

# s-Step Orthomin and GMRES implemented on parallel computers

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## Abstract

The Orthomin ( **Omin** ) [19] and the Generalized Minimal Residual method ( **GMRES** ) [13] are commonly used iterative methods for approximating the solution of nonsymmetric linear systems. The s-step generalizations of these methods enhance their data locality parallel and properties by forming  $s$  simultaneous search direction vectors. Good data locality is the key in achieving near peak rates on memory hierarchical supercomputers. The theoretical derivation of the s-step Arnoldi and Omin has been published in [3], [9]. Here we derive the s-step GMRES method. We then implement s-step Omin and GMRES on the Cray-2 hierarchical memory supercomputer.

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# 1 Introduction

Several algorithms which improve the data locality for dense linear algebra problems have been suggested for shared memory systems (e.g.see [4] , [10], [14]). These algorithms are based on BLAS3 (Basic Linear algebra level 3). BLAS3 consist of submatrix block operations and they have been proven highly efficient for parallel and vector computers One very important advantage of these algorithms over the standard ones is that their very low ratio of memory references over floating point operations. This allows efficient use of vector registers and local memories. It also reduces the need for frequent synchronizations of the processors. Linear algebra algorithms which improve data locality on distributed memory systems have also been studied (e.g.see [11], [12]).

In the area of iterative methods for solving the linear system

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

with nonsingular BLAS2 modules implementations consisting of one or more single vector operations have been studied in [16],[17]. The  $s$ -step iterative methods [1],[2],[3],[9] use BLAS3 operations. Other authors have considered BLAS3 approaches for iterative methods [6], [15]. The  $s$ -step methods form independent direction vectors using repeated matrix vector multiplication of the coefficient matrix with a single direction or residual vector. This provides coarser granularity and increases the parallelism by computing simultaneously the  $2s$  inner products involved in the evaluation of parameters used in advancing the iterations.

The ratio of memory references per floating point operations becomes of the order  $1/s$  of that of the standard methods in operations consisting of linear combinations and dot products. This also holds true for matrix times vector operations with narrow banded matrices. Such an important class of matrices is the block tridiagonal matrices obtained from discretization of partial differential equations on regular domains. To solve iteratively linear systems with these coefficient matrices on a hierarchical memory supercomputer the  $s$ -step methods would require only  $1/s$  of the number of main memory sweeps required by the standard methods. Also, the  $2s$  inner products required for one  $s$ -step are executed simultaneously. This reduces the need for frequent global communication in a parallel system and will increase delivered performance.

In this article we outline the s-step Omin and Arnoldi methods. We then derive the s-step GMRES method. We compare the s-step methods with the standard methods. The implementation on the Cray-2 parallel vector processor shows that the s-step methods are more efficient than the standard ones. In section 2 we review the Omin and GMRES methods. In section 3 we present the s-step Omin method. In section 4 we review the s-step Arnoldi method and we derive the s-step GMRES method. In sections 5 and 6 we present numerical tests and results. In section 7 we draw conclusions.

## 2 Omin and GMRES

In this section we describe Omin and GMRES [5], [13], [19]. Let  $x_0$  be an initial guess to the solution of (1) and let  $r_0 = b - Ax_0$  be the initial residual. The Omin(k) algorithm can be summarized as follows.

### Algorithm 2.1 Omin(k)

Compute  $r_0$  and set  $p_0 = r_0$ .

**For**  $i = 0, 1, \dots$  **until** convergence **do**

1.  $a_i = \frac{r_i^T Ap_i}{(Ap_i)^T Ap_i}$
2.  $x_{i+1} = x_i + a_i p_i$
3.  $r_{i+1} = r_i - a_i Ap_i$
4.  $b_j^i = \frac{(Ar_{i+1})^T Ap_j}{(Ap_j)^T Ap_j}$  for  $j_i \leq j \leq i$
5.  $p_{i+1} = r_{i+1} - \sum_{j=j_i}^i b_j^{(i)} p_j$
6.  $Ap_{i+1} = Ar_{i+1} - \sum_{j=j_i}^i b_j^{(i)} Ap_j$

**EndFor**

In this algorithm  $j_i = \min(0, i - k + 1)$  for Omin(k). Fixing  $j_i = 0$  yields the Generalized Conjugate Residual algorithm (**GCR**) [5] which is equivalent to GMRES. For Computational cost we count only vector operations as inner products, vector updates and matrix vector products (**Mv**). For Omin(k) each iteration (with  $k \leq i - 1$ ) needs:  $k + 2$  inner products,  $2k + 2$  vector updates and 1 Mv.

The GMRES method [13] is based on the Arnoldi procedure for computing an  $l_2$ -orthonormal basis  $q_1, q_2, \dots, q_j$  of the Krylov subspace  $\mathbf{K}_m = \text{span}\{q_1, Aq_1, \dots, A^{m-1}q_1\}$ . If  $Q_j$  is the  $n \times j$  matrix whose columns are the  $l_2$ -orthonormal basis  $\{q_1, q_2, \dots, q_j\}$ , then  $H_j = Q_j^T A Q_j$ , is the upper  $j \times j$  Hessenberg matrix whose entries are the scalars  $h_{i,l}$  generated by the Arnoldi method. GMRES consists of an Arnoldi procedure and an error minimization step. We next present one cycle of the restarted GMRES( $m$ ) method. The norm of the residual is monitored for the convergence check.

**Algorithm 2.2** GMRES( $m$ )

Compute  $r_0$  and set  $q_1 = \frac{r_0}{\|r_0\|}$

**For**  $j = 1, \dots, m - 1$

1.  $h_{i,j} = q_i^T A q_j, 1 \leq i \leq j$
2.  $\hat{q}_{j+1} = A q_j - \sum_{i=1}^j h_{i,j} q_i$
3.  $h_{j+1,j} = \|\hat{q}_{j+1}\|_2$
4.  $q_{j+1} = \hat{q}_{j+1} / \|\hat{q}_{j+1}\|_2$

**EndFor**

Form the approximate solution:  $x_m = Q_m y_m$ , where  $y_m$  minimizes

$$J(y) = \|\beta e_1 - G_m y\| \quad e_1 = [1, \dots, 0]^T. \quad (2)$$

The matrix  $G_m$  is the same as  $H_m$  except for an additional row whose only nonzero element is  $h_{m+1,m}$  in the  $(m+1, m)$  position. Minimizing the error functional  $m$ -dimensional  $J(y)$  is equivalent to solving:

$$\min_{x \in x_0 + \mathbf{K}_m} \|b - Ax\|_2 \quad (3)$$

where  $\mathbf{K}_m = \text{span}\{r_0, Ar_0, \dots, A^{m-1}r_0\}$  is the Krylov subspace of dimension  $m$ . The linear least squares problem (2) is solved by use of the  $QR$  method. More details can be found in [13]. For GMRES each iteration needs:  $i + 2$  inner products,  $i + 1$  vector updates and 1 Mv.

### 3 s-Step Omin

The s-step Minimal Residual (**MR**) method is a simple steepest descent method which computes the following sequence of solution approximations

$$x_{i+1} = x_i + a_i^1 r_i + \dots + a_i^s A^{s-1} r_i,$$

where  $a_i^j$  to minimizes  $\|r_{i+1}\|$  over the affine Krylov subspace

$$\left\{ x_i + \sum_{j=0}^{s-1} a_j A^j r_i : a_j \text{ scalars and } r_i = f - Ax_i \right\}$$

This method is theoretically equivalent to GMRES. Unlike GMRES s-MR is not be stable for large  $s$  because of loss of orthogonality of the direction vectors used.

The s-step MR is used to obtain s-step generalizations for GCR and Omin(k). The details can be found in [3]. To achieve this we form the  $s$  directions  $\{ r_i, \dots, A^{s-1} r_i \}$  and simultaneously  $A^T A$  -orthogonalize to  $k$  preceding blocks of direction vectors  $\{ [p_j^1, \dots, p_j^s] \}_{j=j_i}^{j=i}$ . The norm of the residual  $\|r_{i+1}\|_2$  is minimized simultaneously in all  $s$  new directions in order to obtain  $x_{i+1}$ . The following notation (in BLAS3) facilitates the description of the algorithm.

- Set  $P_i = [p_i^1, \dots, p_i^s]$
- Set  $R_i = [r_i, Ar_i, \dots, A^{s-1} r_i]$ .
- Let  $W_i$  be  $W_i = [ (Ap_i^j)^T Ap_i^l ], 1 \leq j, l \leq s$ .
- Let  $\underline{a}_i, \underline{m}_i$  be the vectors  $\underline{a}_i = [a_i^1, \dots, a_i^s]^T$  and  $\underline{m}_i = [r_i^T Ap_i^1, \dots, r_i^T Ap_i^s]^T$ .
- For  $l = 1, \dots, s$  and  $j = j_i, \dots, i$  let  $\underline{c}_j^l, \underline{b}_j^l$  be the vectors  $\underline{b}_j^l = [b_j^{(l,1)}, \dots, b_j^{(l,s)}]^T$  and

$$\underline{c}_j^l = [A^{(l+1)T} r_{i+1} Ap_j^1, \dots, A^{(l+1)T} r_{i+1}, Ap_j^s]^T.$$

Using BLAS3 operations we summarize s-step Omin(k) in the following algorithm.

**Algorithm 3.1** s-step Orthomin( $k$ )

Compute  $R_0$  and set  $P_0 = R_0$ .

**For**  $i = 0, 1, \dots$  **until** convergence **do**

1. Compute  $\underline{m}_i, W_i$ .
2. (Scalar1) Decompose  $W_i$  and solve  $W_i \underline{a}_i = \underline{b}_i$ .
3.  $x_{i+1} = x_i + P_i \underline{a}_i$
4.  $r_{i+1} = r_i - AP_i \underline{a}_i$
5. Compute  $R_i$ .
6. Compute  $\underline{c}_j^i$ , for  $j = j_i, \dots, i$
7. (Scalar2) Solve  $W_j \underline{b}_j^l = -\underline{c}_j^l$ , for  $j = j_i, \dots, i$  and  $l = 1, \dots, s$ .
8.  $P_{i+1} = R_{i+1} + \sum_{j=j_i}^i P_j \underline{b}_j^l$ .
9.  $AP_{i+1} = AR_{i+1} + \sum_{j=j_i}^i AP_j \underline{b}_j^l$ .

**EndFor**

The value of the index  $j_i$  is  $\min(0, i - k + 1)$ . Fixing  $j_i = 0$  yields the s-step GCR method. For  $s = 1$  we obtain the standard Omin(k) and GCR methods. It is proved in [3] that s-step Omin(1) coincides with s-step GCR if  $A$  is symmetric or skew-symmetric.  $s$  must be kept small (not greater than five) for numerical stability reasons [1]. However if  $R_i$  is made into an  $A^T A$ -orthogonal set (by use of modified Gramm-Schmidt) after it is computed a larger  $s$  can be chosen. In this case it can be easily shown that the linear systems in Scalar1, 2 are diagonal. We do not go into details here because we have not yet implemented this approach.

In [3] it is proved that s-step Omin(k) converges for nonsymmetric definite matrices and for a class of indefinite matrices. In fact since each iteration contains an s-MR iteration it converges for the same class of matrices as GMRES(s).

We give the vector work and storage for Omin(k) and s-step Omin(k) in Table 3.1. Storage includes the matrix  $A$  and the vectors:

$$x, r, AR, \{P_j\}_{j=0}^{j=i+1}, \{AP_j\}_{j=0}^{j=i+1}.$$

More details can be found in [3].

**Table 3.1: Ops/storage for j-iter of Omin(k) and s-Omin(k)**

Vector Ops	Omin(k)	s-Omin(k)
Dotprod	$\min([(j+1)+2], [k+2])$	$\min([(j+1)s^2 + s(s+1)/2], [ks^2 + s(s+1)/2])$
Matvec	1	s
Vect Update	$\min([2(j+1)+1], [2k+2])$	$\min([2(j+1)s^2 + s], [2ks^2 + s(s+1)/2])$
Storage	matr A+(2k+2)vects	matr A+(2ks+s+1)vects

## 4 s-step GMRES

The s-step Arnoldi method has been derived in [9]. Firstly we give an outline the s-step Arnoldi method and then we derive residual error minimization step which yields the s-step GMRES method.

Let us denote by  $k$  the iteration number in the  $s$ -step Arnoldi method. Given the vectors  $\{v_k^1, v_k^2, \dots, v_k^s\}$  (each of dimension  $N$ ) we use  $\bar{V}_k$  to denote the matrix of  $[v_k^1, v_k^2, \dots, v_k^s]$ . Initially we start with a vector  $v_1^1$  and compute  $v_1^2 = Av_1^1$ , ...,  $v_1^s = A^{s-1}v_1^1$ . One way to obtain an  $s$ -step Arnoldi algorithm is to use these  $s$  linearly independent vectors and generate a sequence of block matrices  $\bar{V}_1, \dots$ . To form  $\bar{V}_2$  we compute  $v_2^1 = Av_1^s, v_2^2 = Av_2^1$ , ...,  $v_2^s = A^{s-1}v_2^1$ . Then we orthogonalize  $\bar{V}_2$  against  $\bar{V}_1$ . Inductively we form  $\bar{V}_k$  for  $k > 1$ . The subspaces  $\bar{V}_1, \bar{V}_2, \dots, \bar{V}_k$  are mutually orthogonal, but the vectors  $v_k^1, v_k^2, \dots, v_k^s$  are not orthogonal, that is,  $\bar{V}_k^T \bar{V}_k$  is not a diagonal matrix.

We next summarize the s-step Arnoldi algorithm using BLAS3 operations.

### Algorithm 4.1 s-step Arnoldi

Select  $v_1^1$

Compute  $\bar{V}_1 = [v_1^1, v_1^2 = Av_1^1, \dots, v_1^s = A^{s-1}v_1^1]$

For  $k = 1, \dots, m/s$

1. Call Scalar1
2. Compute  $v_{k+1}^1 = Av_k^s - \sum_{i=1}^k \bar{V}_i [\bar{\mathbf{h}}_{\mathbf{ik}}^1]$ .
3. Compute  $v_{k+1}^2 = Av_{k+1}^1, \dots, v_{k+1}^s = A^{s-1}v_{k+1}^1$

4. Compute  $(A^i v_k^1, v_l^j)$  for  $1 \leq i, j \leq s$  and  $1 \leq l \leq k-1$
5. Compute  $(A^i v_k^1, A^j v_k^1)$  for  $0 \leq i \leq s-1$  and  $i \leq j \leq s$
6. Call Scalar2
7. Compute  $\bar{V}_{k+1} = [v_{k+1}^1, \dots, v_{k+1}^s] - \sum_{i=1}^k \bar{V}_i [0, \mathbf{t}_{\mathbf{ik}}^1, \dots, \mathbf{t}_{\mathbf{ik}}^{s-1}]$

**EndFor**

**Scalar1:** Compute and decompose  $W_i = \bar{V}_i^T \bar{V}_i$ .

solve  $W_i \bar{\mathbf{h}}_{\mathbf{ik}}^q = \mathbf{b}_{\mathbf{ik}}^q$  for  $q = 1, \dots, s$ , where

$$\mathbf{b}_{\mathbf{ik}}^1 = [(v_i^1, Av_{k+1}^1), \dots, (v_i^s, Av_{k+1}^1)]^T, \dots,$$

$$\mathbf{b}_{\mathbf{ik}}^{s-1} = [(v_i^1, A^{s-1}v_{k+1}^1), \dots, (v_i^s, A^{s-1}v_{k+1}^1)]^T$$

**Scalar2:** Solve  $W_i \mathbf{t}_{\mathbf{ik}}^q = \mathbf{b}_{\mathbf{ik}}^q$  for  $1 \leq q \leq s-1$ , where

$$[\mathbf{c}_{\mathbf{ik}}^1, \dots, \mathbf{c}_{\mathbf{ik}}^s] = \bar{V}_i^T A \bar{V}_k$$

It was proven in [3] that the inner products computed in steps 5. and 6. and scalar work can be used in evaluating the coefficients and right hand sides of the linear systems in Scalar 1, 2. The parameters  $\bar{\mathbf{h}}_{\mathbf{ik}}^q$  computed in Scalar 1 are not only important computing  $v_{k+1}^1$  but also they are entries of the upper Hessenberg matrix  $\bar{H}_k$  of the  $s$ -step Arnoldi method. The following matrix equality holds but it is not explicitly computed except for the vector  $v_{k+1}^1$  (in step 2. of algorithm 4.1):

$$A \bar{V}_k = \sum_{j=1}^k \bar{V}_j [\bar{\mathbf{h}}_{\mathbf{jk}}^1, \dots, \bar{\mathbf{h}}_{\mathbf{jk}}^s] + v_{k+1}^1 e_{sk}^T \quad (4)$$

The upper Hessenberg matrix  $\bar{H}_k$  is obtained from matrix  $\bar{H}_{k-1}$  by adding the block column  $[\bar{\mathbf{h}}_{\mathbf{jk}}^1, \dots, \bar{\mathbf{h}}_{\mathbf{jk}}^s]$  for  $j = 1, \dots, k$  down to the diagonal plus an  $s \times s$  subdiagonal block which has the only one nonzero  $\|v_{k+1}^1\|_2^2$  at the position  $(s(k-1) + 1, sk)$ .

To introduce an  $s$ -step GMRES method we use the basis generated by the  $s$ -step Arnoldi method. After  $k$  iterations of  $s$ -step Arnoldi method we have  $v_{k+1}^1$  and a  $(k+1)s \times ks$  matrix  $\bar{G}_k$  generated by the method.  $\bar{G}_k$  is



the same as  $\bar{H}_k$  except for an additional row whose only nonzero element is at the  $(s(k-1) + 1, sk)$  position.

Let  $V_k = [\bar{V}_1, \dots, \bar{V}_k]$  and  $U_k = [V_k, v_{k+1}^1]$  then the matrix  $\bar{G}_k$  satisfies the important relation:

$$AV_k = \bar{G}_k U_k \quad (5)$$

To derive the s-step GMRES we must solve the least squares problem:

$$\min_{z \in K_j} \|f - A[x_0 + z]\| = \min_{z \in K_j} \|r_0 - Az\|. \quad (6)$$

If we set  $z = V_k \bar{y}$ , we can view the norm to be minimized as the following function of  $\bar{y}$ :

$$J(y) = \|v_1^1 - AV_k \bar{y}\| \quad (7)$$

where we have let  $v_1^1 = r_0$  for convenience. Using equation (5)

$$J(y) = \|U_k [e_1 - \bar{G}_k \bar{y}]\|. \quad (8)$$

Here the vector  $e_1 = [1, \dots, 0]^T$ .

Let  $D = W_k^T W_k$ , then  $D = \text{diag}(\bar{V}_1^T \bar{V}_1, \dots, \bar{V}_k^T \bar{V}_k, v_{k+1}^1{}^T v_{k+1}^1)$ . Using Cholesky factorization  $D = L^T L$ , we obtain

$$J(y) = \|[\beta e_1 - L \bar{G}_k \bar{y}]\|. \quad (9)$$

where  $\beta = \|r_0\| = \|v_1^1\|$  because  $L e_1 = \|u_1^1\| e_1$ . Hence the solution of the least squares problem (6) is given by

$$x_k = x_0 + V_k \bar{y}_k \quad (10)$$

where  $\bar{y}_k$  minimizes the functional  $J(y)$ .

Now we describe the restarting s-step GMRES algorithm.

**Algorithm 4.2** s-step GMRES

1. Compute  $r_0$  and set  $v_1^1 = \frac{r_0}{\|r_0\|}$
2. Compute the s-step Arnoldi vectors  $V_1 \dots V_m$
3. Form the approximate solution:  $x_m = x_0 + V_m \bar{y}_m$
4. where  $y_m$  minimizes  $J(y) = \|[\beta e_1 - L \bar{G}_k \bar{y}]\|$ .

5. Restart: Compute  $r_m = f - Ax_m$  and stop if  $\|r_m\| < \epsilon$  else set  $x_0 = x_m$  and  $r_0 = r_m$  and go to 1.

The advantages of  $s$ -step GMRES compared to standard GMRES on parallel computers come from the fact the matrix vector operations, inner products and linear combinations corresponding to  $s$  consecutive steps of the standard GMRES( $m$ ) are grouped together for simultaneous execution. Scalar1 and Scalar2 and the minimization of  $J(y)$  are scalar computations of dimension  $s$ .

**Remark 4.1:** Assume that the degree of the minimal polynomial of  $r_0$  is greater than  $ms$ . Let GMRES( $ms$ ) and  $s$ -step GMRES( $m$ ) start with the same  $x_0$ . Then the iterate  $x_{i(ms)}$  is the same for the  $s$ -step GMRES( $m$ ) and GMRES( $ms$ ).

This result follows from the equivalence of these methods to the  $ms$ -step MR method. We compare the computational work and storage of the  $s$ -step GMRES method to the standard one. We give the vector work for the  $s$ -step and standard GMRES in Table 4.1. We present the storage and vector operations of 1 cycle of the standard GMRES( $sm$ ) compared to 1 cycle of the  $s$ -step GMRES( $m$ ). The details of deriving the formulas are in [13] and [8].

**Table 4.1: Vector Ops of GMRES( $sm$ ) vs  $s$ -GMRES( $m$ )**

Vector Ops	GMRES( $sm$ )	$s$ -GMRES( $m$ )
Dotprod	$ms + [sm(ms + 1)/2]$	$[m(m - 1)s^2]/2 + [s(s + 1)/2 + s]$
Matvec	$(ms+1)$	$s(m+1)$
Vect update	$([m^2s^2 + ms]/2 + 2ms)$	$m(m + 1)s^2$
Storage	Matr A + $(ms + 1)vect$	Matr A + $([s(m + 1)m]/2 + m)vect$

## 5 Numerical Tests

We have discretized a boundary value problems in partial differential equations on a square region by the method of finite differences.

**Problem:**

$$-(b(x, y)u_x)_x - (c(x, y)u_y)_y + (d(x, y)u)_x + (e(x, y)u)_y + f(x, y)u = g(x, y), \quad (11)$$

$$\Omega = (0, 1) \times (0, 1) \tag{12}$$

where  $b(x, y) = e^{-xy}$ ,  $c(x, y) = e^{xy}$ ,  $d(x, y) = \beta(x + y)$   
 $e(x, y) = \gamma(x + y)$ ,  $f(x, y) = \frac{1}{(1+xy)}$ ,  
 $u(x, y) = xe^{xy} \sin(\pi y) \sin(\pi y)$ ,

This problem is a standard elliptic test problem which can be found in [13] and the right hand side function is constructed so that the analytic solution is known. The right hand side function  $g(x, y)$  is obtained by applying the differential operator to  $u(x, y)$ . Dirichlet boundary conditions are imposed. By controlling  $\gamma$  and  $\beta$ , we could change the degree of nonsymmetry of the discretization matrix. We set  $\gamma = 50.0$ ,  $\beta = 1.0$ . We have used the five point difference operator for the Laplacian, central difference for the first derivative. For initial value, we have chosen  $x(i) = 0.05 * \text{mod}(i, 50)$ .

For a nonsingular matrix  $K$  then the transformed system

$$[AK]K^{-1}x = f \tag{13}$$

is a right preconditioned form of the original linear system. We use right preconditioning, since it minimizes the residual norm rather than minimizing the norm of  $r_i$ , where  $r_i$  is the  $i$ -th residual vector. We use ILU(0) preconditioning in vectorizable form [16].

## 6 Results

We used the Cray-2 supercomputer at the Minnesota Supercomputer Institute. The Cray-2 is a four-processor (MIMD) supercomputer. All processors have equal access to a central memory of 512 Megawords. Each Cray-2 processor has 8 vector registers (each 64 words long) and has data access through a single path between its vector registers and main memory. Each processor has 16 Kwords of local memory with no direct path to central memory but with a separate data path between local memory and its vector registers, and the six parallel vector pipelines: common memory to vector register (LOAD/STORE), vector register to local memory (LOAD/STORE), floating point ADD/SUBTRACT, MULTIPLY/DIVIDE, Integer ADD/SUBTRACT and LOGICAL elines. It is possible to design assembly language kernels which exhibit a performance commensurate with the 4.2 nanosecond cycle time of the Cray-2 if the computations allow it.

This means that a rate of 459 Megaflops is possible on one processor if all arithmetic pipelines can be kept busy.

The maximum performance of the Cray-2 for specific applications comes from data movement minimization, good vectorization and division into processing tasks. Because of single paths between vector register and central or local memory on the Cray-2 system, memory transfers constitute a severe bottleneck for achieving maximum performance. Therefore, minimization of data movement results in faster execution times.

The termination criterion used was  $\|r_i\|^{1/2} < 10^{-6}$ . The number of grid point in the  $x$  and  $y$  directions taken is  $nx = 64, 128, 192, 256$ .

The termination criterion used was  $\|r_{subi}\|_{sup1/2} < 10_{sup} - 6$ . The number of grid point in the  $x$  and  $y$  directions taken is  $nx = 32, 64, 128, 192, 256$ .

The selection of  $s$  and  $k$  in s-Omin(k) minimizes the number of iterations for each problem. Since in each iteration of s-GMRES(m) there is an overhead of one matrix vector multiplication (see table 4.1)  $s$  must be chosen as large as possible. So we chose first  $m$  in GMRES(m) and then choose  $s$  and  $mbar$  (in s-GMRES(  $mbar$  )) so that  $m = mbar s$ . In our tests the number of iterations in GMRES(10) equals (in almost all cases) the number of iterations 5-GMRES(2). This is expected from remark 4.1. This is not always true with Orthomin((k+1)s-1) and s-step Orthomin(k). The residual error is minimized on the same number of independent vectors. However, these vectors do not generate the same affine subspace. Actually, s-Omin(k) may converge for indefinite problems for which Orthomin(k) fails [3].

Tables 6.1-6.4 contain the no. of iterations and total execution times for convergence of the methods. The performance gain is about 1.5 for 2-Orthomin(2) and 1.3 for 2-GMRES(5). The 2-GMRES(5) has one additional matrix vector operation and since the preconditioner has low Megaflop rate it offsets the gains made from the other types of operations. This accounts for the low rate of 2-GMRES(5) in the preconditioned case. In terms of programmer optimizations we have unrolled the linear combinations as single GAXPY operations. Unrolling loops for BLAS3 operations did not lead to a faster rate.

**Table 6.1:s-Omin(k) vs s-GMRES(m): Iter's ILU(0) preconditioned.**

dimension	s=1,k=4	s=2,k=2	s=1,m=10	s=2,m=5
64	193	98	30	30
128	335	167	60	59
192	509	252	93	95
256	660	340	146	146

**Table 6.2:Omin(4) vs 2-Omin(2) times(sec) Cray-2 p-PEs**

dimension	p=1	p=4	p=1	p=4
64	0.289	0.602	0.229	0.503
128	1.947	1.503	1.495	1.138
192	7.169	3.113	5.175	2.168
256	17.523	6.873	12.374	4.827

**Table 6.3:GMRES(10) vs 2-GMRES(5) times(sec) Cray-2 p-PEs**

dimension	p=1	p=4	p=1	p=4
64	0.534	1.069	0.381	0.560
128	3.495	2.392	2.782	1.471
192	12.253	5.831	9.183	3.855
256	33.741	12.378	25.978	9.051

**Table 6.4:s-Omin(k) vs s-GMRES(m):time(sec), p=1, Cray-2**

dimension	Omin(4)	2-Omin(2)	GMRES(10)	2-GMRES(5)
64	0.137	0.079	0.223	0.205
128	0.899	0.613	1.487	1.326
192	3.216	1.827	4.863	3.893
256	7.372	4.519	10.917	9.074

## 7 Conclusions

We reviewed the standard and s-step Omin and Arnoldi methods (which are derived in [3], [9]). We have derived the s-step GMRES method. We then used these methods to solve nonsymmetric systems arising from the finite difference discretization of partial differential equations. The s-step methods showed similar convergence properties as the standard methods with gains in

execution time. The gains would have been much higher with use of BLAS3 modules to utilize the local memory of the Cray-2 processor. If the matrix vector multiplication is more costly then the gains from the s-step methods are reduced. However one could program computers with local memory to make matrix vector multiplication with block tridiagonal matrices very fast. On the Cray-2 this has to be done in Cray Assembly language (CAL). We are currently implementing (in CAL) a matrix vector multiplication module which utilizes efficiently the local memory of the Cray-2. This is expected to increase the speed of the matrix vector operations for this type of block tridiagonal matrices.

## References

- [1] A.T.Chronopoulos and C.W.Gear, "s-step iterative methods for symmetric linear systems", *Journal of Computational and Applied Mathematics* 25, pp. 153-168, 1989.
- [2] A. T. Chronopoulos and C. W. Gear "Implementation of Preconditioned s-Step Conjugate Gradient Methods on a Multiprocessor System with Memory Hierarchy" *Parallel Computing* 11 (1989) 37-53.
- [3] A. T. Chronopoulos, "s-step Iterative Methods for (Non)symmetric (In)definite Linear Systems" *SIAM J. on Num. Analysis* Vol. 28, No. 6, 1991.
- [4] J. J. Dongarra, D. C. Sorensen, "Linear Algebra on High-Performance Computers" *Parallel Computing* 85, M. Feilmeier, G. Joubert and U. Schendel (eds.), Elsevier Science Publishers B.V.
- [5] S.C. Eisenstat, H. C. Elman and M. H. Schultz "Variational iterative methods for nonsymmetric systems of linear equations", *SIAM J. Numer. Anal.* 20, (1983) 345-357.
- [6] J. F. Grcar, "Operator Coefficient Methods for Linear Equations" Sandia Rep. SAND89-8691.
- [7] M. Hestenes and E. Stiefel, "Methods of conjugate gradients for solving linear systems," *J. Res. NBS* 49 (1952) 409-436.

- [8] S.K.Kim and A.T.Chronopoulos, "An Efficient Parallel Algorithm for Extreme Eigenvalues of Sparse Nonsymmetric Matrices", International Journal of High Performance Computing Applications, Vol. 6, Issue 4, Dec 1992.
- [9] S.K.Kim and A.T.Chronopoulos, "The s-step Lanczos and Arnoldi Methods on Parallel Computers" In: Proc. of the 1991 Intern. Conf. on parallel Processing, Vol. III, pp.167- 170.
- [10] W. Jalby and U. Meier, "Optimizing Matrix Operations on a Parallel rocessor with a Memory Hierarchy." Proceed. of ICPP, (1986).
- [11] .F.Lucas, T.Blank, and J.J.Tiemann, "A Parallel Solution Method for Large Sparse Systems of Equations", IEEE Transactions on Computer-Aided Design, Vol. CAD-6, No. 6, (1987).
- [12] O.A.McBRYAN and E.F.van de Velde, "Matrix and vector operations on hypercube parallel processors", Parallel Computing 5, (1987), pp. 117-125.
- [13] Y. Saad and M. Schultz, "GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems," SIAM J. SCI. STAT. COMPUT., Vol. 7, (1986).
- [14] K. Gallivan, R. Plemmons, and A. Sameh "Parallel Algorithms for Dense Linear Algebra Computations", SIAM Review, 32, (1990), pp. 54-135.
- [15] P E. Saylor, "Leapfrog Variants of Iterative Methods for Linear Algebraic Equations", Journal of Computational and Applied Mathematics 24, (1988), pp. 169-193.
- [16] H. Van Der Vorst, " A Vectorizable Variant Of Some ICCG Methods" SIAM Sci.Stat Comp, Vol.3(1982), pp. 350-356.
- [17] H. A. Van Der Vorst, "The Performance of FORTRAN Implementations for Preconditioned Conjugate Gradients on Vector Computers" Parallel Computing 3 (1986), pp. 49-58.

- [18] H. A. Van Der Vorst, "Iterative Solution Methods for Certain Sparse Linear Systems with a Non-symmetric Matrix Arising from PDE-Problems" J. Comp. Physics, 44 (1981), pp. 1-9.
- [19] P. Vinsome, "An iterative method for solving sparse sets of simultaneous equations", Society of Petroleum Engineers of AIME, SPE 5729, 1976.