

Numerical Methods for Hyperbolic and Parabolic Conservation Laws

Linear System Solver

Part III: Preconditioning

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Outline

- Methods for symmetric, positive definite Matrices
 - Method of steepest descent
 - Method of conjugate directions
 - CG-scheme
- Methods for non-singular Matrices
 - GMRES
 - BiCG, CGS and BiCGSTAB
- Preconditioning
 - ILU, IC, GS, SGS, ...

Preconditioning

Goal: Convergence acceleration and stabilization

Condition number

Let $A \in \mathbb{R}^{nxn}$ be non-singular, then

$$\text{cond}_a(A) = \|A\|_a \|A^{-1}\|_a$$

is called the condition number of A w.r.t. $\|\cdot\|_a$

Alternatives:

Let $P_L, P_R \in \mathbb{R}^{nxn}$ be non-singular, then

$$\begin{aligned} P_L A P_R y &= P_L b \\ x &= P_R y \end{aligned}$$

is called a preconditioned system associated with $Ax = b$.

Left preconditioning:

$$P_L \neq I$$

Right preconditioning:

$$P_R \neq I$$

Two-sided preconditioning:

$$P_L \neq I \neq P_R$$

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Two-sided preconditioning:

$$P_L \neq I \neq P_R$$

Preconditioning

Properties of the condition number:

- $\text{cond}(I) = \|I\| \|I^{-1}\| = 1 \cdot 1 = 1$
- $\text{cond}(A) = \|A\| \|A^{-1}\| \geq \|A \cdot A^{-1}\| = \|I\| = 1$
- Let A be normal (d.h. $A^T A = AA^T$), then

$$\text{cond}_2(A) = \frac{|\lambda_n|}{|\lambda_1|}$$

where λ_1, λ_n are both eigenvalues with the smallest and largest absolute value, respectively.

(A symmetric \implies A normal)

Preconditioning

Crucial points:

- P_L, P_R easy to calculated (or more precisely matrix-vector-products with P_L, P_R easy to calculated).
- A sparse $\implies P_L, P_R$ sparse.
- $P_L A P_R \approx I$, such that

$$\text{cond}(P_L A P_R) \approx \text{cond}(I) \ll \text{cond}(A)$$

as good as possible.

Scaling

Choose: $P_L = D$ or $P_R = D$ with $D = \text{diag}\{d_{11}, \dots, d_{nn}\}$

Possibilities:

- Scaling using the diagonal element

$$d_{ii} = a_{ii}^{-1}, i = 1, \dots, n \quad (a_{ii} \neq 0 \forall i)$$

- Scaling row- or columnwise w.r.t. the 1-Norm

$$d_{ii} = \left(\sum_{j=1}^n |a_{ij}| \right)^{-1}, \quad d_{jj} = \left(\sum_{i=1}^n |a_{ij}| \right)^{-1}$$

- Scaling row- or columnwise w.r.t. the 2-Norm

$$d_{ii} = \left(\sum_{j=1}^n a_{ij}^2 \right)^{-\frac{1}{2}}, \quad d_{jj} = \left(\sum_{i=1}^n a_{ij}^2 \right)^{-\frac{1}{2}}$$

- Scaling row- or columnwise w.r.t. the ∞ -Norm

$$d_{ii} = \left(\max_{j=1, \dots, n} |a_{ij}| \right)^{-1}, \quad d_{jj} = \left(\max_{i=1, \dots, n} |a_{ij}| \right)^{-1}$$

Advantage: → Easy to calculate, low storage requirements

Disadvantage: → Usually very low acceleration of the convergence

Model problem: Convection-Diffusion-Equation

Given: $\beta = (\cos(\alpha), \sin(\alpha))$, $\alpha = \frac{\pi}{4}$, $\epsilon = 0.1$, $\Omega = (0, 1) \times (0, 1)$

Sought after: $u \in C^2(\Omega) \cap C(\bar{\Omega})$ with

$$\beta \cdot \nabla u - \epsilon \Delta u = 0 \text{ in } \Omega \text{ and } u(x, y) = x^2 + y^2 \text{ on } \partial \Omega$$

Discretization:

- $N = 100$, $h = x_{i+1} - x_i = y_{i+1} - y_i = \frac{1}{N+1}$
- Central differences for $\Delta u = \partial_x^2 u + \partial_y^2 u$
- One-sided differences for $\nabla u = (\partial_x u, \partial_y u)^T$
- Yields $A u = b$ with

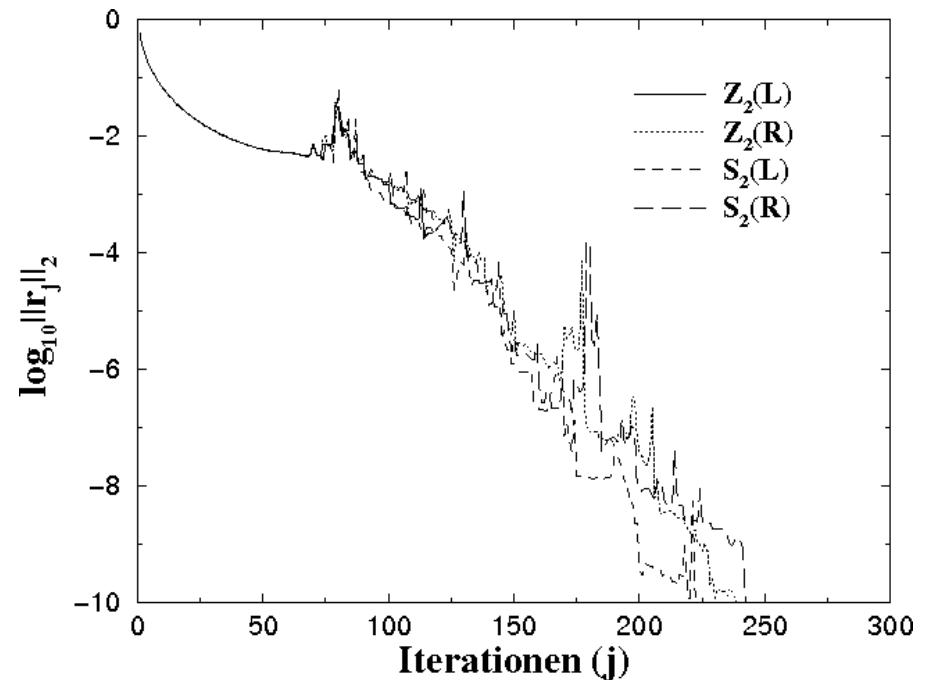
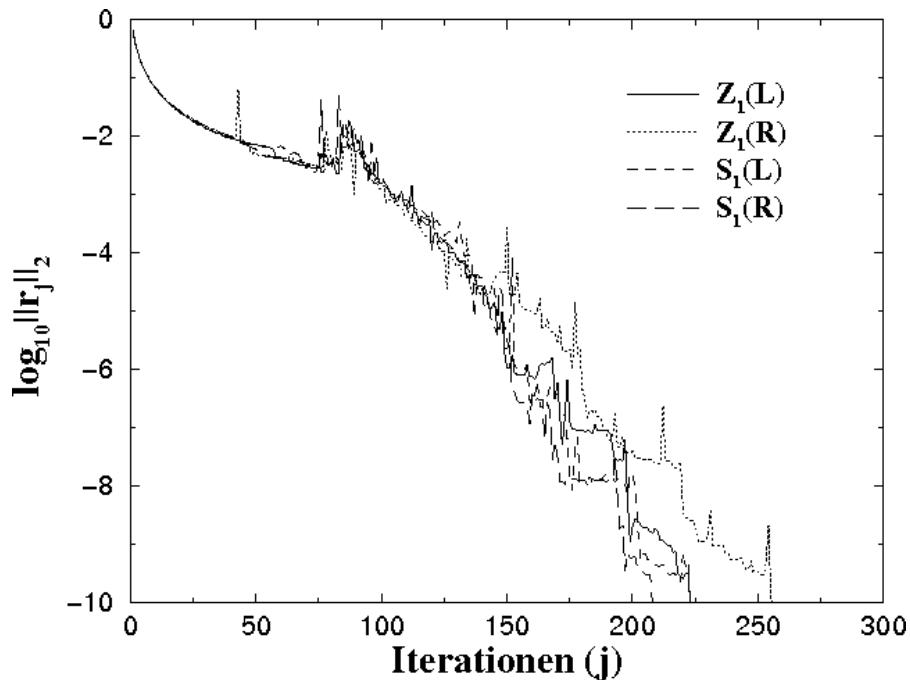
$$A = \text{tridiag}\{D, B, -\epsilon I\} \in \mathbb{R}^{N^2 \times N^2}$$

$$B = \text{tridiag}\{-\epsilon - h \cos \alpha, 4\epsilon + h(\cos \alpha + \sin \alpha), -\epsilon\} \in \mathbb{R}^{N \times N}$$

$$D = \text{diag}\{-\epsilon - h \sin \alpha\} \in \mathbb{R}^{N \times N}$$

Results of different Preconditioners based on scaling

- **L/R:** Left/Right Preconditioning
- **Z/S:** Scaling row- (Z) or columnwise (S)
- **1/2:** Scaling w.r.t. the 1-/2-Norm



- Iterative Solution Method: BiCGSTAB

Splitting-associated preconditioners

Splitting method: $x_{m+1} = B^{-1} (B - A) x_m + B^{-1} b$
with $B \approx A$ and $B^{-1}x$ simple to calculate.

Idea: Choose $P_{L/R} = B^{-1}$

Types: $A = D + L + R$

- Jacobi - method $\rightarrow P = D^{-1}$
- Gauß - Seidel - method $\rightarrow P = (D + L)^{-1}$
- SOR - method $\rightarrow P = \omega (D + \omega L)^{-1}$
- Symm. Gauß - Seidel - method \rightarrow
 $P = (D + R)^{-1} D (D + L)^{-1}$
- SSOR - method \rightarrow
 $P = \omega (2 - \omega) (D + \omega R)^{-1} D (D + \omega L)^{-1}$

Advantages:

- No additional storage requirements
- No calculations
- often good acceleration of the convergence

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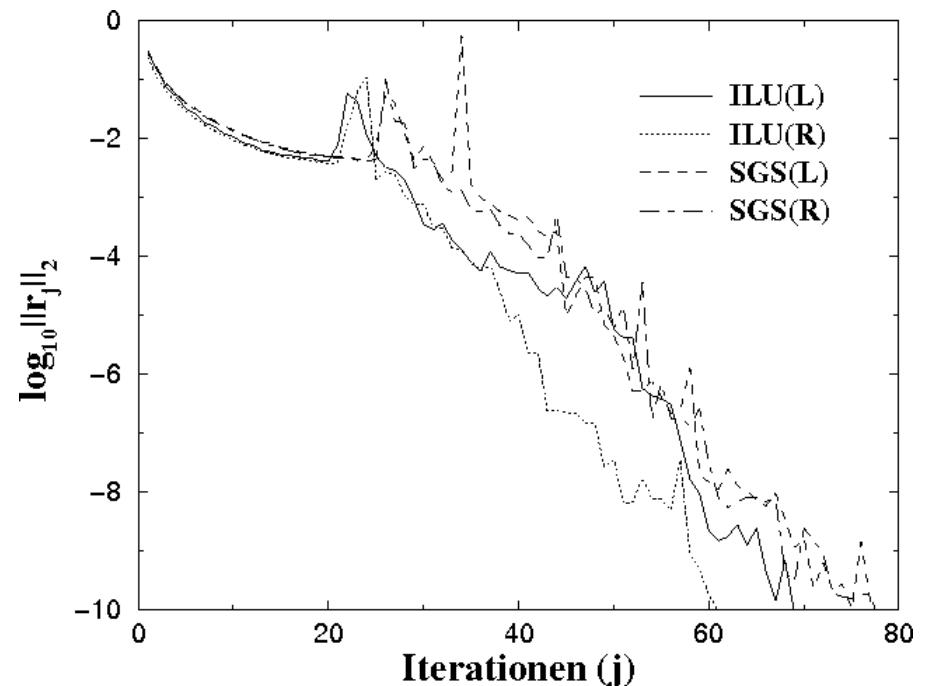
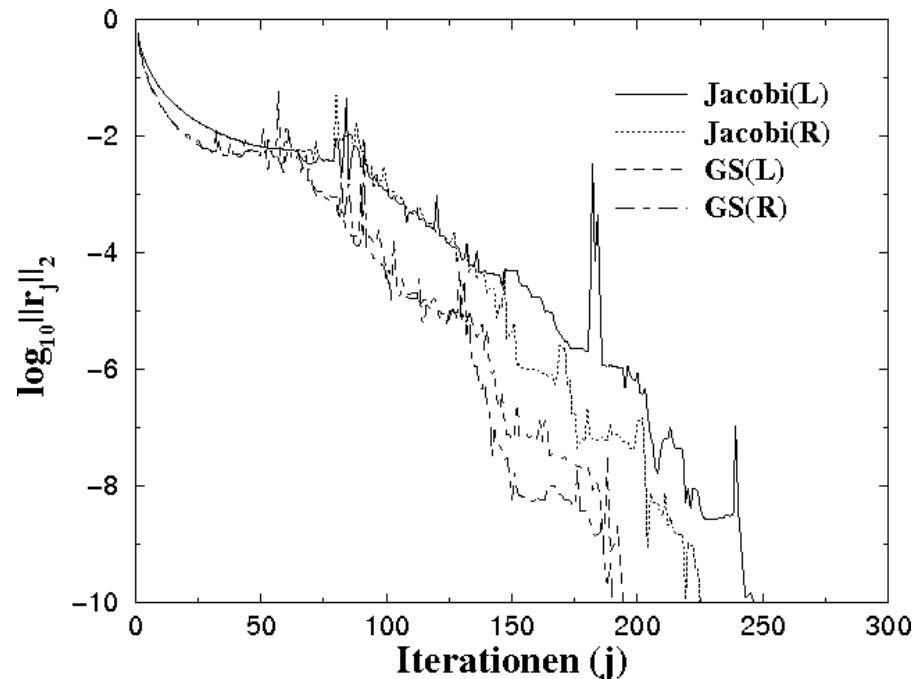
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Results of Splitting-associated preconditioner

- L/R: Left/Right Preconditioning



- Iterative Solution Method: BiCGSTAB

Incomplete LU-Factorization

Standard Gaussian elimination yields $A = L \cdot R$

Problems w.r.t. large, sparse matrices:

- Huge computational effort and storage requirements
- Rounding errors

Idea:

- Calculate $A = L \cdot R + F$, with
 - $r_{ii} = 1, i = 1, \dots, n$
 - $l_{ij} = r_{ij} = 0$, if $a_{ij} = 0$
 - $l_{ij} = r_{ji} = 0$, if $i < j$
 - $(L \cdot R)_{ij} = a_{ij}$, if $a_{ij} \neq 0$

Properties:

- $f_{ij} = 0$, if $a_{ij} \neq 0$
- Storage of A = Complete storage of L and R
- Low computational effort compared to standard Gaussian elimination

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Incomplete LU-Factorization

Procedure: $a_{ki} = (L \cdot R)_{ki}$ for $a_{ki} \neq 0$ directly yields

$$a_{ki} = \sum_{m=1}^n l_{km} r_{mi} \quad \begin{matrix} r_{mi}=0, m>i \\ = \end{matrix} \sum_{m=1}^i l_{km} r_{mi} \quad \begin{matrix} r_{ii}=1 \\ + \end{matrix} \sum_{m=1}^{i-1} l_{km} r_{mi} + l_{ki}$$

Concerning the i-th column of L one gets

$$l_{ki} = a_{ki} - \sum_{m=1}^{i-1} l_{km} r_{mi}, \quad k = i, \dots, n, \text{ mit } a_{ki} \neq 0$$

Analogously, the i-th row of R is given by

$$r_{ik} = \frac{1}{l_{ii}}(a_{ik} - \sum_{m=1}^{i-1} l_{im} r_{mk}), \quad k = i+1, \dots, n, \text{ mit } a_{ik} \neq 0$$

Preconditioner: $P = R^{-1} L^{-1}$

Advantage: Good improvement of the convergence

Disadvantage: Low additional computational effort
and storage requirements

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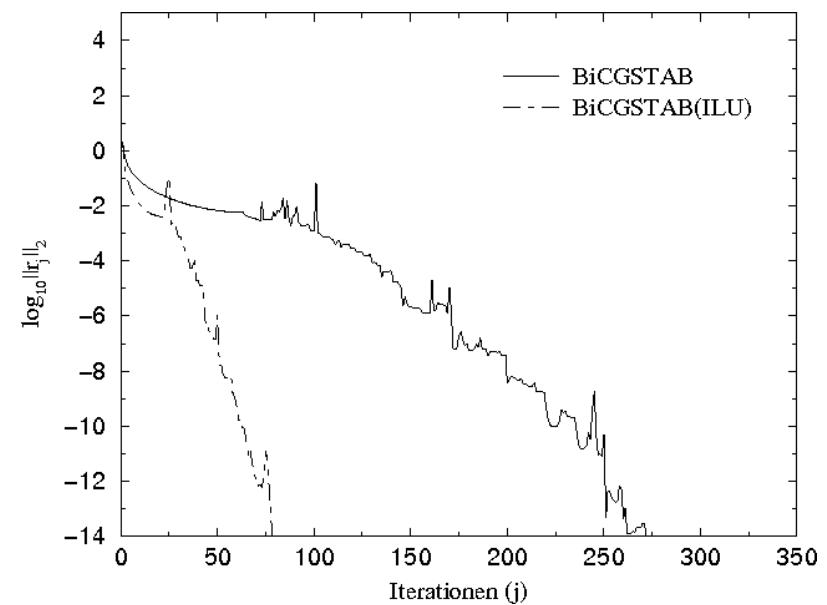
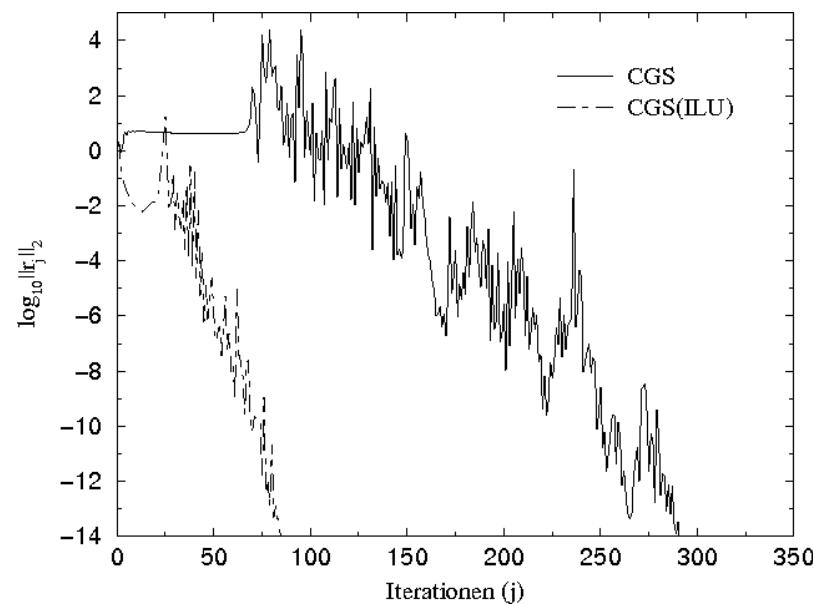
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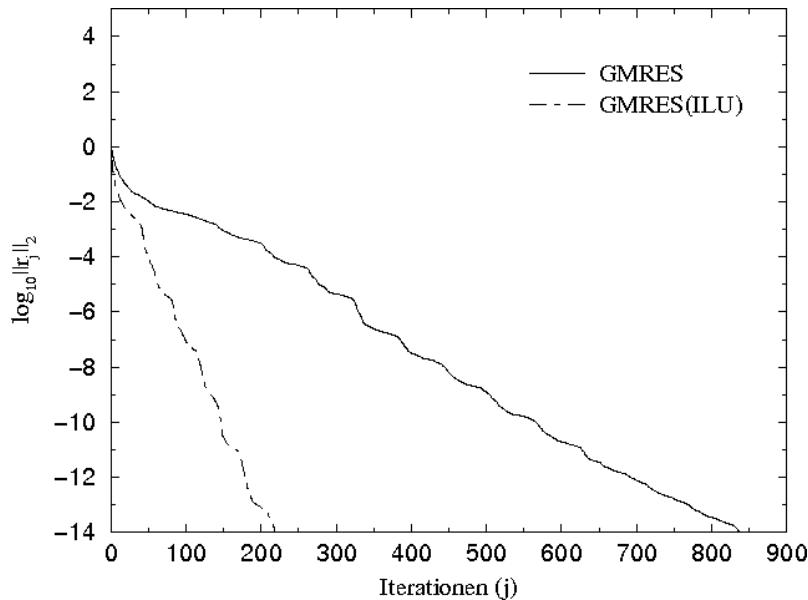
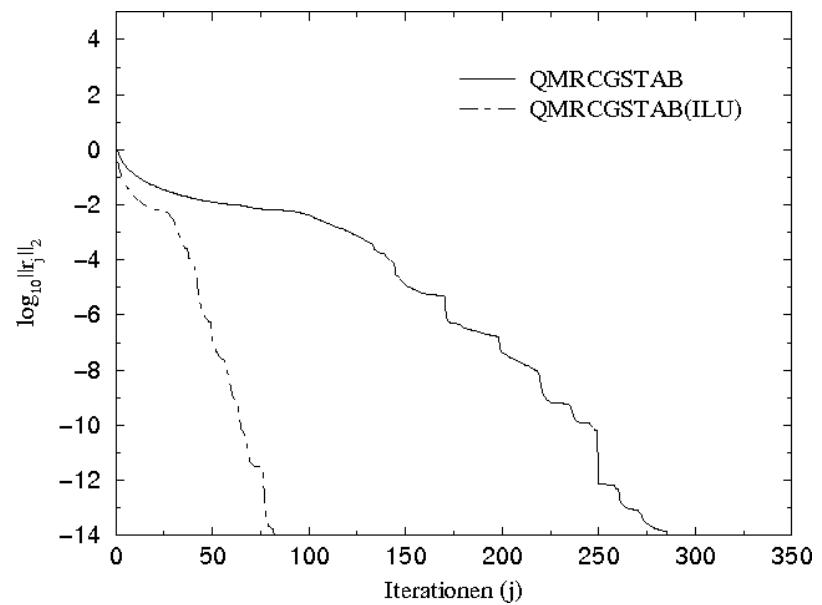
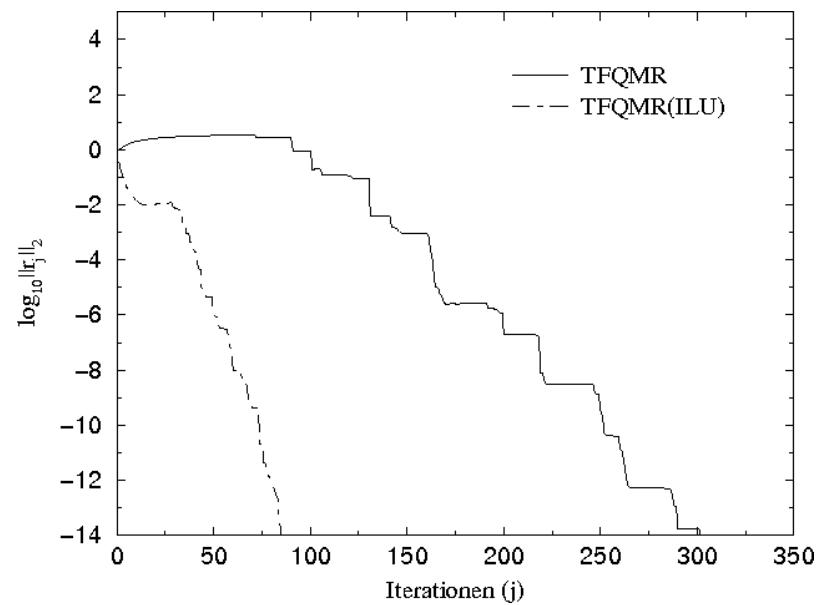
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Results of the ILU-Factorization

- L/R: Convection-Diffusion-Equation: $\epsilon = 0.01$



Results of the ILU-Factorization



Preconditioned CG-scheme (PCG)

Given: $A x = b$, where A symmetric, positive definite

Form of the PCG-scheme:

$$\underbrace{P_L A P_R}_{=A^p} x^p = P_L b$$
$$x = P_R x^p$$

Assumption concerning the applicability of CG:

A^p symmetric, positive definite

Preconditioned CG-scheme (PCG)

Proceeding:

Employ $P_R = P_L^T$ to obtain

$$\begin{aligned} \text{(a)} \quad (A^p)^T &= (P_L A P_L^T)^T = (P_L^T)^T A P_L^T \\ &= P_L A P_L^T = A^p \end{aligned}$$

→ A^p symmetric

(b) Since $y = P_L^T x \neq 0$ for all $x \neq 0$ one gets

$$\begin{aligned} (x, A^p x) &= x^T A^p x = x^T P_L A P_L^T x \\ &= (P_L^T x)^T A P_L^T x = y^T A y > 0 \end{aligned}$$

→ A^p positive definite

Preconditioners for PCG

Incomplete Cholesky-Factorization:

- Procedure is equivalent to the ILU approach
- Benefit from the symmetry of A
- Form

$$A = L L^T + F$$

- Symmetric Preconditioning

$$\begin{aligned} P_L A P_R x^p &= P_L b \\ x &= P_R x^p \end{aligned}$$

with

$$P_L = L^{-1} \text{ and } P_R = L^{-T}$$

Preconditioners for PCG

Symmetric Gauß-Seidel method:

- Classical splitting in terms of $A = L + D + R$
- Basic formulation of the preconditioner

$$P_{SGS} = (D + R)^{-1} D (D + L)^{-1}$$

- Principles of symmetric preconditioners

$$A \text{ symmetric} \implies D + R = D + L^T = (D + L)^T$$

$$A \text{ positive definite} \implies a_{ii} = (e_i, A e_i) > 0, \\ e_i = i\text{-th canonical basis vector}$$

$$\implies D = \text{diag}\{a_{11}, \dots, a_{nn}\} = D^{1/2} D^{1/2}$$

$$\text{with } D^{1/2} = \text{diag}\{a_{11}^{1/2}, \dots, a_{nn}^{1/2}\}$$

- Determination of the symmetric preconditioner

$$\begin{aligned} P_{SGS} &= (D + L)^{-T} D^{1/2} D^{1/2} (D + L)^{-1} \\ &= \underbrace{(D^{1/2} (D + L)^{-1})^T}_{P_L :=} \underbrace{D^{1/2} (D + L)^{-1}}_{P_R :=} = P_L P_R \end{aligned}$$

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Preconditioners in practical applications

Applications:

- Simulation of inviscid fluid flow
Euler equations
- Simulation of viscous fluid flow
Navier-Stokes equations

Numerical method:

- Finite-Volumen method using unstructured grids
- Implicit time integration scheme
 - Solution of a (non-)linear system of equations $Ax = b$ each timestep
 - Properties of the matrix $A \in \mathbb{R}^{nxn}$
 - large: $n \approx 10^4 - 10^6$
 - sparse ($\approx 0.1\%$)
 - unsymmetric
 - badly conditioned

BiNACA0012-profil

Ma= 0.55, Angle of attack 6°, inviscid,
Triangulation: 13577 points

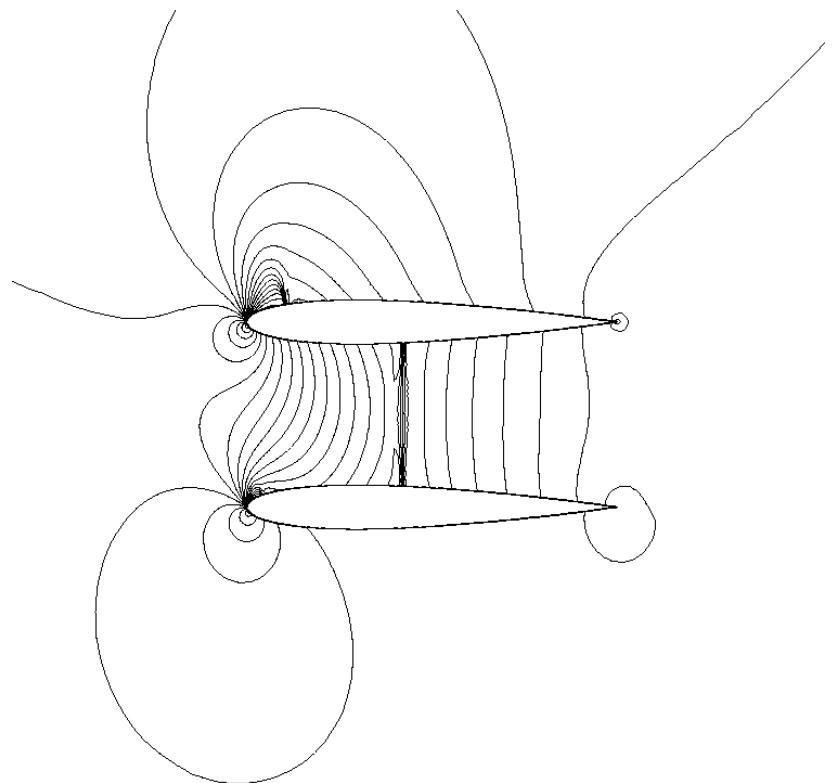
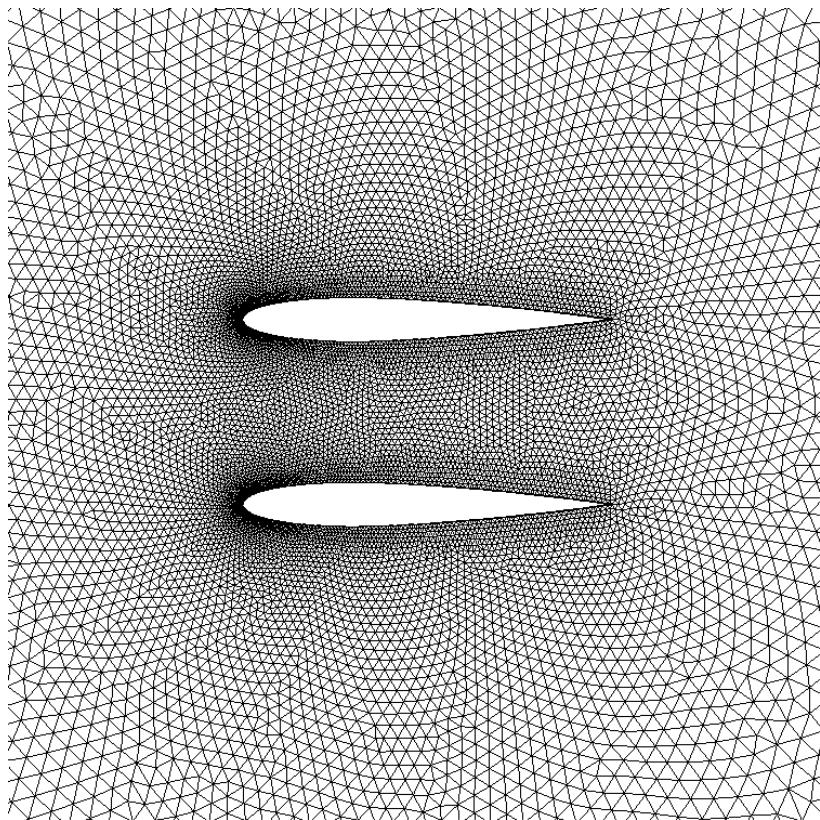
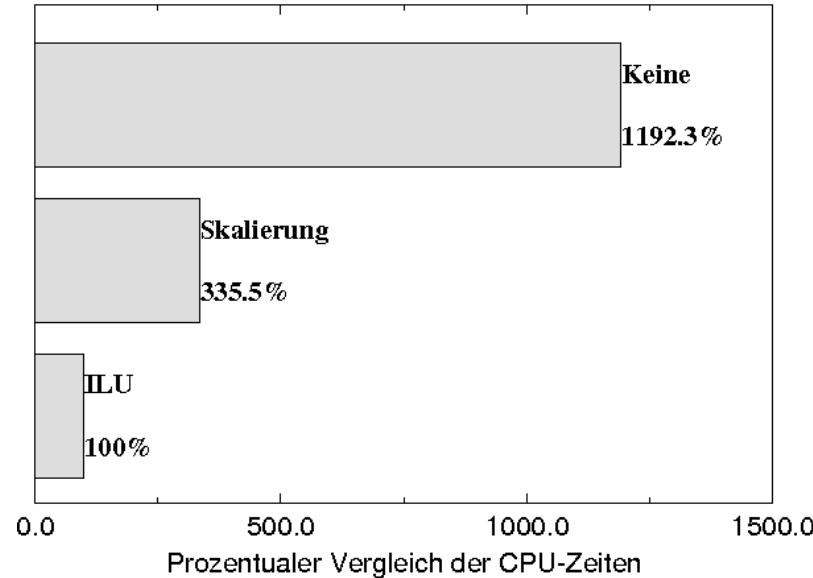


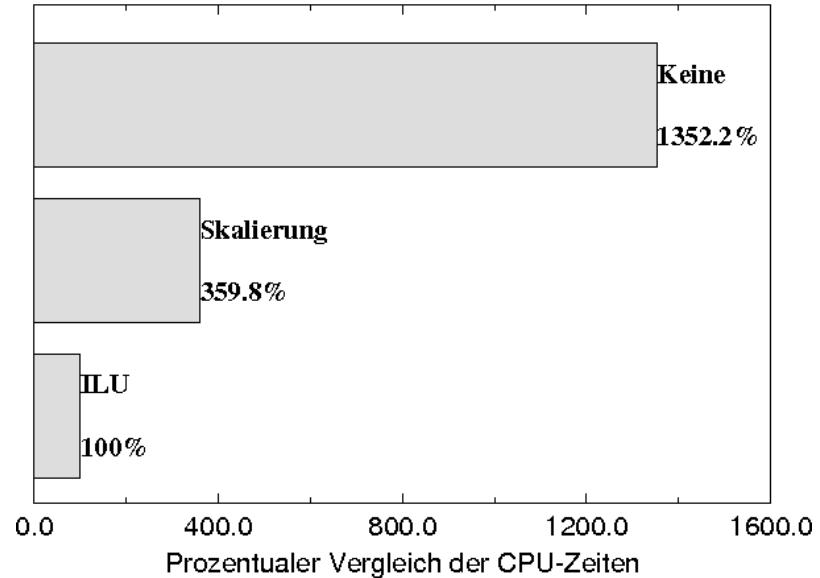
Fig.: Triangulation and isolines of the density distribution

BiNACA0012-profil

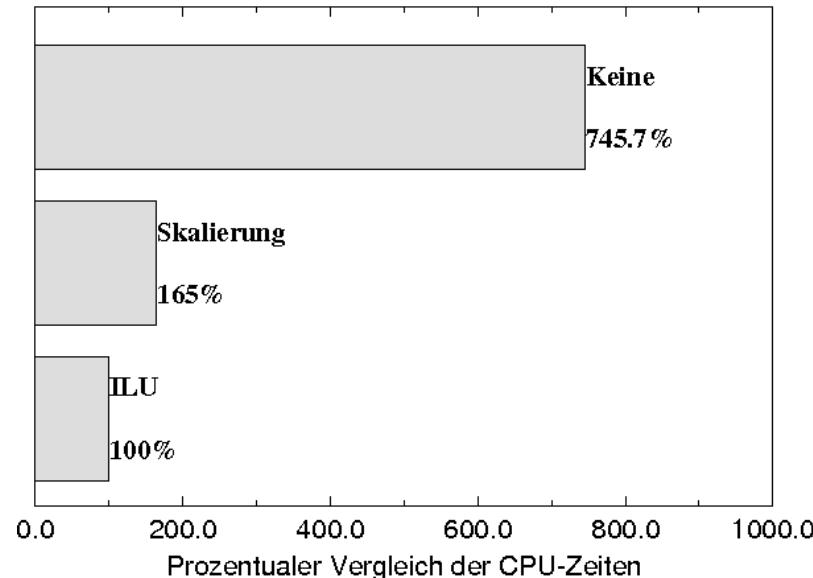
BiCGSTAB



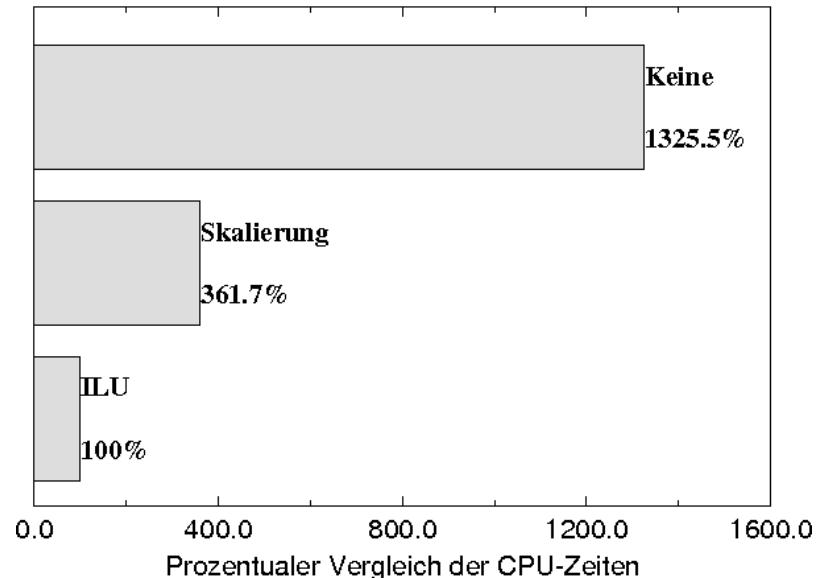
CGS



TFQMR



QMRCGSTAB



NACA0012-profil

$Re = 500$, $Ma = 0.85$, Angle of attack 0° , Triangulation: 8742 points

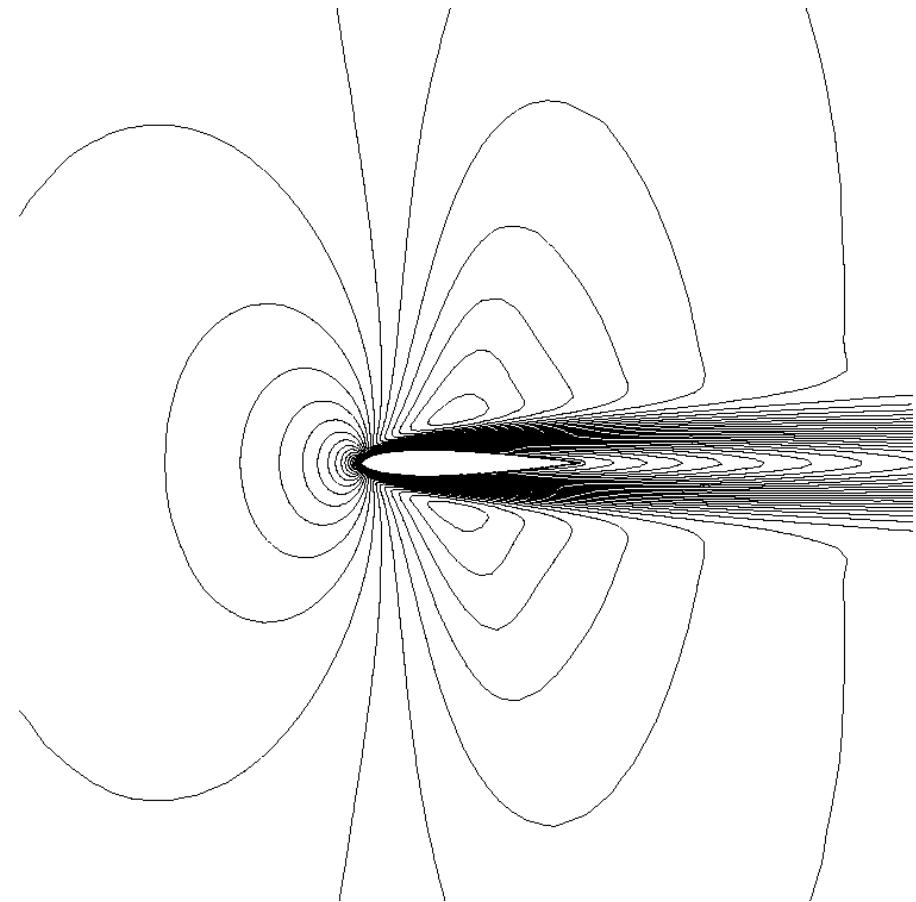
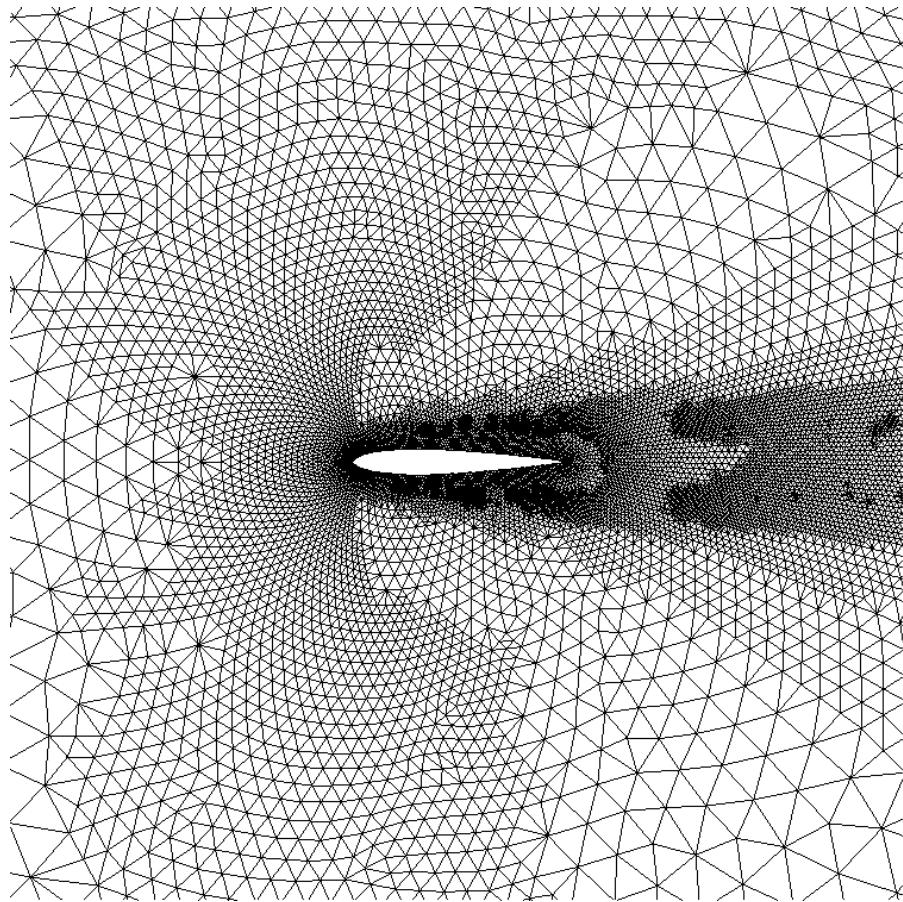
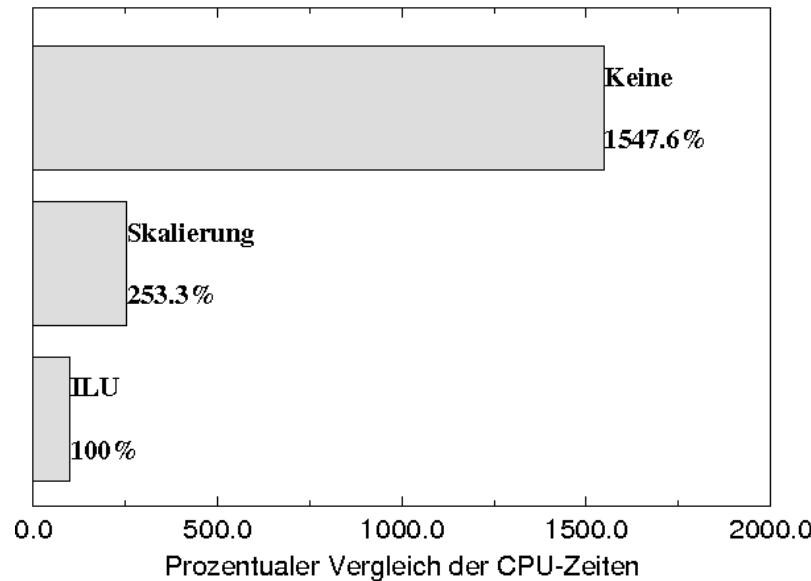


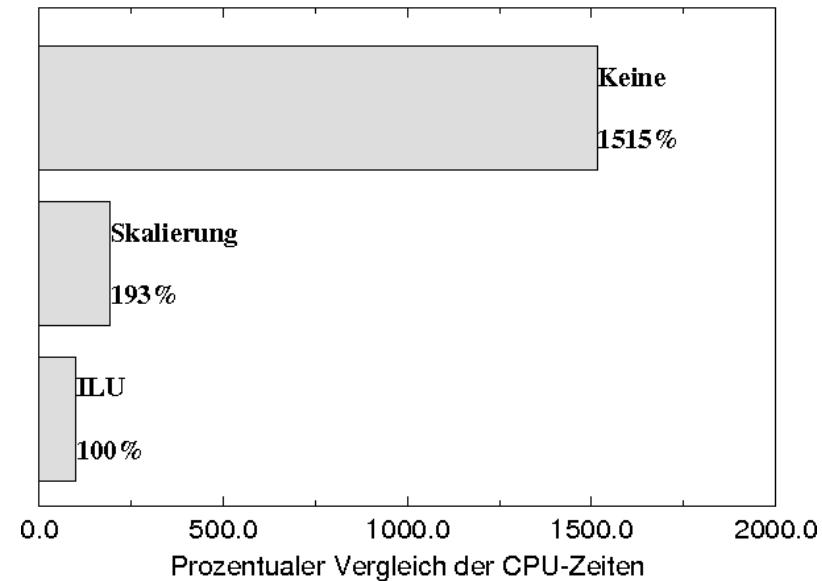
Fig.: Triangulation and isolines of the Mach number distribution

NACA0012-profil

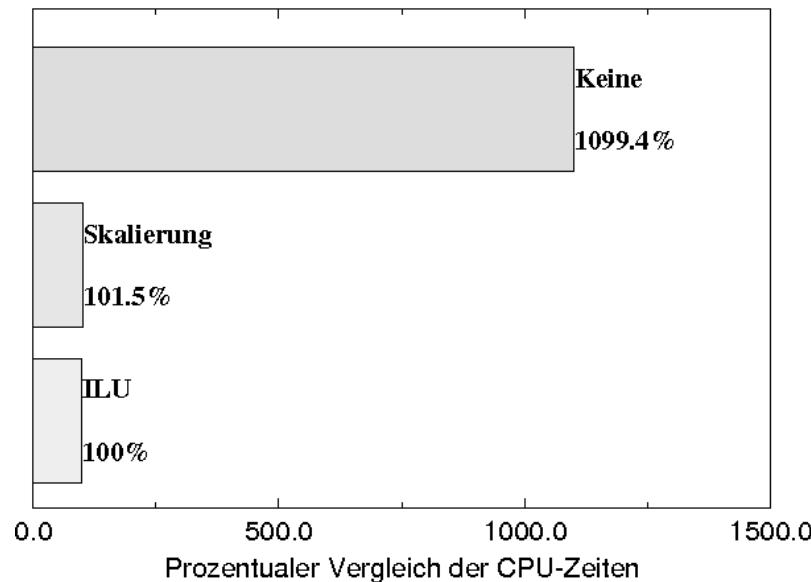
BiCGSTAB



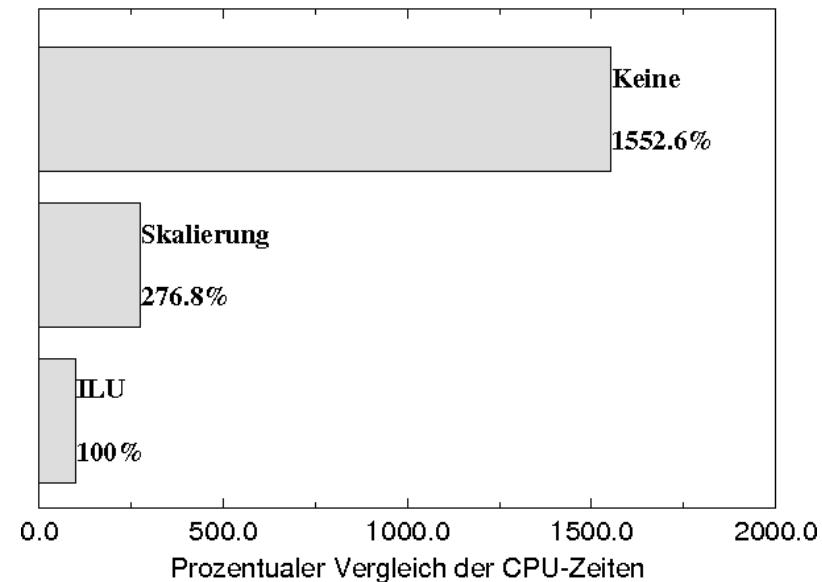
CGS



TFQMR



QMRCGSTAB



Laminar flow about a flat plate

$Re = 6 \cdot 10^6$, $Ma = 5.0$, Angle of attack 0°

Triangulation: 7350 points

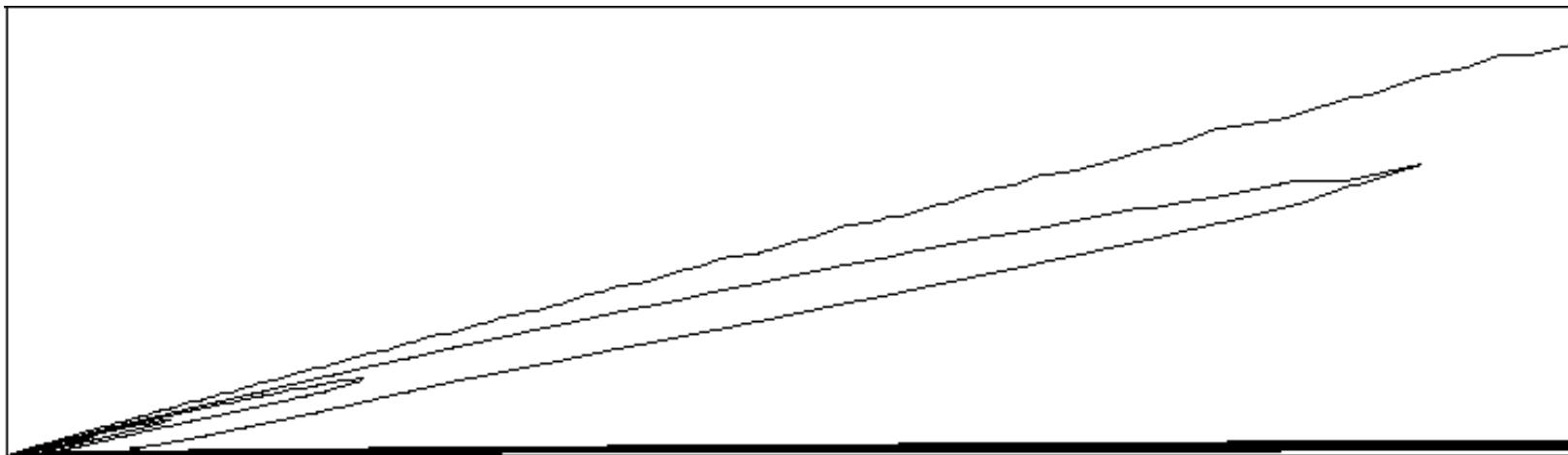
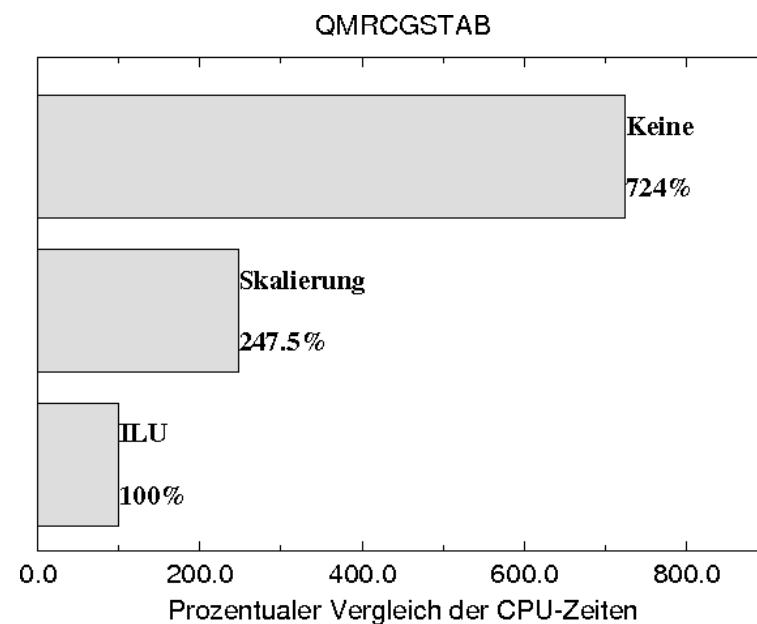
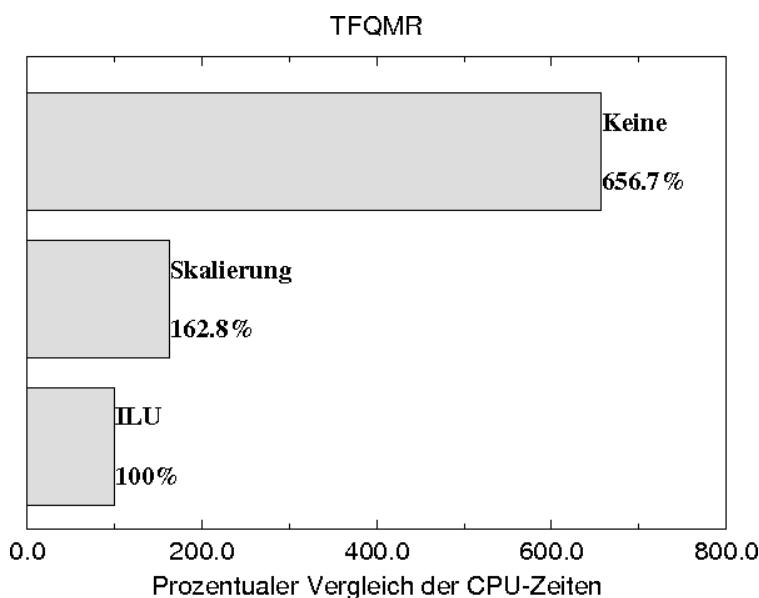
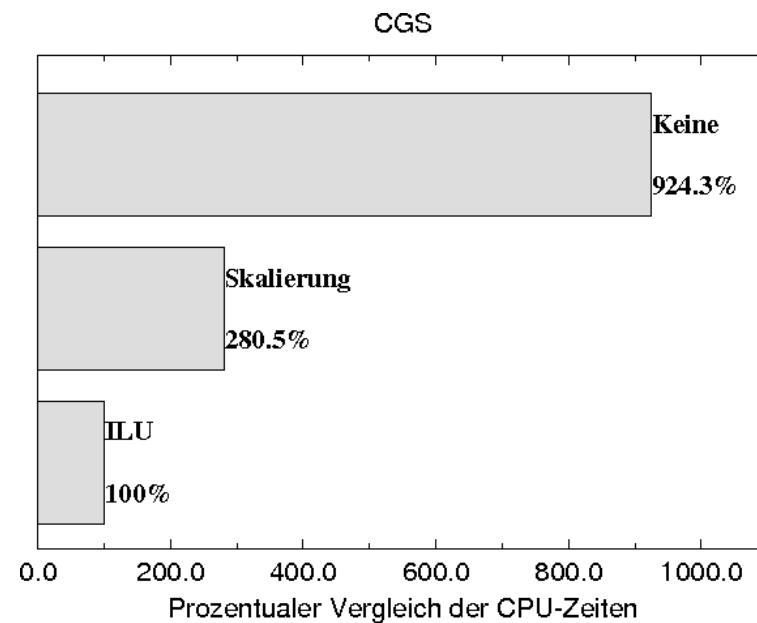
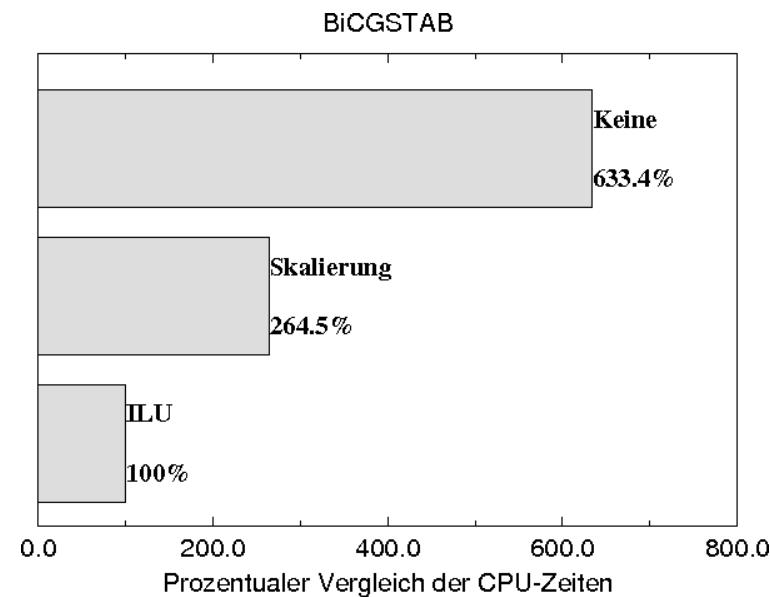


Fig.: Isolines of the Mach number distribution

Laminar flow about a flat plate



RAE 2822-profil

Ma= 0.75, Angle of attack 3°, inviscid

Triangulation: 9974 triangles, 5071 points

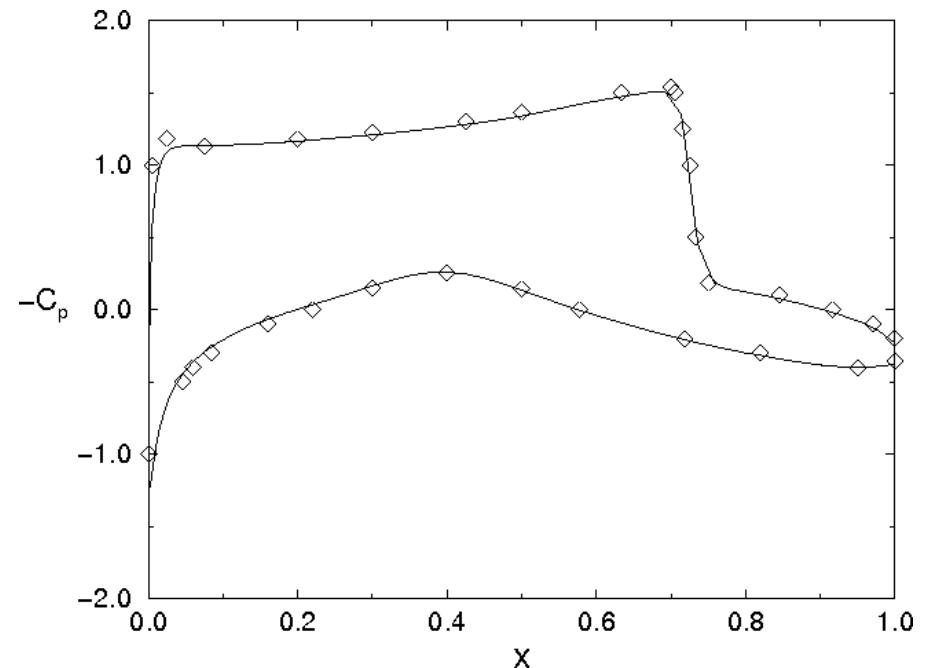
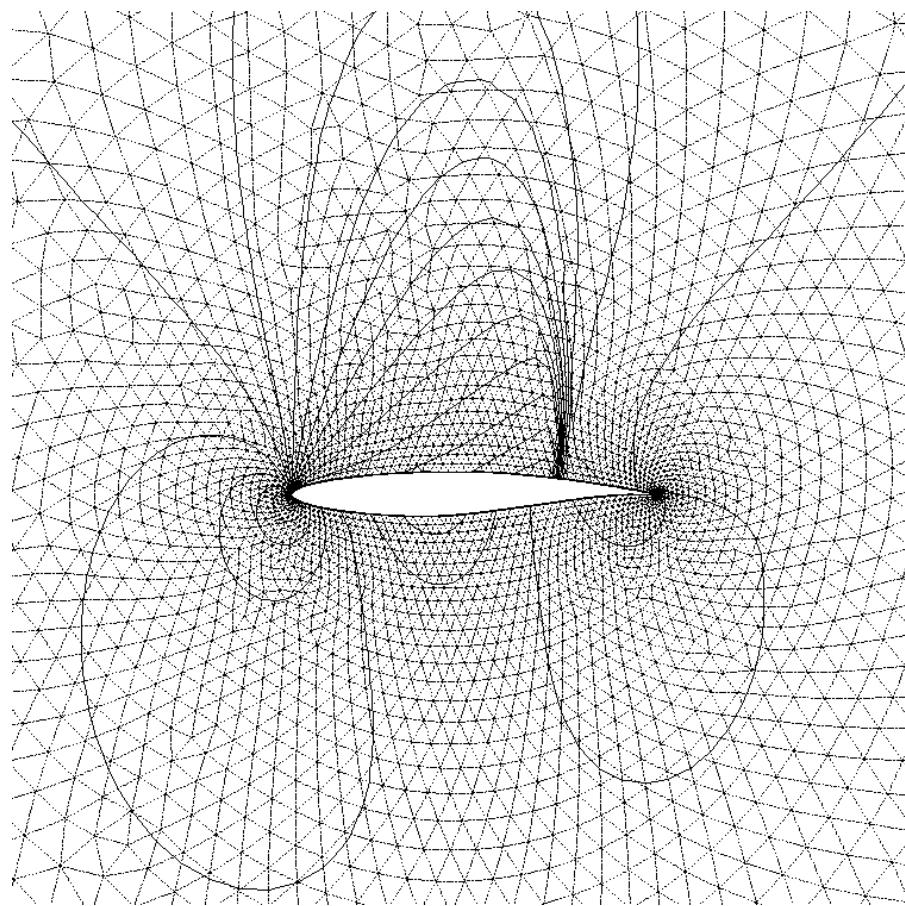


Fig.: Density and C_p -distribution

Explicit scheme	Implicit scheme	
	Scaling	Incomplete LU(5)
3497%	852%	100%

Tab.: Percentage comparison of the CPU-time

Ma= 0.65, Angle of attack 3°, inviscid
Triangulation: 46914 triangles, 23751 points

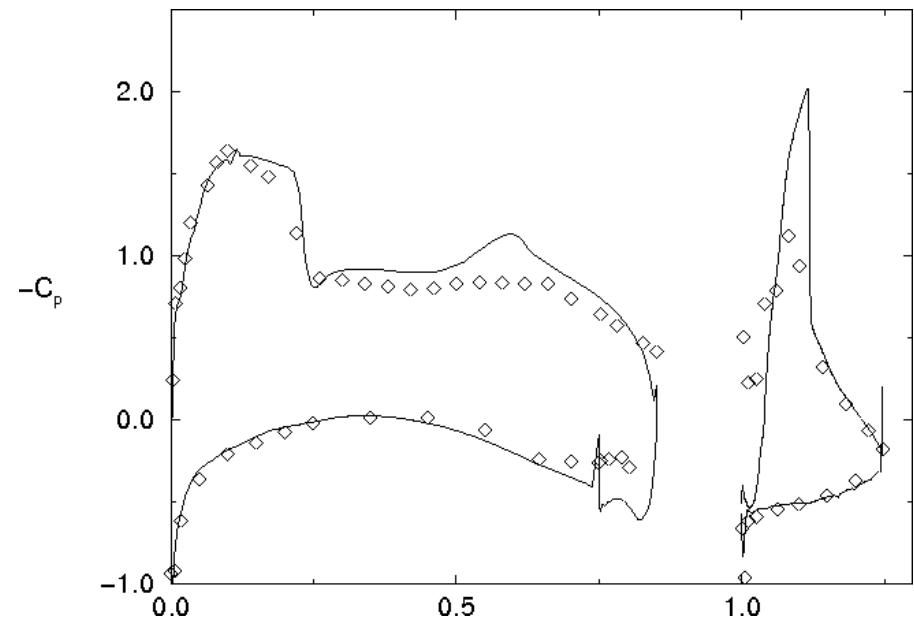
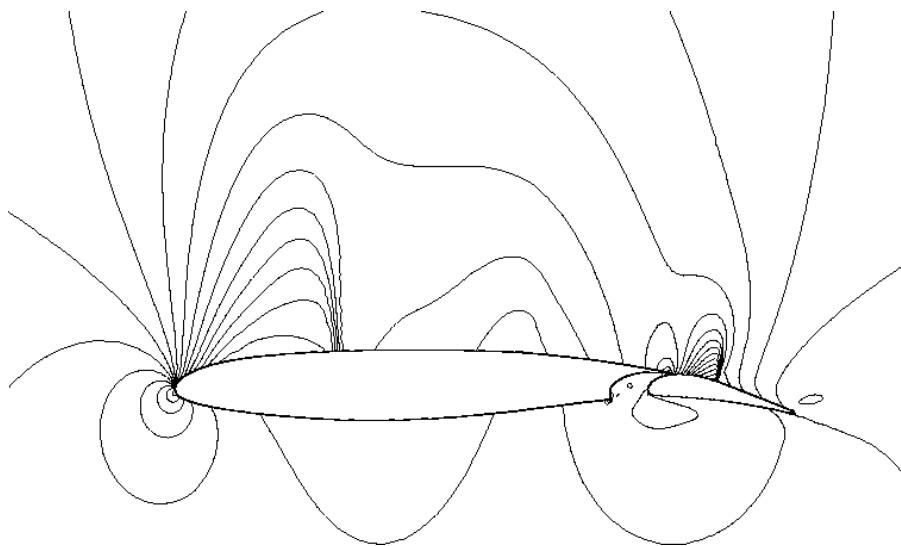


Fig.: Density and C_p -distribution

Explicit scheme	Implicit scheme	
	Scaling	Incomplete LU(5)
1003%	688%	100%

Tab.: Percentage comparison of the CPU-time

Summary

Preconditioning: General procedure

$$A x = b \iff \begin{cases} P_L A P_R y = P_L b \\ x = P_R y \end{cases}$$

Goal: Convergence acceleration and stabilization

Alternatives:

- Scaling
- Splitting-associated preconditioners (Gauß-Seidel, SOR, ...)
- Incomplete Factorization (ILU, IC)

PCG-scheme:

- $P_R = P_L^T \implies P_L A P_R$ symm. pos. def., if A symm. pos. def.
- Symmetric Gauß-Seidel-scheme, IC

Results for FVM: Acceleration up to a factor of 10 by using ILU

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