Spectral methods

- We have seen, so far, **Finite Differences Methods** (FDM) to solve **Partial Differential Equations** (PDE).
- In this approach, we approximated the spatial derivatives in a point with linear combinations of the values of the functions in the points nearby.
- This is a **“local”** method, in the sense that **the precision depends on how many points we consider** in the approximations.

Spectral methods

- **Spectral methods** use a completely different approach.
- Let us suppose we have to solve an equation:

$$\frac{\partial u}{\partial t} = F(u), \quad u(x, t = 0) = u_0(x)$$

where:

  - $u = u(x,t), \qquad x \in [a,b], \quad t > 0$
  - $F(u)$ is an operator containing **spatial derivatives** of u **only**.
  - some kind of **boundary conditions** are given and $u_0(x)$ is the **initial condition**.

Spectral methods

- We suppose the solution $u(x,t)$ belong to some **Hilbert space** H_2, that is:

$$\int_a^b |u|^2 dx < \infty$$

- Let $\{\phi_n(x)\}$ be a **basis** of such function space. Then, we can write:

$$u(x,t) = \sum_{n=0}^{\infty} a_n(t)\phi_n(x)$$

where $a_n(t)$ are the **expansion coefficients** of u on the basis functions ϕ_n.

Spectral methods

- Let us suppose, for the moment, that the basis functions $\{\phi_n(x)\}$ are **chosen** in such a way **to satisfy the boundary conditions** to impose.
- Since $F(u)$ is another **function belonging to** H_2, it will have its own expansion on the basis $\{\phi_n(x)\}$ with some coefficients $c_n(t)$:

$$F(u) = \sum_{n=0}^{\infty} c_n(t)\phi_n(x)$$

- In general, the c_n **depend** on the a_n!

Spectral methods

- We can then substitute the developments of the functions in the equations:

$$\frac{\partial}{\partial t}\sum_{n=0}^{\infty} a_n(t)\phi_n(x) = \sum_{n=0}^{\infty} c_n(t)\phi_n(x)$$

$$\sum_{n=0}^{\infty} \frac{da_n(t)}{dt}\phi_n(x) = \sum_{n=0}^{\infty} c_n(t)\phi_n(x)$$

$$\sum_{n=0}^{\infty} \left[\frac{da_n(t)}{dt} - c_n(t)\right]\phi_n(x) = 0$$

Spectral methods

- Since the $\{\phi_n(x)\}$ are basis functions, we have:

$$\frac{da_n(t)}{dt} = c_n(t), \qquad n = 0, \dots, \infty$$

- We know that, at $t=0$:

$$u(x, t=0) = \sum_{n=0}^{\infty} a_n(t=0)\phi_n(x) = U(x) = \sum_{n=0}^{\infty} U_n \phi_n(x)$$

because $U(x)$ also belongs to H_2 and therefore can be developped on the basis $\{\phi_n(x)\}$.

Spectral methods

- Therefore, we write the original equation as the system:

$$\frac{da_n(t)}{dt} = c_n(t), \qquad n = 0, \ldots, \infty$$

with initial conditions: $a_n(t=0) = U_n, \quad n = 0, \ldots, \infty$

namely we have **transformed** the **partial differential equation** (PDE) in an infinite **set of ordinary differential equations** (ODE), that can be solved analytically (in the simplest cases, almost none!) or numerically with one of the **schemes** we know for solving ODEs (Euler, Runge-Kutta, etc.)!

Spectral methods

- Once we know how to find the coefficients $a_n(t)$ (starting from the initial condition $a_n(t=0)=U_n$), we can reconstruct the $u(x,t)$ at any subsequent time $t>0$, through the relation between $u(x,t)$ and the a_n:

$$u(x,t) = \sum_{n=0}^{\infty} a_n(t)\phi_n(x)$$

- A simple example: the parabolic diffusion equation:

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}, \quad x \in [0, L]$$

Spectral methods

- With initial conditions: $u(x, t=0) = U(x)$
- Boundary conditions: $u(x,t)|_{x=0} = u(x,t)|_{x=L} = 0$
- A suitable base for which boundary conditions are automatically satisfied is: $\phi_n(x) = \sin[n(\pi/L)x]$
- Then, we have: $u(x,t) = \sum_{n=0}^{\infty} a_n(t) \sin(n\frac{\pi}{L}x)$

$$F(u) = \nu \frac{\partial^2 u}{\partial x^2} = \nu \frac{\partial^2}{\partial x^2} \sum_{n=0}^{\infty} a_n(t) \sin(n\frac{\pi}{L}x) =$$

$$= \sum_{n=0}^{\infty} (-n^2 \frac{\pi^2}{L^2}) a_n(t) \sin(n\frac{\pi}{L}x) = \sum_{n=0}^{\infty} c_n \sin(n\frac{\pi}{L}x)$$

Spectral methods

- The original PDE becomes the set of infinite equations:

$$\frac{da_n(t)}{dt} = -\nu n^2 (\frac{\pi}{L})^2 a_n(t), \qquad n = 0, \ldots, \infty$$

- From the initial condition:

$$u(x,t)|_{t=0} = \sum_{n=0}^{\infty} a_n(0) \sin(n \frac{\pi}{L} x) = U(x) = \sum_{n=0}^{\infty} U_n \sin(n \frac{\pi}{L} x)$$

$$\Rightarrow a_n(0) = U_n$$

- That is: $a_n(t) = a_n(0) e^{-\nu n^2 (\pi^2/L^2) t} = U_n e^{-\nu n^2 (\pi^2/L^2) t}$

Spectral methods

- And, finally, the solution:

$$u(x,t) = \sum_{n=0}^{\infty} U_n e^{-\nu n^2 (\pi^2/L^2) t} \sin(n \frac{\pi}{L} x)$$

- Notes:

1) This is an **exact** (**"global"**!!!) **solution**!!!

2) The coefficients c_n depend on a_n in a simple way, then we could find an analytical solution. In the general case we should have applied a numerical time scheme.

Spectral methods

- A more complicated case: the Burger's equation with $\nu = 0$:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0, \quad x \in [0, 2\pi]$$

- In this case, we have to choose periodic boundary conditions, then a "natural" basis is the Fourier basis: $\phi_n(x) = e^{inx}$

- We have:

$$F(u) = -u\frac{\partial u}{\partial x} = -\left(\sum_{l=0}^{\infty} a_l e^{ilx}\right)\left(\frac{\partial}{\partial x}\sum_{k=0}^{\infty} a_k e^{ikx}\right) =$$

$$= -\sum_{l=0}^{\infty}\sum_{k=0}^{\infty}(ik)a_l a_k e^{i(l+k)x} = -\sum_{n=0}^{\infty}\left[\sum_{n=l+k} ika_l a_k\right] e^{inx}$$

Spectral methods

- In this case: $c_n = -\sum_{n=l+k} ik a_l a_k$
- This case is **more difficult** because the equation is **non-linear**!
- Problems:
  1) Numerically, we cannot use an expansion from 0 to infinity!
  2) General method for computing the coefficients for a generic basis $\{\phi_n(x)\}$;
  3) How to compute the non-linear terms?
  4) Boundary conditions?

Spectral methods

- In general, we do not need information on each point of the domain x, but we can consider a limited number $N+1$ of grid-points x_j which are representative of the behavior of the unknown $u(x,t)$ on each point x_j.
- In this simplified view, we can use only $N+1$ basis functions to approximate the unknown $u(x,t)$:

$$u(x,t) \sim u_N(x,t) = \sum_{n=0}^{N} a_n(t)\phi_n(x)$$

- A first problem in this approach is to understand the error due to the truncation...

Spectral methods

- We postpone this problem for later…
- **How to compute the coefficients** a_n **in this approximation?**
- We have chosen $N+1$ points: $x_j = a + j\,\Delta x,\ j=0,\dots N$

$$u_N(x_j) = \sum_{n=0}^{N} a_n \phi_n(x_j) = \sum_{n=0}^{N} M_{jn} a_n$$

that is, it is possible to compute the $u_N(x_j)$, once the a_n are known through a **simple matrix-vector multiplication** and vice-versa.

Fourier Spectral methods

- A new problem is that **this computation requires** $(N+1)^2$ **multiplications**…
- However, there is at least **one case in which the number of operations can be drastically reduced**, that is the **Fourier basis for periodic functions**, where the FFT algorithm allows to compute the coefficients of the expansion (or, vice-versa, the values of the function starting from the coefficients) in $N\, lg_2 N$ operations!

Fourier Spectral methods

- For this reason, **if the boundary conditions allow this**, namely if we have periodicity at the boundaries, we will **always use the Fourier basis** for the application of the spectral method!
- Another problem is due to the fact that, when **non-linear terms** are present **in the equation**, **the computation** of the c_n terms **requires** anyway N^2 **operations**, due to the products in the spectral space.

Fourier Spectral methods

- This problem can be overcome by using the so-called **pseudo-spectral method**, that consists in **computing the non-linear terms in the physical space, instead of the spectral space**!
- This allows the computation of the non-linear terms in a **number of operations proportional to** $N\,lg_2 N$.
- Practically, we compute the coefficients of the first derivative of u (N multiplications), inverse transform them ($N\,lg_2 N$ operations), multiply the quantity by u (N multiplications), then transform again the result in the Fourier space (another $N\,lg_2 N$ operations).

Fourier Spectral methods

- Finally, we can show that the Fourier coefficient a_n decreases with n faster than any power of n:

$$u(x) = \sum_{n=-N/2}^{+N/2} a_n e^{inx}$$

$$u''(x) = \sum_{n=-N/2}^{+N/2} (-n^2) a_n e^{inx} \Rightarrow a_n'' = -n^2 a_n$$

$$u^{IV}(x) = \sum_{n=-N/2}^{+N/2} (+n^4) a_n e^{inx} \Rightarrow a_n^{IV} = n^4 a_n$$

$$\ldots$$

$$|a^{2p}| = n^{2p} |a_n| \quad \forall p = 1, 2, \ldots \qquad \Rightarrow |a_n| = \frac{1}{n^{2p}} |a^{2p}|$$

Fourier Spectral methods

- Where a^{2p}_n represents the Fourier coefficients of the $2p$-th derivative and a_n the coefficients of the original function $u(x)$.
- Therefore, if we can derive $u(x)$ an infinite number of times ($p \to \infty$), this shows that a_n **tends to zero faster than any integer power of** $1/n$, that is a_n decreases quickly with n!
- This ensures that the approximation is really very good, that is **spectral methods are really very precise**, with respect to FDM!

Fourier Spectral methods

- A practical example: the dissipative Burgers equation: $$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$
- In this case: $F(u) = -u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}$
- Suppose the following expansions hold:

$$u(x,t) = \sum_{n=-N/2}^{+N/2} a_n e^{inx}$$

$$F(u) = \sum_{n=-N/2}^{+N/2} c_n e^{inx}$$

Fourier Spectral methods

- We arrive to the following system of ODEs:

$$\frac{da_n}{dt} = c_n \qquad n = -N/2, \ldots, +N/2$$

  where the values of a_n at $t=0$ are known from the initial condition for $u(x,t=0)$.

- Let us solve numerically this system of equations with a simple Forward Euler time scheme:

$$a_n^{k+1} = a_n^k + hc_n^k, \quad n = -N/2, \ldots, +N/2, \quad k = 0, 1, 2, \ldots$$

  where h is the time step and k the time index.

Fourier Spectral methods

- We can split the computation of c_n into two parts, the first related to the **non-linear term**, the second to the **dissipative term**: $c_n = c'_n + c''_n$
- To compute c'_n, we have to use the pseudo-spectral method:

1) compute the Fourier coefficients of the first derivative:

$$a'_n = ika_n$$

2) FFT^{-1} these coefficients to find the first derivative in the physical space

3) multiply u for the first derivative

4) FFT again the result to get the c'_n

Fourier Spectral methods

- The computation of c''_n is straightforward:

$$a''_n = -\nu n^2 a_n$$

- Adding up the two terms we get the c_n and, therefore, the a_n at the subsequent time step, and so on…
- All this requires a **number of operations proportional to $N\, lg_2 N$!**
- Of course, all considerations made for FDM concerning **stability** of the numerical scheme and **evaluation of the dissipation**, still hold:

$$h \leq \frac{2\nu}{c^2 + \nu^2 k^2} \qquad\qquad u\frac{\partial u}{\partial x} \sim \nu \frac{\partial^2 u}{\partial x^2} \Rightarrow \nu \sim u \Delta x$$

Chebyshev Spectral methods

- All the considerations made above are valid when we have **periodic boundary conditions**.
- What to do when this simple assumption is not satisfied, namely we have, for instance, **Dirichlet** or **Neumann** (or mixed) boundary conditions?
- Problems:
  1) Is there a **basis** where it is possible to keep into account the boundary conditions we want to impose?
  2) Does this basis allow a **fast and efficient evaluation of the coefficients**?

Chebyshev Spectral methods

- The answer to all these questions is **positive** and the basis is the one formed by the **Chebyshev's polynomials**!

$$T_n(x) = \cos(n\theta), \quad \theta = \arccos x, \quad x \in [-1, +1]$$

- It is easy to show they are indeed polynomials:

$$T_0(x) = 1$$
$$T_1(x) = \cos[\arccos(x)] = x$$
$$T_2(x) = \cos[2 \arccos(x)] = 2 \cos^2[\arccos(x)] - 1 = 2x^2 - 1$$

and, from the recurrence relation:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

one obtains that $T_n(x)$ is indeed a n-**degree polynomial**!

Chebyshev Spectral methods

- It is possible to show they are solution of the following **eigenvalue problem**:

$$\frac{1}{W(x)}\frac{d}{dx}\left[p(x)\frac{dT_n(x)}{dx}\right] = -n^2 T_n(x)$$

where the functions $W(x)$ and $p(x)$ are defined as:

$$W(x) = \frac{1}{\sqrt{1-x^2}}, \quad p(x) = \sqrt{1-x^2}$$

- The T_n are **orthogonal** in the norm:

$$\int_{-1}^{+1} W(x)T_n(x)T_m(x)dx = c_n\delta_{nm}, \quad c_0 = \pi, c_n = \pi/2, \text{ for } n > 0$$

Chebyshev Spectral methods

- This allows to compute the coefficients as:

$$a_n = \frac{1}{c_n} \int_{-1}^{+1} W(x)\, u(x)\, T_n(x)\, dx, \quad n = 0, 1, 2, \ldots$$

- The **very nice property** of Chebyshev's polynomials is that a suitable (uneven!) **choice of the grid points** in the domain allows the computation of the coefficients a_n in terms of a (cosine) **Fourier transform**!
- This allows the use of the **FFT algorithm to compute the coefficients**!

Chebyshev Spectral methods

- Let us consider in the interval *[-1,+1]*, *N +1* grid-points, arranged as follows:

$$x_j = \cos\left(\frac{j\pi}{N}\right)$$

- This is called Gauss-Lobatto distribution of grid-points. An alternative is the Gauss distribution:

$$x_j = \cos\left[\frac{(2j+1)\pi}{2N+2}\right]$$

- In the former, the points are **more dense on the boundaries**, in the latter **at the center**.

Chebyshev Spectral methods

- In the first case, for instance, the values:

$$\theta_j = \arccos(x_j) = \frac{j\pi}{N}$$

are evenly distributed in the interval *[0, π]*.

- Therefore, by changing the variable from x to θ in the Chebyshev coefficient a_n:

$$a_n = \frac{1}{c_n}\int_{-1}^{+1} \frac{1}{\sqrt{1-x^2}}\, u(x)\, \cos[n \arccos(x)]\, dx =$$

$$= \frac{1}{c_n}\int_{\pi}^{0} u(\cos\theta)\, \cos(n\theta)\, d\theta = \frac{1}{2c_n}\int_{-\pi}^{\pi} u(\cos\theta)\, \cos(n\theta)\, d\theta =$$

$$= \frac{1}{2c_n}\int_{-\pi}^{\pi} u(\cos\theta)\, \Re(e^{in\theta})\, d\theta$$

Chebyshev Spectral methods

- Notice that the grid in θ is indeed evenly spaced, as required by the FFT algorithm!
- For a correct evaluation of the coefficients of the RHS $F(u)$ of the equation, we need to know an expression for the Chebyshev coefficient of the first and second derivatives of a generic function $u(x)$.
- From the recurrence relation:

$$b_n \frac{T'_{n+1}}{n+1} - d_{n-2} \frac{T'_{n-1}}{n-1} = 2T_n, \quad n = 0, 1, 2, \ldots$$

Chebyshev Spectral methods

- Where: $$b_n = \begin{cases} 2 & n = 0 \\ 1 & n > 0 \end{cases} \qquad d_n = \begin{cases} 0 & n < 0 \\ 1 & n \geq 0 \end{cases}$$
- We get finally the expressions between the Chebyshev coefficients of the first (a_n') and second derivatives (a_n'') of $u(x)$ as a function of the coefficients an of $u(x)$:

$$a'_n = \begin{cases} \frac{2}{b_n} \sum_{p=n+1}^{N} p a_p S_{p-(n+1)} & n = 0, \ldots, N-1 \\ 0 & n \geq N \end{cases}$$

$$a''_n = \begin{cases} \frac{1}{b_n} \sum_{p=n+2}^{N} p(p^2 - n^2) a_p S_{p-(n+2)} & n = 0, \ldots, N-2 \\ 0 & n \geq N-1 \end{cases}$$

Chebyshev Spectral methods

- Where:

$$S_p = \begin{cases} 0 & p \text{ odd} \\ 1 & p \text{ even} \end{cases}$$

- Notice that in *a'*, the coefficients for n greater than *N-1* and *N-2* in *a''* are vanishing! This is where the **boundary conditions come into play**!
- In fact, if we did not use the boundary conditions, **the first and second derivatives** would **play no role in the evolution**, and **this is wrong**!

Chebyshev Spectral methods

- To keep into account the boundary conditions we have to evolve in time only the coefficients up to N-2. The latter two coefficients will be computed by imposing the boundary conditions!
- We know from the properties of the Chebyshev polynomials (see, e.g., slides on the boundary value problems!) that:

$$T_n(+1) = 1 \qquad T_n(-1) = (-1)^n$$

$$T_n'(+1) = n^2 \qquad T_n'(-1) = (-1)^n n^2$$

Chebyshev Spectral methods

- For instance, for Dirichlet b.c., if

$$u(+1) = u_+ \qquad u(-1) = u_-$$

we have to evolve the equations up to *N-2* for the Chebyshev coefficients, and then use the b.c. to find the last two coefficients at next time step as a function of the others. For instance, for a Forward-Euler scheme:

$$a_n^{k+1} = a_n^k + hc_n^k \qquad n = 0, \ldots, N-2$$

$$u^{k+1}(+1) = \sum_{n=0}^{N} a_n^{k+1} T_n(+1) = \sum a_n^{k+1} = u_+$$

$$u^{k+1}(-1) = \sum_{n=0}^{N} a_n^{k+1} T_n(-1) = \sum (-1)^n a_n^{k+1} = u_-$$

Chebyshev Spectral methods

- From the last two equations (supposing N is even!), we get:

$$a_{N-1}^{k+1} + a_N^{k+1} = u_+ - \sum_{n=0}^{N-2} a_n^{k+1}$$

$$-a_{N-1}^{k+1} + a_N^{k+1} = u_- - \sum_{n=0}^{N-2} (-1)^n a_n^{k+1}$$

where the coefficients a_n^{k+1} are obtained by solving the time scheme (first relations in the previous slide) for $n = 0,\ldots,N\text{-}2$!

Chebyshev Spectral methods

- In other words:

1) We solve the equations of the scheme for a_n up to $n=N-2$;

2) We combine these coefficients in the sums at RHS of the last two equations and we solve the 2x2 system for the coefficients a_{N-1} and a_N.

- A similar calculation is possible for Neumann and mixed b.c. (one has to use relations for $T_n(+1)$, $T_n(-1)$ and $T'_n(+1)$, $T'_n(-1)$, instead!).

Chebyshev Spectral methods

- Final remark: to use the FFT to evaluate the Chebyshev coefficients we have to use a **non-evenly spaced grid** and that can give a **very strict CFL condition for the time evolution**!

- This problem often needs to be solved by using **implicit time schemes**, with all the difficulties involved.