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For a few iterations less

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The purpose of this talk is to give a method that solves a large linear systems with multiple right-hand sides efficiently. We focus on Block Generalized Minimum Residual-like methods.

Given an m-by-m nonsingular matrix A and an initial set r_0 of p_0 residuals, at step n of the algorithm, the (Block) Krylov subspace $\mathcal{K}_n(A, r_0) = [r_0, Ar_0, A^2 r_0, ..., A^n r_0]$ is constructed and an approximate (Block) solution x_n is given to realize

$$\min_{x \in \mathcal{K}_n(A, r_0)} = \|r_0 - Ax\|_{frobenius}.$$

We note r_n the residual associated to x_n and observe that $\mathcal{K}_n(A, r_0) = [r_0, Ar_0, Ar_1, \ldots, Ar_{n-1}]$.

During the iterations, residuals tend to be colinear. In exact arithmetic, if the residuals become rank deficient ($r_n = u_n s_n$ with u_n an m-by-p_n nonsingular matrix and s_n a p_n-by-p_0 matrix with $p_n < p_0$), then it amounts that the Krylov expansion at step $(n+1)$ can be made via u_n instead of r_n (or $A^{n-1} r_0$). This reduction of the size of the block used in the expansion process is called *deflation* and enables to save useless matrix-vector products (in Block CG and Block QMR, it also have the interest of stabilizing the method). A short bibliography of may be : Block CG [1], Block GMRES [2], Block QMR [4].

In this talk, the question of deflation is addressed in several points :

1. In exact arithmetic, Block GMRES enables deflations; and that even if the Krylov basis is not directly based upon the residuals. If at step n, the residuals become linearly dependent, the associated Krylov block also; and reciprocally.

2. We report numerical results where, while the block residuals become strongly deficient, the expansion vectors in Block GMRES are still well conditioned. Therefore no obvious deflation appears. This violates first item.

3. If aggressive deflation is performed in the Krylov basis upon the loss of independency of the residuals (several strategies are tried), the convergence is noticeably delayed.

4. A simple way to have a stable algorithm with deflation is to use Block GCR since the expansion is based directly on the residuals.

5. We give a criterion to deflate the block-residual in Block-GCR while maintaining stability (numerical experiments are provided)

6. Finally, an algorithm based on an "expansion on the principal direction of the residuals" is given and tested. Numerical experiments let think that this algorithm is the strategy that enables to converge in the less matrix-vector products for Block GCR. This algorithm is a variant to the block GCR given by Paul Soudais [3].

Two last points. First, the main drawback of GCR opposed to GMRES is that GCR needs twice as memory as GMRES. However, we intend to use this algorithm in an inner–outer scheme. In that case FlexibleGMRES(outer)/GMRES(inner) versus GCR(outer)/GMRES(inner) have the same storage requirements. Second, item 1 and 2 have also been remarked by Mickaël Robbé and Miloud Sadkane [5], some French colleagues, they also propose an alternative to Block-GMRES that performs deflation while maintaining the convergence rate. The resulting algorithm is more close to Block GCR than BlockGMRES. Some comparisons between our work and their work is under way.

1. Dianne P. O'Leary. The Block Conjugate Gradient Algorithm and Related Methods. *Linear Algebra and its Applications*, 29:293–32, 1980.

2. Brigitte Vital. *Étude de quelques méthodes de résolution de problèmes linéaires de grande taille sur multiprocesseur*. Ph.D. dissertation, Université de Rennes, November 1990.

3. Paul Soudais. Iterative solution of a 3–D scattering problem from arbitrary shaped multidielectric and multiconducting bodies. *IEEE Antennas and Propagation Magazine*, 42(7):954–959, 1994.

4. Roland W. Freund and Manish Malhotra. A Block QMR Algorithm for Non-Hermitian Linear Systems With Multiple Right-Hand Sides". *Linear Algebra and its Applications*, 254(1–3):119–157, 1997.

5. Mickaël Robbé and Miloud Sadkane. Theoretical numerical analysis of breakdown in block versions of FOM and GMRES methods. Personnal communication, 2003.