



Numerics of Partial Differential Equations

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Mathematical Description of Fluid Dynamics

- Classification of partial differential equations
- Classification of the Euler and Navier-Stokes equations
- Flow phenomena: Shocks, rarefaction, contact discontinuity
- Numerical schemes



Classification of Partial Differential Equations

- Second-order Partial Differential Equations (PDE)
 - Elliptic, parabolic, hyperbolic
- Conservation equations
- Transport equations





Second-Order PDEs

au_{xx} + bu_{xy} + cu_{yy} = h(u, u_x, u_y, x, y)
notation:
$$u_{xx} = \frac{\partial^2 u}{\partial x^2}, \ u_{xy} = \frac{\partial^2 u}{\partial x \partial y}, u_{yy} = \frac{\partial^2 u}{\partial y^2}$$

a, b,
$$c \in \Re$$
constant coefficients $a = a(x, y), b = b(x, y), c = c(x, y)$ linear $a = a(u), b = b(u), c = c(u)$ quasilinear $a = a(u, u_x, u_y, x, y), b, c$ analognon-linear

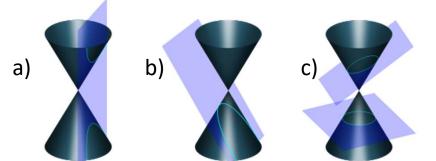


Classification of Second-Order PDEs

$$au_{xx} + bu_{xy} + cu_{yy} = h(u, u_x, u_y, x, y)$$

Criteria:

a) hyperbolic : $b^2 - 4ac > 0$ b) parabolic : $b^2 - 4ac = 0$ c) elliptic : $b^2 - 4ac < 0$ Analog: conic section $ax^2 + bxy + cy^2 = r$





Elliptical Differential Equations

- Physics:
 - Stationary problems: heat transport, potential flow, electric potential
 - Stationary subsonic flows
 - Membrane deflection
- Mathematical model:
 - \circ Laplace equation $u_{xx} + u_{yy} = 0$
 - Poisson equation

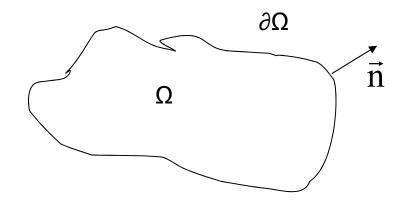
• Helmholtz equation $u_{xx} + u_{yy} + ku = 0$

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



Constraints on Elliptical Differential Equations

• Boundary value problem





Parabolic Differential Equations

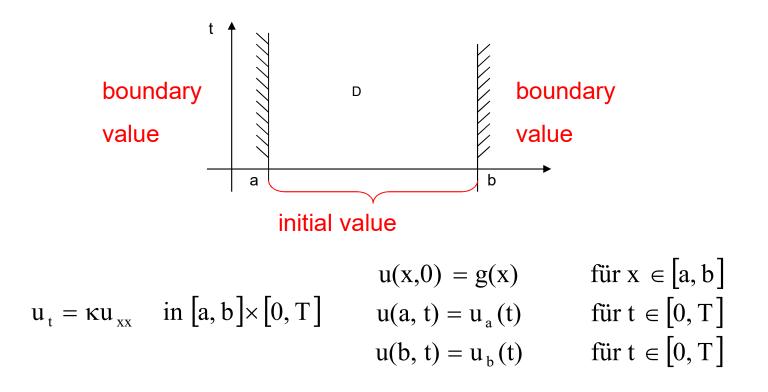
- Physics:
 - $_{\odot}$ Heat transport, diffusion processes
 - Friction-viscosity
 - Transient processes
- Mathematical model:
 - Heat equation $u_t = \kappa \Delta u$
 - \circ Heat equation 1D $u_t = \kappa u_{xx}$
- Limit for stationary processes (u_t=0): Parabolic → elliptic





Constraints on Parabolic Differential Equations

• Initial value and boundary value problem

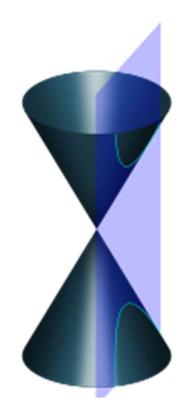




Hyperbolic Differential Equation

- Physics:
 - $_{\odot}$ Wave propagation, acoustic
 - Electromagnetic waves
 - Gas dynamics
- Mathematical model:
 - Wave equation
 - Wave equation 1D $u_{tt} = c^2 u_{xx}$

transport velocity : $c \neq 0$



 $u_{tt} = c^2 \Delta u$



Constraints on Hyperbolic Differential Equations

• Initial value problem

 $u(x,0) = g(x) \quad \forall \ x \in \Re$

Annotation: In practical simulations, the flow depends on initial values and boundary values (e.g. flow around an airfoil). The boundary values are not fixed, but depend on the solution of the flow. Boundary values have to satisfy compatibility conditions.



Hyperbolic Differential Equations of 1. Order

Wave equation 1D: $u_{tt} - c^2 \cdot u_{xx} = 0$ Transformation in system of first order: New variables: $p = c \cdot u_x$, $q = u_t$ Resulting in two equations of first order

$$q_t - c \cdot p_x = 0$$
 system of first order
 $p_t - c \cdot q_x = 0$



Hyperbolic Differential Equations of 1. Order

• Simplest hyperbolic equation in 1D:

 $U_t + aU_x = 0$ Linear transport equation

• Simplest hyperbolic equation in 2D:

 $u_t + au_x + bu_y = 0$

• Simplest quasi-linear hyperbolic equation

 $U_t + UU_x = 0$ Burgers' equation





Conservation Law in 1D

- Burgers' equation $u_t + uu_x = 0$ quasi-linear $u_t + \left(\frac{1}{2}u^2\right)_x = 0$ conservation form
- In general: $u_t + f(u)_x = 0$ u,f,g are scalars or vectors.

$$u_t + Au_x = 0$$
 quasi-linear
 $A = \frac{\partial f(u)}{\partial (u)}$ Jacobian matrix



Conservation Law in 2D

• In general $u_t + f(u)_x + g(u)_y = 0$ conservation form u,f,g are scalars or vectors

> $u_t + Au_x + Bu_y = 0$ quasi-linear $A = \frac{\partial f(u)}{\partial (u)}, \quad B = \frac{\partial g(u)}{\partial (u)}$ Jacobian matrix



Compressible Navier-Stokes Equation

$$\rho_{t} + \nabla \cdot (\rho v) = 0$$

$$(\rho v)_{t} + \nabla \cdot ((\rho v) \circ v) + \nabla p = \nabla \cdot \tau + f$$

$$e_{t} + \nabla \cdot (v(e+p)) = \nabla (\tau \cdot v) - \nabla \cdot q + f \cdot v + Q$$
conservation of energy

 ρ density

V

е

- p pressure
- τ viscosity
- energy

velocity

q heat flux

equation of state

$$p = (\gamma - 1)\rho\varepsilon$$
, $e = \rho\varepsilon + \frac{1}{2}\rho(v \cdot v) + \rho gh$

ideal gas

inner kinetic potential energy

system of conservation laws/ equations

HPCFD03 - Numerics of	Partial Differential		
Equations			





Euler Equations

$$\rho_t + \nabla \cdot (\rho v) = 0$$
$$(\rho v)_t + \nabla \cdot ((\rho v) \circ v) + \nabla p = 0$$
$$e_t + \nabla \cdot (v(e+p)) = 0$$

conservation of mass conservation of momentum conservation of energy

 $\rho \quad \text{ density} \quad$

p Pressure

v velocity

e energy

equation of state

$$p = (\gamma - 1)\rho\varepsilon$$
, $e = \rho\varepsilon + \frac{1}{2}\rho(v \cdot v)$

ideal gas inner kinetic energy

system of conservation laws/ equations

HPCFD03 - Numerics of	Partial Differential		
Equations			



Theory of Characteristics

• Has to satisfy linear transport equation

$$u_t + au_x = 0$$

$$C = \left\{ x = x(t) \text{ with } \frac{dx(t)}{dt} = a \right\} \implies \frac{du(x(t), t)}{dt} = u_t + u_x \frac{dx}{dt} = u_t + au_x$$

Comparison of coefficients

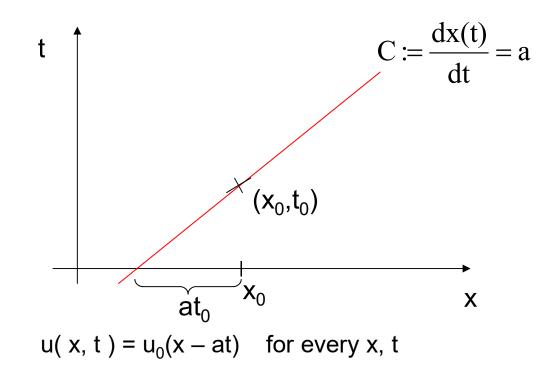
$$\Rightarrow C: \frac{dx}{dt} = a(x, t)$$

a = const. \rightarrow C is linear u = const. on C \rightarrow u(x, t) = u(x - at, 0)





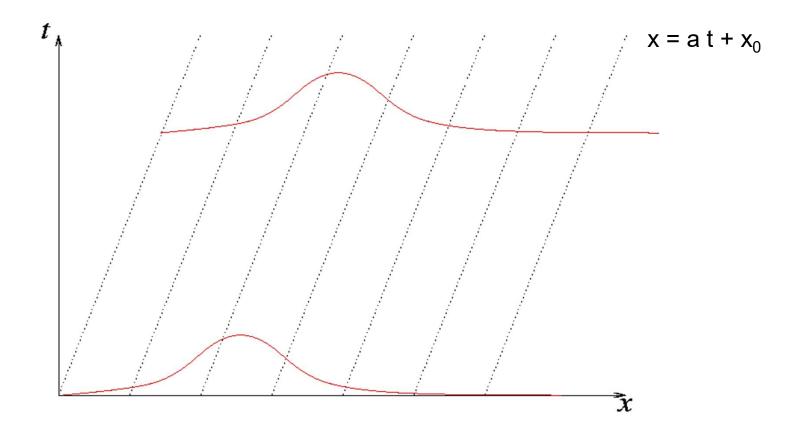
Solution of Initial Value Problem for Linear Transport Euqations



Information is transported along characteristics.



Solution is Constant along a Characteristic



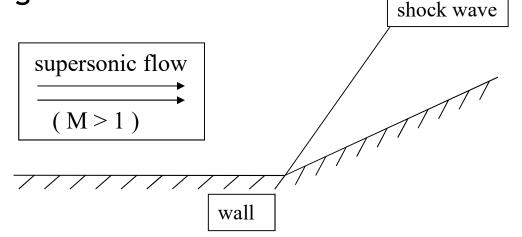




Euler Equations - Flow Phenomena

The non-linear Euler equations allow for discontinuities in the solution, known as shocks. Shocks can be generated out of smooth initial values.

Example: The compression of a supersonic flows in front of a wall generates a shock.

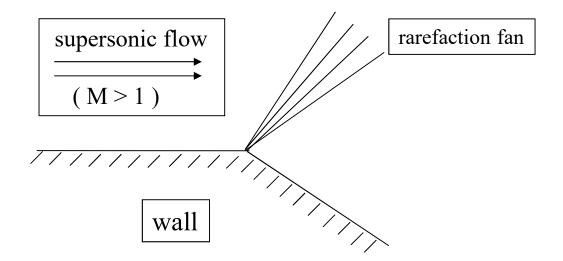




Euler Equations - Flow Phenomena II

The non-linear Euler equations allow for smooth solutions, too. These phenomena are known as rarefaction fans.

Example: Rarefaction of supersonic flows close to walls.



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Euler Equations - Flow Phenomena III

The non-linear Euler equations allow for material interfaces (e.g. water-air, hot and cold fluid,..). These phenomena are called contact discontinuities.

Example: Separation of hot and cold fluids.





Properties of the Euler Equation

- The Euler equations are hyperbolic equations non-linear wave equations.
- Problems: Shocks and Rarefaction

Characteristics of non-linear equations depend on the solution and can intersect: The solution cannot be differentiated \rightarrow The differential system of equations is not longer valid.

The numerical method must handle all phenomena: Shock capturing



Compressible Navier-Stokes Equation - Type

- $\rho_{t} + \nabla \cdot (\rho v) = 0$ conservation of mass $(\rho v)_{t} + \nabla \cdot ((\rho v) \circ v) + \nabla p = \nabla \cdot \tau + f$ conservation of momentum $e_{t} + \nabla \cdot (v(e+p)) = \nabla (\tau \cdot v) - \nabla \cdot q + f \cdot v + Q$ conservation of energy
 - density ρ
 - velocity V
 - е energy

viscosity τ heat flux q

pressure

Parabolic – Hyperbolic!!!

equation of state

 $\rho = (\gamma - 1)\rho\varepsilon$, $\Theta = \rho\varepsilon + \frac{1}{2}\rho(\mathbf{V}\cdot\mathbf{V}) + \rho \mathrm{gh}$

ideal gas

р

inner kinetic potential energy

system of conservation laws/ equations

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Equations			



Properties of the Navier-Stokes Equation

- The Navier-Stokes equations are hyperbolicparabolic equations.
- Problems:

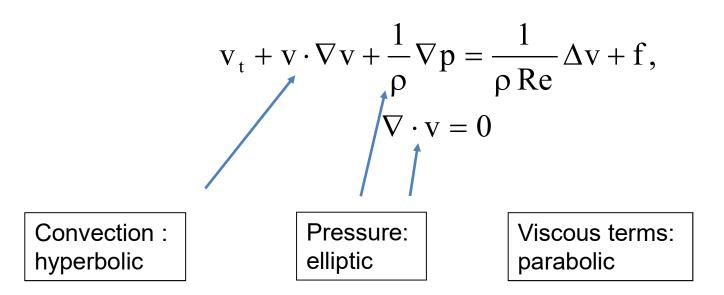
Small viscous terms and heat flux (high Re): hyperbolic terms dominate: Shocks and Rarefaction

The numerical method must handle all phenomena: Shock capturing





Incompressible Navier-Stokes Equation - Type



The incompressible Navier-Stokes equations are parabolic-elliptic. At high Reynolds numbers, the hyperbolic terms are dominating.





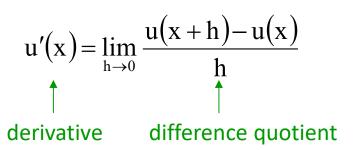
Numerical Schemes

- Numerical methods for solving partial differential equations
 - 1. Finite Difference (FD) methods
 - 2. Finite Element (FE) methods
 - 3. Finite Volume (FV) methods



Differences Methods (Finite Differences - FD)

• Idea:



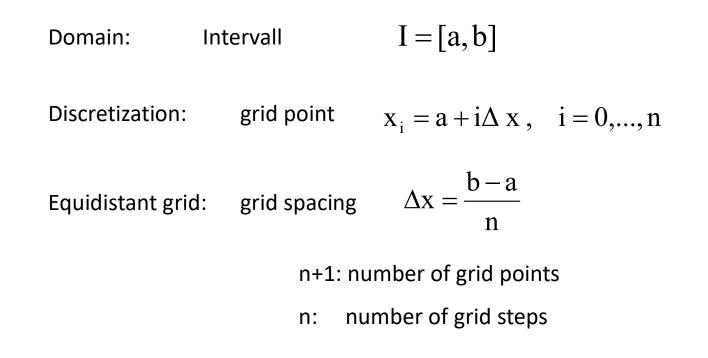
Exchange the derivatives by difference quotients.

Partial differential equation =>

System of differential equations are evaluated at grid points.



Step 1: Discretization of Computational Domain





Step 2: Difference Quotient

Taylor series

(1)
$$u(x_{i-1}) = u(x_i) - \Delta x u_x(x_i) + \frac{\Delta x^2}{2} u_{xx}(x_i) - \frac{\Delta x^3}{6} u_{xxx}(x_i) + \dots$$

(2) $u(x_{i+1}) = u(x_i) + \Delta x u_x(x_i) + \frac{\Delta x^2}{2} u_{xx}(x_i) + \frac{\Delta x^3}{6} u_{xxx}(x_i) + \dots$

For each derivative insert difference quotient

(2)-(1)
$$u(x_{i+1}) - u(x_{i-1}) = 2\Delta x u_x(x_i) + \frac{2\Delta x^3}{6} u_{xxx}(x_i) + O(\Delta x^5)$$
$$\frac{u(x_{i+1}) - u(x_{i-1})}{2\Delta x} = u_x(x_i) + \frac{\Delta x^2}{6} u_{xxx}(x_i) + O(\Delta x^4)$$





Step 2: Difference Quotient II

$$\frac{u(x_{i+1}) - u(x_{i-1})}{2\Delta x} = u_x(x_i) + O(\Delta x^2)$$
Central difference quotient
2. order

$$\frac{u(x_{i+1}) - u(x_i)}{\Delta x} = u_x(x_i) + O(\Delta x)$$
right-hand difference quotient
1. order

$$\frac{u(x_i) - u(x_{i-1})}{\Delta x} = u_x(x_i) + O(\Delta x)$$
left-hand difference quotient
1. order

$$\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} = u_{xx}(x_i) + O(\Delta x^2)$$
Central difference quotient
2. order

- Difference quotient of higher order requires more than 3 points
- Difference quotient of different order and type
- Non-equidistant: terms are more complicate



FD Methods: Procedure

- 1. Step: Discretization of computational domain, grid
- 2. Step: Selection of difference quotient, derivatives are substituted by difference quotients
- 3. Step: Reordering of the difference equation
- 4. Step: Solving the difference equation linear system





FD - Poisson-Equation

$$\mathbf{u}_{\mathrm{xx}} + \mathbf{u}_{\mathrm{yy}} = f$$

Domain : [a,b] x [c,d]

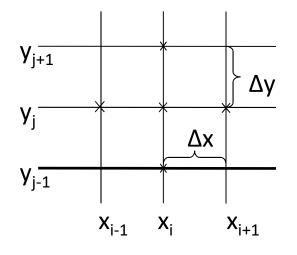
Boundary value (Dirichlet):

$$u(a,y)=u_a(y)$$
 for $x \in [a,b]$
 $u(b,y)=u_b(y)$
 $u(x,c)=u_c(x)$ for $y \in [c,d]$
 $u(x,d)=u_d(x)$



1. Step: Discretization

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equidistant grid spacing

$$\Delta x = \frac{b-a}{n_1}, \quad \Delta y = \frac{d-c}{n_2}$$

grid points

$$\mathbf{x}_i = \mathbf{a} + \mathbf{i}\Delta \mathbf{x}, \quad \mathbf{i} = 0, \dots, n_1$$

$$y_j = c + j\Delta y$$
, $j = 0,..., n_2$



2. Step: Difference Quotient

$$\frac{\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}}{\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2}} \text{ appr. } u_{xx}(x_i, y_j)$$

Insert the finite differences into differential equation of the Poisson equation:

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f_{i,j}$$

at each inner grid point x_i , y_i

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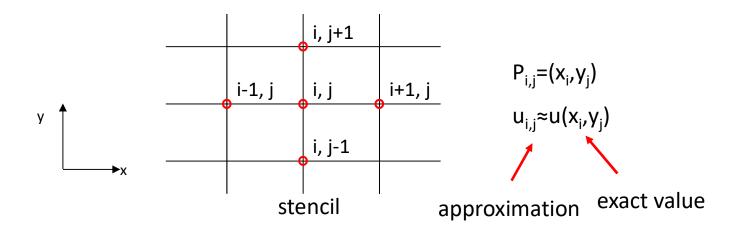


3. Step: Rearranging of the Equations

Equation at each inner grid point

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

$$i = 1, \dots, n_1 - 1, j = 1, \dots, n_2 - 1$$





3. Step: Construction of Linear System

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

$$i = 1, \dots, n_1 - 1, j = 1, \dots, n_2 - 1$$

Special treatment: boundary values

$$a_{i,j}u_{i,j-1} + b_{i,j}u_{i-1,j} + c_{i,j}u_{i,j} + d_{i,j}u_{i+1,j} + e_{i,j}u_{i,j+1} = \overline{f}_{i,j}$$

$$i = 1, \dots, n_1 - 1, j = 1, \dots, n_2 - 1$$

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Form of Linear System

 $a_{i,j}u_{i,j-1} + b_{i,j}u_{i-1,j} + c_{i,j}u_{i,j} + d_{i,j}u_{i+1,j} + e_{i,j}u_{i,j+1} = \overline{f}_{i,j} \quad \text{für} \quad i = 1, \dots, n_1 - 1, \ j = 1, \dots, n_2 - 1$

	$\left(\mathbf{u}_{11} \right)$)	$\left(\mathbf{c}_{11} \right)$	d ₁₁			e ₁₁)	<u> </u>
	u ₂₁		b ₂₁	c ₂₁	d ₂₁			e ₂₁						Pe	ent	a d	iag	ona	al
u =	u ₃₁			b_{31}	\mathbf{c}_{31}	d ₃₁			e ₃₁					LS			0		
	u ₄₁				b_{41}	\mathbf{c}_{41}				e ₄₁)				
	u ₁₂		a ₁₂				c ₁₂	d ₁₂			e ₁₂								
	u ₂₂			a ₂₂			b ₂₂	c ₂₂	d ₂₂			e ₂₂							
	u ₃₂				a ₃₂			b ₃₂	c ₃₂	d ₃₂			e ₃₂						
	<u>u</u> ₄₂	A =				a ₄₂			b ₄₂	c ₄₂				e ₄₂					
	u ₁₃						a ₁₃				c ₁₃	d ₁₃			e ₁₃				
	u ₂₃							a ₂₃			b ₂₃	c ₂₃	d ₂₃			e ₂₃			
	u ₃₃								a ₃₃			b ₃₃	c ₃₃	d ₃₃			e ₃₃		
	u ₄₃									a ₄₃			b ₄₃	c ₄₃				e ₄₃	
	u ₁₄										a ₁₄				c ₁₄	d_{14}			
	u ₂₄											a ₂₄			b ₂₄	c ₂₄	d ₂₄		
	u ₃₄												a ₃₄			b_{34}	c ₃₄	d ₃₄	
	(u ₄₄)	J												a ₄₄			b_{44}	c ₄₄)	



Step 4: Solving the Linear System

Numerical Methods
 Gauss-Algorithm
 Drawbacks: expensive, computes with all zero
 More suitable: Iterative methods
 Solving LS to a certain accuracy

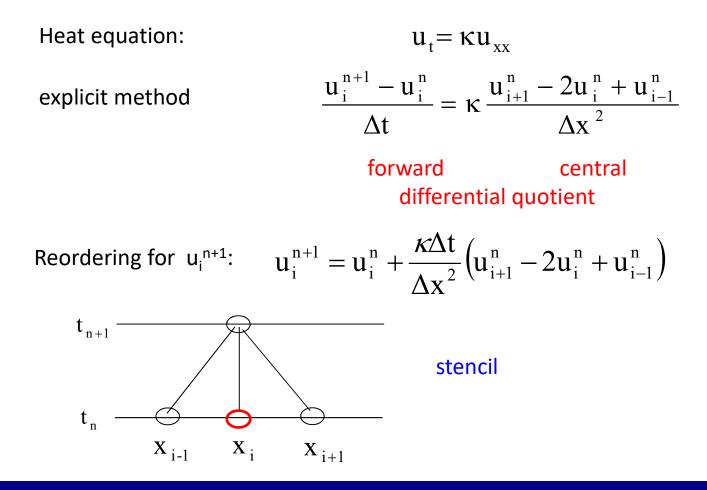


Iterative Methods for Sparse Linear Systems

- Classical iterative methods: Jacobi-, Gauß-Seidel-, SOR-Method ill conditioned systems with small steps. Only for small systems.
- CG-method (Method of conjungent gradients) Matrices are symmetric and positive definite
- Methods of general residual, Krylov-subspace methods Generalization of the CG-Method: GMRES, BIGSTAB
- **Multigrid-methods** Surpasses the disadvantage of classical iterative methods by solving the equation on different fine grids. Fast, but depending on parameters.

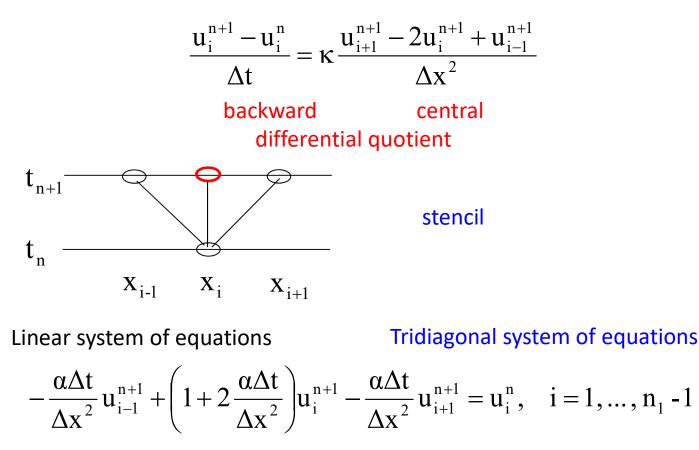


Finite Differences for Heat Equation: Explicit





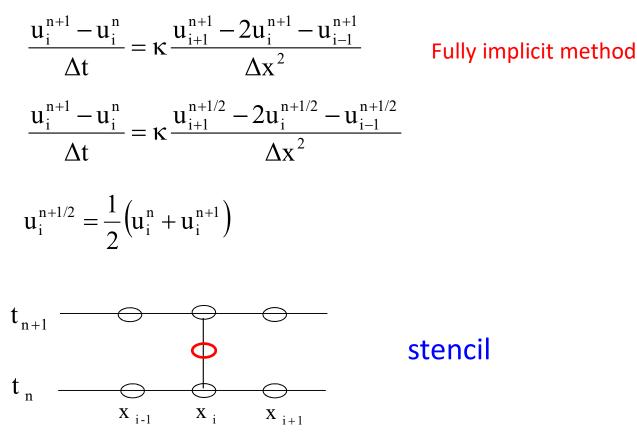
Finite Differences for Heat Equation: Implicit I







Implicit Methods





FD for Parabolic Differential Equations -Summary

Explicit methods

The explicit method $O(\Delta t, \Delta x^2)$ is conditionally stable and requires

$$\kappa \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2^d} \quad \Longrightarrow \Delta t \sim \Delta x^2$$

The stability constrain leads to a practical accuracy of $O(\Delta x^2)$ which correspondence to a method of second order in space and time.

Implicit methods

The implicit method $O(\Delta t, \Delta x^2)$ or the Crank-Nicolson-method $O(\Delta t^2, \Delta x^2)$ are unconditionally stable.



FD for Hyperbolic Differential Equations

 $u_t + au_x = 0$, $a \in \Re$

Linear system of transport equations

Explicit difference method

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \qquad O\left(\Delta t, \Delta x^2\right)$$
$$u_i^{n+1} = u_i^n - a \frac{\Delta t}{2\Delta x} \left(u_{i+1}^n - u_{i-1}^n\right)$$

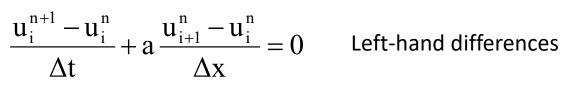
A Neumann stability analyze leads to: Unconditionally unstable !!!!

or





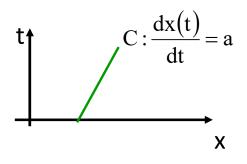
One-Sided Differences



 $\frac{u_i^{n+1} - u_i^n}{\Delta t} + a \frac{u_i^n - u_{i-1}^n}{\Lambda x} = 0 \qquad \text{Right-hand differences}$

Is this method stable?

Case a>0:



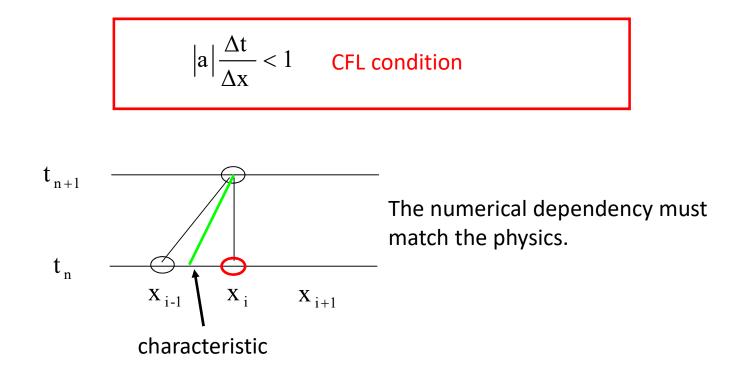
Dependency is motivated by physics!





Upwind Method or CIR-Scheme

von Neumann stability analysis: The CIR- method is conditionally stable under the condition:



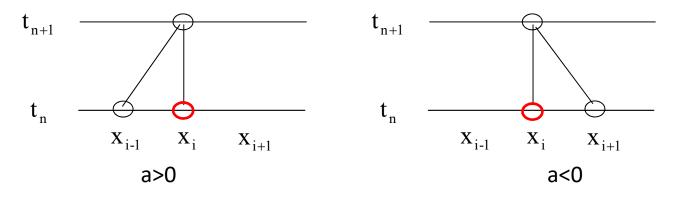


Upwind Method or CIR-Scheme II

$$u_i^{n+1} = u_i^n - a \frac{\Delta t}{\Delta x} \begin{cases} u_i^n - u_{i-1}^n & \text{für } a > 0 \\ u_{i+1}^n - u_i^n & \text{für } a < 0 \end{cases} \quad \begin{array}{l} \text{Courant, Isaacson,} \\ \text{Rees - CIR} \end{cases}$$

Upwind-method:

Design the differences in opposite direction to the information transport. The direction of the characteristic is reflected by the numerical method.



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Implicit Method

Fully implicit

LS, unconditionally stable

$$\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + a \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} = 0$$

Crank – Nicolson - Verfahren LS, unconditionally stable

$$\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + a \frac{u_{i+1}^{n+1/2} - u_{i-1}^{n+1/2}}{2\Delta x} = 0$$

$$u_i^{n+1/2} = \frac{1}{2} \left(u_i^n + u_i^{n+1} \right)^{n+1}$$



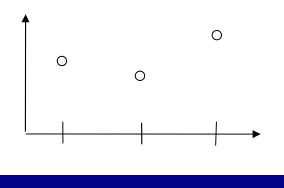
Explicit Methods for Parabolic-Hyperbolic PDEs

- Time step restriction
- **Parabolic** $\Delta t \sim \kappa \Delta x^2$
 - Step size restriction: quadratic
 - Only possible for small κ
- \blacktriangleright Hyperbolic $\Delta t \sim a\Delta x$
 - Step size restriction: linear
 - Generally used for transient problems, stability requires Upwind approximation.



Summary FD

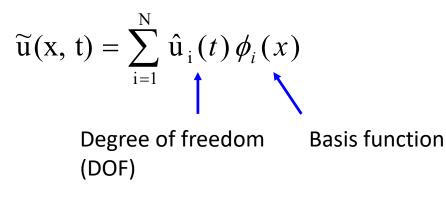
- Finite Differences (FD)
 - Solution is represented by point values
 - Simple coding, even for complex equations
 - Very complex on unstructured grids
 - Problem with discontinuities/strong gradients





Finite Element Method

Different approach: approximation by a continuous function:

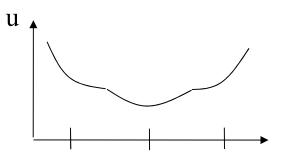


The degree of freedom are chosen in a manner to obtain the best possible approximation.



Summary FE

- Finite Element(FE)
 - Solution is represented by basis functions
 - Even more complex to code than FV
 - Arbitrary, unstructured grids
 - Special techniques at strong gradients





Finite Volume Method

- Approximation of integral mean values
- Standard for conservation lows
- Strong gradients or discontinuities are easy to handle
- Flux calculation between adjoint cells:
 Riemann problem: shock capturing
- Reconstruction, piecewise polynomial

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Comparison of FD, FE, FV

- Finite Difference (FD)
 - Solution is represented by point values
 - Simple coding, even for complex equations
 - Complex on unstructured grids
 - Problems at large gradients (Discontinuities)
- •Finite Volume (FV)
 - Representation as cell mean value
 - More complex to code than FD
 - Arbitrary, unstructured grids
 - No problem at large gradients
- •Finite Element (FE)
 - Solution is superposition of basis functions
 - More complex to code than FV
 - Easy on arbitrary, unstructured grids
 - Requires special techniques at large gradients and shocks

