

# Summary of the lecture

## “Numerische Mathematik 2 für Ingenieure”

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### Abstract

This lecture gives an overview about basic PDE notations, such as classical solutions, classification of solutions, and well-posedness of an abstract PDE problem. Based on this it explains how standard PDEs (linear, scalar, second order) can be solved using finite differences and finite elements. For both methods convergence of discrete solutions to exact solutions is discussed. Finally solution methods for discretized problems will be discussed.

The lecture is divided into four parts: General theory, finite difference method, finite element method, iterative solvers.

**Note:** If you encounter a symbol “!”, then this implies a topic is really important; whereas a symbol “\*” implies a topic is difficult and in-depth knowledge is voluntary.

## Main conceptual questions raised/solved in the lecture

In a physical/engineering/mathematical application you are often provided with a PDE (from a textbook; derived by a practitioner or by experience/expert knowledge, derived from physical laws, ...). Your task might be to solve this PDE. Natural questions which may come to your mind then are:

- In what form is a PDE stated?  
When does the statement make sense?  
How do we define/understand solutions?
- How can we approximate solutions of PDEs via numerical methods?  
smooth solutions  $\Rightarrow$  finite difference methods;  
non-smooth solutions or complicated geometries  $\Rightarrow$  finite element methods  
What are the conceptual differences between finite differences and finite elements?
- Using which assumptions and in which sense do these numerical solution approximate the exact solutions of a well-posed problem? How can this be shown for elliptic problems and parabolic problems in the context of the finite difference method or the finite element method.
- How can we solve the systems of (symmetric, positive definite) linear equations which appear as a result of discretizing a PDE?

## 1 General theory and basics

- ! definitions: space and time domain, configuration space, partial derivatives, abstract definition of a PDE
- some examples: heat equation (house), heat eq., wave eq., Poisson eq., transport eq., \*inviscid Burgers' eq., \*Schrödingers eq., \*Maxwell's eq.,
- ! general form of a linear scalar second order equation and classification (elliptic, parabolic, hyperbolic)
- ! role of boundary conditions (Dirichlet, Neumann, mixed b.c.)
- abstract notation using linear operators  $L$
- ! reason for classification, (the concept of) classical solutions, well-posed problems, ill-posed problems
- general strategies to simplify PDEs
- representation formulas and some exact solutions: fundamental solution, “artificial” solutions, (self-similar) fundamental solution of the heat equation, Duhamels principle, uniqueness of solutions
- \* general existence and uniqueness of classical solutions for sufficiently smooth data and boundaries

## 2 Finite difference method

### 2.1 General strategy and basics

- approximation of first order, second order, higher order derivatives using forward, backward and central differences
- Taylor's theorem and Lagrange form of the remainder
- consistency of  $D_+$ ,  $D_-$ ,  $D_0$ ,  $D_+D_-$  and their domain of definition
- discretization of an elliptic problem in 1D, spaces of discrete “functions”, matrix form of the discrete equation (full matrix and reduced matrix by elimination of unknowns on the boundary), symmetry properties of full and reduced matrix
- treatment of inhomogeneous Dirichlet boundary conditions
- difference stencils and compact notation
- finite differences in higher dimensions (using Taylor's theorem), examples: 5-point stencil in 2D, 7-point stencil in 3D,  $(2n + 1)$ -point stencil in  $n$ D
- lexicographical ordering

### 2.2 Elliptic problems

- Poisson equation and discrete Poisson equation on discretely connected domains

- \* existence and uniqueness of the discrete problem using discrete maximum principle and the stability estimate

$$\max_{\Omega} |u^h| \leq C \max_{\Omega} |f^h| + \max_{\Gamma} |g|$$

- error of discrete solutions in the discrete  $L^2$  and maximum norm, induced matrix norm
- ! consistency of a FDM with respect to a norm, consistency of order  $p > 0$ , convergence of a FDM with respect to a norm, convergence of order  $p > 0$ , interpretation of these definitions, restriction operator
- ! stability of a FDM with respect to a norm
- ! Lax equivalence: consistency and stability imply convergence with the consistency order.
- \* convergence for discrete solutions of the Poisson equation in the maximum norm (using stability estimate)
- convergence for discrete solutions of the Poisson equation in the discrete  $L_2$  norm (using eigenvalues)
- \* eigenvalue problem for the Poisson problem using the Rayleigh quotient, Friedrichs inequality produces a lower bound for the eigenvalues and its implication for stability
- use of eigenvalues/eigenfunctions to compute solutions for parabolic and hyperbolic problems
- higher (consistency) order methods
- ! Neumann boundary conditions and their implementation, non-uniqueness of the Poisson problem with Neumann conditions (zero eigenvalue), symmetry of the matrix

- ! compatibility conditions for data to have existence of solutions for the Neumann problem
- extended equations

$$\begin{pmatrix} A & e \\ e^\top & 0 \end{pmatrix} \begin{pmatrix} \bar{u}^h \\ \lambda \end{pmatrix} = \begin{pmatrix} f^h \\ \sigma \end{pmatrix}$$

and their interpretation for  $\lambda = 0$  and  $\lambda \neq 0$

- mixed boundary conditions (Neumann + Dirichlet)
- periodic boundary conditions, their implementation, non-uniqueness
- outlook: higher order methods, higher order problems, non-trivial geometries, variable coefficients

### 2.3 Parabolic problems

- \* difference between parabolic and elliptic equations (domain of dependence, idea behind time-stepping)
- ! general definition of a parabolic problem using an elliptic operator
- ! two-level time-stepping schemes ( $\theta$ -method, explicit Euler, implicit Euler, Crank-Nicolson method)
- ! consistency orders of  $\theta$  method
- stability of the  $\theta$ -method in discrete  $L^2$  and maximum (and mixed) norm: \*  $M$ -matrices,  $L$ -matrices, strict/weak diagonal dominance; \* norm estimates in maximum norm and CFL

conditions (using  $M$ -matrices etc.); ! norm estimates in  $L^2$  norm and CFL conditions (von Neumann stability)

- discussion of CFL condition as a serious constraint for explicit methods and higher order problems
- convergence of  $\theta$ -scheme

### 3 Finite element method

#### 3.1 Basic concepts

- ! concept of weak solutions
- ! derivation of the variational form/weak form in 1D/2D (Gauss theorem, Green's identities, integration by parts)
- classical solutions are weak solutions; weak solutions are classical solutions, if they are sufficiently smooth
- \* motivation using the fundamental lemma of calculus of variations
- ! Dirichlet boundary conditions as essential boundary conditions
- ! Neumann boundary conditions as natural boundary conditions
- mixed boundary conditions as natural boundary conditions
- ! abstract form of the variational problem using bilinear and linear forms (and their properties)

- ! transformation of a problem with inhomogeneous Dirichlet boundary conditions to a problem with homogeneous boundary conditions

### 3.2 !Galerkin method

- transformation of the problem in an infinite dimensional function space  $V$ , into a problem statement in a finite dimensional space  $V_h$
- alternative statement as a minimization problem for positive symmetric bilinear forms
- Galerkin equations  $A\alpha = f$ , definition of  $A, \alpha, f$
- example: 1D with  $V_h$  generated by Fourier series
- theoretical properties of Galerkin method: uniqueness via positive definiteness

### 3.3 Finite element method

- decompositions and basis function for Galerkin method: elements and finite elements
- admissible decompositions of domains  $\Omega$  with polygonal boundary; non-admissible decompositions
- piecewise polynomials on elements (only supported on few elements)
- ! example: 1D interval with piecewise linear basis functions on subintervals
- \* weak derivative, function spaces  $L^2, H^1, H_0^1, H^2$  and their scalar products and norms, Hilbert spaces



- \* relation of Sobolev-spaces  $H^k$  and  $C^k$  spaces (embedding theorem) in 1D, 2D
- ! example: 2D, counting degrees of freedom  $\dim V_h$  for piecewise linear and quadratic functions, with Dirichlet and natural boundary conditions
- visualization of basis functions
- ! the element-to-point map **e2p**:
- Continuity of basis function via the identification basis functions with points on vertices/edges
- different finite elements in 2D (triangles: linear, quadratic, cubic, bubble; quadrilaterals: bilinear, biquadratic)
- ! construction of the global Galerkin equation (assembly) by transformation on the reference domain  $\Omega_{\text{ref}}$ ; usage of shape functions
- ! transformation  $F_k$ , transformation gradient, integration by substitution, transformation of gradients  $\nabla w_i$

### 3.4 Analysis of FEM

- ! Lax-Milgram (boundedness, coercivity, boundedness)
- examples which fulfill Lax-Milgram
- Galerkin orthogonality
- ! Céas Lemma

- convergence of FEM; assumptions (on regularity of solution, on properties of decomposition, which norm)

### 3.5 Outlook

- treatment of parabolic problems with FEM  
How do we discretize such problems?
- convection diffusion problems  
Are the assumptions of Lax-Milgram theorem fulfilled?
- numerical quadrature  
How and why do we integrate on triangles/intervals?

## 4 Iterative solvers

- linear problems as minimization problems
- steepest descent method (gradient descent method): derivation of the construction, convergence rates, energy norm
- ! SD algorithm
- method of conjugate directions: construction, termination after a finite number of steps, reduction of the error
- construction of conjugate direction using Gram-Schmidt-conjugation and properties; problems, if the construction is made from a general basis  $u_i$

- CG method: construction, Krylov spaces, optimality, termination of finitely many iterations, convergence
- ! CG algorithm
- comparison of steepest descent and conjugate gradients
- preconditioning as a special case of CG where  $\langle \cdot, \cdot \rangle$  is replaced by  $\langle \cdot, \cdot \rangle_B$
- ! PCG algorithm
- choice of preconditioner

#### \*Outlook

- reaction-convection-diffusion problems
- isoparametric elements
- systems of (vector-valued) equations

## 5 Topics covered in the assignments are:

1. some linear algebra, exact solutions, sparse matrices
2. more exact solutions, difference stencils, Taylor expansions and remainder, elliptic problems in 1D, 2D
3. finite differences on nonuniform grids for a singularly perturbed elliptic problem
4. eigenvalue problems on a disc  $B_1$ , boundary conditions (1D)
5. periodic boundary conditions, solvability of Neumann problem,  $\theta$ -scheme
6. even more exact solutions, CFL condition and  $\theta$  scheme, minimization problem, weak form and real weak solutions, stiffness and mass matrix computation
7. building a full finite element program in 1D
8. building a full finite element program in 2D, mesh creation
9. quadratic finite elements in 1D and 2D
10. FEM: elliptic problems with convection, heat equation, integration
11. gradient descent method: theory, practice and implementation
12. CG and PCG method: theory, practice and implementation