# PART IV
# Introduction to Computational Fluid Dynamics

# Agenda

- Classification of linear PDEs in 2D: consider $u : \Omega^2 \to \mathbb{R}$ and $A, B, C \in \mathbb{R}$ such that

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x\,\partial y} + C\frac{\partial^2 u}{\partial y^2} + f(x,y,u) = 0$$

- ELLIPTIC PROBLEMS : $B^2 - 4AC < 0$
  - Poisson equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g(x,y)$$

- PARABOLIC PROBLEMS : $B^2 - 4AC = 0$
  - Heat equation:

$$\frac{\partial u}{\partial t} = a\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + g(x,y)$$

- HYPERBOLIC PROBLEMS : $B^2 - 4AC > 0$
  - Wave equation:

$$\frac{\partial^2 u}{\partial t^2} = a\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + g(x,y)$$

- POISSON EQUATION

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g(x,y) \quad \text{in } \Omega, \quad \Omega \subset \mathbb{R}^2$$

- Assuming $\Delta x = \Delta y = h$, the DISCRETE LAPLACIAN

$$\Delta u = \frac{u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1}}{h^2} + \mathcal{O}(h^2)$$

where $u_{i,j} = u(i\Delta x, j\Delta y)$, $i,j = 1,\dots,N$

- Thus

$$u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = h^2\, g_{i,j}, \qquad i,j = 1,\dots,N$$

- After incorporating boundary conditions (Dirichlet, Neumann) and vectorizing the variables ( $\tilde{g}_{i+(N-1)j} = g_{i,j}$ ), we obtain a sparse algebraic problems with a diagonally-dominant PENTADIAGONAL MATRIX $\Longrightarrow$ straightforward to solve

- HEAT EQUATION
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad \text{in } [0,T]\times[a,b]$$

- CRANK–NICOLSON METHOD $(x_j = j\Delta x, j = 1,\dots,M,\ t = n\Delta t,$
$n = 1,\dots,N)$:
  - spatial derivative: $\left(\frac{\partial^2 u}{\partial x^2}\right)_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} + \mathcal{O}((\Delta x)^2)$
  - time derivative:

$$\left(\frac{\partial u}{\partial t}\right)_j^{n+1} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + \mathcal{O}(\Delta t) = \frac{1}{2}\left[\left(\frac{\partial^2 u}{\partial x^2}\right)_j^{n+1} + \left(\frac{\partial^2 u}{\partial x^2}\right)_j^{n}\right] + \mathcal{O}((\Delta t))$$

$$u_j^{n+1} - u_j^n = \frac{\Delta t}{2(\Delta x)^2}\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} + u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) + \mathcal{O}\left((\Delta x)^2 + (\Delta t)^2\right)$$

  - thus, defining $r = \frac{\Delta t}{(\Delta x)^2}$ ,we have at every time step $n$

$$-ru_{j+1}^{n+1} + 2(1+r)u_j^{n+1} - ru_{j-1}^{n+1} = ru_{j+1}^n + 2(1-r)u_j^n + ru_{j-1}^n$$

which for $U^n = [u_1^n, \dots, u_M^n]^T$ can be written as an algebraic system $(2\mathbf{I} - \mathbf{A})U^{n+1} = (2\mathbf{I} + \mathbf{A})U^n$ , where $\mathbf{A}$ is a tridiagonal matrix

- $\theta$ METHOD
  - allow for a more general approximation in time of the RHS $(\theta \in [0,1])$

$$\left(\frac{\partial u}{\partial t}\right)_j^{n+1} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + \mathcal{O}(\Delta t) = \frac{1}{2}\left[\theta\left(\frac{\partial^2 u}{\partial x^2}\right)_j^{n+1} + (1-\theta)\left(\frac{\partial^2 u}{\partial x^2}\right)_j^{n}\right] + \mathcal{O}(\Delta t)$$

  - special cases
    - $\theta = 0 \implies$ EXPLICIT METHOD: $U^{n+1} = \mathbf{A}_0 U^n$
    - $\theta = \frac{1}{2} \implies$ CRANK–NICOLSON METHOD (see previous slide)
    - $\theta = 1 \implies$ IMPLICIT METHOD: $\mathbf{A}_1 U^{n+1} = U^n$
- Stability:
  - The EXPLICIT SCHEME is STABLE for $r = \frac{\Delta t}{(\Delta x)^2} < \frac{1}{2}$
  - The CRANK–NICOLSON and IMPLICIT SCHEME are STABLE for all $r$

- From now on we will focus on TIME-DEPENDENT (evolution) PDEs and as a model problem will consider the BURGERS EQUATION

$$\begin{cases} \partial_t u + u\partial_x u - \nu\partial_{xx} u = 0 & \text{in } [0,2\pi]\times[0,T] \\ u(x) = u_0(x) & \text{at } t = 0 \end{cases}$$

  Note that steady problems can sometimes be solved as a steady limit of certain time-dependent problems.

- Looking for solution in the form $u_N(x,t) = \sum_{k=-N}^{N} \hat{u}_k(t)e^{ikx}$ . Note that the expansion coefficients $\hat{u}_k(t)$ are now FUNCTIONS OF TIME

- Denote by $u_N^n$ the approximation of $u_N$ at time $t_n = n\Delta t$, $n = 0, 1, \dots$

- Time-discretization of the residual $R_N(x,t)$

$$R_N^n = \frac{u_N^{n+1} - u_N^n}{\Delta t} + u_N^n \partial_x u_N^n - \nu \partial_{xx} u_N^{n+1}$$

Points to note:

  - EXPLICIT treatment of the nonlinear term avoids costly iterations
  - IMPLICIT treatment of the linear viscous term allows one to mitigate the stability restrictions on the time step $\Delta t$
  - here using for simplicity first-order accurate explicit/implicit Euler — can do much better than that

- System of equations obtained by applying the GALERKIN FORMALISM

$$\left(\frac{1}{\Delta t} + \nu k^2\right) \hat{u}_k^{n+1} = \frac{1}{\Delta t}\hat{u}_k^n - i \sum_{\substack{p,q=-N \\ p+q=k}}^{N} q \hat{u}_p^n \hat{u}_q^n, \qquad k = -N, \dots, N$$

Note truncation of higher modes in the nonlinear term.

- Evaluation of the nonlinear $i\sum_{\substack{p,q=-N\\p+q+k}}^{N} q\,\hat{u}_p^n\,\hat{u}_q^n$ term in Fourier space results in a CONVOLUTION SUM which requires $\mathcal{O}(N^2)$ operations – can we do better that that?
- PSEUDOSPECTRAL APPROACH — perform differentiation in FOURIER SPACE and evaluate products in REAL SPACE ; transition between the two representations is made using FFTs which cost "only" $\mathcal{O}(N\log(N))$
  Outline of the algorithm:
  1. calculate (using inverse FFT) $u_N^n(x_j)$, $j=1,\dots,M$ from $\hat{u}_k^n$, $k=-N\dots,N$,
  2. calculate (using inverse FFT) $\partial_x u_N^n(x_j)$, $j=1,\dots,M$ from $ik\hat{u}_k^n$, $k=-N\dots,N$,
  3. calculate the product $w_N^n(x_j)=u_N^n(x_j)\partial_x u_N^n(x_j)$, $j=1,\dots,M$
  4. Calculate (using FFT) $\tilde{w}_k^n$, $k=-N\dots,N$ from $w_N^n(x_j)$, $j=1,\dots,M$
- Note that, because of the ALIASING PHENOMENON , the quantity $\tilde{w}_k^n$ is different from $\hat{w}_k^n=i\sum_{\substack{p,q=-N\\p+q=k}}^{N} q\,\hat{u}_p^n\,\hat{u}_q^n$

- Analysis of aliasing in the PSEUDOSPECTRAL calculation of the nonlinear term

$$w_N^n(x_j) = \sum_{k=-N}^{N} \tilde{w}_k^n e^{ikx_j}, \quad \text{where} \quad w_N^n(x_j) = u_N^n(x_j)\partial_x u_N^n(x_j)$$

- The Discrete Fourier Transform

$$\tilde{w}_k^n = \frac{1}{M}\sum_{j=1}^{M} w_N^n(x_j)e^{-ikx_j} = \frac{1}{M}\sum_{j=1}^{M}\left(\sum_{p=-N}^{N}\hat{u}_p^n e^{ipx_j}\right)\left(\sum_{q=-N}^{N} iq\hat{u}_q^n e^{iqx_j}\right)e^{-ikx_j}$$

$$= \frac{1}{M}\sum_{j=1}^{M}\sum_{p,q=-N}^{N} iq\,\hat{u}_p^n\,\hat{u}_q^n\,e^{i(p+q-k)x_j} = \frac{1}{M}\sum_{p,q=-N}^{N} iq\,\hat{u}_p^n\,\hat{u}_q^n\sum_{j=1}^{M} e^{i(p+q-k)x_j}$$

$$= \hat{w}_k^n + i\sum_{\substack{p,q=-N\\ p+q=k+M}}^{N} q\hat{u}_p^n\hat{u}_q^n + i\sum_{\substack{p,q=-N\\ p+q=k-M}}^{N} q\hat{u}_p^n\hat{u}_q^n \quad k=-N\dots,N$$

The term $\hat{w}_k^n$ is the convolution sum obtained by TRUNCATING the fully spectral Galerkin approach. The terms IN RED are the ALIASING ERRORS .

- Thus, the PSEUDOSPECTRAL GALERKIN equations are

$$\left(\frac{1}{\Delta t} + \nu k^2\right)\hat{u}_k^{n+1} = \frac{1}{\Delta t}\hat{u}_k^n - \tilde{w}_k^n, \quad k=-N,\dots,N$$

- Looking for the solution in the form $u_N(x,t) = \sum_{k=-N}^{N} \hat{u}_k(t) e^{ikx}$, i.e., with the Fourier coefficients $\hat{u}_k$ as unknowns
- Time-discretization of the residual $R_N(x,t)$

$$R_N^n = \frac{u_N^{n+1} - u_N^n}{\Delta t} + u_N^n \partial_x u_N^n - \nu \partial_{xx} u_N^{n+1}$$

- Canceling the residual at the collocation points $x_j$

$$\frac{1}{\Delta t}\left[u_N^{n+1}(x_j) - u_N^n(x_j)\right] + u_N^n(x_j)\partial_X u_N^n(x_j) - \nu \partial_{xx} u_N^{n+1}(x_j) = 0, \;\; j = 1, \dots, M$$

- Straightforward calculation shows that the equation for the Fourier coefficients $\hat{u}_k$ is the same as in the PSEUDOSPECTRAL GALERKIN APPROACH . Thus the two methods are numerically equivalent.
- QUESTION — Show equivalence of pseudospectral Galerkin and collocation approaches to a nonlinear PDE

- "3/2 RULE" — extend the wavenumber range (the "spectrum"), and therefore also the number of collocation points, of the quantities involved in the products, so that the aliasing errors arising in pseudospectral calculations are not present.

- ALGORITHM — consider two $2\pi$-periodic functions

$$a_N(x) = \sum_{k=-N}^{N} \hat{a}_k e^{ikx}, \qquad b_N(x) = \sum_{k=-N}^{N} \hat{b}_k e^{ikx}$$

Calculated in a naive way, the Fourier coefficients of the product $w(x) = a(x)b(x)$ are

$$\tilde{w}_k = \hat{w}_k + \sum_{\substack{p,q=-N \\ p+q=k+M}}^{N} \hat{a}_p \hat{b}_q + \sum_{\substack{p,q=-N \\ p+q=k-M}}^{N} \hat{a}_p \hat{b}_q, \qquad k = -N, \dots, N$$

where $\hat{w}_k$ are the coefficients of the truncated convolution sum that we want to keep (only)

1. Extend the spectra $\hat{a}_k$ and $\hat{b}_k$ to $\hat{a}'_k$ and $\hat{b}'_k$ according to

$$\hat{a}'_k = \begin{cases} \hat{a}_k & \text{if } |k| \le N \\ 0 & \text{if } N < |k| \le N' \end{cases}, \qquad \hat{b}'_k = \begin{cases} \hat{b}_k & \text{if } |k| \le N \\ 0 & \text{if } N < |k| \le N' \end{cases}$$

   The number $N'$ will be determined later.

2. Calculate (via FFT) $a_{N'}$ and $b_{N'}$ in real space on the extended grid $x'_j = \frac{2\pi j}{M'}$, $j = 1, \dots, M'$, where $M' = 2N' + 1$

$$a_{N'}(x'_j) = \sum_{k=-N'}^{N'} \hat{a}'_k e^{ikx'_j}, \qquad b_{N'}(x'_j) = \sum_{k=-N'}^{N'} \hat{b}'_k e^{ikx'_j}$$

3. Multiply $a_{N'}(x'_j)$ and $b_{N'}(x'_j)$: $w'(x'_j) = a_{N'}(x'_j)\, b_{N'}(x'_j), j = 1, \dots, M'$

4. Calculate (via FFT) the Fourier coefficients of $w'(x'_j)$

$$\tilde{w}'_k = \frac{1}{M'} \sum_{j=1}^{M'} w(x'_j) e^{-ikx'_j}, \quad k = -N', \dots, N', \quad M' = 2N' + 1$$

   Taking the latter quantity for $k = -N, \dots, N$ gives an expression for the convolution sum FREE OF ALIASING ERRORS

- Making a suitable choice for $N'$

$$\begin{aligned}\tilde{w}'_k &= \hat{w}_k + \sum_{\substack{p,q=-N' \\ p+q=k+M'}}^{N'} \hat{a}'_p \hat{b}'_q + \sum_{\substack{p,q=-N' \\ p+q=k-M'}}^{N'} \hat{a}'_p \hat{b}'_q \\ &= \hat{w}_k + \sum_{\substack{p,q=-N \\ p+q=k+M'}}^{N} \hat{a}_p \hat{b}_q + \sum_{\substack{p,q=-N \\ p+q=k-M'}}^{N} \hat{a}_p \hat{b}_q\end{aligned}$$

  because $\hat{a}'_p, \hat{b}'_q = 0$ for $|p|, |q| > N$

- The alias terms will vanish, when one of the frequencies $p$ or $q$ appearing in each term of the sum is larger than $N$. Observe that in the first alias term $q = M' + k - p = 2N' + 1 + k - p$, therefore

$$\min_{|k|,|p|\le N}(q) = \min_{|k|,|p|\le N}(2N' + 1 + k - p) = 2N' + 1 - 2N > N$$

  Hence $2N' > 3N - 1$. One may take $N' \geq 3N/2$ (the "3/2 RULE" ) [see the diagram on page 212 in Boyd (2001)]

- Analogous argument for the second aliasing error sum.

- Consider a model ODE problem

$$\mathbf{y}' = \mathbf{r}(\mathbf{y}) + A\mathbf{y}$$

- One would like to use a higher-order ODE integrator with
  - EXPLICIT treatment of nonlinear terms
  - IMPLICIT treatment of linear terms (with high-order derivatives)
- Combining a three-step Runge-Kutta method with the CRANK-NICOLSON METHOD results in the following approach:

$$\left(I - \frac{h_{rk}}{2}A\right)\mathbf{y}^{rk+1} = \mathbf{y}^{rk} + \frac{h_{rk}}{2}A\mathbf{y}^{rk} + h_{rk}\beta_{rk}\mathbf{r}(\mathbf{y}^{rk}) + h_{rk}\zeta_{rk}\mathbf{r}(\mathbf{y}^{rk-1}), \quad rk = 1, 2, 3$$

where

$$h_1 = \frac{8}{15}\Delta t \qquad h_2 = \frac{2}{15}\Delta t \qquad h_3 = \frac{1}{3}\Delta t$$

$$\beta_1 = 1 \qquad \beta_2 = \frac{25}{8} \qquad \beta_3 = \frac{9}{4}$$

$$\zeta_1 = 0 \qquad \zeta_2 = -\frac{17}{8} \qquad \zeta_3 = -\frac{5}{4}$$