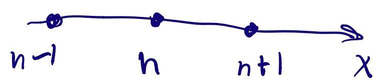
Pseudo-spectral method

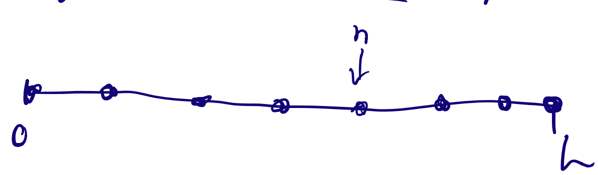
Idea: Let's consider the center difference in finite-differences

$$\partial_x f = \frac{f_{n+1} - f_{n-1}}{2\Delta x} + O(\Delta x^2)$$



for a partial derivative at position n, second-order accurate.

If we use the information at more positions, we can increase the order of accuracy.
The idea behind pseudo-spectral methods is why not use <u>all</u> the points!



Fourier transforms:

The Fourier transform is an operation which transforms one function from one domain (f) to another (F):

space domain $\longrightarrow$ wavenumber domain

time domain $\longrightarrow$ frequency domain

The operators for Fourier transforms and inverse Fourier transforms are

$$\text{FT}: \quad F(k) = \int f(x)\, e^{-ikx}\, dx$$

$$\text{inverse FT}: \quad f(x) = \frac{1}{2\pi} \int F(k)\, e^{ikx}\, dk$$

k: wavenumber
x: spatial position

Note that the derivative is given by

$$\underline{\partial_x f(x)} = \frac{1}{2\pi} \int ik\, F(k)\, e^{ikx}\, dk$$

that is

$$\underbrace{ik\, F(k)}_{\text{wavenumber domain}} \iff \underbrace{\partial_x f(x)}_{\text{space domain}}$$

Discretization: Discrete Fourier transform

$$F(k_\ell) = F(\ell \Delta k) = \sum_{n=0}^{N-1} f(x_n)\, e^{-i k_\ell x_n} \Delta x$$

$$= \sum_{n=0}^{N-1} f(n\Delta x)\, e^{-i \ell \Delta k\, n \Delta x} \Delta x$$

$$= \Delta x \sum_{n=0}^{N-1} f(n\Delta x)\, e^{-i 2\pi n \ell / N}$$

using $x_n = n\Delta x$, $k_\ell = \ell \Delta k$ with $n = 0, .., N-1$; and $\ell = 0, .., N-1$

Similar the discrete inverse Fourier transform

$$f(x_n) = f(n\Delta x) = \frac{1}{N\Delta x} \sum_{\ell=0}^{N-1} F(\ell \Delta k)\, e^{i 2\pi n \ell / N}$$

Putting this together

$$\partial_x f(n\Delta x) = \frac{1}{N\Delta x} \sum_{\ell=0}^{N-1} i(\ell \Delta k)\, F(\ell \Delta k)\, e^{i 2\pi n \ell / N}$$

Note that the boundaries can be an issue, but the advantage is that we reach a very high accuracy of the spatial derivative $\partial_x f$.

$$\Delta k = \frac{2\pi}{N \Delta x}$$ relation between Δk and Δx

<u>Dispersion</u>: Advection equation

$$\partial_t u = -c\,\partial_x u$$

$$\frac{u^{m+1} - u^{m-1}}{2\Delta t} = -c \frac{1}{N\Delta x} \sum_{l=0}^{N-1} i(l\Delta k)\, \underbrace{U^m(l\Delta k)}_{\text{FT of } u^m} e^{i2\pi n l/N}$$

This leads to the stability condition

$$\sin(\omega \Delta t) = \underbrace{2\pi c \frac{\Delta t}{\Delta x} \frac{l}{N}}_{<1}$$

$$c\,\Delta t < \frac{\Delta x}{2\pi} \frac{N}{l} \quad \text{and therefore} \quad \boxed{c\,\Delta t < \frac{\Delta x}{2\pi}} \quad \text{since } l<N$$

compare to $c\Delta t < \Delta x$
for finite-difference

The numerical dispersion become

$$\omega(k_l) = \frac{1}{\Delta t} \arcsin(c\, k_l\, \Delta t)$$

It is controlled by Δt, compared to finite-difference schemes which depend on Δt and Δx.

Note and remarks:

- Fourier transform makes the boundaries periodic

  → non-periodic Chebyshev transforms

  Chebyshev transform ⟷ in depth
  Fourier tranform ⟷ laterally

- computational performance:
  The pseudo-spectral methods involves all points in one direction. This usually is a bottleneck for parallel computations in 2D & 3D.

- Number of gridpoints per wavelength for finite-difference methods is typically 5–10, i.e., smallest wavelength resolved $\lambda_{min} \sim 5\Delta x$.
  With a pseudo-spectral method (Fourier transforms) in principle only 2 points per wavelength are required.