

# PART II

## FINITE DIFFERENCE METHODS FOR DIFFERENTIAL EQUATIONS

# Agenda

## Boundary-Value Problems

- Dirichlet Boundary Conditions
- Neumann Boundary Conditions
- Compact Schemes

## Initial-Value Problems

- Generalis
- Time-Stepping Schemes
- Runge's Principle, Lax Theorem and Conservation Properties

## Finite Differences for PDEs — Review

- Elliptic Problems
- Parabolic Problems
- Hyperbolic Problems

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

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

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

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

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

- ▶ **Endpoint nodes:**

$$y_0 = 0 \quad \implies \quad y_2 - 2y_1 = h^2 g_1$$

$$y_{N+1} = 0 \quad \implies \quad -2y_N + y_{N-1} = h^2 g_N$$

- ▶ 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** :

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

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

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

- ▶ 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 it possible to obtain higher (than 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  $\implies$  **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  $\lambda_r \leq 0$  .

- ▶ **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

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

- ▶ For large  $n$ , the numerical solution remains stable iff

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

- ▶ **CONDITIONALLY STABLE** for real  $\lambda$
- ▶ **UNSTABLE** for imaginary  $\lambda$

# 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** :

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

- ▶ 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):

$$y_{n+1} = y_n + \frac{\lambda h}{2}(y_{n+1} + y_n) \implies y_{n+1} = \left( \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}} \right) y_n$$
$$y_{n+1} = \left( \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}} \right)^n y_0 \triangleq \sigma^n y_0 \implies \sigma = \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}}$$
$$|\sigma| \leq 1 \implies \Re(\lambda h) \leq 0$$

- ▶ **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:

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

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

- ▶ 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 ( $\lambda = \lambda_r$ ):

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

Thus the scheme is **UNCONDITIONALLY UNSTABLE** for diffusion problems!

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

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

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**  $(\xi, \zeta)$  **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:**  $h \rightarrow 0 \implies \text{Local Error} \rightarrow 0$

## Multistep Procedures (II)

### Theorem

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

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  $|z_i| \leq 1$  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  $E(t, h)$  ( $s = \max\{p, q\}$ )

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

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



## Multistep Procedures (IV)

## Proof (Cont.)



$$(\star) \quad \sum_{j=0}^s j^k \alpha_j - k j^{k-1} \beta_j = 0, \quad k = 0, \dots, r$$

- ▶ For the *global error* to vanish we need  $r = 1$ , so that  $\mathcal{O}(h^2)$

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

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



# 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

$$k_1 = f(y_n, t_n)$$

$$k_2 = f(y_n + \beta_1 h k_1, t_n + \alpha_1 h)$$

$$k_3 = f(y_n + \beta_2 h k_1 + \beta_3 h k_2, t_n + \alpha_2 h)$$

⋮

- ▶ Choose  $\gamma_i$ ,  $\beta_i$  and  $\alpha_i$  to match as many expansion coefficients as possible in

$$y(t_{n+1}) = y(t_n) + h y'(t_n) + \frac{h^2}{2} y''(t_n) + \frac{h^3}{6} y'''(t_n) \dots$$

$$y' = f$$

$$y'' = f_t + f f_y$$

$$y''' = f_{tt} + f_t f_y + 2 f f_{yt} + f^2 f_{yt} + f^2 f_{yy}$$

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

## Runge-Kutta Methods (II)

- ▶ **RK4** — an ODE “workhorse”:

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

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

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

- ▶ 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  $t = t_0 + 2nh$ :

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

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<sup>1</sup>

- ▶ 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  $\mathcal{C}(h)$  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**

<sup>1</sup>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  $u = |u|e^{i\varphi}$ )

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

- ▶ In the discrete setting:  $|u_h(nh)| = |u_h((n-1)h)| = \dots = |u_h(0)|$
- Necessary and sufficient condition for discrete conservation:  $\exists h, |\sigma(h)| = 1$

## Conservation Properties (II)

- ▶ Implicit Euler —

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

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

- ▶ Fourth-Order Runge-Kutta —

$$\begin{aligned} |\sigma| &= \left| 1 + i\lambda_i h - \frac{\lambda_i^2 h^2}{2} - i \frac{\lambda_i^3 h^3}{6} + \frac{\lambda_i^4 h^4}{24} \right| = \frac{1}{24} \sqrt{576 - 8\lambda_i^6 h^6 + \lambda_i^8 h^8} \\ &= 1 - \frac{1}{144} \lambda_i^6 h^6 + \dots < 1 \text{ for small } h \end{aligned}$$

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

- ▶ Leapfrog —  $|\sigma_{1/2}| \equiv 1$  for all  $h < \frac{1}{|\lambda_j|}$

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  $u : \Omega^2 \rightarrow \mathbb{R}$  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

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

- ▶ 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
- $\implies$
- 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:

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

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

▶ 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 ( $\theta \in [0, 1]$ )

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

- ▶ 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:

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

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

▶ Stability for  $\frac{(\Delta t)^2}{(\Delta x)^2} \leq 1$

▶ REMARK: need two initial conditions!