Iteratieve methoden

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Inhoud

1. Iteratieve methoden
2. Preconditioneringen
3. Deflatie
4. Parallelle methoden

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1. Iteratieve methoden

LSQR	Paige and Saunders
GMRES	Saad and Schultz
CGS	Sonneveld
Bi-CGSTAB	Van der Vorst and Sonneveld

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1. Iteratieve methoden

LSQR	Paige and Saunders
GMRES	Saad and Schultz
CGS	Sonneveld
Bi-CGSTAB	Van der Vorst and Sonneveld
GCR	Eisenstat, Elman and Schultz
GMRESR	Van der Vorst and Vuik

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GCR and GMRESR

Preconditioned GCR

$k = 0,\ r_0 = b - Ax_0$

while $\|r_k\|_2 > \varepsilon$ **do**

  $k = k + 1$, solve $Ms_k = r_k$

  $v_k = As_k$

  for $j = 1, \ldots k - 1$ **do**

    $\alpha = (v_k, v_j), v_k = v_k - \alpha v_j, s_k = s_k - \alpha s_j$

  end

  $v_k = v_k / \|v_k\|_2, s_k = s_k / \|v_k\|_2$

  $x_k = x_{k-1} + (r_{k-1}, v_k) s_k$

  $r_k = r_{k-1} - (r_{k-1}, v_k) v_k$

end while

GCR and GMRESR

Preconditioned GMRESR

$k = 0,\ r_0 = b - Ax_0$

while $\|r_k\|_2 > \varepsilon$ **do**

$k = k + 1$, solve with GMRES(m): $AMs_k = r_k$

$v_k = As_k$

for $j = 1, \ldots k - 1$ **do**

$\alpha = (v_k, v_j), v_k = v_k - \alpha v_j, s_k = s_k - \alpha s_j$

end

$v_k = v_k / \|v_k\|_2, s_k = s_k / \|v_k\|_2$

$x_k = x_{k-1} + (r_{k-1}, v_k) s_k$

$r_k = r_{k-1} - (r_{k-1}, v_k) v_k$

end while

Preconditioneringen

- Standaard iteratieve methoden
- Multigrid
- ILU
  - ordening
  - fill in
  - lumping
  - blok varianten
- Sparse Approximate Inverse

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Toepassingen

- Poisson op een vierkant met EDM

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- Poisson: EEM, EVM, gebied, randvoorwaarden, coëfficiënten
- Convectie-diffusie

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- Ontkoppelde Navier-Stokes
- Gekoppelde Navier-Stokes

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- Poisson op een vierkant met EDM
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- Convectie-diffusie
- Ontkoppelde Navier-Stokes
- Gekoppelde Navier-Stokes
- Mechanica problemen
- Helmholtz/Maxwell problemen
- . . .

2. Preconditioneringen

If A is SPD the Choleski decomposition LL^T exists.
Only the lower triangular part of A is stored in memory.

Incomplete Choleski (IC) decomposition

Compute L which satisfies:

- $l_{ij} = 0$ for $a_{ij} = 0$ and $i > j$
- $(LL^T)_{ij} = a_{ij}$ for $a_{ij} \neq 0$ and $i \geq j$

This preconditioner exists if A is an M-matrix.

$$a_{ij} \leq 0, \;\; j \neq i \text{ and } A^{-1} \geq 0.$$

Break down IC preconditioner

Suppose A is not an M-matrix.

$$l_{ii}^2 = a_{ii} - \sum_{j=1}^{i-1} l_{ij}^2$$

Break down when right-hand side is negative.

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Break down when right-hand side is negative.

Typical examples

- large convection and central differences
- linear elements with bad triangles
- quadratic elements
- coupled problems: mechanical problems, Navier-Stokes

Solution strategies

1. Use LDL^T and MINRES
2. Replace right-hand side by a small positive number ($a_{ii}/100$)
3. Use IC of $A + \gamma I$ or $A + \gamma\text{diag}(A)$ with a suitable chosen $\gamma > 0$.
4. Construct $\hat{A}$ such that $\hat{A} \approx A$ and $\hat{A}$ is an M-matrix. Use IC of $\hat{A}$.

Lumped IC preconditioners

Suppose A is SPD but not an M-matrix. Construct $\hat{A}$ as follows:

for $i = 1, n$
  $\hat{a}_{ii} = a_{ii}$
  for $j = 1, i-1$
    if $a_{ij} < 0$ **then**
      $\hat{a}_{ij} = a_{ij}$
    else
      $\hat{a}_{ij} = 0$, $\hat{a}_{ii} = \hat{a}_{ii} + a_{ij}$, $\hat{a}_{jj} = \hat{a}_{jj} + a_{ij}$
    end if
  end for
end for

$\hat{A}$ is an M-matrix. Its IC decomposition exists and is used as a preconditioner for $Ax = b$.

Convection diffusion equation

- square domain, diffusion coefficient $\mathbb{D}$
- angle α, central scheme, 100×100 grid

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Convection diffusion equation

- square domain, diffusion coefficient $\mathbb{D}$
- angle α, central scheme, 100×100 grid

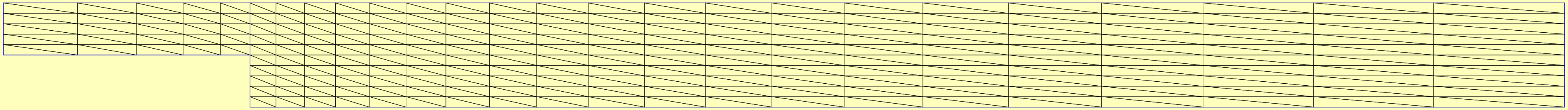
Number of matrix vector products angle is 45^o

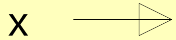
$\mathbb{D}$	Bi	Bi-CGSTAB	GMRES	GMRESR(10)
10^{-3}	42	8	7	7
10^{-4}	nc	52	48	47
10^{-5}	nc	392	207	189
10^{-6}	nc	nc	438	350
10^{-7}	nc	nc	$>$ 500	389

Convergence for lumped ILU is only weakly dependent on the angle

Backward Facing Step

Coupled Navier-Stokes problem





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Backward Facing Step

No convergence without lumping

Backward Facing Step

No convergence without lumping
Stokes

grid	Bi-CGSTAB matvec	CPU	GMRES matvec	CPU	GMRESR matvec	CPU
10×25	484	2.02	1293	6.16	315	1.77
20×50	1398	24.59	497	10.33	485	12.25

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Backward Facing Step

No convergence without lumping

Stokes

grid	Bi-CGSTAB matvec	CPU	GMRES matvec	CPU	GMRESR matvec	CPU
10×25	484	2.02	1293	6.16	315	1.77
20×50	1398	24.59	497	10.33	485	12.25

Navier-Stokes

grid	Bi-CGSTAB matvec	CPU	GMRES matvec	CPU	GMRESR matvec	CPU
10×25	2138	9.38	7828	37	2195	12.36
20×50	4592	85	11107	228	3895	98

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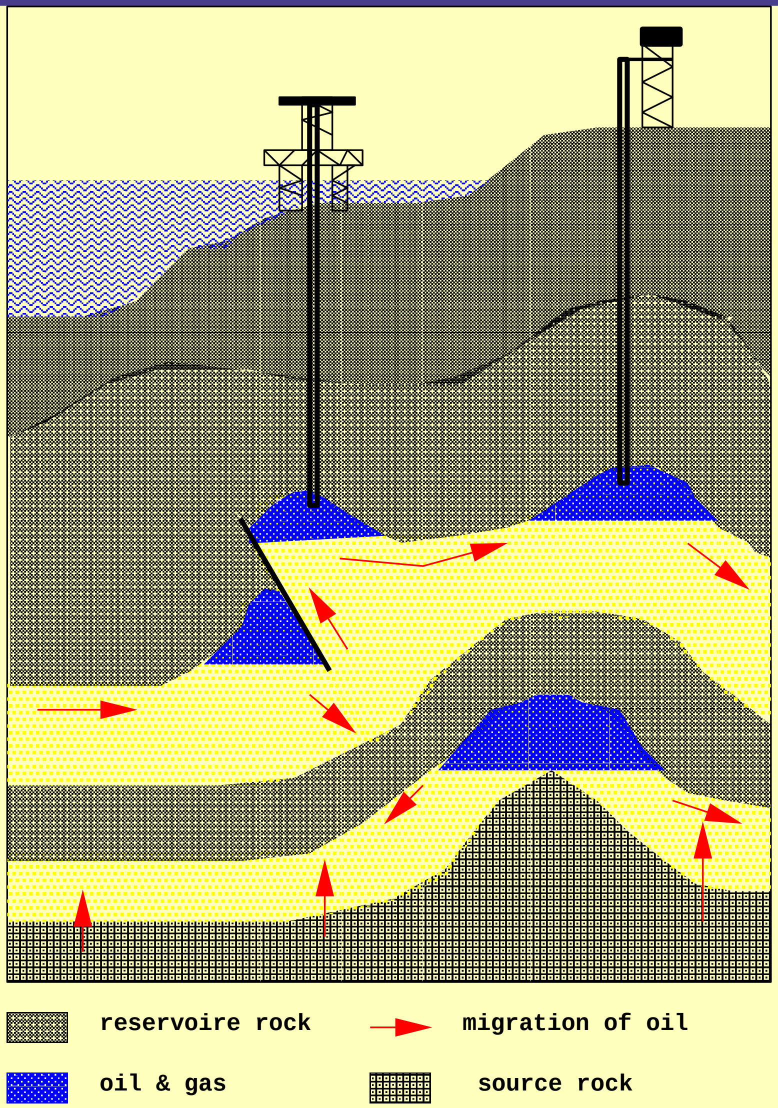
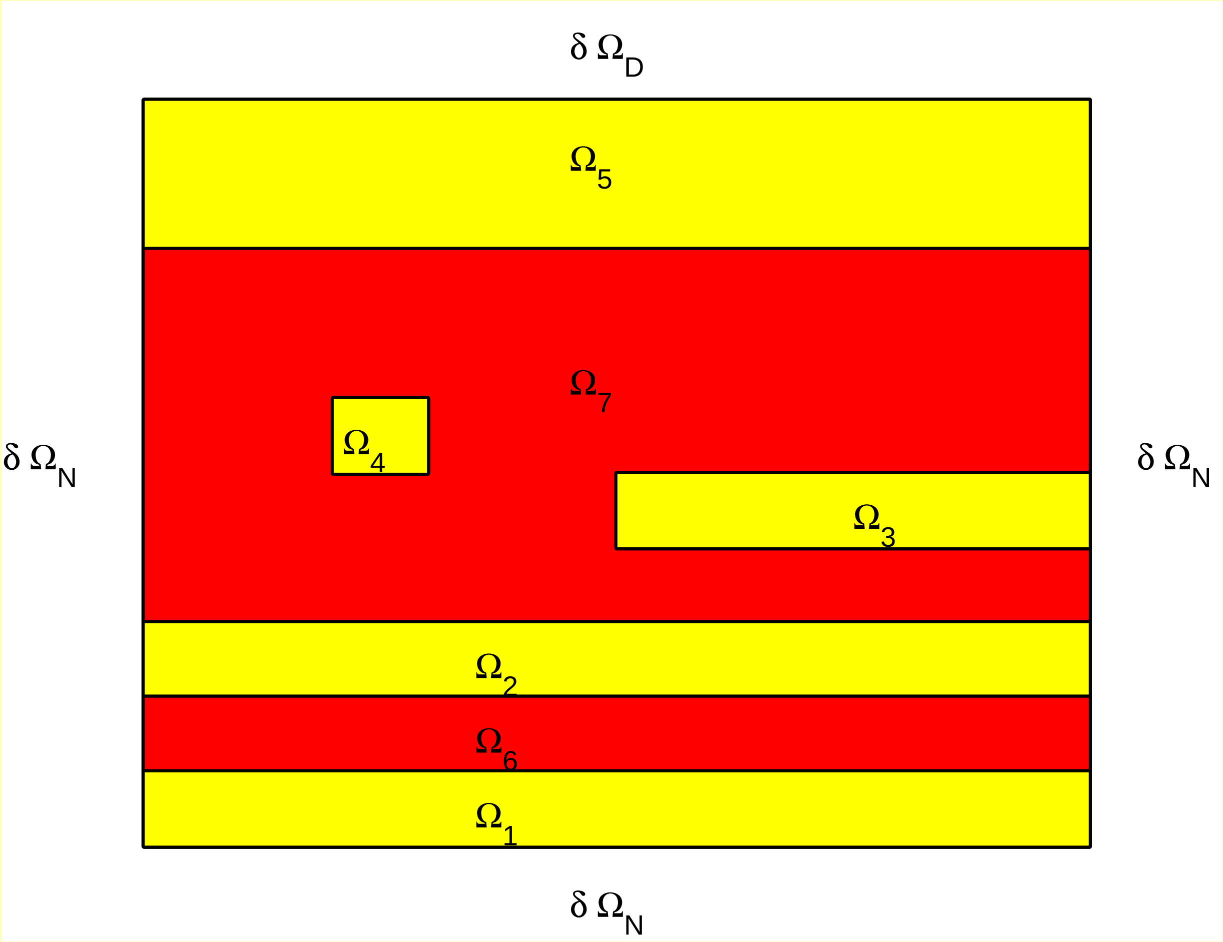
3. Deflatie



Mathematical model: computation of fluid pressure

$-\text{div}(\sigma \nabla p(x)) = 0$ on Ω, p fluid pressure, σ permeability



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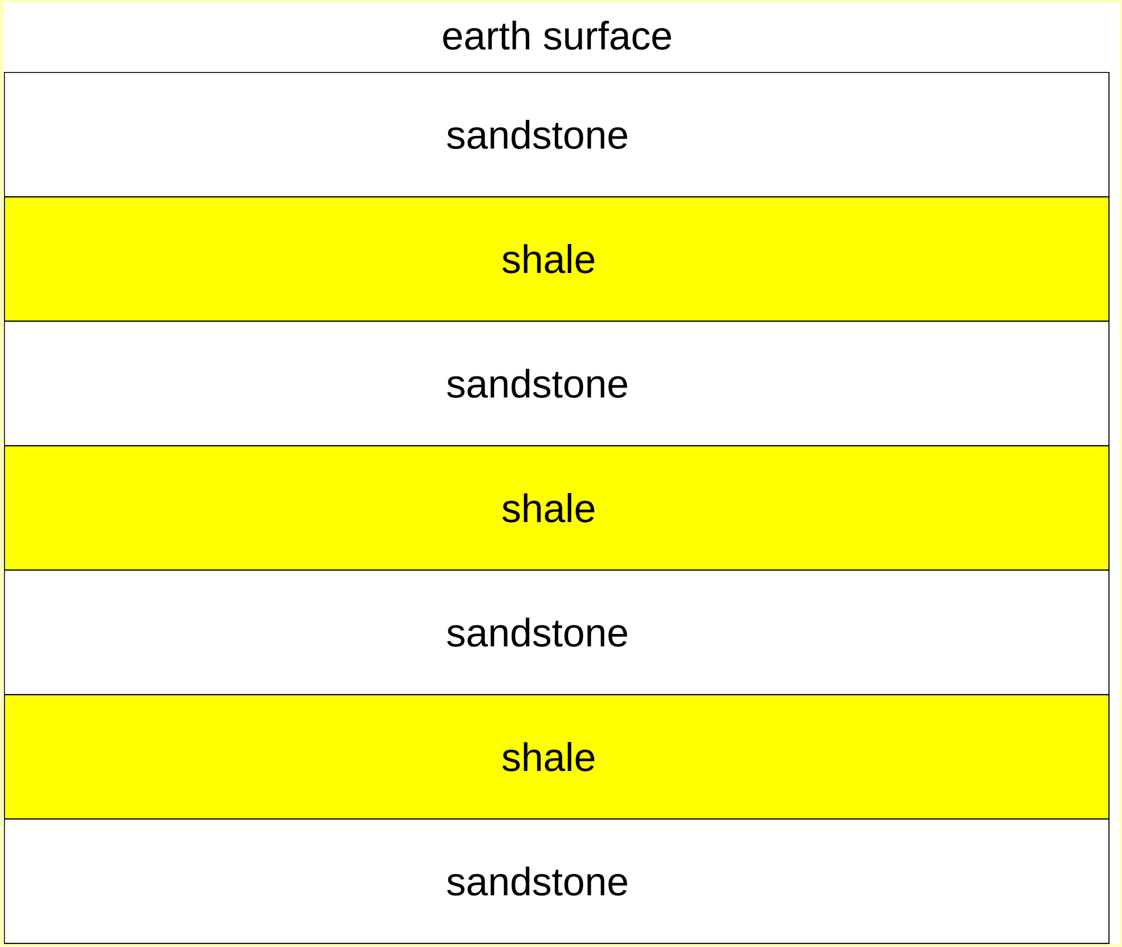
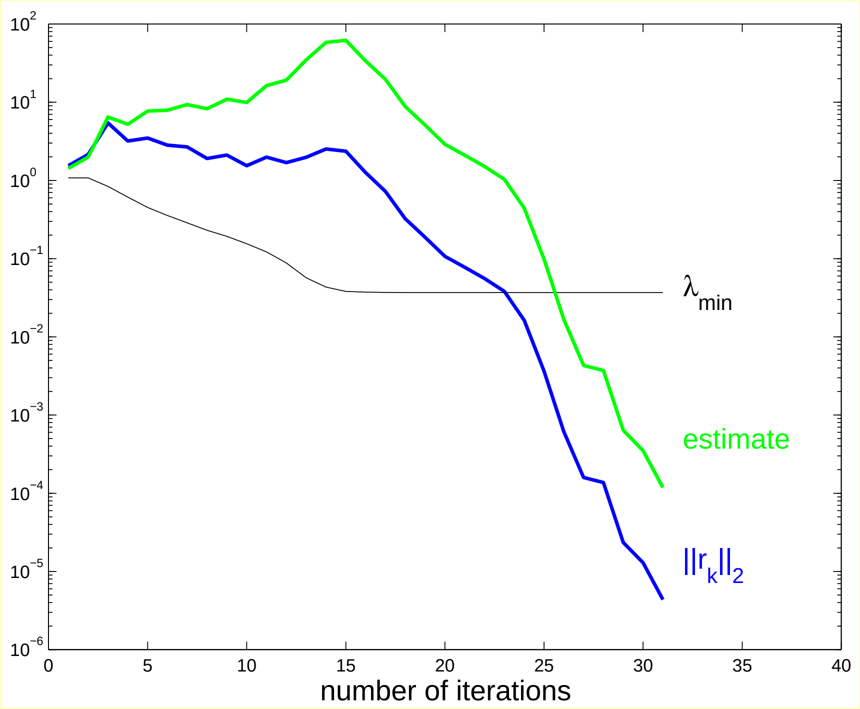
Test problem



Configuration with 7 straight layers

Convergence CG, without preconditioning



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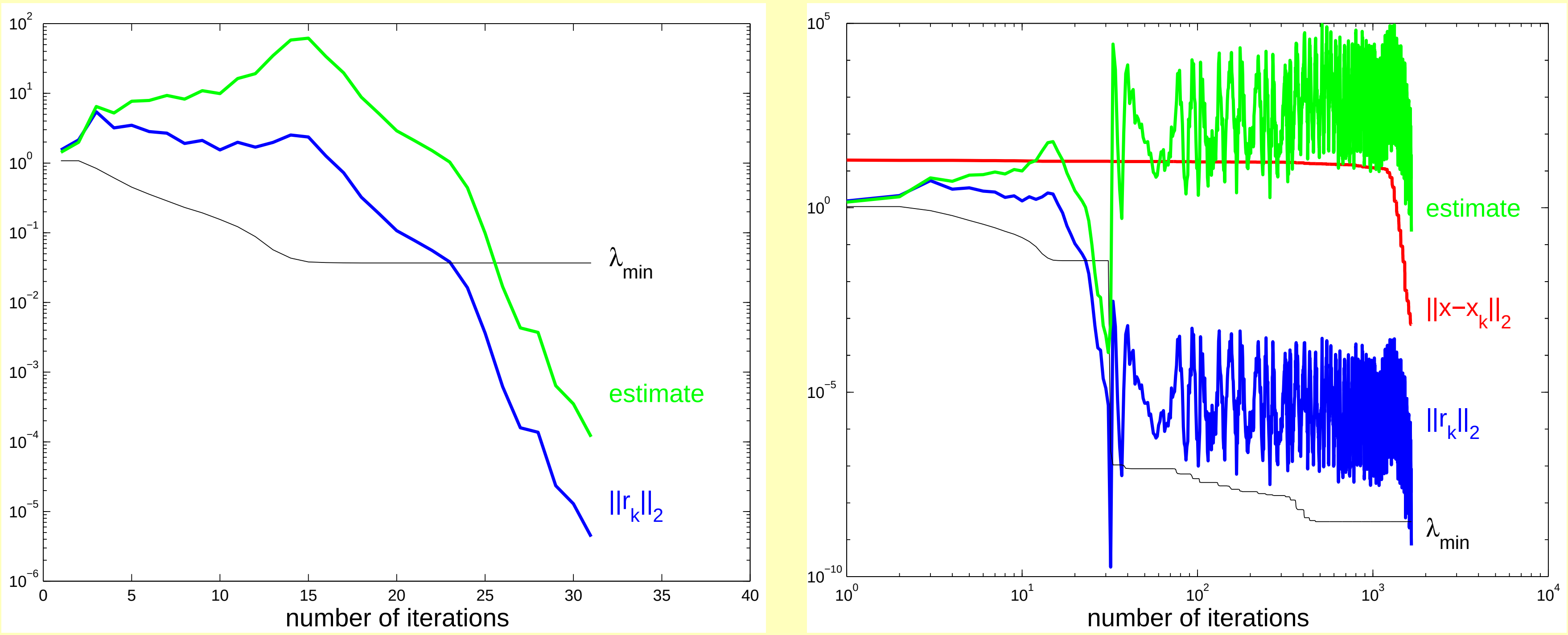
Convergence CG, without preconditioning



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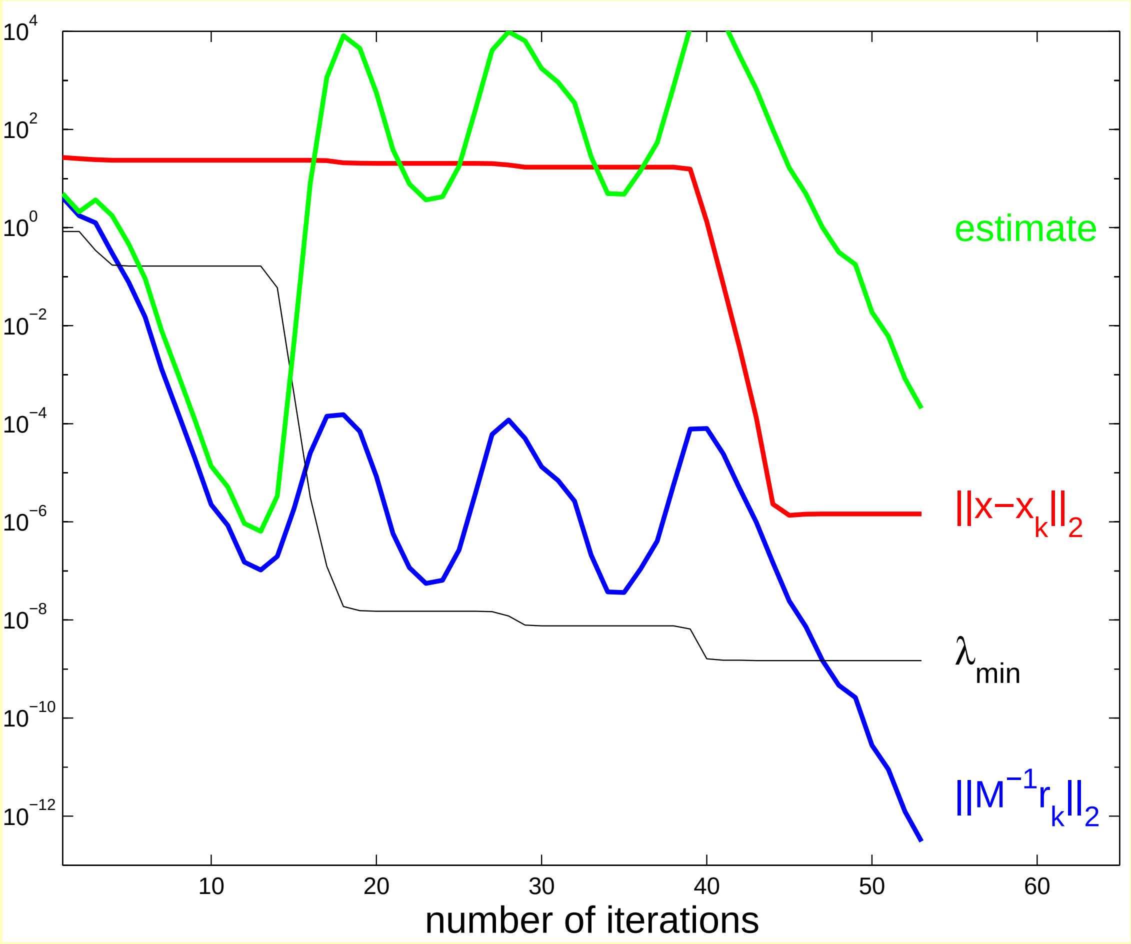
Convergence CG, with IC preconditioning



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Deflated ICCG

A is SPD, Conjugate Gradients

$$P = I - AZE^{-1}Z^T \text{ with } E = Z^T AZ$$

and $Z = [z_1 ... z_m]$, where $z_1, ..., z_m$ are independent deflation vectors.

Properties

1. $P^T Z = 0$ and $PAZ = 0$
2. $P^2 = P$
3. $AP^T = PA$

Deflated ICCG

$$x = (I - P^T)x + P^T x$$

$(I - P^T)x = ZE^{-1}Z^T Ax = ZE^{-1}Z^T b$ and $AP^T x = PAx = Pb$

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Deflated ICCG

$$x = (I - P^T)x + P^T x$$

$$(I - P^T)x = ZE^{-1}Z^T Ax = ZE^{-1}Z^T b \text{ and } AP^T x = PAx = Pb$$

DICCG

$k = 0,\ \hat{r}_0 = Pr_0,\ p_1 = z_1 = L^{-T}L^{-1}\hat{r}_0;$

while $\|\hat{r}_k\|_2 > \varepsilon$ **do**

$k = k + 1;$

$\alpha_k = \frac{(\hat{r}_{k-1}, z_{k-1})}{(p_k, PAp_k)};$

$x_k = x_{k-1} + \alpha_k p_k;$

$\hat{r}_k = \hat{r}_{k-1} - \alpha_k PAp_k;$

$z_k = L^{-T}L^{-1}\hat{r}_k;$

$\beta_k = \frac{(\hat{r}_k, z_k)}{(\hat{r}_{k-1}, z_{k-1})};$ $\qquad p_{k+1} = z_k + \beta_k p_k;$

end while

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Physical deflation vectors

k is number of subdomains

$\Omega_i, i = 1, ..., k^s$ high-permeability subdomains without a Dirichlet b.c.;
$i = k^s + 1, ..., k^h$ remaining high-permeability subdomains

- $z_i = 1$ on $\bar{\Omega}_i$ and $z_i = 0$ on $\bar{\Omega}_j, j \neq i,$
  $i \in \{1, ..., k^s\}$ and $j \in \{1, ..., k^h\}$
- z_i satisfies equation:

$$-\text{div}(\sigma_j \nabla z_i) = 0 \text{ on } \Omega_j, j \in \{k^h + 1, ..., k\},$$

  with appropriate boundary conditions

Sparse vectors, Subproblems are cheap to solve

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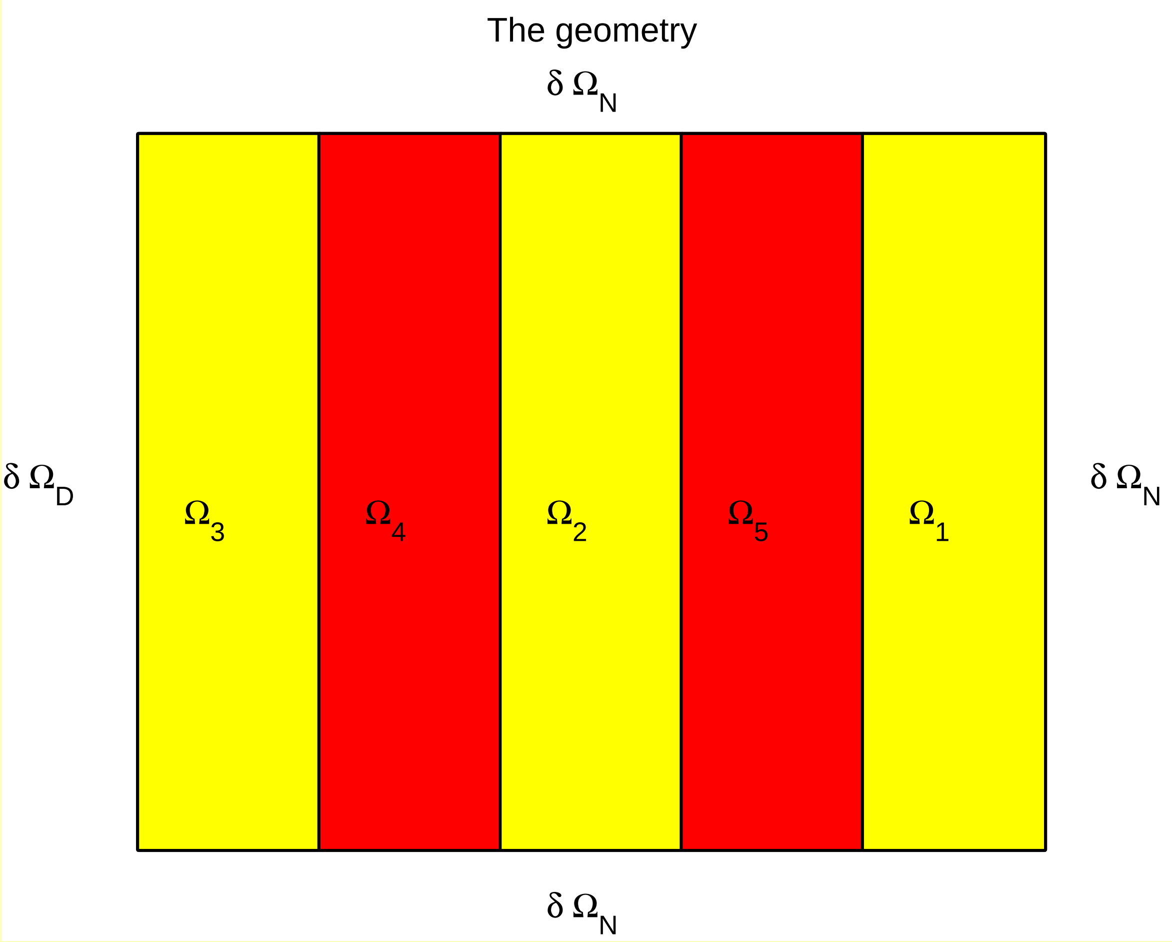
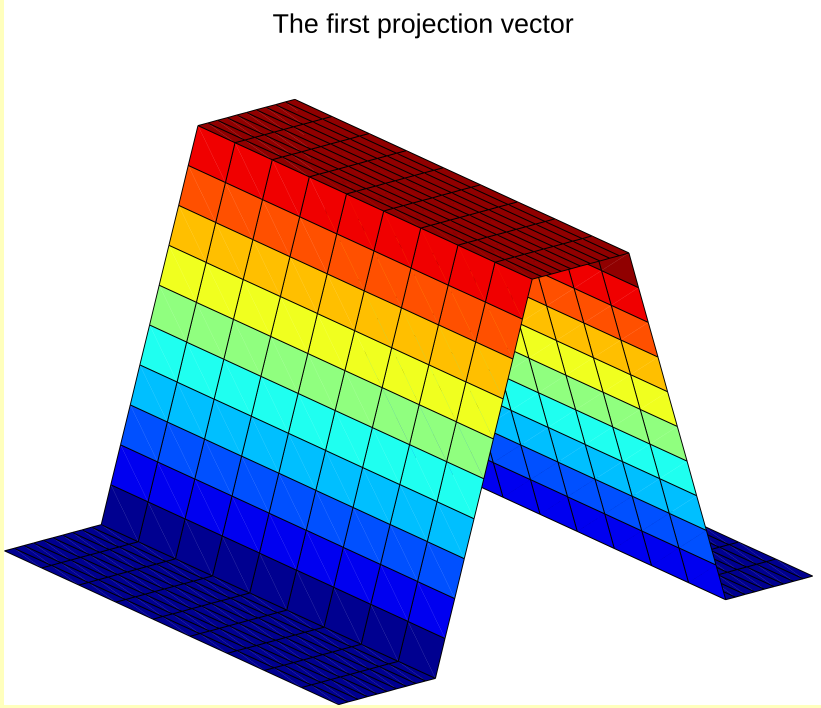
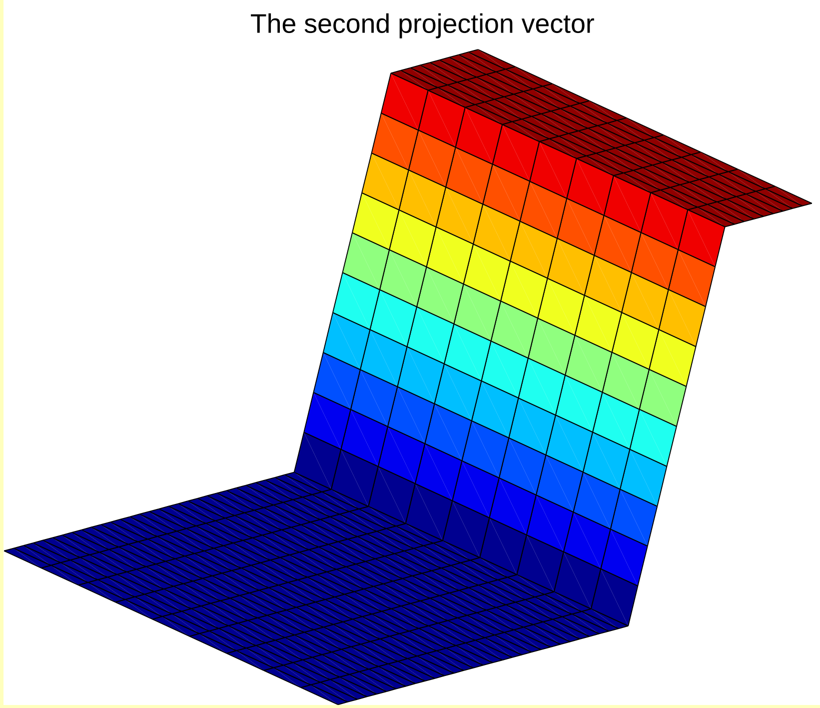
Physical deflation vectors



Physical deflation vectors





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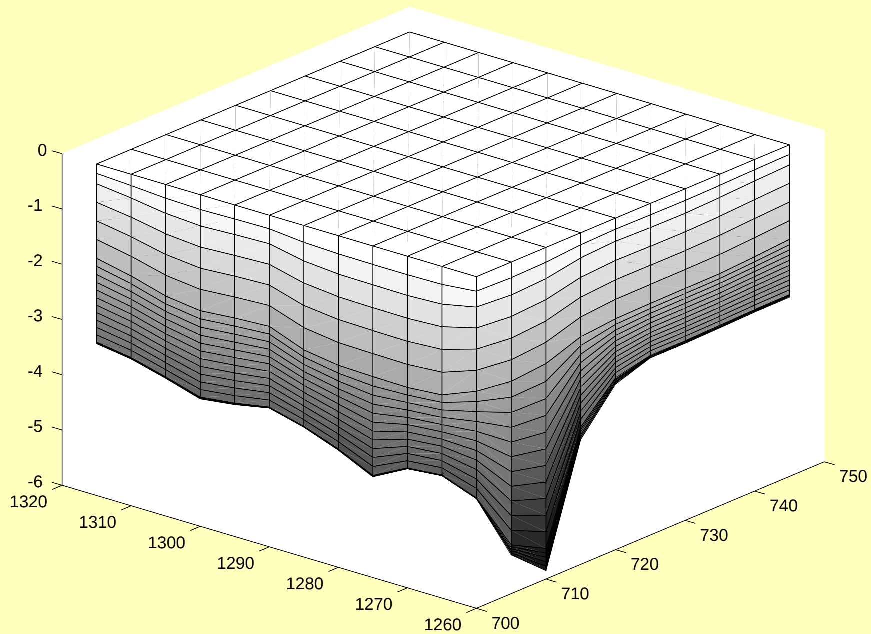
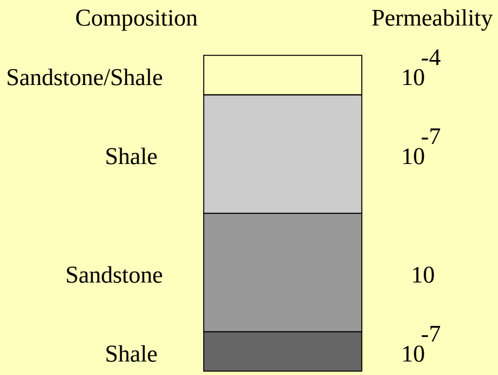
Geometry oil flow problem





A three-dimensional test problem

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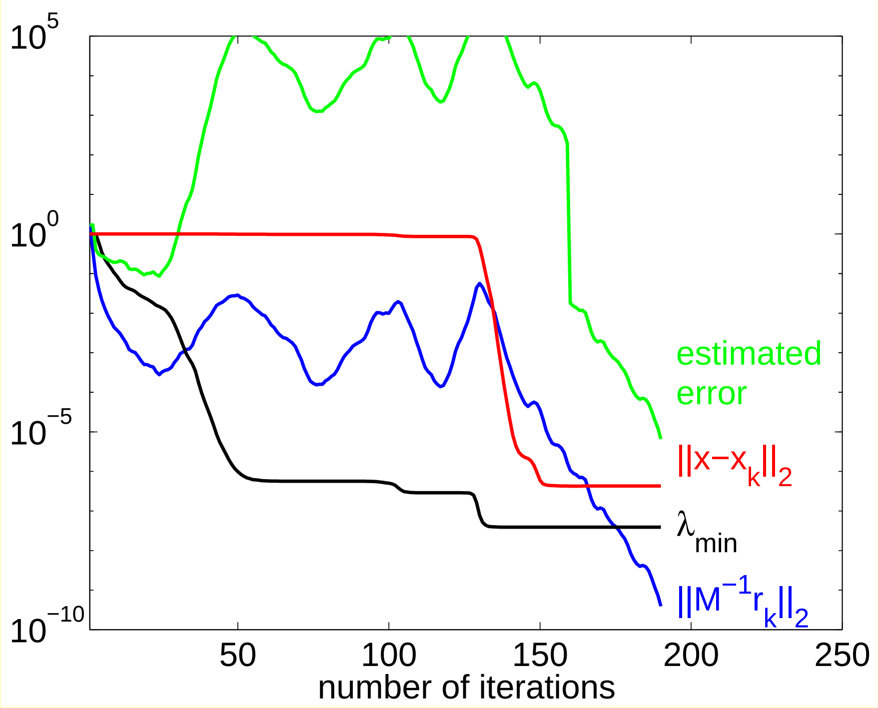
Results oil flow problem

The convergence behavior for ICCG



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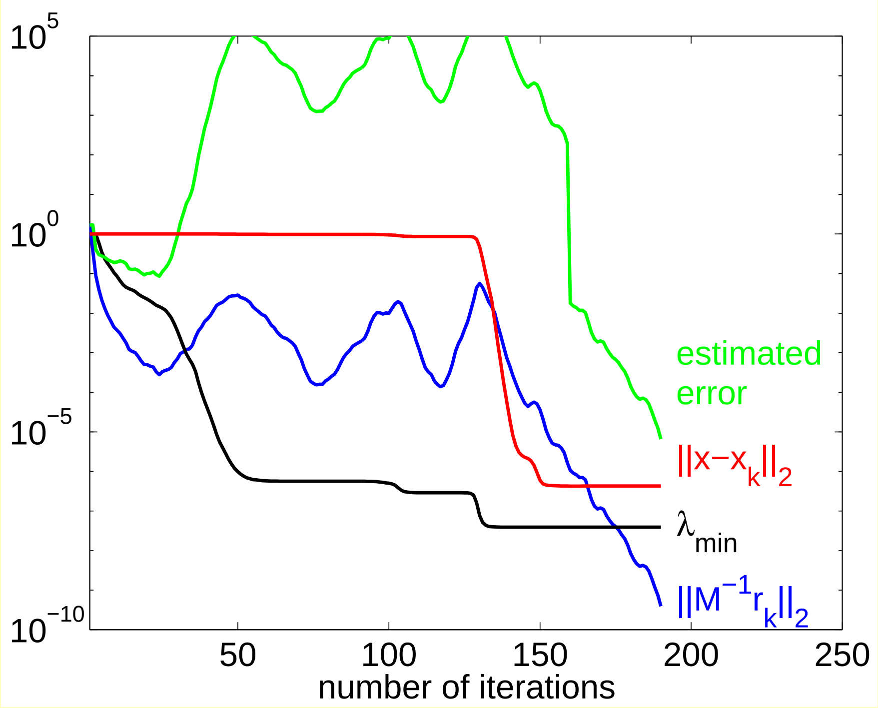
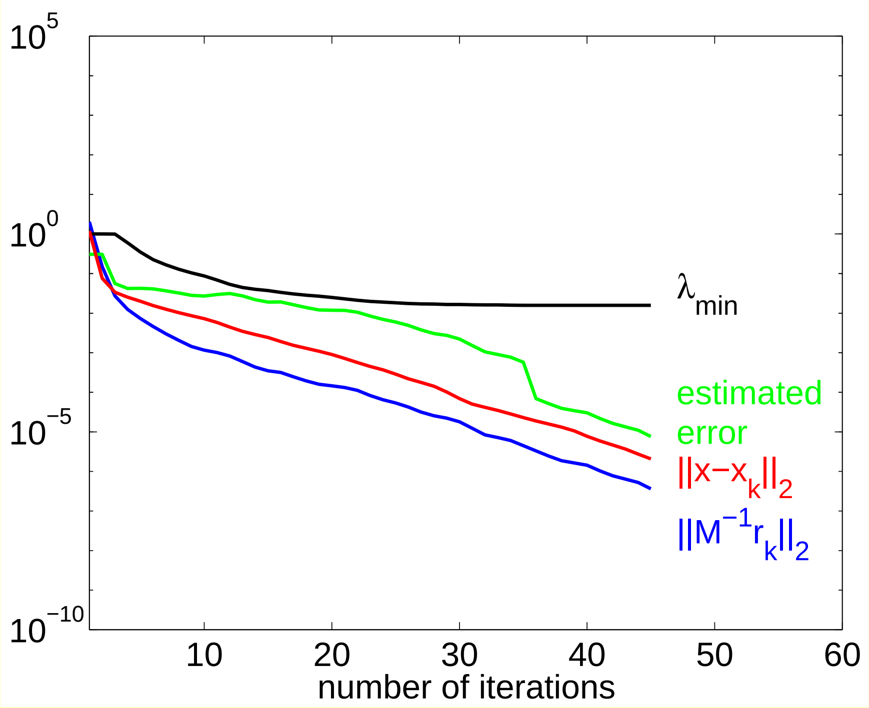
Results oil flow problem

The convergence behavior for ICCG and DICCG





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Subdomain deflation

k is number of subdomains

$z_1, ..., z_k$ deflation vectors

- $z_i = 1$ on $\bar{\Omega}_i$
- $z_i = 0$ on $\Omega \setminus \bar{\Omega}_i$

Remarks

- The matrix E is sparse
- $K_{eff}(PA)$ decreases for increasing k
- Work to invert E increases for increasing k
- Optimal value of k?

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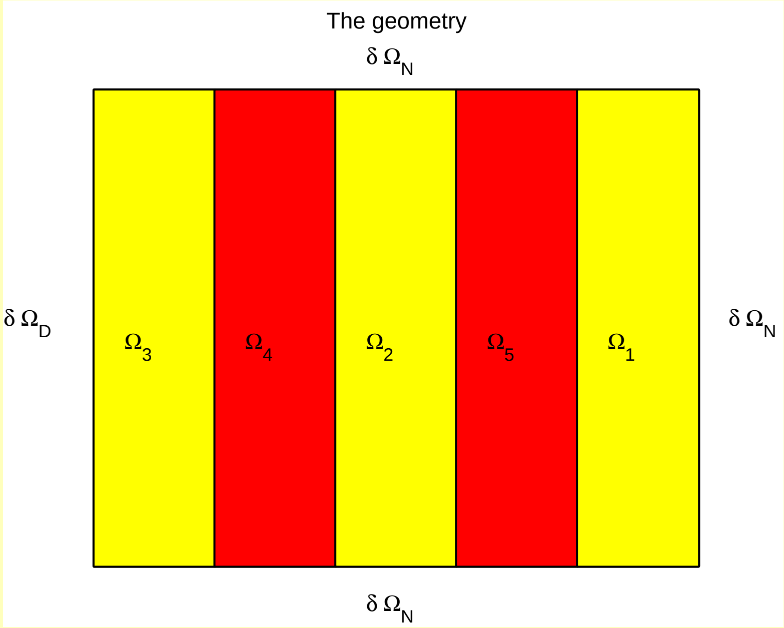
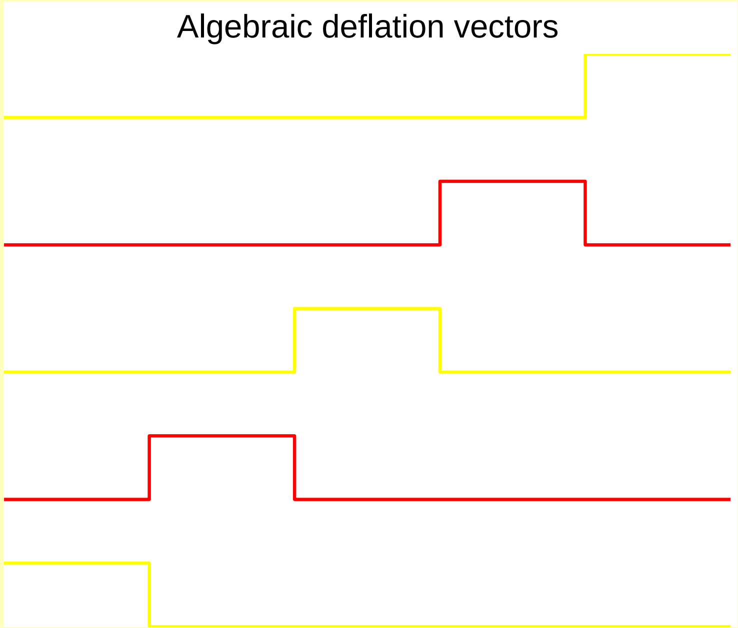
Algebraic deflation vectors





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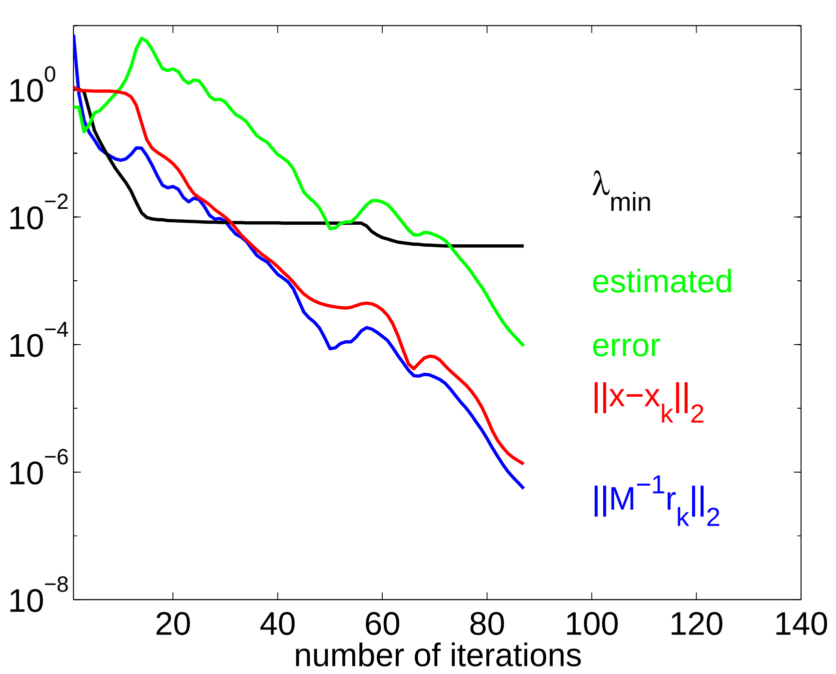
Results (discontinuous coefficients)

Physical deflation vectors



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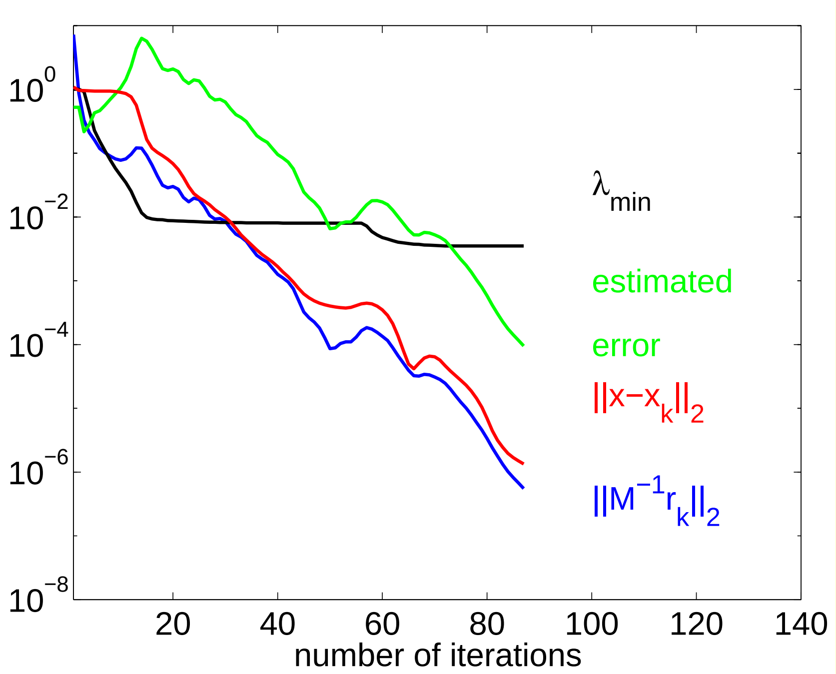
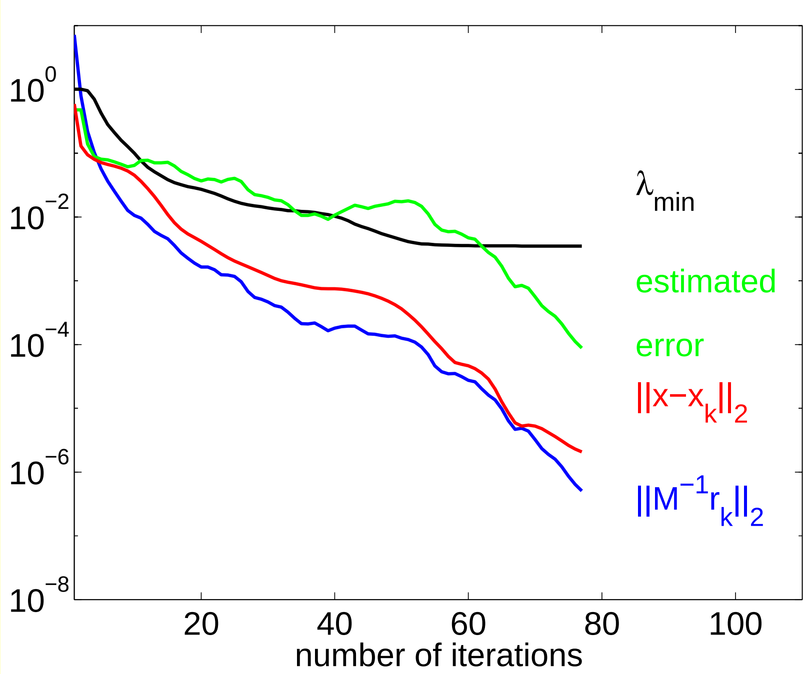


Algebraic deflation vectors



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4. Parallelle methoden

Fixed grid 300×300

Number of iterations

p	1	4	25
GMR6	1 (160)	80 (69)	168 (26)
GMR2	3 (50)	86 (16)	192 (11)
GMR1	6 (24)	139 (14)	303 (6)
RILU	160 (1)	341 (1)	437 (1)

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RILU	160 (1)	341 (1)	437 (1)

Wall clock time Cray T3E

1	4	25
81	685	79
75	167	37
70	222	39
119	65	15

Parallelization of DICCG

Compute and store the sparse vectors

$$c_j = Az_j$$

Compute $E^{-1} = (Z^T AZ)^{-1}$ and store it on each processor
To compute PAv:

1. $w = Av$

2. Compute the inner products $\tilde{w} = Z^T w$

3. $\tilde{e} = (Z^T AZ)^{-1}\tilde{w}$ on each processor

4. form $v - [c_1 ... c_m]\tilde{e}$

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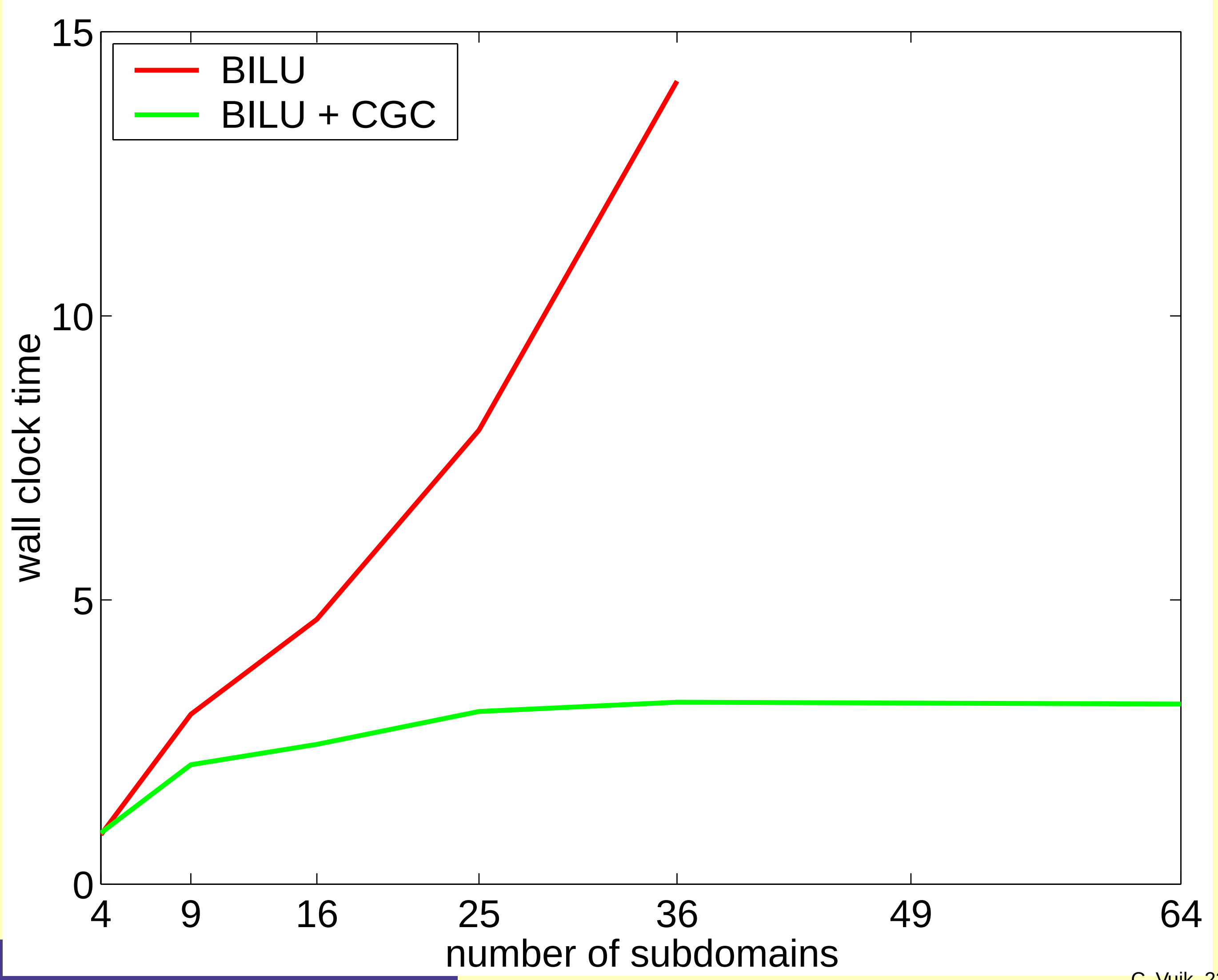
Parallel scalability, subdomain 50×50*, Cray T3E*



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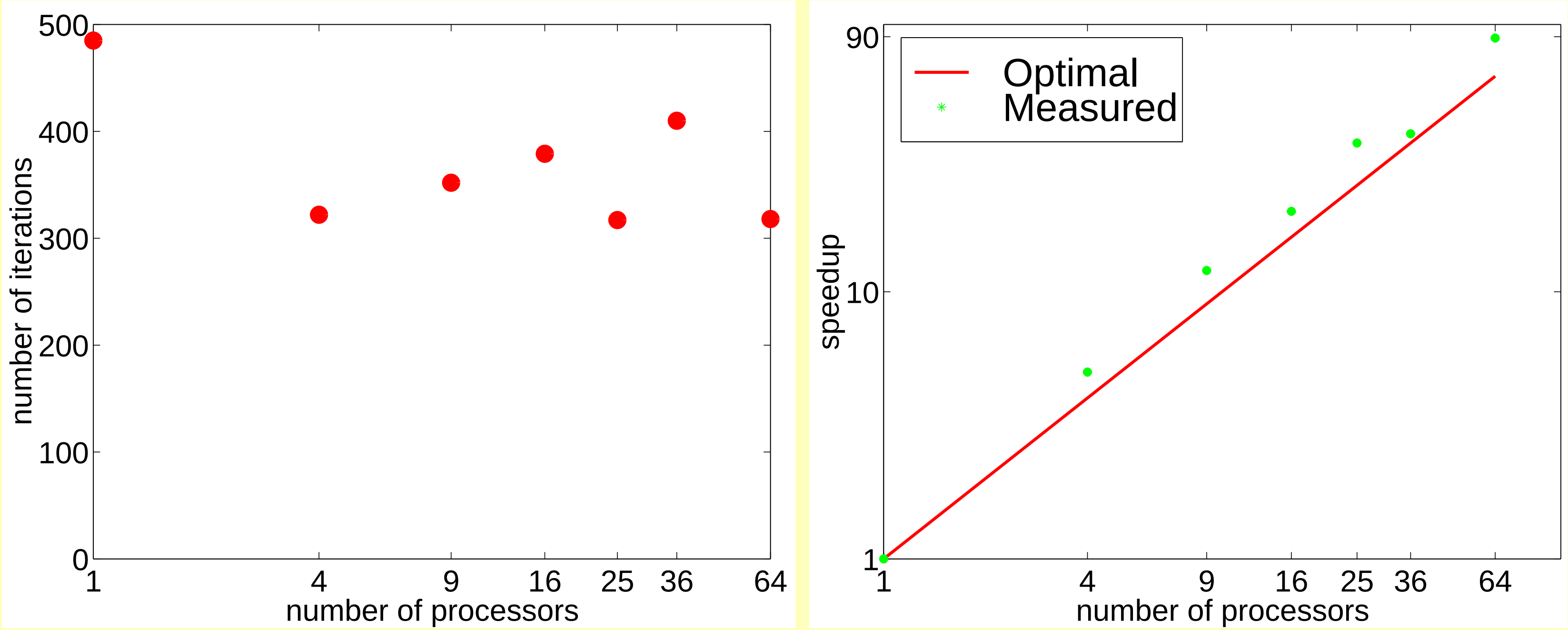
Parallel speedup, 480×480 grid, Cray T3E



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