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Block GMRES With a New Deflation Strategy

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In the last ten years there has been considerable interest in iterative solvers for linear systems of equations with multiple right-hand sides. There exist mainly two basic approaches: (i) using a seed system that reduces cost when a "normal" Krylov space method is subsequently applied to other right-hand sides and (ii) generalizing Krylov space methods to block Krylov space methods that treat all right-hand sides simultaneously (which requires all to be available at once). A typical and seemingly straightforward method of the second kind is block GMRES.

Block Krylov space methods have two major potential advantages over ordinary Krylov space methods. Firstly, when they are applied to a system with, say, s right-hand sides, typically s matrix-vector products can be computed at once. On most of today's computers, even on those with a single processor, this takes considerably less time than to compute s times a single matrix-vector product.

Secondly, after n iterations with a total of ns matrix-vector products, the dimension of the search space for the approximate solutions can be up to s times larger than if we apply the ordinary Krylov space solver individually to all s right-hand sides. Therefore the cost per system may asymptotically decrease by as much as a factor of s. Unfortunately, in practice we often see little benefit from this potential speedup.

There is, however, another closely related aspect: the s approximate solutions obtained after n steps may approximately live in an affine space of much smaller dimension than ns, because the corresponding residuals may be approximately linear dependent. By detecting this dependency and taking appropriate action (normally called "deflation", although this notion is used in other situations too), we can reduce the number of matrix-vector products needed significantly.

In exact arithmetic, deflation and its effect on the minimum dimension of the block Krylov space that contains the exact solution is well understood. It is related to the so-called block grade of the system, which was the topic of our talk at Copper Mountain in 2006. It is also known how, in exact arithmetic, deflation can be built into block GMRES. In particular, deflation can be checked for and taken care of in the block Arnoldi process; there is no need to check directly (at high cost) for the linear dependence of the s residuals except at the beginning and at restarts. However, Julien Langou pointed out at the above mentioned talk that, in practice, i.e., in finite precision arithmetic, block GMRES is not as effective as one would hope for, even if the deflation process is adapted to treat nearly linear dependent situations in an analogous way. (He had pointed out this before in his talk at Copper Mountain in 2004.) We had observed similarly disappointing outcomes in small examples we had tried.

In this talk we will propose a completely different deflation strategy based on checking the block quasi-residuals for approximate linear dependence. To achieve a reduction of the number of matrix-vector products deflation still needs to be enforced in the block Arnoldi process, however.