A PARALLEL IMPLEMENTATION OF THE RESTARTED GMRES ITERATIVE METHOD FOR NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS

RUDNEI DIAS DA CUNHA * AND TIM HOPKINS †

Abstract. We describe the parallelisation of the GMRES(c) method and its implementation on distributed-memory architectures, using both networks of transputers and networks of workstations under the PVM message-passing system. The test systems of linear equations considered are those derived from five-point finite-difference discretisations of partial differential equations.

A theoretical model of the computation and communication phases is presented which allows us to decide for which values of the parameter c our implementation executes efficiently. The results show that for reasonably large discretisation grids the implementations are effective on a large number of processors.

AMS(MOS) subject classifications. 65F10, 65N22, 65Y05, 65Y20

1. Introduction. In [17] Saad and Schultz describe the Generalised Minimum Residual (GMRES) iterative method for the solution of *nonsymmetric* non-singular systems of n linear equations,

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

GMRES was developed to solve (1) when A is not positive real (i.e., the symmetric part of A, $1/2(A + A^T)$, is not positive definite). Two other methods, the Generalised Conjugate Residual (GCR) [11] and ORTHODIR [19] often fail to solve such systems; GCR sometimes suffers from breakdown (i.e., a variable becomes undefined due to a division by zero) and ORTHODIR is less numerically stable than GCR. GMRES never breaks down, unless it has already converged to a solution and requires substantially less storage and arithmetic operations than GCR.

One difficulty that may arise with GMRES in extreme cases is that, because the storage space required by the method increases with the number of iterations, it may be impossible to obtain a solution on a particular hardware system. For some systems, it is possible to use a restarted version, GMRES(c), which considerably reduces the amount of storage required.

In this paper, we consider parallelising the restarted version. We provide analytical and experimental results obtained for the two parallel implementations developed: one using `occam2` on transputers and the other using Fortran77 on a network of Sun workstations, under the PVM message-passing system [1].

A brief overview of the paper is as follows. Section 2 describes the GMRES(c) method and its properties. The parallelisation of the method and different approaches proposed by

* CENTRO DE PROCESSAMENTO DE DADOS, UNIVERSIDADE FEDERAL DO RIO GRANDE DO SUL, BRASIL AND COMPUTING LABORATORY, UNIVERSITY OF KENT AT CANTERBURY, U.K.

† COMPUTING LABORATORY, UNIVERSITY OF KENT AT CANTERBURY, U.K.

other authors are discussed in §3 and results and a complexity analysis of the parallel implementations are given in §4. Finally we give our conclusions in §5.

2. Description of GMRES(c). We first consider the non-restarted GMRES algorithm. It is a modification of the Full Orthogonalisation method [16] which uses the Arnoldi process to compute an orthonormal basis $\{v_1, v_2, \ldots, v_k\}$ of the Krylov subspace $\mathcal{K}_k(A, v_1, k)$. The solution $x^{(k)}$ is taken as $x^{(0)} + Vy^{(k)}$, where V is the matrix whose columns are the vectors v_k computed by the Arnoldi process. The vector $y^{(k)}$ is obtained by solving the system $H^{(k)}y^{(k)} = \beta^{(k)}e_1$, where $H^{(k)}$ is a $k \times k$ upper Hessenberg matrix, whose entries are generated during the Arnoldi orthogonalisation, $\beta^{(k)} = ||\, r^{(0)} \,||_2$, $r^{(0)} = b - Ax^{(0)}$, and e_1 is the canonical vector $(1, 0, \ldots, 0)^T$ of dimension k.

GMRES possesses four important characteristics

1. It never breaks down unless convergence has already been achieved [17, Proposition 2, pp. 865],
2. It converges in at most n iterations [17, Corollary 3, pp. 865],
3. Convergence is monotonic, i.e., $||\, r^{(k+1)} \,||_2 \leq ||\, r^{(k)} \,||_2$. Strict monotonicity is possible if the field of values of A lie in the open right half-plane (see [15, pp. 9]), and
4. The number of vectors of order n that need to be stored grows linearly with k and the number of multiplications grows quadratically.

The last item above is the motivation for the use of a restarted version of GMRES. Instead of generating an orthonormal basis of dimension k, one chooses a value c, $c \ll n$, and generates an approximation to the solution using an orthonormal basis of dimension c. Clearly with this scheme the amount of storage needed may be estimated beforehand and kept within the limits available.

Although GMRES(c) does not break down [17, pp. 865], it may, depending on the system and the value of c, produce a stationary sequence of residuals, thus not achieving convergence. A result given by Saad and Schultz [17, Corollary 6, pp. 867] shows that if A is positive real GMRES(c) converges for any $x^{(0)}$ provided that c is larger than a certain minimum value. This bound on c is not sharp and GMRES(c) may converge even if c is less than the minimum. Determination of this minimum value involves knowledge of the eigenvalue distribution of A and is thus useful in special cases only. It should be noted that the rate of convergence of GMRES(c) increases or remains constant when c is increased.

The two compute intensive operations in GMRES(c) are the Arnoldi process and the solution of the least-squares problem

$$\bar{H}^{(c)}y^{(c)} = \beta^{(k)}e_1 \tag{2}$$

The first is rich in vector-vector operations and the implications of this property for the parallelisation of the method are discussed more fully in §3. The solution of (2) is obtained using the QR factorisation of $\bar{H}^{(c)}$; $y^{(c)}$ being the solution of the triangular system

$$Ry^{(c)} = g, \quad g = Q\beta^{(k)}e_1 \tag{3}$$

where R is a $(c+1) \times c$ triangular matrix whose last row is zero, and Q is a $(c+1) \times (c+1)$ matrix. The matrix Q is the product of the Givens' rotation matrices $G_c \cdot \ldots \cdot G_j \cdot \ldots \cdot G_1$

where $G_j = G(j, j+1, \theta_j)$. Since Q is multiplying $\beta^{(k)}e_1$ we note that the vector g is of the form

$$g_j = \beta^{(k)} \left(\prod_{i=1}^{j-1} \xi_i \right) \eta_j, \quad j = 1, 2, \ldots, c$$

where $\eta_j = \cos\theta_j$ and $\xi_j = \sin\theta_j$.

During the j-th step of the Arnoldi process a new column of $\bar{H}^{(c)}$ is produced (note that $\bar{H}^{(c)}$ is stored in the factored form R). The matrix R is then updated by applying the previous Givens' rotations to the first $j-1$ rows of the new column and a new Givens' rotation is applied to zero the $(j+1, j)$-th element. Initialising g as $(\beta^{(k)}, \beta^{(k)}, 0, \ldots, 0)^T$ we may update the vector g using the steps below in the order shown

$$\begin{aligned} g_j &= \eta_j g_j \\ g_{j+1} &= \xi_j g_{j+1} \\ g_{j+2} &= g_{j+1} \end{aligned}$$

thus avoiding the need to compute Q explicitly with the corresponding savings in arithmetic operations and storage.

A feature of both GMRES and GMRES(c) is that the residual norm of the approximate solution can be obtained without explicitly computing $x^{(k)}$. The norm of the residual is given by

$$||\, \beta^{(k)}e_1 - \bar{H}^{(c)}y^{(c)} \,|| = ||\, Q(\beta^{(k)}e_1 - \bar{H}^{(c)}y^{(c)}) \,|| = ||\, g - Ry^{(c)} \,||$$

and by (3) this norm is $|\, g_{k+1} \,|$ since the last row of R is zero.

2.1. Preconditioning. We consider here the use of GMRES(c) applied to the *left*-preconditioned system,

$$N_m^{-1}Ax = N_m^{-1}b$$

where N_m^{-1} is the preconditioning matrix obtained by the Neumann incomplete series,

$$N_m^{-1} = \left(\sum_{i=1}^{m} (I - D^{-1}A)^i \right) D^{-1} \tag{4}$$

where $D = diag(A)$.

This preconditioner was first introduced by Dubois *et al.* [10] in the solution of symmetric positive-definite systems. In [4] and [9] we provide evidence that this polynomial preconditioner with $m = 1$ is effective for nonsymmetric systems as well. The main advantage of this preconditioner is that it is easily parallelised since it may be expressed as a sequence of matrix-vector products and vector accumulations.

2.2. Algorithmic formulation of GMRES(c). We present below an algorithmic formulation of GMRES(c).

GMRES(c):
1. $r^{(0)} = b - N_m^{-1} A x^{(0)}$
2. $\beta^{(0)} = || \, r^{(0)} \, ||_2$

for $k = 0, 1, \ldots$

3. $g = (\beta^{(k)}, \beta^{(k)}, 0, \ldots, 0)^T$
4. $V_1 = r^{(k)} / \beta^{(k)}$

   for $j = 1, 2, \ldots, c$

5. $R_{i,j} = V_i^T N_m^{-1} A V_j, \quad i = 1, 2, \ldots, j$
6. $\hat{v} = N_m^{-1} A V_j - \sum_{i=1}^{j} R_{i,j} V_i$
7. $R_{j+1,j} = || \, \hat{v} \, ||_2$
8. $V_{j+1} = \hat{v} / R_{j+1,j}$
9. % Apply previous Givens' rotations to column j of R
10. % Compute Givens' rotation to zero element $R_{j+1,j}$
11. % Update g

   endfor

12. Solve $R y^{(c)} = g$
13. $x^{(k+1)} = x^{(k)} + V y^{(c)}$
14. if $| \, g_{k+1} \, |$ satisfies tolerance *stop*.
15. $r^{(k+1)} = b - N_m^{-1} A x^{(k+1)}$
16. $\beta^{(k+1)} = || \, r^{(k+1)} \, ||_2$

endfor

where the subscript in V indicate the appropriate columns.

3. Parallelisation of GMRES. The parallelisation of GMRES has been studied by several authors [3][12][13][14][18]. The main approach is to use another formulation to compute the orthonormal basis, in order to avoid the large number of vector-vector operations found in the Arnoldi process. Joubert and Carey [13] generate non-orthogonal bases of Krylov spaces which are then orthogonalised. The least-squares problem (2) is solved using normal equations; since normal equations tend to have a larger condition number than that of the original problem, loss of accuracy and/or a reduced rate of convergence may occur. The hybrid algorithms proposed require a smaller computational effort than the original formulation of GMRES due to the use of shorter, three-term recurrences instead of the Arnoldi procedure.

Calvetti *et al*. propose that the orthonormal vectors are generated using a Newton basis. A QR factorisation is used to factorise a matrix with block structure; the factorisation is carried in each block independently. Results are reported for an IBM3090-600S VF computer; speed-ups for a system of order $n = 40000$ and an orthonormal basis of dimension 10 are 1.58 and 2.00 using 2 and 4 processors respectively. Johan *et al*. used the GMRES(c) method on Finite-Element problems using a Connection Machine CM-2/CM-200 computer. The system (1) is preconditioned using a Cholesky factorisation; symmetric preconditioning is used. The dimension of the Krylov basis for the fluid flow problems solved is small (5 to 15). The solution of the least-squares problem (2) is made locally on the front-end computer. Parallelism is expressed using the data-parallel constructions found in Fortran90.

More recently, Xu *et al*. have proposed a new version, α-GMRES, which increases the rate of convergence of GMRES. The method is a multilevel iterative scheme composed of an outer and an inner iteration; the system formed at each step of the outer iteration is then solved by GMRES. A block diagonal preconditioner and a damping factor, α, were used to enhance the convergence of GMRES. The least-squares problem (2) is solved locally in each processor. Results are given for an implementation on a Meiko Computing Surface for 2, 3 and 4 processors solving a system of order $n = 4805$ with speed-ups of 1.9, 2.8 and 3.5 respectively.

3.1. Details of our parallel implementation. A parallel version of GMRES(c) was obtained using parallel versions of the linear algebra operations which define the method (§2.2) – matrix-vector products, inner-products, vector 2-norms, vector scalings and vector accumulations. Such a set of parallel linear algebra subroutines for distributed-memory architectures has been implemented on a transputer-based multiprocessor machine (see [6] and [7] for details). These have been successfully used to implement other iterative methods, for example, PCG, CGS and Bi-CGSTAB. The same algorithms developed for the transputer implementations were used to generate the Fortran 77/PVM versions and we found that little effort was needed for the conversion process.

The implementation of GMRES(c) defined here was developed to solve systems derived from the five-point, finite-difference discretisation of partial differential equations (PDEs). Discretising using square grids of $l \times l$ internal points leads to sparse systems of order $n = l^2$.

In the next sections we describe the environments in which the implementations were developed and the parallelisation of the linear algebra operations including the partitioning of data among the processors.

3.1.1. Description of the environments. The `occam2` implementation of GMRES(c) was developed under TDS2 on a Meiko Computing Surface using square grids of up to 25 T800-20 transputers each with 4Mbytes of memory. The linear algebra operations were implemented using loop-unrolling techniques, the loops being unrolled to 16 levels [8].

The Fortran 77/PVM version used up to 8 Sun SPARC 2 workstations each with 32Mbytes of memory and a cache memory of 64Kbytes under SunOS 4.1.3 using Ethernet connections. This implementation was developed using the Sun Fortran 77 compiler and PVM version 2.4.1; code was compiled in optimised mode. Our applications use the PVM `vsnd/vrcv` routines which implement the *send/receive* operations. These are faster than the usual *snd/rcv* routines and allow a point-to-point exchange of data between the processes through UNIX TCP sockets without using the PVM dæmons.

3.1.2. Vector-vector operations. We consider here the distributed computation of vector updates (scalings and accumulations) and inner-products. For both implementations, the vectors (of length n) described in the GMRES(c) algorithm, are partitioned into segments of contiguous elements; each processor holds a segment of at most $\lceil n/p \rceil$ elements.

Vector scalings and accumulations are *disjoint element-wise*; the operations performed in each element of the vector operands are independent of the others. Thus, the execution of such operations on a distributed-memory machine incurs no communication overhead between the processors.

For the Fortran 77/PVM implementation the inner-product is computed using a recursive-doubling algorithm for both the accumulation of the partial sums (computed locally in each processor) and the broadcast of the inner-product to the processors. These two phases are completed in $2\lceil \log_2 p \rceil$ steps. We stress here that with PVM 2.4.1 the broadcast operation for the `vsnd` operation is not implemented as a recursive-doubling algorithm but as $p-1$ *send* operations which is an unacceptable overhead.

The inner-product implemented in `occam2` uses an algorithm similar to recursive-doubling, except that the number of steps required for completion of the accumulation and broadcast phases is $4\lfloor \sqrt{p}/2 \rfloor$. We note that for $1 < p < 64$, the number of steps required by this algorithm is less than or equal to that needed using the recursive-doubling algorithm.

3.1.3. Matrix-vector operation. For the `occam2` version we want to exploit the four communication links available on the transputer. This leads us to use grids of $p = p_r \times p_c$ processors (for simplicity we will consider only square grids of $\sqrt{p} \times \sqrt{p}$ processors). Such a topology maps ideally onto the physical discretisation of the PDE. The vectors containing the coefficients that implicitly form A are partitioned using *geometric distribution* by *blocks*. Each processor holds at most $\lceil l/\sqrt{p}\, \rceil \times \lceil l/\sqrt{p}\, \rceil$ elements of each of the coefficient vectors. This distribution allows the use of *nearest-neighbour* communication between the processors when computing matrix-vector products; i.e., each processor exchanges information with at most four neighbouring processors depending on the position of the processor in the grid. The number of grid points exchanged with each neighbour is $\lceil l/\sqrt{p}\, \rceil$.

In the Fortran 77/PVM version the hardware used has just one connection with the Ethernet network. In this case we use *geometric distribution* by *panels* and the processors (workstations) are logically connected as a linear processor array. Each processor then holds at most $l \times \lceil l/p \rceil$ elements of each of the coefficient vectors. Again nearest-neighbour communications are used but each processor has at most two neighbours and, due to the partitioning used, each processor exchanges l grid points with its neighbour(s).

Figure 1 shows the two data partitioning schemes used. The black squares represent points of the PDE discretisation and the white surrounding squares and rectangles represent the processors. The interaction between the processors is indicated by the arrows.

3.1.4. Other considerations. For the solution of the least-squares problem (2) we need a triangular system solver. Triangular solvers are known to offer less efficiency than other linear algebra operations on distributed-memory machines. Our experiences have shown that efficiencies higher than 50% can only be obtained on such machines for large systems (more than 1000 equations) – see [2] and [5]. This rules out the use of a parallel triangular solver in our implementation, since c is usually small. Our approach to this problem was to let each processor have its own copy of R, $y^{(c)}$ and g and to solve the triangular system $Ry^{(c)} = g$ locally. This approach is similar to that used by Xu *et al.* [18].

The update of x in step 13 can be regarded as a sequence of vector scalings and sums by rewriting $x^{(k+1)} = x^{(k)} + Vy^{(c)}$ as $x^{(k+1)} = x^{(k)} + y_j^{(c)} V_j, \quad j = 1, \ldots, c$. These operations can then be performed independently in each processor.

The Arnoldi orthonormalisation process (steps 3–11) makes substantial use of vector-vector operations with low granularity, requiring $(c^2 + c)/2$ inner-products and c vector 2-

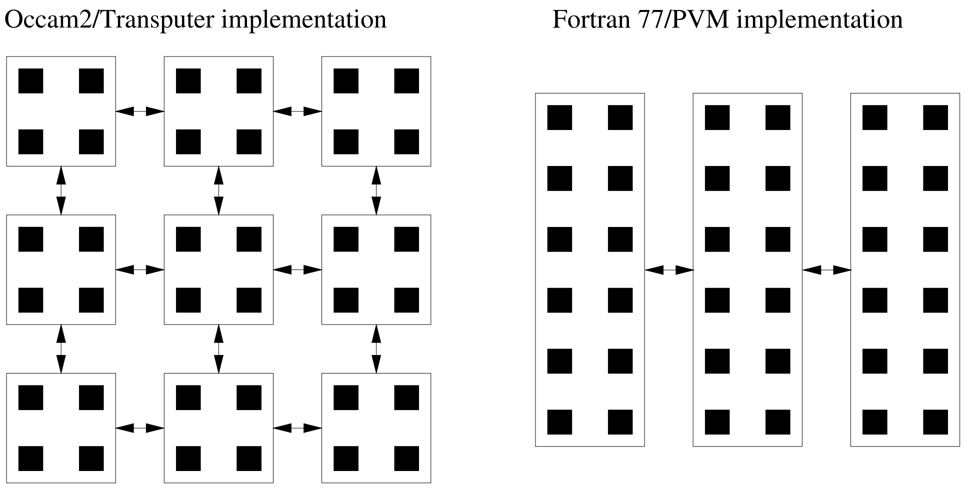


FIG. 1. *Data partitioning and exchange for matrix-vector product.*

norms. Due to the low granularity of these operations, the process has a large overall communication overhead which may only be overcome for large n. The communication load during the Arnoldi process is however minimised since a number of the operations in steps 6, 8, 12 and 13 are executed locally.

4. Results. The test problem used is the system derived from discretising

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + \frac{1}{2}\left(\frac{\partial a u}{\partial x} + a\frac{\partial u}{\partial x}\right) = 1 \tag{5}$$

on the unit square $R = (0,0) \times (1,1)$, where $a = 20e^{3.5(x^2+y^2)}$. Dirichlet conditions $u = 0$ are imposed on ΩR and the first order terms are discretised using central differences.

Equation (5) was discretised on grids with $l = 64$ and 128, the order of the corresponding systems being $n = 4096$ and 16384.

4.1. Scalability of the implementation. In Tables 1 and 2 we list the number of iterations required for convergence and the execution time (in seconds) for the `occam2` and Fortran 77/PVM implementations. The execution time of the `occam2` implementation for $n = 16384$ and $p = 1$ is an estimated time, since the data does not fit in the memory size available; for the same reason we do not list the results for $p = 4$. Note that while increasing c reduces the number of iterations the execution time may still increase. In terms of execution times, the Fortran 77/PVM implementation is considerably faster than the `occam2` implementation due to the more powerful SPARC 2 processor, even at the expense of a higher communication latency in the Ethernet network (see §4.2).

In Figure 2 we show the speed-ups ($S_p = T_1/T_p$) of the parallel implementation of GMRES(c) for the solution of (5) with $c = 10$, 20 and 30, where T_1 is the execution time of a sequential implementation of GMRES(c) and T_p is the execution time of the parallel implementation on p processors.

We note that as n increases the amount of local computation and, hence, the speed-up increases. On the other hand increasing c increases the amount of data communicated

c	k^*	$n = 4096$				
		$p = 1$	$p = 4$	$p = 9$	$p = 16$	$p = 25$
10	611	2902.51	878.43	487.65	284.25	264.88
20	171	2302.04	700.88	391.89	231.58	219.01
30	96	2517.07	771.87	433.14	257.73	245.55
c	k^*	$n = 16384$				
		$p = 1$	$p = 4$	$p = 9$	$p = 16$	$p = 25$
10	4032	77612.87	–	10924.62	5916.36	4590.86
20	1258	68252.86	–	9756.82	5286.04	4138.55
30	469	49846.94	–	7150.41	3875.06	3047.14

TABLE 1

Number of iterations and execution times (in seconds) of the `occam2` *implementation.*

c	k^*	$n = 4096$			
		$p = 1$	$p = 2$	$p = 4$	$p = 8$
10	611	1477.09	640.02	397.15	253.56
20	171	1119.20	477.52	271.89	202.21
30	96	1192.80	522.72	301.20	210.00
c	k^*	$n = 16384$			
		$p = 1$	$p = 2$	$p = 4$	$p = 8$
10	4032	45491.04	23052.96	12075.84	6017.76
20	1258	39148.96	19980.19	10145.77	5009.99
30	469	28192.76	14397.13	7348.06	3640.61

TABLE 2

Number of iterations and execution times (in seconds) of the Fortran 77/PVM implementation.

between the processors (more matrix-vector products, inner-products and vector 2-norms are required per iteration) and thus decreases the speed-up.

The graphs for the Fortran 77/PVM implementation show a superlinear effect which we attribute to the presence of the cache memory.

4.2. Complexity analysis of the parallel implementation. For fixed l and p, we would like to know which values of c will ensure an efficient solution. To help answer this we have developed an analytical model that describes the time taken to perform the floating-point operations and the communication within GMRES(c). For the `occam2` model we consider only square grids of processors. If we consider the *analytical* speed-up

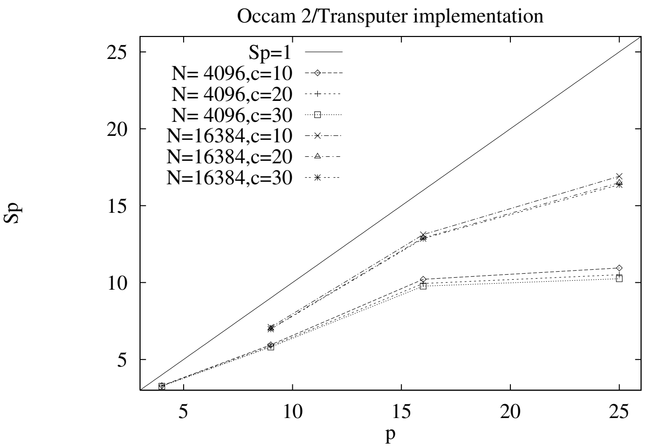
$$S_p^a = \frac{T_{\mathit{flop}}^{\mathit{seq}}}{T_{\mathit{flop}}^{\mathit{par}} + T_{\mathit{comm}}} \tag{6}$$

then we should be able to gain some insight into which values of c an implementation is scalable with respect to the number of processors.

The model for the floating-point operations is taken as

$$T_{\mathit{flop}} = O_* T_* + O_+ T_+ + (kc + 2k + 1) T_{\sqrt{\cdot}} \tag{7}$$

where T_*, T_+ and $T_{\sqrt{\cdot}}$ are the time taken to perform a double-precision multiplication, sum and square-root respectively, taking into account the overhead of addressing the operands.



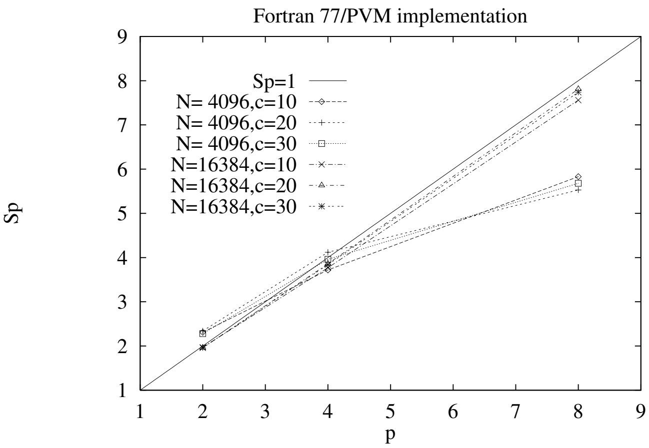


FIG. 2. *Speed-ups of GMRES(c).*

Due to the partitioning of data, the number of arithmetic operations differs between the processors, especially for matrix-vector products, and depends on their relative positions within the processor grid. The expressions for O_* and O_+ for the parallel implementations are obtained for the processors with the highest number of operations. In the `occam2` version these are processors which are not adjacent to an edge of the grid; for the Fortran 77/PVM implementation these processors are those not at the ends of the linear array.

Sequential

$$\begin{aligned} O_* = \quad & (kc^2/2 + 17kc/2 + 6m(kc+k+1) + 9k + 8)l^2 - \\ & 4(m+1)(kc+k+1)l + 3kc^2 + 3kc + k, \\ O_+ = \quad & (kc^2/2 + 13kc/2 + 6m(kc+k+1) + 8k + 6)l^2 - \\ & 4(m+1)(kc+k+1)l - 2kc - 2k - 1, \end{aligned}$$

`occam2`

$$\begin{aligned} O_* = \quad & (kc^2/2 + 7kc/2 + m(kc+k+1) + 4k + 3)\lceil l^2/p \rceil + \\ & 5(m+1)(kc+k+1)\lceil l/\sqrt{p} \rceil^2 + 3kc^2 + 3kc + k, \\ O_+ = \quad & (kc^2/2 + 5kc/2 + 2m(kc+k+1) + 4k + 2)\lceil l^2/p \rceil + \\ & 4(m+1)(kc+k+1)\lceil l/\sqrt{p} \rceil^2 - 3kc - 4k + 2\lfloor \sqrt{p}/2 \rfloor - 2, \end{aligned}$$

$$T_* = 4.364 \cdot 10^{-6}\mathrm{s}, \quad T_+ = 4.114 \cdot 10^{-6}\mathrm{s}, \quad T_{\sqrt{\cdot}} = 1.269 \cdot 10^{-5}\mathrm{s}$$

Fortran 77/PVM

$$\begin{aligned} O_* = \quad & (kc^2/2 + 7kc/2 + m(kc+k+1) + 4k + 3)\lceil l^2/p \rceil + \\ & (kc+k+1)(5lm + 5l - 2m - 2)\lceil l/p \rceil + 3kc^2 + 3kc + k, \\ O_+ = \quad & (kc^2/2 + 5kc/2 + 2m(kc+k+1) + 4k + 2)\lceil l^2/p \rceil + \\ & (kc+k+1)(4lm + 4l - 2m - 2)\lceil l/p \rceil - 3kc - 4k + 2\lceil \log_2 p \rceil - 2, \end{aligned}$$

$$T_* = 1.7 \cdot 10^{-6}\mathrm{s}, \quad T_+ = 1.65 \cdot 10^{-6}\mathrm{s}, \quad T_{\sqrt{\cdot}} = 8.1 \cdot 10^{-6}\mathrm{s}$$

For the communication model, we assume that the time taken to transmit x 64-bit words may be given in the form $T_w(x) = \alpha + \beta x$, where α is the startup time of the communication and β is the time to transfer each word. These parameters are dependent on the communication software and hardware used and were determined by sending messages of different lengths between two processors. The total communication time for the parallel implementations is given by

`occam2`

$$T_{comm} = \begin{array}{l}(kc^2/2 + 3kc/2 + 2k + 1)4\lfloor\sqrt{p}/2\rfloor T_w(1)+ \\ (m+1)(kc+k+1)4T_w(\lceil l/\sqrt{p}\rceil)\end{array} \tag{8}$$

$$\alpha = 2.81 \cdot 10^{-4}\text{s}, \quad \beta = 8.66 \cdot 10^{-6}\text{s},$$

where the terms $4\lfloor\sqrt{p}/2\rfloor T_w(1)$ and $4T_w(\lceil l/\sqrt{p}\rceil)$ represent the time taken to transfer the data during the calculation of the inner-products and matrix-vector products respectively.

Fortran 77/PVM

$$T_{comm} = \begin{array}{l}(kc^2/2 + 3kc/2 + 2k + 1)2\lceil log_2 p\rceil T_w(1)+ \\ (m+1)(kc+k+1)2T_w(l)\end{array} \tag{9}$$

$$\alpha = 2.70 \cdot 10^{-4}\text{s}, \quad \beta = 1.22 \cdot 10^{-5}\text{s},$$

where the terms $2\lceil log_2 p\rceil T_w(1)$ and $2T_w(l)$ represent the time taken to transfer the data during the calculation of the inner-products and matrix-vector products respectively.

We note that Equation (8) is an *upper-bound* for the communication time since it does not take into account the fact that use of the communication links in the grid of processors is not synchronous – for example, it is possible that while one link is transferring data for a matrix-vector product another is transferring data for an inner-product.

To obtain the values of c, we may consider that an acceptable speed-up is obtained if $S_p^a \geq p/2$. If we consider $S_p^a = p/2$ then we may compute the roots of the quadratic equation in c

$$2T_{flop}^{seq} - p(T_{flop}^{par} + T_{comm}) = 0 \tag{10}$$

The roots of (10) then give the desired information about scalability

- If the roots are complex, then there is no value of c for which $S_p^a \geq p/2$ is satisfied.
- If the roots are both negative, then for any value of c we achieve $S_p^a \geq p/2$.
- If one root is negative and the other is positive: select the positive root c^+ since $c > 0$ and take any number $c \leq \lfloor c^+\rfloor$.
- Equation (10) cannot have two positive roots. Writing Equation (10) in the form $Ec^2 + Fc + G = 0$ where E, F and G are functions of p, note that there can be two positive roots iff

$$(E < 0 \wedge F > 0 \wedge G < 0) \vee (E > 0 \wedge F < 0 \wedge G > 0) \tag{11}$$

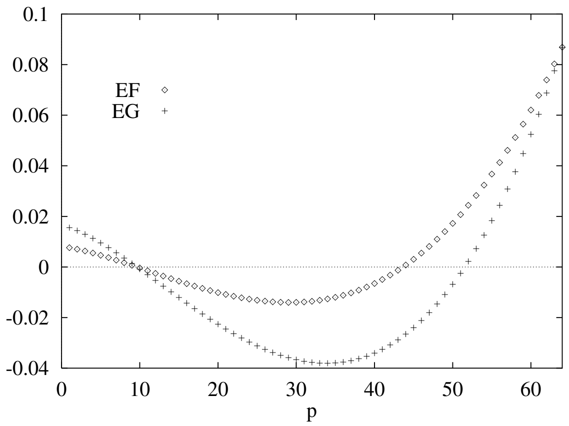


FIG. 3. *Format of curves EF and EG.*

If either $EF > 0$ or $EG < 0$ then the condition above is not satisfied. It can be shown (with the aid of MAPLE) that EF and EG have two real roots (p'_{EF}, p''_{EF}, p'_{EG} and p''_{EG} respectively) where $p'_{EF} = p'_{EG}$ and that, for p large, EF is positive. Figure 3 shows the format of the curves EF and EG. Since the interval $[\, p'_{EF},\, p''_{EF}\,]$ is contained in $[\, p'_{EG},\, p''_{EG}\,]$ it follows that when $EF < 0$, EG is also negative. Thus Condition (11) is not satisfied and Equation (10) cannot have two positive roots.

In Table 3 we list the values of c obtained from the roots of (10) for some values of p and l with $k = 1$ and $m = 1$; the numerical values indicate the maximum c that can be chosen to obtain at least 50% of efficiency. Note that for the `occam2` implementation the values of c are larger than those of the Fortran 77/PVM version. In addition the `occam2` implementation is more effective than the Fortran 77/PVM version for small l. For large l, both implementations are capable of providing good scalability for any value of c with the number of processors, p, considered.

Figure 4 shows the graphs of Equation (6) for different values of l, c and p ($k = 1$ and $m = 1$) using the corresponding equations for the models of the implementations. It can be seen that as the problem size increases it is possible to solve the system efficiently on an increasing number of processors with a larger value of c (note that c is always chosen to be considerably smaller than n). This in turn may allow for a reduction in the overall execution time due to the smaller number of iterations required for convergence when using higher dimensions in the orthonormal basis.

5. Conclusion. A parallel version of GMRES(c) has been implemented using parallel implementations of a set of linear algebra operations, using distributed-memory computers. The parallel algorithm was tested using a transputer-based machine and a network of workstations using the PVM message-passing system. The implementations have been shown to be scalable with respect to the number of processors, especially for large problems.

A theoretical model for the computation and communication phases has been developed and based on this model we show that the communication overheads imposed by Arnoldi orthonormalisation process may be overcome for large n. The `occam2` implementation is more

occam2 implementation										
		p								
l	n	4	9	16	25	36	49	64	81	100
32	1024	299	12	1	N	N	N	N	N	N
64	4096	A	A	19	8	2	1	N	N	N
128	16384	A	A	A	A	29	16	6	4	2
256	65536	A	A	A	A	A	A	355	70	21
512	262144	A	A	A	A	A	A	A	A	A
1024	1048576	A	A	A	A	A	A	A	A	A
Fortran 77/PVM implementation										
		p								
l	n	4	9	16	25	36	49	64	81	100
32	1024	52	N	N	N	N	N	N	N	N
64	4096	A	160	7	N	N	N	N	N	N
128	16384	A	A	A	60	12	2	N	N	N
256	65536	A	A	A	A	A	A	A	58	9
512	262144	A	A	A	A	A	A	A	A	A
1024	1048576	A	A	A	A	A	A	A	A	A

TABLE 3
Values of c for which $S_p^a = p/2$: A="any", N="none".

efficient for smaller problem sizes, mainly due to the small latency of communication. For larger problems, both the occam2 and the Fortran 77/PVM versions are capable of providing speed-ups of more than $p/2$ regardless of the value chosen for c. The main implication of this is that, for the parallel algorithm presented here, it is possible to effectively use networks of workstations even with high latency communications hardware.

An effect that has been detected only in the Fortran 77/PVM implementation is that of superlinearity. We attribute this to the existence of a cache memory on the SPARC2 processor. Thus it may be possible to use this implementation with a larger value of c than that predicted by the model and still obtain a good speed-up.

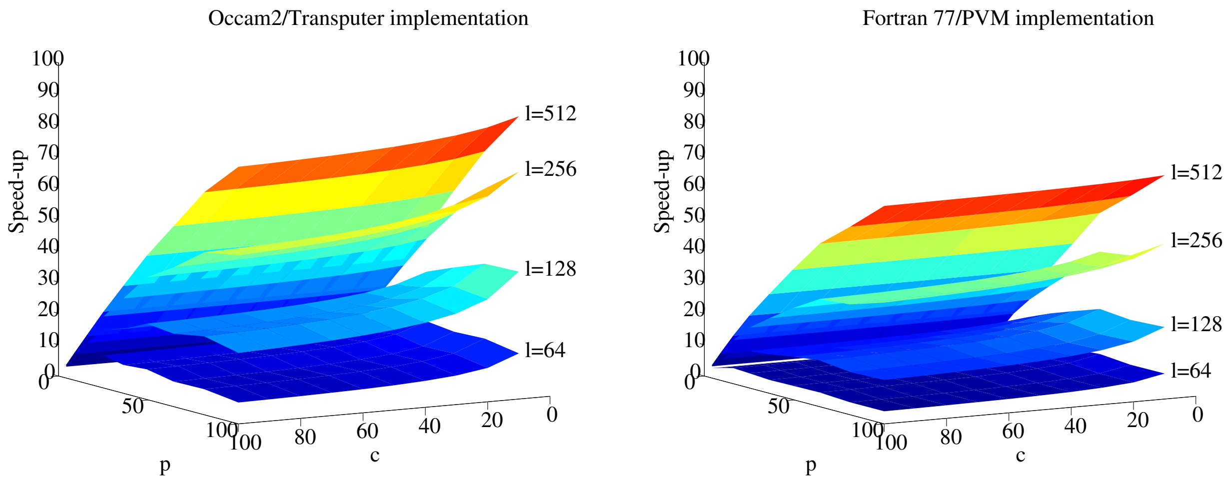


FIG. 4. *Analytical speed-up of GMRES(c).*

As a final note we have also implemented parallel versions of GMRES(c) for generic systems and for problems derived from the seven-point finite-difference discretisation of PDEs in three dimensional regions and have obtained a behaviour similar to that discussed here.

REFERENCES

[1] A. Beguelin, J. Dongarra, A. Geist, R. Manchek, and V. Sunderam, *A user's guide to PVM – Parallel Virtual Machine*, Research Report ORNL/TM-11826, Oak Ridge National Laboratory, 1992.

[2] R. Bisseling and J. van de Vorst, *Parallel triangular system solving on a mesh network of transputers*, SIAM Journal of Scientific and Statistical Computing, 12 (1991), pp. 787–799.

[3] D. Calvetti, J. Petersen, and L. Reichel, *A parallel implementation of the GMRES method*, Research Report ICM-9110-16, Institute for Computational Mathematics, Department of Mathematical Sciences, Kent State University, 1991.

[4] R. da Cunha, *A Study on Iterative Methods for the Solution of Systems of Linear Equations on Transputer Networks*, PhD thesis, Computing Laboratory, University of Kent at Canterbury, July 1992.

[5] R. da Cunha and T. Hopkins, *The parallel solution of triangular systems of linear equations*, in High-Performance Computing II – Proceedings of the Second Symposium on High Performance Computing, Durand, M. and El Dabaghi, F., ed., Amsterdam, October 1991, North-Holland, pp. 245–256. Also as Report No. 86, Computing Laboratory, University of Kent at Canterbury, U.K.

[6] ——, *The Parallel Solution of Partial Differential Equations on Transputer Networks*, Transputing for Numerical and Neural Network Applications, IOS Press, Amsterdam, 1992, pp. 96–109. Also as Internal Report No. 17-92, Computing Laboratory, University of Kent at Canterbury, U.K.

[7] ——, *The Parallel Solution of Systems of Linear Equations using Iterative Methods on Transputer Networks*, Transputing for Numerical and Neural Network Applications, IOS Press, Amsterdam, 1992, pp. 1–13. Also as Internal Report No. 16-92, Computing Laboratory, University of Kent at Canterbury, U.K.

[8] ——, *Increasing the performance of* `occam` *using loop-unrolling*, Internal Report No. 4-93, Computing Laboratory, University of Kent at Canterbury, April 1993. To appear in "Transputer Communications".

[9] ——, *Parallel preconditioned Conjugate-Gradients methods on transputer networks*, Transputer Communications, 1 (1993), pp. 111–125. Also as Internal Report No. 5-93, Computing Laboratory, University of Kent at Canterbury, U.K.

[10] P. Dubois, A. Greenbaum, and G. Rodrigue, *Approximating the inverse of a matrix for use in iterative algorithms on vector processors*, Computing, 22 (1979), pp. 257–268.

[11] S. Eisenstat, H. Elman, and M. Schultz, *Variational iterative methods for nonsymmetric systems of linear equations*, SIAM Journal of Numerical Analysis, 20 (1983), pp. 345–357.

[12] Z. Johan, T. Hughes, K. Mathur, and S. Johnsson, *A data parallel finite-element method for computational fluid-dynamics on the Connection Machine system*, Computer Methods in Applied Mechanics and Engineering, 99 (1992), pp. 113–134.

[13] W. Joubert and G. Carey, *Parallelizable restarted iterative methods for nonsymmetric linear-systems 1 – theory*, International Journal of Computer Mathematics, 44 (1992), pp. 243–267.

[14] ——, *Parallelizable restarted iterative methods for nonsymmetric linear-systems 2 – Parallel implementation*, International Journal of Computer Mathematics, 44 (1992), pp. 269–290.

[15] N. Nachtigal, S. Reddy, and L. Trefethen, *How fast are nonsymmetric matrix iterations?*, numerical analysis report, 90-2, Department of Mathematics, Massachusetts Institute of Technology, March 1990.

[16] Y. Saad, *Krylov subspace methods for solving large unsymmetric systems*, Mathematics of Computation, 37 (1981), pp. 105–126.

[17] Y. Saad and M. Schultz, *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM Journal of Scientific and Statistical Computing, 7 (1986), pp. 856–869.

[18] X. Xu, N. Qin, and B. Richards, *Alpha-GMRES – a new parallelizable iterative solver for large sparse nonsymmetrical linear-systems arising from CFD*, International Journal for Numerical Methods in Fluids, 15 (1992), pp. 613–623.

[19] D. YOUNG AND K. JEA, *Generalized Conjugate-Gradient acceleration of nonsymmetrizable iterative methods*, Linear Algebra and its Applications, 34 (1980), pp. 159–194.