Scientific Computing WS 2017/2018

Lecture 29

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Iterative solver complexity I

- Solve linear system iteratively until $||e_k|| = ||(I - M^{-1}A)^k e_0|| \leq \epsilon$

$$\rho^k e_0 \leq \epsilon$$
$$k \ln \rho < \ln \epsilon - \ln e_0$$
$$k \geq k_\rho = \left\lceil \frac{\ln e_0 - \ln \epsilon}{\ln \rho} \right\rceil$$

- Assume $\rho < \rho_0 < 1$ independent of h resp. N, A sparse and solution of $Mv = r$ has complexity $O(N)$.
  $\Rightarrow$ Number of iteration steps k_ρ independent of N
  $\Rightarrow$ Overall complexity $O(N)$.

Iterative solver complexity II

- Assume $\rho = 1 - h^\delta \Rightarrow \ln\rho \approx -h^\delta$
- $k = O(h^{-\delta})$
- d: space dimension, then $h \approx N^{-\frac{1}{d}} \Rightarrow k = O(N^{\frac{\delta}{d}})$
- Assume $O(N)$ complexity of one iteration step
  $\Rightarrow$ Overall complexity $O(N^{\frac{d+\delta}{d}})$
- Jacobi: $\delta = 2$, something better with at least $\delta = 1$?

dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
1	$O(N^3)$	$O(N^2)$	$O(N)$	$O(N)$
2	$O(N^2)$	$O(N^{\frac{3}{2}})$	$O(N^{\frac{3}{2}})$	$O(N\log N)$
3	$O(N^{\frac{5}{3}})$	$O(N^{\frac{4}{3}})$	$O(N^2)$	$O(N^{\frac{4}{3}})$

- In 1D, iteration makes not much sense
- In 2D, we can hope for parity
- In 3D, beat sparse matrix solvers with $\rho = 1 - O(h)$?

Multigrid: Iterative solver with O(N) complexity

Idea: combine classical preconditioners with coarse grid correction

- Assume embedded finite element spaces $V_0 \dots V_l$ such tha $V_0 \subset V_1 \subset \dots V_l$
- V_k is produced from V_{k-1} by subdividing each triangle into four. Alternative: finite difference refinement
- $\Rightarrow$ interpolation operator $I_{k-1}^k : V_{k-1} \to V_k$
- $\Rightarrow$ restriction operator $R_{k-1}^k = (I_{k-1}^k)^T : V_k \to V_{k-1}$
- Discretization matrix A_k on each level $k = 0 \dots l$
- "Smoother" (Jacobi, ILU, ...) M_k on each level $k = 1 \dots l$
- Number of smoothig steps n_s
- Coarse grid solver
- Number of coarse grid correction steps γ

Multigrid Algorithm

```
Procedure Multigrid(l, u_l, f_l)
  if l = 0 then
    u_0 = A_0^{-1} f_0                          // coarse grid solution
  else
    for i = 1, n_s do
      u_l = u_l - M_l^{-1} A_l (u_l - f_l)       // pre-smoothing
    end
    f_{l-1} = R^l_{l-1} (A_l u_l - f_l)          // restriction
    u_{l-1} = 0
    for i = 1, γ do
      Multigrid(l - 1, u_{l-1}, f_{l-1})         // coarse grid corr.
    end
    u_l = u_l - I^l_{l-1} u_{l-1}                // interpolation
    for i = 1, n_s do
      u_l = u_l - M_l^{-1} A_l (u_l - f_l)       // post-smoothing
    end
  end
end
```

Multigrid remarks

- Use as a preconditioner in CG methods
- First development in early 60ies by Bakhvalov, Fedorenko
- Works well for hierarchically embedded grid systems and smooth problem coefficients: $O(N)$ solution complexity
- Other variant can use embedding of FEM spaces of growing polynomial degree
- "Algebraic multigrid": define coarse grid, interpolations in an algebraic way by choosing coarse grid points and an interpolation from matrix entries
- Hybrid variant: structured grid, matrix dependent transfer operators for problems with strongly varying coefficients (my PhD. thesis)

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Final remarks

Rear view

- I Architectures and Languages
  - C++, a bit of Python
- II Linear Algebra
  - Sparse matrices, iterative methods, some theory behind
- III Finite elements+ Finite volumes on triangular grids
  - Heat/Diffusion equation (stationary + time dependent)
  - Stationary convection diffusion
  - Nonlinear diffusion
  - Triangulations
  - Finite elements + convergence rate estimates
  - Finite volumes
  - Structural properties discretized systems
- IV Parallelization
  - Shared/Distributed memory, GPU
  - Threads, OpenMP, MPI
- Four separate A4 printable pdfs now on course page

Where to go from here: problem classes

- Systems of PDEs
  - Elasticity: deformation of bodies under external forces
  - Stokes/Navier Stokes equations of fluid mechanics
  - Maxwell equations of electrodynamics
  - Charge transport in self-consistent electric field
  - Reaction-Diffusion systems (we have seen one)
- Coupling between them
- Models and discretizations consistent to basic thermodynamic principles
  - Energy conservation
  - Entropy production (second law of thermodynamics)
- Optimization
- Uncertainty quantification
- Reduced order methods

Where to go from here: discretization methods

- Finite differences (not covered intentionally. . .)
- Discontinuous Galerkin methods
- Finite volume methods on general grids
- Precise and oscillation free discretizations for convection-diffusion
- Linear implicit time discretization for nonlinear problems
- Spectral methods
- Isogeometric finite elements (NURBS based)
- Boundary elements
- Criteria
  - Convergence
  - Matrix structures
  - Structural consistency (to basic physical/thermodynamical principles)

Where to go from here: meshing

- 3D meshing with anisotropic resolution of boundary layers

Where to go from here: efficient linear solution methods

- Domain decomposition methods

Where to go from here: languages + code

- Legacy: Fortran + C
- Future (?): JIT based
  - Julia
  - Python/Numba
- Visualization
  - MathGL
  - vtk/paraview
- Parallel programming environments
  - PetsC
  - Trilinos
- Open Source FEM environments
  - Deal II
  - DUNE
  - FENics
- Commercial
  - COMSOL
  - ANSYS /FLUENT

Where to go from here: something completely different

... but Scientific computing as well

- Molecular dynamics, density functional theory
- Machine learning, neuronal networks (?)

Exams

- Room: MA379
- Consultations: This Thursday 10:00-12:00 MA269
- Focus questions on course page
- *Please do not forget your Prüfungsanmeldung*
- Beisitzer:
  - Rene Kehl
  - Olivier Seté
  - Prof. Nabben

Examination dates

2018-02-26	10:00	Ntokas Konstantin
	10:30	Raabe Dominik
	11:00	Blaschke Lana
2018-03-05	10:00	Bender Wilhelm
	10:30	Masuku Amanda
	11:00	Rominger Marvin
	11:30	Zhu Ruidong
2018-03-12	10:00	Beddig Rebekka
	10:30	Beersing-Vasavez Kiran
	11:00	Cejudo José Eduardo
	11:30	Samad Azlaan Mustafa
	12:00	Sheriff Waseem
	12:30	Sun Peng
2018-03-14	10:00	Anker Felix
	10:30	Abdel Dilara
	11:00	Deinert Hendrik
	11:30	Eleftheriadou Ioanna Iro
	12:00	Özge Sahin
	13:30	Palacios Joaquin
	14:00	Scharton Anton
	14:30	Siedler Frederik
	15:00	Vasalakis Matthas
	15:30	Weltsch André
2018-03-26	10:00	Bartels Tinko
	10:30	Baumann Felix
	11:00	Bolz Marie
	11:30	Gabrysch Sven
	12:00	Meyer Sybille
	12:30	Riegger Franziska
	13:00	Runge Daniel