

Scientific Computing WS 2018/2019 Focus Topics

Part I: Sequential hardware, languages.

- Basic principles of the von Neumann Architecture for sequential processors
- Memory Hierarchy and Cache
- Working cycle with compiled languages
- Basic constructs in C++ (control, functions, classes, methods . . .)
- Preprocessor, how to emulate modules
- “Plain” arrays vs. array classes vs. vectors
- Stack, heap, scopes
- Templates
- Inheritance
- Pointers, references, smart pointers in C++
- How to design matrix and vector classes
- The idea behind expression templates

Part II: Linear algebra.

- Computer representation of floating point numbers
- Gaussian elimination, LU factorization, partial pivoting
- Tridiagonal matrix algorithm
- Sparse matrix storage, sparse direct solvers
- Basic iterative methods, simple preconditioners
- Sufficient condition for convergence of iterative methods
- Perron-Frobenius theorem
- Regular splittings, M-Matrices, convergence of iterations based on regular splittings
- Gershgorin circles, Taussky theorem, irreducible matrices
- Matrix theory: (irreducibly) diagonally dominant matrices, nonsingularity criterion,
- Jacobi iteration convergence, M-Matrix criterion
- Incomplete LU factorizations
- The method of conjugate gradients

Part III: Discretization methods.

- Conformal Triangulations
- Shape regularity
- Delaunay triangulation, Voronoi diagram
- Voronoi finite volume discretization, solvability of the discrete problem
- Stiffness matrix assembly for FVM
- Hilbert spaces of square integrable functions
- Strong and weak formulations for heat conduction
- Lax - Milgram lemma
- Cea’s lemma
- Galerkin method, matrix equations
- Lagrangian finite elements
- Barycentric coordinates
- Local basis functions vs global basis functions for P1 FEM
- Convergence rates for linear finite elements for H2-regular problems
- Stiffness matrix assembly for FEM
- Mass matrices, stiffness matrices, condition numbers
- Implementation of Dirichlet boundary values (Penalty method, elimination)
- What is the role of quadrature rules in the finite element method ?
- Time dependent problems, implicit/explicit Euler method
- Convection-diffusion problem, upwinding, exponential fitting
- Nonlinear diffusion, finite volume discretization, Newton method

Part IV.

- Basic paradigms for parallel computing architectures
- Shared Memory vs Distributed Memory programming
- Shared memory: what are write conflicts and how to prevent them
- Structure of parallel program using C++11 threads
- Structure of parallel program using OpenMP
- Main operations for MPI
- Structure of parallel program using MPI
- Main ideas for parallelization on GPU