Accumulating Householder Transformations, Revisited

THIERRY JOFFRAIN and TZE MENG LOW
The University of Texas at Austin
ENRIQUE S. QUINTANA-ORTÍ
Universidad Jaume I
and
ROBERT VAN DE GEIJN and FIELD G. VAN ZEE
The University of Texas at Austin

A theorem related to the accumulation of Householder transformations into a single orthogonal transformation known as the compact WY transform is presented. It provides a simple characterization of the computation of this transformation and suggests an alternative algorithm for computing it. It also suggests an alternative transformation, the UT transform, with the same utility as the compact WY Transform which requires less computation and has similar stability properties. That alternative transformation was first published over a decade ago but has gone unnoticed by the community.

Categories and Subject Descriptors: G.1.3 [**Numerical Analysis**]: Numerical Linear Algebra; G.4 [**Mathematical Software**]: *Efficiency*

General Terms: Algorithms; Performance

Additional Key Words and Phrases: Linear algebra, Householder transformation, compact WY transform, QR factorization

1. INTRODUCTION

Given a nonzero vector $u \in \mathbb{R}^m$, a *Householder transformation* (or *reflector*) is defined by $H = I - \frac{uu^T}{\tau}$, where I denotes the (square) identity matrix and

This research was partially sponsored by NSF grants ACI-0305163 and CCF-0342369 and an equipment donation from Hewlett-Packard. Dr. Quintana-Orti was partially supported by a J. Tinsley Oden Visiting Research Fellowship from the UT-Austin Institute for Computational Engineering and Sciences. Access to the NEC SX-6 server was arranged by NEC Solutions (America), Inc.
Authors' addresses: T. Joffrain, T. M. Low, R. Van de Geijn, and F. G. Van Zee, Department of Computer Sciences, The University of Texas at Austin, Austin, TX 78712; email: {joffrain,itm,rvdg,field}@cs.utexas.edu; E. S. Quintana-Ortí, Departamento de Ingeniería y Ciencia de Computadores, Universidad Jaume I, Campus Riu Sec, 12.071—Castellón, Spain; email: quintana@icc.uji.es.

$\tau = \frac{u^T u}{2}$ [Householder 1958]. It is an orthogonal matrix ($H^T H = HH^T = I$) and its own transpose ($H^T = H$). This transformation has wide application in the solution of linear least-squares problems, the computation of orthonormal bases, and the solution of the algebraic eigenvalue problem.

Two transforms that capture the action of multiple Householder transformations and cast it in terms of high-performance matrix-matrix products were proposed in the late 1980s, the WY transform [Bischof and Van Loan 1987] and the compact WY transform (CWY) [Schreiber and Van Loan 1989]. A third such transform was proposed and published by Walker in 1988 [Walker 1988] in the setting of a GMRES algorithm based on Householder transformations and rediscovered by Puglisi in 1992 in the setting of the QR factorization [Puglisi 1992][1]. Yet few in the numerical analysis community appear to be aware of these results as they relate to the CWY [Sun 1996]. It was a brief brainstorming session involving the authors of this article that independently rediscovered this result once again. We believe the result to be of sufficient importance that it warrants republishing.

In Section 2, we review the traditional way in which the CWY is computed. In Section 3, we present the main theorem that characterizes the accumulation of Householder transformations. In Section 4, we discuss opportunities that appear due to the alternative characterization. Remarks on how to modify LAPACK to accommodate the insights are given in Section 5. Experimental results are presented in Section 6, followed by concluding remarks in the final section.

2. COMPUTING THE COMPACT WY TRANSFORM

The following theorem presents the traditional formula for accumulating Householder transformations into a CWY:

THEOREM 1. *Let the matrix $U_{k-1} \in \mathbb{R}^{m\times k}$ have linearly independent columns. Partition U by columns as*

$$U_{k-1} = (u_0 | u_1 | \cdots | u_{k-1}),$$

and consider the vector $t = (\tau_0, \tau_1, \ldots, \tau_{k-1})^T$ with $\tau_i \neq 0$, $0 \leq i < k$. Then, there exists a unique nonsingular upper triangular matrix $S_{k-1} \in \mathbb{R}^{k\times k}$ such that

$$\left(I - \frac{u_0 u_0^T}{\tau_0}\right)\left(I - \frac{u_1 u_1^T}{\tau_1}\right)\cdots\left(I - \frac{u_{k-1} u_{k-1}^T}{\tau_{k-1}}\right) = \left(I - U_{k-1} S_{k-1} U_{k-1}^T\right).$$

The matrices $S_0, S_1, \ldots, S_{k-1}$ can be computed via the recurrence

$$S_0 = 1/\tau_0 \quad and \quad S_i = \left(\begin{array}{c|c} S_{i-1} & -S_{i-1} U_{i-1}^T u_i / \tau_i \\ \hline 0 & 1/\tau_i \end{array}\right), \quad 1 \leq i < k. \tag{1}$$

PROOF. The recurrence gives the standard algorithm for computing the accumulation of Householder transformations into a CWY. It is proved by induction

[1] We emphasize that, while we will often refer to Puglisi's paper in this article, it is Walker who should be given credit for first proposing the methodology discussed in this article.

Partition $U \rightarrow \left(U_L \,\middle|\, U_R \right)$, $t \rightarrow \left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right)$, $S \rightarrow \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right)$

where U_L has 0 columns, t_T has 0 rows, and S_{TL} is 0×0

while $m(S_{TL}) < m(S)$ **do**

Repartition

$\left(U_L \,\middle|\, U_R \right) \rightarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right)$,

$\left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right) \rightarrow \left(\begin{array}{c} t_0 \\ \hline \tau_1 \\ \hline t_2 \end{array} \right)$, $\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$

where u_1 has one column, and τ_1, σ_{11} are scalars

$s_{01} := U_0^T u_1$

$\sigma_{11} := 1/\tau_1 \;(= 2/u_1^T u_1)$

$s_{01} := -S_{00} s_{01} \sigma_{11}$

Continue with

$\left(U_L \,\middle|\, U_R \right) \leftarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right)$,

$\left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right) \leftarrow \left(\begin{array}{c} t_0 \\ \hline \tau_1 \\ \hline t_2 \end{array} \right)$, $\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$

endwhile

Fig. 1. Traditional algorithm for computing S.

on k. (In our theorem, we lift the restriction that each transformation must be a Householder transformation, a generalization that we will not use subsequently in the article.) □

An algorithm for computing this transformation based on (1) is given in Figure 1.

3. CENTRAL RESULT

We now state a theorem that will give a simpler characterization of the relation between U and S.

THEOREM 2. *Let $U \in \mathbb{R}^{m \times k}$ have linearly independent columns. Then, there exists a unique nonsingular upper triangular matrix $S \in \mathbb{R}^{k \times k}$ such that $I - USU^T$ is an orthogonal matrix. This matrix S satisfies $S = T^{-1}$ with $T + T^T = U^T U$, where $T \in \mathbb{R}^{k \times k}$ is itself a unique nonsingular upper triangular matrix.*

PROOF. We first prove existence. Consider U partitioned by columns as $U = (u_0 | \cdots | u_{k-1})$, and let $\tau_i = u_i^T u_i / 2$, $0 \le i < k$. We then recognize $\tau_i \neq 0$, and each $(I - \frac{u_i u_i^T}{\tau_i})$ is a Householder transformation. Multiplying these Householder transformations together results in an orthogonal matrix. From this, Theorem 1 yields the desired nonsingular upper triangular matrix S.

Since $I - USU^T$ is orthogonal,

$$\begin{aligned} 0 &= I - (I - USU^T)(I - USU^T)^T = I - (I - USU^T)(I - US^T U^T) \\ &= I - (I - US^T U^T - USU^T + USU^T US^T U^T) \\ &= U[(S^T + S) - SU^T US^T]U^T. \end{aligned}$$

Thus, $S^T + S = SU^TUS^T$ since U has full column rank. Now, as matrix S is required to be nonsingular, $S^{-1}(S^T + S)S^{-T} = S^{-1}SU^TUS^TS^{-T}$, and therefore

$$S^{-1} + S^{-T} = U^TU. \tag{2}$$

Finally, replacing S^{-1} by T in (2), we find that $T = \text{striu}(U^TU) + \frac{1}{2}\text{diag}(U^TU)$ uniquely defines the upper triangular matrix T. Here striu(A) denotes the part of matrix A that lies strictly above the diagonal of that matrix, and diag(A) equals the diagonal matrix that has the same diagonal as A. □

Under the assumptions of this theorem, S can be computed by the following three steps:

(1) $S :=$ the upper triangular part of U^TU;
(2) Divide the diagonal elements of S by two;
(3) $S := S^{-1}$.

An algorithm for the first step is given in the top part of Figure 2, while an algorithm that combines the last two steps is given in the bottom part of that figure.

NOTE 1. *Puglisi arrived at the result in Theorem 2 by applying the Woodbury-Morrison formula to $I - USU^T$. We believe our proof is simpler and more revealing.*

The two algorithms in Figure 2 together implement *exactly* the same computation as the traditional algorithm in Figure 1 except that, rather than computing σ_{11} in three steps ($\sigma_{11} := u_1^Tu_1$; $\sigma_{11} := \sigma_{11}/2$; $\sigma_{11} := 1/\sigma_{11}$), the traditional algorithm simply sets σ_{11} to τ_1, which has the same net result.

Update in Figure 1	Update in Figure 2
$s_{01} := U_0^Tu_1$ $\sigma_{11} := 1/\tau_1 \left(= 2/\left(u_1^Tu_1\right)\right)$ $s_{01} := -S_{00}s_{01}\sigma_{11}$	$s_{01} := U_0^Tu_1$ $\begin{cases}\sigma_{11} := u_1^Tu_1\\ \sigma_{11} := \sigma_{11}/2\\ \sigma_{11} := 1/\sigma_{11}\end{cases}$ $s_{01} := -S_{00}s_{01}\sigma_{11}$

Other than one additional recomputation of $u_1^Tu_1/2$ per diagonal element of S, the two algorithms perform the same operations. Therefore, they will have very similar cost and numerical stability. This additional computation is an artifact of the fact that the level 3 Basic Linear Algebra Subprograms (BLAS) routine DSYRK [Dongarra et al. 1990], which would typically be used to compute U^TU, also recomputes the diagonal of the result. Clearly, σ_{11}, the diagonal element of S, could simply be set to $1/\tau_1$ in Figure 2. The computation of U^TU and the inversion of S can be implemented using any algorithm for those operations, not just the ones in Figure 2.

NOTE 2. *Puglisi makes the same connection between the traditional algorithm for computing S and the separate steps just mentioned.*

Partition $U \rightarrow \left(U_L \,\middle|\, U_R \right)$, $S \rightarrow \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right)$
  where U_L has 0 columns and S_{TL} is 0×0

while $m(S_{TL}) < m(S)$ **do**
  Repartition

$$\left(U_L \,\middle|\, U_R \right) \rightarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right), \quad \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$$

  where u_1 is a column and σ_{11} is a scalar

$s_{01} := U_0^T u_1$
$\sigma_{11} := u_1^T u_1$

  Continue with

$$\left(U_L \,\middle|\, U_R \right) \leftarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right), \quad \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$$

endwhile

Partition $S \rightarrow \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right)$
  where S_{TL} is 0×0

while $m(S_{TL}) < m(S)$ **do**
  Repartition

$$\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$$

  where σ_{11} is a scalar

$\sigma_{11} := \sigma_{11}/2$
$\sigma_{11} := 1/\sigma_{11}$
$s_{01} := -S_{00} s_{01} \sigma_{11}$

  Continue with

$$\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$$

endwhile

Fig. 2. Computing S as proposed in Section 3. Top: Compute $S := U^T U$ (upper triangular part only). Bottom: Divide the diagonal elements of S by 2 and compute $S := S^{-1}$.

4. OPPORTUNITIES

While the result in the previous section provides a simple theoretical characterization of the relation between the Householder vectors and the CWY, we now show how it provides opportunities for performance and numerical stability.

4.1 Potential Impact on Performance

The traditional algorithm in Figure 1 is rich in matrix-vector products, a level 2 BLAS [Dongarra et al. 1988] operation. By contrast, Steps (1)–(3) in Section 3 can inherently attain high performance: Step (1) can be implemented by a call to an optimized implementation of the level 3 BLAS routine DSYRK, while the LAPACK routine DTRTRI can be used for Step (3). Typically, k is small enough so that the inversion of the $k \times k$ matrix in Step (3) will keep that matrix in cache memory, making that operation inherently efficient.

NOTE 3. *Puglisi makes the same observation.*

4.2 The UT Transform

$I - UT^{-1}U^T$ represents an alternative expression for the accumulation of the Householder transformations. This formulation eliminates the need for the k^3 floating-point operations (flops) required to compute $S := T^{-1}$. We call this formulation *the UT transform*.

The CWY is typically formed so that it can be applied to a matrix $A \in \mathbb{R}^{m\times n}$, as in the computation $A := (I - USU^T)A$. One can instead compute $(I - UT^{-1}U^T)A$. The parentheses in the following expressions indicate the order in which operations in these two approaches are typically performed:

$$A := A - U[S\ \underbrace{[U^T A]}_{W}\ ] \quad \text{versus} \quad A := A - U[T^{-1}\ \underbrace{[U^T A]}_{W}\ ].$$

The computation of SW and $T^{-1}W$, via the level 3 BLAS routines DTRMM and DTRSM, respectively, requires *exactly* the same number of flops. Thus, avoiding the inversion of matrix T translates directly into k^3 fewer flops being performed.

NOTE 4. *Puglisi makes the same observation.*

For different implementations of the BLAS, DTRSM may attain better or worse performance than DTRMM. This would influence whether to compute and use the UT transform or the CWY.

4.3 Potential Impact on Numerical Stability

Householder transformations are inherently used because of their exceptional stability properties. The CWY is known to inherit these properties. Nonetheless, it is also well known that computing $W := T^{-1}W$ as a triangular solve with multiple right-hand sides is numerically more stable than computing $W := SW$ after explicitly inverting $S := T^{-1}$. Thus, the UT transform is at least as stable as the CWY, and possibly more stable.

NOTE 5. *Puglisi makes a similar comment regarding stability.*

5. MODIFICATIONS TO LAPACK

We now give details of how minor modifications to LAPACK can be made to incorporate the insights in this article.

A detail that is not made obvious in the previous discussion is that the matrix U that stores the Householder vectors as they are computed during a QR factorization has the form $U = \binom{U_1}{U_2}$, where U_1 is unit lower triangular. Thus, the computation $S = U^T U$ can be broken down into $S := U_1^T U_1$, followed by

$S := \mathrm{triu}(U_2^T U_2)$

Partition $U_1 \rightarrow \left(U_L \,\middle|\, U_R \right)$, $t \rightarrow \left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right)$, $S \rightarrow \left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right)$

where U_L has 0 columns, t_T has 0 rows, and S_{TL} is 0×0

while $m(S_{TL}) < m(S)$ **do**

Repartition

$\left(U_L \,\middle|\, U_R \right) \rightarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right)$,

$\left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right) \rightarrow \left(\begin{array}{c} t_0 \\ \hline \tau_1 \\ \hline t_2 \end{array} \right)$, $\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$

where u_1 has one column, and τ_1, σ_{11} are scalars

Compute S:	**Compute** $T = S^{-1}$ **in** S:
$s_{01} := s_{01} + U_0^T u_1$	$s_{01} := s_{01} + U_0^T u_1$
$\sigma_{11} := 1/\tau_1$	$\sigma_{11} := \tau_1$
$s_{01} := -S_{00} s_{01} \sigma_{11}$	

Continue with

$\left(U_L \,\middle|\, U_R \right) \leftarrow \left(U_0 \,\middle|\, u_1 \,\middle|\, U_2 \right)$,

$\left(\begin{array}{c} t_T \\ \hline t_B \end{array} \right) \leftarrow \left(\begin{array}{c} t_0 \\ \hline \tau_1 \\ \hline t_2 \end{array} \right)$, $\left(\begin{array}{c|c} S_{TL} & S_{TR} \\ \hline & S_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} S_{00} & s_{01} & S_{02} \\ \hline & \sigma_{11} & s_{12}^T \\ \hline & & S_{22} \end{array} \right)$

endwhile

Fig. 3. Modification of traditional algorithm for computing S and T.

$S := S + U_2^T U_2$, computing only the upper triangular part. The term $U_2^T U_2$ is a simple call to DSYRK. The problem is that there is no routine in the BLAS or LAPACK that computes only the upper triangular part of $S = U_1^T U_1$, while taking advantage of the special structure of U_1.

To overcome this, let us examine routine DLARFT from LAPACK, which computes the matrix S via the algorithm in Figure 1. Now, S can be computed by initializing it to the upper triangular part of $U_2^T U_2$, changing the update $s_{01} := U_0^T u_1$ to $s_{01} := s_{01} + U_0^T u_1$ in Figure 1, and executing this modified algorithm with U_1 rather than all of U. Thus, first S is set to $U_2^T U_2$, after which the remaining computations are all accomplished by the modification given in Figure 3 (left). This approach casts most computations in terms of $U_2^T U_2$ (DSYRK) and, in one sweep, performs the remaining computation with matrices that are small enough to remain in cache. This is coded by modifying DLARFT, adding a call to DSYRK with U_2 before the loop, changing the upper limit of the loop from `N` (the row dimension of U) to `K` (the row dimension of U_1), and changing a `ZERO` to a `ONE` in the call to DGEMV so that the result of the matrix-vector multiply is added to s_{01}. Let us call the result DLARFT_NEW.

The new routine DLARFT_NEW can then be turned into a computation of T by further changing the algorithm in Figure 1, replacing $\sigma_{11} = 1/\tau_1$ by $\sigma_{11} = \tau_1$, and deleting the update $s_{01} = -S_{00} s_{01} \sigma_{11}$, as illustrated in Figure 3 (right). This translates to a change in one line of DLARFT_NEW and the deletion of one call to DTRMV. Applying the UT transform so computed requires only that a single call to DTRMM be changed to a call to DTRSM in DLARFB.

6. EXPERIMENTS

We demonstrate the potential of the alternative approaches by modifying the LAPACK routines for computing and applying the CWY, DLARFT and DLARFB, and measuring its effect on the LAPACK QR factorization routine, DGEQRF.

6.1 Implementation

Three different implementations were examined: **LAPACK**, the standard LAPACK implementation; **CWY-alt**, the modified LAPACK implementation based on the algorithm in Figure 3 (left); and **UT**, the modified LAPACK implementation based on the UT transform as described in Figure 3 (right).

6.2 Performance

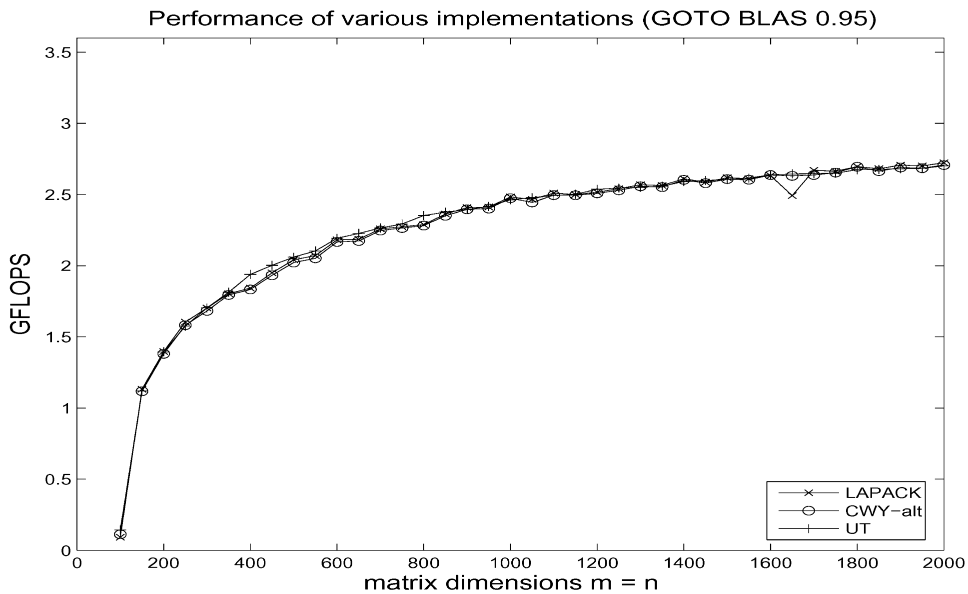
The impact of the described modifications was measured by computing the QR factorization of matrices of various sizes and using the result to solve a linear system (with a single right-hand side). The first target platform was an Intel Itanium 2 (900MHz) processor-based workstation, using the GOTO BLAS library, Release 0.95 [Goto 2005]. The results are reported in Figure 4. In all experiments, a blocksize of $k = 32$ was used.

Casting most computation in DLARFT in terms of DSYRK yields a slight degradation in performance. We speculate that is due to inefficiencies in the implementation of that routine for the specific matrix dimensions that are encountered in our computation. By switching to the implementation based on the UT transform, modest performance improvements are observed. As part of a QR factorization, the amount of computation that is performed in the routines that were optimized constitutes a lower order term so modest improvements are all that can be expected. The performance results in Figure 4 highlight the importance of how well the different kernels that are used by the algorithm are tuned.

NOTE 6. *Puglisi also comments on the inefficiency of the* DSYRK *operation in similar experiments.*

In Figure 5, we report performance attained on an eight CPU NEC SX-6 SMP server with a peak of 8 GFLOPS per CPU. Each CPU of this architecture is a vector processor, making it possible to highly and (more importantly) equally optimize any of the level 3 BLAS. While on a single CPU, no benefit is observed from computing the triangular matrix via SYRK, on multiple CPUs, a noticeable performance improvement results. This is because SYRK parallelizes better than the traditional algorithm for computing S which is rich in matrix-vector multiplication. Since the explicit inversion of the triangular matrix constitutes very little computation relative to the overall QR factorization, CWY-alt and UT attained essentially the same performance.

NOTE 7. *Walker originally proposed this methodology to improve parallelism and reduce communication on distributed memory architectures.*



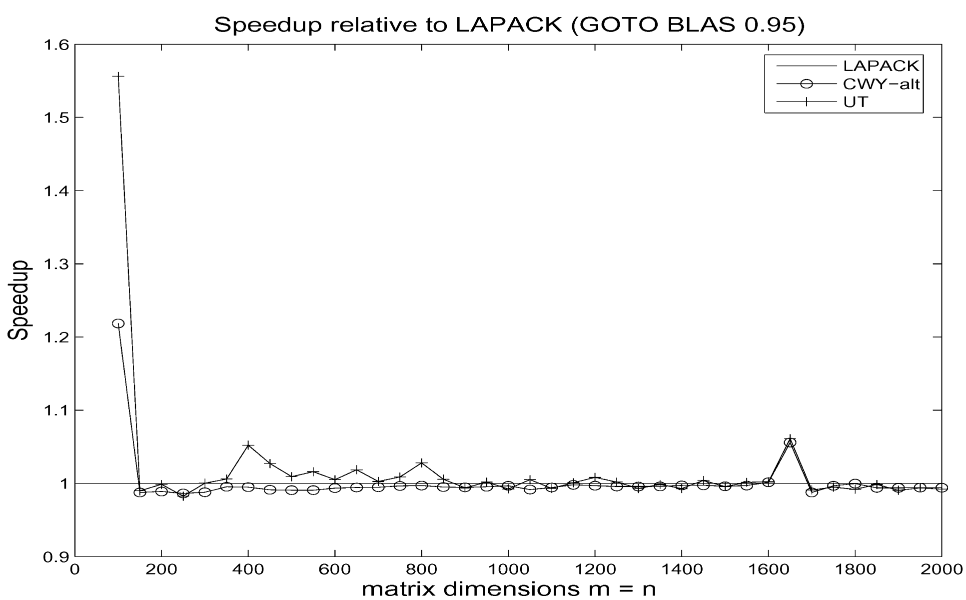


Fig. 4. Performance of the various implementations on an Intel Itanium 2 (900MHz) server (single CPU), linked to GOTO BLAS release 0.95.

6.3 Numerical Stability

The effects of the modifications on numerical stability were also experimentally examined and no meaningful improvements or degradations in the quality of the residual were observed.

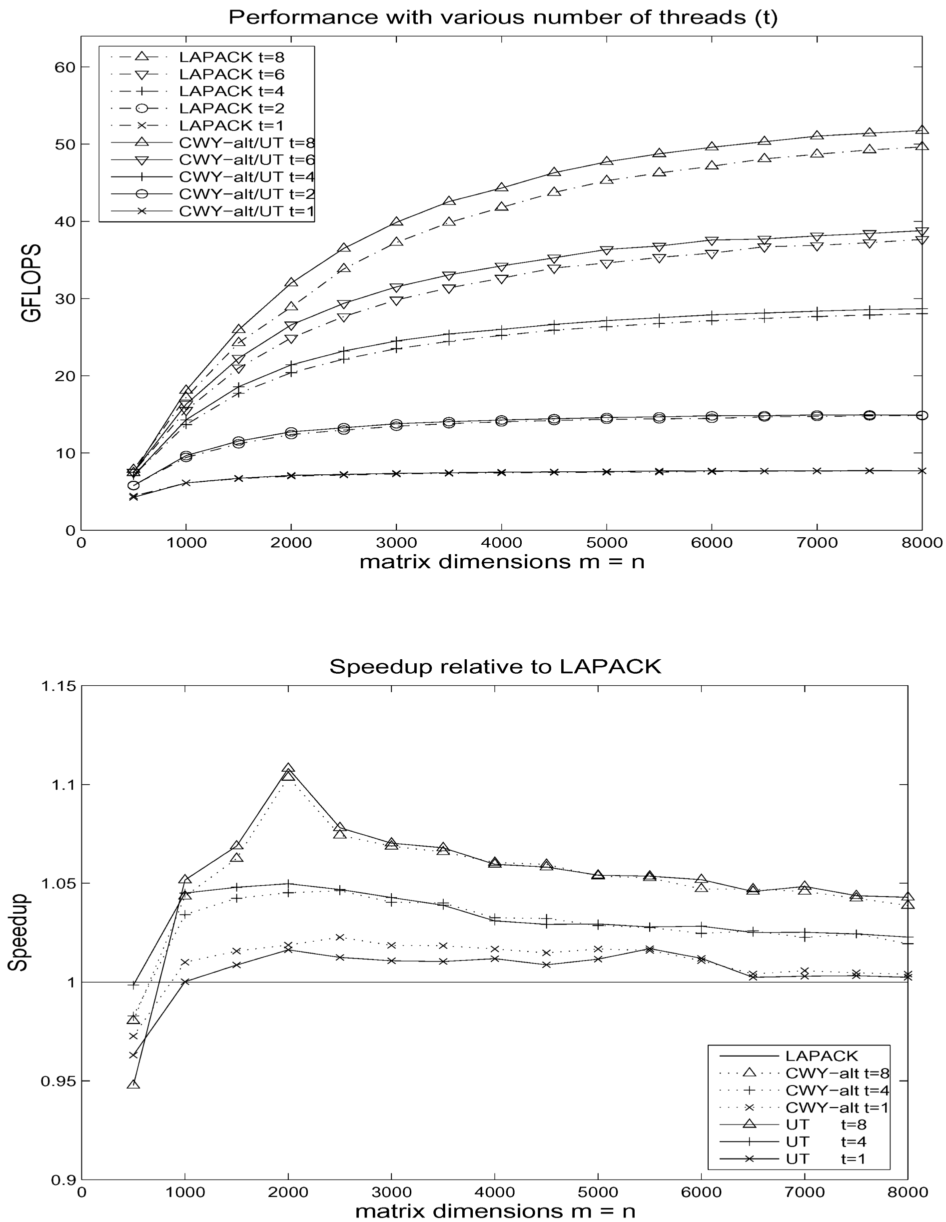


Fig. 5. Performance of LAPACK and UT on a NEC SX-6 SMP server. Note: the performance of CWY-alt and UT was virtually indistinguishable on this architecture.

7. CONCLUSION

In this article, an alternative characterization of the compact WY transform was given. The characterization suggests a simple approach to computing that transform and an alternative way of accumulating Householder transformations, the UT transform, which eliminates the cost of the inversion of a triangular matrix. This alternative transform was already proposed, first by Walker and again by Puglisi, a result that appears to have been lost to the community. On sequential systems, the benefits of the methodology is highly dependent on the tuning of the BLAS library. Performance gains can be expected to be more significant on SMP and distributed memory architectures.

ACKNOWLEDGMENTS

We thank Thuan Cao for performing the experiments on the NEC SX-6 and Dr. Robert Schreiber for his encouragement.

REFERENCES

BISCHOF, C. AND VAN LOAN, C. 1987. The WY representation for products of Householder matrices. *SIAM J. Sci. Stat. Comput. 8*, 1 (Jan.), 2–13.

DONGARRA, J. J., DU CROZ, J., HAMMARLING, S., AND DUFF, I. 1990. A set of level 3 basic linear algebra subprograms. *ACM Trans. Math. Soft. 16*, 1 (Mar.), 1–17.

DONGARRA, J. J., DU CROZ, J., HAMMARLING, S., AND HANSON, R. J. 1988. An extended set of FORTRAN basic linear algebra subprograms. *ACM Trans. Math. Soft. 14*, 1 (Mar.), 1–17.

GOTO, K. 2005. `http://www.cs.utexas.edu/users/kgoto/`.

HOUSEHOLDER, A. S. 1958. Unitary triangularization of a nonsymmetric matrix. *J. ACM 5*, 339–342.

PUGLISI, C. 1992. Modification of the Householder method based on the compact wy representation. *SIAM J. Sci. Stat. Comput. 13*, 723–726.

SCHREIBER, R. AND VAN LOAN, C. 1989. A storage-efficient WY representation for products of Householder transformations. *SIAM J. Sci. Stat. Comput. 10*, 1 (Jan.), 53–57.

SUN, X. 1996. Aggregations of elementary transformations. Tech. Rep. Tech. rep. DUKE-TR-1996-03, Duke University.

WALKER, H. F. 1988. Implementation of the GMRES method using Householder transformations. *SIAM J. Sci. Stat. Comput. 9*, 1, 152–163.

Received August 2004; revised July 2005; accepted August 2005