LECTURE 9

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

NATALIA K. NIKOLOVA

talia@mcmaster.ca

CRL 223, ext. 27141

1. Outline

- finite differences for derivative approximation
- the wave equation in 1-D
  - initial/boundary conditions and excitation sources
- generalisation 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] A. Taflove, *Computational Elertodynamics: the Finite-Difference Time-Domain Method*, Artech, 1995

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

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

[5] Kane 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

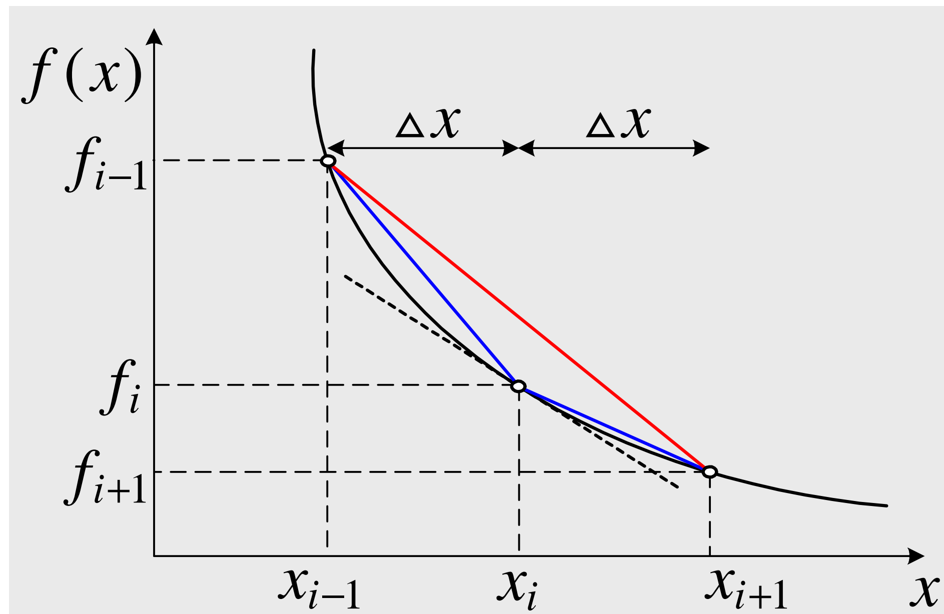
$$\frac{df(x_i)}{dx} = \frac{df_i}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}$$

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 $x_i + \Delta x$

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

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

at $x_i - \Delta x$

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

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

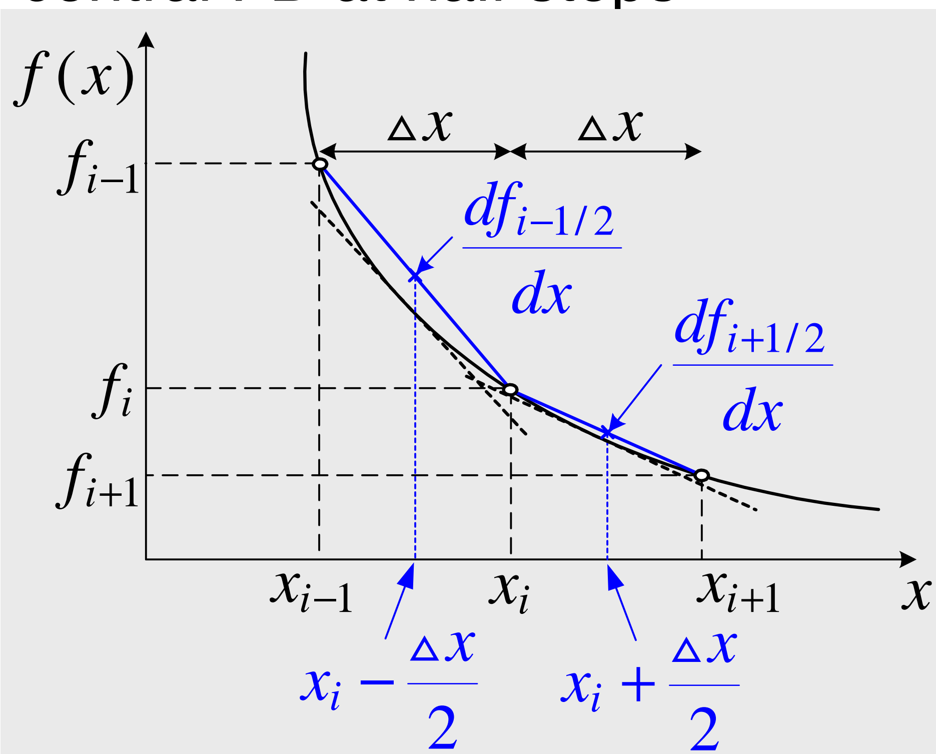
forward and backward FDs have 1st order accuracy

3. Finite differences for derivative approximation – cont.

accuracy: central FDs have 2nd order accuracy!

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

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

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

<u>2nd order derivatives</u>

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

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

+

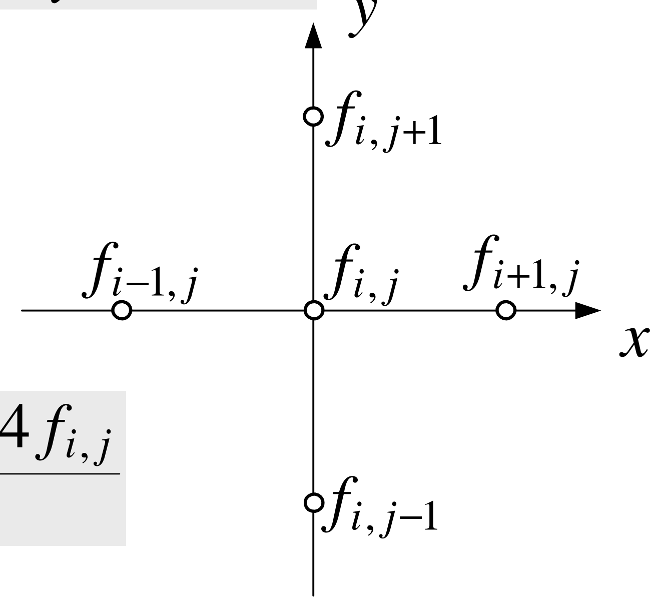
$$\frac{d^2 f}{dx^2} = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2} + O^2$$

3. Finite differences for derivative approximation – cont.

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

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

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



if $\triangle x = \triangle y = \triangle h$

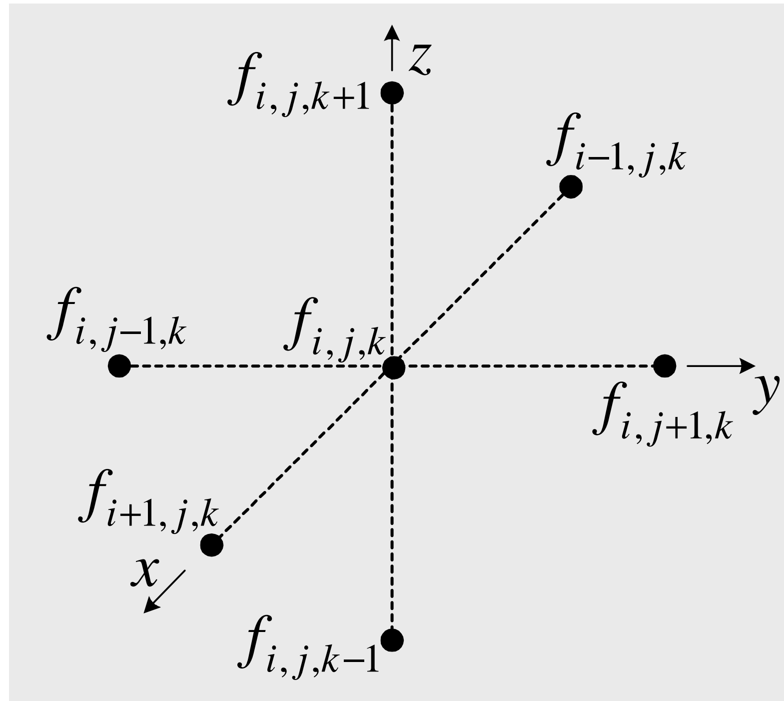
$$\nabla^2_{xy} f \approx \frac{f_{i-1,j} + f_{i+1,j} + f_{i,j-1} + f_{i,j+1} - 4f_{i,j}}{\triangle h^2}$$

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

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

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, one needs
2 boundary conditions:

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

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

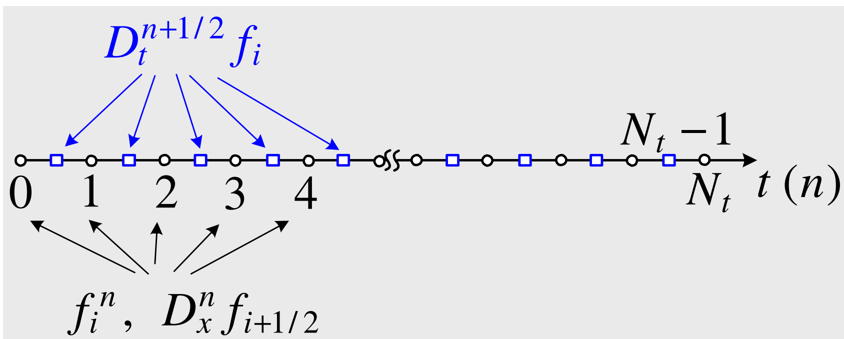
$\underline{\text{at} \quad x = x_{\max}}$

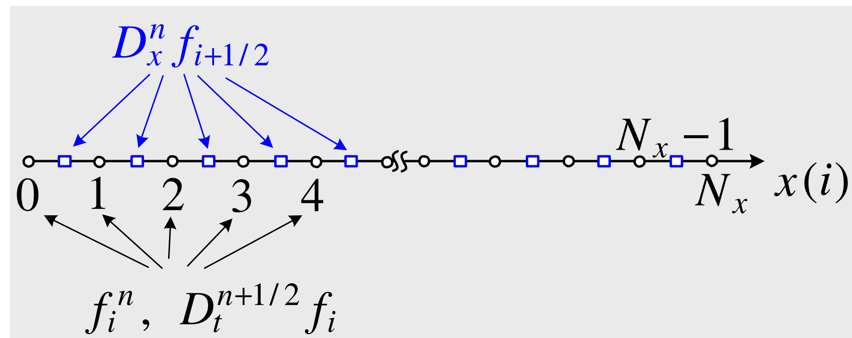
$f(x_{\max},t) \quad \text{or} \quad \left.\frac{\partial f}{\partial x}\right|_{x=x_{\max}}$

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

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

<u>Discretization</u> notations





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

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

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

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

the discretized 1-D wave equation

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

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

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

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: $f_i, D_t f_i$.

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

Implementation of boundary conditions

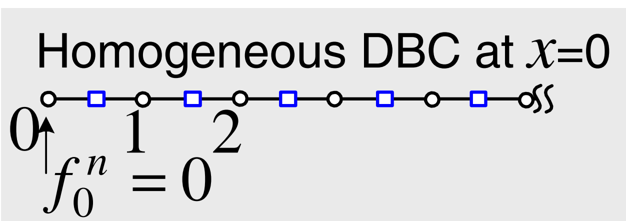
(a) Dirichlet BC (DBC)
prescribes the function value at the boundary

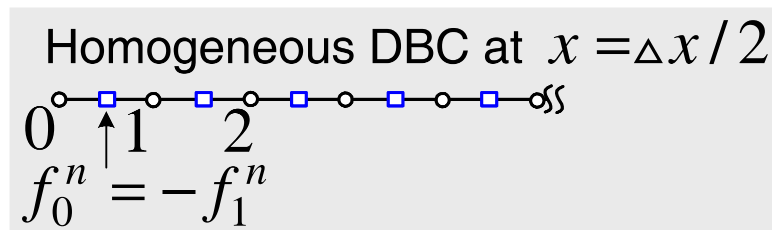
$$f_0^n = b_0, \quad n = 1, 2, \ldots$$

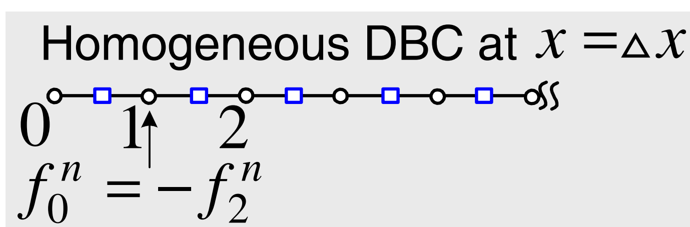
$$f_{N_x}^n = b_N, \quad n = 1, 2, \ldots$$

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)

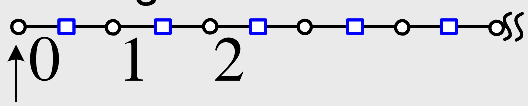
prescribes the boundary value of the function derivative

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

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

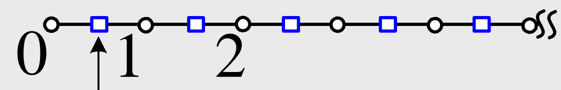
Example: *homogeneous NBCs on a discrete mesh*

Homogeneous NBC at x=0



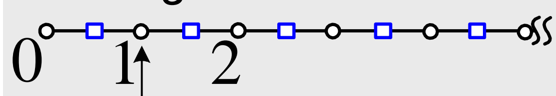
$f_0^n = (4 f_1^n - f_2^n)/3$

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 *L*

<u>Discretized wave equation</u>

α

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

where L is the discrete Laplace operator, and

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

<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.

in 2-D

when $\triangle x = \triangle y = \triangle h$

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

in 3-D

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

$\triangle x = \triangle y = \triangle z = \triangle h$

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

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.

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

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

The discretized wave is

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

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

$$\frac{f_{i-1}^{n} - 2f_i^{n} + f_{i+1}^{n}}{\triangle h^2} = \frac{2}{\triangle h^2}(\cos \beta \triangle h - 1)\sin(\beta i \triangle h - \omega n t)$$

In order both derivatives to be equal

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

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

$$\beta \triangle h \le 0.35$$

In terms of wavelength

$$\triangle h \le \lambda / 18, \quad \lambda = 2\pi / \beta$$

7. Time quantization – minimal time step

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

$$\Delta t \leq T/18, \quad T = 2\pi/\omega$$

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 criterion – cont.

Consider the numerical eigenvalue Λ generated by the numerical time derivative

$$\frac{\partial^2 f_i^n}{\partial t^2} \approx \frac{f_i^{n-1} - 2 f_i^n + f_i^{n+1}}{\Delta t^2} = \Lambda f_i^n$$

We define a constant growth factor at the point i as

$$q_i = \frac{f_i^{n+1}}{f_i^n} \approx \frac{f_i^n}{f_i^{n-1}} \quad \text{for all} \quad n$$

When there are no sources ($g = 0$), stability requires that $|q_i| \leq 1$.

$$(q_i)^2 - (2 + \Lambda \Delta t^2) q_i + 1 = 0$$

$$q_i = (2 + \Lambda \Delta t^2)/2 \pm \sqrt{[(2 + \Lambda \Delta t^2)/2]^2 - 1}$$

8. Stability criterion – cont.

The requirement $|q_i| \leq 1$ is fulfilled if $[(2+\Lambda \Delta t^2)/2]^2 \leq 1$

$$q_i = (2+\Lambda \Delta t^2)/2 \pm j\sqrt{1-[(2+\Lambda \Delta t^2)/2]^2} \quad \Rightarrow \boxed{|q_i| = 1}$$

$$[(2+\Lambda \Delta t^2)/2]^2 \leq 1 \Rightarrow -1 \leq (2+\Lambda \Delta t^2)/2 \leq 1$$

$$\Rightarrow \boxed{-4/\Delta t^2 \leq \Lambda \leq 0}$$

This is the eigenvalue spectrum of a stable marching in time algorithm!

We consider next the eigenvalues of the discrete Laplace operator. They are related to the eigenvalues of the 2nd order time derivative through the wave equation.

$$c^2 L f_i^n = \Lambda f_i^n$$

8. Stability criterion – cont.

At any time step, the instantaneous distribution of the field in space can be Fourier-transformed with respect to the three spatial axes to produce its 3-D spatial spectrum, or the plane-wave eigenmodes of the 3-D grid. Each mode is represented as

$$\tilde{f}_i^n = f_0 e^{j(\beta_x I \Delta x + \beta_y J \Delta y + \beta_z K \Delta z)}$$

The total field is a superposition of all possible modes. We consider one such mode and look for the possible range of values of the characteristic numbers $\beta_x, \beta_y, \beta_z$. Upon substitution in the discrete Laplace operator and factoring out $f_0 e^{j(\beta_x I \Delta x + \beta_y J \Delta y + \beta_z K \Delta z)}$, we obtain

8. Stability criterion – cont.

$$c^2\left[\frac{e^{-j\beta_x \Delta x} - 2 + e^{j\beta_x \Delta x}}{\Delta x^2} + \frac{e^{-j\beta_y \Delta y} - 2 + e^{j\beta_y \Delta y}}{\Delta y^2} + \frac{e^{-j\beta_z \Delta z} - 2 + e^{j\beta_z \Delta z}}{\Delta z^2}\right] = \Lambda$$

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

It is now obvious that the eigenvalues Λ are bound within

$$-4c^2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right) \le \Lambda \le 0$$

Compare with $-4/\Delta t^2 \le \Lambda \le 0$

8. Stability criterion – cont.

To guarantee numerical stability for any spatial mode, the range of eigenvalues for the spatial modes

$$-4c^2\left(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2}\right)\le \Lambda \le 0$$

must be contained completely within the stable range of the time-stepping eigenvalues

$$-4/\Delta t^2 \le \Lambda \le 0$$

$$\Rightarrow \quad (c\Delta t)^2 \le \left(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2}\right)^{-1}$$

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

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

8. Stability criterion – cont.

<u>3-D</u>

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

<u>2-D</u>

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

<u>1-D</u>

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

In a 1-D problem, if the accuracy criterion of the spatial quantization $\Delta h \le \lambda / 18$ is observed, then the accuracy criterion of the time quantization $\Delta t \le T / 18$ is automatically satisfied provided that the stability criterion is enforced.
Note: For 2-D and 3-D problems, the accuracy criterions should be adjusted accordingly, e.g.,

$$\Delta h \le \lambda / (18\sqrt{3}) \approx \lambda / 32$$