = 1 + \frac{\sigma_q}{\mathrm{j}\,\omega\epsilon_2}\,,\ \bar{s}_q = 1 + \frac{\bar{\sigma}_q}{\mathrm{j}\,\omega\mu_2}\,,\ q = x, y$$



For $r_H = 0$ $(\sigma_x/\epsilon_2 = \bar{\sigma}_x/\mu_2)$:

$$\sqrt{s_x} = \sqrt{\bar{s}_x}$$

Amplitude reflection and transmission coefficients $(k_s = \omega\sqrt{\epsilon_s\,\mu_s}\,)$:

$$r_H = \frac{\frac{k_{1x}}{\omega\epsilon_1} - \frac{k_{2x}}{\omega\epsilon_2}\sqrt{\frac{\bar{s}_x}{s_x}}}{\frac{k_{1x}}{\omega\epsilon_1} + \frac{k_{2x}}{\omega\epsilon_2}\sqrt{\frac{\bar{s}_x}{s_x}}} = \left\{ \begin{array}{c} \epsilon_1 = \epsilon_2\,,\ \mu_1 = \mu_2\,,\ s_x = \bar{s}_x\,, \\ k_{1\,x,y} = k_{2\,x,y}\,,\ \sigma_x/\epsilon_2 = \bar{\sigma}_x/\mu_2 \\ (\text{directional-independent}) \end{array} \right\} = 0,$$

$$t_H = 1 + r_H$$

evanescent decay in medium 2

2D Plane Waves and Berenger´s PML Medium

Split-field $H_z = H_{z\,x} + H_{z\,y}$:

$$s_q = 1+\frac{\sigma_q}{\mathrm{j}\,\omega\epsilon_2}\,,\quad \bar{s}_q = 1+\frac{\bar{\sigma}_q}{\mathrm{j}\,\omega\mu_2}\,,\quad q = x, y$$

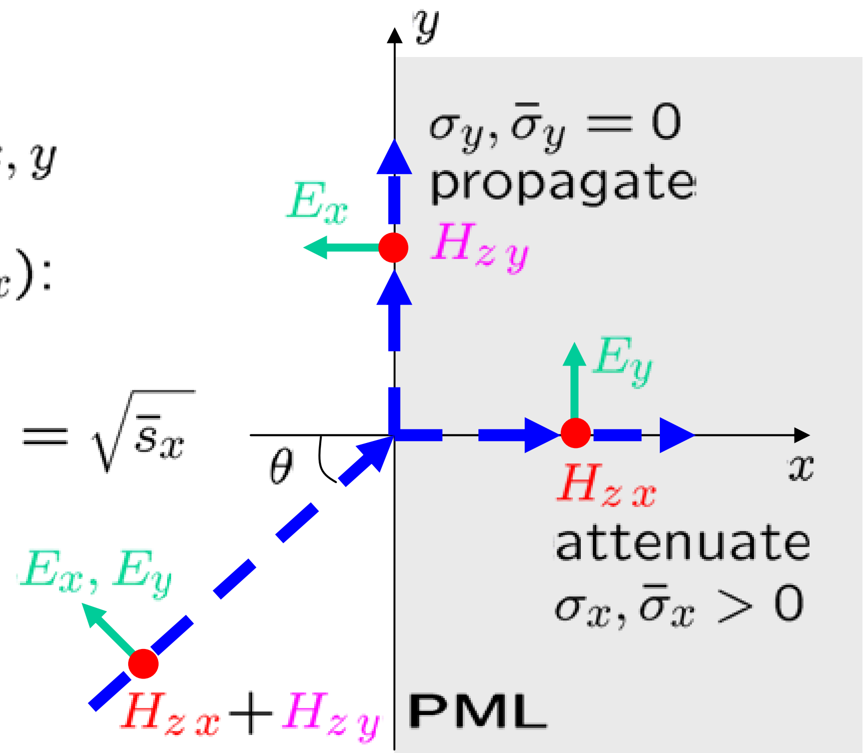
For $r_H = 0$ $(\sigma_x/\epsilon_2 = \bar{\sigma}_x/\mu_2,\ s_x = \bar{s}_x)$:

$$\sqrt{s_x} = \sqrt{1+\left(\frac{\sigma_x}{\omega\epsilon_2}\right)^2}\ \mathrm{e}^{-\frac{1}{2}\arctan\frac{\sigma_x}{\omega\epsilon_2}} = \sqrt{\bar{s}_x}$$

$$\sqrt{s_x\,\bar{s}_x} = s_x = 1-\mathrm{j}\,\frac{\sigma_x}{\omega\epsilon_2}$$

Incident wave:

$$k_{1x} = k_1 \cos\theta$$



Solution in PML medium $(k_s = \omega\sqrt{\epsilon_s\,\mu_s}\,)$:

$$\frac{1}{s_x\bar{s}_x}\,\partial_x^2 H_z + \frac{1}{s_y\bar{s}_y}\,\partial_y^2 H_z + k_2^2 H_z = 0 \qquad H_z = H_{2z}\,\mathrm{e}^{-\mathrm{j}\sqrt{s_x\,\bar{s}_x}\,k_{2x}x}\,\mathrm{e}^{-\mathrm{j}\,k_{2y}y}$$

$$H_z = H_{2z}\exp\left(-\cos\theta\,\sqrt{\frac{\mu_1}{\epsilon_1}}\,\sigma_x\,x\right)\exp\left[-\mathrm{j}(k_{1x}x+k_{1y}y)\right]\quad (k_{1\,x,y} = k_{2\,x,y})$$

Symmetric and Anti-Symmetric Boundary Conditions

Symmetric (even) boundary conditions assume that one or more field components have a symmetry about one or more planes of reflection, e. g., $x = 0$:

$$u(x) = u(-x) \qquad \text{implying an extremal } u \text{ at } x = 0$$

Anti-symmetric (odd) boundary conditions assume that one or more field components have anti-symmetry about one or more planes of reflection, e. g., $x = 0$:

$$u(x) = -u(-x) \qquad \text{implying a zero } u \text{ at } x = 0$$

Periodic Boundary Conditions (PBC)

PBC equivalently describe an infinite structure, comprising the elementary domain ("unit cell" size D_x, D_y, D_z), which is translated and thereby infinitely repeated in all directions with a so-called lattice vector $\vec{R} = n_x D_x\,\vec{e}_x + n_y D_y\,\vec{e}_y + n_z D_z\,\vec{e}_z$ (integers $n_{x,y,z}$).

Bloch's theorem (Floquet theorem in microwaves) states that in a periodic medium the eigenmodes have the property:

$$\vec{E}_{\vec{k}}(\vec{r}\,) = \vec{u}_{\vec{k}}(\vec{r}\,)\,\mathrm{e}^{-\mathrm{j}\,\vec{k}\cdot\vec{r}}, \qquad \vec{H}_{\vec{k}}(\vec{r}\,) = \vec{v}_{\vec{k}}(\vec{r}\,)\,\mathrm{e}^{-\mathrm{j}\,\vec{k}\cdot\vec{r}}$$

$$\vec{u}_{\vec{k}}(\vec{r} + \vec{R}\,) = \vec{u}_{\vec{k}}(\vec{r}\,), \qquad \vec{v}_{\vec{k}}(\vec{r} + \vec{R}\,) = \vec{v}_{\vec{k}}(\vec{r}\,)$$

Consequence (assume $n_{x,y,z} = 1$ for primitive vector $\vec{R}$):

$$\Rightarrow \quad \vec{E}_{\vec{k}}(\vec{r} + \vec{R}\,) = \vec{E}_{\vec{k}}(\vec{r}\,)\,\mathrm{e}^{-\mathrm{j}\,\vec{k}\cdot\vec{R}}, \qquad \Rightarrow \quad \vec{H}_{\vec{k}}(\vec{r} + \vec{R}\,) = \vec{H}_{\vec{k}}(\vec{r}\,)\,\mathrm{e}^{-\mathrm{j}\,\vec{k}\cdot\vec{R}}$$

Only if $k_x D_x$, $k_y D_y$, $k_z D_z$ happen to equal 2π, then the phasors $\vec{E}_{\vec{k}}(\vec{r} + \vec{R}\,)$, $\vec{H}_{\vec{k}}(\vec{r} + \vec{R}\,)$ do *not* experience a phase shift.

Kittel, C.: Introduction to solid state physics, 3rd ed. New York: John Wiley & Sons 1966 (Bloch's theorem: Chapter 9 p. 259 ff.)
Myers, H. P.: Introductory solid state physics. New Delhi: Viva Books Private Ltd. 1998 (Bloch's theorem: Sect. 7.6 p. 190 ff.)
Morse, P. M.; Feshbach, H.: Methods of theoretical physics, Band 1 und 2. New York: McGraw-Hill 1953 (Floquet theorem: Vol. 1 Sect. 5.2 p. 557)

Periodic Boundary Conditions — Formulation

Analytic signal $\underline{\Psi}(t,\vec{r}) = A(t,\vec{r})\,\mathrm{exp}[\mathrm{j}(\omega_0 t - \vec{k}\cdot\vec{r})]$. Real part $\Psi(t,\vec{r}) = E_q(t,x,y,z), H_q(t,x,y,z)$ $(q = x,y,z)$ stands for any field component.

PBC and propagation in z-direction only for simplification:

$$\underline{\Psi}(t, z + D_z) = \underline{\Psi}(t,z)\,\mathrm{exp}(-\mathrm{j}\,k_z D_z)$$

Wrap-around update:

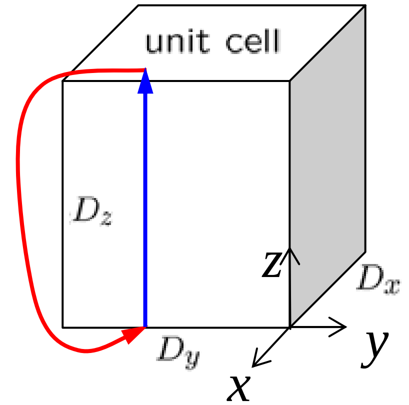
$$\underline{\Psi}(t,z) = \underline{\Psi}(t, z + D_z)\,\mathrm{exp}(\mathrm{j}\,k_z D_z)$$

Ingenious idea by Ko and Mittra (1993): Propagate real signal $\Psi(t,\vec{r})$ and imaginary signal $\Psi_i(t,z)$ with parallel FDTD runs. Excitation of unit cell by $A(t,z) = |A(t,z)|\,\mathrm{exp}[\mathrm{j}\,\varphi(t,z)]$ at $z = z_0$:

$$\Psi(t,z_0) = |A(t,z_0)|\cos[\omega_0 t - k_z z_0 + \varphi(t,z_0)]$$
$$\Psi_i(t,z_0) = |A(t,z_0)|\,\sin[\omega_0 t - k_z z_0 + \varphi(t,z_0)]$$

Ko, W. L.; Mittra, R.: Implementation of Floquet boundary condition in FDTD for FSS analysis. IEEE APS Int. Symp. Dig., June 28-July 2 (1993), vol. 1, pp. 14–17.

Periodic Boundary Conditions — Procedure



- Excite unit cell at $z = 0$ with $\Psi(t,z), \Psi_i(t,z)$ of modulated plane wave (spectrum near $f = f_0$).
- Propagate inititial fields according to FDTD update equations until boundary $z = D_z + \Delta z$.
- Calculate update fields at $z = 0$ by:

$$\Psi(t,0) = \Re\{[\Psi(t, D_z + \Delta z) + \mathrm{j}\,\Psi_i(t, D_z + \Delta z)]\,\exp(\mathrm{j}\,k_z D_z)\},$$
$$\Psi_i(t,0) = \Im\{[\Psi(t, D_z + \Delta z) + \mathrm{j}\,\Psi_i(t, D_z + \Delta z)]\,\exp(\mathrm{j}\,k_z D_z)\}$$

- Repeat updating and wrapping until stationary state is reached.
- Fourier transform stationary time sequence and analyze for resonances (eigenfrequencies) f_ℓ belonging to chosen k_z.
- The spatial distributions associated with the various f_ℓ are the eigenfields or modes of the periodic arrangement.

Ko, W. L.; Mittra, R.: Implementation of Floquet boundary condition in FDTD for FSS analysis. IEEE APS Int. Symp. Dig., June 28–July 2 (1993), vol. 1, pp. 14–17
Harms, P.; Mittra, R.; Ko, W.: Implementation of the periodic boundary condition in the finite-difference time-domain algorithm for FSS structures. IEEE Trans. Antennas Prop. 42 (1994) 1317–1324
Turner, G.; Christodoulou, C.: Broadband periodic boundary condition for FDTD analysis of phased array antennas. IEEE APS Int. Symp. Dig., June 21–26 (1998), vol. 2, pp. 1020–1023

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Dispersive and Nonlinear Media

Lossy and dispersive materials:

- More realistic models (Debye, Lorentz)
- Wave propagation in a plasma

Nonlinear modeling:

- High-power pulses (Kerr, Raman, self-steepening)
- Design of switches
- Design of wavelength converters (e. g., FWM)

Problems and solutions:

- Stability issues
- ABC so far not well established
- PML applicable, also to higher-order FD methods
- Implemented with auxiliary differential equations (ADE)

Fujii, M.; Tahara, M; Sakagami, I; Freude, W.; Russer, P.: High-order FDTD and auxiliary differential equation formulation of optical pulse propagation in 2D Kerr and Raman nonlinear dispersive media. IEEE J. Quantum Electron. 40 (2004) 175–182

Fujii, M.; Omaki, N.; Tahara, M.; Sakagami, I.; Poulton, C.; Freude, W.; Russer, P.: Optimization of nonlinear dispersive APML ABC for the FDTD analysis of optical solitons. IEEE J. Quantum Electron. 41 (2005) 448–454

Fujii, M,; Koos, C.; Poulton, C.; Sakagami, I.; Leuthold, J.; Freude, W.: A simple and rigorous verification technique for nonlinear FDTD algorithm by optical parametric four-wave mixing. Microwave and Optical Technol. Lett. 48 (2006) 88–91

Fujii, M; Koos, C.; Poulton, C.; Leuthold, J.; Freude, W.: Nonlinear FDTD analysis and experimental validation of four-wave mixing in InGaAsP/InP racetrack micro-resonators. IEEE Photon. Technol. Lett. 18 (2006) 361–363

Nonlinear and Dispersive Media Examples — ADE Method

Optical Kerr effect

polarization: $P_K(t) = \varepsilon_0 \; \chi_K^{(3)} \; E^3(t)$ ⇨ finite difference eq.

⇧ const. nonlinear susceptibility

Lorentz dispersion

polarization: $\tilde{P}_L(\omega) = \tilde{\chi}_L(\omega)\tilde{E}(\omega) = \dfrac{\varepsilon_0 \Delta\varepsilon_L \, \omega_L^2}{\omega_L^2 + 2j\delta_L\omega - \omega^2}\tilde{E}(\omega)$

⇩ $\mathcal{F}^{-1}$

$$\omega_L^2 P_L(t) + 2\delta_L \frac{dP_L(t)}{dt} + \frac{d^2 P_L(t)}{dt^2} = \varepsilon_0 \Delta\varepsilon_L \, \omega_L^2 E(t)$$

⇨ finite difference eq.

⇨ solved with Yee's leapfrog algorithm

Fujii, M.; Koos, C.; Poulton, C.; Leuthold, J.; Freude, W.: FDTD modelling and experimental verification of FWM in semiconductor micro-resonators. Proc. 15th International Workshop on Optical Waveguide Theory and Numerical Modelling (OWTNM'06), Varese, Italy, April 20–21, 2006, p. 79

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Scalar Solution of Maxwell´s Equations

Problem classes where vector nature of fields not relevant:

1. Reflection/refraction at plane boundary, no difference E / H-polarization for small $\Delta \ll 1$
2. Diffraction independent of field polarization, if objects $\gg \lambda/n$, and observation $\sim \lambda/n$ away from object of no interest.
3. Electromagnetic field associated with passage of natural light through optical instrument of moderate aperture and conventional design such that intensity represented as single complex scalar wave function.

Normal waveguides weakly guiding $\rightarrow$ z-components of fields negligible, differences TE / TM-waves disappear, grad $\ln n^2$ negligible:

$$|\Delta n|_\lambda / n \ll 1\,, \qquad |\Delta(\mathrm{grad}\, n)|_\lambda / |\mathrm{grad}\, n| \ll 1\,,$$

$$\nabla^2 \vec{E} - \frac{n^2(\vec{r})}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0, \qquad \nabla^2 \vec{H} - \frac{n^2(\vec{r})}{c^2}\frac{\partial^2 \vec{H}}{\partial t^2} = 0$$

Scalar Paraxial Wave Equation

Extracting another rapidly varying phase factor ("arbitrary" β_0):

$$\Psi(t,x,y,z) = \Psi(x,y,z)\,\mathrm{exp}(\mathrm{j}\,\omega_0 t) = a(x,y,z)\,\mathrm{exp}(-\mathrm{j}\,\beta_0 z)\,\mathrm{exp}(\mathrm{j}\,\omega_0 t)$$

Helmholtz equation, alternative formulation ($k = n(x,y,z)k_0$):

$$\left(\partial_x^2 + \partial_y^2 + \partial_z^2 + k^2(x,y,z)\right) a(x,y,z)\,\mathrm{exp}(-\mathrm{j}\,\beta_0 z) = 0\,,$$

$$\left(\partial_x^2 + \partial_y^2 + \underbrace{\partial_z^2}_{0,\ \text{paraxial}} - \mathrm{j}\,2\beta_0\,\partial_z + k^2(x,y,z) - \beta_0^2\right) a(x,y,z) = 0$$

Paraxial approximation, $a(x,y,z)$ varies slowly along z: $\partial_z^2 \ll 2\beta_0\partial_z$, i. e., $|\partial_z^2 a| \ll 2\beta_0|\partial_z a|$, or relative z-variation $|(\partial_z a)/a|$ small compared to angular spatial frequency β_0 of reference wave along z:

$$\partial_z a(x,y,z) = \frac{1}{\mathrm{j}\,2\beta_0}\left(\partial_x^2 + \partial_x^2 + k^2(x,y,z) - \beta_0^2\right) a(x,y,z)$$

Elliptic Helmholtz approximated by parabolic PDE, SVA $a(x,y,z)$. Solution simpler: z-grid may be coarser, no 2nd-order boundary value problem with eigenvalue analysis or iteration needed.

Scalar Paraxial Beam Propagation Method

Advantages

- Straighforward, easy to understand and use by non-expert users
- Numerically efficient, fast response time
- Guided and radiated waveguide fields included
- Mode coupling and mode conversion covered automatically

Drawbacks

- Monochromatic waves only
- Paraxiality requirement
  - Fields propagate essentially along the z-axis
  - Restrictions on possible contrast
- Rapid phase variations (e. g., in MMI devices) not accurate
- Reflections ignored
- Polarization disregarded

Mitigation

- Bi-directional non-paraxial non-iterative BPM
- Semi-vectorial and full-vectorial BPM

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Formal Operator Solution

Paraxially approximated Helmholtz equation:

$$\partial_z a(x,y,z) = \frac{1}{\mathrm{j}\,2\beta_0}\left(\partial_x^2 + \partial_x^2 + k^2(x,y,z) - \beta_0^2\right) a(x,y,z), \qquad \partial_z a = \mathcal{L} a\,,$$

$$\mathcal{L}(x,y,z) = \underbrace{\frac{1}{\mathrm{j}\,2\beta_0}\left(\partial_x^2 + \partial_x^2\right)}_{\mathcal{L}_1} + \underbrace{\frac{1}{\mathrm{j}\,2\beta_0}\left(k^2(x,y,z) - \beta_0^2\right)}_{\mathcal{L}_2}$$

Linear operator $\mathcal{L}(z)$ describes (paraxial) wave propagation $\mathcal{L}_1$ in homogeneous medium with refractive index $n_0 = \beta_0/k_0$, and phase change $\mathcal{L}_2$ due to $(k^2 - \beta_0^2)/(2\beta_0) \approx (n - n_0)k_0$. Initial value operator problem (implied (x,y)-dependencies).

Error in hand-out

$\mathcal{L}(z)$ assumed to be slowly varying. May be regarded constant for length Δz, solution like $\frac{\mathrm{d}f}{\mathrm{d}z} = Lf \rightarrow f(z) = \mathrm{e}^{Lz} f(0)$:

$$\begin{aligned} a(z+\Delta z) &= \exp\left[\mathcal{L}(z)\Delta z\right] a(z) = \exp\left[(\mathcal{L}_1 + \mathcal{L}_2)\Delta z\right] a(z) \\ &= \exp\left[\mathcal{L}_1 \Delta z\right] \exp\left[\mathcal{L}_2 \Delta z\right] a(z) + \mathcal{O}(\Delta z^2) \\ &= \exp\left[\tfrac{1}{2}\mathcal{L}_1 \Delta z\right] \exp\left[\mathcal{L}_2 \Delta z\right] \exp\left[\tfrac{1}{2}\mathcal{L}_1 \Delta z\right] a(z) + \mathcal{O}(\Delta z^3) \end{aligned}$$

Split-Step Fourier Method

Solution of paraxial wave equation, $k = n(x,y,z)k_0$, $\beta_0 = n_0 k_0$:

$$a(x,y,z+\Delta z) = \exp\left[\tfrac{1}{2}\mathcal{L}_1\Delta z\right]\exp\left[\mathcal{L}_2\Delta z\right]\exp\left[\tfrac{1}{2}\mathcal{L}_1\Delta z\right]a(x,y,z)$$

$\mathcal{L}_1$: Propagator $\exp\left[-\mathrm{j}\,\frac{1}{2\beta_0}\left(\partial_x^2+\partial_y^2\right)\frac{\Delta z}{2}\right]$ of field in homogeneous medium with n_0 over distance $\Delta z/2$ (paraxial wave propag.) Operator $\mathcal{L}_1$ and SVA $a(x,y,z)$ in spatial Fourier domain:

$$\mathcal{L}_1 \overset{\mathcal{F}}{\circ\!\!-\!\!\bullet}\ \tilde{\mathcal{L}}_1 = -\mathrm{j}\,\frac{1}{2\beta_0}\left[(\mathrm{j}\,2\pi\xi)^2+(\mathrm{j}\,2\pi\eta)^2\right],$$

$$a(x,y,z) \overset{\mathcal{F}}{\circ\!\!-\!\!\bullet}\ \tilde{a}(\xi,\eta,z) = \iint_{-\infty}^{+\infty} a(x,y,z)\,\mathrm{e}^{\mathrm{j}\,2\pi(\xi x+\eta y)}\,\mathrm{d}x\,\mathrm{d}y$$

$$\mathrm{e}^{\mathcal{L}_1\frac{\Delta z}{2}}\,a(x,y,z) = \mathcal{F}^{-1}\left\{\mathrm{e}^{\overbrace{\mathrm{j}\,\frac{(2\pi)^2}{2\beta_0}\left(\xi^2+\eta^2\right)}^{\tilde{\mathcal{L}}_1}\frac{\Delta z}{2}}\,\tilde{a}(\xi,\eta,z)\right\}$$

$\mathcal{L}_2$: Propagator $\exp\left[-\mathrm{j}\,\frac{1}{2\beta_0}\left(k^2-\beta_0^2\right)\Delta z\right] \approx \exp[-\mathrm{j}\,(k-\beta_0)\,\Delta z]$ of field in medium with $n(x,y,z)-n_0$ over distance Δz (phase change, applied directly)

Complexity of SSFM and FD-BPM

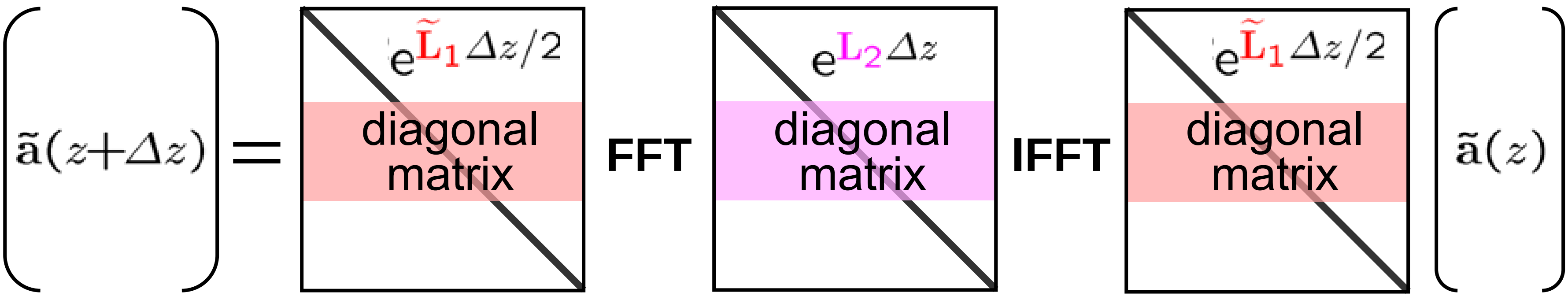
Split-step solution of paraxial wave equation:

$$a(x,y,z+\Delta z) = \exp\left[\tfrac{1}{2}\mathcal{L}_1\Delta z\right]\exp\left[\mathcal{L}_2\Delta z\right]\exp\left[\tfrac{1}{2}\mathcal{L}_1\Delta z\right]a(x,y,z)$$

$N_x \times N_y$ discretizing x, y: $\tilde{\mathcal{L}}_1$, $\mathcal{L}_2$ $\rightarrow$ diagonal matrices $\tilde{\mathbf{L}}_1$, $\mathbf{L}_2$

$\tilde{a}(\xi,\eta,z)$, $a(x,y,z)$ $\rightarrow$ column matrices $\tilde{\mathrm{a}}(i\Delta\xi, j\Delta\eta, z)$, $\mathrm{a}(i\Delta x, j\Delta y, z)$

Split-step Fourier method (SSFM):



3D complexity per z-step: $\mathcal{O}\left(N^2 \log_2 N\right)$ [full wave $\mathcal{O}(N^3)$]

Implicit Crank-Nicholson FD-BPM: $\mathcal{O}(N^2)$ today's standard

Press, W. H.; Flannery, B. P.; Teuklsky, S. A.; Vetterling, W. T.: Numerical Recipes: The Art of Scientific Computing. Cambridge Univ., New York 1986

Scarmozzino, R.; Osgood, Jr., R. M.: Comparison of finite-difference and Fourier-transform solutions of the parabolic wave equation with emphasis on integrated-optics applications. J. Opt. Soc. Amer. A 8 (1991) 724–731

Kremp, T.; Freude, W.: Fast split-step wavelet collocation method for WDM system parameter optimization. J. Lightwave Technol. 23 (2005) 1491–1502

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Boundary Conditions

Computational domains are always finite, but practical problems have to be solved in unbounded regions.

Dirichlet Field is required to be zero on boundary. Reflects radiation back into computational domain.

TBC Transparent boundary condition. Lets radiation pass the boundary and leave the computational domain.

Simple: Recommended for highly multimode problems

Full: May behave poorly with large amount of radiation, then simple TBC can perform better.

ABC Absorbing boundary conditions

PML Perfectly matched layer boundary conditions

Hadley, G. R.: Transparent boundary condition for the beam propagation method. Opt. Lett. 16 (1991) 624–626

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Yevick, D.: A guide to electric field propagation techniques for guided-wave optics. Opt. Quant. Electron. 26 (1994) S185–S197

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Huang, W. P.; Xu, C. L.; Lui, W.; Yokoyama, K.: The perfectly matched layer (PML) boundary condition for the beam propagation method. IEEE Photon. Technol. Lett. 8 (1996) 649–651

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Agrawal, Arti; Sharma, Anurag: Perfectly matched layer in numerical wave propagation: factors that affect its performance. Appl. Opt. 43 (2004) 4225–4231

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Mode Solving with Imaginary Distance BPM

Expanding a scalar field $\Phi(x,y,z)$ in guided and radiation modes:

$$\Phi(x,y,z) = \sum\!\!\!\!\!\!\int_m c_m \Psi_m(x,y)\,\mathrm{e}^{-\mathrm{j}\,\beta_m z} = \left\{z = \mathrm{j}\,z'\right\} = \sum\!\!\!\!\!\!\int_m c_m \Psi_m(x,y)\,\mathrm{e}^{\beta_m z'}$$

Fundamental mode $m = 0$ has largest β_m and grows fastest $\rightarrow$ field $\Psi_0(x,y)$ dominates in superposition $\sum\!\!\!\!\!\!\int_m$ after a short imaginary propagation distance $z' = -\mathrm{j}\,z$.

Helmholtz equation with $\mathcal{L} = \nabla_t^2 + k_0^2 n^2(x,y,z)$, $\nabla_t^2 = \partial_x^2 + \partial_y^2$:

$$\mathcal{L}\Psi_0(x,y) - \beta_0^2 \Psi_0(x,y) = 0 \quad \Rightarrow \quad \beta_0^2 = \frac{\iint_{-\infty}^{+\infty} \Psi_0^* \left(\mathcal{L}\Psi_0\right) \mathrm{d}x\,\mathrm{d}y}{\iint_{-\infty}^{+\infty} \Psi_0^* \Psi_0 \,\mathrm{d}x\,\mathrm{d}y}$$

Higher-order modes by orthogonalization procedure to subtract contributions from lower order modes while propagating.

Feit, M. D.; Fleck, J. A.: Computation of mode properties in optical fiber waveguides by a propagating beam method. Appl. Opt. 19 (1980) 1154–1164

Yevick, D.; Hermansson, B.: New formulations of the matrix beam propagation method: Application to rib waveguides", IEEE J. Quantum Electron. 25 (1989) 221–229

Jüngling, S.; Chen, J. C.: A study and optimization of eigenmode calculations using the imaginary-distance beam-propagation method. IEEE J. Quantum Electron. 30, (1994) 2098–2105

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Mode Solving with BPM and Correlation Method

Excite waveguide field $\Phi(x,y,z)$ with arbitrary initial field $\Phi_0(x,y,0)$, correlation with modes $\Psi_m(x,y)\exp(-\mathrm{j}\,\beta_m z)$ in $0 \le z \le L$:

$$P(z) = \iint_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\, \Phi_0^*(x,y,0)\, \Phi(x,y,z)$$

$$= \iint_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y \sum\nolimits_m c_m^* \Psi_m^*(x,y) \sum\nolimits_n c_n \Psi_n(x,y)\, \mathrm{e}^{-\mathrm{j}\,\beta_n z}$$

$$= \sum_m \sum_n c_m^*\, c_n\, \mathrm{e}^{-\mathrm{j}\,\beta_n z} \iint_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\, \Psi_m^*(x,y)\, \Psi_n(x,y)$$

$$= \sum_{m,n} c_m^*\, c_n\, \mathrm{e}^{-\mathrm{j}\,\beta_m z}\, N\delta_{mn} = N \sum_m |c_m|^2\, \mathrm{e}^{-\mathrm{j}\,\beta_m z}$$

Spatial Fourier transform in limited range $0 \le z \le L$ (resolution!):

$$\tilde{P}(\zeta) = \int_{-\infty}^{+\infty} P(z)\, \mathrm{e}^{\mathrm{j}\,2\pi\zeta z}\, \mathrm{d}z \approx N \sum_m |c_m|^2 \int_0^L \mathrm{e}^{\mathrm{j}\,2\pi[\zeta - \beta_m/(2\pi)]}\, \mathrm{d}z$$

$$\approx N \sum_m |c_m|^2\, \delta[\zeta - \beta_m/(2\pi)] \quad \Rightarrow \quad \beta_m = 2\pi\, \zeta_{\text{peaks}}$$

Modal field from:

$$\Psi_m(x,y) = \frac{1}{L} \int_0^L \Phi(x,y,z)\, \mathrm{e}^{+\mathrm{j}\,\beta_m z}\, \mathrm{d}z$$

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Polarization Effects with Full-Vectorial BPM

$$\nabla^2 \vec{E} + \mathrm{grad}\left((\mathrm{grad} \ln n^2) \cdot \vec{E}\right) = -n^2 \frac{\omega_0^2}{c^2} \vec{E} \,,$$

$$\nabla^2 \vec{H} + (\mathrm{grad} \ln n^2) \times \mathrm{curl}\, \vec{H} = -n^2 \frac{\omega_0^2}{c^2} \vec{H}$$

Weak $n(z)$, $2(\partial_z n)/n \ll 1$, $\mathrm{grad}_z \ln n^2 E_z$ neglected, (x, y)-plane (transverse) components only, $\vec{X}_t = \vec{\hat{X}}_t \exp(-\mathrm{j}\, \beta_0 z)$, $k_0 = \omega_0 / c$:

$$\nabla^2 \vec{\hat{E}}_t - \mathrm{j}\, 2\beta_0\, \partial_z \vec{\hat{E}}_t + \left(n^2 k_0^2 - \beta_0^2\right) \vec{\hat{E}}_t = -\,\mathrm{grad}_t\left((\mathrm{grad}_t \ln n^2) \cdot \vec{E}_t\right) \mathrm{e}^{\mathrm{j}\, \beta_0 z},$$

$$\nabla^2 \vec{\hat{H}}_t - \mathrm{j}\, 2\beta_0\, \partial_z \vec{\hat{H}}_t + \left(n^2 k_0^2 - \beta_0^2\right) \vec{\hat{H}}_t = -\left((\mathrm{grad}_t \ln n^2) \times \mathrm{curl}\, \vec{H}\right)_t \mathrm{e}^{\mathrm{j}\, \beta_0 z}$$

Slowly varying amplitude approximation (SVA), $|\partial_z^2 \vec{\hat{X}}_t| \ll 2\beta_0 |\partial_z \vec{\hat{X}}_t|$, leads to paraxial vector wave equations:

$$\mathrm{j}\, \partial_z \hat{E}_x = \mathcal{A}_{xx} \hat{E}_x + \mathcal{A}_{xy} \hat{E}_y \,, \qquad \mathrm{j}\, \partial_z \hat{H}_x = \mathcal{B}_{xx} \hat{H}_x + \mathcal{B}_{xy} \hat{H}_y \,,$$

$$\mathrm{j}\, \partial_z \hat{E}_y = \mathcal{A}_{yx} \hat{E}_x + \mathcal{A}_{yy} \hat{E}_y \,, \qquad \mathrm{j}\, \partial_z \hat{H}_y = \mathcal{B}_{yx} \hat{H}_x + \mathcal{B}_{yy} \hat{H}_y$$

$\mathcal{A}_{ij}, \mathcal{B}_{ij}$ with $i, j = x, y$ are complicated differential operators.

Huang, W. P.; Xu, C. L.: Simulation of three-dimensional optical waveguides by a full-vector beam propagation method. IEEE J. Quantum Electron. 29 (1993) 2639–2649

Outline

- Finite-difference time-domain (FDTD) method
  - Maxwell's equations, PDE classes, plane waves, sampling
  - Yee's leapfrog algorithm
  - Numerical dispersion, stability, accuracy and examples
  - Boundary conditions: PML, symmetries, periodicity
  - Dispersive and nonlinear media
- Beam propagation method (BPM)
  - Scalar Helmholtz equation
  - Split-step algorithm
  - Boundary conditions: Dirichlet, TBC, ABC, PML
  - BPM mode solving: Imaginary distance, correlation
  - Full-vectorial and semi-vectorial BPM
  - Wide-angle and bi-directional BPM
- Further reading

Wide-Angle and Bi-Directional BPM

Paraxiality requirement and neglected ∂_z^2 places restrictions on bend radii, index-contrast, multimode propagation, and reflections. Relaxed by advanced methods, which also provide high computational efficiency (IIT Delhi group):

- Split-step method for non-paraxial wave equation is inherently bidirectional since the second order wave equation is solved directly.
- Highly accurate, fast, non-iterative, stable with large step sizes and easy to implement.
- Implementations in collocation and finite-difference method

Sharma, Anurag; Agrawal, Arti: Perfectly matched layer in numerical wave propagation: factors that affect its performance. Appl. Opt. 43 (2004) 4225–4231

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Sharma, Anurag; Agrawal, Arti: Non-paraxial split-step finite-difference method for beam propagation. Opt. Quantum Electron. (2006), in press

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Further Reading

General

[1] Huang, W. P. (Ed.): Methods for simulation of guided-wave optoelectronic devices: Part II: Waves and interactions. In: PIER 11 — Progress in Elctromagnetic Research, Chief Editor: J. A. Kong. Cambridge (MA): EMW Publishing 1995

[2] Scarmozzino, R.; Gopinath, A.; Pregla, R.; Helfert, S.: Numerical techniques for modeling guided-wave photonic devices. IEEE J. Sel. Topics Quantum Electron. 6 (2000) 150–162

Stability according to the Courant-Friedrichs-Lewy condition

[3] Lakshmikantham, V.; Trigiante, D.: Theory of difference equations: Numerical methods and applications. Boston: Academic Press 1988

Large-scale FDTD modeling

[4] Freude, W.; Poulton, C.; Koos, C.; Brosi, J.; Glckler, F.; Wang, J.; Chakam, G.-A.; Fujii, M.: Design and fabrication of nanophotonic devices. Proc. 6th Intern. Conf. on Transparent Optical Networks (ICTON'04), July 48, 2004, Wroclaw, Poland. Mo.A.4 vol. 1 pp. 4–9

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FDTD staircasing error mitigation

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Wavelet FDTD leads to low dispersion and coarser grids

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Multiscale analysis

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Replacing explicit Yee leapfrogging by *a*lternating *d*irection *i*mplicit scheme

[13] Rao, H.; Scarmozzino, R.; Osgood, Jr., R. M.: An improved ADI-FDTD method and its application to photonic simulations IEEE Photon. Technol. Lett. 14 (2002) 477–479

What Should You Have Learned?

Numerical analysis has become easy, however:

- Blind trust in numerical data is dangerous.
- Some basic understanding of the algorithm is necessary.
- Often one operates at the limits of resources.
- So always double-check the reliability of results!

A Selection of topics was discussed:

- Basics of the FDTD algorithm (stability, dispersion, BC)
- Fundamentals of the BPM (paraxiality, mode solving)
- The hands-on exercises will demonstrate practical issues.
- Not all material from this course has been orally presented.