Finite differences for wave equations (Lecture 2)
(Book pp 27-33)
The *approximation properties* of difference approximation to derivatives are characterized by the order of accuracy p, and the error coefficient C; Let the grid be$\{x_i\}$, $x_i - x_i = h$ (equidistant, meshsize h) and approximate the derivative $f'(x_i)$ for a smooth function f by some difference formula

$$(Lf)(x_i) = \frac{1}{h}\sum_{k=-s}^{s}\alpha_k f(x_{i+k})$$

The error is then

$$e = f'(x_i) - (Lf)(x_i) = Ch^p f^{(p+1)}(x_i) + o\left(h^{p+1}\right)$$

Examples,

$$f'(x_i) - \underbrace{\frac{1}{h}\left(f_{i+1} - f_i\right)}_{D_+ f_i} = \frac{1}{2}hf'' + o(h^2) \qquad \text{Forward}$$

$$f'(x_i) - \underbrace{\frac{1}{h}\left(f_i - f_{i-1}\right)}_{D_- f_i} = -\frac{1}{2}hf'' + o(h^2) \qquad \text{Backward}$$

$$f'(x_i) - \underbrace{\frac{1}{2h}\left(f_{i+1} - f_{i-1}\right)}_{D_0 f_i} = \frac{1}{6}h^2 f^{(3)} + o(h^4) \qquad \text{Central}$$

$$\left.\begin{aligned} f'(x_i) - \frac{1}{h}(f_{i+1/2} - f_{i-1/2}) &= \frac{1}{24}h^2 f^{(3)} + o(h^4) \\ f'(x_{i+1/2}) - \frac{1}{h}(f_{i+1} - f_i) &= \frac{1}{24}h^2 f^{(3)} + o(h^4) \end{aligned}\right\} \text{Central on staggered grid}$$

The two "different" staggered grid formulas differ only by numbering of points; if values of f are available on the grid, we obtain values for the derivative at $x_{i+1/2}$ (midway between neighbor points) with step h, and at points x_i with step $2h$ (the D_0 formula).

But there is more than approximation to solving differential equations. We replace them by difference equations to obtain approximations u_i to the solution (say $u(x)$) at the gridpoints, so the error is

$$e_i = u(x_i) - u_i$$

Because our focus is on waves, we use a model problem with typical wave solutions: Look for solutions to

$$u' = \mathrm{i}ku,$$

to obtain the harmonic $u = A\exp(\mathrm{i}kx)$ with wave number

$$k = 2\pi/\lambda\ ,\ \lambda = \text{wavelength}.$$

Examples
1. Forward differences

$$u_{m+1} - u_m = hiku_m \Rightarrow u_m = u_0 G^m, G = 1 + hik = 1 + i\theta$$

is called the *amplification factor*, the growth of the solution over one step.

The exact growth factor is $H = \exp(i\theta)$, and $H - G = e^{i\theta} - 1 - i\theta = -\frac{\theta^2}{2} + O(h^3)$.

If the solutions match at $x = 0$ the errors become

$$\frac{e_m}{u_0} = H^m - G^m = H^m\left(1 - e^{m(\ln(1+ikh) - ikh)}\right) = H^m \left(1 - e^{m\left(ikh - \frac{k^2h^2}{2} + \ldots - ikh\right)}\right)$$

$$= H^m \left(1 - e^{-\frac{x_m k^2 h}{2} + ..}\right) \approx H^m \frac{kh}{2} \cdot kx_m \text{ if } |hk| \text{ is small}$$

Thus, if $|kh|$ is small (<<1), the *error grows approximately linearly* with m, and is first order in h; note that *the numerical solution grows*, whereas the exact solution does not.

2. Central differences
The analysis is more complicated because the general solution to the difference equation, which is now a two-step recursion, is a linear combination of two different geometric sequences:

$$u_{m+1} - u_{m-1} = 2i\theta u_m \Rightarrow u_m = AG_1^m + BG_2^m,$$

$$\text{Characteristic equation}: G^2 - 2i\theta G + 1 = 0 : G = i\theta \pm \left(1 - \theta^2\right)^{1/2}$$

$$G_1 = 1 + i\theta - \frac{\theta^2}{2} + O(\theta^3) = e^{i\theta} + O(\theta^3)$$

$$G_2 = -1/G_1 = -\left(e^{-i\theta} + O(\theta^3)\right), G_2^m \approx (-1)^m \text{ for small } \theta$$

The G_1-term approximates the exact solution with second order error: so far so good. And as s long as $|kh| \le 1$, $|G_{1,2}| = 1$, and the numerical solutions neither grow nor decay. The G_2-term is a “spurious” solution, with wavelength $\approx 2h$, the shortest wavelength the grid can support. It has nothing to do with the solutions to the *differential* equation and is responsible for the “wiggles” associated with central difference solutions to first order wave equations.

If $|kh| > 1$, on the other hand, both G’s become purely imaginary, and the numerical solution would grow exponentially with m if we were to use the difference scheme for propagating the wave along the x-axis. Such catastrophical error growth is called *numerical instability*, and the mesh size is limited by the stability requirement $|kh| \le 1$.

3. Central differences for second order “Helmholtz” equation

In contrast to the schemes discussed above, this is an extremely successful scheme. For a time-harmonic solution $v(x,t) = e^{i\omega t}u(x)$ to the wave equation $v_{tt} = c^2 v_{xx}$, with wave number $k = \omega/c$ it gives

$$u'' + k^2 u = 0 : u_{m+1} - 2u_m + u_{m-1} + h^2 k^2 u_m = 0$$

$$\text{Characteristic equation: } G^2 - (2-\theta^2)G + 1 = 0$$

$$G_{1,2} = 1 - \frac{\theta^2}{2} \pm \left(\theta^4/4 - \theta^2\right)^{1/2} = 1 - \frac{\theta^2}{2} \pm i\theta\left(1 - \theta^2/4\right)^{1/2}$$

$$= 1 \pm i\theta - \frac{\theta^2}{2} + O(\theta^3) = e^{\pm i\theta} + O(\theta^3)$$

The exact solution is $Ae^{ikx} + Be^{-ikx} = C\cos kx + D\sin kx$. Subject to the (stability) stepsize requirement $|kh| \le 2$, the numerical solutions are of the exactly the same form but with slightly modified wave numbers,

$$h \cdot k_{num} = \arccos\left(1 - \frac{k^2h^2}{2}\right) \Rightarrow k_{num} = k \cdot \left(1 + O(k^2h^2)\right)$$

Violation of the stepsize limit again gives catastrophic growth of error in attempts to propagate the wave.

Lecture FDTD

Book Ch 5: FDTD

FD = finite difference, TD = time domain

“FDTD” is now used to mean specifically the scheme popularized by Kane S. Yee in 1966, with a grid staggered in time and space. This allows centered differences for all variables, in time and space. We look first at the staggered grid scheme for 1D Maxwell w/o dissipation (lossless material)

$$\varepsilon E_t = H_x, \mu H_t = E_x$$

Grid: Vertical time, horizontal *x*. Usually time index set as superscript, space index as subscript.

```
n+1     + H       H       H       H  …
        |         |
n+1/2   +     E---+---E       E       E …
        |         |           |
n       + H       H       H---+---H
        |                     |
n-1/2   +     E       E       E
        |
n-1     +-H-------H-------H-------H …
         j-1      j      j+1     j+2
```

Update formulas:

$$H_j^{n+1} - H_j^n = \frac{\Delta t}{\mu \Delta x}(E_{j+1/2}^{n+1/2} - E_{j-1/2}^{n+1/2})$$

$$E_{j+1/2}^{n+1/2} - E_{j+1/2}^{n-1/2} = \frac{\Delta t}{\varepsilon \Delta x}(H_{j+1}^n - H_j^n)$$

This first order system of difference equations is equivalent to

$$u_j^{n+1} - 2u_j^{n+1} + u_j^{n+1} = \sigma^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \sigma = \frac{c\Delta t}{\Delta x}$$

where *u* can be *E* or *H*, just like either of *E*(*x*,*t*) and *H*(*x*,*t*) satisfy the wave equation

$$u_{tt} = c^2 u_{xx}, c^2 = \frac{1}{\varepsilon\mu}$$

σ is called the Courant number, the ratio between the distance traveled by the wave in a timestep and the cell size.

Dispersion: Phase speed depends on wavelength

The discretized equation has wave-solutions $u_j^n = U_n e^{ikx_j}$ - because exponential functions are eigenfunctions of constant coefficient difference as well as differential operators. Substitute the ansatz in the difference equation,

$$(U_{n+1} - 2U_n + U_{n-1})e^{ikx_j} = \sigma^2 U_n (e^{ik(x_j+\Delta x)} - 2e^{ikx_j} + e^{ik(x_j-\Delta x)})$$

$$U_{n+1} - 2U_n + U_{n-1} = \sigma^2 U_n (e^{ik\Delta x} - 2 + e^{-ikx}) = -4\sigma^2 U_n \sin^2\frac{\theta}{2}, \theta = k\Delta x$$

This difference equation has solutions of type $U_n = \xi^n$ where ξ satisfies the characteristic equation

$$\xi - (2 - 4\sigma^2 \sin^2 \frac{\theta}{2}) + \xi^{-1} = 0$$

The general solution is $U_n = a\xi_1^{\,n} + b\xi_2^{\,n}$ where ξ_i are the roots of the characteristic equation. For this wave NOT to grow, the moduli of ξ_1 and ξ_2 must be <= 1. But the product of roots is 1, so in that case both roots have modulus 1, $\xi_1 = \exp(i\alpha)$, $\xi_2 = \exp(-i\alpha)$ and

$$\cos\alpha = 1 - 2\sigma^2 \sin^2 \frac{\theta}{2}$$

or

$$\sin\frac{\alpha}{2} = \pm\sigma \sin\frac{\theta}{2}$$

which is possible (with real α) if $\sigma^2 \sin^2 \frac{\theta}{2} \le 1$ for all wave numbers θ, i.e., $\sigma <= 1$.

Now, this means that the wave phase changes by α per timestep Δt,

$$u_j^n = e^{i(\frac{\alpha t}{\Delta t} + kx_j)} = e^{i(\omega t + kx_j)}$$

so the phase speed of the wave is

$$c_{num} = \omega/k = \alpha/(k\Delta t) = \alpha c/(\sigma\theta)$$

or

$$c_{num}/c = \alpha/(\sigma\theta)$$

We see that the wave speed depends on

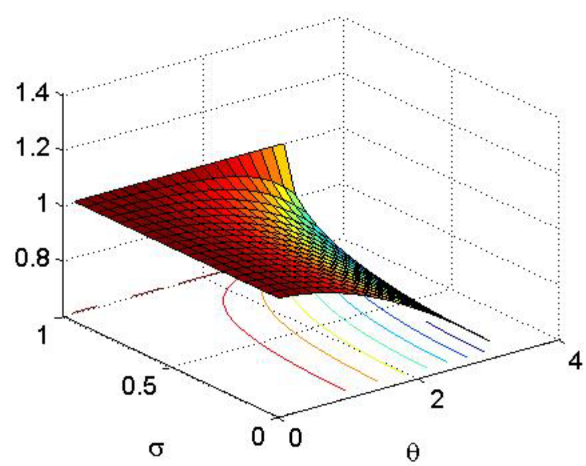
spatial resolution: $2\pi/\theta$ is the number of cells per wavelength.

temporal resolution: σ is the number of cells traveled in a timestep

and this *dispersion* is the most important error in the solution. The waves are NOT *dissipative* because the amplitude is constant: $|\xi| = 1$ when the time-step is limited to $\sigma <= 1$.

The plot shows c_{num}/c as function of σ and θ.

- The error vanishes as $\theta \to 0$: the scheme converges for any stable σ.
- It is correct *independent* of θ if $\sigma = 1$: The magic time-step.
- The error seems never no be worse than 40% and the wave always is too slow;
- Short waves (larger θ) run more slowly that longer.



The error in phase speed could be fixed for monochromatic waves by modifying the material data so the numerical speed matches the desired, but the Magic time-step not possible anyway in 2 & 3D for stability reasons.

Anisotropy and stability

In 2D and 3D the numerical wave speed varies also with the direction of the wave. Consider the 2D case; the Yee scheme is equivalent to the central difference discretization of the wave equation, and assuming the wave travels with a wavefront normal (cos ϕ, sin ϕ) we obtain after a manipulation much like the 1D above that the phase shift per time step α satisfies

$$\sin^2\frac{\alpha}{2} = \sigma^2\left(\sin^2\frac{\theta\cos\phi}{2} + \sin^2\frac{\theta\sin\phi}{2}\right)$$

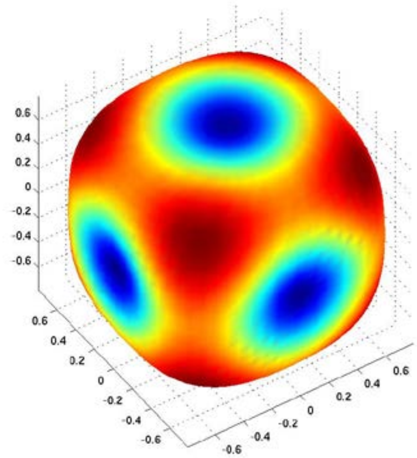
and for 3D

$$\sin^2\frac{\alpha}{2} = \sigma^2\left(\sin^2\frac{\theta\cos\phi_1}{2} + \sin^2\frac{\theta\cos\phi_2}{2} + \sin^2\frac{\theta\cos\phi_3}{2}\right)$$

where the $\cos\phi_k$ are the direction cosines of the wavefront normal. There must be a real α for all wavenumbers θ, and all wave directions, so the max. over ϕ and θ of the RHS must not exceed 1. Thus, the time step is limited to

$$\frac{c\Delta t}{\Delta x} \le \frac{1}{\sqrt{D}}$$

in D space dimensions, assuming equal mesh increments in all dimensions. The waves travel fastest along the main diagonals, and most slowly along the grid lines.



The colored die is a representation of the anisotropy in a 3D FDTD model. The wave speeds depend on the wave direction. A point on the die represents the corresponding propagation direction, its distance to the origin (and its color) shows the wave speed c_{num}/c, with 12 cells per wavelength and a CFL-number of 0.99/sqrt(3).

Complexity and error

Armed with a formula for the dispersion error we can estimate the work for solving a diffraction problem over a domain of size L (L^2 in 2D, L^3 in 3D).
Suppose a phase error of E (compared to the exact solution) is acceptable. The waves travel L and have wavelength λ and accumulate phase error

$$(1-\frac{c_{num}}{c})\frac{L}{\lambda} < E$$

For small θ, we obtain

$$\frac{\alpha}{\sigma\theta} = 1 - \frac{\theta^2}{6} + O(\theta^4)$$

so it is necessary that

$$E > \frac{L}{\lambda}\frac{\theta^2}{6} = \frac{4\pi^2 L}{6\lambda^3}\Delta x^2$$

The number of time-steps to travel L is $n = L/(\sigma\,\Delta x)$ and in D space dimensions there are $(L/\Delta x)^D$ cells so the total work is

$$\frac{1}{\sigma}\left(\frac{L}{\Delta x}\right)^{D+1} W_D > \frac{1}{\sigma}\left(\frac{L \cdot L^{1/2}}{\sqrt{\frac{6E}{4\pi^2}}\lambda^{3/2}}\right)^{D+1} = Const.\frac{\sqrt{D}W_D}{E^{\frac{D+1}{2}}}\left(\frac{L}{\lambda}\right)^{\frac{3(D+1)}{2}}$$

where W_D is the work to for one time step on one cell. In 3D, for example, the work grows as the *sixth power* of the electrical size L/λ and as the inverse square of the phase error accepted.
The table below shows the phase error in ^{o} for a range of L/λ and 2^k cells per wavelength, $k = 1\ldots7$, errors of more than 360^o replaced by 360^o. A common recommendation is $O(10)$ cells per wavelength, but as we see, electrically large cases require much more than that.

Table1: Phase error, degrees; N = #cells per wavelength, Size = L/wavelength

N / Size	2	4	8	16	32	64	128	256
1	74.85	8.68	1.85	0.44	0.11	0.03	0.01	0.00
10	360.00	86.79	18.47	4.45	1.10	0.27	0.07	0.02
100	360.00	360.00	184.72	44.49	11.02	2.75	0.69	0.17
1000	360.00	360.00	360.00	360.00	110.21	27.49	6.87	1.72
10000	360.00	360.00	360.00	360.00	360.00	274.90	68.69	17.17

Table 2, 10log(W)

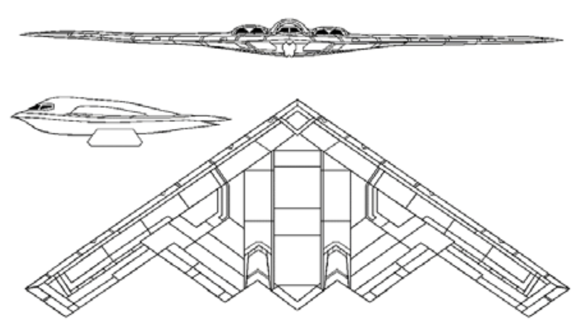
N / Size	2	4	8	16	32	64	128	256
1	0.90	1.81	2.71	3.61	4.52	5.42	6.32	7.22
10	3.90	4.81	5.71	6.61	7.52	8.42	9.32	10.22
100	6.90	7.81	8.71	9.61	10.52	11.42	12.32	13.22
1000	9.90	10.81	11.71	12.61	13.52	14.42	15.32	16.22
10000	12.90	13.81	14.71	15.61	16.52	17.42	18.32	19.22

Suppose 10^o phase error is acceptable:

Size	1	10	100	1000
N	4	12	32	100
#cells	64	1.7M	33G	1P
10logW	2	6	10	15

(M,G,T,P = Mega,Giga,Tera,Peta = $10^{6,9,12,15}$)

Clearly, for this accuracy requirement, $L/\lambda = 10^3$ is out of reach at present, but L/λ a few 100's is possible on a large computer. $L/\lambda = 10$ is easy on your PC.



The wing-span of a Spirit (B2) is 52m and search radars have λ $O(0.1\text{m})$. The craft was designed in the late eighties, on machines (like the Cray XMP/48) capable of 100 Mflops with 64 M words memory.
Obviously, other techniques than second order FDTD were used! We shall see later how the integral equation methods would fare. The rectilinear planform is typical of early stealth

designs, like the F117 NightHawk, which was made of all flat surfaces.

Improvements?

Higher order difference formulas are effective for wave propagation, on a regular grid. But the Yee scheme staircase approximations to oblique boundaries would destroy the potential higher accuracy. Also, construction of higher order accurate and stable boundary conditions is not easy. The most successful attempts are the “summation by parts” operators developed at TDB, Uppsala (Gustafsson, Strand, Nordström & al), and the Embedded Boundary schemes (Leveque, Kreiss, Petersson). Most codes still rely on the second order formulas, and use various types of mesh refinement and/or triangular/tetrahedral meshes close to boundaries to mitigate the staircase effects.

div D = 0, div B = 0? Yee guarantees

Scattering problems: Near vs. far field, Radiation pattern

Excitation: Point source, Plane wave, Huygens surface
Boundary conditions: PEC, PMC BC.
Non-reflecting BC (time domain):
1. Characteristic,
example for Maxwell,“Mur”, Sommerfeld radiation

2. Sponge layers: termination of transmission line; 1D example
Oblique waves.
PML, UPML

About lab 1