Spectral methods – a quick review

For very simple functions, C^∞

in very simple geometries, Cartesian

Remarkably accurate

- error decreases like e^{-kN}
- only 3 modes per wave for 1% accuracy
  cf FD 40 pts at $O(\Delta x^2)$, 20 pts at $O(\Delta x^4)$

Differentiation exact to shortest mode

Trivial Poisson solver

time consuming transform and nonlinear terms
Sometimes FAST transform + less modes needed → competitive

Two ideas - as in FE

Spectral representation

$$u(x,t) = \sum^N \hat{u}_n(t)\phi_n(x)$$

with amplitudes $u_n(t)$ and basis functions $\phi_n(x)$, e.g. Fourier

Galerkin approximation "weighted residuals". For PDE

$$A(u) = f$$

require residue to be orthogonal to each ϕ_m:

$$\langle A(u) - f, \phi_m \rangle = 0 \quad \text{for} \quad m = 1, \dots, N$$

Local vs Global

E.g. for Fourier

$$u(x) = \int e^{ikx}\hat{u}(k)\, dk \qquad \hat{u}(k) = \frac{1}{2\pi}\int e^{-ikx}u(x)\, dx$$

Differentiation - global operator in real space

$$\widehat{\frac{du}{dx}} = ik\hat{u}(k) \quad \text{local in Fourier space}$$

Exact to shortest mode, cf FD $f_i' = \frac{f_{i+1}-f_{i-1}}{2\Delta x} = 0$ for $f_i = (-1)^i$.

Poisson problem

$$\frac{d^2u}{dx^2} = \rho \quad \text{expensive global problem in real space}$$

$$-k^2\hat{u} = \hat{\rho} \quad \text{local in Fourier space}$$

Local/Global continued

Nonlinear terms and spatially vary coefficients

$$u(x)v(x) \quad \text{local in real space}$$

$$\widehat{uv}(k) = \frac{1}{2\pi}\int_{l+m=k} \hat{u}(l)\hat{v}(m) \quad \text{global in Fourier}$$

Numerically

local = cheap global = expensive

Navier-Stokes has both local & global in real or Fourier – need compromise

Pseudo-spectral

combines Fourier and real space operations

Evaluate the nonlinear term in real space, and in Fourier space evaluate derivatives and invert the Poisson problem.
Needs three transforms $\rightarrow$

$$\begin{array}{llll} \hat{u} & \rightarrow & u & \\ \hat{u} \rightarrow \widehat{\nabla u} & \rightarrow \nabla u & u \cdot \nabla u & \\ \uparrow & & \downarrow & \\ \dot{\hat{u}} & \leftarrow \hat{p} & \leftarrow \widehat{u \cdot \nabla u} & \end{array}$$

Choose real points optimally.

Alternative method of satisfying PDE at collocation points rather than in Galerkin projection.

Choice of spectral basis function $\phi_n(x)$

1. complete
2. orthogonal for some weight w

$$\langle \phi_n \phi_m \rangle = \int \phi_n \phi_m w(x)\, dx = N_n \delta_{nm}$$

3. smooth
4. fast convergence
5. FAST transform
6. satisfy boundary conditions

Strongly recommend

- Fully periodic $\rightarrow$ Fourier, $e^{in\theta}$
- Finite interval $\rightarrow$ Chebyshev $T_n(\cos\theta) = \cos n\theta$

Chebyshev polynomials

$$T_n(\cos\theta) = \cos n\theta$$

Orthogonal with weight $w(x) = 1/\sqrt{1-x^2}$

$$\int_{-1}^{1} T_m(x) T_n(x) w(x)\, dx = \begin{cases} 0 & \text{if } n \neq m \\ \pi & \text{if } n = m = 0 \\ \frac{\pi}{2} & \text{if } n = m \neq 0 \end{cases}$$

$$T_0(x) = 1, \qquad T_1(x) = x, \qquad T_2(x) = 2x^2 - 1$$
$$T_3(x) = 4x^3 - 3x, \qquad T_4(x) = 8x^4 - 8x^2 + 1$$

$$(1-x^2)\, T_n'' - x\, T_n' + n^2\, T_n = 0$$
$$T_{n+1} = 2xT_n - T_{n-1}$$
$$2T_n = \tfrac{1}{n+1} T_{n+1}' - \tfrac{1}{n-1} T_{n-1}'$$

Fourier series

Fully periodic (really defined on a circle):

$$f^{(k)}(0+) = f^{(k)}(2\pi -) \quad \text{for all } k$$

Then Fourier series

$$f(\theta) = \sum_{n=-\infty}^{\infty} \hat{f}_n e^{in\theta}$$

with

$$\hat{f}_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-in\theta}\, d\theta$$

– awkward $\frac{1}{2}a_0$ if use sines and cosines.

Rates of convergence

If $f(\theta)$ has k-derivatives, integrate by parts k times

$$\hat{f}_n = \frac{1}{2\pi}\frac{i^k}{n^k}\int_0^{2\pi} f^{(k)}(\theta)e^{-in\theta}\,d\theta$$

Thus series converges rapidly with $\hat{f}_n = o(n^{-k})$ (RLL).

If $f^{(k)}$ has one discontinuity, $\hat{f}_n = O(n^{-k-1})$

If $f \in C^\infty$, $\hat{f}_n = e^{-kn}$ – exponential convergence

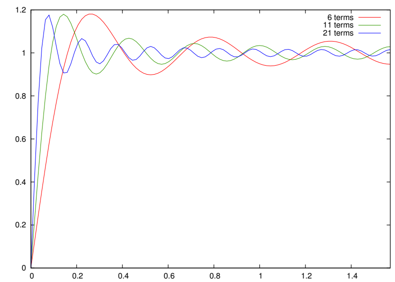
E.g.

$$f(\theta) = \sum_{m=-\infty}^{\infty} \frac{1}{(\theta - 2\pi m)^2 + a^2} \quad \to \quad \hat{f}_n = \frac{\pi}{a} e^{-|n|a}$$

– convergence controlled by singularity of $f(\theta)$ in complex θ-plane

Gibbs phenomenon

Discontinuity $\to$ poor $\sum \frac{\pm 1}{n}$ convergence



with point-wise convergence
but 14% overshoot within $\frac{1}{N}$ of discontinuity

Finite interval

If $f^{(k)}(0+) \neq f^{(k)}(2\pi-)$, then hidden discontinuity at boundary
$\to$ Gibbs problem, with slow convergence.

Use Chebyshev $T_n(x) = \cos n\theta$

Stretch $x = \cos\theta$ makes odd derivatives vanish

$$\tilde{f}(\theta) = f(\cos\theta) \quad \to \quad \frac{d\tilde{f}}{d\theta} = \sin f'$$

Hence function $|\,x\,|$ on $-1 < x < 1$
becomes fully 2π periodic in $-\pi < \theta < 0$

Discrete Fourier Transform (DFT)

Odd $N = 2M + 1$.
Equi-spaced collocation points $\theta_j = \frac{2\pi j}{N}$ for $j = 1, \ldots, N$

Discrete approximation $\tilde{f}_n$ to Fourier $\hat{f}_n$

$$\tilde{f}_n = \frac{1}{N}\sum_{j=1}^{N} f(\theta_j)e^{-in\theta_j} \qquad n = -M, \ldots, M$$

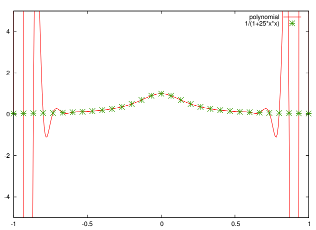
Note for later: $e^{-i(N+k)\theta_j)} \equiv e^{-ik\theta_j}$, so $f_{N+k} = f_k$

Let $\omega = e^{i2\pi/N}$ the N-th root of 1, so $\sum_{-M}^{M}\omega^n = 0$
Then

$$\sum_{n=-M}^{M} \tilde{f}_n e^{in\theta} = \sum_{j=1}^{N} f(\theta_j)\left[\frac{1}{N}\sum_{n=-M}^{M} e^{in(\theta-\theta_j)} = \begin{cases} 1 & \text{if } \theta = \theta_j \\ 0 & \text{if } \theta = \theta_k \neq \theta_j \end{cases}\right]$$
$$= f(\theta_j) \quad \text{if } \theta = \theta_j$$

Runge phenomenon

Fitting polynomial through equi-spaced points can be badly wrong in between fitting points.



However DFT well behaved, because effectively Chebyshev polynomials fitted at points $x_j = \cos(\pi j/N)$ – crowed at ends.

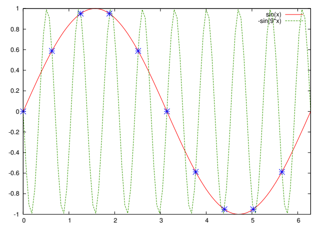
Aliasing

– counter rotating wagon wheels in strobe light

High $(N+k)$ frequency, e.g. $g(\theta) = e^{i(N+k)\theta}$,
appears in DFT to be erroneous low k frequency:

$$\tilde{g}_k = \frac{1}{N}\sum_{j=1}^{N} g(\theta_j) e^{-ik\theta_j} = 1$$

E.g. $N = 10$ equispaced points cannot distinguish between $\sin\theta$ and $-\sin 9\theta$



De-aliasing

Aliasing makes high frequency tail

of exact Fourier modes $\hat{f}_n$ in $n > M$

appear to DFT $\tilde{f}_n$

as low frequency modes at $-M + n$.

De-alias: Chop spectrum to $-\frac{2}{3}M < n < \frac{2}{3}M$,

so nonlinear terms can produce new $\frac{2}{3}M < n < \frac{4}{3}M$

which are then chopped so as not transfer to low frequencies.

In 3D throw away $\frac{19}{27}$ of the modes.

Fast Fourier Transform

DFT calculation for $n = -\frac{1}{2}N, \dots, \frac{1}{2}N$

$$\tilde{f}_n = \sum_{j=1}^{N} f(\theta_j)\omega^{nj}, \quad \text{with } \theta_j = \frac{2\pi j}{N} \text{ and } \omega = e^{i\theta_1}$$

looks like N coefficients $\times$ sum of N terms $= N^2$ operations.

But

$$= \sum_{k=1}^{N/2} f(\theta_{2k})\omega_2^{nk} + \omega^{-1}\sum_{k=1}^{N/2} f(\theta_{2k-1})\omega_2^{nk} \quad \text{with } \omega_2 = \omega^2$$

which is 2 lots of DFT on $\frac{1}{2}N$ points $2(\frac{1}{2}N)^2 = \frac{1}{2}N^2$ operations

If $N = 2^K$, can half K times $\to N \ln_2 N$ operations.

Program: identify even/odd at each 2^n-level $n = 1, \dots, K$,
i.e. binary representation of j

Orzsag speed up in two dimensions

$$\sum_{m=1}^{M}\sum_{n=1}^{N} a_{mn}\phi_m(x_i)\phi_n(y_j)$$

looks line MN terms to sum at MN points (x_i, y_j)

But

$$\sum_{m=1}^{M} a_{mn}\phi_m(x_i)$$

is common to each $(x_i, *)$ point, $\rightarrow$ save factor of M operations.

Also FFT speed up

Differential Matrix

To differentiate data with exponential accuracy

$$f(\theta_j) \xrightarrow{\text{transform}} \tilde{f}_n \xrightarrow{\text{differentiate}} n\tilde{f}_n \xrightarrow{\text{transform}} f'(\theta_j)$$

But transforming is a linear sum, so

$$f'(\theta_i) = D_{ij} f(\theta_i) \quad \text{with differentiation matrix } D$$

FFT factorisation can make $N \ln N$ instead of N^2

$$\begin{aligned} &\text{2pts} \rightarrow \text{2nd order in FD} \rightarrow \text{error} \quad N^{-2} \\ &\text{4pts} \rightarrow \text{4th order in FD} \rightarrow \text{error} \quad N^{-4} \\ &\text{Npts} \rightarrow \qquad\qquad\qquad \rightarrow \text{error} \quad N^{-N} \end{aligned}$$

NB $D^{(2)} \neq DD$

Navier-Stokes

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}$$

Fourier transform

$$i\mathbf{k} \cdot \hat{\mathbf{u}} = 0$$

$$\frac{\partial \hat{\mathbf{u}}}{\partial t} + \widehat{\mathbf{u} \cdot \nabla \mathbf{u}} = -i\mathbf{k}\hat{p} - \nu k^2 \hat{\mathbf{u}}$$

Eliminate pressure

$$\frac{\partial \hat{\mathbf{u}}}{\partial t} = -\left(\mathbf{I} - \frac{\mathbf{kk}}{k^2}\right) \cdot \widehat{\mathbf{u} \cdot \nabla \mathbf{u}} - \nu k^2 \hat{\mathbf{u}}$$

with $\widehat{\mathbf{u} \cdot \nabla \mathbf{u}}$ by pseudo-spectral real space evaluation

Boundary conditions

If homogeneous BCs, recombine to satisfy BCs

$$\phi_{2n} = T_{2n} - T_0 \quad \text{and} \quad \phi_{2n-1} = T_{2n-1} - T_1$$

OR impose BC ("tau" method)

$$\sum_{n-1}^{N} \tilde{f}_n T_n(\pm 1) = \mathrm{BC}$$

Crowding of points $\rightarrow$ time-step limitation

$$\text{For} \quad u_t = D u_{xx} \quad \text{on } [-1, 1]$$

$1/N^2$ crowding of $x_j = \cos\theta_j$ near ± 1
$\rightarrow$ stability if $\Delta t < D/N^4$

Bridging the gap

Local			Global
	Finite Elements	FE h^p	
Finite Differences point data			Spectral whole interval
	Splines global points	Wavelets local waves	