Multi-phase Systolic Algorithms for Spectral Decomposition

by K.J.R. Liu and K. Yao

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ABSTRACT

In this paper, we propose two multi-phase systolic algorithms to solve the spectral decomposition problem based on the QR algorithm. The spectral decomposition is one of the most computationally intensive modern signal processing operations. While the QR algorithm is well known to be an effective method to solve the eigenvalue problem, there is still no single systolic array architecture that can compute the unitary Q matrix readily and perform the QR algorithm efficiently. Previous methods using the QR algorithm had communication problems among different architectures. In this paper, two arrays, a triangular and a rectangular, are presented to implement the multi-phase algorithms. Details on these multi-phase operations of the QR algorithm as well as architectural consequences and performance evaluation are discussed in the paper. Efficient fault-tolerant schemes for these multi-phase operations are also considered.

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1 Introduction

Computing the spectral decomposition of a matrix is an important issue in many modern signal processing and system applications. The feasibility of real-time processing for sophisticated modern signal processing systems depends crucially on efficient implementation of parallel processing of the algorithms and associated architectures needed to perform these operations [4,21]. While many variations exist in the literature for solving these matrix problems, all these iterative methods are based either on the Jacobi-Hestennes method or the QR algorithm [10,40,43]. While there are some fundamental differences between these two approaches, both algorithms have good numerical stability and convergence rate properties and thus are desirable for possible implementation. Since present VLSI technology is capable of building a multiprocessor system on a chip, many researchers have proposed different parallel processing architectures to solve eigenvalue and singular value decomposition (SVD) problems.

For any complex-valued $m \times n$ matrix A, the classical spectral decomposition [41] of the $n \times n$ Hermetian matrix $A^H A$, is given by

$$A^{H}A = \sum_{i=1}^{n} \lambda_{i} \underline{v}_{i}^{H} = V \Lambda V^{H}, \tag{1}$$

where $V = [\underline{v}_1, \dots, \underline{v}_n]$ is an $n \times n$ unitary matrix, $\Lambda = diag[\lambda_1, \dots, \lambda_n]$, and H is the complex conjugate transpose operator. The $\lambda_i's$ are the eigenvalues satisfying $\lambda_1 \geq \lambda_2 \dots \geq \lambda_n \geq 0$ and the $v_i's$ are the eigenvectors satisfying $A^H A \underline{v}_i = \lambda_i \underline{v}_i$. The decomposition of $A^H A$ follows from the SVD [10] of A given by

$$A = USV^H \tag{2}$$

where $U = [\underline{u}_1, \dots, \underline{u}_n]$ is an $m \times n$ matrix with orthogonal column vectors, $S = diag[s_1, \dots, s_n]$, and V is an $n \times n$ unitary matrix. The $s_i's$ are the singular values satisfying $s_1 \geq s_2 \geq \dots \geq s_n \geq 0$ and are the positive square roots of $\lambda_i's$ such that $\Lambda = S^2$. In this paper, we shall use spectral decomposition in the broad sense of not only including the decompositions of (1) and (2), but also including the eigenvalue decomposition of an arbitrary complex-valued $n \times n$ matrix A given by

$$AX = \Lambda X,\tag{3}$$

where X is an $n \times n$ matrix of eigenvectors and $\Lambda = diag[\lambda_1, \dots, \lambda_n]$ is the matrix of eigenvalues of A.

Luk [24], Brent [3], and Gao and Thomas [7] have used effectively the Jacobi-like method to solve these problems for either a multiprocessor system or systolic array. The basic problem concerns the diagonalization of a 2×2 matrix by the rotation matrices $J(\theta)$ and $K(\phi)$ in

$$J(\theta)^T \begin{bmatrix} w & x \\ y & z \end{bmatrix} K(\phi) = \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix}, \tag{4}$$

where w, x, y, and z are elements in two corresponding rows and columns of A. A two-stage procedure is then used to find θ and ϕ [24]. To find the SVD of a square matrix A, an appropriate sequence of 2×2 matrices is computed by using the basic Jacobi transformation in

$$T_{ij}: A \leftarrow J_{ij}^T A K_{ij} \tag{5}$$

where J_{ij} and K_{ij} are rotations in the (i,j) plane chosen to annihilate the (i,j) and (j,i) elements of A respectively [24]. While the Jacobi-like method, as considered in [24], is currently known as one of the most effective parallel SVD algorithm for full dense matrices, the computations required to obtain the rotational matrices needed in this approach to obtain the singular vectors are not simple (either through broadcast in the array or by slowing down the operations) [24]. Moreno and Lang [29] also considered some alternatives to the algorithms in [3].

On the other hand, other researchers have used the QR algorithm to solve the eigenvalue problems. Heller and Ipsen [13,17] performed the QR iteration for banded matrix based on an orthogonal systolic network and Schreiber [35] combined their network with Gentleman and Kung's QR array to compute the QR algorithm. These methods required the computation of the unitary matrix Q. However, problems exist in the concurrent computation of Q and the pipeline operation of the QR iteration [17]. In [28], Moldovan et al. studied the mapping of a large QR algorithm onto a fixed size array. Torralba and Navarro [42] further purposed a size-independent linear array for QR iteration and Hessenberg reduction. While this approach can provide an efficient computation of one iteration of the QR iteration, it is not obvious how to pipeline the iteration.

For some system applications, such as matrix rank determination and system identification [20], the efficient computation of singular values is sufficient, while in other applications such as antenna beamformation [27,38], spectral estimation [19,34], direct finding [11,30], etc., the eigenvectors are crucially needed. This makes practical implementation of systolic arrays discussed above difficult for many applications since they either cannot compute the eigenvector or cannot obtain the eigenvector without broadcast. For example, for the MUSIC algorithm [12], once we determine the signal subspace and noise subspace from the eigenvectors, the sample spectrum is then determined by

$$S(\omega) = \frac{1}{s^H(\omega)X_N X_N^H s(\omega)},$$

where X_N is the matrix of eigenvectors which generate the noise subspace and

$$s(\omega) = [1, e^{-j\omega}, \cdots, e^{-j\omega(K-1)}],$$

with K being the dimension of the matrix X_N . A system which consists of several systolic modules to compute the MUSIC algorithm has been proposed in [33]. However, communication problems among the modules and the difficulty of matching the pipeline rates and timings among different modules may pose difficulties for practical implementation.

Presently, there is no known simple efficient systolic array approach for the generation of eigenvectors. The main reason is that there is no single architecture that is capable of handling all the steps required in the algorithm such that we can pipeline the successive iteration readily. The communication cost among different architectures is high and the interface problem for an efficient data flow is demanding. In this paper, we propose two multi-phase systolic algorithms to solve the spectral decomposition problem based on the QR algorithm. By multi-phase operations we mean that the processing cells can perform different arithmetic operations in different phase of the computations. Two systolic arrays, one triangular and the other rectangular, are designed based on the multi-phase concept. A key feature in our method for the successfully application of the QR algorithm is that the

Q matrix of the QR decomposition can be computed explicitly by multi-phase operations. With the proper feedback of this Q matrix, the QR algorithm can be computed and pipelined effectively in a single systolic array. From the accumulation of those Q matrices in another array, eigenvectors can be computed without needing global communication inside the array.

In Section 2, some preliminary matrix operations useful for the multi-phase operations are discussed. In Section 3, we review the QR algorithm and show the evaluation of the eigenvector from cumulative multiplications of the Q matrices. Then two multi-phase systolic arrays for the QR algorithm and the Hessenberg reduction are presented in Section 4. Their performances, numerical stabilities, and convergence rates are studied in Section 5. Finally, some efficient fault-tolerant schemes that can be incorporated with the arrays are discussed in Section 6. A brief conclusion is given in Section 7.

2 Systolic Array Matrix Processing

In this section, we consider some preliminary matrix and associated systolic array operations needed in the multi-phase systolic algorithms for spectral decompositions.

A. QR Decomposition

A non-degenerate $m \times n$ rectangular matrix A can be factored into two matrices Q and R such that A = QR, where Q is an $m \times m$ unitary matrix and R is an $m \times n$ upper triangular matrix. The matrix Q can be computed using sequences of Givens rotations. An elementary Givens transformation has the form of

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 & r_i & r_{i+1} & \cdots & r_k \\ 0 & \cdots & 0 & x_i & x_{i+1} & \cdots & x_k \end{bmatrix} = \begin{bmatrix} 0 & \cdots & 0 & r'_i & r'_{i+1} & \cdots & r'_k \\ 0 & \cdots & 0 & 0 & x'_{i+1} & \cdots & x'_k \end{bmatrix}$$
(6)

where

$$c = \frac{r_i}{\sqrt{r_i^2 + x_i^2}}, \quad s = \frac{x_i}{\sqrt{r_i^2 + x_i^2}}.$$

Several different QR systolic arrays have been considered by Gentleman and Kung [9], Heller and Ipsen [14], and Luk [25]. In particular, the computation of the Q matrix without broadcast is difficult for the array considered in [24, pp.266]. On the other hand, [9] has shown that a triangular systolic array can be used to obtain the upper triangular matrix R based on sequences of Givens rotations. This approach also leads to an efficient method for performing recursive least-squares computation [26], and is also useful for finding the singular value of a matrix [8]. This systolic array is shown in Fig.1 and the operations of the cells are described in the first column (i.e., Phase 1) of Table 1. While the rotation parameters are propagated to the right, the Q matrix will not appear directly at the right as originally suggested by [36]. In order to demonstrate this point, denote G_{ij} as the Givens rotation matrix of the (i, j) plane. Then matrix Q can be obtained as

$$Q^{T} = \coprod_{i=m-1}^{1} \prod_{j=i+1}^{m} G_{ij}, \tag{7}$$

where \coprod is an ordered matrix product defined by $\coprod_{i=m-1}^{1} C_i = C_{m-1}C_{m-2}\cdots C_1$, while \coprod denotes a conventional product, where the ordering of the terms are not relevant. From Table 2, we can see, for a $n \times n$ QR triarray, the first rotation parameter coming out at

the right edge occurs at time n+1. After that, rotation parameters for different plane rotation come out successively. If assuming that the operation of \prod discussed above can be obtained immediately, then there are m-1 operations of \coprod to be processed when all of \prod are available and need to be multiplied. This observation leads to the conclusion that we cannot obtain the Q matrix by cumulatively multiplying the rotation parameters propagated to the right edge unless an additional rectangular array is used to accumulate the rotation matrices. Thus, this is not an efficient way to obtain the Q matrix.

B. Computation of $R^{-T}x$

In [6], Comon and Robert presented a rectangular systolic array for the computation of $B^{-1}A$, where B and A are square and rectangular matrices respectively. The computation takes two phases. First, the matrix B is fed into the array and B^{-1} is computed. In the second phase, the matrix A is input to produce $B^{-1}A$. For the special case where B is an upper triangular matrix denoted by R, instead of a full dense matrix, McWhirter and Shepherd [27] used the property that a triangular array can compute $R^{-T}\underline{x}$ in one phase with the matrix R prestored in the triarray. Since this property is needed in Phase 2 of our work, and no full derivation was given in [27], we present a brief derivation of this result. Define $r_{ij} = (R)_{ij}$ and $r'_{ij} = (R^{-1})_{ij}$, where $r_{ij} = 0$ and $r'_{ij} = 0$ for i > j, then it can be shown that

$$r'_{ij} = \begin{cases} 1/r_{ii}, & i = j, \\ -\sum_{k=i}^{j-1} r'_{ik} r_{kj} / r_{jj}, & i < j \le n. \end{cases}$$
 (8)

Let $[y_1, \dots, y_n]^T = R^{-T}\underline{x}$, then

$$y_j = \sum_{i=1}^{j} x_i r'_{ij}, \quad j = 1, \dots, n.$$
 (9)

In particular, y_i can be expressed in terms of r_{ij} as

$$y_{j} = \frac{1}{r_{jj}} \cdot (x_{j} - \sum_{i=1}^{j-1} x_{i} \sum_{k=i}^{j-1} r'_{ik} r_{kj})$$

$$= \frac{1}{r_{jj}} \cdot (x_{j} - \sum_{k=1}^{j-1} \sum_{i=1}^{k} x_{i} r'_{ik} r_{kj}).$$
(10)

From (9), y_j is given by

$$y_j = \underbrace{\frac{1}{r_{jj}}}_{(1)} \underbrace{(x_j - \sum_{k=1}^{j-1} y_k r_{kj})}_{(2)} \tag{11}$$

Thus, y_i can be computed recursively according to the above equation in the following algorithm:

Recursive Algorithm for Computing $y = R^{-T}\underline{x}$

$$y_1 = \frac{1}{r_{11}} \cdot x_1$$

for $j = 2$ to n

```
egin{aligned} \mathbf{begin} \ z_j &= x_j \ \mathbf{for} \ k &= 1 \ \mathbf{to} \ j - 1 \ z_j &= z_j - y_k r_{kj} \ y_j &= z_j / r_{jj} \end{aligned} end
```

The corresponding systolic array to implement the above algorithm is the same as the one shown in Fig.1. The operations of the cells are shown in the second column of Table 1. The first part of (11), *i.e.*, the division, is performed by the boundary cell while the second part of (11) is accumulated by the internal cells. With R pre-stored in the triarray, Fig.2 shows the data flow of the input \underline{x} and the output y.

C. Triangular-Matrix Multiplication

The multiplication of a triangular matrix R and an rectangular full dense matrix B is given by

$$(C)_{ij} = (RB)_{ij} = \sum_{k=i}^{n} r_{ik} b_{kj},$$
(12)

where r_{ik} and b_{kj} are elements of matrices R and B. Using the same array as in Fig.1, with R prestored in the triarray and the operations shown in the third column of Table 1, this multiplication can be easily obtained if B is input row by row as in Fig.3.

D. Matrix Multiplication

There are many ways to implement a full matrix-matrix multiplication in a systolic array [21]. In Fig.4, we show a typical architecture that can be incorporated with the multi-phase operations to obtain eigenvectors. With input matrices Q and A arranged as in Fig.4, the matrix B^T , where B = AQ, will reside in the rectangular array when the computation is completed. Details on this issue will be discussed in later sections.

3 QR Algorithm

In this section we review briefly the basic operation of the QR algorithm and show the evaluation of the eigenvectors from the cumulative multiplication of successive Q matrices. For a complex-valued $n \times n$ matrix A, it states that there is a unitary transform U such that $R = UAU^H$ is a upper triangular matrix with diagonal eigenvalues of descending order. This follows from the QR Algorithm [10,40,43] where by setting $A_1 = A$, we have $A_k = Q_k R_k$ and $A_{k+1} = R_k Q_k = Q_k^H A_k Q_k$, $k = 1, \cdots$, with unitary Q_k and upper triangular R_k . Furthermore, A_k converges to the upper triangular matrix with diagonal eigenvalue elements. However, it is not obvious how to compute the eigenvectors from those Q_k and R_k we have calculated. With a derivation similar to that used in [43], here we shows how to obtain the eigenvector associated with the largest eigenvalue from cumulative multiplications of Q_k . From the above discussions, we have

$$A_{k+1} = Q_k^H Q_{k-1}^H \cdots Q_1^H A_1 Q_1 Q_2 \cdots Q_k.$$
 (13)

Define

$$\tilde{Q}_k = \coprod_{i=1}^k Q_i = Q_1 Q_2 \cdots Q_k,$$

$$\tilde{R}_k = \coprod_{i=k}^1 R_i = R_k R_{k-1} \cdots R_1.$$
 (14)

Then we have

$$\tilde{Q}_k A_{k+1} = A_1 \tilde{Q}_k. \tag{15}$$

Thus the multiplication of $\tilde{Q}_k \tilde{R}_k$ can be expressed as

$$\tilde{Q}_{k}\tilde{R}_{k} = Q_{1}Q_{2}\cdots Q_{k}R_{k}R_{k-1}\cdots R_{1}
= \tilde{Q}_{k-1}A_{k}\tilde{R}_{k-1} = A_{1}\tilde{Q}_{k-1}\tilde{R}_{k-1} = A_{1}^{k} = A^{k}.$$
(16)

Let the eigenvalues of A satisfy, $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$. Denote the matrix eigenvectors and eigenvalues of A by X and Λ respectively. Then A^k is given by

$$A^k = X\Lambda^k X^{-1}. (17)$$

Let the QR decomposition of X be X = QR and the LU decomposition of X^{-1} be $X^{-1} = LU$, where L is an unit-lower triangular matrix. Then

$$A^{k} = QR\Lambda^{k}LU = QR(\Lambda^{k}L\Lambda^{-k})\Lambda^{k}U, \tag{18}$$

where

$$\Lambda^k L \Lambda^{-k} = I + E_k, \tag{19}$$

and

$$(E_k)_{ij} = \begin{cases} l_{ij}(\lambda_i/\lambda_j)^k, & i > j, \\ 0, & \text{otherwise.} \end{cases}$$
 (20)

Since, we have $\lim_{k\to\infty} E_k = 0$ and thus $\Lambda^k L \Lambda^{-k}$ approaches the identity matrix. Then (18) can be rewritten as

$$A^k \to QR\Lambda^k U.$$
 (21)

Since the term $R\Lambda^k U$ is an upper triangular matrix, comparing to (16) we can see that $\tilde{Q}_k \to Q$ when k is large. That is, the Q matrix of the QR decomposition of A^k approaches that of the Q matrix of the QR decomposition of the matrix of eigenvector X. Define

$$\tilde{Q}_{k} = [\underline{\tilde{q}}_{1}, \underline{\tilde{q}}_{2}, \cdots, \underline{\tilde{q}}_{n}],
X = [\underline{x}_{1}, \underline{x}_{2}, \cdots, \underline{x}_{n}],$$
(22)

and r_{ij} as the (i,j) element of R. From $\tilde{Q}_k \to X$, we find $r_{11}\tilde{\underline{q}}_1 \to \underline{x}_1$ when k is large. Since \underline{x}_1 is the eigenvector associated with the largest eigenvalue, we conclude that the first column of the matrix \tilde{Q}_k approaches the eigenvector associated with the largest eigenvalue of matrix A when k is large. If the matrix A is symmetric, which is often the case for signal processing applications, the similar transformation $A_{k+1} = \tilde{Q}_k^H A \tilde{Q}_k$ is also symmetric. Since A_{k+1} approaches the upper triangular matrix by the QR algorithm, A_{k+1} approaches a diagonal matrix. That is

$$A_k \to \Lambda,$$
 (23)

and

$$\tilde{Q}_k \Lambda \to X.$$
 (24)

In this case, for large k, the columns of \tilde{Q}_k become proportional to the columns of eigenvector in X.

If A is real, then A_k will converge to a real block upper triangular matrix with 1×1 and 2×2 main diagonal blocks. The complex conjugate pairs of eigenvectors of the 2×2 blocks can be solved easily using the quadratic formula. When A is not a square matrix, the singular values and vectors are of interest. For a $m \times n$ matrix B, where m > n, the SVD of B shows $B = U \Sigma V^T$, where U is a $m \times n$ matrix of orthogonal columns, V is a $n \times n$ unitary matrix, and Σ is a $n \times n$ diagonal matrix with diagonal singular values given in descending order. For many situations where high condition numbers are not encountered, a simple symmetric $n \times n$ matrix $C = B^T B$ can be formed and the matrix V can be found by direct use of the QR algorithm. Similarly, U can be found by using $D = BB^T$.

4 Multi-phase Systolic Algorithms

In this section, we introduce the multi-phase systolic algorithms to compute the QR algorithm. Two arrays, triangular and rectangular, can be used to compute the QR algorithm with some advantages and disadvantages for each. We shall show that our methods compute the Q matrix explicitly without requiring any global communication within the array. Before we consider the multi-phase algorithms, two communication switches are first discussed. A circular multiplexer is a device which takes its inputs and distributes them in different output positions as shown in Fig.5. We use a skewed row to represent the circular multiplexor. A first in/first out (FIFO) buffer is a buffer which takes its input to output in a first in first out manner as shown in Fig.6. Both devices are commonly used in computer and microprocessor systems for data arrangement [16]. The computation of a QR algorithm consists of two basic steps. Initially, set $A_1 = A$.

- (1) for $k = 1, 2, \dots$, compute $A_k = Q_k R_k$;
- (2) compute $A_{k+1} = R_k Q_k$, stop if converge, otherwise go back to step (1).

4.1 Multi-phase Triangular Systolic Array

The QR Decomposition triarray proposed by Gentleman and Kung [9] is used in our approach. The R matrix is stored in the triarray after the computation. To compute the matrix A_{k+1} in step (2), the Q_k matrix has to be computed first. Let us call the computations in step (1) and step (2) an iteration. Several iterations are required for A_k to converge. For each iteration, we propose a three phase operation on a triarray as follows:

- Phase 1: QR decomposition for A_k Compute the QR decomposition of the matrix $A_k = Q_k R_k$, with the upper triangular matrix R_k being stored in the triarray [9]. The data in A_k is input row by row and skewed in time as shown in Fig.7.
- Phase 2: Computing the Q_k matrix From the QR Decomposition, we have $R_k^{-T}A_k^T = Q_k^T$. Let the i^{th} column of matrices A_k^T and Q_k^T be denoted by \underline{a}_i and \underline{q}_i respectively. Then

$$R_k^{-T}[\underline{a}_1, \underline{a}_2, \cdots, \underline{a}_n] = [\underline{q}_1, \underline{q}_2, \cdots, \underline{q}_n]. \tag{25}$$

Section 2 showed that $R_k^{-T}\underline{x}$ can be computed in the same triarray that was used in Phase 1. Since the i^{th} column of A_k^T is the i^{th} row of A_k , then with A_k input row by row skewed in time as shown in Fig.8, the operations of the processing cells are given in the second column of Table 1. The triarray computes the Q_k matrix of A_k . The matrix Q_k is then output row by row as shown in Fig.8. In order to start Phase 3, the matrix Q_k has to be in the form of Fig.9. Observe that the output Q_k of Phase 2 shares the same snap-shot order as the desired arrangement of Q_k in Phase 3 after a transpose operation. A circular multiplexer is used to distribute each column output of Q_k into row input as indicated in Fig.8.

• Phase 3: Computing R_kQ_k

With the operations of the processing cell as shown in the third column of Table 1 and the Q_k obtained in Phase 2, Fig.9 shows the computation of $A_{k+1} = R_k Q_k$ in the triarray. Then the matrix A_{k+1} comes out column by column from the right side of the triarray. Again, we observe that A_{k+1} shares the same snap-shot order as the desired arrangement of A_k in Phase 1 after a transpose operation. If not convergent, a new iteration is repeated by feeding back A_{k+1} into the triarray after using a circular multiplexer as shown in Fig.9. Then Phase 1 operation begins as in Fig.7.

An attractive property of this multi-phase operation is that the feedback requirements of the matrices in different phases are identical. Thus, only a circular multiplexer is needed for each row outside the array. Observe that each column of the matrices input in all of the phases needs n time steps to process and the next phase can be started at time n+1. We find once the result is output at the right hand side of the triarray, after passing through the circular multiplexer, it can be piped into the array for the next phase computation without suffering any delay. If we assume the multiplexer is ideal such that the delay through it can be ignored, it takes 3n+(2n-1)=5n-1 system clocks for one iteration. The (2n-1) term represents the initial time to feed the data into the array. If the number of iterations required for convergence is S, then the total number of system clocks needed is 3Sn+(2n-1). Thus, the converge rate of this algorithm is of the order of O((3S+2)n). After the convergence of the A_k matrix, those values on the boundary cell are the eigenvalues of the A matrix.

4.2 Multi-phase Rectangular Systolic Array

The above method requires the use of the R^{-T} operation in the computations. From a numerical stability point of view, we may want to consider an alternative that uses a square matrix for cumulative multiplication of the rotation parameters. Fig.10 shows a square matrix which is an extended version of the Gentleman-Kung's triangular array with two delay elements (represented by black dots in Fig.10) in the vertical communication links of the lower triangular part of the array. The processors in the lower triangular part are identical to the internal cells in the upper triangular part. In [32], Reilly et al. used the same array for a QRD array processing application. Denote

$$[A//I] = [\underline{\alpha}_1; \underline{e}_1, \underline{\alpha}_2; \underline{e}_2, \cdots, \underline{\alpha}_n; \underline{e}_n]$$
 (26)

as the parallel combination of matrix A and I, where $A = [\underline{\alpha}_1, \underline{\alpha}_2, \cdots, \underline{\alpha}_n]$ and I is a $n \times n$ identity matrix with \underline{e}_i as its i^{th} column. The square array takes the input [A//I]. While

rotating A into an upper triangular matrix, it uses I to accumulate the rotation parameters by

$$Q[A//I] = [R//Q]. \tag{27}$$

We note that processors in the upper triangular part not only rotate the matrix A but also cumulatively multiply the rotation parameters with I. Thus, its work load is, in general, twice as that of Gentleman-Kung's internal cell. Processors in the lower part, on the other hand, only accumulate Q from the propagated rotation parameters. A two phase operation for QR iteration is proposed as follows:

- Phase 1: QR decomposition Compute the QR decomposition of matrix $A_k = Q_k R_k$; both Q_k and R_k are obtained and stored. Then each row of Q_k is piped out and fed back to the array through a FIFO buffer as shown in Fig.10.
- Phase 2: Computing R_kQ_k In this phase, the operation is identical to that of the Phase 3 in the triangular array. A circular multiplexer is used to transform A_{k+1} from row output into column input. Continue this iteration until converged.

Due to the delay elements at the lower triangular part of the array and the work load of each processor (except those in the lower triangular part) being twice as that of the triangular array, the time to obtain the i^{th} row of the Q_k matrix, t_i , is

$$t_i = \max(2(n+3i-3), 2(2n+i-2)),$$

where 2(n+3i-3) is the time for the left-most cell of the i^{th} row to obtain its Q element and 2(2n+i-2) is the time for the right-most cell to finish. Obviously, when $i \geq \lceil \frac{n+1}{2} \rceil$, $t_i = 2(n+3i-3)$. Thus, the time required to obtain the whole Q matrix is $t_n = 8n-6$. By assuming that it takes time n to sequentially pipe out the Q_k matrix, this algorithm takes (9n-6)+n+(2n-1) to complete an iteration in the worst case. Again, denoting the number of iteration as S, this algorithm converge in the order of O(S(10n-6)+2n-1) = O((10S+2)n). Of course, the performance can be improved by piping out each row of Q matrix when it is available instead of waiting for the whole Q matrix to be available. With this, the performance can reach to the order of O((9S+2)n).

4.3 The Hessenberg Reduction

In order to perform the QR algorithm efficiently in conventional Von Neumann type serial computers, we usually transform the data matrix A into an upper Hessenberg matrix before applying the QR iteration. With this transformation, the amount of work per iteration is reduced from $O(n^3)$ to $O(n^2)$ [10]. However, this motivation may not be relevant for parallel processing architectures. The reasons are two folds:

1. Due to the hardware resources in a parallel processing architecture, the computations can be performed concurrently without hindering the processing time. For example, the computation times of the two multi-phase arrays discussed above are of the order O(n).

2. The data matrix is usually not in the Hessenberg form. The pre-processing of the data matrix to Hessenberg form may not be able to be incorporated with the following computations. That is, the pre-processing must be done separately.

Both reasons may lead to the conclusion that the Hessenberg form is not of practical interest in parallel processing of the QR algorithm unless the Hessenberg form can be obtained easily by using the same parallel processing architecture. Many prior works avoid this issue by assuming that the Hessenberg form (or sometimes the tridiagonal form) is already available from the beginning. Fortunately, the Hessenberg form can be obtained easily in conjunction with the above proposed multi-phase algorithms and architectures.

To obtain the Hessenberg form, we can choose a unitary similarity transformation U such that $A_1 = U^H A U$ is a upper Hessenberg matrix [10]. The transformation U can be obtained from sequences of Givens rotations. Denote G_i as the product of the Givens rotation matrices which zero out the proper positions of the i^{th} column. Since the first i rows will not be affected by G_i , the matrix G_i is of the form $G_i = diag(I_i, \bar{G}_i)$, where I_i is an identity matrix of dimension i. Suppose the Hessenberg form through its first k-1 columns has been obtained

$$(G_1 \cdots G_{k-1})^H A(G_1 \cdots G_{k-1}) = \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ 0 & B_{32} & B_{33} \end{bmatrix},$$
 (28)

where B_{11} and B_{33} are $(k-1) \times (k-1)$ and $(n-k) \times (n-k)$ matrices respectively. Then

$$(G_1 \cdots G_k)^H A(G_1 \cdots G_k) = \begin{bmatrix} B_{11} & B_{12} & B_{13}\bar{G}_k \\ B_{21} & B_{22} & B_{23}\bar{G}_k \\ 0 & \bar{G}_k^H B_{32} & \bar{G}_k^H B_{33}\bar{G}_k \end{bmatrix}$$
(29)

is a Hessenberg form through its first k columns. Thus

$$A_1 = (G_1 \cdots G_{n-1})^H A(G_1 \cdots G_{n-1})$$
(30)

is an upper Hessenberg matrix and

$$U = G_1 \cdots G_{n-1} = \begin{bmatrix} 1 & \underline{0}^T \\ \underline{0} & G \end{bmatrix}. \tag{31}$$

Denote

$$A = \begin{bmatrix} \underline{a}^T \\ \bar{A} \end{bmatrix} = U\tilde{A} = \begin{bmatrix} 1 & \underline{0}^T \\ \underline{0} & G \end{bmatrix} \cdot \begin{bmatrix} \underline{a}^T \\ \tilde{R} \end{bmatrix}, \tag{32}$$

where $\bar{A} = G\tilde{R}$ and \tilde{R} is of the form of an upper triangular matrix without the lowest right element. Then $A_1 = \tilde{A}U = U^H A U$. Obviously, this is similar to the computations in the QR iteration. To obtain G and \tilde{R} , let

$$\hat{A} = \begin{bmatrix} \bar{A} \\ ----- \\ 0, 0, \cdots, 1 \end{bmatrix}. \tag{33}$$

The QRD of \hat{A} is

$$\hat{A} = \hat{Q}\hat{R} = \begin{bmatrix} G & \underline{0}^T \\ \underline{0} & 1 \end{bmatrix} \cdot \begin{bmatrix} \tilde{R} \\ 0, 0, \dots, 1 \end{bmatrix}. \tag{34}$$

Now, we can use the multi-phase operations to obtain the upper Hessenberg form. We call this Phase 0, with three internal operations.

- Phase 0: The Hessenberg Reduction.
 - (1) Use Phase 1 Operation for QRD of \hat{A} . from $\hat{A} = \hat{Q}\hat{R}$, we obtain \tilde{R} in the triarray.
 - (2) Use Phase 2 Operation for computing the G matrix. From $\hat{Q} = \hat{R}^{-T}\hat{A}^{T}$, we obtain matrix G.
 - (3) Use Phase 3 Operation for computing the Hessenberg matrix A_1 . By forming

 $\tilde{A} = \left[\begin{array}{c} \underline{a}^T \\ \tilde{R} \end{array} \right]$

and

$$U = \left[\begin{array}{cc} 1 & \underline{0}^T \\ \underline{0} & G \end{array} \right],$$

we obtain the Hessenberg matrix $A_1 = \tilde{A}U$.

4.4 Computing the Eigenvectors

To compute an eigenvector, a matrix multiplication systolic array can be incorporated with the multi-phase array such that those matrices Q_1, \cdots, Q_k are accumulated to form the \tilde{Q}_k matrix. Noted that $\tilde{Q}_k = \tilde{Q}_{k-1}Q_k$ and the matrix \tilde{Q}_{k-1} is available at the start of the k^{th} iteration, while the matrix Q_k is coming out at Phase 2 operation of the k^{th} iteration. Then \tilde{Q}_k is obtained by multiplying \tilde{Q}_{k-1} and Q_k as shown in Fig.4. A system configuration for triangular array is shown in Fig.11a and that for rectangular is shown in Fig.11b. As discussed in Section 3, for a symmetric A matrix, when A_k converged, \tilde{Q}_k yields the matrix of eigenvectors. For a non-symmetric A matrix, the first column of \tilde{Q}_k yields the eigenvector associated with the largest eigenvalue.

5 Performance Comparisons

5.1 Comparisons of the arrays

Although there are three phases of operations, the arithmetic operations in Phase 2 and Phase 3 form a subset of the operations executed in Phase 1. Therefore we do not increase the cell complexity in the multi-phase arrays. The performance and characteristics of both triangular and rectangular arrays considered above are summarized in Table 3. The advantages of the triangular array are: it requires less computational time and fewer cells, I/O ports, and communication devices. Furthermore, all of the processing cells are fully utilized. However, due to the computation of R^{-T} in Phase 2 of the operation, it may be numerically

less stable for certain highly ill-conditioned data. For example, consider the matrix given by

$$\begin{bmatrix} 0.7601 & -0.3967 & 0.6060 \\ -0.3967 & 1.7475 & -0.1962 \\ 0.6060 & -0.1962 & 0.4924 \end{bmatrix}$$

with eigenvalues $\{2.0, 1.0, 10^{-12}\}$. If the triarray algorithm (which uses R^{-T} to obtain Q^T) is used, the eigenvalues are obtained as $\{2.0, 1.0, 3.6818 \cdot 10^{-6}\}$. On the other hand, based on the rectangular array (where the R^{-T} is not explicitly computed), the eigenvalues are obtained as $\{2.0, 1.0, 9.9999 \cdot 10^{-13}\}$. All these results are obtained using MATLAB with double precision computations. As a result, we have a complexity versus numerical stability tradeoff for the two multi-phase arrays.

5.2 Rate of Convergence

As in Luk [24], by convergence of the upper triangularity of A, we mean the parameter $of f(A_k)$ defined as

$$off(A_k) = \frac{\sum_{i < j} a_{ij(k)}^2}{N},\tag{35}$$

where N is a number of off-diagonal elements, has fallen below some prechosen tolerance value. As indicated in [24], it is difficult to monitor $off(A_k)$ in the parallel computation. Luk then proposed that the iteration be stopped after a sufficiently large number S of iterations. In the studies of Brent and Luk [3,24], they found that $S \leq 9$ for random symmetric matrices of order $n \leq 230$ and $S \leq 6$ for $n \leq 24$. Therefore, they chose S = 10 for $n \leq 100$ for the Jacobi-like method. Similar to their approach, we apply the QR algorithm to random $n \times n$ symmetric matrices (a_{ij}) , where the elements a_{ij} for $1 \leq i \leq j \leq n$ were uniformly and independently distributed in [-1,1]. The tolerance to meet the stopping condition is $off(A_k) \leq 10^{-10}$. We can see from Fig.12 that the number of iterations for a QR algorithm to converge is in the order of 10 for matrix size smaller than 20×20 . Even though we can reduce the matrix to Hessenberg form for full dense matrix or tridiagonal form for symmetric matrix, and the QR iteration with origin shift can accelerate the convergence rate [15,39,44], the number of iterations is still on the order of 10. As an example, the 4×4 tridiagonal matrix

$$\left[\begin{array}{cccc} 1 & 2 & 0 & 0 \\ 2 & 3 & 4 & 0 \\ 0 & 4 & 5 & 6 \\ 0 & 0 & 6 & 7 \end{array}\right]$$

still requires eight iterations to converge when the symmetric QR algorithm is used [10, pp.424] This kind of property is not desirable for parallel processing implementation. It is known that the Jacobi-like method may require more flops than the symmetric QR algorithm. However, due to parallel implementation, many rotations may take place at the same time. The computations involved in QR algorithm and Jacobi-like method are generally of the same complexity. From these discussions, the one which requires fewer iterations is more attractive from the parallel implementational point of view. Furthermore,

the convergence rate of a QR iteration depends on the ratio of the eigenvalues. In our simulations, in more than 10% of the cases, the randomly generated symmetric matrices required significantly more iterations to converge. As pointed out before, it is difficult to monitor the quantity $off(A_k)$ to decide when the algorithm converges in the parallel computations. Since the convergence rate is highly dependent on the ratio of eigenvalues, there is no general rule for choosing a sufficient number of iterations S to insure convergence. This is an undesirable intrinsic property of the QR algorithm for parallel implementation as compared to the Jacobi-like method.

6 Efficient Fault-tolerance Schemes

Reliable implementation is quite essential in parallel processing architectures. For a complex parallel processing system, a single fault from any part of the system can make the whole system useless. For various critical applications using spectral decomposition, highly-reliable computations are demanded. Fault-tolerance is therefore needed in many of these problems. A simple and cost effective fault-tolerant scheme is the checksum and weighted checksum proposed by Abraham et al [1]. This scheme is one of the typical examples of the algorithm-based fault-tolerance which has been applied to various signal processing and linear algebra operations [22]. Defining the checksum vector $\underline{e}^T = [1, 1, \dots, 1]$, the column, row and full checksum matrices A_c , A_r and A_f of a square n-by-n matrix A are defined as

$$A_{c} = \begin{bmatrix} A \\ \underline{e}^{T} A \end{bmatrix},$$

$$A_{r} = \begin{bmatrix} A & A\underline{e} \end{bmatrix},$$

$$A_{f} = \begin{bmatrix} A & A\underline{e} \\ \underline{e}^{T} A & \underline{e}^{T} A\underline{e} \end{bmatrix}.$$

If any fault occurs during the computation, the checksum criterion is not met and thus the fault is detected. The weighted checksum scheme can be further used to correct errors [18]. It has been suggested in [5] that a (weighted) checksum scheme can be incorporated into the QR iteration for error detection. These properties as well as others are considered here for the multi-phase arrays.

Since there are different operations in different phases, the inherent natures of the operations of each phase are thus different and should be examined for possible fault-tolerant implementation individually. The fault-tolerant schemes for each phase of the multi-phase triangular array are given as follows:

• Phase 1: As pointed out in [5,22], row checksum is invariant for the QR decomposition. It can be seen

$$A_r = \left[\begin{array}{cc} A & A\underline{e} \end{array} \right] = Q \left[\begin{array}{cc} R & R\underline{e} \end{array} \right] = QR_r. \tag{36}$$

This means that the QR decomposition of a row checksum matrix results in a row checksum upper triangular matrix. Fig.13 shows the implementation of this scheme.

• Phase 2: Due to the nature of computations in this phase, row checksum is no longer valid. Fortunately, column checksum is possible as given by

$$R^{-T}A_c^T = R^{-T} \begin{bmatrix} A^T & A^T \underline{e} \end{bmatrix} = \begin{bmatrix} Q^T & Q^T \underline{e} \end{bmatrix} = Q_c^T.$$
 (37)

An implementation of this scheme is shown in Fig.14.

• Phase 3: Although a row checksum upper triangular matrix R_r and a column checksum unitary matrix Q_c are obtained in the above phases, unfortunately, R_rQ_c does not yield any relevant use. By defining the *trace* operation as the sum of the diagonal elements in a square matrix, we obtain Tr[AB] = Tr[BA], where A and B are square matrices. Therefore,

$$Tr[A_{k+1}] = Tr[R_k Q_k] = Tr[Q_k R_k] = Tr[A_k] = \sum_{i=1}^n \lambda_i,$$
 (38)

where λ_i is the eigenvalue of matrix A_k . This invariant property can be used to check the result of the Phase 3 operation. If the trace of A_k is different from the trace obtained before, a fault is then detected during the Phase 3 computation.

For the rectangular array, the Phase 2 operation is the same as the Phase 3 operation of the triangular array. For its Phase 1 operation, an interesting feature of this computation is given by

$$Q[A_r//I_r] = [R_r//Q_r]. (39)$$

That is, a row checksum of the parallel combination of matrices A and I gives a row checksum of the upper triangular matrix R_r and a row checksum of the unitary matrix Q_r .

7 Conclusions

The multi-phase systolic algorithms proposed in this paper can be used efficiently to solve the eigenvalue and SVD problems based on the QR algorithm. In particular, the eigenvectors can be obtained without global communication within the arrays using the multi-phase operations. We showed that the QR algorithm can achieve a parallel implementation on a single architecture. Two systolic arrays, a triangular and a rectangular, are proposed for multi-phase implementation. Efficient algorithm-based fault-tolerance schemes can be incorporated with both arrays easily. Since the operations in each phase belong to the same types of computation, the cell complexity is thus not increased by multi-phase operations. There is a tradeoff between numerical stability and complexity for both arrays. Each iteration takes O(n) time units while the time required for convergence is O(Sn), where S is the number of iterations. Unlike the Jacobi-like method, the convergence rate of the QR algorithm depends on the ratio of the eigenvalues. As a consequence, S may vary for matrices of the same size, with or without origin shift to accelerate the convergence. Generally, S is in the order of 10 for the QR algorithm. From the parallel processing point of view, we have demonstrated the advantage of the QR algorithm that can yield two multi-phase systolic algorithms implementable on single architectures without requiring global connections, while from the intrinsic convergence rate point of view, the QR algorithm is somewhat less attractive as compared to the Jacobi-like method. Depending on specific system and

hardware requirements, one approach may be more desirable than the other. Of course, it is most meaningful to have two basic approaches to choose from for real-time VLSI signal processing based on spectral decomposition.

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Figure Captions:

Fig.1 Triangular systolic array for QR decomposition.

Fig.2 Computation of $R^{-T}\underline{x}$ using a triarray.

Fig.3 Multiplication of a triangular matrix R and an rectangular full dense matrix B with C = RB using a triarray.

Fig.4 Matrix-matrix multiplication in a rectangular array.

Fig.5 A circular multiplexor.

Fig.6 A first in/first out buffer.

Fig. 7 Phase 1: The QR decomposition.

Fig.8 Phase 2: Computing the Q matrix.

Fig.9 Phase 3: Computing the matrix product RQ.

Fig.10 Multi-phase rectangular array for the QR iteration.

Fig.11a System configuration of the multi-phase triarray.

Fig. 11b System configuration of the multi-phase rectangular array.

Fig.12 The number of iterations for a QR algorithm to converge versus the matrix size.

Fig.13 Row checksum for $A_r = QR_r$.

Fig.14 Column checksum for $R^{-T}A_c^T = Q_c^T$.

Table 1 Operations of the processing cells for different phases.

Table 2 The timing table for the rotation parameters to reach the right edge of the QR triarray.

Table 3 Comparisons of the multi-phase triarray and rectangular array.

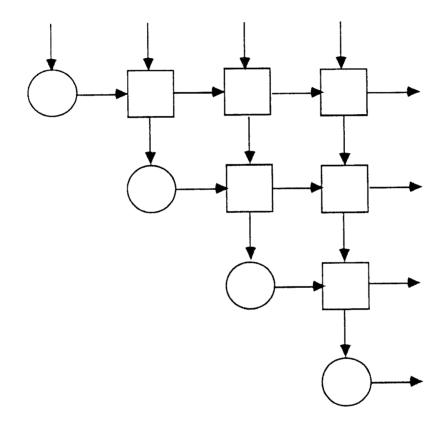


Fig.1

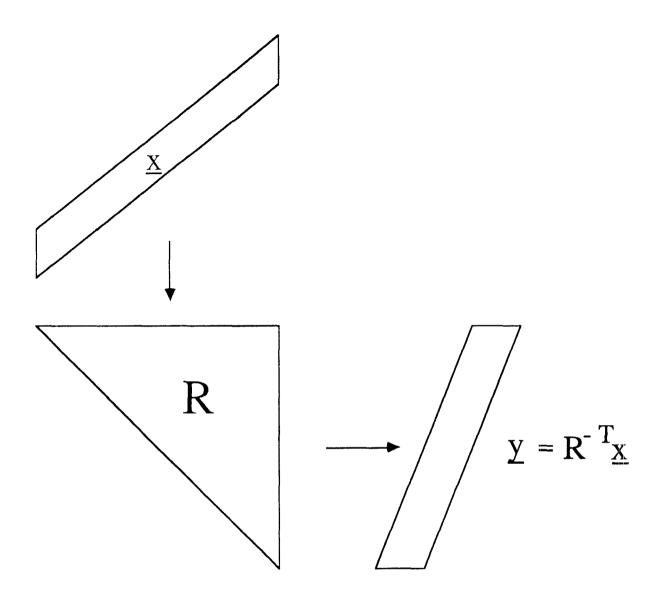


Fig.2

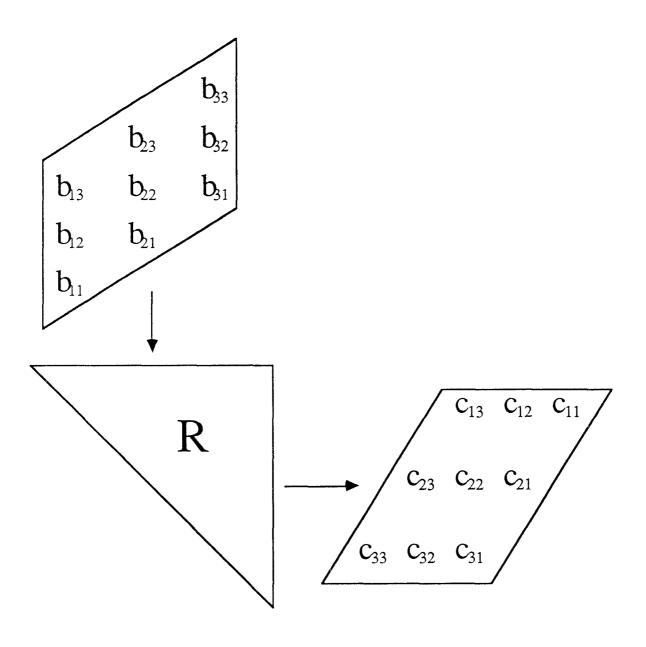


Fig.3

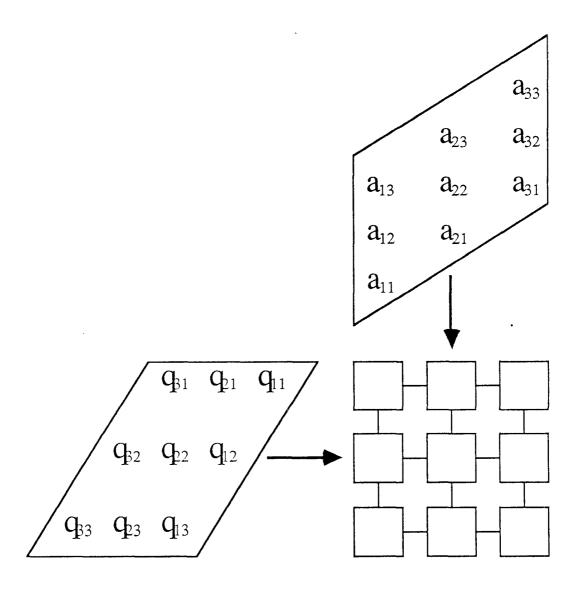


Fig.4

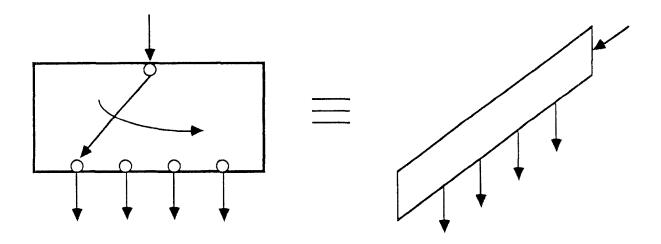


Fig.5

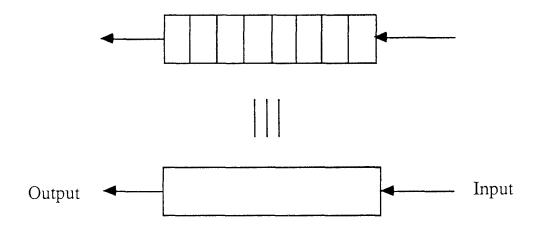


Fig.6

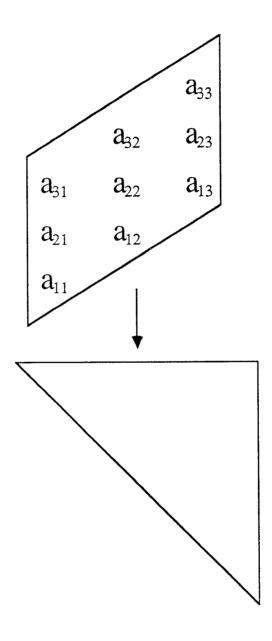


Fig.7

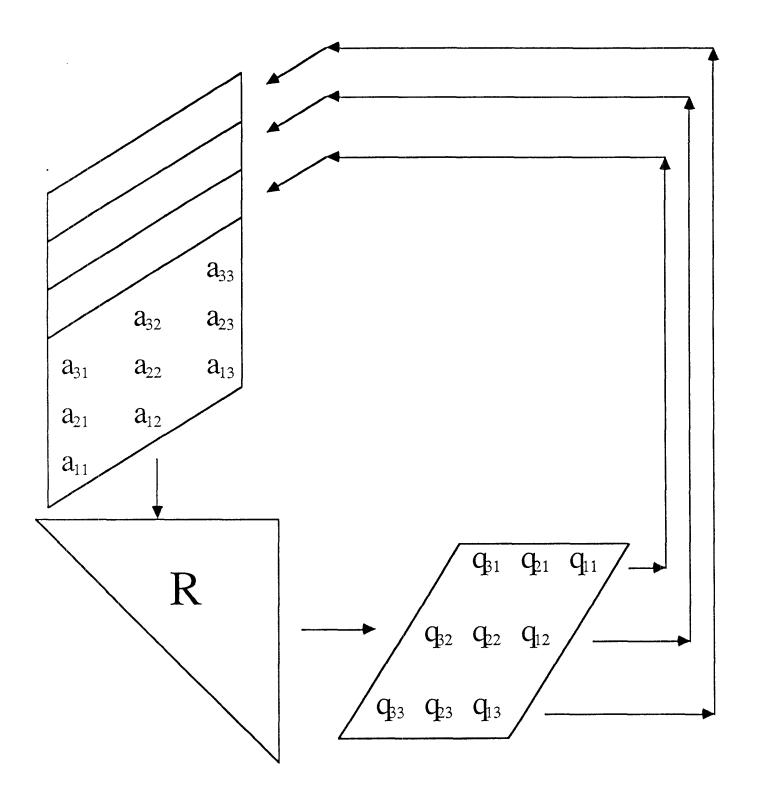


Fig.8

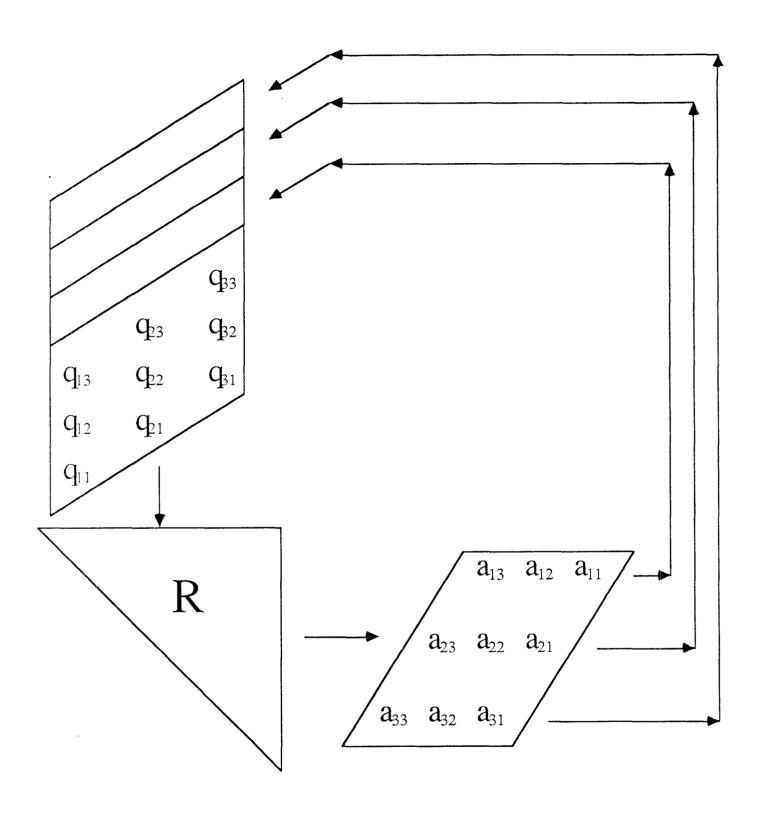


Fig.9

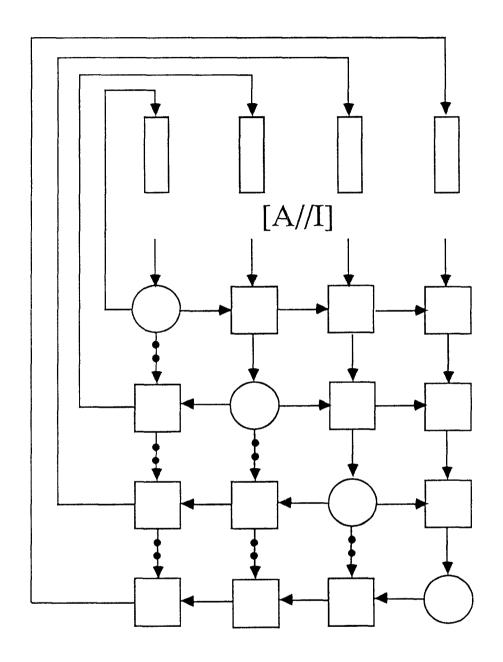


Fig.10

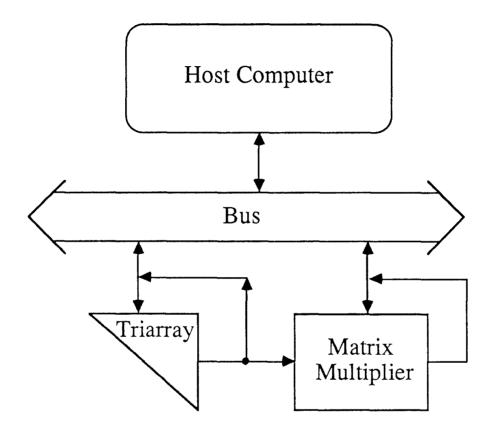


Fig.11a

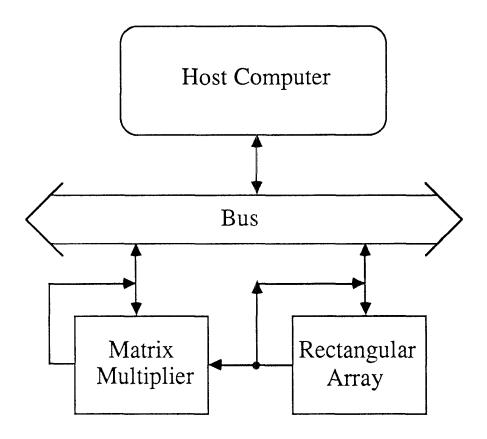


Fig.11b

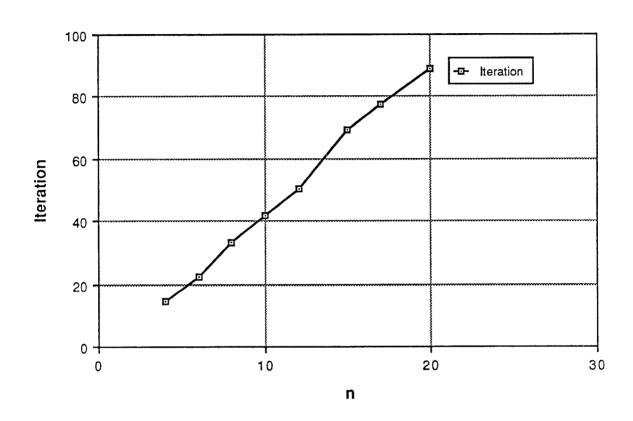


Fig. 12

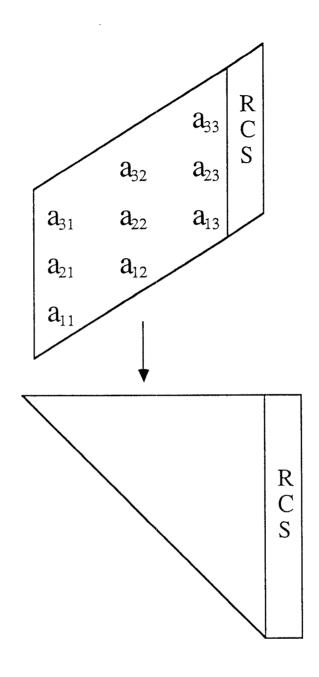


Fig.13

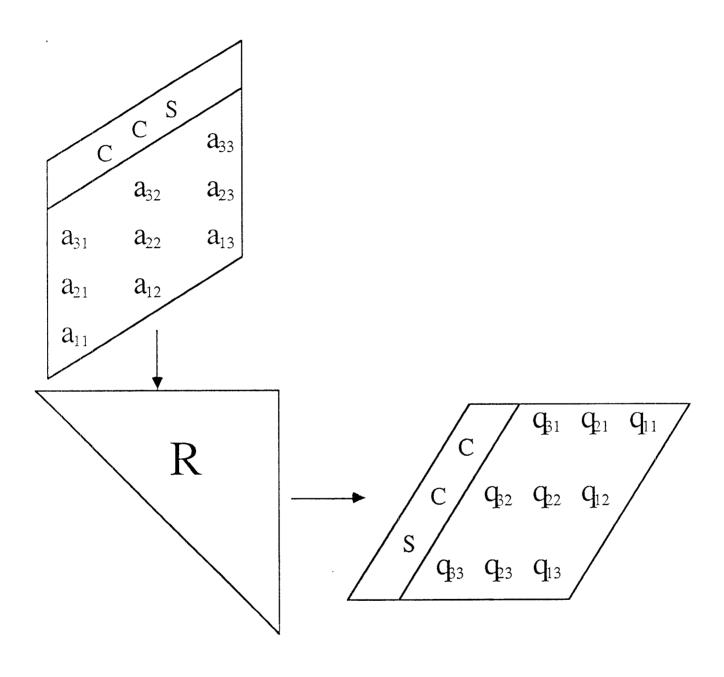


Fig.14

Phase 3	$s \leftarrow x_{in}r$	$s_{out} \leftarrow s_{in} + x_{in}r$	
Phase 2	$s \leftarrow x_{in}/r$	$x_{out} \leftarrow x_{in} - sr$	
Phase 1	If $x_{in}=0$ then $c\leftarrow 1;\ s\leftarrow 0;$ otherwise $r'=\sqrt{r^2+x_{in}^2};$ $c\leftarrow r/r';\ s\leftarrow x_{in}/r'$ end	$x_{out} \leftarrow cx_{in} - sr$ $r \leftarrow sx_{in} + cr$	
Phase Cell	x_{in} (c, s)	(c,s) r x_{out}	

Table 1

Time	n+1	n+2	n+3	n+4	n+5	n+6
First row	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
Second row			(2,3)	(2,4)	(2,5)	(2,6)
Third row					(3,4)	(3,5)

Table 2

	Triangular array	Rectangular array
Computation time	O((3S+2)n)	O((10S+2)n) worst case
Numerical stability	fair	stable
Number of cells	<u>n(n+1)</u> 2	n ² plus (n ² -n) d-elements
I/O ports	2n	3n
Utilization	1	<1
Communication devices	1	2

Table 3