Fourier Derivatives

$$f(x) = \int_{-\infty}^{\infty} F(k)\, e^{-ikx}\, dk$$

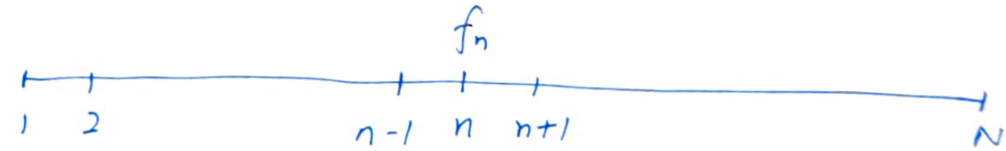
$$\partial_x f(x) = \int_{-\infty}^{\infty} -ik\, F(k)\, e^{-ikx}\, dk$$

Let us write $f(x) = f_x$ & $F(k) = \hat{f}_k$

$$f_x \xrightarrow{FT} \hat{f}_k \xrightarrow{-ik} -ik\,\hat{f}_k \xrightarrow{IFT} \partial_x f_x$$

Since we have to solve it numerically, so

$f(x)$



$x \longrightarrow$

$$f_n = \sum_{k=-\frac{N}{2}}^{N/2} \hat{f}_k\, e^{-2\pi i \left(\frac{kn}{N}\right)} \qquad \text{(DFT)}$$

$$f_n \xrightarrow{DFT} \hat{f}_k$$

$$DFT[\{\partial_x f_n\}]_k = \left(-2\pi i \frac{k}{N}\right) \hat{f}_k$$

$$DFT[\{\partial_{xx} f_n\}]_k = -4\pi^2 \left(\frac{k}{N}\right)^2 \hat{f}_k$$

Poisson Eqn 1D

$$\nabla^2 \psi = -\omega \Rightarrow \partial_{xx}\psi = -\omega$$

ω_n $[n = 1, \dots N]$ Known

ψ_n $[n = 1, \dots N]$ Unknown

DFT

$$-k^2 \hat{\psi}_k = -\hat{\omega}_k \Rightarrow \hat{\psi}_k = + \frac{\hat{\omega}_k}{k^2}$$

$$\omega_n \xrightarrow{DFT} \hat{\omega}_k \xrightarrow{\nabla^2} -\frac{\hat{\omega}_k}{k^2} \xrightarrow{DFT^{-1}} -\psi_n$$

$$-\frac{\hat{\omega}_k}{k^2} \downarrow -\hat{\psi}_k$$

Home Work: Compare FD vs Spectral

Time Dependent Problem:

1 D diffusion eqn $\partial_t u = \nu \, \partial_{xx} u$ PDE

u_n $[n = 1, \dots N]$ are known at $t = 0$.

Apply spatial DFT $\Rightarrow \partial_t \hat{u}_k = -\nu k^2 \hat{u}_k$

$k = [-\frac{N}{2}, \dots \frac{N}{2}]$

Set of N ODEs; One can solve it using any time marching method (Euler/RK2/RK4).

$$u_n \xrightarrow{DFT} \hat{u}_k \xrightarrow[\text{in FS}]{\text{Temporal evolution}} \hat{u}_k^+ \xrightarrow{DFT^{-1}} u_n^+$$

$$\hat{u}_k + \Delta t(-\nu k^2 \hat{u}_k)$$

How to handle non-linear term?

$$\rho(x)\, u(x)$$

We are working in FS so at a given time we have $\hat{\rho}$ & $\hat{u}$.

Now (ρu) corresponds to convolution in FS
$\downarrow$
Expensive (CPU time)
$\downarrow$
Must be avoided (N^2)

$$\widehat{\rho u} \neq \hat{\rho}\,\hat{u} \xrightarrow{\text{IFT}} \rho * u$$

$$\rho * u = \int_{-\infty}^{\infty} \rho(x)\, u(x-l)\, dl$$

Steps
a> At time t $\hat{\rho}_k$ & $\hat{u}_k$

b> $\rho_n = DFT^{-1}(\hat{\rho}_k)$ & $u_n = DFT^{-1}(\hat{u}_k)$

c> $w_n = \rho_n u_n$

d> $DFT(w_n) = \hat{w}_k = \widehat{(\rho u)}_k$

To summarise

$$\begin{array}{ccc} \hat{\rho}_k,\ \hat{u}_k & \xrightarrow{DFT^{-1}} & \rho_n,\ u_n \\ & & \Big\downarrow \text{Multiply} \\ \widehat{(\rho u)}_k & \xleftarrow[DFT]{} & (\rho_n u_n) \end{array}$$

Aliasing Effect:

The fourier modes are

$$e^{-ik_j x_n} \qquad k_j = \frac{j\,2\pi}{N\Delta};\ \left[j = -\frac{N}{2}+1; \ldots, 0, 1, 2, \ldots, \frac{N}{2}\right]$$

$$\cong e^{-i2\pi\left(\frac{jn}{N}\right)} \qquad x_n = n\Delta;\ [n = 1, 2, \ldots N] \ \&\ \Delta = \frac{2\pi}{N} \text{ in general}$$

$$\equiv e^{-i2\pi\left(\frac{j+lN}{N}\right)n} \qquad \text{Where } l = [0, 1, \ldots]$$

Modes k_j will contribute to DFT as if they had $k_j = \frac{2\pi j}{N\Delta}$

$$\boxed{k_j = 2\pi\left(\frac{j+lN}{N\Delta}\right)}$$

i.e. high k modes bias/alias the amplitude of lower k modes

e.g. $N = 8$; Domain $L = 2\pi \Rightarrow \Delta = \frac{2\pi}{8}$

$k_j = -3, -2, -1, 0, 1, 2, 3, 4$

if we consider modes 9, 17, --- will contribute to mode $k = 1$. i.e., The modes that we model outside k range will bias the modeled k.

Plot $\sin(x)$ & $\sin(9x)$ on a grid $N = 8$, $L = 2\pi$.
It appears as same function when sampled.

$\Rightarrow$ Any function provided has to be superpositions of the explicitly available modes.

Aliasing & Nonlinearity (P4)

Let us say $f(x) = \sin(k_1 x)$ & $u(x) = \sin(k_2 x)$

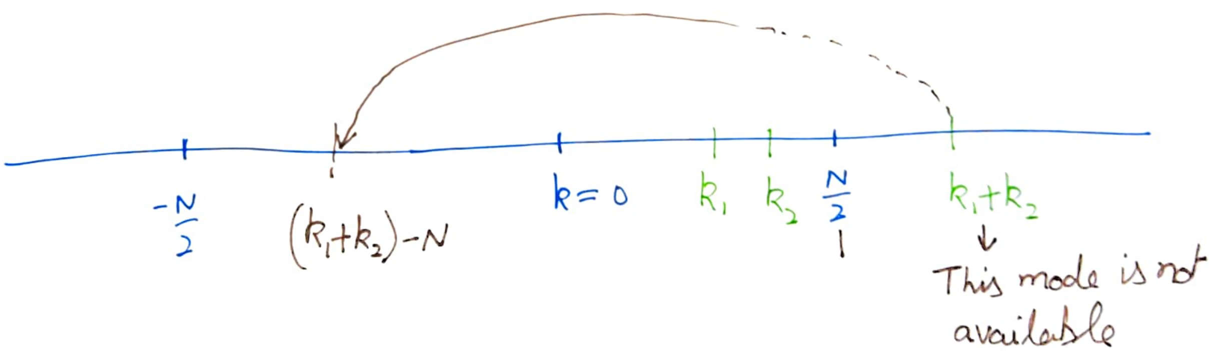
$$-\frac{N}{2} < k_1, k_2 < \frac{N}{2}$$

Now $$f(x)\,u(x) = \sin(k_1 x) \cdot \sin(k_2 x)$$

$$= -\cos[(k_1+k_2)x] + \cos[(k_1-k_2)x]$$

Now in this scenario (k_1+k_2) might be $> \frac{N}{2}$ and available fourier modes might be aliased.

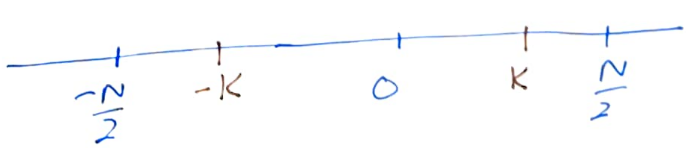
i.e. if $(k_1+k_2) \geq \frac{N}{2} \Rightarrow (k_1+k_2) \cong (k_1+k_2) - N$



Dealiasing: To avoid dealiasing one needs to kill a part of high wave number amplitudes prior to multiplication.

Set $\hat{u}_k = 0$ for $k = [-\frac{N}{2}+1, -K]$ & $[K, \frac{N}{2}]$

& $\hat{u}_k = \hat{u}_k$ for $k = [-K, K]$



if $k_1+k_2 > \frac{N}{2} \Rightarrow k_1+k_2-N$ will be aliased.

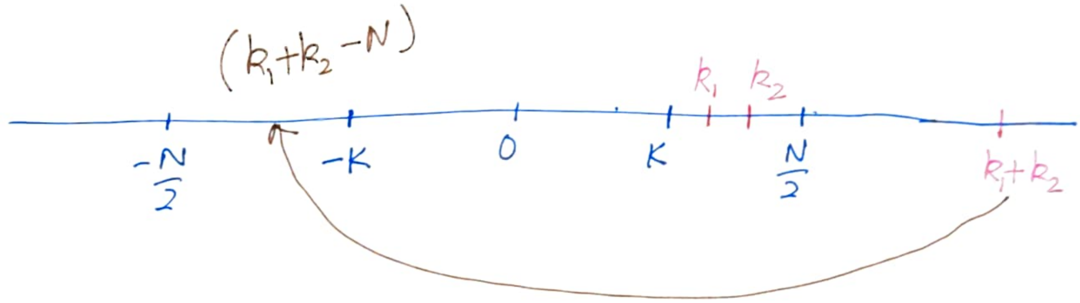
We want this wave number to be $<-K$.

$$k_1+k_2-N < -K$$

Since $\{k_1, k_2\}_{max} = K \Rightarrow K+K-N = -K$

$$\Rightarrow K = \frac{N}{3} = \frac{2}{3}\left(\frac{N}{2}\right)$$

Known as '$\frac{2}{3}$ dealiasing' rule.



The rang $[-K,K]$ is free of aliasing.

Since NS $\rightarrow$ 2nd order nonlinearity

$K = \frac{2}{3}\left(\frac{N}{2}\right)$ works fine.

What if the nonlinearity is of 3rd order or higher?

<u>Summary</u>

Fourier Space	Direct Space
$\hat{\rho}_k$, $\hat{u}_k$	
$\hat{\rho}_k, \hat{u}_k = 0$ for $\lvert k\rvert > \frac{N}{3}$ $\xrightarrow{DFT^{-1}}$	ρ_n, u_n
	$\downarrow$
$\hat{\omega}_k = \widehat{(\rho u)}_k$ $\xleftarrow{DFT}$	$\omega_n = (\rho_n u_n)$

1D Burger's Eqn

$$\partial_t u + u\,\partial_x u = \nu\,\partial_{xx} u + f \longrightarrow \text{Forcing} = 0$$

a> Initialize velocity field

$$u(x) = \sin(x)\ ;\quad x \in [0, 2\pi]\ ;\quad u_n = \sin(x_n)$$

$$x_n = n\Delta\ ;\quad n = [0, 1, \ldots N-1]$$

$$\Delta = \frac{2\pi}{N}$$

b> Calculate the derivatives in FS

$$u_n = \sum_{k=-\frac{N}{2}}^{N/2} \hat{u}_k\, e^{-2\pi i \left(\frac{kn}{N}\right)}$$

$$\hat{u}_k \longrightarrow -ik\,\hat{u}_k = \widehat{(\partial_x u)}_k$$

$$\hat{u}_k \longrightarrow k^2\,\hat{u}_k$$

c> Nonlinear term

$$\hat{u}_k \ \&\ \widehat{(\partial_x u)}_k \xrightarrow[2/3]{\text{Dealiase}} \hat{u}_k^*,\ \widehat{(\partial_x u)}_k^*$$

$$\Big\downarrow\ \text{DFT}^{-1}$$

$$\widehat{(u\partial_x u)}_k \xleftarrow{\text{DFT}} (u\,\partial_x u) \xleftarrow{\text{Multiply}} u^*,\ \partial_x u^*$$

d> Time Marching : Euler/RK2/RK4

$$\partial_t \hat{u}_k + \cancel{u\partial_x}\,\widehat{(u\partial_x u)}_k = -\nu k^2\,\hat{u}_k$$

$$\Rightarrow \partial_t \hat{u}_k = -\nu k^2\,\hat{u}_k - \widehat{(u\partial_x u)}_k = \widehat{RHS}_k$$

Evolve $\hat{u}_k$ in FS.

Number of arrays:

u ; ~~$\partial_x u$~~ $\partial_x u / u\partial_x u$; RHS

$u \to$ old, New

2 ; 1 ; 1

4 Arrays

Choice of Δt & Δx

a> $\frac{2D}{\Delta x^2}\Delta t < 1$

b> $\{u\}_{max}\Delta t < \Delta x$ [Courant-Friedrichs-Lewy] Stability criterion.

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

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}\right]$$

Amplification factor $\xi = 1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)$

stability condn $|\xi| < 1 \Rightarrow \frac{2D\Delta t}{(\Delta x)^2} \leq 1$

Physical interpretation is

$\sqrt{D\Delta t} \leq \Delta x$

$\hookrightarrow$ Diffusion length in time Δt.

$$\boxed{\nabla^2 \psi = -\omega} \qquad (x, y) \in [0, 2\pi]^2$$

$$\omega = \sin 5x \quad \Rightarrow \quad \psi = \frac{1}{25} \sin 5x$$

$$(u_x, u_y) = [+\partial_y \psi, -\partial_x \psi] = [0, -\frac{1}{5} \cos 5x]$$

$$\omega = \nabla \times u = \hat{k}\,[\partial_x u_y - \partial_y u_x] = \hat{k}\,[-\partial_{xx}\psi - \partial_{yy}\psi]$$

$$= \hat{k}\, -\nabla^2 \psi$$