THE FINITE-DIFFERENCE TIME-DOMAIN (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.

$$E_{x_{i,j,k}}^{n+1} = k_E^E \cdot E_{x_{i,j,k}}^{n} + k_H^E \cdot \left[\frac{H_{z_{i,j,k}}^{n+0.5} - H_{z_{i,j-1,k}}^{n+0.5}}{\triangle y} - \frac{H_{y_{i,j,k}}^{n+0.5} - H_{y_{i,j,k-1}}^{n+0.5}}{\triangle z} - J_{ex_{i,j,k}}^{i\,n+0.5} \right]$$

$$E_{y_{i,j,k}}^{n+1} = k_E^E \cdot E_{y_{i,j,k}}^{n} + k_H^E \cdot \left[\frac{H_{x_{i,j,k}}^{n+0.5} - H_{x_{i,j,k-1}}^{n+0.5}}{\triangle z} - \frac{H_{z_{i,j,k}}^{n+0.5} - H_{z_{i-1,j,k}}^{n+0.5}}{\triangle x} - J_{ey_{i,j,k}}^{i\,n+0.5} \right]$$

$$E_{z_{i,j,k}}^{n+1} = k_E^E \cdot E_{z_{i,j,k}}^{n} + k_H^E \cdot \left[\frac{H_{y_{i,j,k}}^{n+0.5} - H_{y_{i-1,j,k}}^{n+0.5}}{\triangle x} - \frac{H_{x_{i,j,k}}^{n+0.5} - H_{x_{i,j-1,k}}^{n+0.5}}{\triangle y} - J_{ez_{i,j,k}}^{i\,n+0.5} \right]$$

$$k_E^E = \frac{1 - \dfrac{\sigma_e \triangle t}{2\varepsilon}}{1 + \dfrac{\sigma_e \triangle t}{2\varepsilon}} \qquad k_H^E = \frac{\dfrac{\triangle t}{\varepsilon}}{1 + \dfrac{\sigma_e \triangle t}{2\varepsilon}} \qquad \sigma_e \neq 0$$

11. Yee's discrete algorithm – cont.

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

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

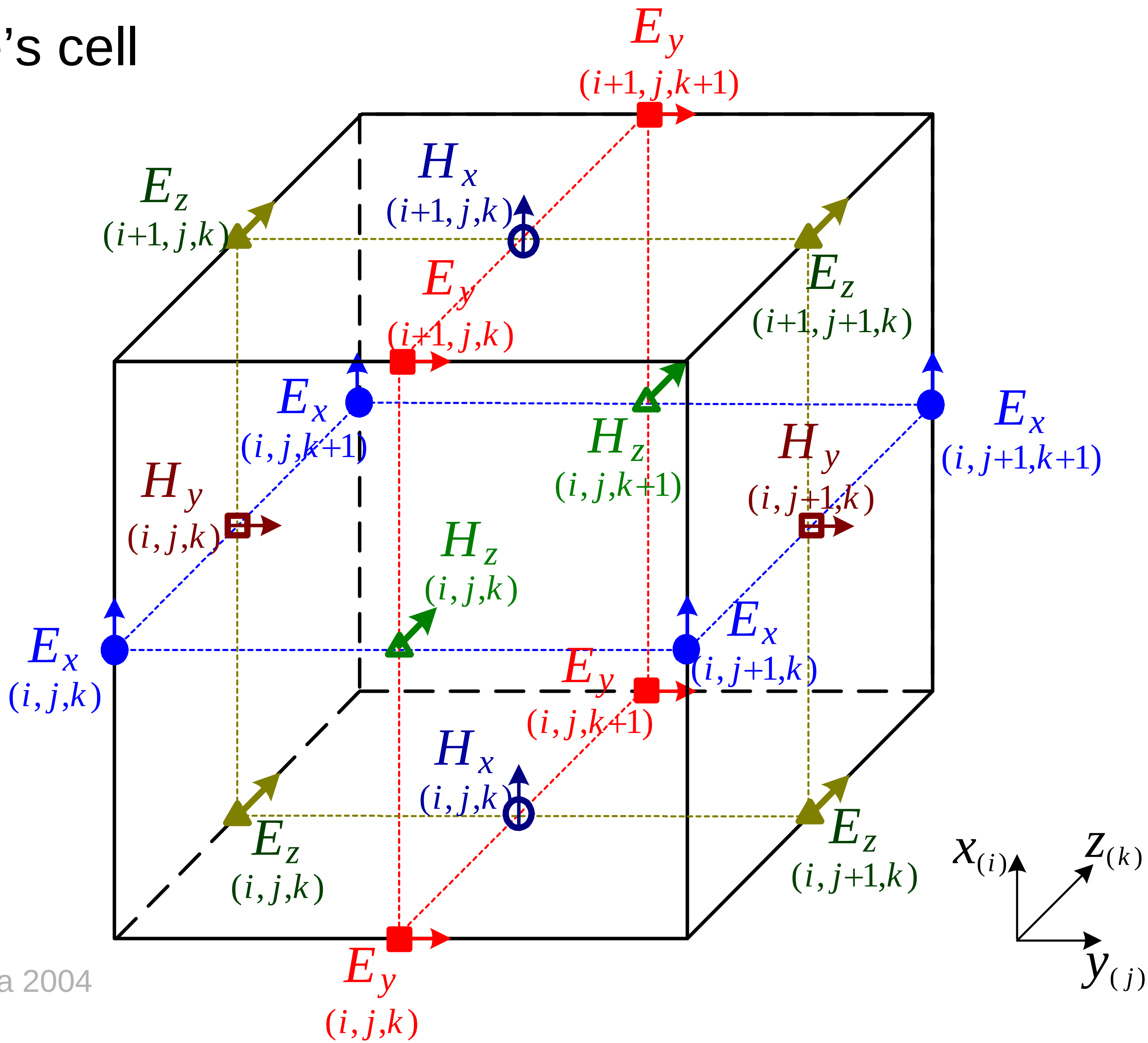
$$\varepsilon \frac{E_{x_{i,j,k}}^{n+1} - E_{x_{i,j,k}}^{n}}{\triangle t} + \sigma_e \frac{E_{x_{i,j,k}}^{n+1} + E_{x_{i,j,k}}^{n}}{2} =$$

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

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.

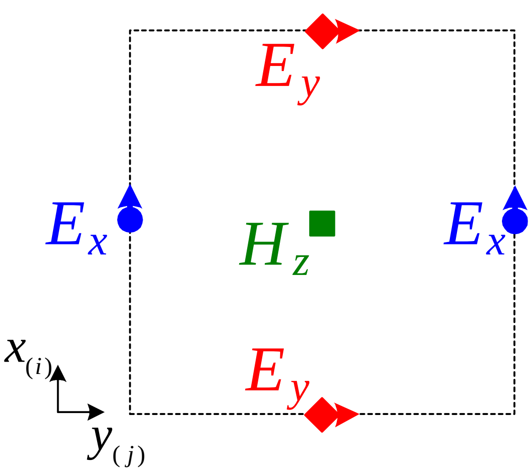
2-D problems and their discretization

The 2-D TE_z mode

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

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

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

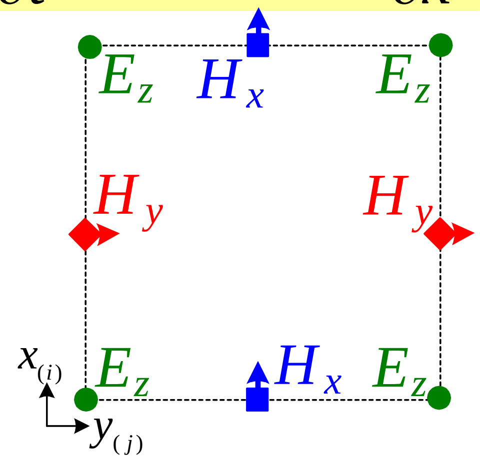


The 2-D TM_z mode

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

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

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



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 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 one-way 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:

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

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

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

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

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*.

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

$$L^- f = \frac{\partial f}{\partial x} - \frac{1}{c}\frac{\partial f}{\partial t} = 0$$

Solution: $f(x+ct)$

$$L^+ f = \frac{\partial f}{\partial x} + \frac{1}{c}\frac{\partial f}{\partial t} = 0$$

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

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

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

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

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

 Multiplying by ∂_t

12. ABCs – cont.

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

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

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

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

etc.

12. ABCs – cont.

<u>Mur's ABC of 2nd order</u> (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^+ and 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 *f* is evaluated at integer spatial grid positions (*i*,*j*,*k*) and time positions *n*.

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

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.

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

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

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

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

12. ABCs – cont.

Substitute all the FD approximations above in

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

The result is

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

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

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

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:

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

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

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 2^{nd} 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 known 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:

$$
\begin{aligned}
&m=1 \quad f_1 = f\left(x_{\max} - \alpha c \triangle t, t\right)\\
&m=2 \quad f_2 = f\left(x_{\max} - 2\alpha c \triangle t, t - \triangle t\right)\\
&m=3 \quad f_3 = f\left(x_{\max} - 3\alpha c \triangle t, t - 2\triangle t\right)\\
&\vdots\\
&m=N \quad f_N = f\left(x_{\max} - N\alpha c \triangle t, t - (N-1)\triangle t\right)
\end{aligned}
$$

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

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

12. ABCs – cont.

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

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

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

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

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

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

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

$$\vdots$$

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

We denote the discrete functions, which go back in space and time as (see previous slide)

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

12. ABCs – cont.

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

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

However, it is usually more efficient (and easy) to program the recursive calculations shown in the previous slide.

12. ABCs – cont.

We can expressed (interpolate) the function in terms of the backward finite differences at f_1 as

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

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

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

This is Liao's ABC.

12. ABCs – cont.

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.

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

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_F(:,:,ix2)=AX(:,:,3)
A3_F(:,:,ix3)=AX(:,:,4)
A4_F(:,:,ix4)=AX(:,:,5)
```

```
*************************************************************************************
subroutine LIAO

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
```