Spectral methods

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Objectives

Main objective of the lecture is to give an introduction to spectral and spectral-element methods for the discretisation of PDEs. I will

- give a fast motivating introduction
- introduce you to the bases adopted
- introduce the main operations on the basis
- give an idea of advantages and drawbacks

Outline

Why spectral methods?

Consider the truncated discrete Fourier Transform of $u(x)$, $\check{u}_k$.

Theorem

If $u(x)$ is m-times continuously differentiable in $[0, 2\pi]$ ($m \geq 1$), and if $u^{(j)}$ is periodic for all $j \leq m - 2$, then

$$\check{u}_k = O(k^{-m}),$$

If $u(x)$ is infinitely differentiable and periodic with all its derivatives on $[0, 2\pi]$, $\check{u}_k$ decays faster than any negative power of k.

The main advantage of spectral methods is their extreme accuracy for smooth problems.

The heat equation in a periodic box

Let us consider the 1D heat equation with constant diffusion parameter ν, discretised by a first-order time-discretisation scheme:

$$U^{n+1} = U^n + \nu \Delta t \frac{\partial^2 U^n}{\partial x^2}$$

with periodic conditions in the interval $(0, L)$. Let us set $U^n(x) = \sum_{k=-\infty}^{+\infty} U_k^n e^{i2\pi\kappa x/L}$, then

$$U_k^{n+1} = U_k^n - \frac{4\pi^2\kappa^2\nu\Delta t}{L^2} U_k^n$$

The solution is very, very simple, since each Fourier mode evolves independently.

The same holds for the 2D and 3D heat equation.

The Navier–Stokes equations in a periodic box

Let us Fourier transform the Navier–Stokes equation in space $\boldsymbol{u}(\boldsymbol{r},t)=\sum_{\boldsymbol{\kappa}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\check{\boldsymbol{u}}(\boldsymbol{\kappa},t)$ and $p(\boldsymbol{r},t)=\sum_{\boldsymbol{\kappa}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\check{p}(\boldsymbol{\kappa},t)$.

$$\frac{d\check{\boldsymbol{u}}}{dt}+\nu\boldsymbol{\kappa}^2\check{\boldsymbol{u}}=-(1-\frac{\boldsymbol{\kappa}}{\boldsymbol{\kappa}^2}\boldsymbol{\kappa}\cdot)\check{G},$$

where $\check{G}$ is the Fourier transform of the nonlinear term.

Matters of efficiency: the FFT

When hierarchical bases are employed, the presence of nonlinear terms that are treated pseudo-spectrally requires to compute the point values from the coefficients and viceversa.
These operations require in general N^{d+1} operations using matrix multiplication.
For sinusoidal functions (and Chebyshev polynomials), they can be accomplished in just $CN^d \log N$ operations using the recursive Fast Fourier Transform (FFT) algorithm first proposed by Cooley and Tuckey for $N = 2^n$ points, and then extended to more general numbers of points (see www.fftw.org).
Exploiting FFT quasi-optimal spectral methods can be obtained.

Pseudospectral treatment of the nonlinear term

Let us compute the Fourier Transform of the product of two functions $\check{G} = \mathcal{F}(uv)$ starting from $\check{u}$ and $\check{v}$ described with N coefficients:

$$\mathcal{F}(uv) = \mathcal{F}\left(\sum_{j=-N/2}^{N/2-1} \check{u}_j e^{2\pi i j x/L} \sum_{l=-N/2}^{N/2-1} \check{v}_l e^{2\pi i l x/L} \right)$$

$$= \mathcal{F}\left(\sum_{m=-N/2}^{N/2-1} \left(\sum_{j+l=m} \check{u}_j \check{v}_l \right) e^{2\pi i m x/L} \right)$$

the convolution requires N^{d+1} ops in d dimensions.
Pseudospectral treatment: cost reduced to $O(N^d \log N)$ ops:

1. transform $\check{u}$ and $\check{v}$ to the physical space by FFT ($O(N^d \log N)$ ops)
2. compute the product $u(x_k)v(x_k)$ for all points k ($O(N^d)$ ops)
3. transform $u(x_k)v(x_k)$ to Fourier space by FFT ($O(N^d \log N)$ ops)

Aliasing error

Fact

The product of two truncated expansions involves a doubled number of harmonics (since $2\sin(\alpha x)\cos(\alpha x) = \sin(2\alpha x)$).

Aliasing error

The pseudospectral treatment leads to an error when the expansion of the term uv is truncated as u and v $\rightarrow$ energy associated with discarded wavenumbers summed to retained wavenumbers.

Dealiasing

1. transform $\check{u}$ and $\check{v}$ to the physical space on $3N/2$ points
2. compute the product $u(x_k)v(x_k)$ for all points $3N/2$ points
3. transform $u(x_k)v(x_k)$ to $3N/2$ Fourier harmonics
4. discard harmonics with wavenumber larger that $N/2$

Fourier and homogeneous directions

The Fourier approximation is spectrally accurate in an interval only if periodic boundary conditions can be applied in fact:

- to obtain spectral accuracy the interpolated function must be infinitely differentiable
- a function defined on a finite interval can be made periodic by translating it an infinite number of times
- only very peculiar functions (almost only periodic functions) will be infinitely smooth when made periodic in this way

Conclusion

Fourier methods are employed almost only when periodic boundary conditions can be applied (in invariant directions).

Extension to compact intervals

Question

Can the good approximation properties shown by Fourier expansion be obtained on compact intervals?

Answer

Yes, if special high order polynomials are employed.

The polynomials suitable to obtain spectral accuracy in the approximation of $C^\infty(\Omega)$ functions are the eigenfunctions $u(x)$ of the singular Sturm–Liouville equation:

$$-(p(x)u')' + q(x)u = \lambda w(x)u, \quad x \in (-1, 1).$$

The Sturm-Liouville equation is singular if $p(-1) = p(1) = 0$.

Orthogonal polynomials and their properties

The general eigenfunctions of the singular Sturm–Liouville equation are the Jacobi polynomials:

$$
\begin{aligned}
P_n^{(\alpha,\beta)}(z) &= \frac{(-1)^n}{2^n n!}(1-z)^{-\alpha}(1+z)^{-\beta}\frac{d^n}{dz^n}\left[(1-z)^{\alpha+n}(1+z)^{\beta+n}\right] \\
&= \frac{1}{2^n}\sum_{k=0}^{n}\binom{n+\alpha}{k}\binom{n+\beta}{n-k}(z-1)^{n-k}(z+1)^k
\end{aligned}
$$

that are eigenfunctions of the singular Sturm-Liouville equation

$$
\left(1-x^2\right)y'' + (\beta-\alpha-(\alpha+\beta+2)x)y' + n(n+\alpha+\beta+1)y = 0.
$$

Some properties

The Jacobi polynomials are orthogonal in the interval $(-1, 1)$ with respect to the weighted inner product

$$(u, v)_{\alpha,\beta} \equiv \int_{-1}^{1} u(x)v(x)(1-x)^{\alpha}(1+x)^{\beta} dx.$$

Particular choices of the indices α and β lead to well known orthogonal polynomials:

- $\alpha = \beta = 0 \rightarrow$ Legendre polynomials
- $\alpha = \beta = -1/2 \rightarrow$ Chebyshev polynomials

Some properties

Symmetry:

$$P_n^{(\alpha,\beta)}(-z) = (-1)^n P_n^{(\beta,\alpha)}(z);$$

Derivatives:

$$\frac{d^k}{dz^k} P_n^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha+\beta+n+1+k)}{2^k \Gamma(\alpha+\beta+n+1)} P_{n-k}^{(\alpha+k,\beta+k)}(z).$$

Recurrence:

$$\begin{aligned}
&2n(n+\alpha+\beta)(2n+\alpha+\beta-2)P_n^{(\alpha,\beta)}(z) = \\
&= (2n+\alpha+\beta-1)\left\{(2n+\alpha+\beta)(2n+\alpha+\beta-2)z+\alpha^2-\beta^2\right\}P_{n-1}^{(\alpha,\beta)}(z) \\
&- 2(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)P_{n-2}^{(\alpha,\beta)}(z),
\end{aligned}$$

for $n = 2, 3, \ldots$.

Accuracy properties and other properties

The main advantages of this kind of polynomials are:
Their orthogonality, which assures:

- stable approximations
- better conditioned discrete operators
- sparsity of simple discrete operators

The spectral accuracy of the approximation, stated by the following

Theorem

For any $v \in H^r_{(\alpha,\beta)}$ and $r \geq 0$,

$$\|P_{N,\alpha,\beta}(v) - v\|_{(\alpha,\beta)} \leq cN^{-r}\|v\|_{(\alpha,\beta)}.$$

Outline

Start: the NS equations in a box

We consider the time-dependent incompressible Navier–Stokes equations. The domain is $\Omega = (0,1)^2$. The problem can be formulated as: Find a velocity $\boldsymbol{u}$ and a pressure p (up to a constant) so that

$$\begin{cases} \dfrac{\partial \boldsymbol{u}}{\partial t} - \nu \nabla^2 \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} + \boldsymbol{\nabla} p = \boldsymbol{0}, \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \\ \boldsymbol{u}_{|\partial\Omega} = \boldsymbol{b}, \\ \boldsymbol{u}_{|t=0} = \boldsymbol{u}_0, \end{cases}$$

where ν is viscosity, $\boldsymbol{b}$ is the velocity b.c. and $\boldsymbol{u}_0$ is the divergence-free initial velocity.

A mixed-basis spectral-projection method

The problem is discretized in time by a second-order, pressure-correction scheme, with end-of-step velocity eliminated. The viscous step for BDF scheme reads:

$$\begin{cases} \dfrac{3\boldsymbol{u}^{k+1} - 4\boldsymbol{u}^{k} + \boldsymbol{u}^{k-1}}{2\Delta t} - \nu\nabla^2\boldsymbol{u}^{k+1} = -(\overline{\boldsymbol{u}}^{k+1}\cdot\boldsymbol{\nabla})\overline{\boldsymbol{u}}^{k+1} \\ \qquad\qquad\qquad\qquad\qquad\qquad -\frac{1}{3}\boldsymbol{\nabla}(7p^{k} - 5p^{k-1} + p^{k-2}), \\ \boldsymbol{u}^{k+1}{}_{|\partial\Omega} = \boldsymbol{b}^{k+1}, \end{cases}$$

Then, the incremental projection step reads:

$$\begin{cases} -\widehat{\nabla}^2(p^{k+1} - p^{k}) = -\dfrac{3}{2\Delta t}\,\boldsymbol{\nabla}\cdot\boldsymbol{u}^{k+1}, \\ \dfrac{\partial(p^{k+1} - p^{k})}{\partial n}_{|\partial\Omega} = 0. \end{cases}$$

Spatial discretisation

Owing to the different boundary conditions, we introduce two different bases for the approximation of velocity and pressure.

The velocity is solution of a Helmholtz–Dirichlet problem, a suitable basis for the n-dimensional problem is the direct product of the following polynomial basis:

$$L_0^*(x) = 1, \quad L_1^*(x) = \frac{x}{\sqrt{2}}, \quad L_i^*(x) = \frac{L_{i-2}(x) - L_i(x)}{\sqrt{2(2i-1)}}. \quad i \geq 2,$$

The pressure is solution of a Poisson–Neumann problem. A convenient basis for this problem is obtained by the direct product of Legendre polynomials normalized to obtain a unit mass matrix.

$$L_{i_h}^{\diamond}(x) = \sqrt{i_h + \tfrac{1}{2}}\, L_{i_h}(x). \qquad i_h \geq 0.$$

Spatial discretisation

We introduce the expansions for ($\boldsymbol{u}_N$ and $p_{\hat{N}}$)

$$\boldsymbol{u}_N(t,x,y) = \sum_{i=2}^{N} L_i^*(x)\, \boldsymbol{U}_{i,j}(t)\, L_j^*(y) \sum_{j=2}^{N},$$

$$p_{\widehat{N}}(t,x,y) = \sum_{i_h=0}^{N-2} L_{i_h}^{\diamond}(x)\, P_{i_h,\hat{\jmath}}(t)\, L_{\hat{\jmath}}^{\diamond}(y) \sum_{\hat{\jmath}=0}^{N-2},$$

($\sum$ is used to denote summation on the second index).
By the Galerkin method, we obtain the following algebraic problem:

$$\boldsymbol{U}^{k+1} M^* + M^* \boldsymbol{U}^{k+1} + \gamma M^* \boldsymbol{U}^{k+1} M^* = \boldsymbol{F}^{k+1},$$
$$D^{\diamond} (P^{k+1} - P^k) + (P^{k+1} - P^k) D^{\diamond} = G^{k+1},$$

where $\gamma = 1/(\nu \Delta t)$.

Right-hand sides

The right-hand sides of the previous equations are:

$$\nu\, \boldsymbol{F}_{i,j}^{k+1} = \frac{1}{\Delta t}\left(L_i^*(x)L_j^*(y), \boldsymbol{u}_N^k\right) + \left(L_i^*(x)L_j^*(y), \boldsymbol{f}^{k+1}\right)$$
$$- \left(L_i^*(x)L_j^*(y), \nabla(2p_{i_h}^k - p_{i_h}^{k-1})\right) - \left(L_i^*(x)L_j^*(y), (\boldsymbol{u}_N^k\cdot\nabla)\boldsymbol{u}_N^k\right),$$

$$G_{i_h,\hat{\jmath}}^{k+1} = -\frac{1}{\Delta t}\left(L_{i_h}^\diamond(x)L_{\hat{\jmath}}^\diamond(y), \nabla\cdot\boldsymbol{u}_N^{k+1}\right),$$

where $\widetilde{p} = 7p^k - 5p^{k-1} + p^{k-2}$.
The matrices corresponding to $\left(L_i^*(x), L_{i_h}^\diamond{}'(x)\right)$ and $\left(L_{i_h}^\diamond(x), L_i^*{}'(x)\right)$ representing the first derivatives can be evaluated analytically and are sparse with only the two first rows and one codiagonal different from zero. Similarly, the ‘matrices $\left(L_i^*(x), L_{i_h}^\diamond(x)\right)$ and $\left(L_{i_h}^\diamond(x), L_i^*(x)\right)$ needed to evaluate the gradient and the divergence are sparse with only the diagonal and one codiagonal different from zero.

Discrete operators: an example

The mass matrix M^* is pentadiagonal with only three diagonals different from zero:

$$
M^* = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ \vdots \\ N-2 \\ N-1 \\ N \end{array}
\begin{array}{c}
\begin{array}{ccccccc} 0 & 1 & 2 & \cdots & N-2 & N-1 & N \end{array} \\
\begin{pmatrix}
c_0 & 0 & a_0 & & & & \\
0 & c_1 & 0 & \ddots & & & \\
a_0 & 0 & c_2 & \ddots & \ddots & & \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & \\
 & & \ddots & \ddots & \ddots & \ddots & a_{N-2} \\
 & & & \ddots & \ddots & \ddots & 0 \\
 & & & & a_{N-2} & 0 & c_N
\end{pmatrix}
\end{array}
$$

where:

$$
\begin{aligned}
a_0 &= \sqrt{\frac{2}{3}}, & a_1 &= \frac{1}{3\sqrt{5}}, & a_i &= \frac{-1}{(2i+1)\sqrt{(2i-1)(2i+3)}}, & i \geq 2, \\
c_0 &= 2, & c_1 &= \frac{1}{3}, & c_i &= \frac{2}{(2i-3)(2i+1)}, & i \geq 2.
\end{aligned}
$$

Alternative forms of the nonlinear term

There are several possible formulations for the nonlinear term that are not equivalent.

Table : Formulation of the nonlinear term (here $\otimes$ denotes the tensor product and $\boldsymbol{\omega} = \boldsymbol{\nabla} \times \boldsymbol{u}$ is the vorticity).

Convective	$\left(v, (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u}\right)$
Rotational	$\left(v, \boldsymbol{\omega} \times \boldsymbol{u}\right)$
Skew-symmetric	$\frac{1}{2}\left(v, (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u}\right) - \frac{1}{2}\left(\boldsymbol{u} \cdot \nabla v, \boldsymbol{u}\right)$
Divergence	$\left(v, \boldsymbol{\nabla} \cdot (\boldsymbol{u} \otimes \boldsymbol{u})\right)$

The skew-symmetric form is the only one which is stable and conserves energy in presence of aliasing.
The divergence form is not stable even for dealiased pseudospectral treatments (for coarse discretizations).

Outline

Some references

- C. Canuto, M.Y. Hussaini, A. Quarteroni & T.A. Zang, *Spectral methods in fluid dynamics*, Springer, 1988.
- J. Shen, T. Tang & L. Wang, *Spectral methods: algorithms, analysis and applications*, Springer, 2011.