Fourier Error Analysis (Lomax 3.5)

- So far we discussed truncation error
- Now, we will introduce the resolving power of finite diff.
  For dynamic problems the resolving power is more important than truncation error

We will consider periodic functions

Fourier representation $u(x) = \sum_n a_n e^{i k_n x}$ ← sum of sines and cosines with different wavelengths

The quantity e^{ikx} forms the building block of the problem. We will analyze using e^{ikx}

Exact derivative: $\frac{d}{dx} e^{ikx_i} = ik\, e^{ikx_i}$

Finite difference derivative: $\delta_x u|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \text{error}(\Delta x^2)$

$$= \frac{e^{ik\Delta x(i+1)} - e^{ik\Delta x(i-1)}}{2\Delta x}$$

$$= \frac{(e^{ik\Delta x} - e^{-ik\Delta x})}{2\Delta x} e^{ikx_i}$$

remember that $e^{ikx} = \cos kx + i \sin kx$

$$\rightarrow \delta_x u|_i = \frac{1}{2\Delta x}\left[\cos k\Delta x + i\sin k\Delta x - \cos(-k\Delta x) - i\sin(-k\Delta x)\right] e^{ikx_i}$$

$$\rightarrow \delta_x u|_i = \frac{1}{2\Delta x}\left[\cancel{\cos k\Delta x} + i\sin k\Delta x - \cancel{\cos k\Delta x} + i\sin k\Delta x\right] e^{ikx_i}$$

$$\delta_x u|_i = \underbrace{i \frac{\sin k\Delta x}{\Delta x}}_{\text{modified wavenumber } k^*} e^{ikx_i} \qquad \text{exact is } \frac{\partial u}{\partial x} = i\,k\,e^{ikx_i}$$

$$k^* = \frac{\sin k\Delta x}{\Delta x} = k \underbrace{- \frac{k^3 \Delta x^2}{6}}_{\substack{\text{error in approximation of } k \\ 2^{nd} \text{ order approximation}}} + \cdots$$

- k^* is an approximation of k
- k^* depends on the numerical approximation!
  It is different for different schemes

"Flow physics" using one-dimensional convection

- Use periodic or infinite domains

PDE: $\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0$

look for solutions with form $u(t,x) = f(t) e^{ikx}$

put into PDE: $\frac{df}{dt} e^{ikx} + a f(t)\, i k\, e^{ikx} = 0$

ODE for $f(t)$: $\frac{df}{dt} = -iakf$

Solve ODE to find $f(t)$: $\int_0^t \frac{df}{f}\, dt = \int_0^t -iak\, dt$

$\log f(t) - \log \underbrace{f(0)}_{\text{initial condition}} = -iakt$

$f(t) = f(0)\, e^{-iakt}$

Put $f(t)$ into $u(t,x)$ form:

$$u(t,x) = f(0)\, e^{ik(x-at)}$$

phase speed

it is constant

initial condition

All wavelengths travel with speed a

Repeat the process using $\frac{u_{i+1}-u_{i-1}}{2\Delta x}$ in the place of $\frac{\partial u}{\partial x}$

$$\frac{df}{dt} e^{ikx_i} + a\,\frac{u_{i+1}-u_{i-1}}{2\Delta x} = 0$$

⋮

math

⋮

$$+\, a\, i \left(\frac{\sin k\Delta x}{\Delta x}\right) f\, e^{ik\Delta x}$$

I get this instead of k

modified phase speed

$$u_{numerical}(x,t) = f(0)\, e^{ik(x-a^* t)}$$

$$a^* = a\,\frac{\sin k\Delta x}{k\Delta x}$$

$$a^* = a\,\frac{\overbrace{\sin k\Delta x}^{k^*}}{k\Delta x}$$

$$\frac{a^*}{a} = \frac{k^*}{k}$$

Super Important:

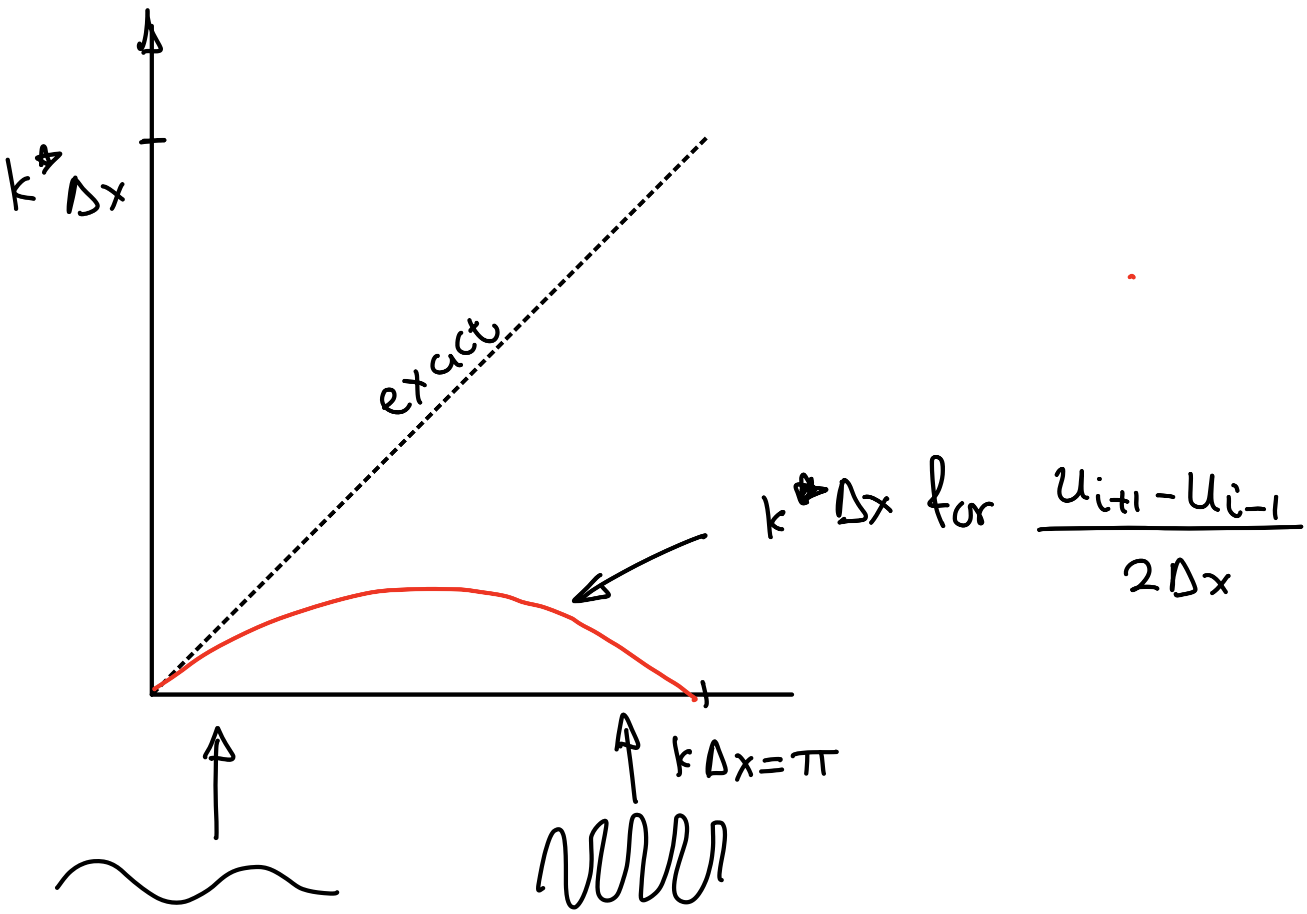
Phase speed depends on k!

Propagation speed depends on wavelength

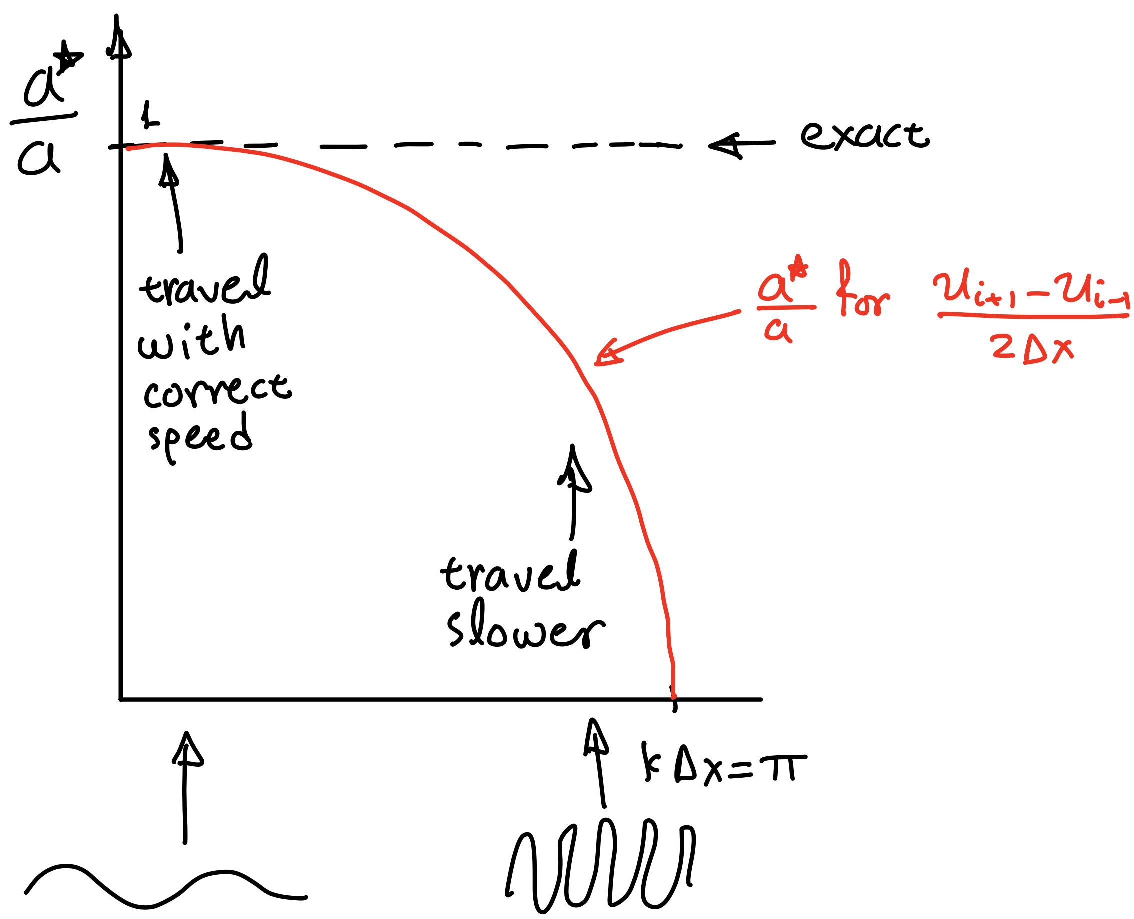
This is called dispersion

Shapes are not preserved

Shapes change as they are convected



$k^* \Delta x$
exact
$k^* \Delta x$ for $\frac{u_{i+1} - u_{i-1}}{2\Delta x}$
$k\Delta x = \pi$



$\frac{a^*}{a}$
1
exact
travel with correct speed
$\frac{a^*}{a}$ for $\frac{u_{i+1} - u_{i-1}}{2\Delta x}$
travel slower
$k\Delta x = \pi$

remember : $\text{length} = \dfrac{2\pi}{k}$

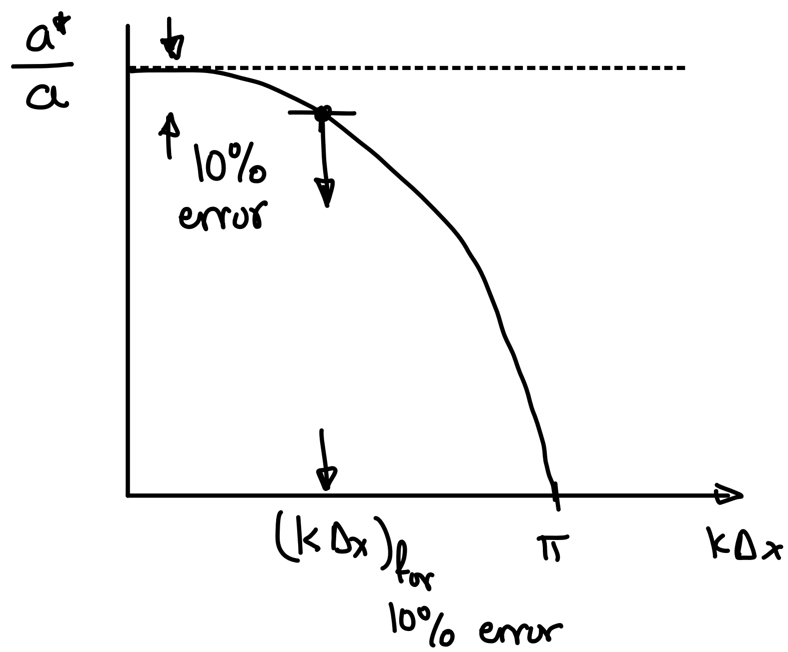
minimum wavelength on the grid: $2\Delta x = \dfrac{2\pi}{k_{max}}$

$$\Rightarrow k_{max}\Delta x = \pi$$

Also: $\text{wavelength} = \dfrac{2\pi}{k}$

$$\frac{\text{wavelength}}{\Delta x} = \frac{2\pi}{k\Delta x}$$

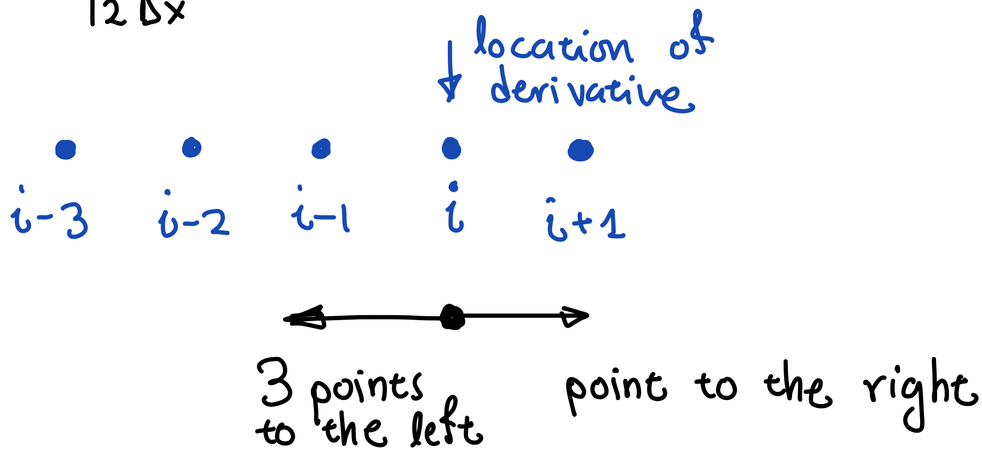
number of grid points per wavelength $= \dfrac{2\pi}{k\Delta x}$



number of grid points per wavelength $= \dfrac{2\pi}{(k\Delta x)_{10\% \text{ error}}}$

Example:

$$\delta_x u_i \simeq \frac{1}{12\Delta x}\left(-u_{i-3}+6u_{i-2}-18u_{i-1}+10u_i+3u_{i+1}\right) + O(\Delta x^4)$$



- 5-point stencil
- one-side-biased (more points to the left)

$$\delta_x u\big|_i = \underbrace{\delta_x^a u\big|_i}_{\text{anti-symmetric}} + \underbrace{\delta_x^s u\big|_i}_{\text{symmetric}}$$

$$\delta_x^a u\big|_i = \frac{1}{12\Delta x}\left[\frac{1}{2}\left(u_{i+3}-u_{i-3}\right)-3\left(u_{i+2}-u_{i-2}\right)+\frac{21}{2}\left(u_{i+1}-u_{i-1}\right)\right]$$

$$\delta_x^s u\big|_i = \frac{1}{12\Delta x}\left[-\frac{1}{2}\left(u_{i+3}+u_{i-3}\right)+3\left(u_{i+2}+u_{i-2}\right)-\frac{15}{2}\left(u_{i+1}+u_{i-1}\right)+10u_i\right]$$

Important: Any one-side-biased FD operator has a symmetric component

Finite difference operators (Lomax Chapter 3.5)

$\delta_x u|_i$ e.g. $\delta_x u|_i = \dfrac{u_{i+1} - u_{i-1}}{2\Delta x}$ with u_i periodic

Operator:

$$\underbrace{\frac{1}{2\Delta x}\begin{bmatrix} 0 & 1 & & & -1 \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & -1 & 0 \end{bmatrix}}_{B_p} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_M \end{bmatrix}$$

In general any matrix $M \times M$ can be written as

$$B_p = \underbrace{\tfrac{1}{2}\left(B_p - B_p^T\right)}_{\text{anti-symmetric}} + \underbrace{\tfrac{1}{2}\left(B_p + B^T\right)}_{\text{symmetric}}$$

centered schemes

e.g. $\dfrac{u_{i+1} - u_{i-1}}{2\Delta x}$

Similarly, $\delta_x|_i = \underbrace{\delta_x^a|_i}_{\text{anti-sym.}} + \underbrace{\delta_x^s|_i}_{\text{symmetric}}$

Modified PDE & Numerical Dissipation

(Lomax Chapters 11.1 and 11.2)

Approximation for first derivative

$$\delta_x u|_i = +\frac{1}{2\Delta x}\Big[\underbrace{(u_{i+1} - u_{i-1})}_{\text{anti-symmetric}} + b\underbrace{(-u_{i+1} + 2u_i - u_{i-1})}_{\text{symmetric}}\Big]$$

Taylor expansions (about poin i)

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 u}{\partial x^2} + \frac{1}{6}\Delta x^3 \frac{\partial^3 u}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 u}{\partial x^4} \cdots$$

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 u}{\partial x^2} - \frac{1}{6}\Delta x^3 \frac{\partial^3 u}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 u}{\partial x^4} \cdots$$

$$+\frac{1}{2\Delta x}(u_{i+1} - u_{i-1}) = +\frac{1}{2\Delta x}\left(2\Delta x \frac{\partial u}{\partial x} + \frac{2}{6}\Delta x^3 \frac{\partial^2 u}{\partial x^3} + \cdots\right)$$

All even derivatives cancel out

$$\frac{b}{2\Delta x}(-u_{i+1} + 2u_i - u_{i-1}) =$$

$$= \frac{b}{2\Delta x}\left(-\Delta x^2 \frac{\partial^2 u}{\partial x^2} + \frac{2}{24}\Delta x^4 \frac{\partial^4 u}{\partial x^4} + \cdots\right)$$

All odd derivatives cancel out

Consider $\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0$

Use $\delta_x u|_i$ in (neglecting H.O.T.)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = -\frac{a}{6}\Delta x^3 \frac{\partial^3 u}{\partial x^3} + \frac{a b}{2}\Delta x \frac{\partial^2 u}{\partial x^2} - \frac{a b}{24}\Delta x^3 \frac{\partial^4 u}{\partial x^2}$$

(we deal with $\frac{\partial u}{\partial t}$ later...)

Is it consistent? Yes, because

$\Delta x \to 0 \Rightarrow \text{RHS} \to 0$

We are really solving something like:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + \gamma \frac{\partial^3 u}{\partial x^3} + \tau \frac{\partial^4 u}{\partial x^4}$$

Looking for solutions of form: $u(t,x) = e^{\underline{i}kx} e^{(r+\underline{i}s)t}$

Solution is: $u(t,x) = \underbrace{e^{-k^2(\nu - \tau k^2)}}_{\substack{\text{amplitude} \\ \text{even derivatives}}} \underbrace{e^{\underline{i}k[x-(a+\gamma k^2)t]}}_{\substack{\text{phase} \\ \text{odd derivatives}}}$

Form of dissipation

"Numerical dissipation"

Dealing with the time derivative (not in Lomax)

$$\underbrace{\frac{u_i^{n+1}-u^n}{\Delta t}}_{\text{approximation for } \frac{\partial u}{\partial t}} + \frac{1}{2\Delta x}\left[(u_{i+1}-u_{i-1}) + b(-u_{i+1}+2u_i-u_{i-1})\right] = 0$$

$$u_i^{n+1} = u_i^n + \Delta t \frac{\partial u}{\partial t} + \frac{1}{2}\Delta t^2 \frac{\partial^2 u}{\partial t^2} + \frac{1}{6}\Delta t^3 \frac{\partial^3 u}{\partial t^3} + \cdots$$

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = \frac{\partial u}{\partial t} + \frac{1}{2}\Delta t \frac{\partial^2 u}{\partial t^2} + \frac{1}{6}\Delta t^2 \frac{\partial^3 u}{\partial t^3} + \cdots$$

We will replace time derivatives with space derivatives

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\frac{\partial u}{\partial t}$$

use PDE: $\frac{\partial u}{\partial t} = -\frac{\partial u}{\partial x}$

use PDE again

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial t}\frac{\partial u}{\partial x} = -\frac{\partial}{\partial x}\frac{\partial u}{\partial t} = +\frac{\partial}{\partial x}\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2}$$

Similarly: $$\frac{\partial^3 u}{\partial t^3} = -\frac{\partial^2}{\partial t^2}\frac{\partial u}{\partial x}$$

$$\frac{\partial^3 u}{\partial t^3} = -\frac{\partial}{\partial x}\frac{\partial^2 u}{\partial t^2} = -\frac{\partial^3 u}{\partial x^3}$$

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = \frac{\partial u}{\partial t} + \frac{1}{2}\Delta t \frac{\partial^2 u}{\partial x^2} - \frac{1}{6}\Delta t^2 \frac{\partial^3 u}{\partial x^3}$$

Big Conclusion:

Finite differences are <u>always</u> dispersive and <u>can be</u> dissipative (if they include a symmetric component)

Implicit Filtering Property

↳ Do NOT confuse this with implicit schemes

$$\delta_x u = \underbrace{\frac{d}{dx}\int_{-\infty}^{\infty} G(x-x')\,u(x')\,dx'}_{\text{exact derivative filtered } u(x)}$$

approximation of first derivative

$$i k^* \hat{u} = i k \hat{G} \hat{u}$$

$$\hat{G}(k) = \frac{k^*}{k}$$

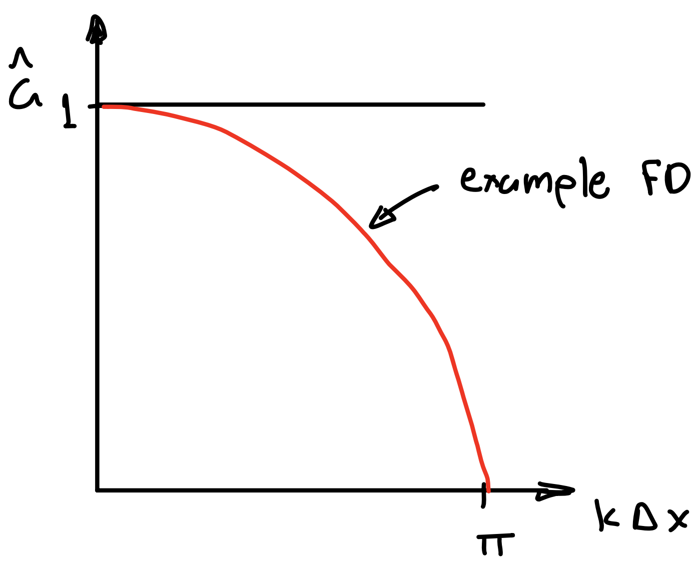
Definition of implicit filter transfer function

What is the exact value of $\hat{G}(k)$?

exact derivative $\frac{du}{dx} = \frac{1}{dx}\int_{-\infty}^{\infty} \delta(x)\,u(x')\,dx'$

Dirac Delta function

$\hat{G}_{exact} = \hat{\delta} = 1$ independent of k !

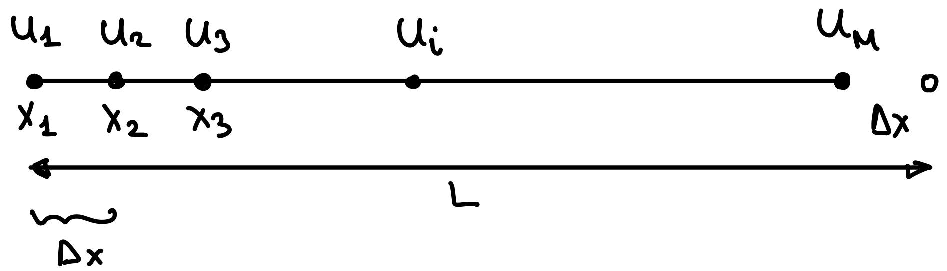


Spectral Methods: no dispersion - no dissipation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \qquad u(t,x) \text{ is periodic on } [0, L]$$

$$u(t=0, x) = u_0(x)$$

Discretization



PDE becomes: $\frac{d}{dt}\vec{u}_i + \left.\overrightarrow{\frac{\partial u}{\partial x}}\right|_i = 0$

or $\frac{d}{dt}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_i \\ \vdots \\ u_M \end{bmatrix} + \begin{bmatrix} \left.\frac{\partial u}{\partial x}\right|_1 \\ \left.\frac{\partial u}{\partial x}\right|_2 \\ \vdots \\ \left.\frac{\partial u}{\partial x}\right|_i \\ \\ \left.\frac{\partial u}{\partial x}\right|_M \end{bmatrix} = 0$ ← Here we have $x_i - u_i$ pairs and the x-derivative at locations x_i

Take the Discrete Fourier Transform:

$$\frac{d}{dt}\vec{\hat{u}}_n + \underline{i}\,\underbrace{\vec{k}_n \odot}_{\text{element-wise multiplication}} \vec{\hat{u}}_n = 0$$

Now we have pairs $k_n - \hat{u}_n$ with $n = 0, 1, \dots, M-1$

wavenumber (k_n) Fourier coefficient ($\hat{u}_n$)

or...

$$\frac{d}{dt}\begin{bmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_i \\ \vdots \\ \\ \hat{u}_{M-1} \end{bmatrix} + \underline{i}\begin{bmatrix} k_0\hat{u}_0 \\ k_1\hat{u}_1 \\ \vdots \\ k_i\hat{u}_i \\ \vdots \\ \\ k_{M-1}\hat{u}_{M-1} \end{bmatrix} = 0$$

$$\frac{d}{dt}\begin{bmatrix}\hat{u}_0\\ \hat{u}_1\\ \vdots\\ \hat{u}_i\\ \vdots\\ \hat{u}_{M-1}\end{bmatrix} = -i\underbrace{\begin{bmatrix}k_0\hat{u}_0\\ k_1\hat{u}_1\\ \vdots\\ k_i\hat{u}_i\\ \vdots\\ k_{M-1}\hat{u}_{M-1}\end{bmatrix}}_{\text{RHS}}$$

Recipe:

1. Discretize : x_i and u_i
2. Initialize u_i with the initial condition $u_i = f(x_i)$
3. Take discrete Fourier transform $\vec{\hat{u}}_n = \mathrm{DFT}(\vec{u}_i)$
4. Form wavenumber vector k_n
5. Numerically integrate in time $\frac{d}{dt}\vec{\hat{u}}_n = -i\, k_n \vec{\hat{u}}_n$ using Runge-Kutta with $\Delta t = \Delta x/2$

   The time-integration evolves the Fourier coefficients in time! Make new $\hat{u}_n$ at later times

6. After time integration reached tend take inverse DFT $\vec{u}_i = i\mathrm{DFT}(\vec{\hat{u}}_n)$

   at $t = $ tend

Boundary conditions for periodic functions

→ Spectral method imply periodic functions
No need to set boundary conditions

Finite differences

derivative here $= \dfrac{u_2 - u_M}{2\Delta x}$

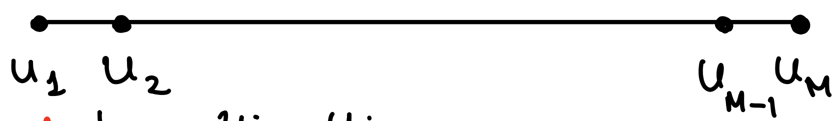
different formula near boundary

derivative here $\dfrac{u_3 - u_1}{2\Delta x}$

Dealing with discrete periodicity

There are two main appoaches to apply periodic BCs

A: Modify FD near the boundary

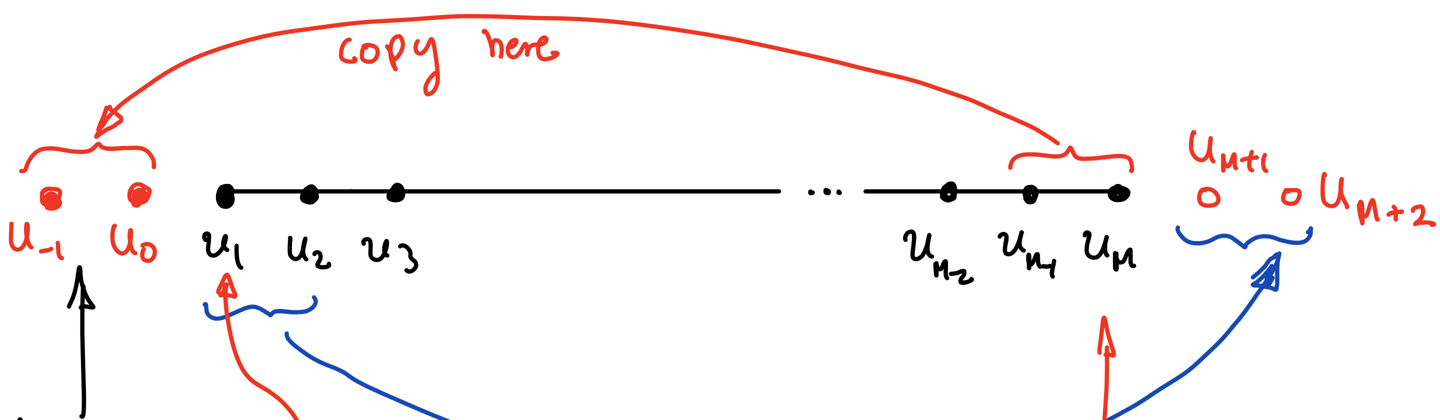


M unique points

using $\frac{du}{dx} = \frac{u_{i+1} - u_{i-1}}{2\Delta}$

$$\left.\frac{du}{dx}\right|_1 = \frac{u_2 - u_M}{2\Delta x} \qquad \left.\frac{du}{dx}\right|_M = \frac{u_1 - u_{M-1}}{2\Delta x}$$

B: Use ghost points to set BCs



$$\left.\frac{du}{dx}\right|_1 = \frac{u_2 - u_0}{2\Delta x} \qquad \left.\frac{du}{dx}\right|_M = \frac{u_{M+1} - u_{M-1}}{2\Delta x}$$

Ghost Points:

- help set boundary condition
- the number depends on stencil width
- advantage: No special code to compute FD near boundary
- disadvantage: shift in physical domain indixes
  index "bookkeeping"

Thus... boundary condition means setting the values of ghost points