On a Black-Box Preconditioner Update for Solving Sequences of Nonsymmetric Linear Systems in Matrix-free Environment

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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 ?

Below we list some known strategies.

- Very simple trick: Hot starts, i.e. use the solution of the previous system as initial guess. A little more sophisticated is extrapolation of the current solution.

- If the linear solver is a Krylov subspace method, strategies to recycle information gained from previously generated Krylov subspaces can be beneficial in many applications [Parks, de Sturler, Mackey, Johnson, Maiti - 2006], [Giraud, Gratton, Martin - 2007], [Frank, Vuik - 2001].

1. Introduction: Efficient solution of sequences

- Sometimes exact updating of the LU decompositions for large problems is feasible: Rank-one updates of LU factorizations have been used since decades in the simplex method where the change of one system matrix to another is restricted to one column [Bartels, Golub, Saunders - 1970; Forrest, Tomlin - 1972 ; Suhl, Suhl - 1993].

- In nonlinear systems solved with a Newton-type method one can 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.

1. Introduction: Efficient solution of sequences

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

- 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].

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

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

We would like M^+ to be an update of M that is as powerful as M itself.

If $||A - M||$ is the accuracy of the preconditioner M for A, we will try to find an updated M^+ for A^+ with comparable accuracy,

$$||A - M|| \approx ||A^+ - M^+||.$$

2. The considered preconditioner updates

Let M be factorized as

$$M = LDU \approx A,$$

then the choice

$$M^+ = LDU - B$$

would give $||A - M|| = ||A^+ - M^+||$.

We will approximate this ideal update $LDU - B$ in two steps, similarly to the techniques in [Benzi, Bertaccini - 2003, Bertaccini - 2004]. First we use

$$LDU - B = L(DU - L^{-1}B) \approx L(DU - B) \quad \text{or}$$

$$LDU - B = (LD - BU^{-1})U \approx (LD - B)U$$

depending on whether L is closer to identity or U. Define the standard splitting

$$B = L_B + D_B + U_B.$$

2. The considered preconditioner updates

Then the second approximation step is

$$L(DU - B) \approx L(DU - D_B - U_B) \equiv M^+$$

(upper triangular update) or

$$(LD - B)U \approx (LD - L_B - D_B)U \equiv M^+$$

(lower triangular update). Then 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 $L, U, triu(B)$	$A^+, triu(A), L, U$

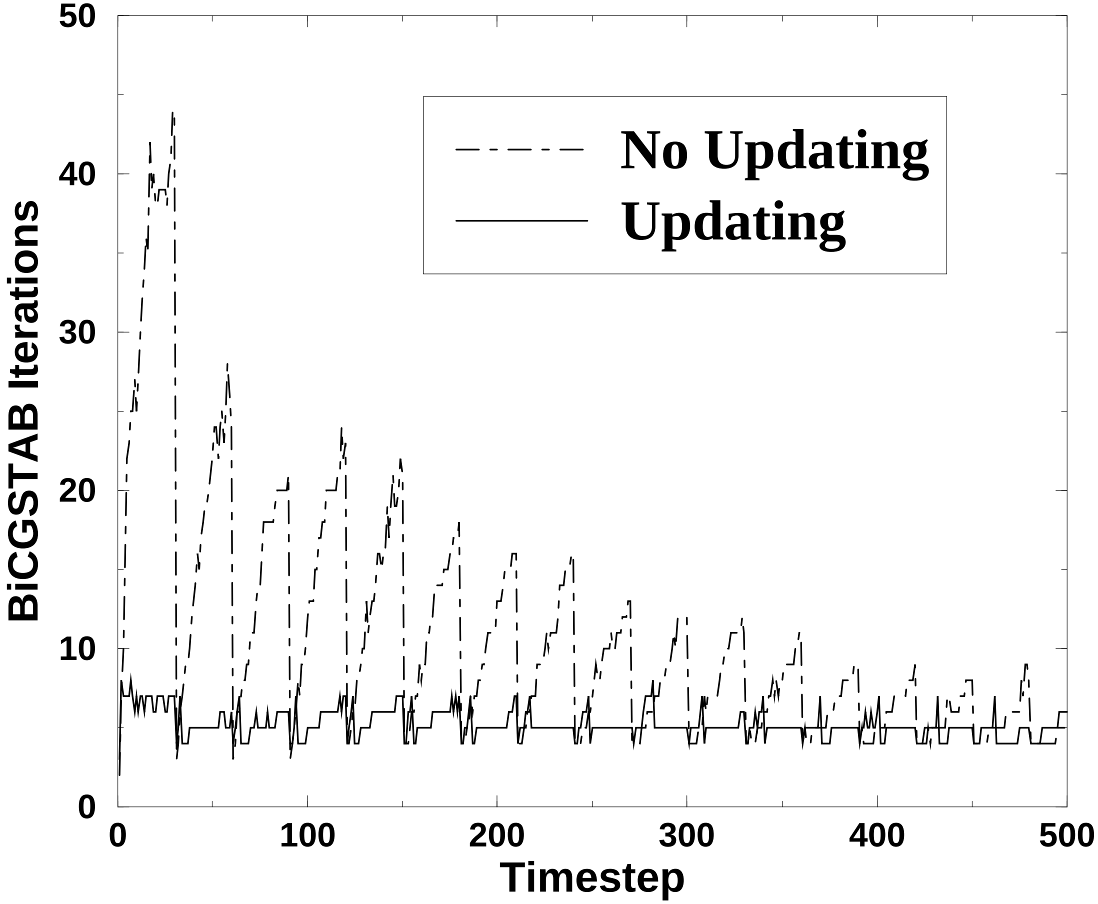
- This is the basic idea; more sophisticated improvements are possible
- Ideal for upwind/downwind modification but our experiments cover broader spectrum of problems

2. The considered preconditioner updates

Consider the following CFD problem (compressible supersonic flow):

- Frontal flow with Mach-number 10 around a cylinder, which leads to a steady state.
- 500 steps of the implicit Euler method are performed.
- The grid consists of 20994 points, we use Finite Volume discretization and system matrices are of dimension 83976. The number of nonzeroes is about 1.33$\cdot 10^6$ for all matrices of the sequence.
- In the beginning, a strong shock detaches from the cylinder, which then slowly moves backward through the domain until reaching the steady state position.
- The iterative solver is BiCGSTAB with stopping criterion 10^{-7}, the implementation is in C++.

2. The considered preconditioner updates



BiCGSTAB iterations for the first 500 systems in the cylinder problem

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, one uses 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 leads to 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

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

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

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

Table 1: *Sequence from structural mechanics problem of dimension 4.936 solved by preconditioned GMRES(40).*

ILUT(0.001,20), Psize $\approx$ 404 000						
Matrix	Recomp		Freeze		Updated	
	its	fevals	its	fevals	its	fevals
$A^{(0)}$	187	89	187	89	187	89
$A^{(1)}$	89	89	393	0	146	25
$A^{(2)}$	126	89	448	0	182	25
$A^{(3)}$	221	89	480	0	184	25
$A^{(4)}$	234	89	513	0	190	25
$A^{(5)}$	193	89	487	0	196	25
$A^{(6)}$	178	89	521	0	196	25
$A^{(7)}$	246	89	521	0	196	25
overall fevals	2 186		3 639		1 966	

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 separable function components, 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

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

3. Updates in matrix-free environment

In

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

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, we have 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, $triu(B)$, 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

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

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 $R = 50$ and a 91×91 grid.
- We use a Newton-type method and solve the resulting 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

Table 2: *Sequence from nonlinear convection-diffusion problem of dimension 8 281 with Reynolds number 50 solved with preconditioned BiCGStab with flexible stopping criterion. The reference preconditioner is ILU(0).*

	Freeze	Recomp.	Lower tr. update	Upper tr. update
linear solver iterations	410	122	153	186
Newton iterations	9	9	9	9
overall time in seconds	4.39	4.29	2.25	2.73

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.
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Thank you for your attention!

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