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Computers and Structures 83 (2005) 2414–2422

Computers & Structures

www.elsevier.com/locate/compstruc

New implementation of QMR-type algorithms

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Received 25 November 2003; accepted 17 March 2005
Available online 22 August 2005

Abstract

Quasi-minimal residual algorithms, these are QMR, TFQMR and QMRCGSTAB, are biorthogonalisation methods for solving nonsymmetric linear systems of equations which improve the irregular behaviour of BiCG, CGS and BiCG-STAB algorithms, respectively. They are based on the quasi-minimisation of the residual using the standard Givens rotations that lead to iterations with short term recurrences. In this paper, these quasi-minimisation problems are solved using a different direct solver which provides new versions of QMR-type methods, the modified QMR methods (MQMR). MQMR algorithms have different convergence behaviour in finite arithmetic although are equivalent to the standard ones in exact arithmetic. The new implementations may reduce the number of iterations in some cases.

In addition, we study the effect of reordering and preconditioning with Jacobi, ILU, SSOR or sparse approximate inverse preconditioners on the performance of these algorithms.

Some numerical experiments are solved in order to compare the results obtained by standard and modified algorithms.

Keywords: Nonsymmetric linear systems; Sparse matrices; Krylov subspace methods; Quasi-minimal residual methods; Preconditioning; Reordering

1. Introduction

The application of discretization techniques to obtain approximate solutions of partial differential equations generally leads to large and sparse linear systems of equations,

$$Ax = b \tag{1}$$

Direct solvers have the disadvantage of producing the fill-in effect which affects the memory requirements and the computational cost. However, iterative methods based on Krylov subspaces present some advantages with respect to direct ones and other iterative solver.

For systems with symmetric positive definite matrix, the conjugate gradient algorithm [20] is in general the best choice. Nevertheless, for nonsymmetric systems, there exist different families of methods [23], each of them with its own characteristics of robustness and efficiency. Orthogonalisation methods such as GMRES [25] are constructed using a minimisation procedure in a Krylov subspace generated by A, what produces a smooth monotonic convergence but at the expense of

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0045-7949/$ - see front matter
doi:10.1016/j.compstruc.2005.03.026

increasing cost and memory requirements per iteration. The biconjugate gradient method (BiCG) [9], reference of all biorthogonalisation methods, does not increase the computational cost and memory requirements along the iterations. The procedure is defined by a Galerkin condition instead of a minimisation as GMRES. This leads to an erratic convergence behaviour with strong oscillation of the residual norm. In addition, this algorithm includes a matrix-vector product with A^{T} per iteration and there exists a double possibility of break-down. Sonneveld [26] proposes a transpose-free algorithm, the conjugate gradient squared (CGS), a faster converging alternative to BiCG when the latter converges, but with the same convergence problems. In order to improve and smooth the convergence of the previous biorthogonalisation methods, van der Vorst [28] presents the BiCGSTAB which has a better performance in most of the cases but does not eliminate the break-downs.

Freund and Nachtigal [12] propose another biorthogonalisation approach, the quasi-minimal residual method (QMR), which solves the rest of the BiCG problems, although it is not transpose free. Each iteration is characterised by a quasi-minimisation of the residual norm, leading to a smoother convergence without strong oscillations. The break-down in BiCG due to nonexistent iterates is avoided. On the other hand, this method uses a look-ahead variant of the nonsymmetric Lanczos algorithm [13,14] for generating the basis of the Krylov subspace, which eliminates the other case of possible break-down of BiCG. However, in some applications A is only accessible by approximations and not explicitly. In such cases, A^{T} is not readily available. The transpose-free QMR algorithm (TFQMR) [11] is a quasi-minimal residual version of the CGS algorithm that smoothes its convergence without involving A^{T}-vector products. Following the same procedure, Chan et al. [5] propose a QMR variant of the BiCGSTAB algorithm (QMRCGSTAB), which simultaneously takes advantage of the quasi-minimisation of the residual and the transpose-free characteristic of BiCGSTAB. Nevertheless, the differences between TFQMR and CGS is more appreciable than those between QMRCGSTAB and BiCGSTAB due to the smoother behaviour of the latter compared to CGS. The relation between both families of algorithms is well illustrated in [29], where the quasi-minimal residual methods are derived by using residual smoothing techniques in BiCG, CGS and BiCGSTAB algorithms, respectively.

The behaviour of these methods improves considerably when preconditioning is used [1,24,4,27]. These techniques consist of transforming the original system (1) into another $\overline{A}\bar{x} = \bar{b}$, which provides the same solution, where $\overline{A}$ has a lower condition number. Implicit preconditioners construct approximations of matrix A that are easily reversible or suitable to factorise, for example, Jacobi, SSOR and ILU. More recently, the possibilities of parallel computing have led to explicit preconditioners that directly approximate the inverse of A. In [19,22] it is obtained such approximate inverse M by minimising the Frobenius norm of matrix $AM - I$. Also a factorised approximate inverse is proposed in [2].

The effect of reordering techniques on the convergence of preconditioned Krylov methods has been studied by several authors. In [7,3] it is observed that reordering has not a beneficial effect in the convergence behaviour of the conjugate gradient method with incomplete factorisation preconditioning. However, these techniques considerably improve the convergence of other Krylov subspace methods for solving nonsymmetric linear systems [8,3,10].

In Section 2 we summarise the formulation of the standard QMR algorithm and introduce its modified version. Next, in Sections 3 and 4, respectively, the modified TFQMR and QMRCGSTAB methods are developed. Section 5 is devoted to some numerical experiments in order to compare the proposed algorithms with other Krylov subspace methods, including the standard QMR-type algorithms. Finally, in Section 6 we present the concluding remarks of this paper.

2. Modified QMR method

The approximate solution using the standard QMR method for the Krylov subspace of order k is

$$x_k = x_0 + V_k u \tag{2}$$

where u minimises the norm,

$$\|\gamma e_1 - \overline{T}_k u\|_2 \tag{3}$$

which is a simplification of the residual norm,

$$\|r\|_2 = \|V_{k+1}(\gamma e_1 - \overline{T}_k u)\|_2 \tag{4}$$

where V_k is the matrix which columns are the vectors v_i, $i = 1, \ldots, k$, obtained by Lanczos biorthogonalisation procedure, $\gamma = \|r_0\|_2$, and matrix $\overline{T}_k$ is

$$\overline{T}_k = \begin{pmatrix} T_k \\ \delta_{k+1} e_k^t \end{pmatrix} \tag{5}$$

with

$$T_k = \begin{pmatrix} \alpha_1 & \beta_2 & & \cdot & & & \\ \delta_2 & \alpha_2 & \beta_3 & \cdot & & & \\ & \delta_3 & \alpha_3 & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & \cdot & \alpha_{k-2} & \beta_{k-1} & \\ & & & \cdot & \delta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & \cdot & & \delta_k & \alpha_k \end{pmatrix} \tag{6}$$