THE FINITE-DIFFERENCE TIME-DOMAIN (FDTD) METHOD – PART I

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1. Outline

- finite differences for derivative approximation
- the wave equation in 1-D

  initial/boundary conditions and excitation sources
- generalization to 2-D and 3-D
- Maxwell's equations; 2-D problems: TM and TE modes
- Yee's algorithm in 3-D space
- Yee's algorithm in 2-D space
- introduction to absorbing boundary conditions
- PROJECT: determine the modes of a rectangular waveguide

2. References and recommended further reading

[1] R.C. Booton, *Computational Methods for Electromagnetics and Microwaves*, Wiley, 1992, pp. 59-73

[2] M.N.O. Sadiku, *Numerical Techniques in Electromagnetics*, CRC Press, 2001, pp. 159-192

[3] W. Yu *et al*., *Parallel Finite Difference Time Domain Method*, Artech, 2006

[3] A. Taflove, *Computational Elertodynamics: the Finite-Difference Time-Domain Method*, Artech, 1995

[4] A. Taflove and S.C. Hagness, *same as above,* 2nd ed., Artech, 2000

[5] K. Kunz and R. Luebbers, *Finite-Difference Time-Domain Method for Electromagnetics*, CRC Press, 1993

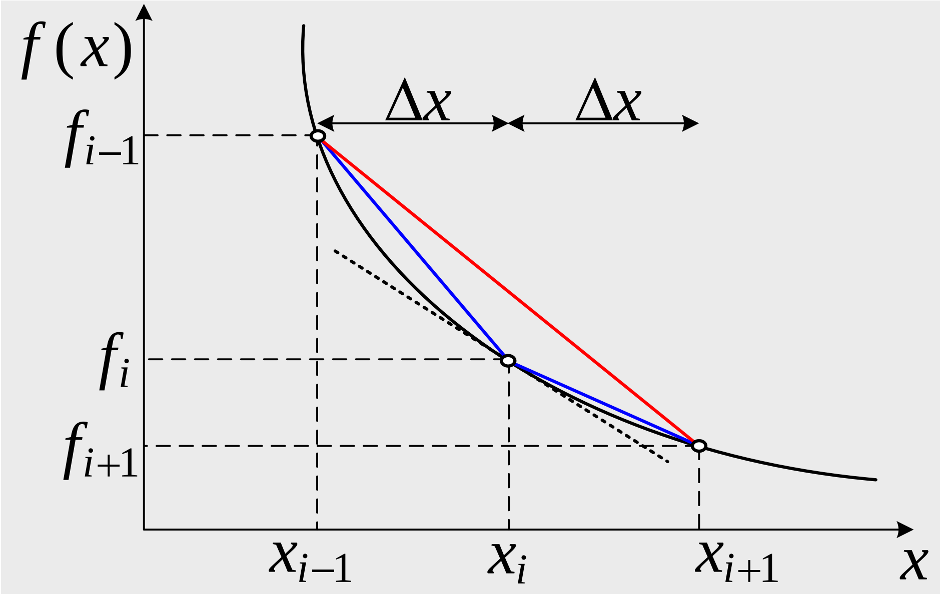
[6] K.S. Yee, "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media," *IEEE Trans. Antennas Propagat.*, vol. AP-14, No. 3, pp. 302-307, May 1966

3. Finite differences for derivative approximation

1st order derivatives

forward FD

$$\frac{df(x_i)}{dx} = \frac{df_i}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}$$



backward FD

$$\frac{df(x_i)}{dx} = \frac{df_i}{dx} \approx \frac{f_i - f_{i-1}}{\Delta x}$$

central FD

$$\frac{df(x_i)}{dx} = \frac{df_i}{dx} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

3. Finite differences for derivative approximation – cont.

accuracy

Taylor expansions

- at $x_i + \Delta x$

$$f(x_i + \Delta x) = f_{i+1} = f_i + \Delta x \frac{df_i}{dx} + \frac{1}{2}\Delta x^2 \frac{d^2 f_i}{dx^2} + \frac{1}{6}\Delta x^3 \frac{d^3 f_i}{dx^3} + O^4$$

$$\frac{df_i}{dx} = \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x)^1$$

- at $x_i - \Delta x$

$$f(x_i - \Delta x) = f_{i-1} = f_i - \Delta x \frac{df_i}{dx} + \frac{1}{2}\Delta x^2 \frac{d^2 f_i}{dx^2} - \frac{1}{6}\Delta x^3 \frac{d^3 f_i}{dx^3} + O^4$$

$$\frac{df_i}{dx} = \frac{f_i - f_{i-1}}{\Delta x} + O(\Delta x)^1$$

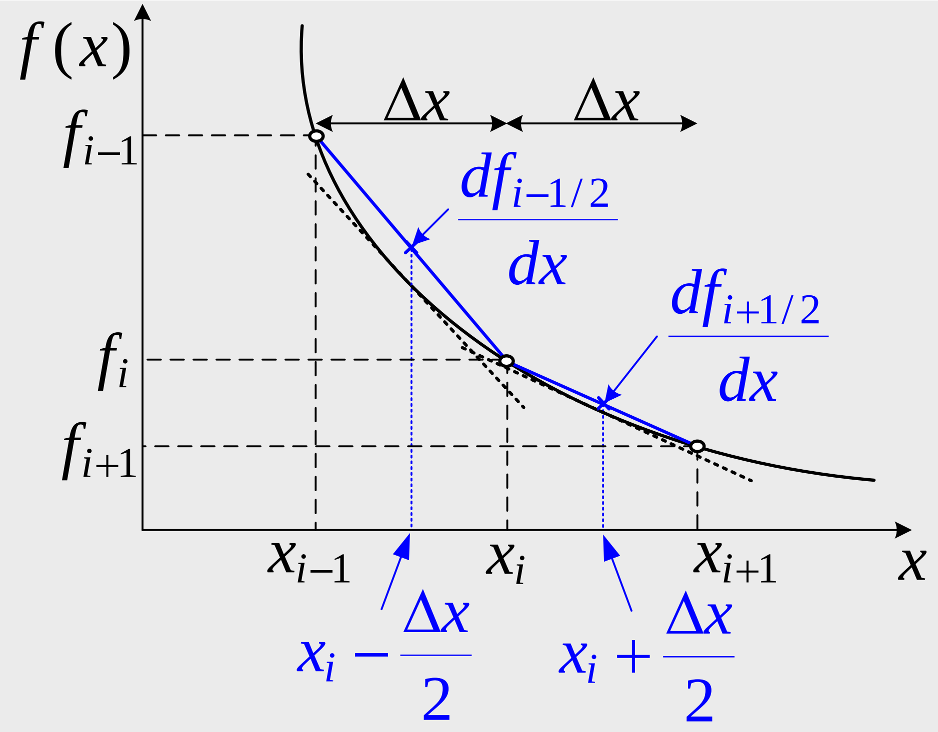
forward and backward FDs have 1st order accuracy

3. Finite differences for derivative approximation – cont.

accuracy: central FDs have 2nd order accuracy

combine both expansions to obtain: $\dfrac{df_i}{dx} = \dfrac{f_{i+1} - f_{i-1}}{2\Delta x} + O^2$

central FD at half steps



$$\frac{df(x_i + \Delta x/2)}{dx} = \frac{df_{i+1/2}}{dx} = \frac{f_{i+1} - f_i}{\Delta x} + O^2$$

3. Finite differences for derivative approximation – cont.

second-order accurate backward/forward approximations of 1st order derivatives

$$\frac{df_i}{dx} \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{\Delta x} \qquad\qquad \frac{df_i}{dx} \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\Delta x}$$

<u>2nd order derivatives</u>

$$f_{i+1} = f_i + \Delta x \frac{df_i}{dx} + \frac{1}{2}\Delta x^2 \frac{d^2 f_i}{dx^2} + \frac{1}{6}\Delta x^3 \frac{d^3 f_i}{dx^3} + O^4$$

$$+$$

$$f_{i-1} = f_i - \Delta x \frac{df_i}{dx} + \frac{1}{2}\Delta x^2 \frac{d^2 f_i}{dx^2} - \frac{1}{6}\Delta x^3 \frac{d^3 f_i}{dx^3} + O^4$$

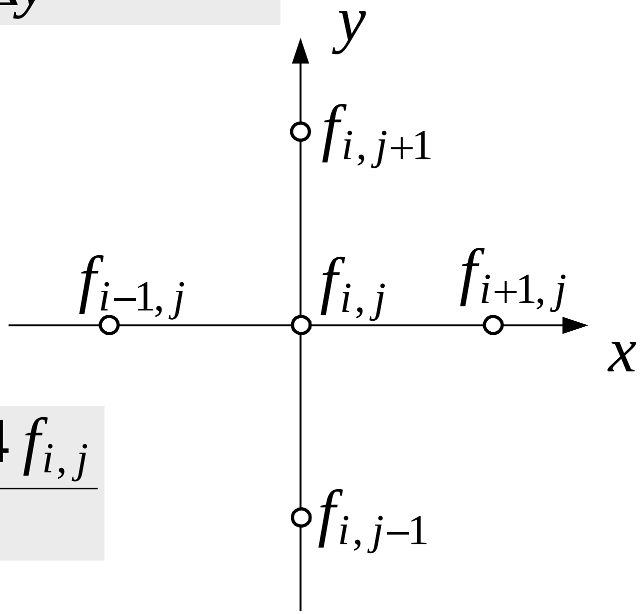
$$\boxed{\frac{d^2 f}{dx^2} = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2} + O^2}$$

3. Finite differences for derivative approximation – cont.

Laplace operator in 2-D space: (x, y)

$$\nabla^2_{xy} f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

$$\nabla^2_{xy} f \approx \frac{f_{i-1,j} + f_{i+1,j} - 2 f_{i,j}}{\Delta x^2} + \frac{f_{i,j-1} + f_{i,j+1} - 2 f_{i,j}}{\Delta y^2}$$



if $\quad \Delta x = \Delta y = \Delta h$

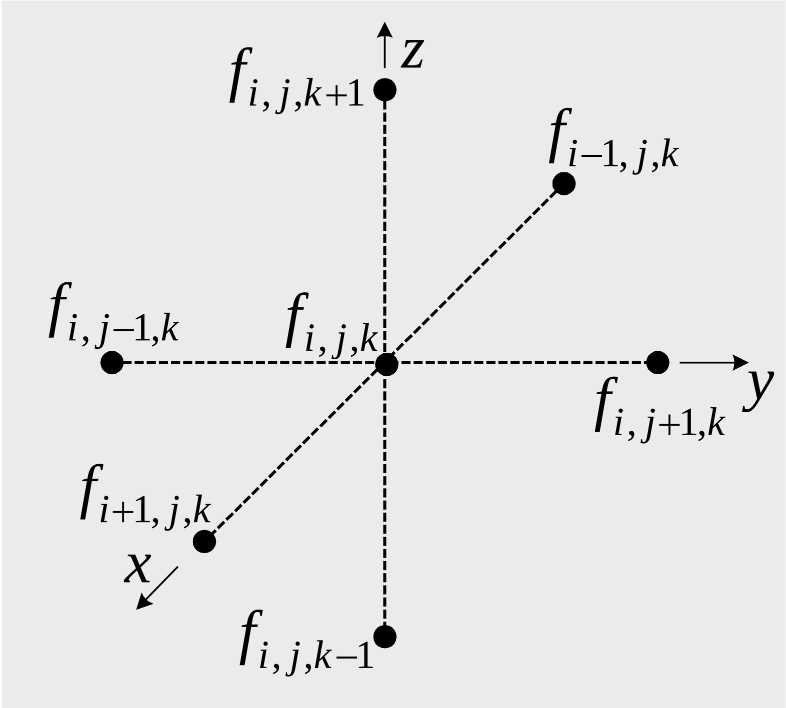
$$\nabla^2_{xy} f \approx \frac{f_{i-1,j} + f_{i+1,j} + f_{i,j-1} + f_{i,j+1} - 4 f_{i,j}}{\Delta h^2}$$

3. Finite differences for derivative approximation – cont.

Laplace operator in 3-D space (x, y, z)

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

$$\nabla^2 f \approx \frac{f_{i-1,j,k} + f_{i+1,j,k} - 2f_{i,j,k}}{\Delta x^2} + \frac{f_{i,j-1,k} + f_{i,j+1,k} - 2f_{i,j,k}}{\Delta y^2} + \frac{f_{i,j,k-1} + f_{i,j,k+1} - 2f_{i,j,k}}{\Delta z^2}$$



if $\Delta x = \Delta y = \Delta z = \Delta h$

$$\nabla^2 f \approx \frac{f_{i-1,j,k} + f_{i+1,j,k} + f_{i,j-1,k} + f_{i,j+1,k} + f_{i,j,k-1} + f_{i,j,k+1} - 6f_{i,j}}{\Delta h^2}$$

4. The wave equation in 1-D space

$$\frac{\partial^2 f}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 f}{\partial t^2} = -g(x,t)$$

general solution

$$f(x,t) = f^{+}(x-ct) + f^{-}(x+ct)$$

wave traveling in the $+x$ direction   wave traveling in the $-x$ direction

to determine the particular solution, we need

• 2 *boundary conditions*:

$\underline{\text{at} \quad x = 0}$

$$f(0,t) \quad \text{or} \quad \left.\frac{\partial f}{\partial x}\right|_{x=0}$$

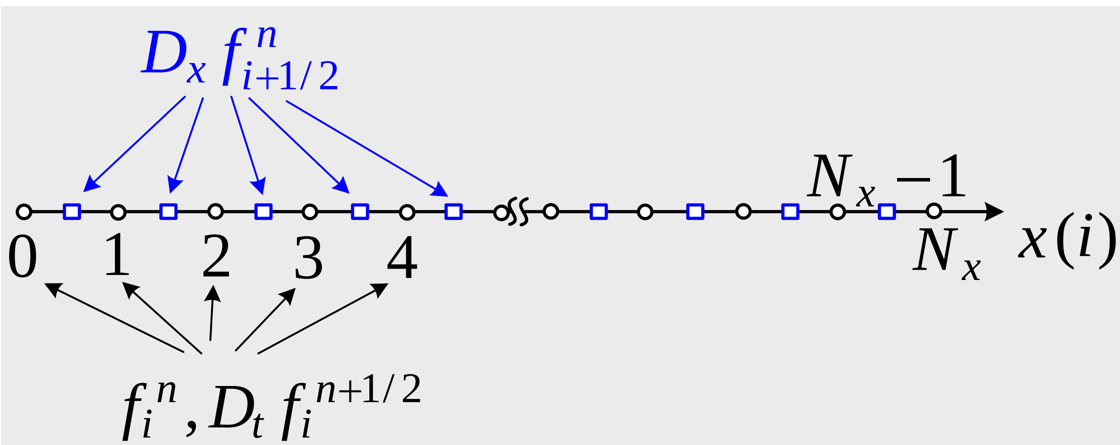
$\underline{\text{at} \quad x = x_{\max}}$

$$f(x_{\max},t) \quad \text{or} \quad \left.\frac{\partial f}{\partial x}\right|_{x=x_{\max}}$$

4. The wave equation in 1-D space – cont.

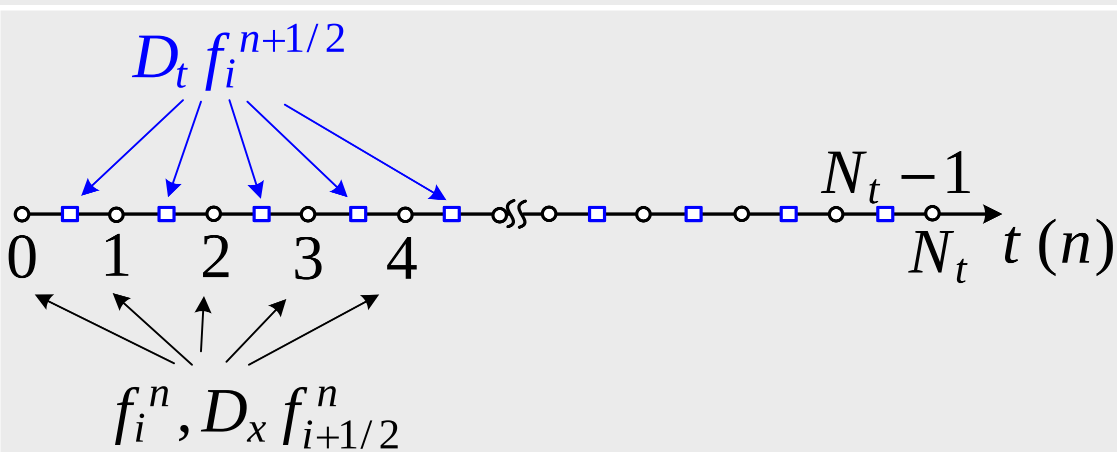
- 2 *initial conditions*: $f(x,0)$ and $\left.\dfrac{\partial f}{\partial t}\right|_{t=0}$

<u>Discretization</u>



$$f(i\Delta x, n\Delta t) = f_i^n$$

$$D_x f_{i+1/2}^n = f_{i+1}^n - f_i^n \approx \Delta x \left.\frac{\partial f}{\partial x}\right|_{\substack{x=(i+1/2)\Delta x,\\ t=n\Delta t}}$$



$$D_t f_i^{n+1/2} = f_i^{n+1} - f_i^n \approx \Delta t \left.\frac{\partial f}{\partial t}\right|_{\substack{x=i\Delta x,\\ t=(n+1/2)\Delta t}}$$

4. The wave equation in 1-D space – cont.

the discretized 1-D wave equation:

$$\frac{D_t f_i^{n+1/2} - D_t f_i^{n-1/2}}{(c\Delta t)^2} = \frac{f_{i+1}^n - 2 f_i^n + f_{i-1}^n}{\Delta x^2} + g_i^n$$

$$D_t f_i^{n+1/2} = D_t f_i^{n-1/2} + \underbrace{\left(\frac{c\Delta t}{\Delta x}\right)^2}_{\alpha} \Big(\underbrace{f_{i+1}^n - 2 f_i^n + f_{i-1}^n}_{D_{xx} f_i^n} + \Delta x^2 g_i^n \Big)$$

$$f_i^{n+1} = f_i^n + D_t f_i^{n+1/2}$$

The above update scheme requires: (i) the function values at the n-th moment of time, and (ii) the derivative values from the previous step at the ($n-1/2$) moment of time.

Thus, for each point of space, two numbers are stored in the computer memory: $f_i^n, D_t f_i^{n+1/2}$.

4. The wave equation in 1-D space – cont.

<u>Implementation of boundary conditions</u>

(a) Dirichlet BC (DBC)

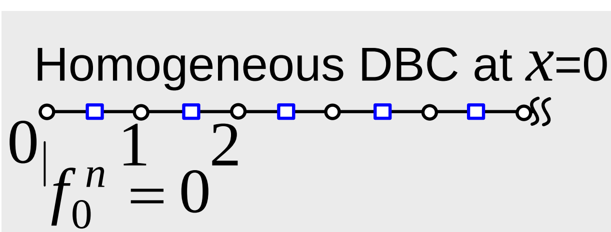
prescribes the function value at the boundary

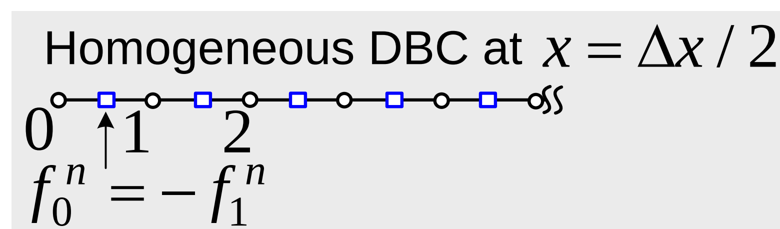
$$f_0^n = b_0, \quad n = 1, 2, \ldots$$

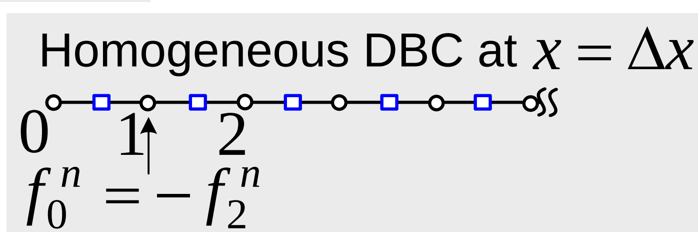
$$f_{N_x}^n = b_N, \quad n = 1, 2, \ldots$$

If the function boundary value is zero: *homogeneous BC*

Example: *homogeneous DBCs on a discrete mesh*







4. The wave equation in 1-D space – cont.

(b) Neumann BC (NBC)

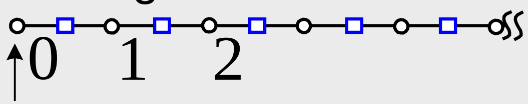
prescribes the boundary value of the function derivative

$$\frac{\partial f_0^n}{\partial x} = B_0, \quad n = 1, 2, \ldots$$

$$\frac{\partial f_{N_x}^n}{\partial x} = B_N, \quad n = 1, 2, \ldots$$

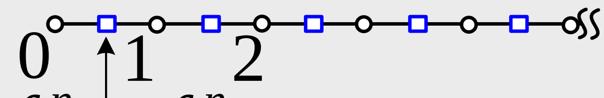
Example: *homogeneous NBCs on a discrete mesh*

Homogeneous NBC at x=0



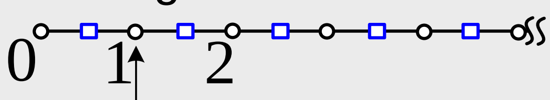
$$f_0^n = (4 f_1^n - f_2^n)/3$$

Homogeneous NBC at $x = \Delta x / 2$



$$f_0^n = f_1^n$$

Homogeneous NBC at $x = \Delta x$



$$f_0^n = f_2^n$$

5. The wave equation in 2-D and 3-D space

The only difference with the 1-D wave equation is that the second-order derivative wrt x is replaced by the Laplace operator $\Delta = \nabla^2$.

<u>Discretized wave equation</u>

$$D_t^{n+1/2} f_{i,j,k} = D_t^{n-1/2} f_{i,j,k} + \underbrace{\left(\frac{c\Delta t}{\Delta h}\right)^2}_{\alpha} \left(Lf_{i,j,k}^{n} + \Delta h^2 g_{i,j,k}^{n} \right)$$

where L is the discrete Laplace operator, and

$\Delta h = \min(\Delta x, \Delta y, \Delta z)$

$$Lf \approx \Delta h^2 \nabla^2 f$$

<u>in 2-D</u>

$$Lf = \left(\frac{\Delta h}{\Delta x}\right)^2 (f_{i+1,j}^{n} - 2 f_{i,j}^{n} + f_{i-1,j}^{n}) + \left(\frac{\Delta h}{\Delta y}\right)^2 (f_{i,j+1}^{n} - 2 f_{i,j}^{n} + f_{i,j-1}^{n})$$

5. The wave equation in 2-D and 3-D space – cont.

<u>in 2-D</u>

when $\Delta x = \Delta y = \Delta h$

$$Lf = (f^n_{i+1,j} + f^n_{i-1,j} + f^n_{i,j+1} + f^n_{i,j-1} - 4 f^n_{i,j})$$

<u>in 3-D</u>

$$Lf = \left(\frac{\Delta h}{\Delta x}\right)^2 (f^n_{i+1,j,k} - 2 f^n_{i,j,k} + f^n_{i-1,j,k}) +$$
$$\left(\frac{\Delta h}{\Delta y}\right)^2 (f^n_{i,j+1,k} - 2 f^n_{i,j,k} + f^n_{i,j-1,k}) +$$
$$\left(\frac{\Delta h}{\Delta z}\right)^2 (f^n_{i,j,k+1} - 2 f^n_{i,j,k} + f^n_{i,j,k-1})$$

$\Delta x = \Delta y = \Delta z = \Delta h$

$$Lf = (f^n_{i+1,j,k} + f^n_{i-1,j,k} + f^n_{i,j+1,k} + f^n_{i,j-1,k} + f^n_{i,j,k+1} + f^n_{i,j,k-1} - 6 f^n_{i,j})$$

6. Space quantization – minimal spatial step

The size of the minimal spatial step Δh is crucial for the accuracy of the algorithm.

Consider a sinusoidal wave propagating along +*x* in free space.

$$f(x,t) = \sin\left(\beta x - \omega t\right)$$

$\beta = \omega / c$ - wave number (phase constant)

The discretized sine wave is

$$f_i^n = \sin\left(\beta i \Delta h - \omega n \Delta t\right)$$

The 2-nd order *x*-derivative of the continuous sine wave is

$$\frac{\partial^2 f}{\partial x^2} = -\beta^2 \sin(\beta x - \omega t)$$

6. Space quantization – minimal spatial step, cont.

The 2-nd order *x*-derivative of the discretized sine wave is

$$\frac{f_{i-1}^{n} - 2f_{i}^{n} + f_{i+1}^{n}}{\Delta h^2} = \frac{2}{\Delta h^2} \cdot \left(\cos \beta\Delta h - 1\right) \cdot \sin(\beta i \Delta h - \omega n t)$$

In order both derivatives to be equal

$$\cos \beta\Delta h - 1 = -\frac{\beta^2 \Delta h^2}{2}$$

must hold. The above equality is accurate to about 1% if

$$\beta\Delta h \le 0.69 \approx \pi / 4.5$$

In terms of the wavelength

$$\Delta h \le \lambda / 9, \quad \lambda = 2\pi / \beta$$

For sufficient accuracy in 1-D problems, $\boxed{\Delta h \le \lambda_{\min} / 9}$

7. Time quantization – minimal time step

Similar analysis with respect to the time derivatives of the analog and digital sine wave shows that the time step has to satisfy

$$\boxed{\Delta t \le T_{\min} / 9, \;\; T_{\min} = 2\pi / \omega_{\max}}$$

8. Stability criterion (Courant-Friedrich-Levy criterion)

Explicit time-stepping algorithms for the solution of dynamic problems are prone to ***instabilities*** if certain criteria are not satisfied. Instability is a spurious (nonphysical, due to numerical errors) increase of the numerical values of the field as the time-marching proceeds. Often, this is observed as an exponential increase.

8. Stability (CFL) criterion – cont.

Consider a harmonic plane wave of <u>real-valued</u> frequency ω

$$f(x,y,z,t) = f_0 e^{\mathrm{i}(\omega t - \beta_x x - \beta_y y - \beta_z z)}$$

It satisfies the wave equation in 3-D

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 f}{\partial t^2} = 0$$

When discretized, this wave is represented as

$$f_{i,j,k}^{n} = f_0 e^{\mathrm{i}(\omega n\Delta t - \beta_x i\Delta x - \beta_y j\Delta y - \beta_z k\Delta z)}$$

8. Stability (CFL) criterion – cont.

Applying centrals FDs to the 3-D wave equation, we find that the discretized wave must satisfy

$$\frac{f^n_{i+1,j,k} - 2f^n_{i,j,k} + f^n_{i-1,j,k}}{\Delta x^2} + \frac{f^n_{i,j+1,k} - 2f^n_{i,j,k} + f^n_{i,j-1,k}}{\Delta y^2} + \frac{f^n_{i,j,k+1} - 2f^n_{i,j,k} + f^n_{i,j,k-1}}{\Delta z^2} = \frac{f^{n-1}_{i,j,k} - 2f^n_{i,j,k} + f^{n+1}_{i,j,k}}{c^2 \Delta t^2}$$

8. Stability (CFL) criterion – cont.

Substitution of the discretized wave into the discretized 3-D wave equation leads to

$$\frac{e^{-\mathrm{i}\beta_x\Delta x}-2+e^{\mathrm{i}\beta_x\Delta x}}{\Delta x^2}+\frac{e^{-\mathrm{i}\beta_y\Delta y}-2+e^{\mathrm{i}\beta_y\Delta y}}{\Delta y^2}+\frac{e^{-\mathrm{i}\beta_z\Delta z}-2+e^{\mathrm{i}\beta_z\Delta z}}{\Delta z^2}$$

$$=\frac{e^{-\mathrm{i}\omega\Delta t}-2+e^{+\mathrm{i}\omega\Delta t}}{c^2\Delta t^2}$$

which can also be written as

$$\left[\frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right]^2$$

$$=\left[\frac{1}{\Delta x}\sin\left(\frac{\beta_x\Delta x}{2}\right)\right]^2+\left[\frac{1}{\Delta y}\sin\left(\frac{\beta_y\Delta y}{2}\right)\right]^2+\left[\frac{1}{\Delta z}\sin\left(\frac{\beta_z\Delta z}{2}\right)\right]^2$$

8. Stability (CFL) criterion – cont.

Solving for ω gives

$$\omega = \frac{2}{\Delta t}\arcsin\left(c\Delta t\sqrt{T_x + T_y + T_z}\right) \quad \text{where}$$

$$T_\xi = \frac{1}{\Delta\xi^2}\sin^2\left(\frac{\beta_\xi \Delta\xi}{2}\right), \;\; \xi \equiv x, y, z$$

In order ω to be real (so that the wave does not increase or decrease exponentially in magnitude)

$$c\Delta t\sqrt{\frac{1}{\Delta x^2}\sin^2\left(\frac{\beta_x \Delta x}{2}\right) + \frac{1}{\Delta y^2}\sin^2\left(\frac{\beta_y \Delta y}{2}\right) + \frac{1}{\Delta z^2}\sin^2\left(\frac{\beta_z \Delta z}{2}\right)} \le 1$$

This must be fulfilled in the worst-case scenario of all sine-squared functions being 1.

8. Stability (CFL) criterion – cont.

$$\Rightarrow \boxed{\Delta t \le \frac{1}{c\sqrt{\dfrac{1}{\Delta x^2} + \dfrac{1}{\Delta y^2} + \dfrac{1}{\Delta z^2}}}}$$

This condition is known as the Courant-Friedrich-Levy (CFL) or Courant's condition

If $\Delta x = \Delta y = \Delta z = \Delta h,$

$$(c\Delta t)^2 \le \frac{\Delta h^2}{3} \quad \Rightarrow \quad \boxed{\alpha = \frac{c\Delta t}{\Delta h} \le \frac{1}{\sqrt{3}}}$$

8. Stability (CFL) criterion – cont.

3-D $\quad \boxed{(c\Delta t)^2 \le \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1}} \Rightarrow \boxed{\alpha = \frac{c\Delta t}{\Delta h} \le \frac{1}{\sqrt{3}}}$

2-D $\quad \boxed{(c\Delta t)^2 \le \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1}} \Rightarrow \boxed{\alpha = \frac{c\Delta t}{\Delta h} \le \frac{1}{\sqrt{2}}}$

1-D $\quad \boxed{(c\Delta t)^2 \le \Delta x^2} \Rightarrow \boxed{\alpha = \frac{c\Delta t}{\Delta h} \le 1}$

In a 1-D problem, if the accuracy criterion of the spatial quantization $\Delta h \le \lambda / 9$ is observed, then the accuracy criterion of the time quantization $\Delta t \le T / 9$ is automatically satisfied provided that the stability criterion is enforced.

Note: For 2-D and 3-D problems, the accuracy criteria should be adjusted accordingly, e.g.,

$$\Delta h \le \lambda_{\min} / (9\sqrt{3}) \approx \lambda_{\min} / 16$$