LECTURE 11

THE FDTD METHOD – PART III

11. Yee's discrete algorithm

Maxwell's equations are discretized using central FDs. We set the magnetic loss equal to zero. Then,

$$\sigma_m = 0, \quad \mathbf{J}_m^i = 0$$

$$H_{x_{i,j,k}}^{n+0.5} = H_{x_{i,j,k}}^{n-0.5} - \frac{\Delta t}{\mu} \cdot \left[\frac{E_{z_{i,j+1,k}}^n - E_{z_{i,j,k}}^n}{\Delta y} - \frac{E_{y_{i,j,k+1}}^n - E_{y_{i,j,k}}^n}{\Delta z} \right]$$

$$H_{y_{i,j,k}}^{n+0.5} = H_{y_{i,j,k}}^{n-0.5} - \frac{\Delta t}{\mu} \cdot \left[\frac{E_{x_{i,j,k+1}}^n - E_{x_{i,j,k}}^n}{\Delta z} - \frac{E_{z_{i+1,j,k}}^n - E_{z_{i,j,k}}^n}{\Delta x} \right]$$

$$H_{z_{i,j,k}}^{n+0.5} = H_{z_{i,j,k}}^{n-0.5} - \frac{\Delta t}{\mu} \cdot \left[\frac{E_{y_{i+1,j,k}}^n - E_{y_{i,j,k}}^n}{\Delta x} - \frac{E_{x_{i,j+1,k}}^n - E_{x_{i,j,k}}^n}{\Delta y} \right]$$

11. Yee's discrete algorithm – cont.

$$E^{n+1}_{x_{i,j,k}} = k^E_E \cdot E^n_{x_{i,j,k}} + k^E_H \cdot \left[\frac{H^{n+0.5}_{z_{i,j,k}} - H^{n+0.5}_{z_{i,j-1,k}}}{\Delta y} - \frac{H^{n+0.5}_{y_{i,j,k}} - H^{n+0.5}_{y_{i,j,k-1}}}{\Delta z} - J^{i^{n+0.5}}_{ex_{i,j,k}} \right]$$

$$E^{n+1}_{y_{i,j,k}} = k^E_E \cdot E^n_{y_{i,j,k}} + k^E_H \cdot \left[\frac{H^{n+0.5}_{x_{i,j,k}} - H^{n+0.5}_{x_{i,j,k-1}}}{\Delta z} - \frac{H^{n+0.5}_{z_{i,j,k}} - H^{n+0.5}_{z_{i-1,j,k}}}{\Delta x} - J^{i^{n+0.5}}_{ey_{i,j,k}} \right]$$

$$E^{n+1}_{z_{i,j,k}} = k^E_E \cdot E^n_{z_{i,j,k}} + k^E_H \cdot \left[\frac{H^{n+0.5}_{y_{i,j,k}} - H^{n+0.5}_{y_{i-1,j,k}}}{\Delta x} - \frac{H^{n+0.5}_{x_{i,j,k}} - H^{n+0.5}_{x_{i,j-1,k}}}{\Delta y} - J^{i^{n+0.5}}_{ez_{i,j,k}} \right]$$

$$k^E_E = \frac{1 - \frac{\sigma_e \Delta t}{2\varepsilon}}{1 + \frac{\sigma_e \Delta t}{2\varepsilon}} \qquad k^E_H = \frac{\frac{\Delta t}{\varepsilon}}{1 + \frac{\sigma_e \Delta t}{2\varepsilon}} \qquad \sigma_e \neq 0$$

11. Yee's discrete algorithm – cont.

The above coefficients are obtained by averaging the *E*-field, which appears in the loss term. For example,

$$\varepsilon \frac{\partial E_x}{\partial t} + \sigma_e E_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - J_{ex}^i \Rightarrow$$

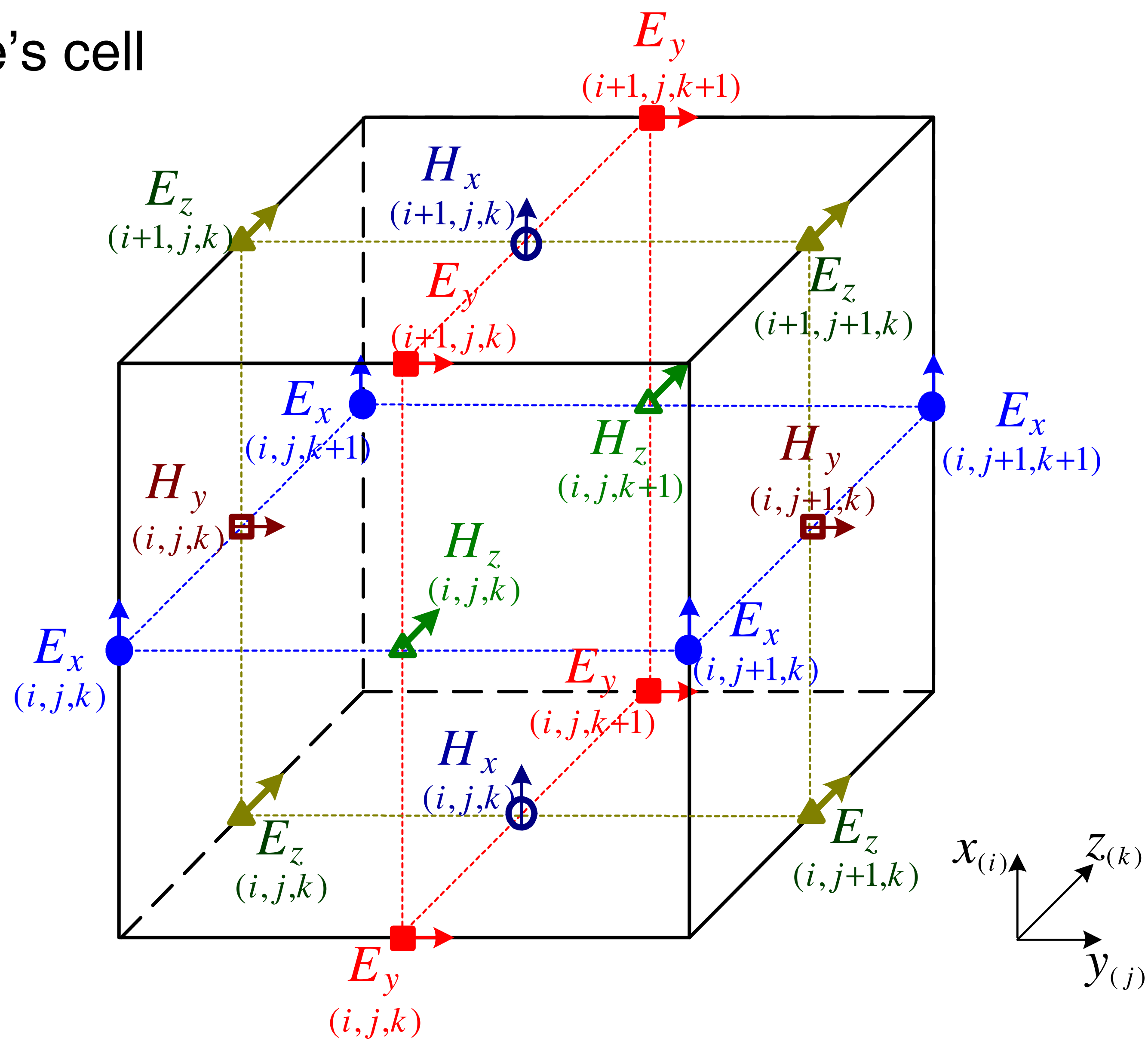
$$\varepsilon \frac{E_{x_{i,j,k}}^{n+1} - E_{x_{i,j,k}}^{n}}{\triangle t} + \sigma_e \frac{E_{x_{i,j,k}}^{n+1} + E_{x_{i,j,k}}^{n}}{2} =$$

$$\frac{H_{z_{i,j,k}}^{n+0.5} - H_{z_{i,j-1,k}}^{n+0.5}}{\triangle y} - \frac{H_{y_{i,j,k}}^{n+0.5} - H_{y_{i,j,k-1}}^{n+0.5}}{\triangle z} - J_{ex_{i,j,k}}^i$$

The discretization steps in time and in space, as well as the numerical constant $\alpha = c\triangle t / \triangle h$ are determined as for the wave equation.

11. Yee's discrete algorithm – cont.

Yee's cell



11. Yee's discrete algorithm – cont.

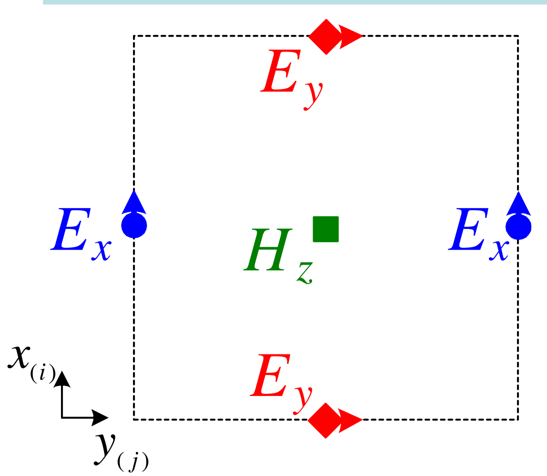
2-D problems and their discretization

The 2-D TE_z mode

$$\mu\frac{\partial H_z}{\partial t}+\sigma_m H_z=-\left(\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}\right)$$

$$\varepsilon\frac{\partial E_x}{\partial t}+\sigma_e E_x=\frac{\partial H_z}{\partial y}-J^i_{ex}$$

$$\varepsilon\frac{\partial E_y}{\partial t}+\sigma_e E_y=-\frac{\partial H_z}{\partial x}-J^i_{ey}$$

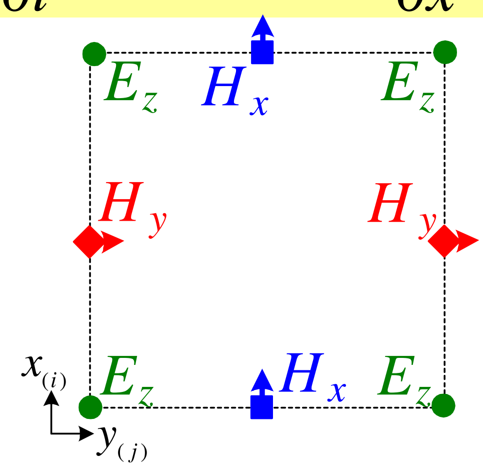


The 2-D TM_z mode

$$\varepsilon\frac{\partial E_z}{\partial t}+\sigma_e E_z=\frac{\partial H_y}{\partial x}-\frac{\partial H_x}{\partial y}-J^i_{ez}$$

$$\mu\frac{\partial H_x}{\partial t}+\sigma_m H_x=-\frac{\partial E_z}{\partial y}$$

$$\mu\frac{\partial H_y}{\partial t}+\sigma_m H_y=\frac{\partial E_z}{\partial x}$$



12. Absorbing (radiation) boundary conditions

ABCs constitute a special type of BCs, which simulate reflection-free propagation out of the computational domain. ABCs are necessary in open (radiation/scattering) problems, as well as in guided-wave problems where matched port terminations are needed.

The simplest to implement ABCs are associated with various approximations of a one-way plane wave propagation.

- One-way wave equation (Mur's ABC)
- Liao extrapolation
- Perfectly Matched Layers – basics
- Others: Higdon operator, Bayliss-Turkel annihilating operators, etc.

12. ABCs – cont.

A. <u>The one-way wave equation</u> (B.Engquist and A.Majda, "Absorbing boundary conditions for the numerical simulation of waves," *Mathematics of Computation*, vol. 31, 1977, pp. 629-651)

This is an equation which permits wave propagation in only one direction. Consider the 3-D scalar wave equation

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

The partial derivative operator is defined as

$$L=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}=\partial_x^2+\partial_y^2+\partial_z^2-c^{-2}\partial_t^2$$

We wish to simulate propagation along –*x* at *x*=0.

12. ABCs – cont.

The partial differential operator *L* can be factored, i.e., represented as sequentially applied two operators:

$$Lf = L^{+}L^{-}f = 0$$

$$L^{-} = \partial_x - c^{-1}\partial_t\sqrt{1-S^2} \qquad S^2 = \left(\frac{\partial_y}{c^{-1}\partial t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial t}\right)^2$$

$$L^{+} = \partial_x + c^{-1}\partial_t\sqrt{1-S^2}$$

The partial differential operators L^{+} and L^{-} are pseudo-differential operators. They cannot be applied directly to a function. Formally, the equation

$$L^{-}f = 0$$

represents a wave traveling along $-x$, while the equation

$$L^{+}f = 0$$

represents a wave traveling along $+x$.

12. ABCs – cont.

This becomes obvious in the case of a plane wave propagating along +/- *x*.

$$\partial_z = 0, \partial_y = 0 \Rightarrow S = 0 \qquad \Rightarrow L^- = \partial_x - c^{-1}\partial_t, \;\; L^+ = \partial_x + c^{-1}\partial_t$$

$$L^- f = \frac{\partial f}{\partial x} - \frac{1}{c}\frac{\partial f}{\partial t} = 0 \qquad \text{Solution: } f(x+ct)$$

$$L^+ f = \frac{\partial f}{\partial x} + \frac{1}{c}\frac{\partial f}{\partial t} = 0 \qquad \text{Solution: } f(x-ct)$$

The radical appearing in L^+ and L^- can be expanded using Taylor series

$$(1-S^2)^{1/2} = 1 - \frac{1}{2}S^2 + O(S^4)$$

12. ABCs – cont.

If S^2 is very small, then $(1-S^2)^{1/2} \approx 1$

The above is a first-order approximation of *S*. This means that the partial derivatives with respect to *y* and *z* are very small when compared with the partial derivative with respect to time scaled by the velocity of propagation *c*.

$$S^2 = \left(\frac{\partial_y}{c^{-1}\partial t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial t}\right)^2$$

This happens when the wave is incident upon the *x*=const. plane almost normally. The L^- operator then becomes

$$L^{-1} = \partial_x - c^{-1}\partial_t$$

$$\Rightarrow \quad L^- f = \partial_x f - c^{-1}\partial_t f = 0$$

12. ABCs – cont.

When the wave, however, impinges upon the *x*=0 boundary wall at larger angles, the 1st order approximation is very inaccurate. At grazing angles, *S* is large! For better accuracy, the second-order approximation can be used

$$(1-S^2)^{1/2} \approx 1-\frac{1}{2}S^2 \longleftarrow S^2 = \left(\frac{\partial_y}{c^{-1}\partial t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial t}\right)^2$$

The *L*- operator now becomes $L^- = \partial_x - c^{-1}\partial_t\left(1-\frac{1}{2}S^2\right)$

$$\Rightarrow L^- = \partial_x - c^{-1}\partial_t\left[1-\frac{1}{2}\left(\frac{\partial_y}{c^{-1}\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial_z}{c^{-1}\partial t}\right)^2\right]$$

$$L^- = \partial_x - \frac{\partial_t}{c} + \frac{1}{2}\frac{c}{\partial_t}\left(\partial_{yy}^2 + \partial_{zz}^2\right)$$

Multiplying by ∂_t

12. ABCs – cont.

$$L^- f = \partial^2_{xt} f - \frac{1}{c}\partial^2_{tt} f + \frac{c}{2}\left(\partial^2_{yy} f + \partial^2_{zz} f\right) = 0 \quad \text{at} \quad x = 0$$

$$L^+ f = \partial^2_{xt} f + \frac{1}{c}\partial^2_{tt} f - \frac{c}{2}\left(\partial^2_{yy} f + \partial^2_{zz} f\right) = 0 \quad \text{at} \quad x = x_{\max}$$

$$L^- f = \partial^2_{yt} f - \frac{1}{c}\partial^2_{tt} f + \frac{c}{2}\left(\partial^2_{xx} f + \partial^2_{zz} f\right) = 0 \quad \text{at} \quad y = 0$$

$$L^+ f = \partial^2_{yt} f + \frac{1}{c}\partial^2_{tt} f - \frac{c}{2}\left(\partial^2_{xx} f + \partial^2_{zz} f\right) = 0 \quad \text{at} \quad y = y_{\max}$$

etc.

12. ABCs – cont.

Mur's ABC of 2^{nd} order (G. Mur, "Absorbing boundary conditions for the finite-difference approximation of the time-domain electromagnetic field equations," *IEEE Trans. Electromagnetic Compatibility*, vol. 23, 1981, pp. 377-382.

Mur implemented the above approximate expressions into finite-difference equations. Mur expands the partial derivatives in the L^+/L^- operators using central finite differences of the field component about an auxiliary grid point displaced half a step along the direction of absorption and along time.

Consider propagation along –*x*, at the *x*=0 boundary. We assume that the scalar function U is evaluated at integer spatial grid positions (*i*,*j*,*k*) and time positions *n*.

$$\partial^2_{xt} f\Big|^n_{1/2,j,k} = \frac{1}{2\Delta t}\left(\frac{f^{n+1}_{1,j,k} - f^{n+1}_{0,j,k}}{\Delta x} - \frac{f^{n-1}_{1,j,k} - f^{n-1}_{0,j,k}}{\Delta x}\right)$$

12. ABCs – cont.

Now, the 2nd order time derivative has to be evaluated ½ step from the boundary as well. Mur averages the time derivatives at *x*=0 and *x*=1.

$$\partial_{tt}^2 f = \frac{1}{2}\left[\frac{f_{0,j,k}^{n+1} - 2f_{0,j,k}^{n} + f_{0,j,k}^{n-1}}{\Delta t^2} + \frac{f_{1,j,k}^{n+1} - 2f_{1,j,k}^{n} + f_{1,j,k}^{n-1}}{\Delta t^2}\right]$$

Now, the 2nd order *y*- and *z*- derivatives also have to be evaluated ½ step from the boundary. Mur averages those as well.

$$\partial_{yy}^2 f = \frac{1}{2}\left[\frac{f_{0,j-1,k}^{n} - 2f_{0,j,k}^{n} + f_{0,j+1,k}^{n}}{\Delta y^2} + \frac{f_{1,j-1,k}^{n} - 2f_{1,j,k}^{n} + f_{1,j+1,k}^{n}}{\Delta y^2}\right]$$

$$\partial_{zz}^2 f = \frac{1}{2}\left[\frac{f_{0,j,k-1}^{n} - 2f_{0,j,k}^{n} + f_{0,j,k+1}^{n}}{\Delta z^2} + \frac{f_{1,j,k-1}^{n} - 2f_{1,j,k}^{n} + f_{1,j,k+1}^{n}}{\Delta z^2}\right]$$

12. ABCs – cont.

Substitute all the FD approximations above in

$$L^- f = \partial^2_{xt} f - \frac{1}{c}\partial^2_{tt} f + \frac{c}{2}\left(\partial^2_{yy} f + \partial^2_{zz} f\right) = 0$$

The result is

$$\begin{aligned} f^{n+1}_{0,j,k} = &-f^{n-1}_{0,j,k} + k_1\left(f^{n+1}_{1,j,k} + f^{n-1}_{0,j,k}\right) + k_2\left(f^{n}_{0,j,k} + f^{n}_{1,j,k}\right) + \\ &+ k_{3y}\left(f^{n}_{0,j-1,k} - 2f^{n}_{0,j,k} + f^{n}_{0,j+1,k} + f^{n}_{1,j-1,k} - 2f^{n}_{1,j,k} + f^{n}_{1,j+1,k}\right) + \\ &+ k_{3z}\left(f^{n}_{0,j,k-1} - 2f^{n}_{0,j,k} + f^{n}_{0,j,k+1} + f^{n}_{1,j,k-1} - 2f^{n}_{1,j,k} + f^{n}_{1,j,k+1}\right) \end{aligned}$$

$$k_1 = \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x} \qquad k_2 = \frac{2\Delta x}{c\Delta t + \Delta x} \qquad k_{3y} = \frac{(c\Delta t)^2 \Delta x}{2\Delta y^2 (c\Delta t + \Delta x)}$$

$$k_{3z} = \frac{(c\Delta t)^2 \Delta x}{2\Delta z^2 (c\Delta t + \Delta x)}$$

12. ABCs – cont.

Mur's ABC of 1st order

To obtain Mur's approximation of

$$L^{-} f = \partial_x f - c^{-1}\partial_t f = 0$$

simply remove the 2nd order *y*- and *z*-derivatives from the formula above.

$$f_{0,j,k}^{n+1} = -f_{0,j,k}^{n-1} + k_1\left(f_{1,j,k}^{n+1} + f_{0,j,k}^{n-1}\right) + k_2\left(f_{0,j,k}^{n} + f_{1,j,k}^{n}\right)$$

$$k_1 = \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x} \qquad k_2 = \frac{2\Delta x}{c\Delta t + \Delta x}$$

In Yee's algorithm, the *E*-field components tangential to the boundary are evaluated at this boundary. For example, at an x=0 boundary wall, the E_y and E_z field components define the boundary values of the EM field problem. Mur's ABC is applied to them.

12. ABCs – cont.

B. <u>Liao's extrapolation</u> (Z.P. Liao, H.L. Wong, B.P. Yang, and Y.F. Yuan, "A transmitting boundary for transient wave analyses," Scientia Sinica (series A), vol. XXVII, 1984, pp. 1063-1076.)

The ABC known as Liao's ABC is easily explained as an extrapolation of the wave in space-time using Newton's backward-difference polynomial. It is an order less reflective than Mur's 2nd order ABC and does not depend strongly on the angle of incidence.

We now consider a boundary wall at x_{max}. We assume that the field values are know for points located along a straight line perpendicular to the boundary. The objective is to find an approximation of the field at the boundary at the next time step $f(x_{\max}, t + \Delta t)$.

12. ABCs – cont.

The field values used for the approximation are obtained by a simultaneous shift in space-time:

$$m=1 \quad f_1 = f\left(x_{\max} - \delta c \Delta t, t\right)$$
$$m=2 \quad f_2 = f\left(x_{\max} - 2\delta c \Delta t, t - \Delta t\right)$$
$$m=3 \quad f_3 = f\left(x_{\max} - 3\delta c \Delta t, t - 2\Delta t\right)$$
$$\vdots$$
$$m=N \quad f_N = f\left(x_{\max} - N\delta c \Delta t, t - (n-1)\Delta t\right)$$

Notice that such representation corresponds to a wave propagating in the +x direction: $f(x-ct)$

We aim at finding $f_0 = f(x_{\max}, t + \Delta t)$

12. ABCs – cont.

We now define backward finite-difference approximation of p^{th} order at the point $\xi_1 = (x_{\max} - \alpha c \triangle t, t)$.

$$D^1 f(\xi_1) \equiv \Delta^1 f_1 = f_1 - f_2$$

$$D^2 f(\xi_1) \equiv \Delta^2 f_1 = \Delta^1 f_1 - \Delta^1 f_2,$$

$$D^3 f(\xi_1) \equiv \Delta^3 f_1 = \Delta^2 f_1 - \Delta^2 f_2,$$

$$\vdots$$

$$D^N f(\xi_1) \equiv \Delta^N f_1 = \Delta^{N-1} f_1 - \Delta^{N-1} f_2$$

$$\Delta^1 f_2 = f_2 - f_3$$

$$\Delta^2 f_2 = \Delta^1 f_2 - \Delta^1 f_3$$

$$\Delta^1 f_3 = f_3 - f_4$$

$$f_m = f(\xi_m) = f\left(x_{\max} - m\delta c \triangle t, t - (m-1)\triangle t\right)$$

12. ABCs – cont.

The *N*-th backward difference can be written in terms of the function values as

$$\Delta^N f_1 = \sum_{m=1}^{N+1} (-1)^{m-1} C_{m-1}^N f_m,$$

where the Newton binomial coefficients are

$$C_{m-1}^N = \begin{pmatrix} N \\ m-1 \end{pmatrix} = \frac{N!}{(N-m+1)!(m-1)!}$$

Alternatively, a function can be expressed (interpolated) in terms of the backward finite differences at f_1

$$f_m \cong f_1 + \beta\Delta^1 f_1 + \frac{\beta(\beta+1)}{2!}\Delta^2 f_1 + \frac{\beta(\beta+1)(\beta+2)}{3!}\Delta^3 f_1 + \cdots$$
$$+ \frac{\beta(\beta+1)\cdots(\beta+N-2)}{(N-1)!}\Delta^{N-1} f_1, \quad 1 \le m \le N, \quad \beta = 1-m$$

12. ABCs – cont.

We now use the above formula to extrapolate the function values, and we set $m = 0$. Then, $\beta = 1$.

$$f_0 = f(t + \triangle t, x_{\max}) \cong f_1 + \Delta^1 f_1 + \Delta^2 f_1 + \Delta^3 f_1 + \cdots \Delta^{N-1} f_1$$

This is Liao's ABC. Liao *et al.* showed that for a sinusoidal plane wave of unit amplitude and wavelength λ, the maximum error is given by

$$|\Delta^N f|_{\max} = 2^N \sin^N(\pi c \triangle t / \lambda)$$

Assuming that

$$\triangle h = 2c\triangle t \quad \text{and} \quad \triangle h = \lambda / 32$$

the error is estimated at 0.1%. Liao's ABC is robust and depends little on the angle if incidence. With orders higher than N=3, however, it sometimes causes instabilities.

12. ABCs – cont.

$$f_0 = f(t + \Delta t, x_{max}) \cong f_1 + \Delta^1 f_1 + \Delta^2 f_1 + \Delta^3 f_1 + \cdots \Delta^{N-1} f_1$$

Liao's ABC is simple to implement.

```
! ABC in MAIN
ix2=nt-((nt-1)/2)*2
ix3=nt-((nt-1)/3)*3
ix4=nt-((nt-1)/4)*4

F0=>AX(:,:,nk);F1=>AX(:,:,nk-1)       ! front, ABC
F2=>A2_F(:,:,ix2);F3=>A3_F(:,:,ix3);F4=>A4_F(:,:,ix4)
call LIAO(ni,nj)
```

```
! before end of cycle
! history
A2_B(:,:,ix2)=AX(:,:,3)
A3_B(:,:,ix3)=AX(:,:,4)
A4_B(:,:,ix4)=AX(:,:,5)
```

```
*******************************************************************************************
subroutine LIAO(dim1,dim2)

D1=F1-F2;D2=F2-F3;D3=F3-F4
DD1=D1-D2;DD2=D2-D3
DDD1=DD1-DD2

F0=F1+D1+DD1+DDD1
return
end subroutine LIAO
```

```
! define variables
real(8),dimension(ni,nj,2),target:: A2_F,A2_B
real(8),dimension(ni,nj,3),target:: A3_F,A3_B
real(8),dimension(ni,nj,4),target:: A4_F,A4_B
real(8),dimension(:,:),pointer:: F0,F1,F2,F3,F4
```

Important topics not discussed in this overview lecture

Perfectly Matched Layer ABC

FDTD on curvilinear grids

FDTD in dispersive and anisotropic media

FDTD in nonlinear and gain materials

Integrating lumped elements with the FDTD full-wave analysis

Near-to-Far-Field transformation for antenna radiation patterns

Modified implicit FDTD schemes – the FDTD-ADI