PART II
Finite Difference Methods for Differential Equations

Agenda

- Solving a TWO-POINT BOUNDARY VALUE PROBLEM with DIRICHLET BOUNDARY CONDITIONS :

$$\frac{d^2y}{dx^2} = g \qquad \text{for } x \in (0, 2\pi)$$
$$y(0) = y(2\pi) = 0$$

- Finite-difference approximation:
  - Second-order center difference formula for the interior nodes:

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} = g_j \text{ for } j = 1, \dots, N$$

    where $h = \frac{2\pi}{N+1}$ and $x_j = jh$
  - Endpoint nodes:

$$y_0 = 0 \quad \Longrightarrow y_2 - 2y_1 = h^2 g_1$$
$$y_{N+1} = 0 \Longrightarrow -2y_N + y_{N-1} = h^2 g_N$$

  - Tridiagonal algebraic system — solved very efficiently with the THOMAS ALGORITHM (a version of the Gaussian elimination)

- Solving a TWO-POINT BOUNDARY VALUE PROBLEM with NEUMANN BOUNDARY CONDITIONS :

$$\frac{d^2y}{dx^2} = g \qquad \text{for } x \in (0, 2\pi)$$
$$\frac{dy}{dx}(0) = \frac{dy}{dx}(2\pi) = 0$$

- Finite-difference approximation:
  - Second-order center difference formula for the interior nodes:

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} = g_j \text{ for } j = 1, \dots, N$$

  - First-order Forward/Backward Difference formulae to re–express endpoint values:

$$\frac{y_1 - y_0}{h} = 0 \implies y_0 = y_1$$
$$\frac{y_{N+1} - y_N}{h} = 0 \implies y_{N+1} = y_N$$

    First-order only — DEGRADED ACCURACY!
  - Tridiagonal algebraic system — Is there any problem? Where?

- In order to retain the SECOND-ORDER ACCURACY in the approximation of the Neumann problem need to use higher-order formulae at endpoints, e.g.

$$y_0' = \frac{-y_2 + 4y_1 - 3y_0}{2h} = 0 \implies y_0 = \frac{1}{3}(-y_2 + 4y_1)$$

- The first row thus becomes

$$\frac{2}{3}y_2 - \frac{2}{3}y_1 = h^2 g_1$$

SECOND–ORDER ACCURACY RECOVERED!

- COMPACT STENCILS — stencils based on three grid points (in every direction) only: $\{x_{j+1}, x_j, x_{j-1}\}$ at the $j-th$ node
- Is is possible to obtain higher (then second) order of accuracy on compact stencils? — YES!
- Consider the central difference approximation to the equation $\frac{d^2y}{dy^2} = g$

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} - \frac{h^2}{12} y_j^{(iv)} + \mathcal{O}(h^4) = g_j$$

- Re-express the error term $\frac{h^2}{12} y_j^{(iv)}$ using the equation in question:

$$\frac{h^2}{12} y_j^{(iv)} = \frac{h^2}{12} g_j'' = \frac{h^2}{12}\left[\frac{g_{j+1} - 2g_j + g_{j-1}}{h^2} - \frac{h^2}{12} g_j^{(iv)} + \mathcal{O}(h^4)\right]$$

- Inserting into the original finite-difference equation:

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} = g_j + \frac{g_{j+1} - 2g_j + g_{j-1}}{12} + \mathcal{O}(h^4)$$

- Slight modification of the RHS $\Longrightarrow$ FOURTH-ORDER ACCURACY!!!

- COMPACT FINITE DIFFERENCE SCHEMES —
  - ADVANTAGES:
    - Increased accuracy on compact stencils
  - DRAWBACKS:
    - need to be tailored to the specific equation solved
    - can get fairly complicated for more complex equations

- Consider the following CAUCHY PROBLEM :

$$\frac{dy}{dt} = f(y,t) \text{ with } y(t_0) = y_0$$

  The independent variable t is usually referred to as TIME .

- Equations with higher-order derivatives can be reduced to systems of first-order equations

- Generalizations to systems of ODEs straightforward

- When the RHS function does not depend on y, i.e.,
  $f(y,t) = f(t)$,
  solution obtained via a QUADRATURE

- Assume uniform time-steps (h is constant)

- ACCURACY — unlike in the Boundary Value Problems, there is no terminal condition and approximation errors may accumulate in time; consequently, a relevant characterization of accuracy is provided by the GLOBAL ERROR

$$\text{(global error)} = \text{(local error)} \times (\# \text{ of time steps}),$$

rather than the LOCAL ERROR .

- STABILITY — unlike in the Boundary Value Problems, where boundedness of the solution at final time is enforced via a suitable terminal condition , in Initial Value Problems there is a priori no guarantee that the solution will remain bounded.

Model Problem (I)

- STABILITY of various numerical schemes is usually analyzed by applying these schemes to the following LINEAR MODEL :

$$\frac{dy}{dt} = \lambda y = (\lambda_r + i\lambda_i)y \text{ with } y(t_0) = y_0,$$

which is stable when $\lambda_r <= 0$.

- EXACT SOLUTION:

$$y(t) = y_0 e^{\lambda t} = \left(1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \dots\right) y_0$$

Model Problem (II)

- MOTIVATION — consider the following ADVECTION-DIFFUSION PDE :

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - a\frac{\partial^2 u}{\partial x^2} = 0$$

Taking Fourier transform yields (k is the wavenumber):

$$\frac{d\hat{u}_k}{dt} + c\,i\,k\,\hat{u}_k + a\,k^2\,\hat{u}_k = 0$$

where

  - the real term $a\,k^2\,\hat{u}_k$ represents DIFFUSION
  - the imaginary term $c\,i\,k\,\hat{u}_k$ represents ADVECTION

Euler Explicit Scheme (I)

- Consider a Taylor series expansion

$$y(t_{n+1}) = y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(t_n) + \dots$$

Using the ODE we obtain

$$y' = \frac{dy}{dt} = f$$
$$y'' = \frac{dy'}{dt} = \frac{df}{dt} = f_t + ff_y$$

- Neglecting terms proportional to second and higher powers of h yields the EXPLICIT EULER METHOD

$$y_{n+1} = y_n + hf(y_n, t_n)$$

- Retaining higher–order terms is inconvenient, as it requires differentiation of f and does not lead to schemes with desirable stability properties.

Euler Explicit Scheme (II)

- Local error analysis:

$$y_{n+1} = (1 + \lambda h)\, y_n + [\mathcal{O}(h^2)]$$

- Global error analysis:

$$(\text{global error}) = Ch^2 \cdot N = Ch^2 \cdot \frac{T}{h} = C' h$$

Thus, the scheme is

- locally second-order accurate
- globally (over the interval $[t_0, t_0 + Nh]$) first-order accurate

Euler Explicit Scheme (III)

- Stability (for the model problem)

$$y_{n+1} = y_n + \lambda h y_n = (1 + \lambda h) y_n$$

- Thus, the solution after n time steps

$$y_n = (1 + \lambda h)^n y_0 \triangleq \sigma^n y_0 \quad \Longrightarrow \quad \sigma = 1 + \lambda h$$

- For large n, the numerical solution remains stable iff

$$|\sigma| \le 1 \quad \Longrightarrow \quad (1 + \lambda_r h)^2 + (\lambda_i h)^2 \le 1$$

  - CONDITIONALLY STABLE for real λ
  - UNSTABLE for imaginary λ

Euler Implicit Scheme (I)

- IMPLICIT SCHEMES — based on approximation of the RHS that involve $f(y_{n+1}, t)$, where y_{n+1} is the unknown to be determined
- IMPLICIT EULER SCHEME — obtained by neglecting second and higher-order terms in the expansion:

$$y(t_n) = y(t_{n+1}) - hy'(t_{n+1}) + \frac{h^2}{2}y''(t_{n+1}) - \dots$$

- Upon substitution $\left.\frac{dy}{dt}\right|_{t_{n+1}} = f(y_{n+1}, t_{n+1})$ we obtain

$$y_{n+1} = y_n + hf(y_{n+1}, t_{n+1})$$

- The scheme is
  - locally SECOND–ORDER accurate
  - globally (over the interval $[t_0, t_0 + Nh]$) FIRST–ORDER accurate

Euler Implicit Scheme (II)

- Stability (for the model problem):

$$y_{n+1} = y_n + \lambda h y_{n+1} \implies y_{n+1} = (1-\lambda h)^{-1} y_n$$

$$y_{n+1} = \left(\frac{1}{1-\lambda h}\right)^n y_0 \triangleq \sigma^n y_0 \implies \sigma = \frac{1}{1-\lambda h}$$

$$|\sigma| \leq 1 \implies (1-\lambda_r h)^2 + (\lambda_i h)^2 \geq 1$$

- Implicit Euler scheme is thus stable for
  - all stable model problems
  - most unstable model problems
- REMARK: When solving systems of ODEs of the form $\mathbf{y} = \mathcal{A}(t)\mathbf{y}$, each implicit step requires solution of an algebraic system: $\mathbf{y}_{n+1} = (I - h\mathcal{A})^{-1}\mathbf{y}_n$
- Implicit schemes are generally hard to implement for nonlinear problems

Crank-Nicolson Scheme (I)

- Obtained by approximating the formal solution of the ODE $y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(y,t)\,dt$ using the TRAPEZOIDAL QUADRATURE :

$$y_{n+1} = y_n + \frac{h}{2}\left[f(y_n, t_n) + f(y_{n+1}, t_{n+1})\right]$$

- The scheme is
  - locally THIRD–ORDER accurate
  - globally (over the interval $[t_0, t_0 + Nh]$) SECOND–ORDER accurate

Crank-Nicolson Scheme (II)

- Stability (for the model problem):

$$y_{n+1} = y_n + \frac{\lambda h}{2}(y_{n+1} + y_n) \implies y_{n+1} = \left(\frac{1+\frac{\lambda h}{2}}{1-\frac{\lambda h}{2}}\right) y_n$$

$$y_{n+1} = \left(\frac{1+\frac{\lambda h}{2}}{1-\frac{\lambda h}{2}}\right)^n y_0 \triangleq \sigma^n y_0 \implies \sigma = \frac{1+\frac{\lambda h}{2}}{1-\frac{\lambda h}{2}}$$

$$|\sigma| \le 1 \implies \Re(\lambda h) \le 0$$

- STABLE for all model ODEs with stable solutions

Leapfrog Scheme (I)

- LEAPFROG as an example of a TWO-STEP METHOD :

$$y_{n+1} = y_{n-1} + 2\,h\,\lambda\,y_n$$

- CHARACTERISTIC EQUATION for the AMPLIFICATION FACTOR ($y_n = \sigma^n y_0$)

$$\sigma^2 - 2\,h\,\lambda\sigma - 1 = 0$$

  where roots give the amplification factors:

$$\sigma_1 = \lambda h + \sqrt{1+\lambda^2 h^2} \simeq \quad 1 + \lambda h + \frac{\lambda^2 h^2}{2} + \dots \quad = \quad e^{\lambda h} + \mathcal{O}(h^3)$$

$$\sigma_2 = \lambda h - \sqrt{1+\lambda^2 h^2} \simeq -(1 - \lambda h + \frac{\lambda^2 h^2}{2} - \dots) = -e^{-\lambda h} + \mathcal{O}(h^3)$$

- Thus, the scheme is
  - locally THIRD–ORDER accurate
  - globally (over the interval $[t_0, t_0 + Nh]$) SECOND–ORDER accurate

Leapfrog Scheme (II)

- Stability for diffusion problems ($\lambda = \lambda_r$):

$$\sigma_1 = \lambda h + \sqrt{1 + \lambda_r^2 h^2} > 1 \quad \text{for all} \quad h > 0$$

  Thus the scheme is UNCONDITIONALLY UNSTABLE for diffusion problems!

- Stability for advection problems ($\lambda = i\lambda_i$):

$$\sigma_{1/2}^2 = 1 \text{ (!!!) for } \quad h < \frac{1}{|\lambda_i|}$$

  Thus, the scheme is CONDITIONALLY STABLE and NON-DIFFUSIVE for advection problems!

- QUESTION — analyze dispersive (i.e., related to $\arg(\sigma)$) errors of the leapfrog scheme.

Multistep Procedures (I)

- General form of a MULTISTEP (ξ, ζ) PROCEDURE :

$$\sum_{j=0}^{p} \alpha_j y_{n+j} = h \sum_{j=0}^{q} \beta_j f(y_{n+j}, t_{n+j})$$

  with characteristic polynomials

$$\xi_p(z) = \alpha_p z^p + \alpha_{p-1} z^{p-1} + \cdots + \alpha_0$$
$$\zeta_q(z) = \beta_q z^q + \beta_{q-1} z^{q-1} + \cdots + \beta_0$$

  - if $p > q$ — EXPLICIT SCHEME
  - if $p \leq q$ — IMPLICIT SCHEME

- CONSISTENCY: $h \to 0 \quad \Longrightarrow \quad \text{Local Error} \to 0$

Multistep Procedures (II)

Theorem

- *Consider an initial-value problem* $\frac{dy}{dt} = f(t, y)$, $y(0) = y_0$, *where* $f\ :\ [0, T] \times \mathbb{R}^n \to \mathbb{R}^n$ *is* r *times continuously differentiable w. r. t. both variables. A* (ξ, ζ) *–procedure converges uniformly in* $[0, T]$, *i.e.,* $\lim_{h\to 0} \max_{t_n \in [0,T]} \|y_n - y(t_n)\| = 0$ *if:*

  1. *the following consistency conditions are verified:* $\xi(1) = 0$ *and* $\xi'(1) = \zeta(1)$ *(* CONSISTENCY CONDITION *)*
  2. *all roots of the polynomial* $\xi(z)$ *are such that* $|z_i| \le 1$ *and the roots with* $|z_k| = 1$ *are simple (* STABILITY CONDITION *)*

Multistep Procedures (III)

Proof (part 1.)

- Taylor expansions

$$y(t+j\,h) = \sum_{k=0}^{r} \frac{y^{(k)}(t)}{k!}\, j^k\, h^k + \mathcal{O}(h^{r+1})$$

$$y'(t+j\,h) = \sum_{k=0}^{r-1} \frac{y^{(k+1)}(t)}{k!}\, j^k\, h^k + \mathcal{O}(h^r) = \sum_{k=1}^{r} k\,\frac{y^{(k)}(t)}{k!}\, j^{k-1}\, h^{k-1} + \mathcal{O}(h^r)$$

- Error $E(t,h)$ $(s = \max\{p,q\})$

$$E(t,h) = \sum_{j=0}^{s} \alpha_j\, y(t+j\,h) - h \sum_{j=0}^{s} \beta_j\, f(t+j\,h, y(t+j\,h)) = \sum_{j=0}^{s} \left[\alpha_j\, y(t+j\,h) - h\,\beta_j\, y'(t+j\,h)\right]$$

$$= \sum_{k=0}^{r} \underbrace{\left[\sum_{j=0}^{s} j^k \alpha_j - k\, j^{k-1}\, \beta_j\right]}_{=0\ (\star)} \frac{y^{(k)}(t)}{k!}\, h^k + \mathcal{O}(h^{r+1})$$

Multistep Procedures (IV)

Proof (Cont.)

- $$(\star) \qquad \sum_{j=0}^{s} j^k \alpha_j - k\, j^{k-1}\, \beta_j = 0, \quad k = 0, \dots, r$$
- For the *global error* to vanish we need $r = 1$, so that $\mathcal{O}(h^2)$

$$k = 0: \qquad \sum_{j=0}^{s} \alpha_j = 0 \qquad \Longrightarrow \qquad \xi(1) = 0$$

$$k = 1: \qquad \sum_{j=0}^{s} j\, \alpha_j = \sum_{j=0}^{s} \beta_j \qquad \Longrightarrow \qquad \xi'(1) = \zeta(1)$$

□

Runge-Kutta Methods (I)

- General form of a FRACTIONAL STEP METHOD :

$$y_{n+1} = y_n + \gamma_1 \, h \, k_1 + \gamma_2 \, h \, k_2 + \gamma_3 \, h \, k_3 + \dots$$

where

$$\begin{aligned} k_1 &= f(y_n, t_n) \\ k_2 &= f(y_n + \beta_1 h k_1, t_n + \alpha_1 h) \\ k_3 &= f(y_n + \beta_2 h k_1 + \beta_3 h k_2, t_n + \alpha_2 h) \\ &\vdots \end{aligned}$$

- Choose γ_i, β_i and α_i to match as many expansion coefficients as possible in

$$\begin{aligned} y(t_{n+1}) &= y(t_n) + hy'(t_n) + \frac{h^2}{2} y''(t_n) + \frac{h^3}{6} y'''(t_n) \dots \\ y' &= f \\ y'' &= f_t + ff_y \\ y''' &= f_{tt} + f_t f_y 2ff_{yt} + f^2 f_{yt} + f^2 f_{yy} \end{aligned}$$

- Runge-Kutta methods are SELF–STARTING with fairly good stability and accuracy properties.

Runge-Kutta Methods (II)

- RK4 — an ODE "workhorse":

$$y_{n+1} = y_n + \frac{h}{6}k_1 + \frac{h}{3}(k_2 + k_3) + \frac{h}{6}k_4$$

$$k_1 = f(y_n, t_n) \qquad k_2 = f(y_n + \frac{h}{2}k_1, t_{n+1/2})$$

$$k_3 = f(y_n + \frac{h}{2}k_2, t_{n+1/2}) \qquad k_4 = f(y_n + hk_3, t_{n+1})$$

- The amplification factor:

$$\sigma = 1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \frac{\lambda^4 h^4}{24}$$

  Thus, stability iff $|\sigma| \leq 1$
- ACCURACY:

$$e^{\lambda h} = \sigma + \mathcal{O}(h^5)$$

  Thus, the scheme is
  - locally FIFTH–ORDER accurate
  - globally (over the interval $[t_0, t_0 + Nh]$) FOURTH–ORDER accurate

Runge's Principle

- Let $(k+1)$ be the order of the local truncation error; denote $Y(t,h)$ an approximation of the exact solution $y(t)$ computed with the step size h; then at $t = t_0 + 2nh$:

$$y(t) - Y(t,h) \simeq C\,2\,n\,h^{k+1} \quad = C(t-t_0)h^k$$
$$y(t) - Y(t,2h) \simeq C\,n\,(2h)^{k+1} = C(t-t_0)2^k\,h^k$$

  Subtracting:

$$Y(t,2h) - Y(t,h) \simeq C(t-t_0)(1-2^k)h^k$$

- Thus, we can obtain an estimate of the ABSOLUTE ERROR based on solution with two step–sizes only:

$$y(t) - Y(t,h) \simeq \frac{Y(t,h) - Y(t,2h)}{2^k - 1}$$

- Runge's principle is very useful for ADAPTIVE STEP SIZE REFINEMENT

Lax Equivalence Theorem[1]

- Consider an INITIAL VALUE PROBLEM

$$\frac{du}{dt} = \mathcal{L}u \quad \text{with} \quad u(t_0) = u_0$$

  and assume that it is well–posed, i.e., it admits solutions which are unique and stable

- Consider a numerical method defined by a finite–difference operator $C(h)$ such that the approximate solution is given by

$$u_h(nh) = \mathcal{C}(h)^n u_0, \quad n = 1, 2, \dots$$

- The above method is CONSISTENT iff $\frac{\mathcal{C}(h)-I}{h}$ is a convergent approximation of the operator $\mathcal{L}$

- LAX THEOREM — For a CONSISTENT difference method STABILITY is equivalent to CONVERGENCE

[1] For a more technical discussion, see \$ 5.2 in Atkinson & Han (2001)

Conservation Properties (I)

- Is ACCURACY and STABILITY all that matters?
- CONSERVATION PROPERTIES — conservation by the numerical method (i.e., in the discrete sense) of various invariants the original equation may possess
  - REMARK — conservation properties are particularly relevant for solution of Hamiltonian / hyperbolic systems
- Example — conservation of the solution norm:
  - In the continuous setting (assume $u = |u|e^{i\varphi}$)

$$\frac{du}{dt} = i\lambda_i u \quad \Longleftrightarrow \quad \begin{cases} \frac{d|u|}{dt} = 0 \quad \Longrightarrow \quad |u(t)| = |u_0|, \\ \frac{d\varphi}{dt} = \lambda_i, \end{cases}$$

  - In the discrete setting: $|u_h(nh)| = |u_h((n-1)h)| = \cdots = |u_h(0)|$

Necessary and sufficient condition for discrete conservation: $\exists h, \ |\sigma(h)| = 1$

Conservation Properties (II)

- Implicit Euler —

$$|\sigma| = \left|\frac{1}{1 - i\lambda_i h}\right| = \frac{1}{\sqrt{1+\lambda_i^2 h^2}} = 1 - \frac{1}{2}\lambda_i^2 h^2 + \cdots < 1 \quad \text{for all } h$$

  The scheme is thus DISSIPATIVE (i.e., not conservative)

- Fourth–Order Runge–Kutta —

$$|\sigma| = \left|1 + i\lambda_i h - \frac{\lambda_i^2 h^2}{2} - i\frac{\lambda_i^3 h^3}{6} + \frac{\lambda_i^4 h^4}{24}\right| = \frac{1}{24}\sqrt{576 - 8\lambda_i^6 h^6 + \lambda_i^8 h^8}$$

$$= 1 - \frac{1}{144}\lambda_i^6 h^6 + \cdots < 1 \quad \text{for small } h$$

  The scheme is thus DISSIPATIVE (i.e., not conservative)

- Leapfrog — $|\sigma_{1/2}| \equiv 1 \quad \text{for all} \quad h < \frac{1}{|\lambda_i|}$
  The scheme is thus CONSERVATIVE for all time–steps for which it is stable!!! Leapfrog is an example of a SYMPLECTIC INTEGRATOR which are designed to have good conservation properties.

- 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 $(x_j = j\Delta x, j = 1, \ldots, M,\ t = n\Delta t,$ $n = 1, \ldots, N)$:
  - 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:

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

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

  - 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 $U^n = [u_1^n, \ldots, u_M^n]^T$ 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

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

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

  - 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

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

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

$$u_j^{n+1} = \frac{(\Delta t)^2}{(\Delta x)^2}\left(u_{j+1}^n + u_{j-1}^n\right) - u_j^{n-1} + 2\left(1 - \frac{(\Delta t)^2}{(\Delta x)^2}\right) u_j^n + \mathcal{O}\left((\Delta x)^2(\Delta t)^2 + (\Delta t)^4\right)$$

- Stability for $\frac{(\Delta t)^2}{(\Delta x)^2} \leq 1$
- Remark: need two initial conditions!