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Report**Author(s):**

Arbenz, Peter; Oettli, Michael

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Wissenschaftliches Rechnen

Peter Arbenz
Michael Oettli

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ETH Zürich
Departement Informatik
Institut für Wissenschaftliches Rechnen
Prof. Dr. W. Gander

Peter Arbenz
Institut für Wissenschaftliches Rechnen
Eidgenössische Technische Hochschule
CH-8092 Zürich
e-mail: arbenz@inf.ethz.ch

Michael Oettli
Institut für Wissenschaftliches Rechnen
Eidgenössische Technische Hochschule
CH-8092 Zürich
e-mail: oettli@inf.ethz.ch

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BLOCK IMPLEMENTATIONS OF THE SYMMETRIC QR AND JACOBI ALGORITHMS

Peter Arbenz and Michael Oettli

*Institute for Scientific Computing,
ETH Zurich, 8092 Zurich, Switzerland*

Abstract

A common approach to solve problems in numerical linear algebra efficiently on modern high speed computers is to redesign the classical algorithm, which was originally developed for serial computers. In this paper, we discuss block variants of QR and Jacobi algorithms for the computation of the complete spectral decomposition of symmetric matrices. We report on numerical tests, which have been performed on a CRAY Y-MP and an ALLIANT FX/80.

1 Introduction

The QR-algorithm is the most widely used algorithm for finding the eigenvalues and eigenvectors of a symmetric matrix. Subroutines, which implement this algorithm (e.g. **TRED2** and **TQL2** from EISPACK [21]) perform very well on sequential computers. But, the classical algorithm may be reorganized to exploit the hardware of high performance computers.

On modern supercomputers with vector- and/or parallel-processing capabilities, it is very important to avoid unnecessary memory references, as moving data between different levels of memory (registers, cache, main memory) is slow compared to arithmetic operations on the data. It has turned out, that on vector-processing computers matrix-vector operations can be efficiently implemented (see [10]). On parallel shared memory computers with cache memory only matrix-matrix operations perform optimally (see [13]). These facts has led to the development of new algorithms and redesign of old ones, which are based on these level 2 (matrix-vector) and level 3 (matrix-matrix) operations. This approach is further motivated by the availability of highly optimized BLAS-2 [8] and BLAS-3 [7] library routines on various supercomputers.

A further very popular algorithm for the computation of the complete eigenvalue problem is the algorithm of Jacobi. This algorithm did not make it into EISPACK. But, a very good implementation in ALGOL by Rutishauser can be found in the ‘Handbuch’ of Wilkinson and Reinsch [18]. We discuss improvements of the original algorithm which concern blocking of Jacobi rotations as well as parallel execution of the blocked rotations.

In this report we examine how these two algorithms may be reorganized to block algorithms and efficiently implemented on high performance computers.

Numerical tests of the algorithms have been made on a CRAY Y-MP and on an ALLIANT FX/80.

2 QR Algorithm

The starting point of this section is a paper by Z. Bai & J. Demmel [2], which describes a block QR algorithm for real *nonsymmetric* matrices based on a multishift iteration.

2.1 The Tridiagonalization

The symmetric QR algorithm requires the initial reduction of the full matrix to tridiagonal form. This operation is usually performed in the following way.

Let $A \in \mathbb{R}^{n \times n}$ be the full, symmetric matrix. The algorithm constructs a sequence $A_0, A_1, \dots, A_{n-2}$ of matrices similar to A , such that A_{n-2} has the required tridiagonal form:

$$\begin{aligned} A_0 &= A, \\ A_k &= P_k^T A_{k-1} P_k, \quad k = 1, \dots, n-2 \end{aligned}$$

Each $P_k = (I - u_k u_k^T)$ with $\|u_k\|_2 = \sqrt{2}$ is a symmetric orthogonal Householder matrix chosen to introduce zeros below the subdiagonal of the k -th column and to the right of the superdiagonal of the k -th row of A_{k-1} (see [14] for how to choose the u_k). Further, the similarity transformation can be expressed as a rank-2 update:

$$A_k = P_k^T A_{k-1} P_k = A_{k-1} - u_k v_k^T - v_k u_k^T$$

where

$$v_k = y_k - \frac{1}{2}(u_k^T y_k) u_k, \quad y_k = A_{k-1} u_k$$

When the eigenvectors are required too, the Householder matrices have to be accumulated

$$Q = P_1 P_2 \cdots P_{n-2}$$

To minimize the number of arithmetic operations the accumulation is performed in reversed order.

$$\begin{aligned} Q_{n-1} &= I, \\ Q_k &= Q_{k+1} - u_k (u_k^T Q_{k+1}), \quad k = n-2, \dots, 1 \end{aligned}$$

This requires only $\frac{4}{3}n^3 + O(n^2)$ flops. A flop or floating point operation is defined here as a floating point add or multiply (see [14]). The complete reduction algorithm requires $\frac{8}{3}n^3 + \frac{3}{2}n^2 + \frac{5}{6}n - 29$ flops.

To achieve better memory utilization on parallel-processing computers with hierarchical memory, Dongarra et al. [11] have proposed to aggregate a sequence of p transformations, so that the matrix will be updated by a rank- $2p$ symmetric matrix. The modified algorithm is as follows: instead of explicitly updating the matrix with the rank two change, only the second column of A_2 , say a_2 is formed. Then a_2 is updated by applying the original rank-2 update:

$$a_2 = a_2 - v_1^{(2)} u_1 - u_1^{(2)} v_1,$$

where $v_1^{(2)}$ and $u_1^{(2)}$ denote the second elements of v_1 and u_1 . From this, u_2 can be computed and y_2 and v_2 are constructed as follows:

$$\begin{aligned} y_2 &= A_2 u_2 = (A_1 - u_1 v_1^T - v_1 u_1^T) u_2, \\ v_2 &= y_2 - \frac{1}{2}(u_2^T y_2) u_2 \end{aligned}$$

Then, A_3 can be formed as a symmetric rank four update:

$$\begin{aligned} A_3 &= A_1 - u_1 v_1^T - v_1 u_1^T - u_2 v_2^T - v_2 u_2^T \\ &= A_1 - [u_1 u_2][v_1 v_2]^T - [v_1 v_2][u_1 u_2]^T. \end{aligned}$$

In general we have a rank- $2p$ update

$$A_{p+1} = A_1 - UV^T - VU^T$$

where

$$U = [u_1, \dots, u_p], \quad V = [v_1, \dots, v_p]$$

Thus A_{p+1} can be formed by a rank- $2p$ update, which is rich in matrix-matrix operations.

The Householder matrices can be accumulated in a blocked fashion by using the storage efficient WY-representation [19]. The product $P_1 \cdots P_p$ of Householder matrices can be written in the form $I - UTU^T$, where U is the matrix of Householder vectors from above and T is a $p \times p$ upper-triangular matrix [19]. Thus, the accumulation is rich in matrix-matrix operations, too:

$$\begin{aligned} Q_m &= I \\ Q_k &= Q_{k+1} - U_k T_k U_k^T Q_{k+1}, \quad k = m-1, \dots, 1, \quad m = n/p \end{aligned}$$

The matrix-matrix operations in this block reduction are paid by additional $(2p - \frac{3}{2})n^2 + O(n)$ flops and extra workspace of size $n \times p$ for V and $p \times p$ for T .

We implemented the algorithm in FORTRAN-77 with calls to BLAS primitives of level two and three as subroutine **BTRED**. An analogous algorithm is implemented in the new library LAPACK [1] as subroutines **SSYTRD**, **DORGQR**. Numerical tests are discussed in section 4.

2.2 Multishift QR Iteration

Given a symmetric tridiagonal matrix $T \in \mathbb{R}^{n \times n}$, the QR algorithm constructs a sequence of similar matrices T_i ($i = 1, 2, \dots$), converging to diagonal form. Let us first look at a step of the usual implicit symmetric QR iteration (see [14]):

- Choose a shift σ . A favourite shift is Wilkinson's (the eigenvalue of T 's trailing 2-by-2 principal submatrix closer to the last diagonal element of T).
- compute first column m_1 of $M = (T_i - \sigma I)$.
- Determine a Givens rotation G_0 , such that $G_0^T m_1 = \mu e_1$, $\mu \in \mathbb{R}$ where e_1 is the first column of the identity matrix
- Perform similarity transformation with G_0 on T_i :

$$G_0^T T_i G_0 = \tilde{T}_i = \begin{bmatrix} \times & \times & + & 0 & 0 \\ \times & \times & \times & 0 & 0 \\ + & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

- Restore tridiagonal form with a sequence of Givens rotations. At any stage, there is only one nonzero entry outside the tridiagonal band.

$$T_{i+1} = G_{n-2}^T \cdots G_1^T \tilde{T}_i G_1 \cdots G_{n-2}$$

This QR step requires about $30n$ flops and additional $6n^2$ flops if the Givens rotations are accumulated.

Now, Bai & Demmel [2] proposed to choose k shifts simultaneously and to perform k steps at a time. The benefit of this modification are fewer iterations and more costly steps, which are however rich in matrix-matrix operations. This implicit multishift algorithm may be formulated for the symmetric case as follows:

- Choose k shifts $\sigma_1, \dots, \sigma_k$. As [2], we shifted by the k eigenvalues of the $k \times k$ trailing principle submatrix.
- Compute the first column m_1 of M , where $M = (T_i - \sigma_1 I)(T_i - \sigma_2 I) \cdots (T_i - \sigma_k I)$
- Determine a Householder reflector $P_0 = I - u_0 u_0^T$, such that $P_0^T m_1 = \mu e_1$, $\mu \in \mathbb{R}$
- Premultiply and postmultiply T_i with P_0 : $P_0^T T_i P_0 = \tilde{T}_i$
- Restore tridiagonal form with a sequence of Householder transformations.

$$T_{i+1} = P_{n-2}^T \cdots P_1^T \tilde{T}_i P_1 \cdots P_{n-2}$$

After pre- and post-multiplying T_i by P_0 , $\tilde{T}_i$ is a triangular matrix with two symmetric $k \times k$ bulges of nonzero elements outside the tridiagonal band, e.g. for $n = 6, k = 2$:

$$\begin{bmatrix} \times & \times & + & + & 0 & 0 \\ \times & \times & \times & + & 0 & 0 \\ + & \times & \times & \times & 0 & 0 \\ + & + & \times & \times & \times & 0 \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

The bulges of nonzero elements are “chased” down the diagonal in the same way as in the case of a single shift. But now, Householder reflectors may be used instead of Givens rotations. Matrix–matrix operations are introduced, if the Householder reflections are aggregated to chase the bulges p columns at a time. The result is a reduction algorithm, which is basically the same algorithm we used to tridiagonalize the full matrix. In fact, only two adjustments are necessary: the length of the Householder vectors depend now on the number of shifts k and the transformations cannot be accumulated in reversed order anymore.

It must be considered however, that the performance of this reduction, which is the core of the QR iteration, depends on a k , that is large enough to exploit the advantages of level 3 operations. But that means additional work of $O(n^2)$ flops per step.

The convergence criterion is the same as in the standard QR algorithm. Negligible small subdiagonal elements are set to zero and the appropriate submatrices are deflated. The algorithm then works on the submatrices. If a submatrix is smaller than some n_0 depending on k , the classical QR algorithm is used to compute its eigenvalues.

We implemented this multishift QR iteration in FORTAN 77 as subroutine **BLKQR** with calls to BLAS primitives. The k shifts are computed by the EISPACK routine **TQL1** and submatrices smaller than n_0 are handled by **TQL2**. To simplify the algorithm, we kept the tridiagonal matrix in the $n \times n$ storage place of the initial full matrix. Furthermore, extra workspace of size $n \times p$ for V and $p \times p$ for T is needed for the reduction (see section 2.1). Numerical experiments are reported in section 4.

3 The Jacobi Algorithm

The Jacobi Algorithm for solving the symmetric eigenvalue problem

$$A\mathbf{x} = \lambda\mathbf{x}$$

was published by Jacobi in 1846 [16]. He proposed to construct a sequence $\{A_k\}_{k=0}^{\infty}$, $A_0 = A$, by

$$A_{k+1} = J_k^T A_k J_k, \quad A_0 = A, \quad (1)$$

where the matrices

$$J_k = J(p_k, q_k, \vartheta_k) = \begin{pmatrix} I_{p_k-1} & & & & \\ & c_k & & s_k & \\ & & I_{q_k-p_k-1} & & \\ & -s_k & & c_k & \\ & & & & I_{n-q_k} \end{pmatrix}$$

are so-called plane or Jacobi rotations. Here, I_m denotes the identity matrix of order m , $c_k = \cos \vartheta_k$ and $s_k = \sin \vartheta_k$. ϑ_k , $|\vartheta_k| < \frac{\pi}{4}$, is chosen such that $a_{p_k, q_k}^{(k+1)} = 0$. In the classical Jacobi algorithm, the pair (p_k, q_k) of rotation indices is chosen to zero the off-diagonal element largest in modulus, i.e. $|a_{p_k, q_k}^{(k)}| = \max_{p>q} |a_{pq}^{(k)}|$. Jacobi proved that with this strategy $\{A_k\}$ converges to a diagonal matrix. Let $V_k = J_0 J_1 \cdots J_k$. The convergence of the Jacobi algorithm implies that the orthogonal matrix $V = \lim_{k \rightarrow \infty} V_k$ diagonalizes A .

While the updates $A_{k+1} = J_k^T A_k J_k$ and $V_{k+1} = V_k J_k$ cost only $12n$ flops, locating the largest off-diagonal requires $(n-1)n/2$ comparisons. To avoid this expensive searching, the rotation index pairs can be chosen cyclically, e.g. row-wise, starting with $(p, q) = (1, 2)$ and ending with $(p, q) = (n-1, n)$. The most elaborate implementation of this algorithm is by Rutishauser [18].

Rutishauser’s Jacobi algorithm is inferior to the QR algorithm with respect to speed on serial computers. QR is about 5 times as fast as Jacobi.

Nevertheless, the Jacobi algorithm has always stayed very popular, on one hand because of its simplicity, on the other hand for its stability and precision [6]. A further reason, why the Jacobi algorithm deserves interest is that it is easily adapted to parallel computation [3, 4, 5, 12]. Indeed, if the rotation index pairs are chosen, for instance, along the antidiagonal, in the so-called modulus ordering [17, 20], each cycle (sweep) of rotations can be subdivided into $\sim n$ stages of $\sim \frac{n}{2}$ Jacobi

updates all of which can be executed in parallel. Figure 1 illustrates this selection of rotation index pairs. In this figure, the matrix of rotation index pairs (p, q) are depicted. Rotations which can be executed in parallel are indicated by the same number. A disadvantage of parallel Jacobi

×	2	3	4	5	6	7
	×	4	5	6	7	1
		×	6	7	1	2
			×	1	2	3
				×	3	4
					×	5
						×

Figure 1: Rotation index pairs of modulus ordering

algorithms is, that the symmetry of the matrices A_k cannot be exploited anymore. The rotations belonging to one stage interfere when they are applied from different sides. Therefore, all rotations of a stage are to be applied as a whole, first on the rows and then on the columns, thus doubling the serial complexity of the parallel algorithm. To avoid this complexity increase, one-sided or implicit Jacobi algorithms have been proposed. We discuss the implementation of Veselić and Hari [23]. One-sided Jacobi algorithms have their origin in the algorithm of Hestenes for the computation of the singular value decomposition of a matrix [15].

Let us assume, that $A = A^T$ is *positive* definite. This is theoretically no restriction as any symmetric matrix can be made positive definite by an appropriate spectral shift. This shift may however worsen the *relative* accuracy of the computed results [6]. When A is positive definite, its Cholesky decomposition

$$A = LL^T \quad (2)$$

exists. Set

$$\tilde{A} = L^T L. \quad (3)$$

$\tilde{A}$ is similar to A . (The step from (2) to (3) is actually one step of the symmetric LR algorithm.) We apply the Jacobi algorithm to $\tilde{A}$, constructing a sequence $\{\tilde{A}_k\}_{k=0}^{\infty}$, $\tilde{A}_0 = \tilde{A}$, which converges towards a diagonal matrix D . We do not work with the $\tilde{A}_k$ explicitly, but with its factor L_k , where $\tilde{A}_k = L_k^T L_k$. Note that L_k is not lower triangular for $k > 0$.

To determine the rotation angle ϑ_k of $J(p_k, q_k, \vartheta_k)$ the elements $\tilde{a}_{p_k p_k}$, $\tilde{a}_{q_k q_k}$ and $\tilde{a}_{p_k q_k}$ must be at hand. While the diagonal elements of $\tilde{A}_k$ are typically stored in an auxiliary vector and thus are readily available, the off-diagonal element $\tilde{a}_{p_k q_k}$ has to be computed as the dot product of the p_k -th and q_k -th column of L_k . The L_k are related through

$$L_{k+1} = L_k J_k = L_k J(p_k, q_k, \vartheta_k).$$

Let $Q_k = J_0 \cdots J_{k-1}$. The Jacobi algorithm constructs a matrix sequence converging towards a diagonal matrix,

$$\tilde{A}_k = L_k^T L_k = Q_k^T L^T L Q_k \longrightarrow D, \quad (k \rightarrow \infty).$$

So, the matrix sequence $\{L_k\}$ tends to a matrix, say $S = LQ$, where $Q = \lim_{k \rightarrow \infty} Q_k$. As the product of orthogonal matrices, Q itself has mutually orthogonal columns. One easily verifies that also $SD^{-\frac{1}{2}}$ is orthogonal. Furthermore,

$$\begin{aligned} ASD^{-\frac{1}{2}} &= LL^T L Q D^{-\frac{1}{2}} \\ &= L Q D^{-\frac{1}{2}} D D^{-\frac{1}{2}} Q^T L^T L Q D^{-\frac{1}{2}} \\ &= L Q D^{-\frac{1}{2}} D = S D^{-\frac{1}{2}} D \end{aligned}$$

So, the columns of $SD^{-\frac{1}{2}}$ are the normalized eigenvectors of A . As the initial Cholesky decomposition of A can be performed in-place, this one-sided Jacobi algorithm needs only the memory for one matrix. The algorithm computes the matrix S from which the eigenvectors of A are obtained

by normalization of its columns. The norms of the columns of S (in practice of L_k for some k) are A 's eigenvalues.

The cost of one iteration step is $8n$ flops, $2n$ for the computation of $a_{p_k q_k}^{(k)}$ and $6n$ for the update of L_k . A complete cycle costs $4n^3$ compared with $6n^3$ of the original cyclic Jacobi algorithm. The one-sided algorithm is not only cheaper but also better suited for parallel implementation as the rotations are applied merely from the right.

The initial Cholesky decomposition costs roughly $\frac{1}{3}n^3$. It can be parallelized in several ways [9].

Further, it is possible to execute Jacobi's algorithm in blocked form [20, 22]. This means that plane rotations are gathered before they are applied on the full matrix. To be more precise, let

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{pmatrix} \in \mathbb{R}^{n \times n}$$

be a $m \times m$ block matrix with blocks $A_{ij} \in \mathbb{R}^{b_i \times b_j}$ and $b_1 + \cdots + b_m = n$. To perform one block-Jacobi step with the (r, s) -block one proceeds as follows:

- Set $\bar{A} = \begin{pmatrix} A_{rr} & A_{sr} \\ A_{rs} & A_{ss} \end{pmatrix} \in \mathbb{R}^{(b_r+b_s) \times (b_r+b_s)}$ and $\bar{V} = I_{b_r+b_s}$.
- Apply plane rotations $J(p, q, \vartheta)$ with $p = 1, \dots, p_1$ and $q = q_0, \dots, b_p + b_q$ on A and V ,

$$\bar{A} \leftarrow J(p, q, \vartheta)^T \bar{A} J(p, q, \vartheta), \quad \bar{V} \leftarrow \bar{V} J(p, q, \vartheta).$$

We set $p_1 = b_p$ if $r < m$, otherwise $p_1 = b_p + b_q$. The value of q_0 is $b_p + 1$ if $s > r + 1$, otherwise $q_0 = p + 1$.

- Finally, the r -th and s -th block rows and columns of A and the r -th and s -th block columns of V are updated,

$$\begin{pmatrix} A_{1r} & A_{1s} \\ \vdots & \vdots \\ A_{m1} & A_{ms} \end{pmatrix} \leftarrow \begin{pmatrix} A_{1r} & A_{1s} \\ \vdots & \vdots \\ A_{mr} & A_{ms} \end{pmatrix} \bar{V}$$

$$\begin{pmatrix} A_{r1} & \cdots & A_{s1} \\ A_{rm} & \cdots & A_{sm} \end{pmatrix} \leftarrow \bar{V}^T \begin{pmatrix} A_{r1} & \cdots & A_{s1} \\ A_{rm} & \cdots & A_{sm} \end{pmatrix}$$

$$\begin{pmatrix} V_{1r} & V_{1s} \\ \vdots & \vdots \\ V_{m1} & V_{ms} \end{pmatrix} \leftarrow \begin{pmatrix} V_{1r} & V_{1s} \\ \vdots & \vdots \\ V_{mr} & V_{ms} \end{pmatrix} \bar{V}.$$

In this way, each off-diagonal element of A is zeroed once per cycle if each off-diagonal block is selected once per block sweep. If the blocks are selected row-wise or in the modulus ordering, the block Jacobi algorithm is equivalent with the (non-blocked) row-cyclic Jacobi algorithm and thus convergent [17, 20].

4 Numerical Tests

Numerical experiments have been carried out on a CRAY Y-MP/464 at Zurich and on an ALLIANT FX/80 at CERFACS.

All new codes have been written in FORTRAN 77 with 64 bit precision and with calls to appropriate BLAS routines. BLAS-1 subroutines are not used, because both compilers optimized the corresponding FORTRAN loops as well. Unless otherwise stated, the test matrices have been generated randomly for the QR algorithm. As our Jacobi implementation works only with positive definite matrices, those tests have been performed with matrices A with $a_{ij} = n - |i - j|$.

4.1 Block Reduction

The execution times of **BTRED**, our implementation of the block tridiagonalization algorithm, **TRED2** and an additional routine **STRED** are shown here. **TRED2** is the unmodified EISPACK routine. The third subroutine **STRED** is an implementation of the classical reduction. It differs from **TRED2** in that as many calls to BLAS-2 primitives as possible were made.

On the CRAY, all three codes were vectorized by the compiler. Furthermore, the level 2 and level 3 BLAS routines, which are included in the scientific library (SCILIB) run in concurrent mode, if several processors are available. Therefore, the execution times t and the speedups s in table 1 are given for one and four processors respectively. The speedup is defined as the ratio of the execution times between the EISPACK routine and the new routines. The timings for one

Size	1 proc.	1 processor					4 processors				
	TRED2 $t(\text{sec})$	STRED $t(\text{sec})$	s	BTRED $t(\text{sec})$	s	(p)	STRED $t(\text{sec})$	s	BTRED $t(\text{sec})$	s	(p)
100	0.037	0.014	2.6	0.016	2.3	(4)	0.024	1.5	0.024	1.5	(10)
200	0.19	0.084	2.3	0.094	2.0	(4)	0.060	3.2	0.077	2.5	(10)
300	0.53	0.27	2.0	0.29	1.8	(4)	0.14	3.8	0.21	2.5	(8)
400	1.1	0.61	1.8	0.65	1.7	(10)	0.27	4.1	0.40	2.8	(8)
500	2.0	1.2	1.7	1.2	1.7	(10)	0.49	4.1	0.71	2.8	(8)

Table 1: Tridiagonalization on CRAY Y-MP

processor in Table 1 show, that the new routines are more than twice as fast as **TRED2** at order 100, but the speedups decrease with increasing orders. Furthermore, **STRED** is slightly faster than **BTRED**. The parameter p is that blocksize used in **BTRED**, for which the best result was obtained. These times on the CRAY confirm, that algorithms with optimal exploitation of matrix-vector operations have an optimal performance on poor vector-processing machines without cache memory and that therefore matrix-matrix operations can only yield small further improvements (compare [10]).

The times of the new routines on four processors show, that BLAS-2 and BLAS-3 primitives are well suited to perform in parallel. They are actually the only part of the algorithm executed in parallel. But **BTRED** is still inferior to **STRED**. This shows, that the CRAY Y-MP has a well balanced architecture, i.e. the memory bandwidth is sufficiently high to keep pace with the cpu.

On the ALLIANT, the codes were compiled using the **-Ogv -AS** options to perform global optimization and vectorization. Optimized BLAS routines are included in the mathematical library, which can be linked to a program using the **-lalgebra -lcommon -lmath** options. This subroutines are not only vectorized but also parallelized. The times in Table 2 for one processor show,

Size	1 proc.	1 processor					8 processors				
	TRED2 $t(\text{sec})$	STRED $t(\text{sec})$	s	BTRED $t(\text{sec})$	s	(p)	STRED $t(\text{sec})$	s	BTRED $t(\text{sec})$	s	(p)
100	0.867	0.805	1.08	0.878	0.99	(5)	0.189	4.59	0.215	4.03	(4)
200	6.20	5.69	1.09	5.62	1.10	(10)	1.20	5.17	1.20	5.17	(4)
300	21.1	18.8	1.12	17.5	1.21	(10)	4.30	4.91	3.83	5.51	(5)
400	51.8	47.9	1.08	40.0	1.30	(15)	11.4	4.54	8.88	5.83	(5)
500	103.0	95.3	1.08	76.6	1.34	(15)	23.4	4.40	17.1	6.02	(5)

Table 2: Tridiagonalization on ALLIANT FX/80

that vectorization causes only minor speedups in both new routines. On eight processors however, concurrency shows a good effect. **STRED** is more than four times as fast as the EISPACK routine. Further, the block algorithm **BTRED** is clearly superior to **STRED** at a problem size greater than 200. The matrix-matrix-operations are needed to exploit the cache memory (see [13]).

4.2 Block QR Iteration

To analyze the performance of our block multishift QR routine **BLKQR**, we compared it with the unmodified EISPACK routine **TQL2**. The block size p and the number of shifts k were chosen to

minimize the running time. Table 3 shows, that **BLKQR** requires about twice the time of **TQL2** on

Size	1 processor		1 processor			
	TQL2		BLKQR			
	$t(\text{sec})$	#it.	$t(\text{sec})$	s	#it.	(p, k)
100	0.0890	207	0.184	0.48	54	(4,8)
200	0.496	399	0.918	0.54	132	(4,6)
300	1.37	583	2.60	0.53	196	(6,6)
400	3.00	773	5.56	0.54	264	(6,6)
500	5.53	960	9.51	0.58	322	(6,6)

Table 3: QR iteration on CRAY Y-MP

one processor of the CRAY. The results on the ALLIANT (see Table 4) are very similar. Minor speedups are only achieved on eight processors. But better speedups up to three are achieved with unmodified **TQL2**, if some loops are executed in vector-concurrent mode. While **TQL2** needs

Size	1 processor		1 processor				8 processors			
	TQL2		BLKQR				BLKQR			
	$t(\text{sec})$	#it.	$t(\text{sec})$	s	#it.	(p, k)	$t(\text{sec})$	s	#it.	(p, k)
100	1.89	213	5.29	0.36	58	(4,8)	3.02	0.63	60	(4,8)
200	13.2	411	28.0	0.47	143	(4,6)	12.3	1.07	143	(4,6)
300	44.7	609	72.0	0.62	204	(6,6)	30.1	1.48	204	(6,6)
400	106.0	797	157.0	0.68	275	(6,6)	58.7	1.81	271	(6,6)
500	205.0	994	285.0	0.72	346	(6,6)	103.0	1.99	347	(6,6)

Table 4: QR iteration on ALLIANT FX/80

about $2n$ iterations, **BLKQR** needs only $\frac{2}{3}n$ iterations. Bai & Demmel counted $\frac{1}{4}n$ iterations for their Hessenberg QR algorithm.

Empirically we observed, that deflation happens with the following scheme. Usually after a few iterations a $k \times k$ -submatrix is deflated at the tail of the matrix. The larger k is, the fewer iterations are needed. However, more iterations are required for larger k until the first submatrix is deflated and afterward the deflation may happen at any place.

The core of the QR iteration is certainly the optimal choice of the shifts. We did not address this problem and simply used the strategy suggested by Bai & Demmel.

4.3 Jacobi

We investigated three variants of Jacobi's algorithm, all written in Fortran 77.

1. A translation of Rutishauser's ALGOL subprogram [18], which incorporates the row-cyclic Jacobi algorithm. This program is used as a reference.
2. A translation and modification of a Pascal program given by Veselić, which is an implementation of the one-sided algorithm by Veselić and Hari [23]. In contrast to the original Pascal program, the modulus ordering of the rotation index pairs is implemented to make parallel execution of the rotations of one stage possible. The stopping criterion was

$$\max_{p \neq q} \frac{|\tilde{a}_{pq}^{(k)}|}{\sqrt{\tilde{a}_{pp}^{(k)} \tilde{a}_{qq}^{(k)}}} < \sqrt{n}\epsilon,$$

where ϵ is the machine precision. With this stopping criterion we obtained results with the one-sided Jacobi algorithm which were about as accurate as with Rutishauser's algorithm.

If $|\tilde{a}_{pq}^{(k)}| < \sqrt{n}\epsilon\sqrt{\tilde{a}_{pp}^{(k)}\tilde{a}_{qq}^{(k)}}$ for some (p, q) , the corresponding rotation was not performed.

3. A block version of the just given one-sided Jacobi algorithm. The blocks are chosen along the antidiagonal in the modulus ordering. So, the block Jacobi rotations can be performed in

parallel. Within the blocks the rotations are chosen row-wise. The updating of the temporary matrices $\tilde{A}$ and $\tilde{V}$ (cf. §3) was done just as in the adaption of the Rutishauser subroutine in 1. As most of the work of one block step is in forming the off-diagonal block of $\tilde{A}$ and in the updating of the block columns of A , all rotations of a sweep have been performed in this algorithm. Furthermore, we did not obtain the desired accuracy, when we performed rotations only if $|\tilde{a}_{ij}|/\sqrt{\tilde{a}_{ii}\tilde{a}_{jj}} > \sqrt{n}\epsilon$, n the order of A .

Size	1 proc.	1 processor			8 processors						1 proc.
	VESELIC $t(\text{sec})$	VESBLK $t(\text{sec})$	s	(p)	VESPAR $t(\text{sec})$	s	VESBLK $t(\text{sec})$	s	(p)	RUTISH $t(\text{sec})$	
100	7.56	12.3	0.61	(12)	2.03	3.72	3.14	2.40	(8)	13.0	
200	62.2	89.1	0.70	(12)	16.9	3.68	19.9	3.13	(8)	106.0	
300	225.0	262.0	0.86	(16)	73.1	3.08	57.4	3.92	(12)	383.0	
400	540.0	583.0	0.93	(20)	194.0	2.78	129.0	4.19	(16)	970.0	

Table 5: Jacobi on ALLIANT FX/80

Table 5 shows the timings we obtained on the ALLIANT FX/80. The comparison of the times for the Rutishauser **RUTISH** and modified Veselić implementation **VESELIC** show the estimated ratio of about 3/2. The ratio is actually a little better which is probably due to the fast Givens rotations used in **VESELIC**. The speedup we obtained with the parallelization is only about 3.5 on the 8 processor machine. It decreases with increasing matrix order.

On one processor, the blocked implementation **VESBLK** is somewhat slower than **VESELIC**, but still considerably faster than **RUTISH**. On eight processors however, it is superior to the unblocked implementation at matrix sizes exceeding 250 and is more than seven times as fast as Rutishauser's implementation **RUTISH** at size 400. Table 6 shows the times we measured on the Cray Y-MP.

Size	1 proc.	1 processor			4 processors						1 proc.
	VESELIC $t(\text{sec})$	VESBLK $t(\text{sec})$	s	(p)	VESPAR $t(\text{sec})$	s	VESBLK $t(\text{sec})$	s	(p)	RUTISH $t(\text{sec})$	
100	0.55	0.80	0.69	(8)	0.18	3.1	0.30	1.8	(8)	0.42	
200	3.0	4.7	0.64	(8)	1.0	3.0	1.7	1.8	(8)	2.8	
300	7.9	13.0	0.61	(8)	2.4	3.3	5.0	1.6	(8)	8.8	
400	17.0	30.0	0.57	(8)	5.2	3.3	12.0	1.4	(8)	20.0	

Table 6: Jacobi on CRAY Y-MP

The overhead for the blocked algorithm is too large to be compensated by the BLAS-3 operations. Interestingly, **RUTISH** is faster than **VESELIC** for matrix orders smaller than 200 on this machine.

4.4 A Comparison of QR and Jacobi Algorithms

Finally, let us make a comparison between the classical algorithms **TRED2/TQL2** and **RUTISH** and the new block algorithms **BTRED/BLKQR** and **VESBLK** to compute the complete spectral decomposition. Positive definite test matrices of the form QDQ^T have been produced, where D is a diagonal matrix with diagonal entries uniformly distributed in $[0, n]$ and Q is the Q-factor of the QR-factorization of a random matrix.

While the classical algorithms ran on one processor of the ALLIANT, the new block algorithms used all eight. The timing results in Table 7 show, that **BTRED/BLKQR** is fastest. The reason is the high speedup in the tridiagonalization. Although, classical Jacobi is not competitive with the QR algorithm, the blocked parallel Jacobi implementation **VESBLK** is even faster than **TRED2/TQL2**.

5 Conclusions

The aim of this work was to learn, how new ideas, which were proposed in different papers, effect the performance of the QR and Jacobi algorithms for symmetric matrices on supercomputers.

Size	Algorithm	$t(\text{sec})$	$\max_i \ Tq_i - \lambda_i q_i\ _2$	$\max_i \ [q_1, \dots, q_n]^T q_i - e_i\ _2$
100	TRED2/TQL2	2.66	0.59093E-12	0.62630E-14
	BTRED/BLKQR	2.97	0.16983E-11	0.64044E-14
	RUTISH	14.9	0.10199E-12	0.26609E-14
	VESBLK	2.79	0.45009E-12	0.26723E-14
200	TRED2/TQL2	19.4	0.22968E-11	0.10263E-13
	BTRED/BLKQR	12.7	0.29786E-11	0.81243E-14
	RUTISH	120.0	0.30690E-12	0.36766E-14
	VESBLK	17.1	0.90176E-12	0.31513E-14
300	TRED2/TQL2	64.5	0.32024E-11	0.12431E-13
	BTRED/BLKQR	36.9	0.78236E-11	0.99906E-14
	RUTISH	439.0	0.58644E-12	0.44042E-14
	VESBLK	47.1	0.17705E-11	0.27981E-14
400	TRED2/TQL2	153.0	0.45461E-11	0.15090E-13
	BTRED/BLKQR	71.5	0.96399E-11	0.11459E-13
	RUTISH	1020.0	0.10427E-11	0.48764E-14
	VESBLK	110.0	0.27734E-11	0.25046E-14

Table 7: Total time and accuracy of results on ALLIANT FX/80

It has turned out, that the blocked tridiagonalization is very fast on larger problem sizes. This algorithm combined with a unblocked version for smaller matrices is a very powerful implementation for high performance computers. Actually, the new linear algebra library LAPACK [1] contains such subroutines (SSYTRD, DORGQR).

Our implementation of the multishift QR iteration from Bai & Demmel is not suited to the symmetric eigenvalue problem. A further reduction of the number of iteration steps would be required to compensate the additional work.

The parallel blocked one-sided Jacobi algorithm turned out to be quite competitive with the QR algorithm on a parallel shared memory computer with cache memory as the ALLIANT FX/80. In situations, where the original matrix is close to diagonal, block Jacobi could be the method of choice.

The CRAY Y-MP has a well balanced architecture, therefore the blocked algorithms are not more efficient than the unblocked ones on this machine.

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