Numerical Techniques 2025–2026

3. Space differencing

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Previously on Numerical Techniques . . .

- Discretization and finite differences
- Consistency, convergence and stability
- Effects of time discretization on oscillation equation:
  - Damping or amplification
  - Acceleration or deceleration
  - Implicitness of 2TL schemes
  - Computational mode of 3TL schemes and filtering

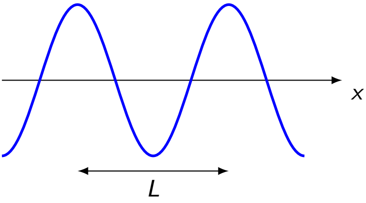
Waves in space and time

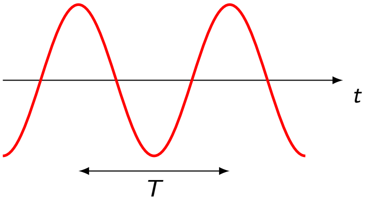
The following function is oscillating in space and time:

$$\psi(x,t) = e^{i(kx-\omega t)}$$

where

- ω is the *frequency*: $\omega = \frac{2\pi}{T}$ with T the period;
- k is the *wavenumber*: $k = \frac{2\pi}{L}$ with L the wavelength.





The dispersion relation

- If $\omega = c\,k$, then $\psi(x,t)$ is a solution to the advection equation

$$\frac{\partial\psi}{\partial t} + c\frac{\partial\psi}{\partial x} = 0$$

- So there is a relation between the frequency ω (or period T), the wavenumber k (or wavelength L) and the propagation speed c.
- We call this relation between ω and k the *dispersion relation*.
- For the advection equation it is simply

$$\omega = ck$$

expressing that all waves propagate at the same speed.

- We define:

$$\text{the phase speed } \frac{\omega}{k} \qquad \text{the group speed } \frac{\partial \omega}{\partial k}$$

- For the particular case of the 1D advection equation,

  group speed $=$ phase speed $= c$.

The discrete dispersion relation

- we will now determine the dispersion relation when discretizing x (not t!): $\omega_d = f(k)$.
- this allows to focus on effect of spatial discretization (cfr. Fourier decomposition to focus on temporal discretization)
- the comparison of the discrete dispersion relation with the exact dispersion relation will tell us
  - amplification: determined by imaginary part of ω_d
  - acceleration: determined by real part of ω_d

since

$$e^{i(kj\Delta x - \omega_d t)} = e^{\omega_i t}\, e^{i(kj\Delta x - \omega_r t)}$$

Dispersion relation with the centered scheme

- Let's consider the centered finite difference scheme,

$$\frac{d\phi_j}{dt} + c\left(\frac{\phi_{j+1} - \phi_{j-1}}{2\Delta x}\right) = 0$$

- Suppose the solution is of the form,

$$\phi_j(t) = e^{i(kj\Delta x - \omega_{2c} t)}$$

- This will be the case if

$$-i\omega_{2c}\phi_j = -c\,\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x}\phi_j$$

or ($e^{i\theta} = \cos\theta + i\sin\theta$),

$$\omega_{2c} = c\,\frac{\sin k\Delta x}{\Delta x}$$

- ω_{2c} is real so there is no amplitude error.
- The phase speed is

$$\frac{\omega_{2c}}{k} = c\frac{\sin k\Delta x}{k\Delta x} \approx c\left[1 - \frac{1}{6}(k\Delta x)^2\right]$$

  This is a function of k, so the waves are *dispersive*.
  - This scheme is second-order in $k\Delta x$.
  - The phase speed is zero for $k\Delta x = \pi$, i.e. for the "$2\Delta x$"-wave.
- The group speed is

$$\frac{\partial \omega_{2c}}{\partial k} = c\cos k\Delta x$$

  The group velocity of the $2\Delta x$ waves is $-c$!

Higher order scheme

- What about a higher-order discretization of $\partial\psi/\partial x$:

$$\frac{d\phi_j}{dt} + c\left[\frac{4}{3}\frac{\phi_{j+1}-\phi_{j-1}}{2\Delta x} - \frac{1}{3}\frac{\phi_{j+2}-\phi_{j-2}}{4\Delta x}\right] = 0$$

- Similar calculations give the following discrete dispersion relation:

$$\omega_{4c} = \frac{c}{\Delta x}\left(\frac{4}{3}\sin k\Delta x - \frac{1}{6}\sin 2k\Delta x\right)$$

which is fourth-order accurate since the phase speed is

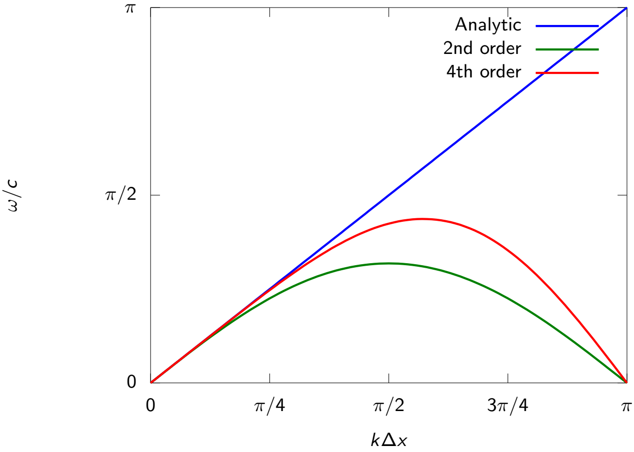
$$c = \frac{\omega_{4c}}{k} \approx c\left[1 - \frac{(k\Delta x)^4}{30}\right]$$

- The group velocity is given by

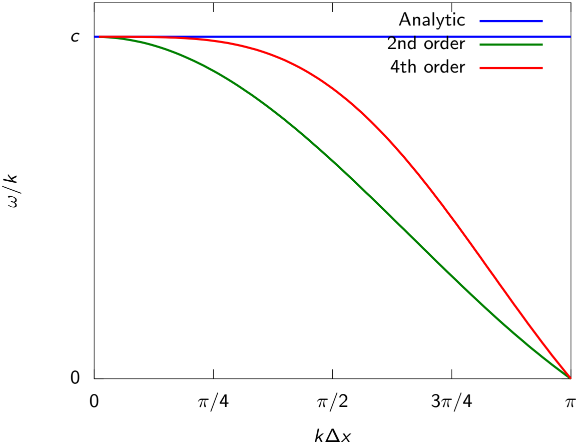
$$\frac{\partial \omega_{4c}}{\partial k} = c\left[\frac{4}{3}\cos k\Delta x - \frac{1}{3}\cos 2k\Delta x\right]$$

Remark: the $2\Delta x$ wave has a group velocity of $-\frac{5}{3}c$, which is even worse than for the second-order scheme !

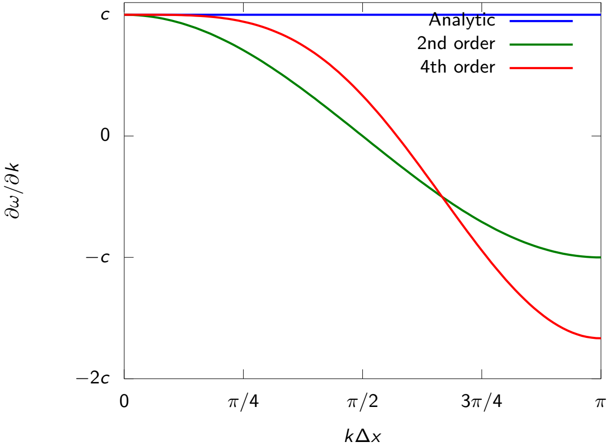
Scaled frequency



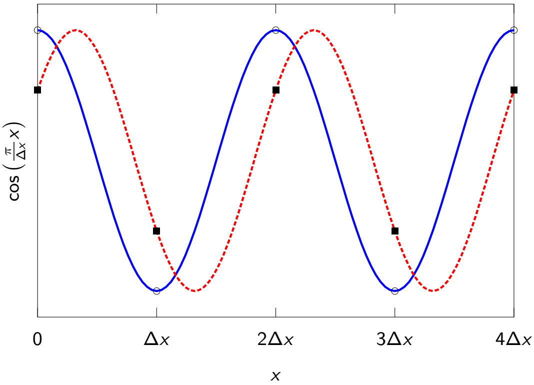
Phase speed


Analytic
2nd order
4th order
c
0
ω/k
0
$\pi/4$
$\pi/2$
$3\pi/4$
π
$k\Delta x$

Group velocity



- There is a fundamental problem with representing the phase of the $2\Delta x$ wave:



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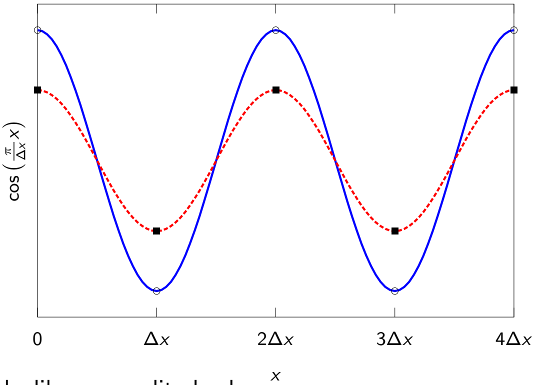
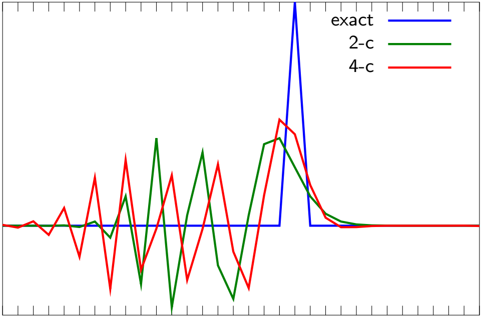


A phase shift looks like an amplitude change.

- Advection of a sharp spike:



- Let us try the one-sided decentered derivatives

$$\frac{d\phi_j}{dt} + c\left(\frac{\phi_j - \phi_{j-1}}{\Delta x}\right) = 0$$

which is the decentered scheme that we have seen before (upstream scheme).

- The discrete dispersion relation becomes

$$\omega_{1s} = \frac{c}{i\Delta x}\left(1 - e^{-ik\Delta x}\right) = \frac{c}{\Delta x}\left[\sin k\Delta x + i\left(\cos k\Delta x - 1\right)\right]$$

- Besides phase errors, there will be amplitude errors due to the imaginary part. The amplitude will grow or decay with a rate

$$\exp\left[-\frac{c}{\Delta x}\left(1 - \cos k\Delta x\right)t\right]$$

In case $c < 0$ this gives rise to an amplification, which is to be expected after what we saw in the first lesson.

- Another one-sided decentered scheme is

$$\frac{d\phi_j}{dt} + \tfrac{1}{6}c\frac{2\phi_{j+1} + 3\phi_j - 6\phi_{j-1} + \phi_{j-2}}{\Delta x} = 0$$

which is third-order.

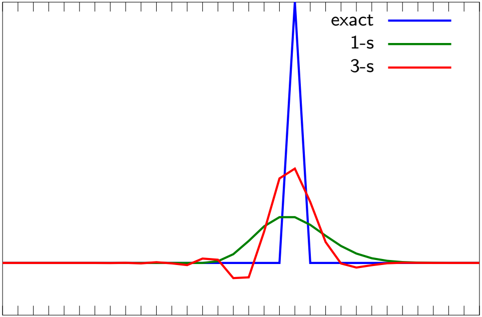
- The discrete dispersion relation becomes

$$\omega_{3s} = \frac{c}{\Delta x}\left[\left(\tfrac{4}{3}\sin k\Delta x - \tfrac{1}{6}\sin 2k\Delta x\right) - \tfrac{i}{3}\left(1 - \cos k\Delta x\right)^2\right]$$

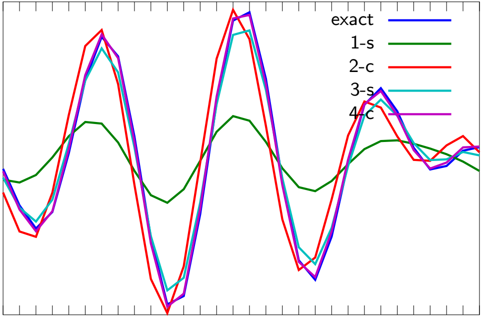
which has the same phase error as the fourth-order scheme, and an amplitude decay

$$\exp\left[-\frac{c}{3\Delta x}\left(1 - \cos k\Delta x\right)^2 t\right]$$

- Advection of a sharp spike:



- Advection of a sum of two waves:



Discussion

- The damping in the decentered schemes can be good or bad;
- In the spike test they damp the spurious trail which makes decentered schemes actually better than the centered ones.
- The third-order scheme somewhat better approximates the analytic solution than the first-order one
- However, the spike test is an extreme test! In the more realistic test with 2 modes it is not clear whether the third-order decentered scheme is better than the second-order centered one:
    - The amplitude is better for the second-order one
    - The third-order one does not make a phase error.

- A qualitative description of the error is obtained by examining the truncated terms; instead of solving the advection equation with zero RHS, we are in fact solving

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = \epsilon_m \frac{\partial^m \phi}{\partial x^m} + \epsilon_{m+1}\frac{\partial^{m+1}\phi}{\partial x^{m+1}} + \dots$$

- an even order m will lead to a dissipative effect:

$$\frac{\partial \xi}{\partial t} = \frac{\partial^m \xi}{\partial x^m} \quad \Rightarrow \quad \xi(x,t) = Ce^{ikx}e^{-\gamma t}$$

- an odd term will lead to a dispersive effect:

$$\frac{\partial \xi}{\partial t} = \frac{\partial^m \xi}{\partial x^m} \quad \Rightarrow \quad \xi(x,t) = Ce^{i(kx-\omega t)}$$

Discussion

- The centered derivatives have *no* numerical dissipation.
  (only odd terms in the truncation error)
- The first and second-order have the same leading-order dispersive terms, so they have the same dispersion! The same holds for the third- and fourth order schemes.
- In fact, the dispersive error in the odd-order schemes are dissipated away!
- So we are compensating one error by another! This is usually a bad idea.
- One way out for the even-order schemes is to introduce some (controlled) artificial dissipation.
- (We will see later that this is in fact also important in nonlinear systems).

Time and space differencing

- Until now we have been isolating the error coming from the *time differencing* and the *space differencing*

- The *fundamental* behaviour of the scheme can sometimes be deduced from the constituents.

  For instance, a combination of a *forward difference scheme* with *centered derivatives* will be a combination of an amplifying time scheme with a neutral space scheme, yielding an amplifying scheme.

- But what will happen if we combine *forward differencing* with an *upstream one-sided space differencing*? Forward differencing will amplify, while the one-side space differencing may damp the mode. Further analysis is needed...

- What if we combine the leapfrog scheme with centered space differencing? Leapfrog is conditionally neutral; centered-space differencing is neutral. But leapfrog is accelerating, whereas centered differencing is decelarating?

- One can consider the solution to the time- and space-discretized equation of the form

$$\phi_j^n = e^{i(kj\Delta x - \omega n \Delta t)}$$

- Substituting this solution in the scheme and solving for ω as a function of k gives the *discrete dispersion relation*.
- In fact, it summarizes the behaviour of a scheme completely: let $\omega = \omega_r + i\omega_i$, then
  - ω_i determines the amplification factor
  - ω_r determines the phase-speed error.

(leave the complex algebra to a computer or a mathematician...)

Summary

- We studied the influence of space discretization through the *dispersion relation*
- The dispersion relation tells how waves propagate; phase speed and group speed.
- All finite difference schemes have difficulties with the $2\Delta x$ wave
- Decentered schemes also show damping, on top of dispersion
- Also combined time-space effects can be studied through the dispersion relation

Exercises

1. Determine the discrete dispersion relation for a 2nd-order centered leapfrog discretization of the advection equation:

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\,\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

   You'll need $\frac{e^{i\theta} - e^{-i\theta}}{2i} = \sin\theta$.

2. Determine the discrete dispersion relation for the upstream scheme:

$$\frac{\phi_j^{n+1} - \phi_j^{n}}{\Delta t} + c\,\frac{\phi_{j}^n - \phi_{j-1}^n}{\Delta x} = 0$$

   You'll need $\log(a + ib) = \frac{1}{2}\log(a^2 + b^2) + i\ \arctan(b, a)$. This is pretty hard to calculate analytically, so use a computer to check the results...
   Does this confirm what we saw in the first lesson?

Exercises: Leapfrog, 2nd order FD

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\,\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Exercises: Leapfrog, 2nd order FD

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\,\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Substituting a harmonic solution, discretized in space and time: $\phi_j^n = e^{i(kj\Delta x - \omega n\Delta t)}$, gives:

$$\frac{e^{i(kj\Delta x - \omega(n+1)\Delta t)} - e^{i(kj\Delta x - \omega(n-1)\Delta t)}}{2\Delta t} + c\,\frac{e^{i(k(j+1)\Delta x - \omega n\Delta t)} - e^{i(k(j-1)\Delta x - \omega n\Delta t)}}{2\Delta x} = 0$$

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

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Dividing both sides by $e^{i(kj\Delta x - \omega n\Delta t)}$, gives:

$$\frac{e^{-i\omega\Delta t} - e^{i\omega\Delta t}}{2\Delta t} + c\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} = 0$$

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Substituting a harmonic solution, discretized in space and time: $\phi_j^n = e^{i(kj\Delta x - \omega n\Delta t)}$, gives:

$$\frac{e^{i(kj\Delta x - \omega(n+1)\Delta t)} - e^{i(kj\Delta x - \omega(n-1)\Delta t)}}{2\Delta t} + c\frac{e^{i(k(j+1)\Delta x - \omega n\Delta t)} - e^{i(k(j-1)\Delta x - \omega n\Delta t)}}{2\Delta x} = 0$$

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$$\frac{e^{-i\omega\Delta t} - e^{i\omega\Delta t}}{2\Delta t} + c\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} = 0$$

Using $e^{i\theta} - e^{-i\theta} = 2i\sin\theta$, this is simplified to

$$\sin\omega\Delta t = \frac{c\Delta t}{\Delta x}\sin k\Delta x$$

The discrete dispersion relation is

$$\omega = \frac{1}{\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta x} \sin k\Delta x\right)$$

So:

- for $\left|\frac{c\Delta t}{\Delta x}\right| < 1$, ω is real. The scheme is stable without amplitude error.
- for $\left|\frac{c\Delta t}{\Delta x}\right| > 1$, ω is complex. The scheme is unstable.
- for $k\Delta x = \pi$, $\omega = 0$. So the scheme is decelerating.

Exercises: upstream scheme

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\,\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\,\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

Substituting a harmonic solution, discretized in space and time: $\phi_j^n = e^{i(kj\Delta x - \omega n \Delta t)}$, and dividing both sides by ϕ_j^n, gives:

$$e^{-i\omega\Delta t} - 1 + \frac{c\Delta t}{\Delta x}\left(1 - e^{-ik\Delta x}\right) = 0$$

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$$e^{-i\omega\Delta t} - 1 + \frac{c\Delta t}{\Delta x}\left(1 - e^{-ik\Delta x}\right) = 0$$

The discrete dispersion relation becomes

$$\omega = \frac{i}{\Delta t}\log\left(1 - \mu\left(1 - \cos k\Delta x + i\sin k\Delta x\right)\right)$$

with μ the Courant number $\mu = \frac{c\Delta t}{\Delta x}$.

Stability is obtained if the imaginary part of ω is smaller than zero, i.e. if

$$\log\left((1-\mu+\mu\cos k\Delta x)^2+(\mu\sin k\Delta x)^2\right)\leq 0$$

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Or

$$\mu(1-\mu)(1-\cos k\Delta x)\leq 0$$

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$$\mu(1-\mu)\leq 0$$

Or if

$$0\leq\mu\leq 1$$