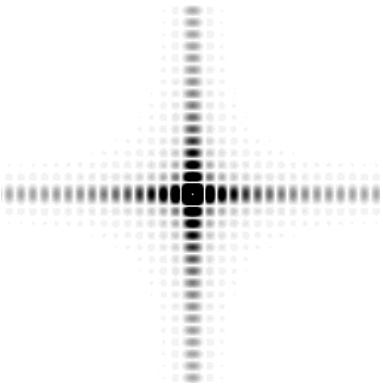

Pseudo-Spectral method

Lecture notes

The Pseudo-Spectral (PS) method is a strong-form method, like the Finite Difference (FD) method which has been discussed in previous classes.

Idea behind the PS method

Let us consider the central difference expansion used in FD, which is second-order accurate:

$$\partial_x f = \frac{f_{n+1} - f_{n-1}}{2\Delta x} + O(\Delta x^2),$$

which gives us the partial derivative at the position n (see Figure 1)

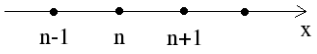

Figure 1: 1D discretization: $x = n \times \Delta x$.

We have seen in previous classes that we can also define higher-order schemes (stencils). For example, using a combination of $f_{n+3/2}$, $f_{n+1/2}$, $f_{n-1/2}$, and $f_{n-3/2}$, we reach a fourth-order accuracy:

$$\partial_x f = \frac{a[f_{n+3/2} - f_{n-3/2}] + b[f_{n+1/2} - f_{n-1/2}]}{\Delta x} + O(\Delta x^4),$$

with $a = -1/24$ and $b = 9/8$. Thus, when we use function information (f) at more positions (n), the order of accuracy can increase.

This is the basic idea behind the PS method: since at any given time step, we have access to all the function points f_n, why not use all these points to determine the (spatial) derivative of f!

PS method implies use of Fourier transforms

The Fourier Transform (FT) is an operation which transforms one function (f) from one domain to an other (usually in the Fourier domain, functions are noted with capital letters F). For example:

- space domain $\rightarrow$ wavenumber domain,
- time domain $\rightarrow$ frequency domain.

An Inverse Fourier Transform operator also exists, which means that you can recover the initial function f from F.

These operators write as:

$$\begin{cases} \text{FT:} & F(k) = \int f(x)\, e^{-ikx}\, \mathrm{d}x \\ \text{inverse FT:} & f(x) = \frac{1}{2\pi} \int F(k)\, e^{ikx}\, \mathrm{d}k \end{cases}$$

where k is a wavenumber and x a spatial position.

The Fourier Transform has some interesting properties. It is easy to show that:

$$\partial_x f(x) = \frac{1}{2\pi} \int ik\, F(k) e^{ikx}\, \mathrm{d}k,$$

meaning that we have the following equivalence in each domain:

$$ik\, F(k) \iff \partial_x f(x),$$

that is, a partial differentiation in the space domain is equivalent to multiplying by ik in the Fourier domain. This is convenient since multiplications are cheap from a numerical point of view.

Discretization

Let us consider the following discretization:

$$\begin{aligned} x_n &= n\Delta x \quad n = 0, ..., N-1 \\ k_l &= l\Delta k \quad\ \ l = 0, ..., N-1 \end{aligned}$$

The length of the interval is thus $N\Delta x$. We recall that $k = \frac{2\pi}{\lambda}$, where λ. Thus, the largest wavelength which can be resolved on this discretized domain is $\lambda = N\Delta x$, such that

$$\Delta k = \frac{2\pi}{N\Delta x} \quad \Rightarrow \quad \Delta k \Delta x = \frac{2\pi}{N}.$$

This gives us a constraint on Δx and Δk, which are not independent from each other. That is, once Δx is chosen, Δk is fixed, and vice versa.

So now we can start discretizing the FT & inverse FT as:

$$\begin{aligned} & F(l\Delta k) = \textstyle\sum_{n=0}^{N-1} f(n\Delta x) \exp(-i\, l\Delta k\, n\Delta x)\Delta x \\ \iff \quad & F(l\Delta k) = \Delta x \textstyle\sum_{n=0}^{N-1} f(n\Delta x) \exp(-i\, 2\pi nl/N) \end{aligned}$$

where we have used the fact that $\Delta k \Delta x = \frac{2\pi}{N}$. The last expression is called the *Discrete Fourier Transform*.

$$\begin{aligned} & f(n\Delta x) = \tfrac{\Delta k}{2\pi} \textstyle\sum_{n=0}^{N-1} F(l\Delta k) \exp(i\, 2\pi nl/N) \\ \iff \quad & f(n\Delta x) = \tfrac{1}{N\Delta x} \textstyle\sum_{n=0}^{N-1} F(l\Delta k) \exp(i\, 2\pi nl/N) \end{aligned}$$

Using the fact that $ikF(k) \iff \partial_x f(x)$, we also have

$$\partial_x f(n\Delta x) = \frac{1}{N\Delta x} \sum_{n=0}^{N-1} i(l\Delta k) F(l\Delta k) \exp(i\, 2\pi nl/N).$$

Notice that with the PS method, boundaries can be an issue. But the advantage of the method is that we reach a very high accuracy of the spatial derivatives, $\partial_x f$, compared to the FD method.

Dispersion of the PS scheme

Let us consider

$$\partial_t u = -c\,\partial_x u.$$

Using a central finite-difference scheme in time and a PS scheme in space yields:

$$\frac{u^{m+1} - u^{m-1}}{2\Delta t} = -\frac{c}{N\Delta x}\sum_{l=0}^{N-1} i(l\Delta k)U^m(l\Delta k)\exp(i\,2\pi nl/N).$$

Let us assume that we have a solution of the type $u(x,t) = f(x)\,e^{-iwt}$. Then, introducing this solution into the previous equation, we get:

$$\frac{\exp[-iw(m+1)t]-\exp[-iw(m-1)t]}{2\Delta t} \quad \times \quad \frac{1}{N\Delta x}\sum_{l=0}^{N-1} F(l\Delta k)\exp(i\,2\pi nl/N) = -\frac{c}{N\Delta x}\sum_{l=0}^{N-1} i(l\Delta k)F(l\Delta k)\exp(i2\pi nl/N)\times\exp(-iwm\Delta t)$$

This expression simplifies, such that for a given l we simply have:

$$\frac{\exp(-iw\Delta t) - \exp(iw\Delta t)}{2\Delta t} = -ic(l\Delta k),$$

and further

$$\frac{\sin(w\Delta t)}{\Delta t} = c\,l\Delta k = c\,l\frac{2\pi}{N\Delta x}.$$

Thus, the stability condition is such that:

$$\sin(w\Delta t) = 2\pi c\,\frac{\Delta t}{\Delta x}\,\frac{l}{N}$$

Now, if

$$\begin{aligned} & 2\pi c\,\tfrac{\Delta t}{\Delta x}\,\tfrac{l}{N} < 1 \\ \iff \quad & c\,\Delta t < \tfrac{\Delta x}{2\pi}\,\tfrac{N}{l} \\ \iff \quad & c\,\Delta t < \tfrac{\Delta x}{2\pi} \quad \text{since } l < N \end{aligned}$$

We recognize that this stability condition is a little bit stricter than the Courant condition met earlier, which stated $c\Delta t < \Delta x$.

From the stability condition, the numerical dispersion writes as:

$$w(k) = \frac{1}{\Delta t}\arcsin(c\,k\Delta t).$$

We see that the dispersion is completely controlled by the time step Δt. So this scheme behaves better than the FD schemes we previously studied (staggered grids, center difference in space & time,...), which depended on both Δt and Δx.

Final remarks

The PS method is very accurate. It allows for better stability and minimal numerical dispersion. However, it starts to get tricky when a model possesses boundaries, because the Fourier Transform makes boundaries periodic. Variations of the PS method use for example Chebychev Transforms, which have a nice discrete form and allow for free surface boundary conditions, as long as the surface is flat. Therefore, it is common in seismology to see people using Chebychev Transforms at depth and Fourier Transforms laterally.

The number of grid points for most popular Finite-Difference (FD) schemes is usually between 5 – 10 points. That is, the smallest wavelength resolved $\lambda_{min} \sim 5 - 10\,\Delta x$. With a Pseudo-Spectral (PS) method (and Fourier Transform) in principle only 2 points per wavelength are required.

Finally, notice that because the PS method involves all points in one direction, this method is not well suited for parallel computations with problems in 2D & 3D.

In the following lectures, you will be introduced to weak methods, and more specifically to the Spectral-Element method (SEM). The SEM offers the flexibility of the Finite-Element method (weak method) and the accuracy of a Pseudo-Spectral method (strong method). Plus, SEM is very well suited for parallel computations as we'll see later on.