Spectral (Fourier) Methods

(1)

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These are some quick notes on FFT-based spectral methods, suitable for periodic domains or simple BCs.

First start from continuum Fourier series:

$$u \in L^2([0, 2\pi]) \Rightarrow$$

$$u = \sum_{n=-\infty}^{\infty} \hat{u}_n \exp(inx)$$

$$\hat{u}_m = \frac{1}{2\pi} \int_0^{2\pi} u(x) \exp(-inx)\,dx$$

The role of the numerical or truncated approximation of $u(x)$ is played by

$$\omega = \{ \hat{u}_n , \quad n = \underbrace{-N \dots N}_{\text{even number often used (more later)}} \}$$

$$u_h(x) = P_N u(x) = \sum_{n=-N}^{N} \hat{u}_n \exp(inx)$$

SPECTRAL ACCURACY (EXPONENTIAL ACC.)

If $u(x)$ is ANALYTIC

$$\boxed{\| u - P_N u \|_2 \sim C e^{-N} \| u \|_2}$$

THIS IS BECAUSE THE FOURIER COEFFICIENTS $\hat{u}_n$ DECAY EXPONENTIALLY WITH n. BUT non-smooth functions exhibit power-law decay, $1/n$ for discontinuous ones. (Gibbs phenomenon) ③

In practice, we use the discrete Fourier transform, which is a way to interpolate periodic functions on a regular grid: trigonometric interpolant

Interpolating polynomial (trig):

$$x_j = \frac{2\pi}{2N+1}, \quad \underbrace{j \in [0, \dots, 2N]}_{\text{grid points}}$$

$$I_N u(x) = \sum_{n=-N}^{N} \tilde{u}_n \exp(inx)$$

$$\tilde{u}_n = \frac{1}{2N+1} \sum_{j=0}^{2N} u(x_j) \exp(-inx_j)$$

DFT done using FFT

Fundamental <u>aliasing</u> problem

$$\exp\left(i(n+2Nm)x_j\right) = \exp(i n x_j)$$

for all $m \in \mathbb{Z}$ and $\forall j$

This gives

$$\boxed{\underset{\substack{\uparrow \\ \text{DFT}}}{\tilde{u}_n} = \underset{\substack{\uparrow \\ \text{continuum FT}}}{\hat{u}_n} + \underbrace{\sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty} \hat{u}_{n+2Nm}}_{\text{Aliasing error}}}$$

Error estimate

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$$\|u - I_N u\|_2^2 = \underbrace{\sum_{n \subseteq N} |\hat{u}_n - \tilde{u}_m||^2}_{\text{aliasing error}}$$

$$+ \underbrace{\sum_{|n|>N} |\hat{u}_n|^2}_{\text{truncation error}}$$

Choose N large enough to make $|\hat{u}_m| / \max_n |\hat{u}_n|$ sufficiently small :
ALWAYS POSSIBLE FOR **SMOOTH** functions

Differentiation just becomes
multiplication in Fourier space.
One issue to deal with in
practice is the odd mode
left without a conjugate partner
for even sized grid (typically
best for FFTs).
See notes by S. G. Johnson (MIT)
for details.

$$y(x) = y_0 + \sum_{0<k<N/2} \left(Y_k e^{i\frac{2\pi}{L}kx} + Y_{N-k} e^{-i\frac{2\pi}{L}kx} \right)$$

$$+ \underbrace{Y_{N/2}}_{\text{Special mode}} \cos\left(\frac{\pi N x}{L}\right)$$

(could be associated with $k = -\frac{N}{2}$)

Unique "minimal oscillation" trigonometric interpolant

SPECTRAL DIFFERENTIATION

Alg 1 : First Derivative

ⓐ $y_n \xrightarrow{FFT} Y_k \,, \quad 0 \le k < N$

ⓑ

$$Y_k \Leftarrow Y_k \cdot \begin{cases} \frac{2\pi i}{L} k & \text{if } k < N/2 \\ \frac{2\pi i}{L} (k-N) & \text{if } k > N/2 \\ 0 & \text{if } k = N/2 \\ & \text{(if } N \text{ even)} \end{cases}$$

ⓒ $Y_k \xrightarrow{iFFT} y_n$

For Second Derivative

$$Y_k \Leftarrow Y_k \cdot \begin{cases} -\left(\frac{2\pi}{L} k\right)^2 & \text{if } k \le N/2 \\ -\left(\frac{2\pi}{L}(k-N)\right)^2 & \text{otherwise} \end{cases}$$

NOTE: Second derivative NOT the same as derivative of derivative:

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DISCRETIZED DIFFERENTIAL OPERATORS, e.g. difference operators or spectral differences do not inherit all of the properties of the continuum operators.

MIMETIC DIFFERENCES: TRY TO KEEP THE CONTINUUM PROPERTIES that are important for the physics/analysis of the PDE

E.g. (from S. G. Johnson)

WHY NOT ALSO MULTIPLY BY ZERO
the mode $N/2$ in the SECOND DERIVATIVE?

<u>Answer</u>: IT WOULD ADD A NONTRIVIAL ELEMENT TO THE NULL SPACE OF THE LAPLACIAN. (a zig-zag high frequency oscillation) which can pollute iterative solutions, lead to instabilities, affect non-linearities, etc.

<u>BAD</u>! BUT spectral accuracy <u>not</u> affected by choice!

CFD MANTRA: <u>ACCURACY IS NOT EVERYTHING</u>!

S. G. Johnson goes through another nice example. (12)

Consider Sturm - Louville operator

$$\underbrace{-\frac{d}{dx} c(x) \frac{d}{dx}}, \quad c(x) > 0$$

$\left\{ \begin{array}{l} \text{Symmetric positive semidefinite} \\ \text{operator with only constants in its} \\ \text{null space} \end{array} \right.$

It is POSSIBLE TO CONSTRUCT a pseudo - spectral method to compute this operator's action and preserve these properties.

BAD IDEA!

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$$\frac{d}{dx}\left(c(x)\frac{du}{dx}\right) = c'u' + cu''$$

compute these spectrally

→ Does not preserve Hermitian property

Algorithm: Compute $(cy')'$ on grid

(1) Compute y' as before but save $Y_{N/2}$

(2) Compute $v_n = c_n y_n'$ on all grid points in real space: PSEUDOSPECTRAL

(3) Compute v_n' using Alg 1, but, before ifft, change $V'_{N/2}$ to

$$V'_{N/2} = -\bar{c}\left(\frac{\pi N}{L}\right)^2 Y_{N/2}$$

Let's consider the

KORTEWEG - de VRIES EQUATION

$$\underbrace{\left(\partial_t \varphi + \partial_{xxx}\varphi\right)}_{\text{linear}} - 6\varphi\left(\partial_x \varphi\right) = 0$$

stiff high-order

nonlinear

Linear part is easy to do spectrally <u>entirely</u> in Fourier Space.

But nonlinear product $\varphi\left(\partial_x \varphi\right)$ is not good for spectral methods.

<u>PSEUDOSPECTRAL</u>: Compute $\varphi\left(\partial_x \varphi\right)$ IN REAL SPACE, then convert to Fourier

Best seems to rewrite

$$\varphi(\partial_x \varphi) = \frac{1}{2} \partial_x (\varphi^2)$$

so compute φ^2 in real space then differentiate spectrally in Fourier space

$$\partial_t \hat{u} = ik^3 \hat{u} - 3ik \widehat{(u^2)}$$

Compute as $\mathrm{FFT}\left(\left(\mathrm{iFFT}(\hat{u})\right)^2\right)$

We can solve this system of ODEs using Exponential temporal integrators (quick aside)

But first we need to discuss aliasing & filtering when dealing with non linearities such as products

$$u(x) = \sum_{k=-m}^{m} \hat{u}_k e^{ikx}$$

$$v(x) = \sum_{k=-m}^{m} \hat{v}_k e^{ikx}$$

How to compute $w(x) = u(x) \cdot v(x)$ in Fourier space, i.e., how to compute $\hat{w}_k$?

Note that

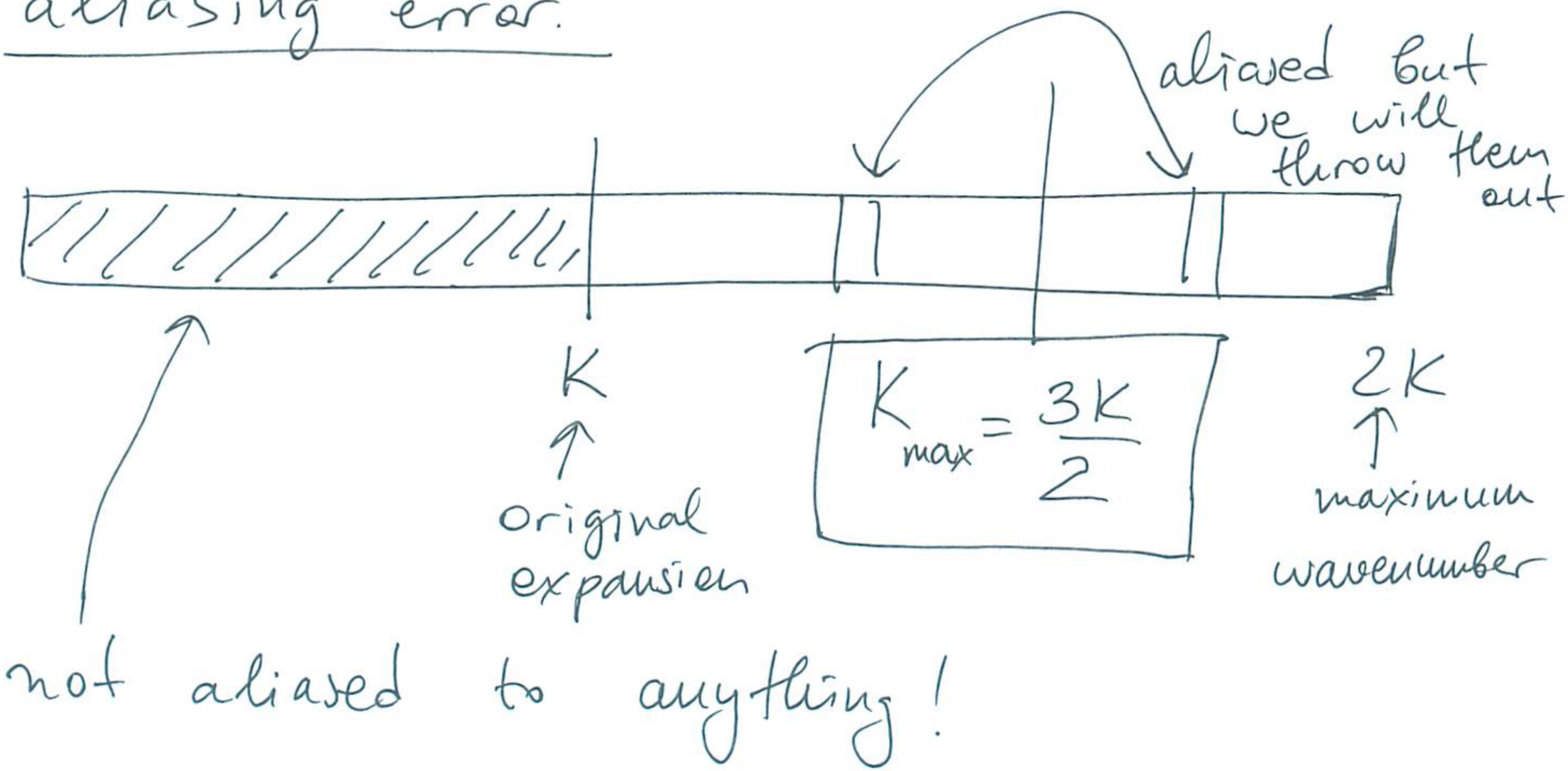
$$w(x) = u(x) \cdot v(x) = \sum_{k=-2m}^{k=2m} w_k e^{ikx}$$

has twice higher frequencies as the original.

This is a general rule : <u>nonlinearities generate high-wavenumber / frequency content</u> and therefore one has to do something about this: <u>FILTERING</u> is the process of removing high frequencies.

If we naively fix the grid size in our FFTs the higher frequencies will be aliased with lower ones and this will introduce

aliasing error.



We can ensure that the K frequencies we do keep are <u>not</u> aliased by <u>padding the FFT</u> grid by $3/2$ more entries.

In 2D this is $(3/2)^2$ more effort!
3D this is $(3/2)^3$ more effort!
$\simeq 3.4$

One can use a <u>smooth low-pass filter</u> as an alternative, especially useful for <u>turbulent flows</u>

Algorithm:

Compute $\hat{w}_k$ for $w = u \cdot v$ using N fourier coefficients only, $M = 3N/2$

(1) $\hat{u}_{padded} = [\ \hat{u}(1:\frac{N}{2})\ \ \text{zeros}(1, M-N)\ \ \hat{u}(\frac{N}{2}+1:\text{end})\ ]$

same for $\hat{w}_{padded}$

(2) $u = \text{ifft}(\hat{u}_{padded})$ (on grid of size M)

same for w

(3) $w = u \cdot v$ in real space

(4) $\hat{w}_{padded} = \text{fft}(w)$

(5) $\hat{w} = \frac{3}{2}\,[\ \hat{w}_{padded}(1:N/2)\ \ \hat{w}_{padded}(M-N/2+1:M)\ ]$

Take the advection equation

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

$$\Rightarrow \frac{da_k}{dt} = -\frac{i}{2\pi} \sum_{n=-N}^{N} n\, a_n \int_{-\pi}^{\pi} c(x,t)\, e^{-i(n-k)x}\, dx$$

if one uses the finite (truncated) Fourier basis.

Now, assume $c(x,t)$ is also approximated (represented) in the finite Fourier basis

$$c(x,t) = \sum_{m=-N}^{N} c_m(t)\, e^{imx}$$

$$\Rightarrow \frac{da_k}{dt} = - \sum_{\substack{m+n=k \\ |m|, |n| \le N}} i n c_m a_n$$

convolution

$$\frac{\partial \hat{\psi}}{\partial t} + \widehat{\left(c(x) \frac{\partial \psi}{\partial x} \right)} = \partial_t \hat{\psi} + \hat{c} \circledast (ik \hat{\psi})$$

Also

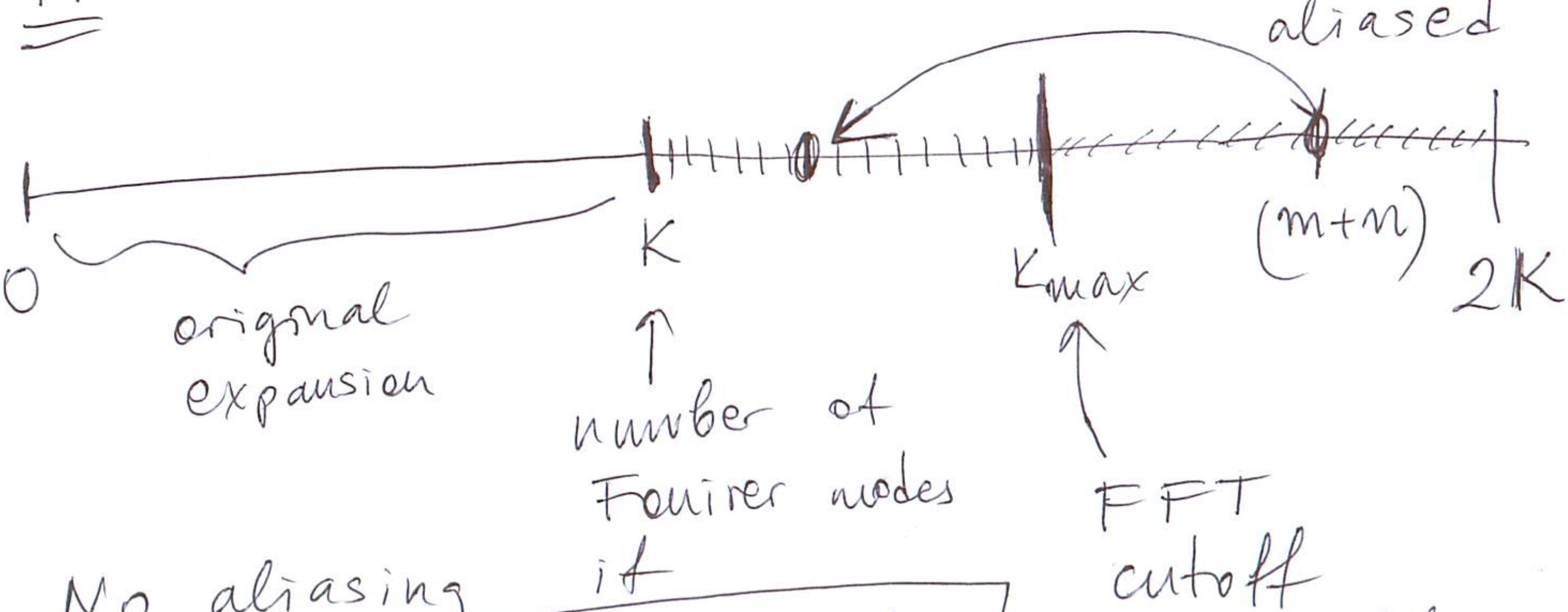
$$\frac{da_k}{dt} = - \sum_{\substack{n \\ (m=k-n) \\ |n|, |m| \le N}} i n a_n c_{k-n}$$

The convolution is expensive to calculate $\rightarrow$ do it in real space (pseudospectral method)

The <u>pseudo spectral</u> approach :

$$\hat{c} \circledast (ik\hat{\psi}) = FFT\left\{ iFFT(\hat{c}) \cdot iFFT(ik\hat{\psi}) \right\}$$

is <u>equivalent</u> to the convolution sum <u>if</u> there are no aliasing errors



$\Rightarrow$ No aliasing if $\boxed{K_{max} = 3K/2}$ as we saw before