Lecture on

Elementary Numerical Mathematics

Winter Term 2019/20

Prof. Dr. Gerhard Wellein
Department for Computer Science
HPC Services, Regionales Rechenzentrum Erlangen (RRZE)

Organization

- **Lecture (4 hrs. each week):**
  - Monday – time: 12:15 -13:45 – room: 0.151-115 (EEI building)
  - Thursday – time: 10:15 -11:45 – room: EE 0.135 (Cauerstr. 4)

PLEASE ASK / INTERRUPT ME WHENEVER NECESSARY

- **Tutorials (2 hrs.):**
  - Monday – time: 10:15 -11:45 – room: 01.153-113

  OR

  - Tuesday – time: 12:15 - 13:45 – room: 01.252-128

  - Weekly exercises (assignments: Monday – Monday)
  - Theoretical and programming exercises

Doing the exercises on a regular basis is the best way to prepare for the written exams

Backup timeslot for lectures (due to my frequent travels…..)

- **On travel: Oct. 21 / Nov. 18.– 21.**

- **At least 3 alternative lectures dates:**

- **Choices:**
  - Tuesday 18:00 – 19:30
  - Wednesday 18:00 – 19:30
  - **Thursday 18:00 – 19:30**

  - What is your preference?

- **Exams:**
  - Mid-term exam (MTE): ???? Week before christmas (December)
  - Final exam (FE): Mid of February (week after end of lectures)
  - **Final mark: Result(MTE) + 2*Result(FE)**
  - Register at www.campus.uni-erlangen.de for the 7,5 ECTS module "`Elementary Numerical Mathematics`" with Prüfungsnummer "494959"
- **Exercises start Monday, October 21st**

Doing the exercises on a regular basis is the best way to prepare for the written exams

- **Lecturers**
  - Gerhard Wellein (gerhard.wellein@fau.de)
  - Georg Hager (georg.hager@fau.de)

- **Tutors**
  - Julian Hammer (julian.hammer@fau.de)
  - ???

- **All information about ElNuMa is available at:**
  - http://moodle.rrze.uni-erlangen.de/moodle/course/view.php?id=404
  - Link is also available in the univis.
  - All students attending the lecture should sign up in moodle!!!!

Motivation

- **Computational Engineering is interdisciplinary**
  - Applied Mathematics
  - ComputerScience
  - Technical Application (Engineering Science)

- **Students have different background**
  - Aim: Bring all to a similar level in all fields

- **This course: Applied Mathematics (Numerical Analysis)**
  - compact course – broad scope
  - some theory/mathematics, more algorithms
  - discuss application relevant issues:
    convergence, accuracy, num. effort,numerical stability)
  - how to compute/calculate solutions to (real) problems
    (often no exact analytic solution → numerical approximation)

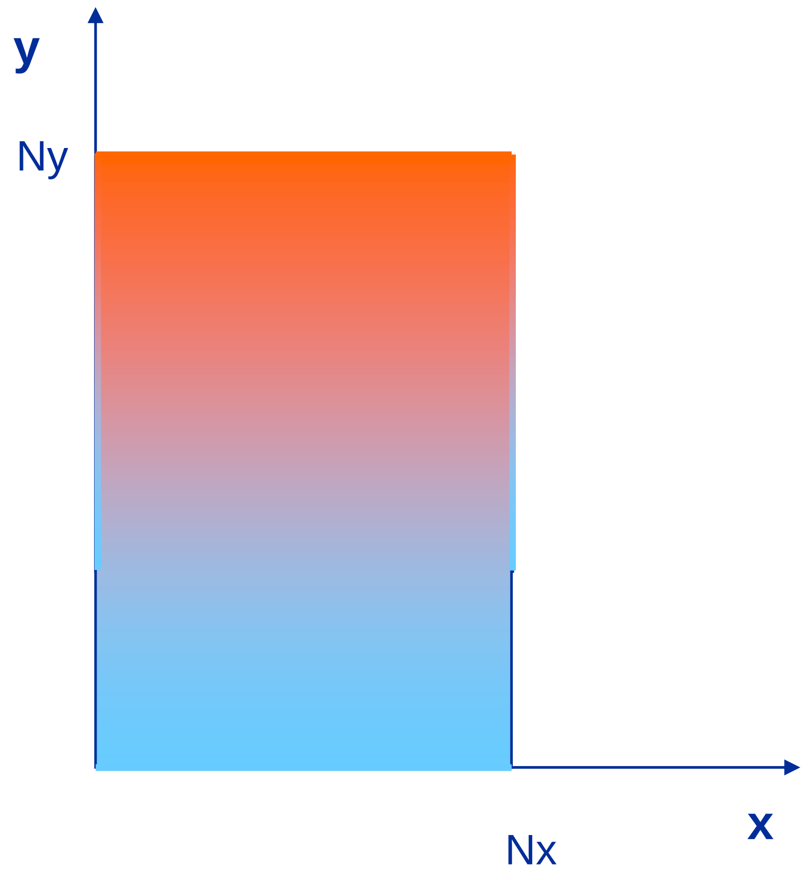
- Solving the heat conduction equation

$$\frac{\partial \Phi}{\partial t} = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2}$$

(Parabolic Partial Differential Equation)

- **Square piece of metal**
  - Temperature $\Phi(x,y,t)$
  - Boundary values:
    $\Phi(x,Ny,t) = 1$,
    $\Phi(x,0,t) = 0$,
    $\Phi(0,y,t) = y = \Phi(Nx,y,t)$
  - Initial values for all x<Nx, y <Ny are zero

- **Temporal evolution:**
  - to stationary state
  - partial differential equation



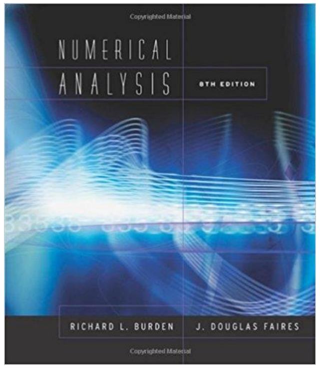
Contents of the lecture

- Mathematical preliminaries (This is what you should be familiar with)

I. Round-off errors and computer arithmetics *(Number representation)*
II. Linear equations – Direct methods *(Gaussian Elimination)*
III. Linear equations – Iterative methods *(Jacobi, Gauss-Seidel)*
IV. Interpolation and polynomial approximation *(Lagrange Polynomial)*
V. Numerical differentiation and integration *(Richardson extrapolation)*
VI. Solutions of equations in one variable *(Fixed Point, Newton)*
VII. Initial value problems for ordinary differential equation *(Euler, Runge-Kutta)*
VIII. Numerical solution to partial differential equations *(Finite-Difference)*

Contents of the lecture

R. L. Burden, J. D. Faires,
Numerical Analysis
Brooks Cole Publishing, 2005 (or later editions)
(see library)



- Further reading:
  - C. F. van Loan**: Introduction to Scientific Computing**
  - J. Stoer, R. Burlisch**: Introduction to Numerical Analysis**
  - **… many others …**

Mathematical Preliminaries - Calculus

- Convergence and limits
- Continuous functions
- Differential calculus
- Integration
- Multivariate functions

Calculus – Convergence and Limits

- Sequence $\{a_n\}_{n=1}^{\infty}$: $\lim_{n \to \infty} a_n$
- Series: $\sum_{k=0}^{\infty} a_k$,e.g., $\sum_{k=0}^{\infty} q^k$
- Functions : $\lim_{x \to a} f(a)$ and $\lim_{x \to oo} f(x)$
- Examples: (1/n), q^n , sign(x), sin(x)/x

Calculus – Continuous functions

- **Definition:**
  - ε–δ– continuity
- **Continuous function defined on closed interval** `f:[a,b]` → `R`
  - Attains minimum and maximum → *Extreme value theorem*
  - *Intermediate value theorem*
    `f(a)<f(b)` and `f(a)<K<f(b)` → There is `c (a<c<b)` with `f(c)=K`
- **Other continuous definitions:**
  - *Uniform continuity*
  - **Lipschitz continuity (brief repetition in ElNuMa)**

Calculus - Differential calculus

- Definition of derivative
- Rules for diff: (sum, product, quotient, chain rule)
- *Theorem of Rolle* and *Mean value theorem*
- Extreme values (min / max) of functions
- **Taylor expansion, ~ Theorem (brief repetition in ElNuMa)**

Calculus - Integration

- Definition (e.g. Riemannian integral) → area
- Rules for integration (sum, partial, substitution)
- Integration and Differentiation

Calculus - Multivariate functions (e.g. $\rho(x,y,z)$)

- Continuity
- Differentiation – total, partial, Jacobi-matrix
- Extreme values
- Iterated integrals

Mathematical Prelimaries - Linear Algebra

- Vectors and Matrices
- Determinant and Inverse of Matrices
- Linear Systems
- Eigenvalues and eigenvectors; characteristic polynmomial
  (brief repetition in ElNuMa)

Linear Algebra

- Rules for sum, product (matrix-matrix, matrix-vector)
- Vector Norm
- **Matrix norm (derived from vector norm) (brief repetition in ElNuMa)**
- Special matrices
  - Dense, diagonal, triangular, sparse,…
  - **Symmetric & positive definite, diagonally dominant (brief repitition in ELNuMa)**

Linear Algebra

- Definition of determinant and rules for calculating
- Invertibility characterized by determinant
  - **A is regular (nonsingular / invertible) if det(A) ≠ 0 → A^{-1} exists**
  - **A is singular (noninvertible) if det(A) = 0**
- Co-factors and inverse
- Rules for determinants
- Characterization of positive definite matrices
  (brief repetition in ElNuMa)

Linear Algebra – Solving linear systems

- Matrix notation
  - Rank of a matrix
  - Uniqueness and existence of solution
  - Square matrices

- How to solve dense linear systems of equations
  - Cramer‘s rule
  - **Gauss elimination**
    (we will start with that – after introduction round-off errors and finite precision arithmetic)