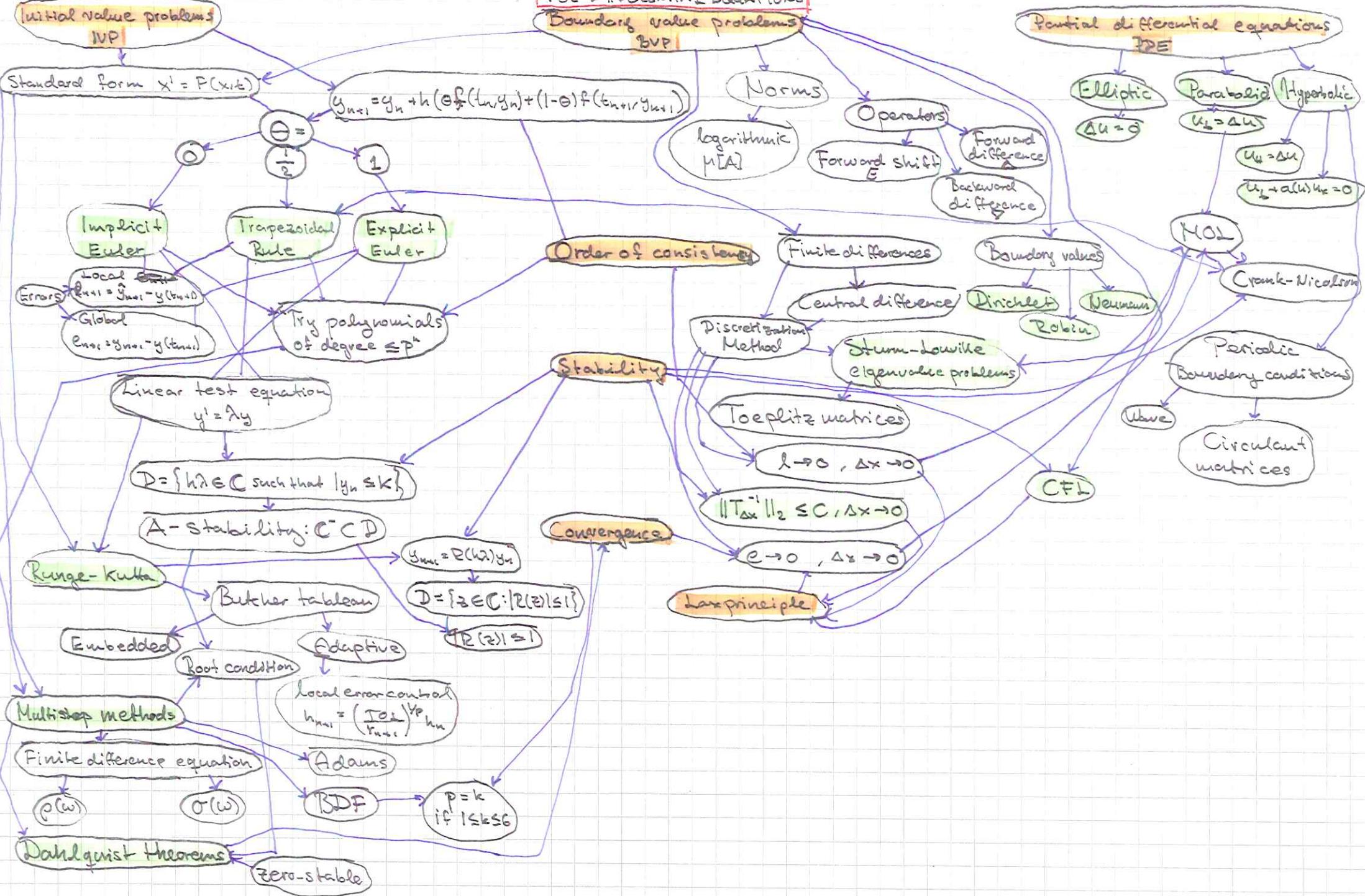


# NUMERICAL METHODS FOR DIFFERENTIAL EQUATIONS



## NUMERICAL METHODS FOR DIFFERENTIAL EQUATIONS

- \* Edsberg: Introduction to computation and modeling for differential equations.
- \* Söderlind/Arevalo - Lectures
- \* Projects

(1) Initial Value Problems in ODEs.

Standard formulation of a system of ODEs:

$$\frac{dy}{dt} = f(t, y) \quad y(0) = y_0 \quad f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m \quad (1).$$

Lipschitz condition:  $\|f(t, u) - f(t, v)\| \leq L[f] \cdot \|u - v\|$  (2)  
 $u, v \in \mathbb{R}^m \quad L[f] < \infty$  Constant.

- If  $f(t, y)$  is continuous for  $t \in [0, T]$  and satisfies (2), then there exists a unique solution to the IVP on  $[0, T]$  for every  $y(0) = y_0$ .

For  $\frac{dy}{dt} = f(t, y, y')$   $y(0) = y_0, y'(0) = y_0'$

$$1) \begin{cases} x_1 = y \\ x_2 = y' \end{cases} \Rightarrow \begin{cases} x_1' = x_2 \\ x_2' = f(t, x_1, x_2) \end{cases} \quad \begin{matrix} x_1(0) = y_0 \\ x_2(0) = y_0' \end{matrix}$$

The Explicit Euler method

$$y' = f(t, y) \quad y(t_0) = y_0$$

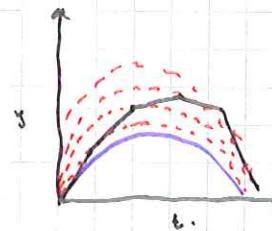
$$\cdot y'(t_n) \approx \frac{y(t_{n+1}) - y(t_n)}{h} \quad (3).$$

$h = t_{n+1} - t_n$  {time step}.

$$\Rightarrow \frac{y_{n+1} - y_n}{h} = f(t_n, y_n) \quad y_0 = y(t_0)$$

Thus:

$$\boxed{\begin{aligned} y_{n+1} &= y_n + h f(t_n, y_n) \\ t_{n+1} &= t_n + h \end{aligned}} \quad (4).$$



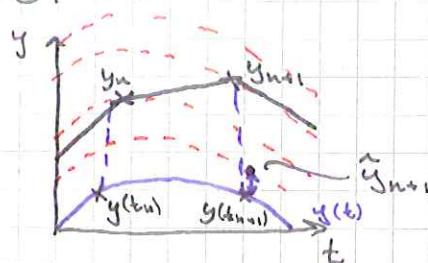
- Each step introduces an error and ends up on a different solution trajectory.

A method is convergent if for every ODE with a Lipschitz function  $f$  and every fixed  $T$ , with  $T = N \cdot h$  it holds that

$$\lim_{N \rightarrow \infty} \|y_{N,h} - y(T)\| = 0.$$

Global error:  $\{e_n = y_n - y(t_n)\}$   
 $\{e_{n+1} = y_{n+1} - y(t_{n+1})\}$

Local error:  $\delta_{n+1} = \hat{y}_{n+1} - y(t_{n+1})$



Def. Given  $y_{n+1} = \Phi_h(f, h, y_0, y_1, \dots, y_n)$

The order of consistency is  $p$  if:  $y(t_{n+1}) - \Phi(f, h, y(t_0), y(t_1), \dots, y(t_n)) = O(h^{p+1})$  as  $h \rightarrow 0$  for every analytic  $f$ .

∴ Local error is then  $O(h^{p+1})$

OR: if:

the formula is exact for all polynomials  $y = P(t)$  of degree  $p$  or less. 2.  
 Explicit Euler  $\rightarrow P = 1$

## The trapezoidal rule

$$y(t) \approx y(t_n) + (t - t_n) \frac{1}{2} [f(t_n, y(t_n)) + f(t_{n+1}, y(t_{n+1}))] \quad (5).$$

So

$$\begin{aligned} t_{n+1} &= t_n + h \\ y_{n+1} &= y_n + \frac{h}{2} [f(t_n, y_n) + f(t_{n+1}, y_{n+1})] \end{aligned} \quad (6)$$

This method is implicit! Of order 2!

Theta methods:

$$y_{n+1} = y_n + h (\theta f(t_n, y_n) + (1-\theta) f(t_{n+1}, y_{n+1})) \quad \theta \in [0, 1] \quad (7)$$

$$\left\{ \begin{array}{l} \theta = 1 : \text{Explicit Euler} \\ \theta = 1/2 : \text{Trapezoidal rule (implicit).} \\ \theta = 0 : \text{Implicit Euler.} \end{array} \right.$$

Implicit Euler method

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

The slope is at the right endpoint  $\rightarrow$  instead of the left!

Def. The linear test equation  $y' = \lambda y$   $y(0) = 1$   $t \geq 0$   $\lambda \in \mathbb{C}$

$$y(t) = e^{\lambda t} \Rightarrow |y(t)| \leq K \Leftrightarrow \operatorname{Re}(\lambda) \leq 0$$

Def. The stability region  $D$  of a method is all  $h \in \mathbb{C}$  such that  $|y_n| \leq K$  when the method is applied to the test equation.

Def. A method is A-stable if its stability region contains ' $C$ '

$$C = \{z \in \mathbb{C} : \operatorname{Re}(z) \leq 0\} \subset D$$

"If the original problem is stable, then an A-stable method will replace that problem numerically." (Usually)

### Stiffness

For A-stable methods there is no stability region restriction on  $h$ . The stepsize is only restricted by accuracy.

Stiff differential equations are characterized by homogeneous solutions being strongly damped  $\text{Ex: } y = \lambda(y - \sin t) + \cos t \quad \{ \lambda \ll -1 \}$ . (\*)

Stability regions of explicit methods are bounded, and  $h \in D$  puts a strong stability restriction requirement on  $h$ .

Ex: EE. applied to (\*) requires  $h \leq -\frac{2}{\lambda} \ll 1$ .

Implicit methods with unbounded stability regions put no restrictions on  $h$ , and the stepsize is only restricted to accuracy requirement.

II

Runge-Kutta  
and linear  
Multi-step  
Methods.

## Runge-Kutta methods

Explicit:

$$y_{n+1} = y_n + \sum_{i=1}^s b_i h f(t_n + c_i h, Y_i) ; Y_i = y_n + \sum_{j=1}^{i-1} a_{ij} h Y_j$$

$\{Y_i\}$  denotes the numerical approximations to  $\{y(t_n + c_i h)\}$ .

$Y_i$  - stage values :  $Y'_i = f(t_n + c_i h, Y_i)$  - stage derivatives. If they are related through

$$Y_i = y_n + \sum_{j=1}^{i-1} a_{ij} h Y_j$$

and the method advances one step through:

$$y_{n+1} = y_n + \sum_{i=1}^s b_i h Y'_i$$

### The Butcher Tableau

$$\begin{array}{c|ccccc} 0 & 0 & 0 & \dots & 0 \\ c_1 & a_{11} & 0 & \dots & 0 \\ \vdots & & & \ddots & \\ c_s & a_{s1} & a_{s2} & \dots & 0 \\ \hline & b_1 & b_2 & \dots & b_s \end{array} \leftrightarrow \begin{array}{c|c} c & A \\ \hline & b \end{array}$$

$A = \{a_{ij}\}$  - RK matrix

$b = [b_1, b_2, \dots, b_s]^T$  - weight vector.

$c = [c_1, c_2, \dots, c_s]$  - nodes.

$s$  number of stages.

- s-stage ERK methods of order  $p=s$  exist only for  $s \leq 4$ .
- An s-stage ERK method has  $s+s(s-1)/2$  coefficients to choose, but the order conditions are many.

Embedded:

We can embed two methods in one Butcher tableau, example:

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{6} (Y'_1 + 2Y'_2 + 2Y'_3 + Y'_4) & (p=4). \\ z_{n+1} &= y_n + \frac{h}{6} (Y'_1 + 4Y'_2 + 2Y'_3). & (p=3) \end{aligned} \quad \left\{ \text{RK34.} \right.$$

The difference  $y_{n+1} - z_{n+1}$  can be used as an error estimate.

Implicit:

$$Y_i = y_n + h \sum_{j=1}^s a_{ij} Y_j$$

$$Y'_i = f(t_n + c_i h, Y_i)$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i Y'_i$$

"Implicit Euler" is of order 1 and "implicit midpoint" method is the only 1-stage ERK of order 2.

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \quad \begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}$$

### The stability function

- For every Runge-Kutta method applied to the linear test equation  $y' = \lambda y$  we have

$$y_{n+1} = R(h\lambda) y_n \quad (8)$$

where the rational function

$$R(z) = 1 + z \mathbf{b}^T (\mathbf{I} - z \mathbf{A})^{-1} \mathbf{1} \quad (9)$$

is called the method's stability function. If the method is explicit, then  $R(z)$  is a polynomial of degree  $s$ .

### A-stability:

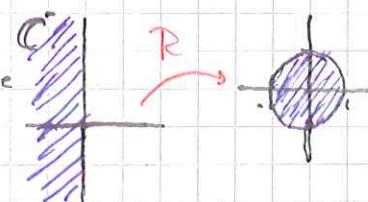
Def. The method's stability region is the set

$$D = \{z \in \mathbb{C} : |R(z)| \leq 1\}$$

- If  $R(z)$  maps all of  $\mathbb{C}$  into the unit circle, then the method is A-stable.

No explicit RK-method is A-stable!

- $|R(z)| \leq 1$  for all  $z \in \mathbb{C}$  if and only if all the poles of  $R(z)$  have positive real parts and  $|R(iw)| \leq 1$  for all  $w \in \mathbb{R}$ . (Complex Analysis, maximum principle)



### Linear Multistep Methods.

Method of the type  $y_{n+1} = \phi(t, h, y_0, y_1, y_2, \dots, y_n)$  using values from previous steps (EB, 10<sup>th</sup> edn).

A k-step multistep method replaces an ODE by a finite difference equation

$$\sum_{j=0}^{k-1} a_{k-j} y_{n+j} = h \sum_{j=0}^k b_j w_j f(t_{n+j}, y_{n+j})$$

$$p(w) = \sum_{j=0}^k a_j w^j$$

$$e(w) = \sum_{j=0}^k b_j w^j$$

Normalization  $a_k = 1$  or  $e(1) = 1$ .

If  $b_k = 0 \Rightarrow$  method is explicit.

$b_k \neq 0 \Rightarrow$  method is implicit.

- A multistep method is of order of consistency  $p$  if the local error is  $O(h^{p+1})$ .

Try the "polynomial method".

### The root condition:

Def: A polynomial  $p$  satisfies the root condition if all of its zeros have moduli less than or equal to 1 and the zeros of unit modulus are simple.

Def: A method is zero-stable if  $p$  satisfies the root condition.

• A multistep method is convergent if and only if it is zero-stable and consistent of order  $p \geq 1$ .

### Dahlquist's first barrier

- The maximal order of an zero-stable k-step method is

$$p = \begin{cases} k & \text{if } k \text{ is odd} \\ k+1 & \text{if } k \text{ is even} \end{cases}$$

explicit methods  
implicit methods

### Backward differentiation formulas

#### Def Backwards difference operator

$$\begin{aligned}\nabla^0 y_{n+k} &= y_{n+k} \\ \nabla^i y_{n+k} &= \nabla^{i-1} y_{n+k} - \nabla^{i-1} y_{n+k-1} \quad i \geq 1.\end{aligned}$$

- The k-step BDF method  $\sum_{i=0}^k \frac{\nabla^i}{i!} y_{n+k} = h f(t_{n+k}, y_{n+k})$  is convergent of order  $p=k$  if and only if  $1 \leq k \leq 6$ .

X BDF methods are suitable for stiff problems.

### A-stability

The characteristic equation  $(z + h\lambda)$

$$p(w) - z(w) = 0 \quad \text{[difference eq., us method]} \quad (16.)$$

which has  $k$  roots  $w_j(z)$ . The method is A-stable if

$$\operatorname{Re} z \leq 0 \Rightarrow |w_j(z)| \leq 1, \quad (\text{root condition}).$$

### Dahlquist's second barrier

- The highest order of an A-stable multistep method is  $p=2$ . Of all 2nd order A-stable multistep methods, the trapezoidal rule has the smallest error.

### Difference Operators

- Shifting the sequence by 1.

Differentiation:  $D: y \rightarrow y'$  where  $D = \frac{d}{dt}$

Forward shift:  $E: y(t) \rightarrow y(t+h)$ .

The forward difference operator:

$$\Delta y(t) = y(t+h) - y(t)$$

$$\Delta y_n = y_{n+1} - y_n$$

$$\Delta^k y_n = \Delta(\Delta^{k-1} y_n)$$

$$E y_n = y_{n+1}.$$

## Finite Difference approximation of derivatives

$$\frac{dy}{dx} \approx \frac{\Delta y}{\Delta x}$$

$$\frac{d^2y}{dx^2} \approx \frac{\Delta y_n / \Delta x - \Delta y_{n-1} / \Delta x}{\Delta x} \approx \frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta x^2} \approx \frac{\Delta^2 y}{\Delta x^2}$$

The Backward difference operator.

$$\nabla y(t) = y(t) - y(t-h)$$

$$\nabla y_n = y_n - y_{n-1}$$

III FDM for  
2p-BVPs and  
Sturm-Liouville  
problems.

### Approximation of derivatives

I-order.

$$\text{FWD} \quad y'(x) \approx \frac{y(x+\Delta x) - y(x)}{\Delta x} + O(\Delta x) \quad (\star) \quad y'(x) = \frac{y(x+\Delta x) - y(x-\Delta x)}{2\Delta x} + O(\Delta x^2) \quad (\star\star)$$

$$\text{BWD} \quad y'(x) \approx \frac{y(x) - y(x-\Delta x)}{\Delta x} + O(\Delta x), \quad y''(x) \approx \frac{y(x+\Delta x) - 2y(x) + y(x-\Delta x)}{\Delta x^2} + O(\Delta x^4) \quad (\star\star\star)$$

Derivatives  $\rightarrow$  finite differences  $\rightarrow$  matrices.

Take  $(\star)$ , introduce  $y = \{y(x_i)\}$  and  $y' = \{y'_i(x_i)\}$

$$\begin{pmatrix} y'_0 \\ y'_1 \\ \vdots \\ y'_N \end{pmatrix} \approx \frac{1}{\Delta x} \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & \ddots & 1 \\ & & & & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{N+1} \end{pmatrix}$$

Forward difference  $\sim (N+1) \times (N+2)$  matrix.  
Nullspace  $y = (1 \ 1 \ 1 \ \dots \ 1)^T$

The central difference.  $(\star)$ .

$$\begin{pmatrix} y'_0 \\ y'_1 \\ \vdots \\ y'_N \end{pmatrix} \approx \frac{1}{2\Delta x} \begin{pmatrix} -1 & 0 & 1 & & & \\ & \ddots & & \ddots & & \\ & & \ddots & & \ddots & \\ & & & \ddots & & \\ & & & & -1 & 0 & 1 \\ & & & & & & y_{N+1} \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{N+1} \end{pmatrix}$$

$N \times (N+2)$   
Nullspace 2D  $\left\{ \begin{matrix} \tilde{y} = (1 \ 1 \ 1 \ \dots \ 1)^T \\ \tilde{y} = (1 \ -1 \ 1 \ -1 \ \dots \ 1)^T \end{matrix} \right.$   
"False" nullspace does not converge to a  $C^1$ -function.

I-order central difference  $(\star\star)$ .

$$\begin{pmatrix} y''_0 \\ y''_1 \\ \vdots \\ y''_N \end{pmatrix} \approx \frac{1}{\Delta x^2} \begin{pmatrix} 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & & \ddots & \\ & & & \ddots & & \\ & & & & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{N+1} \end{pmatrix} \quad N \times (N+2)$$

Nullspace  $\left\{ \begin{matrix} \tilde{y} = (1 \ 1 \ 1 \ \dots \ 1)^T \\ \tilde{y} = (0, 1, 2, 3, \dots, N+1)^T \end{matrix} \right.$

### Finite difference methods for 2p-BVP

If we consider  $y'' = f(x, y)$

$$y(0) = a; y(1) = b$$

$\Rightarrow$  Introduce equidistant grid with  $\Delta x = \frac{1}{N+1}$ .

• Discrete 2p-BVP.

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = f(x_i, y_i) \quad i = 1 \dots N \quad \text{This is a system of equations } F(y) = 0 \text{ for the } N \text{ unknowns } y_1, y_2, \dots, y_N.$$

$$y_0 = a; y_{N+1} = b.$$

Boundary conditions:

\* Dirichlet boundary conditions

$$y(0) = a$$

\* Neumann boundary conditions

$$y'(0) = f$$

\* Robin conditions

$$y(0) + c \cdot y'(0) = b$$

$$F_1(y) = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - f(x_i, y_i)$$

$$F_i(y) = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - f(x_i, y_i)$$

$$F_N(y) = \frac{y_{N+1} - 2y_N + y_0}{\Delta x^2} - f(x_N, y_0)$$

$$y_{N+1} = b$$

{ Neumann and Robin conditions require special attention for the convergence to be preserved! }

## Sturm-Liouville eigenvalue problems

$$\frac{d}{dx} \left( P(x) \frac{dy}{dx} \right) - \lambda y = 0 \quad (12).$$

$$y(a) = 0; \quad y(b) = 0.$$

$$y'' = \lambda y, \quad \Rightarrow \lambda = \frac{\omega^2}{c^2} \quad (13).$$

$$\text{Discretization} \Rightarrow T_{\Delta x} y = \lambda \Delta x y$$

$$P_{i-1/2} y_{i-1} - (p_{i-1/2} + p_i + p_{i+1/2}) y_i + p_{i+1/2} y_{i+1} = \lambda \Delta x^2 y_i$$

$$y_0 = y_{N+1} = 0.$$

$$(1) p_{i+1/2} = \frac{y_{i+1} - y_i}{\Delta x} \quad (14). \\ (2) p_{i-1/2} = \frac{y_i - y_{i-1}}{\Delta x} \quad \left. \begin{array}{l} (1)-(2) \\ \hline \end{array} \right/ \Delta x.$$

Symmetric tridiagonal  $N \times N$  eigenvalue problem

$$T_{\Delta x} y = \lambda \Delta x y$$

There are  $N$  eigenvalues  $\lambda_{n,m} = \lambda_n + O(\Delta x^2)$

- The first few eigenvalues are well approximated, but the approximation gets gradually worse. - Good approximations for first  $\sqrt{N}$  eigenvalues.

Toepplitz matrices.

\* Constant along diagonals \*

Much is known - Eigenvalues, Norms, Inverses etc.

Eigenvalues:

$y_{0,n} = y_{N,n} = y_{N+1,n}$  has the characteristic equation

$$z^2 - \lambda z + 1 = 0$$

The roots are  $z$  and  $1/z \Rightarrow$  general solution:  $y_n = \alpha z^n + \beta z^{-n}$   $\left\{ \begin{array}{l} (z+z)(z-z) = 0 \\ z^2 - (z_1+z_2)z + z_1 z_2 = 0 \end{array} \right.$

Insert the BC  $y_0 = 0 = \alpha + \beta$  into the solution:

$$y_n = \alpha(z^n - z^{-n})$$

$y_{N+1} = 0 = \alpha(z^{N+1} - z^{-(N+1)}) \Rightarrow z^{2(N+1)} = 1 = e^{2\pi i k},$  so the roots:

$$z_k = e^{\frac{2\pi i k}{N+1}}, \quad k=1:N.$$

(15).

The sum of the roots  $\lambda_k = z_k + 1/z_k \Rightarrow \lambda_k = 2 \cos\left(\frac{k\pi}{N+1}\right)$ , thus

$$\boxed{\lambda_k[T] = -4 \sin^2 \frac{k\pi}{2(N+1)}}$$

$\nwarrow$   $N$  real eigenvalues for the  $\begin{pmatrix} T & 0 \\ 0 & -T \end{pmatrix} (-2; 1; 0)$  Toepplitz matrix.

$\Rightarrow$  The eigenvalues for  $T_{\Delta x} := \frac{T}{\Delta x^2}$  are  $\lambda_k[T_{\Delta x}] \approx -k^2 \pi^2$  for  $k \in \mathbb{N}$ .

Norms:

• For a symmetric matrix  $A$ , it holds  $\|A\|_2 = \max_k |\lambda_k|$   
and  $\mu_2[A] = \max_k |\lambda_k|$

$$\text{Def. } \|A\|_2^2 = \max_{\substack{x \neq 0 \\ x^T x \geq 0}} \frac{x^T A^T A x}{x^T x}$$

We get that  $p(x) = \lambda^2$  where  $\lambda$  is  $\text{eig}[A]$ . Therefore  $\|A\|_2 = \max[\lambda[A]]$

$$\text{Def. } \mu_2[A] = \max_{\substack{x \neq 0 \\ x^T x \geq 0}} \frac{x^T A x}{x^T x}$$

We get that  $p(x) = \lambda$  where  $\lambda$  is  $\text{eig}[A]$ . Therefore  $\mu_2[A] = \max[\lambda[A]]$

• The Euclidean norms of  $T_{\Delta x}$  are

$$\|T_{\Delta x}\|_2 \approx \frac{9}{\Delta x^2} \quad \text{and} \quad \mu_2[T_{\Delta x}] \approx \pi^2$$

## Convergence - The Lax Principle

Consistency: local error  $\ell \rightarrow 0$  as  $\Delta x \rightarrow 0$ .

Stability:  $\|T_{\Delta x}^{-1}\|_2 \leq C$  as  $\Delta x \rightarrow 0$ .

Convergence: global error  $e \rightarrow 0$  as  $\Delta x \rightarrow 0$ .

The fundamental theorem of numerical analysis {Lax Principle}.

Consistency + Stability  $\Rightarrow$  Convergence.

$$\begin{array}{ccc} \ell \rightarrow 0 & \|T_{\Delta x}^{-1}\|_2 \leq C & e \rightarrow 0 \\ \hline & \Delta x \rightarrow 0 & \end{array}$$

Sobolev's lemma.

For all functions with  $u(0) = u(1) = 0$  it holds that

$$\|u''\|_2 \geq \pi \|u'\|_2$$

### Differential operators

Def:  $\langle v, Au \rangle = \langle A^* v, u \rangle$  defines the adjoint operator  $A^*$ .

The eigenvalues of adjoint operators are **real** and **orthogonal**.

### Elliptic operators

Def: An operator is elliptic if for all  $u \neq 0$   $\langle u, Au \rangle > 0$ .

"More general":

$$-\frac{d}{dx} \left( p(x) \frac{du}{dx} \right) + q(x) \text{ is elliptic if } p(x) > 0 \text{ and } q(x) \geq 0$$

Def: An operator is positive definite if it is **self-adjoint** and **elliptic**.  
 $\mu_2[-A] < 0$ .

### From finite difference to finite element.

$$Au = f \rightarrow bu.$$

FDM - The main idea:

Replace functions  $u$  and  $f$  by vectors and differential operators  $A$  by matrix to get a linear system of equations.

Galerkin method (FEM) - The main idea:

Approximate function  $u$  by polynomial and keep differential operator  $A$  as is.

## (V)

Partial

differential

equations  
- elliptic and  
parabolic.

### Brief overview of PDE problems

Three basic types, four prototype equations.

- Elliptic  $\Delta u = 0$ ; + BC
- Parabolic  $u_t = \Delta u$ ; + BC  $\equiv$  IC
- Hyperbolic  $\begin{cases} u_{tt} = \Delta u & + BC \equiv IC \\ u_t + a(u)u_x + BC \equiv IC \end{cases}$

### Classification of PDEs

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + L(u_{x,y}, u, x, y) = 0 \quad "L linear in u_x, u_y, u"$$

$$\delta := \det \begin{pmatrix} A & B \\ B & C \end{pmatrix} = AC - B^2$$

$\delta > 0$  Elliptic PDE

$$u_{xx} + u_{yy} = 0$$

$\delta = 0$  Parabolic PDE

$$u_t = u_{xx}$$

$\delta < 0$  Hyperbolic PDE(s)

$$u_{yy} = u_{xx}$$

Laplace equation

$$A=C=1; B=0$$

Diffusion equation

$$A=1; B=C=0$$

Wave equation

$$A=1; B=0; C=-1$$

## Elliptic problems

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\left\{ \begin{array}{l} \text{Laplace equation } \Delta u = 0 \\ \text{Poisson equation } -\Delta u = f \end{array} \right. \quad \left\{ \begin{array}{l} \text{BC: } u = u_0(x, y, z) \\ x, y, z \in \partial \Omega \end{array} \right.$$

The Poisson equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad \text{Dirichlet condition } u(x, y) = 0 \text{ on boundary.}$$

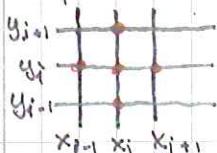
$$\text{Uniform grid } \left\{ \begin{array}{l} \Delta x = \frac{1}{N+1} \\ \Delta y = \frac{1}{M+1} \end{array} \right.$$

Discretization:  $u_{i,j} \approx u(x_i, y_j)$ .

$$u_{i,j} - u_{i,j} = 2u_{i,j} + u_{i,j+1} + u_{i,j-1} \xrightarrow{\Delta x^2} \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f(x_i, y_j).$$

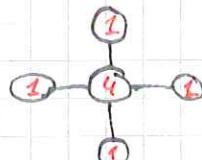
$$\Delta x = \Delta y \quad \left\{ \frac{u_{i-1,j} + u_{i+1,j} - 4u_{i,j} + u_{i,j+1} + u_{i,j-1}}{\Delta x^2} = f(x_i, y_j) \right\}$$

Equidistant mesh



Participating approximations  
and mesh points.

Computational stencil



"five-point operator".

Linear system of equations

$$\frac{1}{\Delta x^2} \begin{pmatrix} T & I & 0 & \dots \\ I & T & I & \dots \\ 0 & I & T & \dots \\ \vdots & \ddots & I & \dots \\ & & & I \end{pmatrix} \begin{pmatrix} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ \vdots \\ u_{1,N} \end{pmatrix} = \begin{pmatrix} f(x_1, y_1) \\ f(x_1, y_2) \\ f(x_1, y_3) \\ \vdots \\ f(x_1, y_N) \end{pmatrix}$$

The Toeplitz matrix:  $T = \text{tridiag}(1, -4, 1)$

$N^2 \times N^2$  - large and very sparse.

## Parabolic problems

$$\text{Diffusion equation } u_t = \Delta u$$

Some applications

\* Diffusive process

Heat conduction  $u_t = d \cdot \nabla^2 u$

\* Chemical reactions

Reaction-diffusion  $u_t = d \cdot \nabla^2 u + f(u)$

Convection-diffusion  $u_t = u_x + \frac{1}{Pe} u_{xx}$

## Method of lines (MOL) discretization

$$\ln u_t = u_{xx}$$

$$\Rightarrow u_{xx} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}$$

Semi-discretization  $u \approx T_{\Delta x} u$   
(system of ODEs).

→ Full FDM discretization

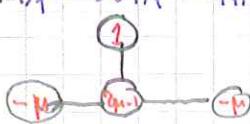
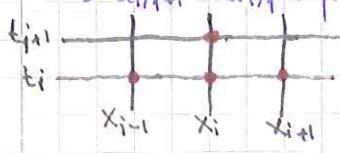
•  $u_i(t) \approx u(x_i, t)$  along the line  $x = x_i$  in  $(x, t)$ -plane  $u \approx \frac{1}{\Delta x} \begin{pmatrix} -2 & 1 \\ 1 & -2 & 1 \\ & \ddots & \ddots & -2 \end{pmatrix} u$

• Time-stepping to solve IVP (EE) with  $u_{i,0} \approx u(x_i, 0)$

$$\frac{u_{i+1,t} - u_{i,t}}{\Delta t} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

Def: Courant number  $\mu = \frac{\Delta t}{\Delta x^2}$

$$\Rightarrow u_{i+1,t} = u_{i,t} + \mu \cdot (u_{i-1} - 2u_i + u_{i+1})$$



## Stability and the CFL condition

Stability requires  $\Delta t \cdot \lambda_k \leq \frac{1}{2}$  for all eigenvalues

$$\Delta t \cdot \lambda_k \in \left[ -\frac{\pi n \Delta x}{\Delta x^2}, -\pi^2 \Delta t \right]$$

Stiffness → the CFL condition can be avoided using A-stable methods.

### Crank-Nicolson method

The Crank-Nicolson method ⇔ Trapezoidal rule for PDES!

- Implicit
- A-stable | Crank-Nicolson is unconditionally stable!  
There is no CFL-condition on the time step  $\Delta t$ .

### Lax Principle

Consistency  $e_{ij} \rightarrow 0 \quad \Delta t, \Delta x \rightarrow 0$

Stability CFL-condition  $\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$

Convergence  $e_{ij} \rightarrow 0 \quad \Delta t, \Delta x \rightarrow 0$

Consistency + Stability ⇒ Convergence.

The order of convergence is  $p=2$ .

## Hyperbolic problems.

"Wave" equations with applications

\* Wave equation  $U_{tt} = U_{xx}$

\* Linear conservation law  $U_t + CU_x = 0$

\* Nonlinear conservation law  $U_t + UU_x = 0$

\* Burgers equation  $U_t + UU_x = U_{xx}$

### Hyperbolic problems

\* Korteweg-de Vries (KdV) equation  $U_t + UU_x = -U_{xxx}$  { dispersion; solitons }

\* Klein-Gordon equation  $U_{tt} = U_{xx} - U$  { dispersion; "telegraph equation"; quantum theory }

\* Schrödinger equation  $iU_t = U_{xx}$  { quantum theory }

\* Beam equation  $U_{tt} = -U_{xxxx}$  { elastic vibration }

### Standard hyperbolic model problems

• Wave equations  $[U_{tt} = C^2 U_{xx}]$  or  $[U_t + CU_x = 0]$

• Conservation laws  $[U_t + (f(U))_x = 0]$  (inviscid flow).

• d'Alembert solution  $[U(x,t) = g(x-ct)]$  (solves  $U_t + CU_x = 0$ ).

## The Advection equation. Some schemes

$$U_t + U_x = 0 \quad 0 \leq x \leq 1 \quad t \geq 0$$

→ ic  $U(x,0) = g(x)$  → bc  $U(0,t) = \phi(t)$ .

$$\textcircled{1} \quad U_x \approx (U_{x+1}^n - U_{x-1}^n) / \Delta x \quad (\text{Backward difference}).$$

$$\textcircled{2} \quad U_x \approx (U_{x+1}^n - U_x^n) / \Delta x \quad (\text{Forward difference}).$$

$$\textcircled{3} \quad U_x \approx (U_{x+1}^n - U_{x-1}^n) / 2\Delta x \quad (\text{Symmetric difference}).$$

$$\textcircled{4} \quad U_x \approx \left( \frac{1}{4}U_{x+1}^n + \frac{5}{6}U_x^n - \frac{3}{8}U_{x-1}^n + \frac{1}{2}U_{x-2}^n - \frac{1}{12}U_{x-3}^n \right) / \Delta x$$

Upwind schemes use more points to the left than to the right of the current point, when the flow is from left to right.

$P=1$  UPWIND As exact solutions is transported to the right at a constant speed, information comes from the left!

(Upwind is necessary for stability).

Construction of FD schemes from SD:

$$U_t + U_x = 0 \quad \rightarrow \mu = \frac{\Delta t}{\Delta x}$$

$$\textcircled{1} \quad U_x \approx (U_x^n - U_{x-1}^n) / \Delta x \quad \Rightarrow U_x \approx (U_{x+1}^{n+1} - U_x^n) / \Delta t \Rightarrow U_x^{n+1} = (1-\mu)U_x^n + \mu U_{x+1}^n \quad [\text{Upwind (Euler) scheme}]$$

$$\textcircled{2} \quad U_x \approx (U_{x+1}^n - U_x^n) / \Delta x \quad \Rightarrow U_x \approx (U_x^{n+1} - U_x^n) / \Delta t \Rightarrow U_x^{n+1} = (1+\mu)U_x^n - \mu U_{x-1}^n \quad [\text{Downwind scheme}]$$

$$\textcircled{3} \quad U_x \approx (U_{x+1}^{n+1} - U_{x-1}^{n+1}) / (2\Delta x) \quad \Rightarrow U_x \approx (U_x^{n+2} - U_x^{n+1}) / (2\Delta t) \Rightarrow U_x^{n+2} = \mu(U_x^{n+1} - U_{x-1}^{n+1}) + U_x^n \quad [\text{Leapfrog method}]$$

Classical FD schemes for  $u_t + au_x = 0$

1. Central difference scheme (always unstable!).

$$u_e^{n+1} = u_e^n + \frac{\alpha\beta}{2}(u_{e-1}^n - u_{e+1}^n)$$

2. The Lax-Friedrichs scheme (convergent,  $p=1$ ).

$$u_e^{n+1} = \frac{u_{e-1}^n + u_{e+1}^n}{2} + \frac{\alpha\mu}{2}(u_{e-1}^n - u_{e+1}^n)$$

$$\text{or } u_e^{n+1} = \frac{1}{2}(1+\alpha\mu)u_{e-1}^n + \frac{1}{2}(1-\alpha\mu)u_{e+1}^n$$

3. The Lax-Wendroff scheme (convergent,  $p=2$ ).

$$u_e^{n+1} = \frac{\alpha\mu}{2}(1+\alpha\mu)u_{e-1}^n + (1-\alpha^2\mu^2)u_e^n - \frac{\alpha\mu}{2}(1-\alpha\mu)u_{e+1}^n$$

{uses auto upwinding dependent on Courant number  $\mu$  and flow direction  $\alpha$ }

4. The Beam-Warming scheme (convergent,  $p=2$ ).

$$u_e^{n+1} = \frac{\alpha\mu}{2}(1-\alpha\mu)(2-\alpha\mu)u_e^n + \alpha\mu(2-\alpha\mu)u_{e-1}^n - \frac{\alpha\mu}{2}(1-\alpha\mu)u_{e+1}^n$$

{genuine upwind scheme: uses no downwind information}

Lax-Wendroff scheme in matrix form

$$U^{n+1} = AU^n \rightarrow \text{Dirichlet boundary conditions}$$

$$A = \begin{bmatrix} 1 - \alpha^2\mu^2 & \frac{\alpha\mu}{2}(\alpha\mu - 1) & & \\ \frac{\alpha\mu}{2}(\alpha\mu + 1) & 1 - \alpha^2\mu^2 & \frac{\alpha\mu}{2}(\alpha\mu + 1) & \\ & \ddots & \ddots & \ddots & \frac{\alpha\mu}{2}(\alpha\mu + 1) & 1 - \alpha^2\mu^2 \end{bmatrix}$$

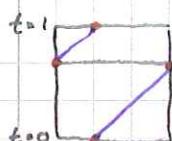
with  $\alpha\mu = 1$ .

$$A = \begin{pmatrix} 0 & 0 & & \\ 1 & 0 & 0 & \\ & \ddots & 0 & 0 \\ & & 1 & 0 \end{pmatrix} \text{ Shift matrix}$$

All eigenvalues  $\lambda_k[A] = 0$ .

Periodic boundary conditions.

Periodicity in  $t$  and  $x$



$$u(0,t) = u(1,t) \quad t \geq 0$$

$$u(x,0) = g(x) \Rightarrow u(x,1) = g(x),$$

Circulant matrices:

$$C(k) = \begin{bmatrix} k_0 & k_1 & \dots & k_{d-1} \\ k_{d-1} & & & \\ \vdots & & & \\ k_1 & k_2 & \dots & k_0 \end{bmatrix} \text{ Circulant matrices are a special class of Toeplitz matrices.}$$

A finite difference scheme with periodic b.c. is stable only if and only if:

$$|\lambda_k[A(\alpha\mu)]| \leq 1$$

1) Convection-diffusion equation ( $u_t = u_{xx} + u_{xxx}$ )  
Parabolic  $\frac{\Delta t}{\Delta x^2} \leq 1$

2) Wave equation ( $u_{tt} = c^2 u_{xx}$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x} \leq 1$

3) Schrödinger equation ( $i u_t = u_{xx}$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x^2} \leq 1$

4) Korteweg-de Vries equation ( $u_t + u u_x = -u_{xxx}$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x^3} \leq 1$

5) Inviscid Burgers equation ( $u_t + u u_x = 0$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x} \leq 1$

6) Reaction-diffusion equation ( $u_t = u_{xx} + f(u)$ )  
Parabolic  $\frac{\Delta t}{\Delta x^2} \leq 1$

7) Advection equation ( $u_t + u u_x = 0$ )  
Parabolic  $\frac{\Delta t}{\Delta x} \leq 1$

8) Viscous Burger equation ( $u_t + u u_x = u_{xx}$ )  
Parabolic  $\frac{\Delta t}{\Delta x^2} \leq 1$

9) Heat conduction equation ( $u_t = \alpha \cdot u_{xx}$ )  
Parabolic  $\frac{\Delta t}{\Delta x^2} \leq 1$

10) Linear conservation law ( $u_t + c u_x = 0$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x} \leq 1$

11) Klein-Gordon equation ( $u_{tt} = u_{xx} - u$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x} \leq 1$

12) Beam equation ( $u_{tt} = -u_{xxxx}$ )  
Hyperbolic  $\frac{\Delta t}{\Delta x^2} \leq 1$