CHAPTER 9

Spectral methods

1. Preliminaries

We have so far used Fourier methods in the theoretical analysis of numerical algorithms. However Fourier methods are also very useful in the *construction* of numerical methods for PDE's. By way of an introduction to spectral methods we shall concentrate on solving time dependent problems with periodic boundary conditions over a finite domain which we take to be $[-\pi, \pi]$, $f(x+2\pi) = f(x)$. If $\|f\|_1 < \infty$ the function $f(x)$ can be expressed as a *Fourier series*

$$f(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ikx} \tag{1.1}$$

with the Fourier coefficients given by

$$\hat{f}_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} dx \ . \tag{1.2}$$

This is the discrete wavenumber equivalent of the continuum Fourier transform introduced previously

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k) e^{i\xi x} d\xi, \ \hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(x) e^{-i\xi x} d\xi. \tag{1.3}$$

Typically we are interested in finding solutions that are smooth, say of class C^1 over $[-\pi, \pi]$ except a finite number of points of discontinuity. The important result from Fourier analysis relevant to this class of problems is:

THEOREM 5. *If f is piecewise smooth with period 2π then the Fourier series of converges to $f(x)$*

$$\lim_{K \to \infty} \sum_{k=-K}^{K} \hat{f}_k e^{ikx} = f(x) \ . \tag{1.4}$$

At a point of discontinuity we extend f by the definition $f(x) = (f(x_-) + f(x_+))/2$.

2. Evaluation of derivatives

Assume that $f \in \mathcal{C}^1$ and periodic over $[-\pi, \pi]$ so that both f and f' have convergent Fourier series. The series expansion of f' is

$$f'(x) = \sum_{k=-\infty}^{\infty} d_k e^{ikx} \ . \tag{2.1}$$

Derivation of the Fourier series of f leads to

$$f'(x) = i \sum_{k=-\infty}^{\infty} k \hat{f}_k e^{ikx} \tag{2.2}$$

so we conclude that

$$d_k = ik\hat{f}_k \ . \tag{2.3}$$

If we know the Fourier coefficients of f, the Fourier coefficients of the derivatives of f are obtained by multiplication with ik. This again is essentially a consequence of the exponential being an eigenfunction of the differentiation operator

$$\partial_x e^{ikx} = ike^{ikx} \ . \tag{2.4}$$

3. Discrete Fourier transform

In practical work we can only use a finite number of wave modes and a finite number of function values. The finite version of the Fourier transform is known as the discrete Fourier transform and is given by

$$f_j = \sum_{k=-N/2+1}^{N/2} \hat{f}_k e^{ikx_j} \tag{3.1}$$

$$\hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j} \tag{3.2}$$

where the function values are known at $x_j = jh - \pi$, $h = 2\pi/N$, $j = 0, 1, \cdots, N-1$ and the wavenumbers run from $-N/2+1$ to $N/2$. Introducing $\omega_N = e^{2\pi i/N}$, the N^{th} root of unity the transformation formulas can be written

$$f_j = \sum_{k=-N/2+1}^{N/2} \hat{f}_k \omega_N^{jk}, \ \hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j \omega_N^{-jk} \ . \tag{3.3}$$

These specify two matrix-vector multiplication operations

$$f = F^{-1}\hat{f}, \ \hat{f} = Ff \tag{3.4}$$

and would seem to require $O(N^2)$ arithmetic operations to carry out. The operation count can be drastically reduced by use of the fast Fourier transform (FFT) algorithm. If N is even, $N = 2P$ we can separate the sequence $\{f_0, f_1, \ldots, f_{2P-1}\}$ into two parts, one containing even indices and the other the odd ones

$$u_j = f_{2j}, \ v_j = f_{2j+1}, \ j = 0, \ldots, P-1 \ . \tag{3.5}$$

The Fourier coeffcients $\hat{f}_k$ are then computed by

$$\hat{f}_k = \frac{1}{2P} \sum_{j=0}^{P-1} \left(u_j \omega_N^{-2jk} + v_j \omega_N^{-(2j+1)k} \right) \tag{3.6}$$

$$= \frac{1}{2P} \left(\sum_{j=0}^{P-1} u_j \omega_P^{-jk} + \omega_N^k \sum_{j=0}^{P-1} v_j \omega_P^{-jk} \right) \tag{3.7}$$

and instead of one matrix-vector multiply costing $O(N^2)$ we obtain two matrix-vector multiplies each costing $O(N^2/4)$ for a total computational effort of $O(N^2/2)$.

FIGURE 1. An example of aliasing. $\sin x$, $\sin 5x$, $\sin 9x$ are the same when sampled on a coarse grid (circles).

The beauty of this approach is that if $N = 2^p$ we can continue the procedure and reduce the operation count down to $O(N \log_2 N)$ a significant improvement over $O(N^2)$. The FFT can be also implemented for N as some composite of other powers of small prime numbers. Through application of the FFT we see that derivatives are economically evaluated using (2.3).

If we do not use a sufficient number of Fourier modes to completely capture all variations in the function, an error known as *aliasing* can occur. The minimum number of points needed to capture all variations in a function is given by the *Nyquist criterion.* If K is the highest wavenumber present in function f then we need at least $N = 2K$ points to completely represent f through a discrete Fourier series. Aliasing is easily understood as an artefact of too coarse a sampling of a function. Consider for instance the case when $N = 4$ so the grid nodes are $x_j = -\pi + j\pi/2$, $j = 0, \dots, 3$. Note that $\sin x$, $\sin 5x$, $\sin 9x$ are indistinguishable on this grid, Fig. 1. Aliasing leads to contamination of low wavenumber modes from higher wavenumbers present in f that are not resolved by the chosen grid resolution. The errors thus introduced can be quite significant since the low wavenumber modes govern the coarse features of f. There exist a number of techniques to eliminate aliasing. Besides the obvious one of ensuring the Nyquist criterion is met filtering the high wavenumbers or using higher resolution in certain stages of a computation are also used.

4. Applications to PDE's

Fourier methods are especially useful in solving problems for which we know the solution is smooth. This is a result of a number of results from Fourier analysis. If f is L^2 then we can state:

THEOREM 6. *If f has $p-1$ continuous derivatives in L^2 for $p \geq 0$ and a p^{th} derivative of bounded variation then*

$$\hat{f}(\xi) = O(|\xi|^{-p-1}) \text{ as } |\xi| \to \infty \ . \tag{4.1}$$

This statement tells us how the Fourier coefficients decay at high wavenumbers. In particular for infinitely differentiable functions the Fourier coefficents decay faster than any polynomial power. This behavior implies that once enough Fourier modes have been introduced to capture the characteristic scales of f the amplitude of higher modes is essentially zero. For numerical work we expect that a finite number of modes will essentially reproduce the exact behavior of the smooth function and its derivatives. It is the combination of accuracy and ease of evaluation of derivatrives that make Fourier methods valuable in solving PDE's numerically. Note however that this is generally the case only when we have smooth functions and for very special boundary conditions such as the periodic boundary conditions considered here.

Let us now sketch how various common PDE's can be solved through Fourier methods. In all cases we shall consider periodic boundary conditions over the interval $[-\pi, \pi]$ along each spatial direction.

4.0.3. *Advection equation.* For the problem

$$q_t + uq_x = 0 \tag{4.2}$$

$$q(x, t = 0) = q_0(x) \tag{4.3}$$

with u constant, we introduce the Fourier series

$$q_j(t) = \sum_{k=-N/2+1}^{N/2} \hat{q}_k(t)\omega_N^{jk} \tag{4.4}$$

giving the values of q at the points $x_j = -\pi + jh$, $h = 2\pi/N$. This is a semi-discretization formulation in which time is kept as a continuous variable at this stage. The values of the x-derivative at x_j are given by

$$\left(\frac{\partial q}{\partial x}\right)_j (t) = \sum_{k=-N/2+1}^{N/2} ik\hat{q}_k(t)\omega_N^{jk} \tag{4.5}$$

The powers of ω_N form a basis for grid functions so replacing the series into (4.2) leads to

$$\frac{d}{dt}\hat{q}_k + iuk\hat{q}_k = 0 \tag{4.6}$$

$$\hat{q}_k(t = 0) = \hat{q}_{0,k} \tag{4.7}$$

for $k = -N/2 + 1, \ldots, N/2$ with $\hat{q}_{0,k}$ the Fourier coefficents of the initial condition. For real q we have $\hat{q}_k = (\hat{q}_{-k})^*$ so the complete Fourier coefficients can be obtained from a knowledge of the positive wavenumbers only. The system of ODE's is thus reduced to $k = 0, 1, \ldots, N/2$. Each equation can be solved analytically

$$\hat{q}_k(t) = \hat{q}_{0,k}\exp(-iukt) \tag{4.8}$$

and the problem is solved. Note that if q is C^∞ and N large enough to capture all the modes present in $q_0(x)$ the solution is essentially exact and we would expect to observe errors on the order of machine zero when carrying out this computation in practice.

For the 2D adevction equation

$$q_t + uq_x + vq_y = 0 \tag{4.9}$$

$$q(x, y, t = 0) = q_0(x, y) \tag{4.10}$$

the procedure is quite similar. We shall employ a double Fourier series representation

$$q_{m,n} = \sum_{k=-M/2+1}^{M/2} \sum_{l=-N/2+1}^{N/2} \hat{q}_{k,l}(t)\omega_M^{mk}\omega_N^{nl} \tag{4.11}$$

to obtain the system

$$\frac{d}{dt}\hat{q}_{k,l} + i(uk + vl)\hat{q}_{k,l} = 0 \tag{4.12}$$

$$\hat{q}_{k,l}(t = 0) = \hat{q}_{0,k,l} \tag{4.13}$$

again easily solvable.

4.0.4. *Diffusion equation.* For the diffusion equation

$$q_t = \alpha q_{xx} \tag{4.14}$$

$$q(x, t = 0) = q_0(x) \tag{4.15}$$

the same procedure leads to the system of ODE's

$$\frac{d}{dt}\hat{q}_k = -\alpha k^2 \hat{q}_k \tag{4.16}$$

$$\hat{q}_k(t = 0) = \hat{q}_{0,k} \tag{4.17}$$

In the 2D case

$$q_t = \alpha(q_{xx} + q_{yy}) \tag{4.18}$$

$$q(x, y, t = 0) = q_0(x, y) \tag{4.19}$$

we obtain

$$\frac{d}{dt}\hat{q}_{k,l} = -\alpha(k^2 + l^2)\hat{q}_{k,l} \tag{4.20}$$

$$\hat{q}_{k,l}(t = 0) = \hat{q}_{0,k,l} \tag{4.21}$$

Note that solving this system of ODE's is quite easy. Compare with the necessity of solving an implicit system of MN equations that would be obtained if we use a standard finite difference formulation such as Crank-Nicolson.

4.0.5. *Variable velocity advection.* Let us now consider

$$q_t + u(x)q_x = 0 \tag{4.22}$$

$$q(x, t = 0) = q_0(x) \tag{4.23}$$

Here things get more complicated since we have to introduce a Fourier series for $u(x)$ also to mimic the procedure followed above. This however would lead to a convolution product in Fourier space and the system of ODE's

$$\frac{d}{dt}\hat{q}_k + i \sum_{l+m=k} \hat{u}_l \hat{q}_m = 0 \tag{4.24}$$

and the solution of this system is no longer immediate; we need to also solve a dense linear system. This costs $O((N/2)^3/3)$ much more than the Fourier transforms or the $O(N)$ cost we would expect from a finite difference method. Instead of adopting this procedure we can carry out the following operations to advance our numerical solution from $\{Q_j^n\}$ to $\{Q_j^{n+1}\}$ (we have reverted to the Q notation since the method is now fully discretized and we no longer will be able to solve the ODE systems that arise analytically):

(1) Compute $\left\{\hat{Q}_k^n\right\}$ from $\{Q_j^n\}$
(2) Compute the Fourier coefficients of the derivative q_x, $\left\{ik\hat{Q}_k^n\right\}$
(3) Carry out the inverse Fourier transform to find $\left\{(Q_x)_j^n\right\}$. We have at this stage completed the evaluation of the derivatives, q_x through a process known as numerical spectral differentiation.
(4) Compute $c_j = u(x_j)\,(Q_x)_j^n$ for $j = 0, \ldots, N-1$
(5) Find the Fourier coefficients of the $\{c_j\}$ grid function, $\{\hat{c}_k\}$

(6) Solve the system of ODE's

$$\frac{d}{dt}\hat{q}_k + ik\hat{c}_k = 0 \tag{4.25}$$

$$\hat{q}_k(0) = \hat{Q}_k^n \tag{4.26}$$

over a time step Δt

$$\hat{q}_k(t^{n+1}) = \hat{Q}_k^n \exp\left(-ik\hat{c}_k\Delta t\right) \tag{4.27}$$

This is known as a pseudo-spectral method since we work both in spectral space to evaluate derivatives and in real space to evaluate products. There arises the problem that the product $u_j(Q_x)_j^n$ might be affected by aliasing errors. This is avoided typically by using a higher resolution at this stage of the algorithm, $3N/2$ instead of N points being used to sample c_j.

4.0.6. *2D incompressible Navier-Stokes equations in $\omega - \psi$ formulation.* Let us conclude with a realistic practical example. The 2D incompressible Navier-Stokes equations

$$u_x + v_y = 0 \tag{4.28}$$

$$u_t + uu_x + vu_y = -p_x + \alpha\left(u_{xx} + u_{yy}\right) \tag{4.29}$$

$$v_t + uv_x + vv_y = -p_y + \alpha(v_{xx} + v_{yy}) \tag{4.30}$$

describe viscous fluid flow with velocity (u, v) and pressure p. They are a widely used model in weather prediction in which periodic boundary conditions apply. The system of 3 PDE's can be reduced to 2 equations through use of the vorticity (ω) stream function (ψ) formulation. The vorticity is defined as the curl of the velocity field. For a 2D flow there is only one non-zero component, perpendicular to the plane of flow

$$\omega = v_x - u_y \tag{4.31}$$

The streamfunction is defined by

$$\psi_y = u,\ \psi_x = -v \tag{4.32}$$

and is constant along a streamline of flow. Taking ∂_y of (4.29) and -∂_x of (4.30) and adding the result leads to the vorticity transport equation

$$\omega_t + u\omega_x + v\omega_y = \alpha(\omega_{xx} + \omega_{yy})\ . \tag{4.33}$$

The vorticity can be expressed in terms of the stream function

$$\omega = (-\psi_x)_x - (\psi_y)_y \tag{4.34}$$

or

$$\nabla^2\psi = -\omega \tag{4.35}$$

Note that velocities obtained from a stream function automatically satisfy the continuity equation (4.28)

$$u_x + v_y = \psi_{yx} - \psi_{xy} = 0\ . \tag{4.36}$$

We can solve (4.33) and (4.35) by the following algorithm:

(1) From the current approximation of the vorticity field $\{\Omega_{ij}^n\}$ compute the Fourier transform $\{\hat{\Omega}_{kl}^n\}$

(2) Solve the Poisson equation for the stream function to find

$$\hat{\Psi}^n_{kl} = \frac{1}{k^2 + l^2}\hat{\Omega}^n_{kl} \tag{4.37}$$

(3) Evaluate the derivatives of the stream function needed to compute the velocities

$$\hat{U}^n_{kl} = il\hat{\Psi}^n_{kl},\ \hat{V}^n_{kl} = -ik\hat{\Psi}^n_{kl} \tag{4.38}$$

(4) Apply the inverse Fourier transform to find the velocity field in real space $\{U^n_{ij}\}$, $\{V^n_{ij}\}$

(5) Compute the derivatives of the vorticity in Fourier space

$$ik\hat{\Omega}^n_{kl},\ il\hat{\Omega}^n_{kl} \tag{4.39}$$

(6) Use the inverse Fourier transform to real space and obtain $\{(\Omega_x)^n_{ij}\}$, $\{(\Omega_y)^n_{ij}\}$

(7) Compute the convection term in real space

$$C^n_{ij} = U^n_{ij}\,(\Omega_x)^n_{ij} + V^n_{ij}\,(\Omega_y)^n_{ij} \tag{4.40}$$

(8) Fourier transform the convection term $\{\hat{C}^n_{kl}\}$

(9) Apply an ODE solver to advance the vorticity forward in time by solving

$$\frac{d}{dt}\hat{\Omega}_{kl} + \hat{C}_{kl} = -\alpha(k^2 + l^2)\hat{\Omega}_{kl} \tag{4.41}$$

The evaluation of the convective term can potentially introduce aliasing errors so this is carried out either with filtering or on an extended grid.