Numerical Methods II (Pseudo)Spectral Methods for PDEs

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Outline

- Convolutions using FFT
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- Solving PDEs using FFTs
- 4 Chebyshev Series via FFTs
- Conclusions

Convolutions using FFT

Filtering using FFTs

- Because FFT is a very fast, almost linear algorithm, it is used often to accomplish tasks in data processing, e.g., noise filtering (see example in previous lecture), computing (auto)correlation functions, etc.
- Denote the (continuous or discrete) Fourier transform with

$$\hat{\mathbf{f}} = \mathcal{F}\left(\mathbf{f}
ight)$$
 and $\mathbf{f} = \mathcal{F}^{-1}\left(\hat{\mathbf{f}}
ight)$.

- Plain FFT is used in signal processing for digital filtering (low-pass, high-pass, or band-pass filters)
- How to do it: Multiply the spectrum by a filter $\hat{S}(k)$ discretized as $\hat{\mathbf{s}} = \left\{\hat{S}(k)\right\}_k$:

$$\mathbf{f}_{\mathsf{filtered}} = oldsymbol{\mathcal{F}}^{-1}\left(\hat{\mathbf{s}} oldsymbol{oldsymbol{G}} \hat{\mathbf{f}}
ight) = \mathbf{f} \circledast \mathbf{s},$$

where \odot denotes element-wise product, and \circledast denotes convolution.

Convolution

• For continuous function, an important type of operation found in practice is **convolution** (smoothing) of a (periodic) function f(x) with a (periodic) **kernel** K(x):

$$(K \circledast f)(x) = \int_0^{2\pi} f(y)K(x-y)dy.$$

• It is not hard to prove the **convolution theorem**:

$$\mathcal{F}(K \circledast f) = \mathcal{F}(K) \odot \mathcal{F}(f)$$
.

Importantly, this remains true for discrete convolutions:

$$(\mathbf{K} \circledast \mathbf{f})_j = \frac{1}{N} \sum_{j'=0}^{N-1} f_{j'} K_{j-j'} \quad \Rightarrow$$

$$\mathcal{F}(\mathsf{K} \circledast \mathsf{f}) = \mathcal{F}(\mathsf{K}) \boxdot \mathcal{F}(\mathsf{f}) \quad \Rightarrow \quad \mathsf{K} \circledast \mathsf{f} = \mathcal{F}^{-1}(\mathcal{F}(\mathsf{K}) \boxdot \mathcal{F}(\mathsf{f}))$$

Proof of Discrete Convolution Theorem

Assume that the normalization used is a factor of N^{-1} in the forward and no factor in the inverse DFT:

$$f_{j} = \sum_{k=0}^{N-1} \hat{f}_{k} \exp\left(\frac{2\pi i j k}{N}\right), \text{ and } \hat{f}_{k} = \frac{1}{N} \sum_{j=0}^{N-1} f_{j} \exp\left(-\frac{2\pi i j k}{N}\right)$$

$$\left[\mathcal{F}^{-1}\left(\mathcal{F}\left(\mathbf{K}\right) \boxdot \mathcal{F}\left(\mathbf{f}\right)\right)\right]_{k} = \sum_{k=0}^{N-1} \hat{f}_{k} \hat{K}_{k} \exp\left(\frac{2\pi i j k}{N}\right) =$$

$$N^{-2} \sum_{k=0}^{N-1} \left(\sum_{l=0}^{N-1} f_{l} \exp\left(-\frac{2\pi i l k}{N}\right)\right) \left(\sum_{m=0}^{N-1} K_{m} \exp\left(-\frac{2\pi i m k}{N}\right)\right) \exp\left(\frac{2\pi i j k}{N}\right)$$

$$= N^{-2} \sum_{l=0}^{N-1} f_{l} \sum_{m=0}^{N-1} K_{m} \sum_{k=0}^{N-1} \exp\left[\frac{2\pi i \left(j-l-m\right) k}{N}\right]$$

contd.

Recall the key discrete orthogonality property

$$\forall \Delta k \in \mathbb{Z} : N^{-1} \sum_{j} \exp \left[i \frac{2\pi}{N} j \Delta k \right] = \delta_{\Delta k} \Rightarrow$$

$$N^{-2} \sum_{l=0}^{N-1} f_l \sum_{m=0}^{N-1} K_m \sum_{k=0}^{N-1} \exp\left[\frac{2\pi i (j-l-m) k}{N}\right] = N^{-1} \sum_{l=0}^{N-1} f_l \sum_{m=0}^{N-1} K_m \delta_{j-l-m}$$
$$= N^{-1} \sum_{l=0}^{N-1} f_l K_{j-l} = (\mathbf{K} \circledast \mathbf{f})_j$$

Computing convolutions requires 2 forward FFTs, one element-wise product, and one inverse FFT, for a total cost $N \log N$ instead of N^2 . We can use this to solve **periodic integro-differential equations** involving convolutions, for example (recall that trapezoidal rule for the convolution is spectrally accurate for analytic functions)!

Spectral Differentiation

Spectral Derivative

- Consider approximating the derivative of a periodic function f(x), computed at a set of N equally-spaced nodes, \mathbf{f} .
- We can differentiate the spectral approximation: Spectral derivative

$$f'(x) \approx \phi'(x) = \frac{d}{dx}\phi(x) = \frac{d}{dx}\left(\sum_{k=0}^{N-1} \hat{f}_k e^{ikx}\right) = \sum_{k=0}^{N-1} \hat{f}_k \frac{d}{dx}e^{ikx}$$
$$= \sum_{k=0}^{N-1} \left(ik\hat{f}_k\right)e^{ikx} = \sum_{k=0}^{N-1} \left(\widehat{\phi'}\right)_k e^{ikx} \implies$$

$$\widehat{(\phi')}_k = ik\widehat{f}_k \quad \Rightarrow \quad \phi' = \mathcal{F}^{-1}\left(i\mathbf{k} \odot \widehat{\mathbf{f}}\right)$$

• Differentiation, like convolution, becomes multiplication in Fourier space.

Indeed
$$-\int f(y)\delta'(x-y)\,dy = \int f'(y)\delta(x-y)\,dy = f'(x).$$

Unmatched mode

- Recall that for even N there is one unmatched mode, the one with the highest frequency and amplitude $\hat{f}_{N/2}$.
- We need to choose what we want to do with that mode; see notes by
 S. G. Johnson (MIT) linked on webpage for details:

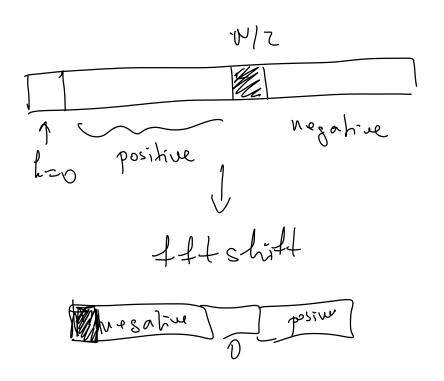
$$\phi(x) = \hat{f}_0 + \sum_{0 < k < N/2} \left(\hat{f}_k e^{ikx} + \hat{f}_{N-k} e^{-ikx} \right) + \hat{f}_{N/2} \cos\left(\frac{Nx}{2}\right).$$

This is the unique "minimal oscillation" trigonometric interpolant.

Differentiating this we get

$$\widehat{(\phi')}_{k} = \widehat{f}_{k} \begin{cases} 0 & \text{if } k = N/2 \\ ik & \text{if } k < N/2 \\ i(k-N) & \text{if } k > N/2 \end{cases}$$

• Real valued interpolation samples result in **real-valued** $\phi(x)$ for all x.



FFT-based differentiation

```
% From Nick Trefethen's Spectral Methods book
% Differentiation of \exp(\sin(x)) on (0,2*pi]:
 N = 8; % Even number!
  h = 2*pi/N; x = h*(1:N)';
  v = \exp(\sin(x)); vprime = \cos(x).*v;
  v_{hat} = fft(v);
  ik = 1i * (0:N/2-1)(0)(-N/2+1:-1)'; % Zero special mode
  w_hat = ik .* v_hat:
```

Differentiation matrices

- Writing g = f' we can denote this in matrix notation $\hat{\mathbf{g}} = \widehat{\mathbf{D}}_1 \hat{\mathbf{f}}$, where $\widehat{\mathbf{D}}_1$ is a **diagonal differentiation matrix** with ik on its diagonal (why does it have to be a matrix?).
- ullet Observe that $\widehat{f D}_1^\star = -\widehat{f D}_1$ (anti-Hermitian).
- In real space $\mathbf{g} = \mathbf{Df}$ and in Fourier space $\hat{\mathbf{g}} = \widehat{\mathbf{Df}}$, related by

$$D = F^{-1}\widehat{D}F = F^{*}\widehat{D}F$$
, $\subset antisyumetric$

where **F** is the unitary DFT matrix. Observe this is a similarity transformation!

• Here **Ff** and $\mathbf{F}^*\hat{\mathbf{f}}$ are computed using the (forward/inverse) FFT in nearly linear time.

Second derivative

Differentiating the interpolant twice we get

$$\widehat{(\phi'')}_k = \widehat{f}_k \begin{cases} -k^2 & \text{if } k < N/2 \\ -(k-N)^2 & \text{if } k \ge N/2 \end{cases}$$

- Similarly, if g = f'' then $\hat{\mathbf{g}} = \widehat{\mathbf{D}}_2 \hat{\mathbf{f}}$, where $\widehat{\mathbf{D}}_2$ has $-k^2$ on its diagonal, $\widehat{\mathbf{D}}_2^* = \widehat{\mathbf{D}}_2$ (Hermitian, same for \mathbf{D}_2).
- Double differentiating is different from differentiating twice in sequence, i.e., $\mathbf{D}_2 \neq \mathbf{D}_1^2$.
- Why is D_2 "better" than D_1^2 ? They have the same spectral accuracy.
- \mathbf{D}_1^2 has a nontrivial null space of $\mathbf{1}$ and $\mathbf{F}^{-1}\mathbf{e}_{N/2}$, while \mathbf{D}_2 has only $\mathbf{1}$.
- So D_2 is closer to the **continuum Laplacian operator** in periodic domains (having only constant functions in its null space). This is important when solving elliptic/parabolic PDEs.

$$\nabla^{2} u(\vec{x}) = f(\vec{x})$$

$$\nabla^{2} u(\vec{x}) = f^{*} \hat{D}_{2} + \hat{D}_$$

Discrete Matrices vs Continuum Operators

- The lesson learned from $D_2 \neq D_1^2$ is quite general: Continuum identities don't always translate to discrete identities.
- Many properties that seem obvious in continuum, may not work for discretizations:
 - Chain and product rules e.g., (cu)' = c'u + cu'.
 - Integration by parts (including boundary terms).
 - Operators commute, e.g., $\partial_x (\partial_y f) = \partial_y (\partial_x f)$.
 - Null spaces, eigenvalue spectrum properties (e.g., positive definiteness, symmetry, etc.).
- Mimetic discretizations try to mimic some of the properties of continuum operators.

Sturm-Louville Problems

 As an example, consider the periodic Sturm-Louville (SL) operator appearing in many boundary-value problems (BVPs):

$$\mathcal{L} = -\frac{d}{dx}c(x)\frac{d}{dx}, \quad c(x) > 0.$$

- From PDE class we know that this is a **symmetric positive semidefinite (SPsD) differential operator** with only constant functions in its null space; proving this uses integration by parts.
- When discretized, this will become a matrix **L**. We want this matrix to be SPsD with only **e** in its null space.
- It is a bad idea is to use the chain rule and discretize:

$$-\mathcal{L}f = \frac{d}{dx}c(x)\frac{d}{dx}f(x) = c'f' + cf''$$

$$-\mathbf{L}\mathbf{f} = (\mathbf{D_1c})\boxdot(\mathbf{D_1f}) + c\boxdot(\mathbf{D_2f}) \quad (\mathsf{BAD!})$$
since this is not an SPsD **L**.

Pseudospectral SL operator

• Another possibility is the **pseudospectral algorithm** that does not use the chain rule:

- In words: Go to Fourier space using the FFT, multiply coefficients by ik, go back to real space with iFFT, multiply by c(x) in real-space, then go back to Fourier space (FFT) and multiply coefficients by -ik, and then go back to real space again (iFFT).
- Why does this work? In matrix notation

$$\mathbf{L} = -\left(\mathbf{F}^{\star}\widehat{\mathbf{D}}_{1}\mathbf{F}\right)\mathbf{C}\left(\mathbf{F}^{\star}\widehat{\mathbf{D}}_{1}\mathbf{F}\right) = \mathbf{D}_{1}\mathbf{C}\mathbf{D}_{1}^{\star},$$

where \mathbf{C} is a diagonal matrix with $\mathbf{c} > 0$ on its diagonal.

This is obviously SPsD since C is SPD (why?).

Pseudospectral SL algorithm

For even N the pseudo-spectral \mathbf{L} has a nontrivial null space just like \mathbf{D}_1^2 does (think c=1), but this can be fixed (see article by Johnson):

- Compute \mathbf{f}' using FFT/iFFT but save the coefficient $\hat{f}_{N/2}$ (two FFTs).
- 2 Compute $\mathbf{g} = \mathbf{c} \cdot \mathbf{f}'$ in real space (pseudospectral part).
- Compute g using FFT.
- **Outpute** (\mathbf{Lf}) in Fourier space as:

$$\widehat{(\mathbf{Lf})}_{k} = \begin{cases} \widehat{c}_{0} \left(\frac{N}{2}\right)^{2} \widehat{f}_{N/2} & \text{if } k = N/2 \\ -ik\widehat{g}_{k} & \text{if } k < N/2 . \\ -i(k-N)\widehat{g}_{k} & \text{if } k > N/2 \end{cases}$$

Compute Lf in real space using an iFFT.

Solving PDEs using FFTs

KdV equation

• Consider as an example the periodic Korteweg – de Vries equation on $[0, 2\pi)$,

 $\partial_t \phi = -\partial_{xxx} \phi + 6\phi \left(\partial_x \phi\right),$

which models waves in a channel and has soliton solutions.

- First note that $\phi \phi_x = \partial_x \left(\phi^2/2 \right)$ and this is the right form to use because **KdV** is a conservation law and $\phi^2/2$ is a flux.
- Not all forms of PDEs equivalent on paper are equivalent numerically! We prefer

$$\partial_t \phi = -\partial_{xxx} \phi + 3\partial_x (\phi^2).$$

The idea is to use a Fourier series representation,

$$\phi(x,t) = \sum_{k} \hat{\phi}_{k}(t) e^{ikx}.$$

Spectral spatial discretization

If we go to Fourier space we get a system of coupled (nonlinear)
 ODEs:

- Note that the unmatched mode N/2 should be set to zero for the third derivative (all odd derivatives in fact).
- This is a **pseudo-spectral spatial discretization** and will be spectrally accurate for analytic solutions.
- In order to actually compute solutions we need methods to solve systems of ODEs (coming up soon)!

Spectral A du antages - Spectral accuracy
Sallows as to use
A a much coarser
grid to reach
a given accuracy (B*) For linear PDts with coust-welly, Matrices are diasonal Nou-periodic domains

Next true

Pisa de an Lages - Using FFTS ouly works with periodic because otherwise hy do not decay fast (algebraicaly) (But orthogonal polynomials work) (B) Matrices are, in general, dense (A*) Fail for non-smooth solutions ~ Do not preserve structure

of PDE

Nonlinear PDEs

- This is called an **exponential temporal integrator** and can be used to build accurate integrators for the nonlinear KdV equation.
- If the equation were linear, then $\hat{\phi}_k(t) = 0$ if $\hat{\phi}_k(0) = 0$: linear PDEs do not generate new Fourier components.
- But this is not true for nonlinear equations: in general, the solution will have nonzero components for all k for sufficiently long times, and aliasing becomes a problem.
- An extreme example is Burger's equation, which develops singularities (shocks), leading to the Gibbs phenomenon and loss of spectral accuracy.

Aliasing

• As an example, consider the product (or square)

$$C(x) \frac{1}{1} v$$

$$w(x) = u(x)v(x) \Rightarrow$$

$$w(x) = \left(\sum_{k''=-n}^{n} \hat{u}_{k''} e^{ik''x}\right) \left(\sum_{k=-n}^{n} \hat{u}_{k'} e^{ik'x}\right) = \sum_{k=-2n}^{2n} \hat{w}_{k} e^{ikx}$$

- So we doubled the number of Fourier modes, and handling this would require growing our FFT grid along the way!
- What we want to compute is the truncated Fourier series

$$w(x) \approx \tilde{w}(x) = \sum_{k=-n}^{n} \hat{w}_k e^{ikx}.$$

• If we do this naively using FFTs on a grid of N = 2n + 1 points, however, we will alias the modes |k| > n with those with |k| < n and this will introduce aliasing error.

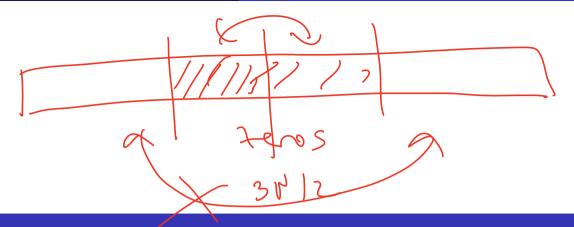
Anti-aliasing via oversampling

- But there is an easy fix using **oversampling**. Take u = v for simplicity and even N: M = 3M/2 M = 3M/2 M = 3M/2
- Evaluate u(x) on a grid of N points, take the FFT to compute $\hat{\mathbf{u}}$.
- 2 Padd the FFT to size M = 2N, avoiding fftshift (see fftinterp):

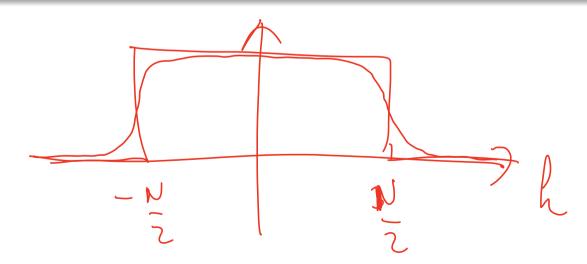
$$(\hat{\mathbf{u}})_{\text{padded}} = [\hat{\mathbf{u}}(1:N/2) \quad \text{zeros}(1,M-N) \quad \hat{\mathbf{u}}(N/2+1:\text{end})].$$

Note: It can be shown that M = 3N/2 also gives the same result.

- 3 Compute an oversampled $u_{os}(x)$ on a grid of size 2N by taking the iFFT of $(\hat{\mathbf{u}})_{padded}$.
- Occupate $\hat{\mathbf{u}}_{os}^{2}$ in real space, and take the FFT to compute $\hat{\mathbf{w}}$.
- Truncate to N Fourier coefficients by returning $[\hat{\mathbf{w}}(1:N/2) \quad \hat{\mathbf{w}}(M-N/2+1:\text{end})].$



Chebyshev Series via FFTs



Chebyshev Polynomials

- If we are solving PDEs on a bounded interval, say [-1,1] for simplicity, we need other orthogonal polynomials, not trig ones.
- Recall from Numerical Methods I the Chebyshev polynomials:

$$T_n(x \in [-1, 1]) = \cos(n\theta)$$
 where $x = \cos(\theta \in [0, 2\pi])$.

$$T_0(x) = 1$$
, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$, $T_3(x) = 4x^3 - 3x$,...

• These are orthogonal with respect to the weighted inner/dot product:

$$\int_{-1}^{1} T_m(x) T_n(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} \pi & m=n=0\\ \pi/2 & m=n>0\\ 0 & m\neq n \end{cases}.$$

Chebyshev Interpolants

We can represent functions using these polynomials as basis functions,

$$f(x) = \sum_{n=0}^{\infty} \breve{f}_n T_n(x) \Rightarrow$$

$$\breve{f}_{n>0} = \frac{2}{\pi} \int_{-1}^{1} f(x) T_n(x) \frac{dx}{\sqrt{1-x^2}}.$$

• We discretize the function pointwise at N+1 Chebyshev nodes

$$\theta_j = j\pi/N, \quad j = 0...N$$

 $x_j = \cos \theta_j$

• This gives us the Chebyshev interpolant (approximation):

$$\phi(x) = \sum_{n=0}^{N} \breve{f}_n T_n(x).$$

Chebyshev Nodes

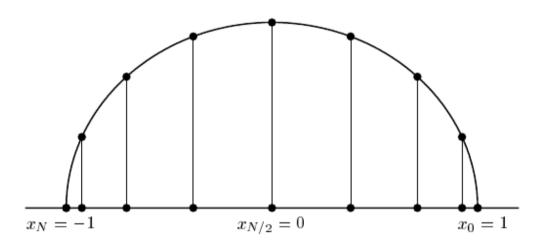


Fig. 5.1. Chebyshev points are the projections onto the x-axis of equally spaced points on the unit circle. Note that they are numbered from right to left.

Chebyshev via Fourier

• Changing variables from x to θ we get

• So if we consider instead of f(x) the function

$$g(\theta) = f(\cos \theta)$$

then we can go from **Fourier coefficients** of g to **Chebyshev** for f:

$$\breve{f}_{n>0} = \hat{g}_{-n} + \hat{g}_n$$

Chebyshev-Fourier transformation

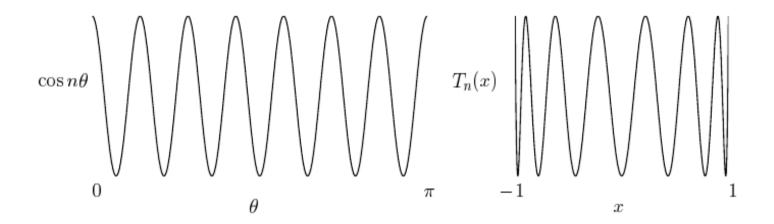


Fig. 8.2. The Chebyshev polynomial T_n can be interpreted as a sine wave "wrapped around a cylinder and viewed from the side".

Chebyshev via FFT

- This means that we can do **FFTs in equispaced points on** $\theta \in [0, 2\pi]$ instead of Chebyshev on non-equispaced nodes.
- Note that we want to extend this to $\theta \in [0, 2\pi]$ to be periodic and not $\theta \in [0, \pi]$, so we **double the number of points** and do the FFTs on vectors of length 2N.
- If f(x) can be extended analytically just outside of [-1, 1], then we get **spectral accuracy**.
- Intuition: Chebyshev polynomials are sine waves "wrapped around a cylinder and viewed from the side".
- One can approximate derivatives using the FFT; all that is needed is change of variables from x to θ using the chain rule.
- The chain of variables adds factors of the form $(1-x^2)^{-p/2}$ (where p is an integer) when converting from Fourier coefficients derivatives of g to derivatives of f.

Conclusions

Function Norms

- Consider a one-dimensional interval I = [a, b]. Standard norms for functions similar to the usual vector norms:
 - Maximum norm: $||f(x)||_{\infty} = \max_{x \in I} |f(x)|$
 - L_1 norm: $||f(x)||_1 = \int_a^b |f(x)| dx$
 - Euclidian L_2 norm: $||f(x)||_2 = \left[\int_a^b |f(x)|^2 dx \right]^{1/2}$
- Different function norms are not equivalent!
- An inner or scalar product (equivalent of dot product for vectors):

$$(f,g) = \int_a^b f(x)g^*(x)dx$$

• Formally, function spaces are **infinite-dimensional linear spaces**. Numerically we always **truncate and use a finite basis**.

Discrete Function Norms

• Consider a set of m nodes $x_i = a + ih$ with a constant grid spacing h = (b - a)/m, and evaluate the function at those nodes pointwise

$$\mathbf{f} = \{f(x_0), f(x_1), \cdots, f(x_m)\}.$$

 We define the discrete "function norms" and "dot products", with periodic BCs:

$$||f(x)||_{2} \approx \left[h \sum_{i=0}^{m-1} |f(x_{i})|^{2}\right]^{1/2} = \sqrt{h} ||\mathbf{f}||_{2},$$

$$||f(x)||_{1} \approx h \sum_{i=0}^{m-1} |f(x_{i})| = h ||\mathbf{f}||_{1},$$

$$||f(x)||_{\infty} \approx \max_{i} |f(x_{i})| = ||\mathbf{f}||_{\infty}$$

$$(f,g) \approx \mathbf{f} \cdot \mathbf{g} = h \sum_{i=0}^{m-1} f(x_{i})g^{*}(x_{i}).$$

Conclusions/Summary

- Convolution in real space becomes multiplication in Fourier space, and vice versa.
- **Spectrally-accurate derivatives** $f^{(\nu)}$ of analytic functions f can be done by multiplication by $(ik)^{\nu}$ in Fourier space, zeroing out the unmatched mode for even N and odd ν .
- Not all forms of operators and PDEs equal on paper are equal numerically. Choose the form that preserves the important properties of the continuum PDE: conservation laws, self-Hermitian operators, completeness (this is where understanding PDEs is crucial beyond superficial: functional analysis).
- Nonlinear PDEs can be discretized spectrally in space to a system of coupled nonlinear ODEs. Non-periodic domains can be handled by using orthogonal polynomials but boundary conditions need to be thought about some more!