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8-TH COPPER MOUNTAIN CONFERENCE ON ITERATIVE METHODS

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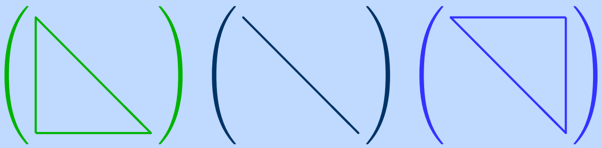
OUTLINE

1. inverse–based ILUs, theoretical background
2. Multilevel algorithms
3. ILUPACK
4. Numerical experiments
5. Conclusions

$$Ax = b$$

INCOMPLETE LU DECOMPOSITION

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = LDU + E \approx$$  , where L, U are unit diagonal.

INVERSE–BASED DROPPING

At elimination step k, drop l_{ik}, u_{kj} if

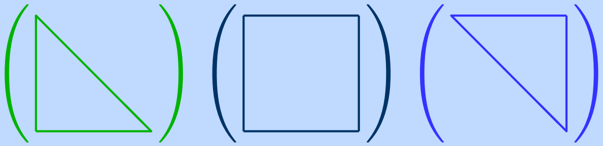
$$|l_{ik}| * \|e_k^\top L^{-1}\| \leqslant \tau |d_{kk}|, \qquad |u_{kj}| * \|U^{-1} e_k\| \leqslant \tau |d_{kk}|,$$

where τ is a drop tolerance [B. '01, '03], [Li, Saad, Chow '03].

$\Longrightarrow L^{-1}$ and U^{-1} serve as approximate inverses

FACTORED APPROXIMATE INVERSE (AINV), **[Benzi, Tůma ’98]**

$$W^\top A Z =$$



$$= D + E$$

$$W \longleftrightarrow L^{-\top}, \quad Z \longleftrightarrow U^{-1}$$

THEOREM [B., Saad ’01]. Suppose that the AINV process and the inverse–based ILU are computed using the same approximate Schur complement.
Let τ be the drop tolerance. Then

$$|(I - WL^\top)_{ij}| \leqslant 2(\mathbf{j} - \mathbf{i})\tau, \quad |(I - ZU)_{ij}| \leqslant 2(\mathbf{j} - \mathbf{i})\tau \quad \forall i < j.$$

Growth of the inverse triangular factors

Problem. $\|L^{-1}\|$ and $\|U^{-1}\|$ may become very large.

$\Rightarrow$ pivoting recommended.

BUT what kind of pivoting is appropriate?

Consider the approximate factorization

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = \underbrace{\begin{pmatrix} L_B & 0 \\ L_E & I \end{pmatrix}}_{L_k} \underbrace{\begin{pmatrix} D_B & 0 \\ 0 & S_C \end{pmatrix}}_{D_k} \underbrace{\begin{pmatrix} U_B & U_F \\ 0 & I \end{pmatrix}}_{U_k} + E_k,$$

where L_k and $U_k^\top$ are unit lower triangular matrices and the leading $k \times k$ part of D_k is diagonal.

Inverse error

$$F_k := L_k^{-1} E_k U_k^{-1}$$

LEMMA. Denote by v_k and w_k the entries in column k of $L_k D_k$ (resp. row k of $D_k U_k$) that are dropped at step k of the incomplete LU decomposition.

1. Suppose that the approximate Schur complement S_C is defined via

$$S_C = C - L_E D_B U_F \quad \text{(S–version)}$$

$$\Rightarrow F_k = \sum_{l \leqslant k} \left(L_k^{-1} v_l e_l^\top U_k^{-1} + L_k^{-1} e_l w_l^\top U_k^{-1} \right)$$

2. Suppose that the approximate Schur complement S_C is defined via

$$S_C = \begin{bmatrix} -L_E L_B^{-1} & I \end{bmatrix} A \begin{bmatrix} -U_B^{-1} U_F \\ I \end{bmatrix} \quad \text{(T–version)}$$

$$\Rightarrow F_k = \sum_{l \leqslant k} \left(L_k^{-1} v_l e_l^\top \qquad + \qquad e_l w_l^\top U_k^{-1} \right)$$

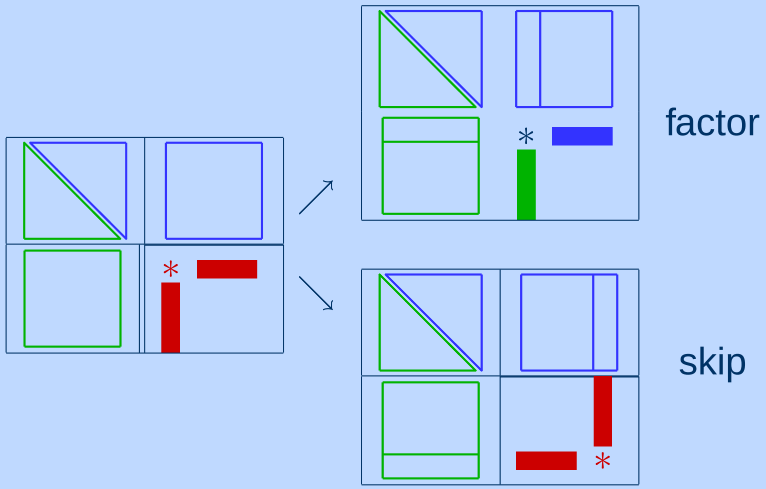
Consequences

- $\|L_k^{-1}\|$ and $\|U_k^{-1}\|$ contribute to the inverse error
- For the S–version even their PRODUCT $\|L_k^{-1}\| \cdot \|U_k^{-1}\|$!

Inverse–based pivoting

Control $\|L^{-1}\|, \|U^{-1}\| \leqslant \kappa$ by a **factor or skip strategy**

At step k :



Rows/columns that exceed the prescribed bound are pushed to the end

Sketch of the templates

1. Compute a static partial reordering

$$A \rightarrow P^\top A Q = \begin{pmatrix} B & F \\ E & C \end{pmatrix}$$

2. Factor $P^\top AQ$ and control $\|L_k^{-1}\|, \|U^{-1}\| \leqslant \kappa$.

$$P^\top A Q \longrightarrow \hat{P}^\top A \hat{Q} = \begin{pmatrix} \hat{B} & \hat{F} \\ \hat{E} & \hat{C} \end{pmatrix} = \begin{pmatrix} L_B & 0 \\ L_E & I \end{pmatrix} \begin{pmatrix} D_B & 0 \\ 0 & S_C \end{pmatrix} \begin{pmatrix} U_B & U_F \\ 0 & I \end{pmatrix}$$

3. Apply strategy recursively to the approximate Schur complement S_C (multilevel scheme)

$$A \xrightarrow{1.} P^\top A Q \xrightarrow{2.} \hat{P}^\top A \hat{Q} \xrightarrow{3.} \left(\begin{array}{c|c} L \cdot D \cdot U & F \\ \hline E & S \end{array}\right)$$

$$S \xrightarrow{1.} P_S^\top S Q_S \xrightarrow{2.} \hat{P}_S^\top S \hat{Q}_S \xrightarrow{3.} \left(\begin{array}{c|c} L_S \cdot D_S \cdot U_S & F_S \\ \hline E_S & T \end{array}\right)$$

$$\ldots$$

TEMPLATE 1. STATIC REORDERINGS

Examples.

- RCM (Reverse Cuthill–McKee), MMD (Multiple Minimum Degree), AMF (Approximate Minimum Fill), INDSET (independent set, ARMS), MC64 (from HSL).
- ddPQ [Saad '03]. Permutations P, Q as a compromise between diagonal dominance and fill

   1. Define numerical weights

   $$\rho_i = \frac{\max_j |a_{ij}|}{\sum_j |a_{ij}|}, \quad \gamma_j = \frac{\max_i |a_{ij}|}{\sum_i |a_{ij}|}$$

   2. define fill weights, e.g.

   $$f_i = |\{j: \; a_{ij} \neq 0\}, \quad g_j = |\{i: \; a_{ij} \neq 0\}, \quad h_{ij} = (f_i - 1)(g_j - 1) + 1, \ldots$$

   3. order ratios in decreasing order, e.g. order

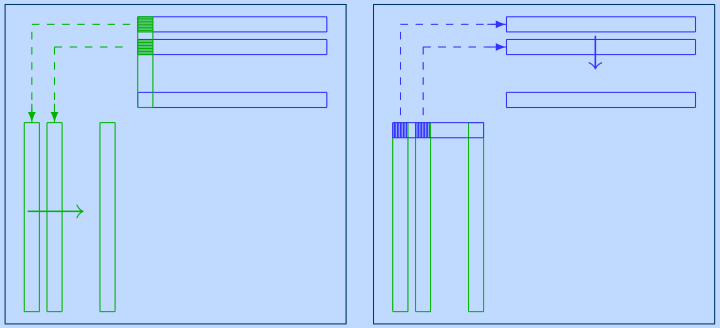
   $$\{\frac{\rho_i}{g_{k_i}} \forall i\}, \quad \{\frac{\gamma_j}{f_{l_j}} \forall j\}, \quad \{\frac{\rho_i \gamma_{k_i}}{h_{i,k_i}} \forall i, \frac{\rho_{l_j} \gamma_j}{h_{l_j,j}} \forall j\}, \ldots$$

   4. use associated indices (i, j) and skip duplicate entries

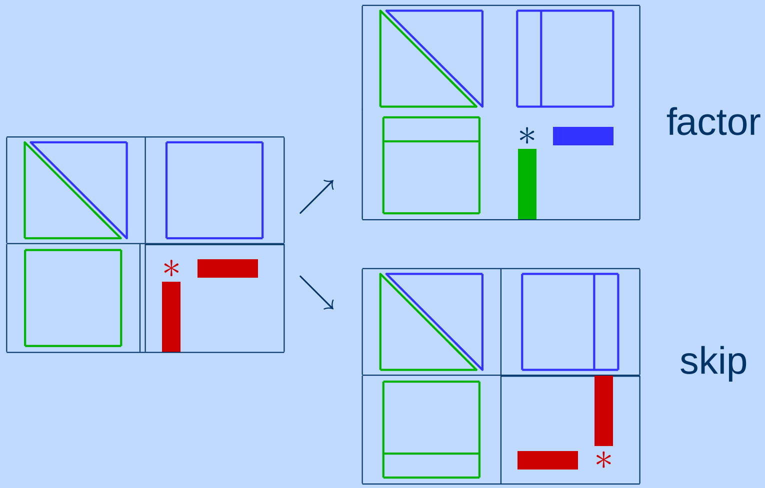
   Further selection criteria, e.g. enforce submatrix to be close to lower triangular

TEMPLATE 2. PILUC — INVERSE-BASED ILU THAT CONTROLS $\|L_k^{-1}\|, \|U_k^{-1}\|$

- ILU (Crout–version)



- $\|L_k^{-1}\|, \|U_k^{-1}\| \leqslant \kappa$ controlled by diagonal pivoting



- $\|L_k^{-1}\|, \|U_k^{-1}\|$ estimated [Cline, Moler, Stewart, Wilkinson ’77], [B. ’03]

TEMPLATE 3. MULTILEVEL SCHEME

$$(\hat{P}^\top A\hat{Q})^{-1} = \begin{pmatrix} B & F \\ E & C \end{pmatrix}^{-1} \approx \left\{ \begin{pmatrix} L_B & 0 \\ L_E & I \end{pmatrix} \begin{pmatrix} D_B & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} U_B & U_F \\ 0 & I \end{pmatrix} \right\}^{-1}$$

$$\approx \begin{pmatrix} \tilde{B}^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -\tilde{B}^{-1}F \\ I \end{pmatrix} S_C^{-1} \begin{pmatrix} -E\tilde{B}^{-1} & I \end{pmatrix}, \text{ where } \tilde{B} = L_B D_B U_B$$

Recursive application to $S_C \longrightarrow$ (additive) algebraic multigrid scheme (or block ILU)

- use concept of ARMS [Saad, Suchomel '99], i.e. skip L_E, U_F.
- After AMG is set up, S_C can be discarded.
- Without L_E, U_F, forward/backward substitution twice as expensive, but more accurate and less memory needed.

Approximate Schur complements

1. $S_C = C - L_E D_B U_F$
   use analogous approximation scheme for $B \approx L_B D_B U_B$ (S–version)

2. $S_C = \begin{bmatrix} -L_E L_B^{-1} & I \end{bmatrix} A \begin{bmatrix} -U_B^{-1} U_F \\ I \end{bmatrix}$
   use analogous approximation scheme for $B \approx L_B D_B U_B$ (T–version)

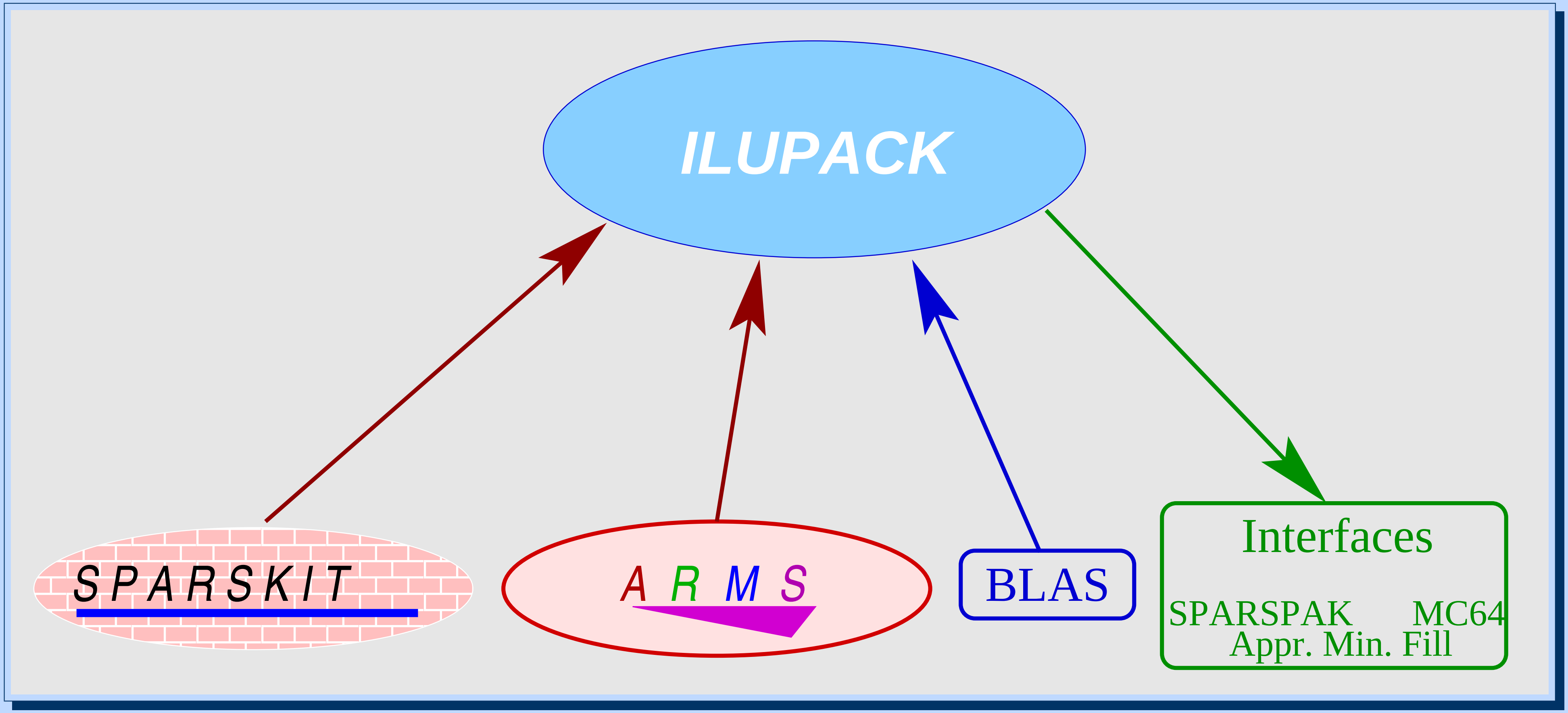
3. Use S–version for the computation of $B \approx L_B D_B U_B$ (M–version)
   Use T–version for the computation of S_C

Approximation order

Denote by τ the drop tolerance and let $B = L_B D_B U_B + E_B$

- If we use 1., then $\|E_B\| = \mathcal{O}(\tau)$, $\|L_B^{-1} E_B U_B^{-1}\| = \mathcal{O}(\tau\kappa^2)$
- if we use 2., then $\|E_B\| = \mathcal{O}(\tau^2)$, $\|L_B^{-1} E_B U_B^{-1}\| = \mathcal{O}(\tau^2\kappa)$
- Similar arguments apply to S_C

Preconditioning software package (C/FORTRAN 77) based on inverse–based multilevel ILUs



Names And Formats

1. ILUPACK currently supports real single/double precision and complex single/double precision.

2. Apart from the arithmetic ILUPACK distinguishes between two classes of matrices, namely general matrices and symmetric (Hermitian) positive definite matrices.

3. matrices are stored in SPARSKIT format (compressed sparse row format).

SPARSKIT, ARMS, . . .

- Several routines from SPARSKIT incorporated (GMRES, FGMRES, ILUT, ILUTP,. . .)
- Reorderings (INDSET, ddPQ) and several tools from ARMS adapted
- Most common reorderings supported or at least interfaces are provided

TEMPLATE 1

- Preconditioner allows three arbitrarily chosen permutation/scaling functions
  1. Initial preprocessing (applied only once)
  2. Regular reordering (applied to any subsequent system)
  3. Final pivoting (if the regular reordering fails)
- Custom reorderings possible

TEMPLATE 2

Partial ILUC (Crout version) with static permutation and diagonal pivoting (F77 core routine)

TEMPLATE 3

- Three different versions of approximate Schur complements are supported (S–, M– and T–version). M–version is default.
- After the computation of the approximate Schur complement the parts L_E and U_F are discarded.
- if the fill exceeds a certain amount, the algorithm switches to full-matrix processing.

PRECONDITIONERS

1. inverse–based multilevel ILU (referred as "ILUPACK")

2. ILUTP

3. ILUC (single–level, inverse–based)

ORDERINGS

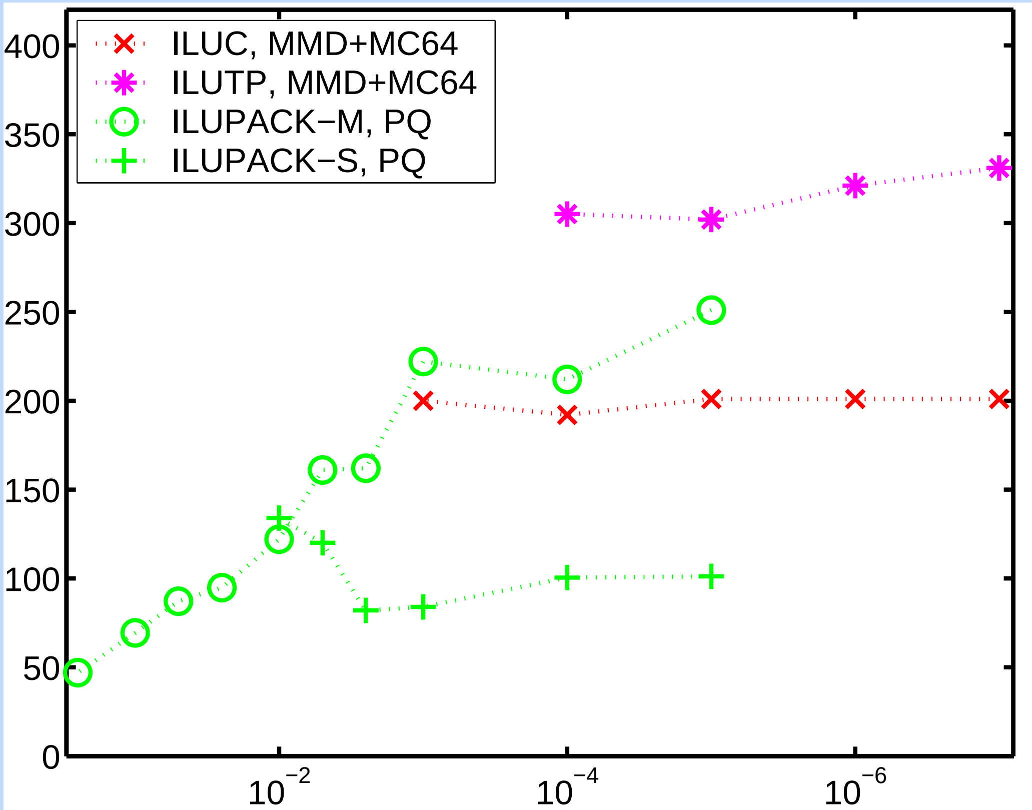
PQ, RCM, $\ldots +$ row/column scaling

ITERATIVE SOLVERS

- GMRES, PCG. Iteration stopped if $\|b - Ax^{(k)}\| \leqslant \sqrt{\text{eps}}\|b - Ax^{(0)}\|$
- Iterative solver treated as failure, if a break down occurred or more than 500 steps were needed.

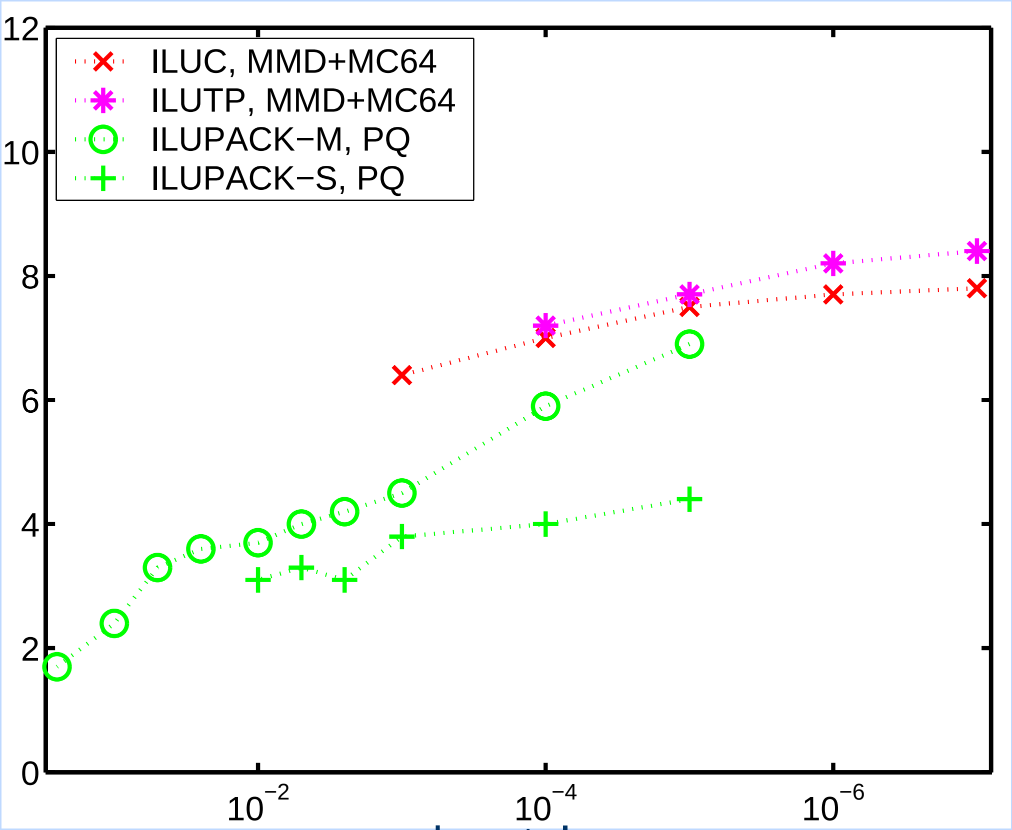
EXAMPLE. **Matrix ATT/TWOTONE**

Computation time



drop tol.

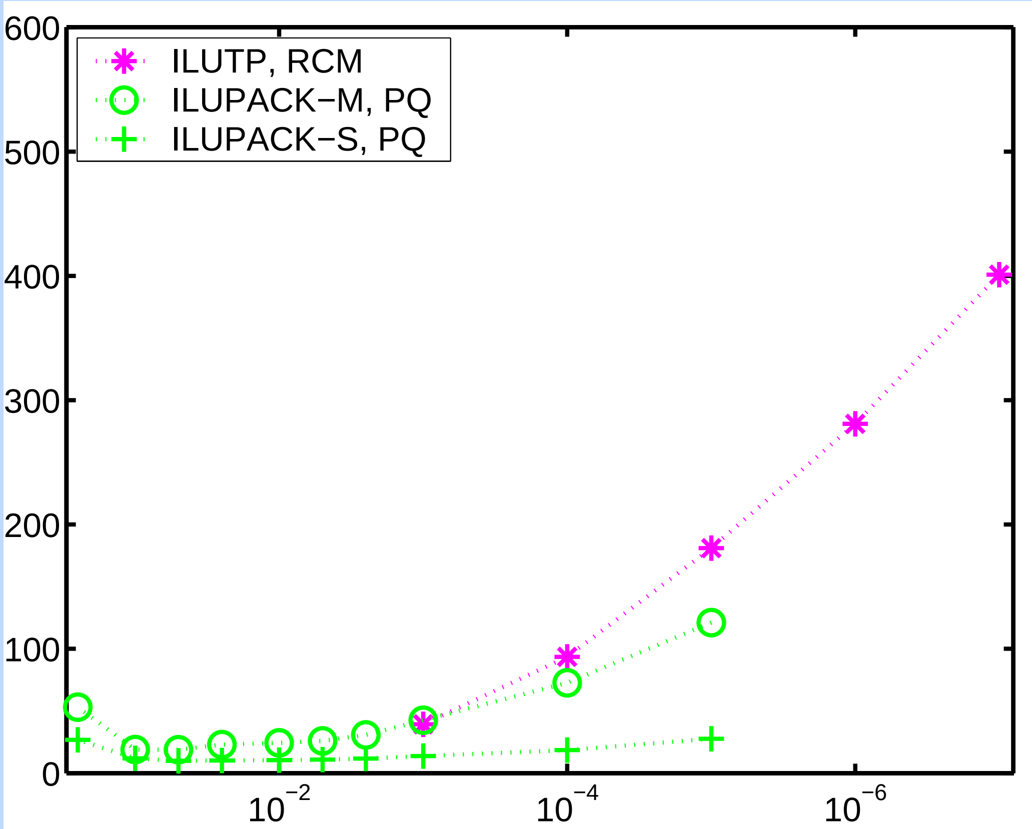
Memory requirement



drop tol.

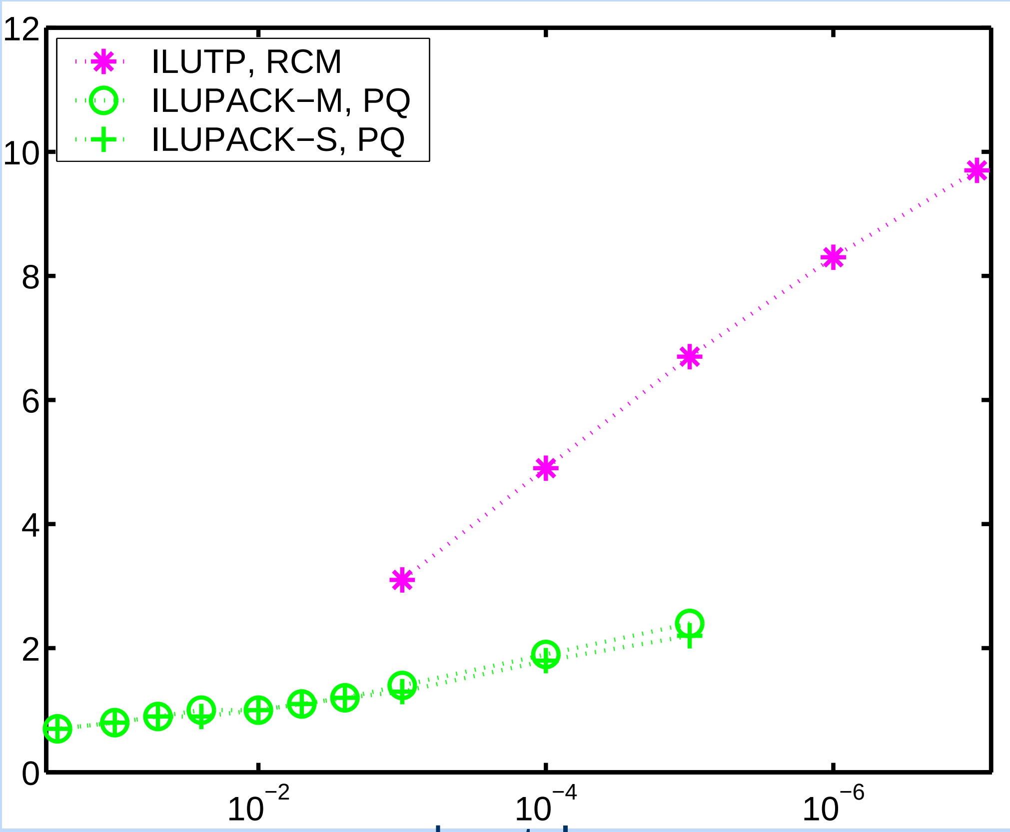
EXAMPLE. **Matrix VAVASIS/AV41092**

Computation time



drop tol.

Memory requirement



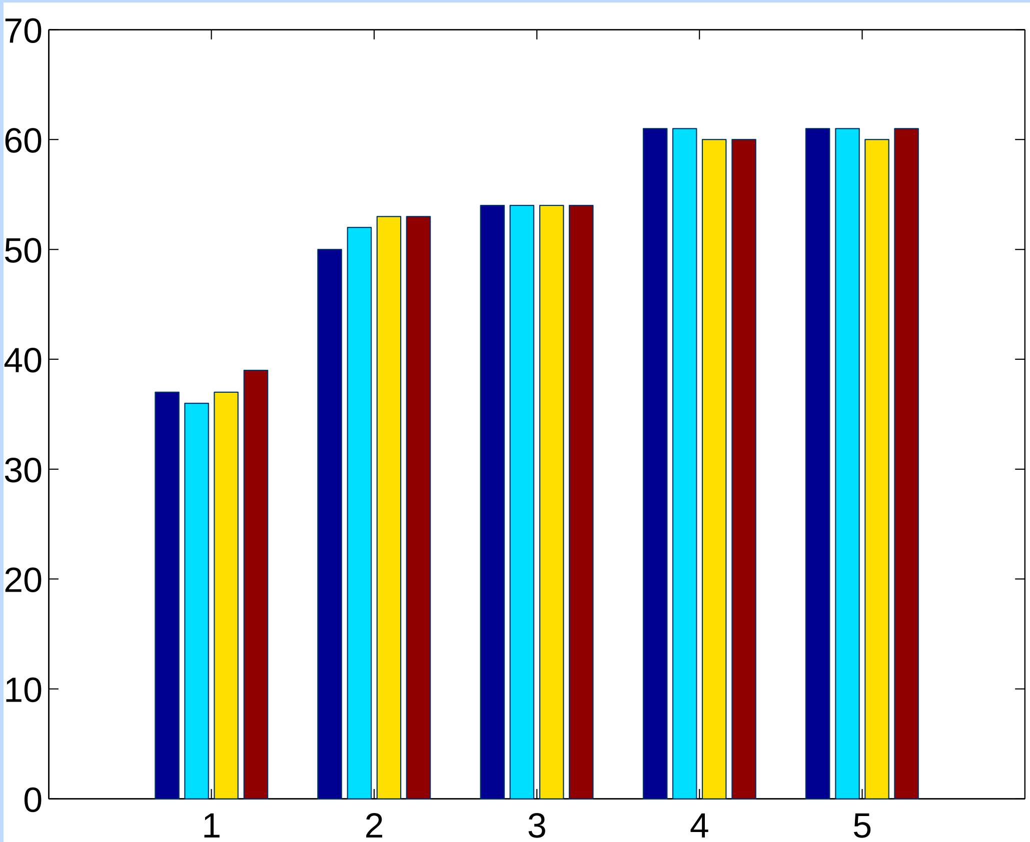
drop tol.

ILUPACK — dependence on inverse bound κ

Almost no difference between $\kappa = 10$, $\kappa = 25$, $\kappa = 50$, $\kappa = 100$

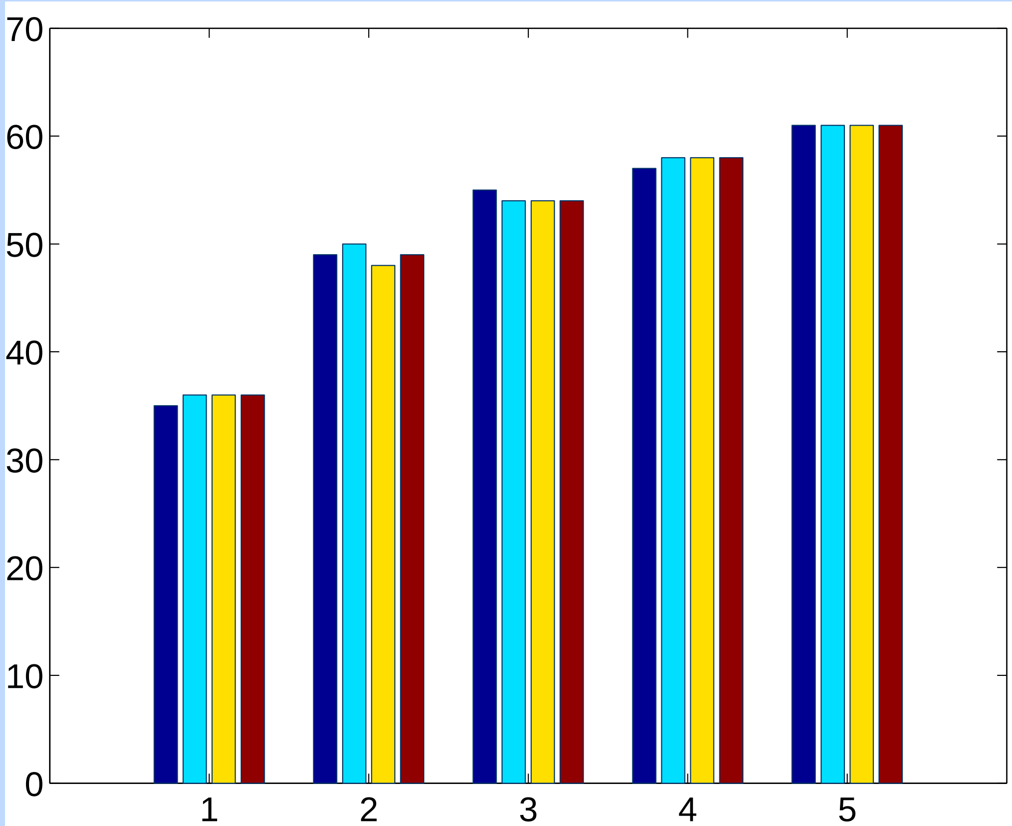
64 LARGE TEST MATRICES, NUMBER OF SUCCESSFUL COMPUTATIONS

ILUPACK M–version



drop tol. $[10^{-*}]$

ILUPACK S–version

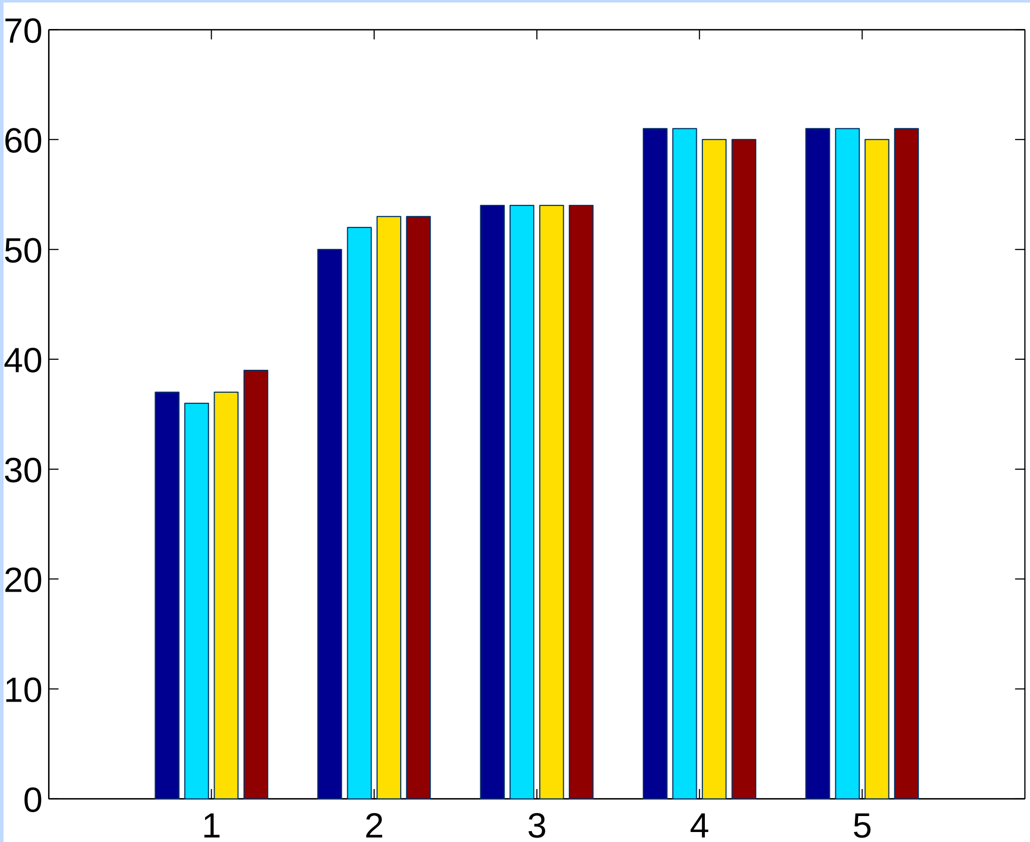


drop tol. $[10^{-*}]$

$\kappa = 10$, $\kappa = 25$, $\kappa = 50$, $\kappa = 100$

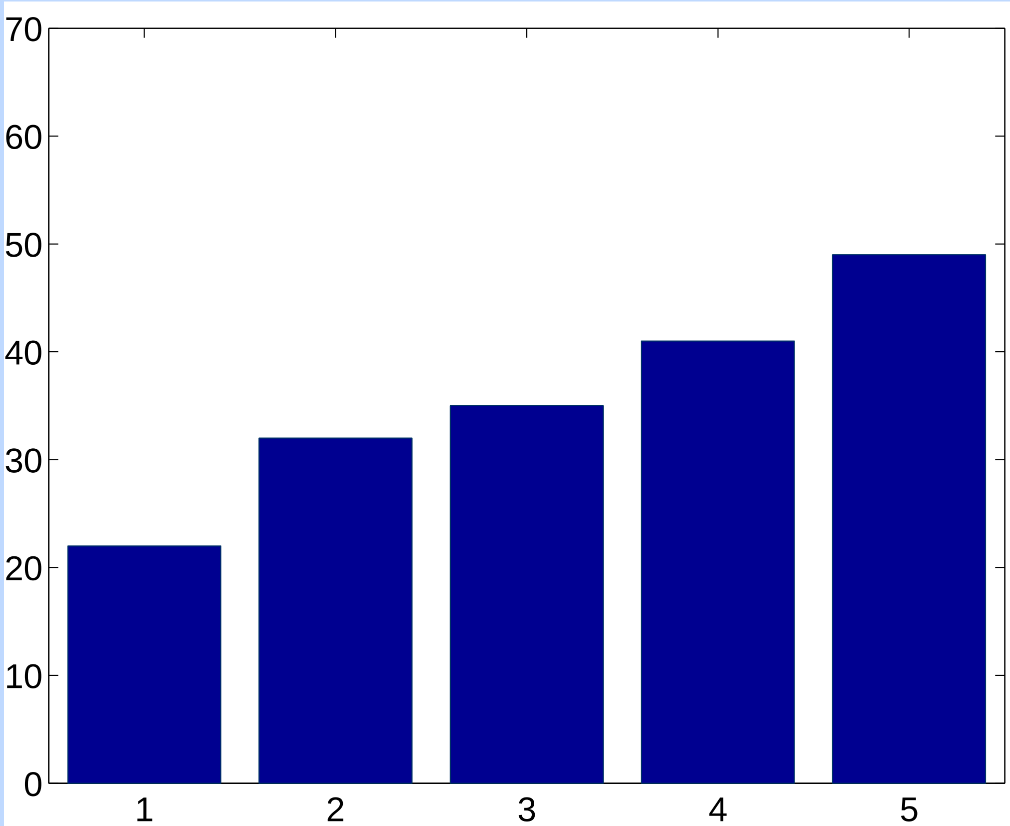
64 LARGE TEST MATRICES, NUMBER OF SUCCESSFUL COMPUTATIONS

ILUPACK M–version



drop tol. $[10^{-*}]$

ILUTP + RCM

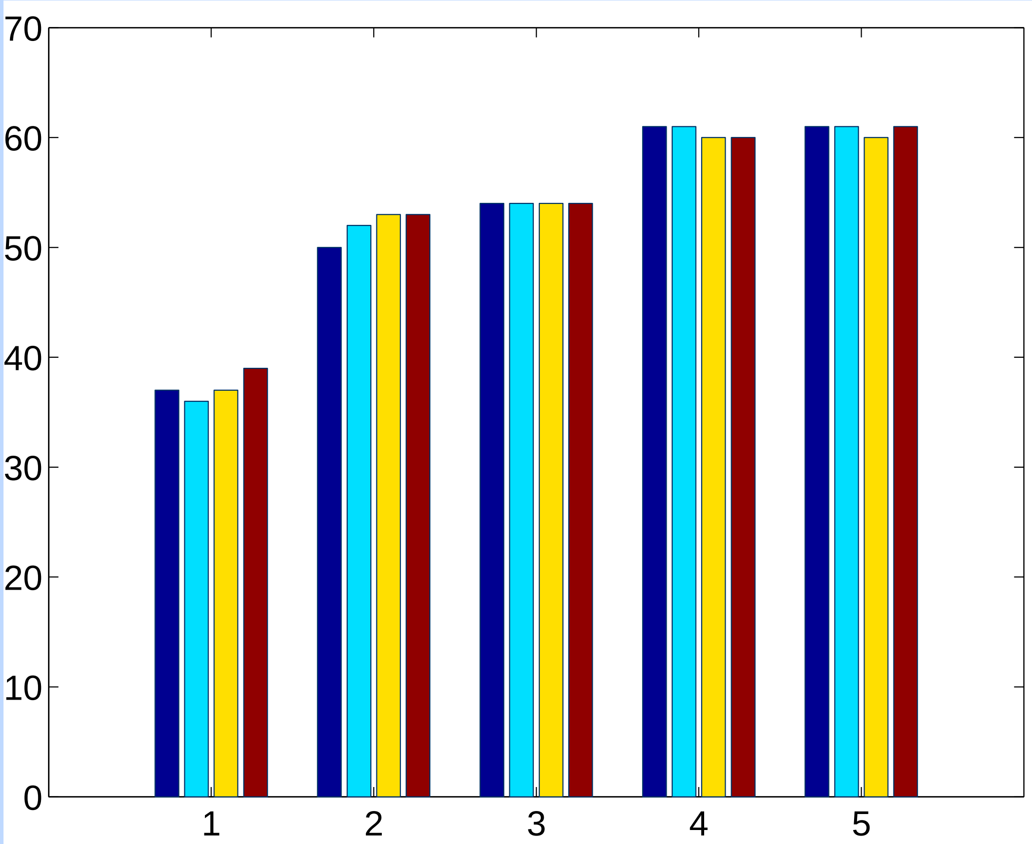


drop tol. $[10^{-*}]$

$\kappa = 10$, $\kappa = 25$, $\kappa = 50$, $\kappa = 100$

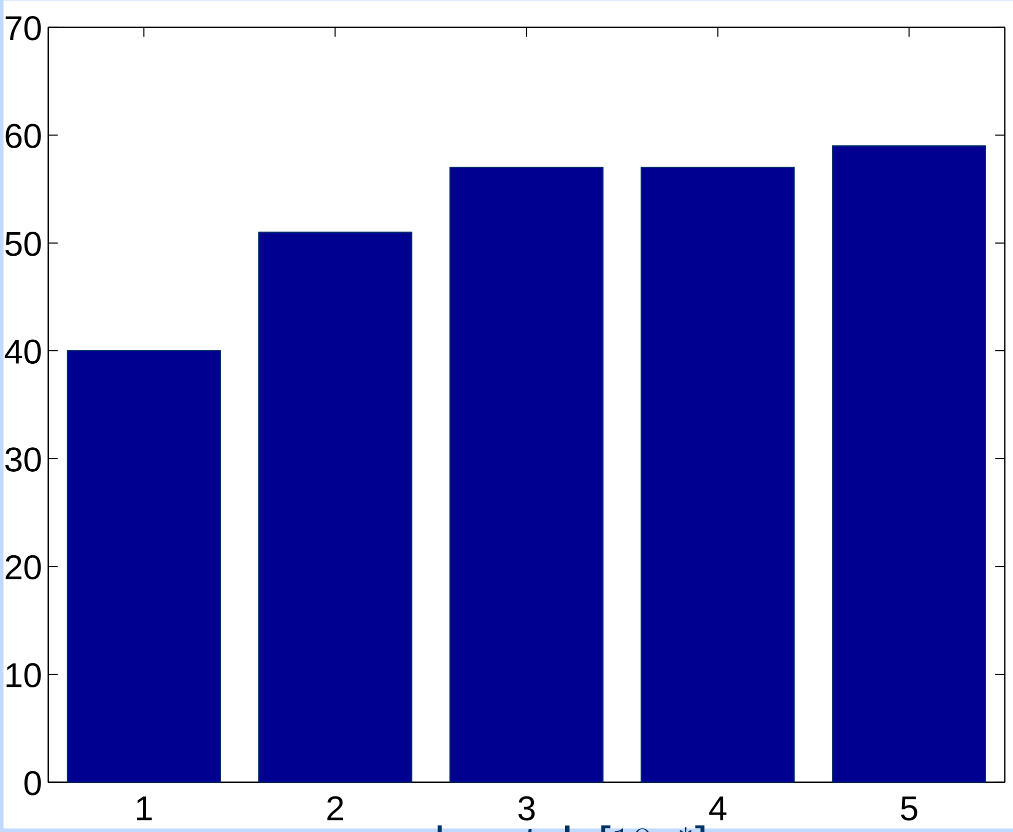
64 LARGE TEST MATRICES, NUMBER OF SUCCESSFUL COMPUTATIONS

ILUPACK M–version



drop tol. $[10^{-*}]$

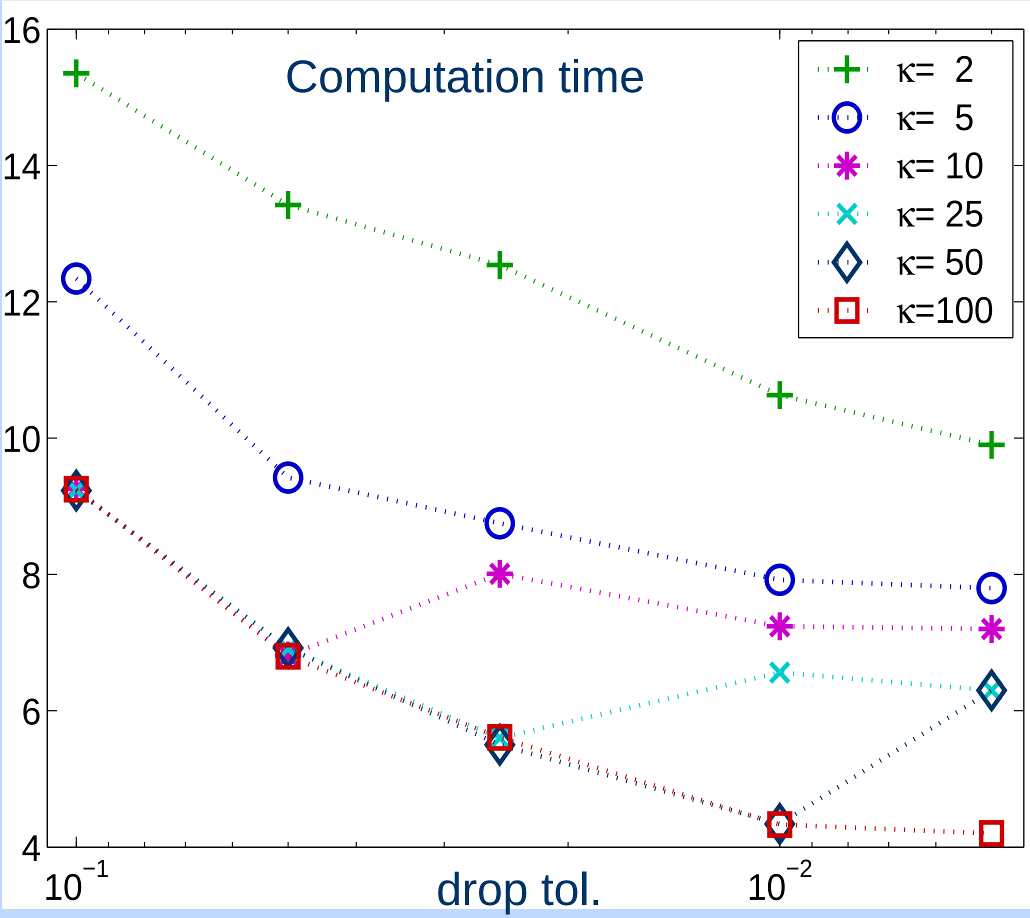
ILUTP + RCM + MC64

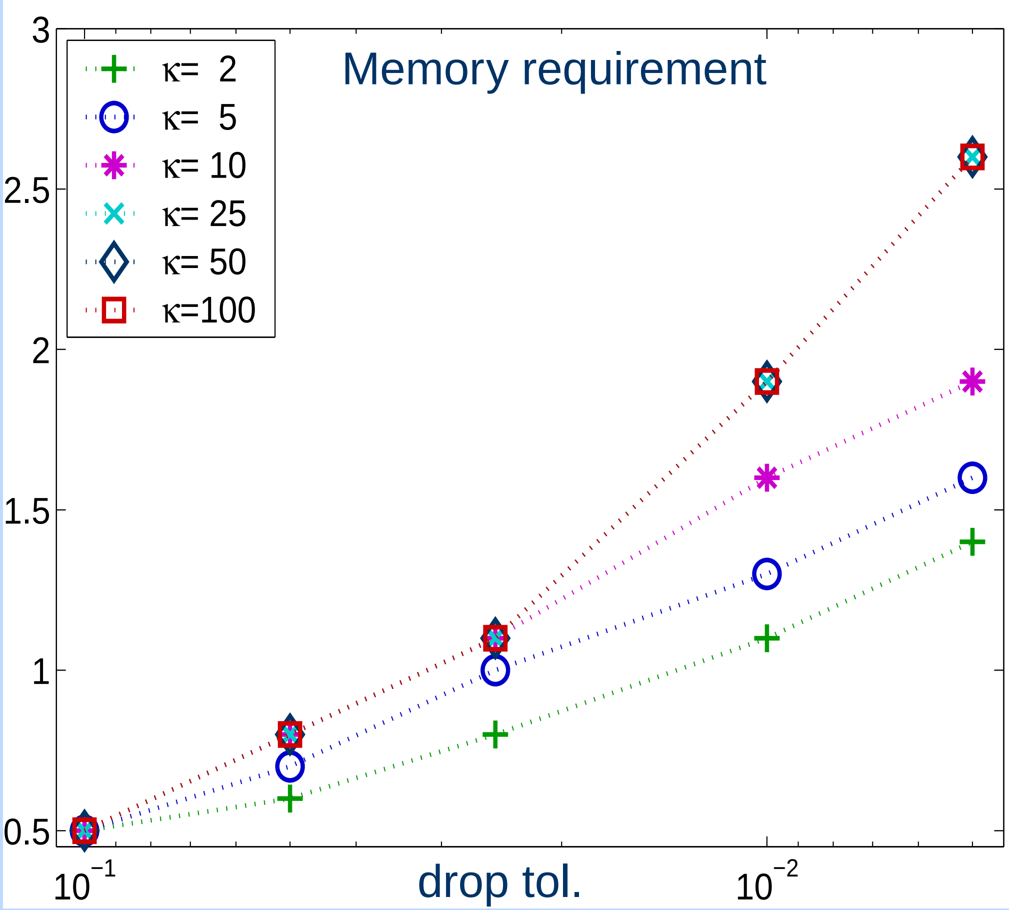


drop tol. $[10^{-*}]$

EXAMPLE. **cylindric shell problem**

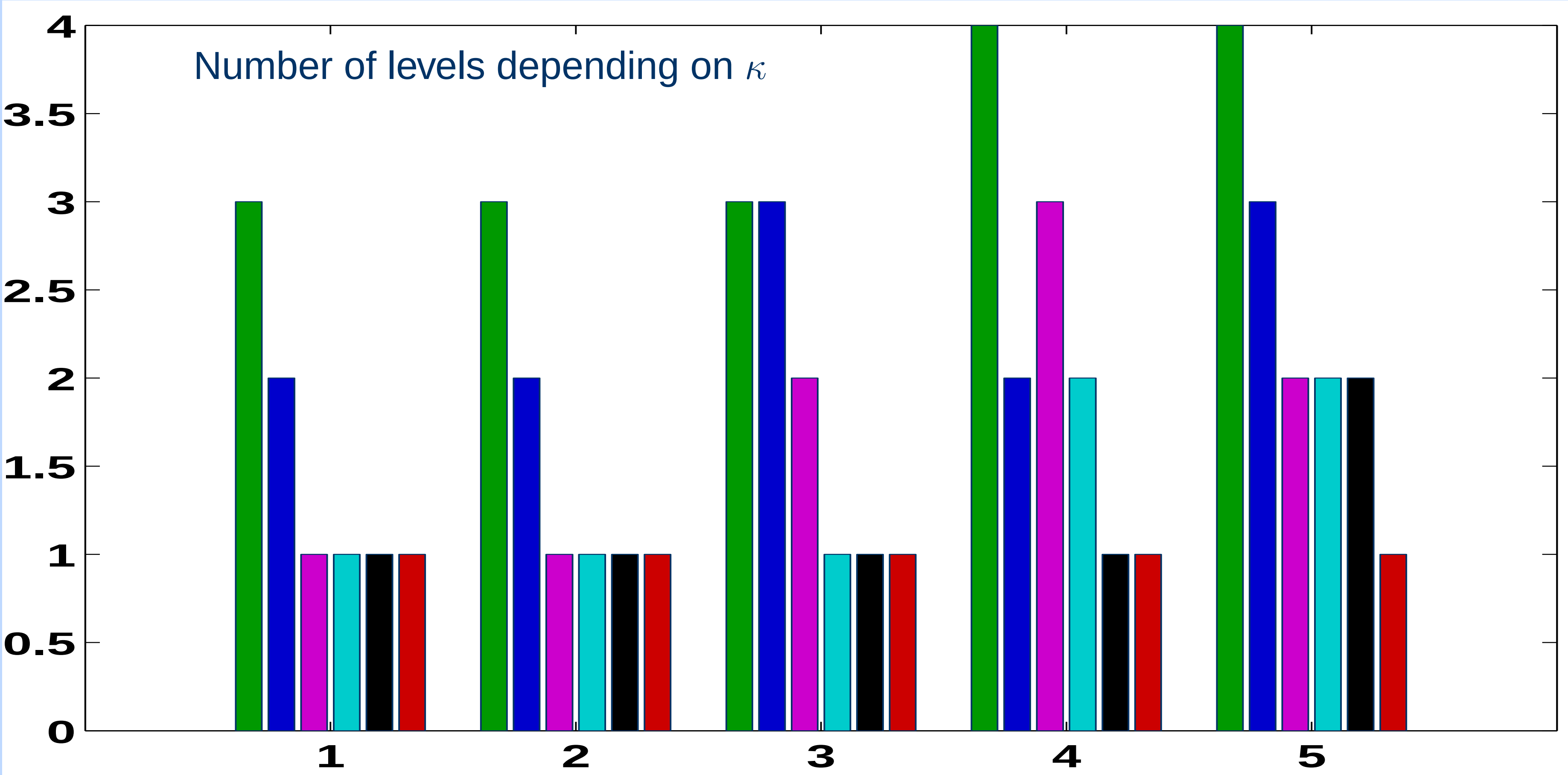
Tight bounds on $\|U^{-1}\| \leqslant \kappa$ implicitly yield FINE GRID/COARSE GRID selection





EXAMPLE. **cylindric shell problem**

Number of levels. $\kappa = 2$, $\kappa = 5$, $\kappa = 10$, $\kappa = 25$, $\kappa = 50$, $\kappa = 100$.



drop tol. 0.1 0.05 0.025 0.01 0.005

Conclusions

1. Multilevel preconditioners using inverse–based ILUs
2. numerical experiments indicate higher robustness with respect to parameter tuning (time dependent problems, nonlinear equations)
3. Main objective: inverse triangular factors are kept bounded
4. AMG-like preconditioners realized in the software package ILUPACK that offers inverse–based multilevel ILUs for a broad class of matrices
5. Still to do: reordering strategies for PDE-type problems

ILUPACK BEING RELEASED BY APRIL/MAY, 2004

http://www.math.tu-berlin.de/ilupack/