On an approximate preconditioner update for sequences of large nonsymmetric linear systems

Jurjen Duintjer Tebbens
Institute of Computer Science
Academy of Sciences of the Czech Republic

joint work with

Miroslav Tůma
Institute of Computer Science
Academy of Sciences of the Czech Republic
and Technical University in Liberec

Modelling 2009, Rožnov pod Radhoštěm, June 25, 2009.

1. Introduction: Efficient solution of sequences

The solution of *sequences* of linear systems arises in numerous applications, e.g. CFD-problems with implicit Euler leads to a number of linear systems in every time-step.

The central question for efficient solution will always be: How can we share part of the computational effort throughout the sequence ?

Some known strategies are using hot starts, Krylov subspace recycling, exact updates of LU-factorizations, etc ...

We concentrate on sequences arising from Newton-type iterations to solve nonlinear equations,

$$J(x_k)(x_{k+1} - x_k) = -F(x_k), \quad k = 1, 2, \dots$$

where $J(x_k)$ is the Jacobian of F evaluated at x_k.

1. Introduction: Efficient solution of sequences

- One option to save costs in a Newton-type method is to skip evaluations of the (approximate) Jacobian during some iterations, leading to Shamanskii's combination of the chord and Newton method [Brent - 1973].

- Another option: Allow changing the system matrices but freeze the preconditioner [Knoll, Keyes - 2004]. Naturally, a frozen preconditioner will deteriorate when the system matrix changes too much.

- To enhance the power of a frozen preconditioner one may also use approximate preconditioner updates.

1. Introduction: Efficient solution of sequences

- In [Meurant - 2001] we find approximate preconditioner updates of incomplete Cholesky factorizations and
- in [Benzi, Bertaccini - 2003, 2004] banded preconditioner updates were proposed for both symmetric positive definite approximate inverse and incomplete Cholesky preconditioners.
- In Quasi-Newton methods the difference between system matrices is of small rank and preconditioners may be efficiently adapted with approximate small-rank preconditioner updates; this has been done in the symmetric positive definite case, see e.g. [Bergamaschi, Bru, Martínez, Putti - 2006, Nocedal, Morales - 2000].
- Approximate preconditioner updates based on approximate inverses are considered in [Calgaro, Chehab, Saad - 2009].

2. The considered preconditioner updates

In this presentation we focus on a preconditioner update proposed recently [DT, Tůma - 2007]:

- A black-box approximate preconditioner update designed for *nonsymmetric* linear systems solved by arbitrary iterative methods.

- Its computation is much cheaper than the computation of a new preconditioner.

- Simple algebraic updates which can be easily combined with other (problem specific) strategies and can be applied in matrix-free environment.

2. The considered preconditioner updates

Notation:

Consider two systems

$$Ax = b, \qquad \text{and} \qquad A^+x^+ = b^+$$

preconditioned by M and M^+ respectively and let the difference matrix be defined as

$$B \equiv A - A^+.$$

Define the standard splitting

$$B = L_B + D_B + U_B$$

and let M be factorized as

$$M = LDU \approx A.$$

2. The considered preconditioner updates

Then the proposed preconditioner updates have the form

$$M^+ \equiv (LD - L_B - D_B)U \quad \text{or} \quad M^+ \equiv L(DU - D_B - U_B).$$

Note that M^+ is for free and its application asks for one forward and one backward solve. Schematically,

type	initialization	solve step	memory
Recomp	$A^+ \approx L^+U^+$	solves with L^+, U^+	A^+, L^+, U^+
Update	—	solves with $L, U, triu(B)$	$A^+, triu(A), L, U$

- This is the basic idea; more sophisticated improvements are possible
- Ideal for upwind/downwind modification but our experiments cover broader spectrum of problems

3. Updates in matrix-free environment

An important advantage of Krylov subspace methods is that they do not require the system to be stored explicitly; a matrix-vector product (matvec) subroutine, based on a function evaluation, suffices.

$\Rightarrow$ important reducing of storage and computation costs.

Standard example: Newton iteration of the form

$$J(x_k)(x_{k+1} - x_k) = -F(x_k), \quad k = 1, 2, \ldots$$

where $J(x_k)$ is the Jacobian of F evaluated at x_k. Then a matvec with $J(x_k)$ is replaced by the standard difference approximation,

$$J(x_k) \cdot v \approx \frac{F(x_k + h\|x_k\|v) - F(x_k)}{h\|x_k\|},$$

for some small h.

3. Updates in matrix-free environment

First note that to compute an incomplete factorization in matrix-free environment at all, the system matrix has to be *estimated by matvecs* ; for example a tridiagonal matrix

$$\begin{pmatrix} * & * & & & & \\ * & * & * & & & \\ & * & * & * & & \\ & & \ddots & \ddots & \ddots & \\ & & & * & * & * \\ & & & & * & * \end{pmatrix}$$

can be easily obtained with matvecs with

$$(1,0,0,1,0,0,\dots)^T,$$
$$(0,1,0,0,1,0,\dots)^T,$$
$$(0,0,1,0,0,1,\dots)^T.$$

3. Updates in matrix-free environment

In general, given the sparsity pattern, one runs a graph coloring algorithm that tries to minimize the number of matvecs for a good estimate [Cullum, Tůma - 2006].

Hence recomputing the preconditioner requires for every linear system:

- A number of additional matvecs to estimate the current matrix
- When the nonzero pattern changes during the sequence: Rerunning the graph coloring algorithm.

Preconditioner recomputation is even more expensive in matrix-free environment !

How about the preconditioner updates ?

3. Updates in matrix-free environment

Recall the upper triangular update is of the form

$$M^+ = L(DU - D_B - U_B)$$

based on the splitting

$$L_B + D_B + U_B = B = A - A^+.$$

Thus the update needs some entries of A and A^+ and repeated estimation is necessary.

However:

- A has been estimated before to obtain the reference ILU-factorization
- Of A^+ we need estimate only the upper triangular part
- Can there be taken any advantage of the fact we estimate only the upper triangular part?

3. Updates in matrix-free environment

Example:

$$\begin{pmatrix} * & & & & * \\ & * & & & * \\ & & \ddots & & \vdots \\ & & & \ddots & * \\ * & * & * & * & * \end{pmatrix}$$

- estimating the whole matrix asks for n matvecs with all unit vectors;
- estimating the upper triangular part requires only 2 matvecs,

$$(1, \ldots, 1, 0)^T \qquad \text{and} \qquad (0, \ldots, 0, 1)^T.$$

The problem of estimating only the upper triangular part is an example of a *partial graph coloring problem* [Pothen et al. - 2007].

3. Updates in matrix-free environment

The graph coloring algorithm for a matrix C works on the *intersection graph*

$$G(C^T C).$$

We can prove: The graph coloring algorithm for $triu(C)$ works on

$$G(triu(C)^T triu(C)) \cup G_K, \qquad \text{where}$$

$$G_K = \cup_{i=1}^n G_i, \quad G_i = (V_i, E_i) = (V, \{\{k, j\}|\ c_{ik} \neq 0\ \wedge\ c_{ij} \neq 0\ \wedge\ k < i \leq j\}).$$

Combined with a priori sparsification, there may be needed significantly less matvecs to estimate $triu(C)$ than to estimate C. Summarizing,

type	initialization	solve step	memory
Recomp	$est(A^+)$, $A^+ \approx L^+U^+$	solves with L^+, U^+	L^+, U^+
Update	$est(triu(A^+))$	solves with $L, U, triu(B)$	$triu(A^+), triu(A), L, U$

3. Updates in matrix-free environment

Example: Structural mechanics problem.

- A small strain metal viscoplasticity model for a rectangular plate of length 100, width 21.2 and height 9.62 cm with a hole in the middle;
- The discretization used 1 350 quadratic elements in most of the domain;
- We apply the Multilevel-Newton algorithm where every time-step contains an inner loop that requires the solution of nonlinear systems;
- We consider here a sequence of linear systems from a randomly chosen time-step in the middle of the simulation process;
- This sequence consists of 8 linear systems of dimension 4 936 with matrices containing about 315 000 nonzeros;
- We use restarted GMRES(40) preconditioned by ILUT.

Kindly provided by Karsten Quint (Universität Kassel).

3. Updates in matrix-free environment

Number of function evaluations for different precondition strategies.

ILUT$(10^{-5}, 50)$, Psize $\approx 812\,000$						
Matrix	Recompute		Freeze		Update	
	GMRES	estimation	GMRES	estimation	GMRES	estimation
$A^{(0)}$	65	89	65	89	65	89
$A^{(1)}$	31	89	128	0	52	25
$A^{(2)}$	35	89	163	0	45	25
$A^{(3)}$	35	89	237	0	45	25
$A^{(4)}$	37	89	167	0	52	25
$A^{(5)}$	38	89	169	0	51	25
$A^{(6)}$	37	89	168	0	51	25
$A^{(7)}$	50	89	168	0	51	25
Total fevals	1 040		1 354		701	

3. Updates in matrix-free environment

An alternative strategy circumvents estimation of A^+:

Let the matvec be replaced with a function evaluation

$$A^+ \cdot v \quad \rightarrow \quad F^+(v), \quad F^+ : \mathbb{R}^n \rightarrow \mathbb{R}^n,$$

e.g. in Newton's method

$$J(x^+) \cdot v \quad \approx \quad \frac{F(x^+ + h\|x^+\|v) - F(x^+)}{h\|x^+\|} \equiv F^+(v).$$

We assume function components are well separable, i.e. we assume it is possible to compute the components $F_i^+ : \mathbb{R}^n \rightarrow \mathbb{R}$,

$$F_i^+(v) = e_i^T F^+(v)$$

at the cost of about one nth of the full function evaluation $F^+(v)$.

Then the following strategy can be beneficial:

3. Updates in matrix-free environment

- The forward solves with L in $M^+ = L(DU - D_B - U_B)$ are trivial.

- For the backward solves, use a mixed explicit-implicit strategy: Split

$$DU - D_B - U_B = DU - triu(A) + triu(A^+)$$

in the explicitly given part

$$X \equiv DU - triu(A)$$

and the implicit part $triu(A^+)$.

We then have to solve the upper triangular systems

$$\left(X + triu(A^+)\right) z = y,$$

yielding the standard backward substitution cycle:

3. Updates in matrix-free environment

$$z_i = \frac{y_i - \sum_{j>i} x_{ij} z_j - \sum_{j>i} a^+_{ij} z_j}{x_{ii} + a^+_{ii}}, \qquad i = n, n-1, \ldots, 1.$$

The sum $\sum_{j>i} a^+_{ij} z_j$ can be computed by the function evaluation

$$\sum_{j>i} a^+_{ij} z_j = e_i^T A^+ (0, \ldots, 0, z_{i+1}, \ldots, z_n)^T \approx F^+_i \left((0, \ldots, 0, z_{i+1}, \ldots, z_n)^T \right).$$

The diagonal $\{a^+_{11}, \ldots, a^+_{nn}\}$ can be found by computing

$$a^+_{ii} = F^+_i(e_i), \qquad 1 \le i \le n.$$

Summarizing, with this technique we can obtain the cost comparison:

type	initialization	solve step	memory
Recomp	$est(A^+)$, $A^+ \approx L^+ U^+$	solves with L^+, U^+	L^+, U^+
Update	$est(diag(A^+))$	solves with L, U, eval($\mathcal{F}$), eval($\mathcal{F}^+$)	L, U

3. Updates in matrix-free environment

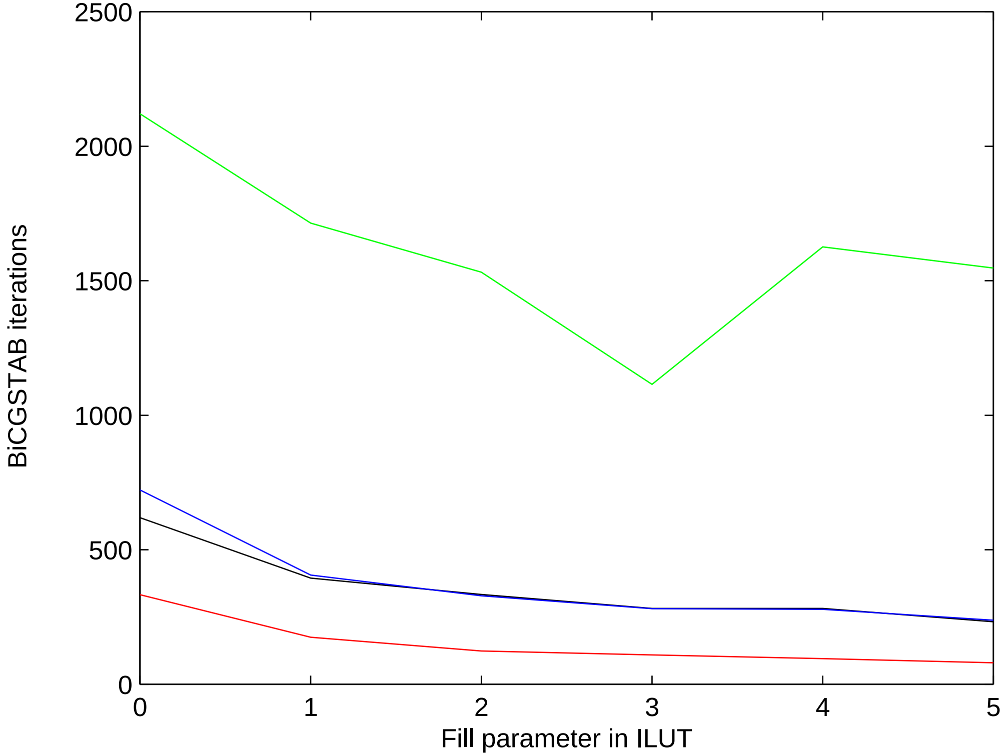
As an example consider a two-dimensional nonlinear convection-diffusion model problem: It has the form

$$-\Delta u + Ru\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\right) = 2000x(1-x)y(1-y), \tag{1}$$

on the unit square, discretized by 5-point finite differences on a uniform grid.

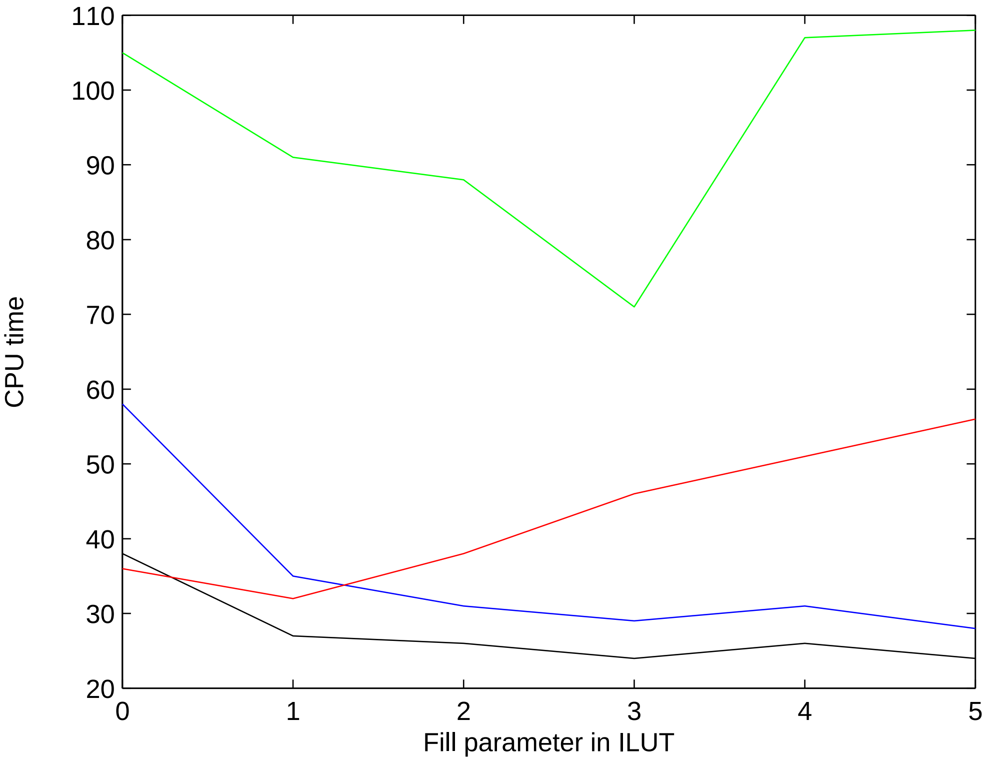
- The initial approximation is the discretization of $u_0(x, y) = 0$.
- We use here $R = 500$ and a 250×250 grid.
- We use a Newton-type method and solve the resulting 10 to 12 linear systems with BiCGSTAB with right preconditioning.
- We use a flexible stopping criterion.
- Fortran implementation (embedded in the UFO - software for testing nonlinear solvers).

3. Updates in matrix-free environment



Green: Freeze; Red: Recompute; Black: Update with partial estimation;
Blue: Update with implicit backward/forward solves.

3. Updates in matrix-free environment



Green: Freeze; Red: Recompute; Black: Update with partial estimation;
Blue: Update with implicit backward/forward solves.

For more details see:

- DUINTJER TEBBENS J, TŮMA M: *Preconditioner Updates for Solving Sequences of Linear Systems in Matrix-Free Environment*, submitted to NLAA in 2008.
- BIRKEN PH, DUINTJER TEBBENS J, MEISTER A, TŮMA M: *Preconditioner Updates Applied to CFD Model Problems*, Applied Numerical Mathematics vol. 58, no. 11, pp.1628–1641, 2008.
- DUINTJER TEBBENS J, TŮMA M: *Improving Triangular Preconditioner Updates for Nonsymmetric Linear Systems*, LNCS vol. 4818, pp. 737–744, 2007.
- DUINTJER TEBBENS J, TŮMA M: *Efficient Preconditioning of Sequences of Nonsymmetric Linear Systems*, SIAM J. Sci. Comput., vol. 29, no. 5, pp. 1918–1941, 2007.

Thank you for your attention!

Supported by project number KJB100300703 of the grant agency of the Academy of Sciences of the Czech Republic.