

# Implementation and performance evaluation of new inverse iteration algorithm with Householder transformation in terms of the compact WY representation

HIROYUKI ISHIGAMI,<sup>†1</sup> KINJI KIMURA<sup>†1</sup>  
and YOSHIMASA NAKAMURA<sup>†1</sup>

A new inverse iteration algorithm that can be used to compute all the eigenvectors of a real symmetric tridiagonal matrix on parallel computers is developed. In the classical inverse iteration, the modified Gram-Schmidt orthogonalization is used, and this causes a bottleneck in parallel computing. In this paper, the use of the compact WY representation is proposed in the orthogonalization process of the inverse iteration with the Householder transformation. This change results in drastically reduced synchronization cost in parallel computing. The new algorithm is evaluated on a 32-core parallel computer, and it is shown that the algorithm is up to 7.46 times faster than the classical algorithm in computing all the eigenvectors of matrices with several thousand dimensions.

## 1. Introduction

The eigenvalue decomposition of a symmetric matrix, i.e., a decomposition into a product of matrices consisting of eigenvectors and eigenvalues, is one of the most important operations in linear algebra. It is used in vibrational analysis, image processing, data searches, etc.

Owing to recent improvements in the performance of computers equipped with multicore processors, we have had more opportunities to perform calculations on parallel computers. As a result, there has been an increase in the demand for an eigenvalue decomposition algorithm that can be effectively parallelized.

The inverse iteration algorithm is an algorithm for computing eigenvectors independently associated with mutually distinct eigenvalues. However, when we use this algorithm, we must reorthogonalize the eigenvectors if some eigenval-

ues are very close to each other. Adding this reorthogonalization increases the computational cost. Moreover, for this reorthogonalization, we have generally used the MGS (modified Gram-Schmidt) algorithm. However, this algorithm is sequential and inefficient for parallel computing. As a result, we are unable to maximize the performance of parallel computers. Hereinafter, we will refer to the inverse iteration algorithm with MGS as the classical inverse iteration.

We can also orthogonalize vectors by using the Householder transformation<sup>9)</sup>, and we call this process the Householder orthogonalization algorithm. While the MGS algorithm is unstable in the sense that the orthogonality of the resulting vectors depends on the condition number of the matrix<sup>10)</sup>, the Householder algorithm is stable because its orthogonality does not depend on the condition number. The Householder algorithm is also sequential and ineffective for parallel computing, and its computational cost are higher than those of MGS.

In 1989, the Householder orthogonalization in terms of the compact WY representation was proposed<sup>8)</sup>. By adopting this orthogonalization, stability and effective parallelization can be achieved. Hereafter, we refer to this algorithm as the compact WY orthogonalization algorithm. In 2010, Yamamoto demonstrated the fact<sup>10)</sup>: When this algorithm is used in the Arnoldi process, the computation time for parallel computation is less than that when the MGS algorithm is used, and the orthogonality of the eigenvectors generated using this algorithm is better than that of the eigenvectors generated using MGS.

In this paper, we consider an implementation of the compact WY orthogonalization to the inverse iteration algorithm for a real symmetric tridiagonal matrix and we evaluate its performance. Thereafter, we present a new inverse iteration algorithm for computing the eigenvectors of a real symmetric tridiagonal matrix.

## 2. Classical inverse iteration and its defect

### 2.1 Classical inverse iteration

We consider the problem of computing eigenvectors of a real symmetric tridiagonal matrix  $T \in \mathbb{R}^{n \times n}$ . Let  $\lambda_j \in \mathbb{R}$  be eigenvalues of  $T$  such that  $\lambda_1 < \lambda_2 < \dots < \lambda_n$ . Let  $\mathbf{v}_j \in \mathbb{R}^n$  be the eigenvector associated with  $\lambda_j$ . When  $\tilde{\lambda}_j$ , an approximate value of  $\lambda_j$ , and a starting vector  $\mathbf{v}_j^{(0)}$  are given, we can compute

---

<sup>†1</sup> Graduate school of Informatics, Kyoto University

an eigenvectors of  $T$ . To this end, we solve the following equation iteratively:

$$(T - \tilde{\lambda}_j I) \mathbf{v}_j^{(k)} = \mathbf{v}_j^{(k-1)}. \quad (1)$$

Here  $I$  is the  $n \times n$  identity matrix. If the eigenvalues of  $T$  are mutually well-separated, the solution of  $\mathbf{v}_j^{(k)}$ , Eq.(1) generically converges to the eigenvector associated with  $\lambda_j$  as  $k$  goes to  $\infty$ . The above iteration method is the inverse iteration. The computational cost of this method is of  $O(mn)$  when we compute  $m$  eigenvectors, and it is less than that of others for eigenvalue decomposition. In the implementation, we have to normalize the vectors  $\mathbf{v}_j^{(k)}$  to avoid overflow.

When some of all the eigenvalues are close together or there are clusters of eigenvalues, we have to reorthogonalize all the eigenvectors associated with such eigenvalues because they need to be orthogonal to each other. In the classical inverse iteration, we apply the MGS to this process and the computational cost of it is of  $O(m^2n)$ . Therefore, when we calculate eigenvectors of the matrix that has many clustered eigenvalues, the total computational cost increases significantly. In addition, the classical inverse iteration is implemented the Peters-Wilkinson method<sup>7)</sup>. In this method, when the distance between the close eigenvalues is less than  $10^{-3}\|T\|$ , we regard them as members of the same cluster of eigenvalues, and we orthogonalize all of the eigenvectors associated with these eigenvalues. The classical inverse iteration algorithm is shown by Fig.1 and  $j_1$  denotes the index of the minimum eigenvalue of some cluster.

## 2.2 The defect of the classical inverse iteration

The inverse iteration is a prominent method for computing eigenvectors, because we can compute eigenvectors independently and this process is easily parallelized by assigning each cluster to each core.

Let us consider the Peters-Wilkinson method in the classical inverse iteration. When the dimension of  $T$  is greater than 1000, most of the eigenvalues are regarded as being in the same cluster<sup>3)</sup>.

In this case, we have to parallelize the inverse iteration with respect to not the cluster but the loop described from lines 2 to 16 in Fig.1. This loop includes the iteration based on Eq.(1) and the orthogonalization of the eigenvectors. This orthogonalization process becomes a bottleneck of the classical inverse iteration with respect to the computational time. The MGS algorithm is mainly based on a BLAS level-1 operation and it is a sequential algorithm. Because of this, when

```

1: for  $j = 1$  to  $n$  do
2:   Generate  $\mathbf{v}_j^{(0)}$  from random numbers.
3:    $k = 0$ .
4:   repeat
5:      $k \leftarrow k + 1$ .
6:     Normalize  $\mathbf{v}_j^{(k-1)}$ .
7:     Eq.(1): Compute  $\mathbf{v}_j^{(k)}$  by using  $\mathbf{v}_j^{(k-1)}$ .
8:     if  $|\lambda_j - \tilde{\lambda}_{j-1}| \leq 10^{-3}\|T\|$ , then
9:       for  $i = j_1$  to  $j - 1$  do
10:         $\mathbf{v}_j^{(k)} \leftarrow \mathbf{v}_j^{(k)} - \langle \mathbf{v}_j^{(k)}, \mathbf{v}_i \rangle \mathbf{v}_i$ 
11:       end for
12:     else
13:        $j_1 = j$ .
14:     end if
15:   until some condition is met.
16:   Normalize  $\mathbf{v}_j^{(k)}$  to  $\mathbf{v}_j$ .
17: end for

```

Fig. 1 Algorithm of classical inverse iteration.

we compute all the eigenvectors in parallel computers, the number of synchronizations is of  $O(m^2)$ . Therefore, the MGS algorithm is ineffective on parallel computing.

In conclusion, the classical inverse iteration is an ineffective algorithm for parallel computing because the MGS algorithm is used in its orthogonalization process.

## 3. Other orthogonalization algorithms

### 3.1 Householder orthogonalization

The Householder orthogonalization, based on the Householder matrices, is one of the alternative orthogonalization methods. When some vectors  $\mathbf{v}, \mathbf{d} \in \mathbb{R}^n$  satisfy  $\|\mathbf{v}\|_2 = \|\mathbf{d}\|_2$ , there exists the symmetric matrix  $H$  satisfying  $HH^\top = H^\top H = I$ ,  $H\mathbf{v} = \mathbf{d}$  defined by  $H = I - t\mathbf{y}\mathbf{y}^\top$ ,  $\mathbf{y} = \mathbf{v} - \mathbf{d}$ ,  $t = 2/\|\mathbf{y}\|_2^2$ . The transformation by  $H$  is called the Householder transformation. We can orthogonalize some vectors by using the Householder transformations. This orthogonalization algorithm is shown in Fig.2. The vector  $\mathbf{y}_j$  is the vector in which the elements from 1 to  $(j-1)$  are the same as the elements of  $\mathbf{v}'_j$  and the elements from  $(j+1)$  to  $n$  are zero. The vector  $\mathbf{e}_j$  is the  $j$ th vector of  $I \in \mathbb{R}^{n \times n}$ . The orthogonality of the vectors  $\mathbf{q}_j$  generated by the Householder orthogonalization does not depend on the condition number of  $T$ . Therefore, the Householder orthogonalization is more

```

1: for  $j = 1$  to  $m$  do
2:   Generate  $\mathbf{v}_j$  from  $\mathbf{q}_1, \dots, \mathbf{q}_{j-1}$ .
3:    $\mathbf{v}'_j = (I - t_{j-1}\mathbf{y}_{j-1}\mathbf{y}_{j-1}^\top) \cdots (I - t_2\mathbf{y}_2\mathbf{y}_2^\top) (I - t_1\mathbf{y}_1\mathbf{y}_1^\top) \mathbf{v}_j$ .
4:   Compute  $\mathbf{y}_j$  and  $t_j$  by using  $\mathbf{v}'_j$ .
5:    $\mathbf{q}_j = (I - t_1\mathbf{y}_1\mathbf{y}_1^\top) (I - t_2\mathbf{y}_2\mathbf{y}_2^\top) \cdots (I - t_j\mathbf{y}_j\mathbf{y}_j^\top) \mathbf{e}_j$ .
6: end for

```

**Fig. 2** Algorithm of Householder orthogonalization.

stable than MGS. On the other hand, being similar to MGS, it is a sequential algorithm that is mainly based on a BLAS level-1 operation. Its computational cost is higher than that of MGS. Thus the Householder orthogonalization is an ineffective algorithm in parallel computing.

### 3.2 Compact WY orthogonalization

In 2010, Yamamoto presented the Householder orthogonalization in the Arnoldi process in terms of the compact WY representation<sup>10)</sup>. This study suggests that the Householder orthogonalization becomes capable of computation with a BLAS level-2 operation in terms of the compact WY representation<sup>8)</sup>. Yamamoto also showed that the computation time for orthogonalization on parallel computers has decreased with the use of the Householder orthogonalization in terms of the compact WY representation, compared to this computational time in the case of the MGS algorithm<sup>10)</sup>.

Now, we consider the Householder orthogonalization in Fig.2 and we introduce the compact WY representation. First, we define  $Y_1 = \mathbf{y}_1 \in \mathbb{R}^{n \times 1}$  and  $T_1 = t_1 \in \mathbb{R}^{1 \times 1}$ . Next, we define matrices  $Y_j \in \mathbb{R}^{n \times j}$  and upper triangular matrices  $T_j \in \mathbb{R}^{j \times j}$  recursively as follows:

$$Y_j = \begin{bmatrix} Y_{j-1} & \mathbf{y}_j \end{bmatrix}, T_j = \begin{bmatrix} T_{j-1} & -t_j T_{j-1} Y_{j-1}^\top \mathbf{y}_j \\ \mathbf{0} & t_j \end{bmatrix}. \quad (2)$$

In this case, the following equation holds

$$H_1 H_2 \cdots H_j = I - Y_j T_j Y_j^\top. \quad (3)$$

As shown by Eq.(3), we can rewrite the product of the Householder matrices  $H_1 H_2 \cdots H_j$  in a simple block matrix form. Here  $I - Y_j T_j Y_j^\top$  is called the compact WY representation of the product of the Householder matrices. Fig.3 shows the compact WY orthogonalization algorithm.

### 3.3 Comparison of the orthogonalization algorithms

The compact WY orthogonalization has a stable orthogonality arising from

```

1: for  $j = 1$  to  $m$  do
2:   Generate  $\mathbf{v}_j$  from  $\mathbf{q}_1, \dots, \mathbf{q}_{j-1}$ .
3:    $\mathbf{v}'_j = (I - Y_{j-1} T_{j-1} Y_{j-1}^\top) \mathbf{v}_j$ .
4:   Compute  $\mathbf{y}_j$  and  $t_j$  by using  $\mathbf{v}'_j$ .
5:   Eq.(2): Update  $Y_j$  and  $T_j$  by using  $t_j, \mathbf{y}_j, T_{j-1}$  and  $Y_{j-1}$ .
6:    $\mathbf{q}_j = (I - Y_j T_j Y_j^\top) \mathbf{e}_j$ .
7: end for

```

**Fig. 3** Algorithm of the compact WY orthogonalization.

**Table 1** Comparison of the orthogonalization methods<sup>1)10)</sup>

orthogonalization	Computation	Synchronization	Orthogonality
MGS	$O(2m^2n)$	$O(m^2)$	$O(\epsilon\kappa)$
Householder	$O(4m^2n)$	$O(m^2)$	$O(\epsilon)$
compact WY	$O(4m^2n)$	$O(m)$	$O(\epsilon)$

$\epsilon$  : machine epsilon     $\kappa$  : condition number of a matrix

the Householder transformations, and its mathematical calculation is mainly performed by BLAS level-2 operations. As a result, this orthogonalization has more stable and sophisticated orthogonality, and it is more effective for parallel computing than MGS. Table 1 displays the differences in performance of the three orthogonalization methods, considered in the above sections. In this table, *Computation* denotes the order of the computational cost. *Synchronization* denotes the order of the number of synchronizations. *Orthogonality* denotes the norm  $\|Q^\top Q - I\|$ , where  $Q = [\mathbf{q}_1 \ \dots \ \mathbf{q}_n]$ .

## 4. Inverse iteration algorithm with compact WY orthogonalization

We present a new inverse iteration algorithm. This new algorithm is described in Fig.4. This algorithm is based on DSTEIN, a LAPACK (Linear Algebra PACKage)<sup>6)</sup> code of the inverse iteration algorithm for computing eigenvectors of a real symmetric tridiagonal matrix code of the classical inverse iteration. Concretely, we change the orthogonalization process of it from MGS to the compact WY orthogonalization. Next, we explain an application of the compact WY orthogonalization to the classical inverse iteration. For the DSTEIN algorithm, we need not know the index  $j_c$  which denotes the  $j_c$ -th eigenvalue of the cluster in computing the  $j_c$ -th eigenvector. However, we must know the index for the compact WY orthogonalization when we compute and update  $T_j, Y_j$ . To overcome

```

1: for  $j = 1$  to  $n$  do
2:   Generate  $\mathbf{v}_j^{(0)}$  from random numbers.
3:    $k = 0$ 
4:   repeat
5:      $k \leftarrow k + 1$ .
6:     Normalize  $\mathbf{v}_j^{(k-1)}$ .
7:     Eq.(1): Compute  $\mathbf{v}_j^{(k)}$  by using  $\mathbf{v}_j^{(k-1)}$ .
8:     if  $|\lambda_j - \tilde{\lambda}_{j-1}| \leq 10^{-3} \|T\|$ , then
9:        $j_c \leftarrow j - j_1$ .
10:      if  $j_c = 1$  and  $k = 1$ , then
11:        Compute  $Y_1 = \mathbf{y}_1$  and  $T_1 = t_1$  by using  $\mathbf{v}_{j_1} (= \mathbf{v}_{j-1})$ .
12:      end if
13:      Normalize  $\mathbf{v}_j^{(k)}$ .
14:      if  $j_c = 1$ , then
15:         $\mathbf{v}'_2 \leftarrow \mathbf{v}_2 - t_1 \langle \mathbf{y}_1, \mathbf{v}_j^{(k)} \rangle \mathbf{y}_1 (= (I - Y_1 T_1^\top Y_1^\top) \mathbf{v}_j^{(k)})$ .
16:        Compute  $\mathbf{y}_2$  and update  $Y_2$  by using  $\mathbf{v}'_2$ .
17:        Compute  $t_2$  and  $T_{1,2} = -t_2 t_1 \langle \mathbf{y}_1, \mathbf{y}_2 \rangle$  and update  $T_2$ .
18:      else
19:         $\mathbf{v}'_{j_c+1} = (I - Y_{j_c} T_{j_c}^\top Y_{j_c}^\top) \mathbf{v}_j^{(k)}$ .
20:        Compute  $\mathbf{y}_{j_c+1}$  and  $t_{j_c+1}$  by using  $\mathbf{v}'_{j_c+1}$ .
21:        Eq.(2): Update  $Y_{j_c+1}$  and  $T_{j_c+1}$  by using  $t_{j_c+1}$ ,  $\mathbf{y}_{j_c+1}$ ,  $T_{j_c}$  and  $Y_{j_c}$ .
22:      end if
23:       $\mathbf{v}_j^{(k)} \leftarrow (I - Y_{j_c+1} T_{j_c+1}^\top Y_{j_c+1}^\top) \mathbf{e}_{j_c+1}$ .
24:    else
25:       $j_1 \leftarrow j$ .
26:    end if
27:  until some condition is met.
28:  Normalize  $\mathbf{v}_j^{(k)}$  to  $\mathbf{v}_j$ .
29: end for

```

Fig. 4 Algorithm of the compact WY inverse iteration.

the above difficulty, we introduce a variable  $j_c$  on line 9, and we can recognize it. This introduction of  $j_c$  enables us to execute the intended program. However, we do not get accurate results because the compact WY orthogonalization algorithm includes many equations with a comparatively large number of elements such as  $Y_{j_c} T_{j_c}^\top Y_{j_c}^\top$  and  $Y_{j_c} T_{j_c} Y_{j_c}^\top$  and they may cause overflow. To overcome this difficulty, we have to normalize  $\mathbf{v}_j^{(k)}$  on line 6, and this normalization excludes overflow.

In the original DSTEIN algorithm, we need not know that  $\lambda_{j_1}$  is the first eigenvalue of the cluster. However, we must compute  $\mathbf{y}_1$  and  $t_1$ . Therefore, at the starting point of the computation of the eigenvector associated with the

Table 2 The specification of Computer 1 and 2

	Computer 1	Computer 2
CPU	AMD Opteron 2.0GHz 32cores(8cores×4)	Intel Xeon 2.93GHz 8cores(4cores×2)
Memory	16GB	32GB
Compiler	Gfortran-4.4.5	Gfortran-4.4.5
LAPACK	LAPACK-3.3.0	LAPACK-3.3.0
BLAS	GotoBLAS2-1.13	GotoBLAS2-1.13

second eigenvalue  $\lambda_j$  ( $j = j_1 + 1$ ), we compute  $\mathbf{y}_1$  and  $t_1$ . At this time, because  $T_1$  is a  $1 \times 1$  matrix, i.e., a scalar, we can omit the computation of some of Eq.(2) and only compute them. In addition, because  $\mathbf{v}_{j-1}$  is a normalized vector so that it equals to  $(I - Y_1 T_1 Y_1^\top) \mathbf{e}_1$ , we need not compute  $\mathbf{y}_1$  it again.

## 5. Numerical experiments

We describe some numerical experiments performed using DSTEIN and DSTEIN-cWY in parallel computers, and we compare the computation time. DSTEIN is implemented in the classical inverse iteration, and DSTEIN-cWY is implemented in the new inverse iteration presented in the previous section.

### 5.1 Contents of the numerical experiments

We report computations of all the eigenvectors associated with eigenvalues of some matrices by using DSTEIN and DSTEIN-cWY on parallel computers, and we compare the calculation time. In these experiments, we compute the approximate eigenvalues by using LAPACK's program DSTEBZ, which is capable of computing them by using the bisection method. We record the calculation time for DSTEIN and DSTEIN-cWY using TIME, which is the internal function of Fortran and returns an integer number of times.

In the experiments, we use two computers equipped with multicore CPUs, and we implement those algorithms by using GotoBLAS2<sup>5)</sup>, which is implemented to parallelize BLAS operations by assigning them to each CPU core. Table 2 shows the specifications of two computers. All the matrices in the experiments are the glued-Wilkinson matrices  $W_g^\dagger$ , which are real symmetric and have dimensions on the order of thousands. More precisely,  $W_g^\dagger$  consists of the block matrix

$W_{21}^\dagger \in \mathbb{R}^{21 \times 21}$  and the scalar parameter  $\delta \in \mathbb{R}^{1 \times 1}$  and is defined as follow:

$$W_g^\dagger = \begin{bmatrix} W_{21}^\dagger & \delta & & & \\ \delta & W_{21}^\dagger & & & \\ & & \delta & & \\ & & & \ddots & \\ & & & & \delta & \\ & & & & & & W_{21}^\dagger \end{bmatrix}, \quad (4)$$

where  $W_{21}^\dagger$  is defined by

$$W_{21}^\dagger = \begin{bmatrix} 10 & 1 & & & & & & & & & \\ 1 & 9 & 1 & & & & & & & & \\ & & & \ddots & & & & & & & \\ & & 1 & & \ddots & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 0 & & & & \\ & & & & & & & \ddots & & & \\ & & & & & & & & \ddots & & \\ & & & & & & & & & 1 & \\ & & & & & & & & & & 10 \end{bmatrix}, \quad (5)$$

and  $\delta$  satisfies  $0 < \delta < 1$  and is also the semi-diagonal element of  $W_g^\dagger$ . Since  $W_g^\dagger$  is real symmetric tridiagonal and its semi-diagonal elements are nonzero, all the eigenvalues of  $W_g^\dagger$  are real and they are divided into 11 clusters of close eigenvalues. When  $\delta$  is small, the distance between the minimum and maximum eigenvalues in any cluster is small. In our experiments, we set  $\delta = 10^{-4}$ .

Computing eigenvalues and eigenvectors of the glued-Wilkinson matrix is one of the benchmark problems of eigenvalue decomposition. For example, the glued-Wilkinson matrix was used to evaluate the performance of the algorithm<sup>2)4)</sup>.

### 5.2 Results of the experiments

Table 3 shows the results of the experiments on Computer 1 that were mentioned in the previous section, and Table 4 shows the results of the experiments on Computer 2. In tables,  $n$  is the dimension of the glued-Wilkinson matrix,  $t$  and  $t_{cwy}$  are computation time by DSTEIN and DSTEIN-cWY respectively. In addition, Fig.5 illustrates the results in Tables 3 and 4 through graphs. The dotted line corresponds to  $t$  and the straight line to  $t_{cwy}$ .

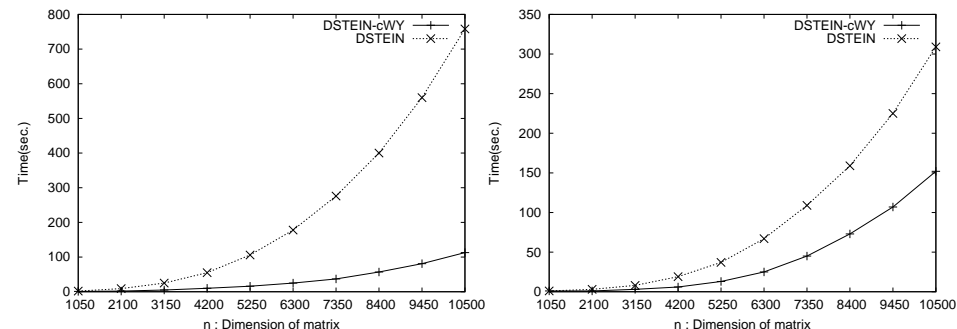
From Table 3 and 4, we see that, on both Computers 1 and 2, all the eigenvectors of the glued-Wilkinson matrix  $W_g^\dagger$  with dimensions of the order of several thousand are computed in parallel.

**Table 3** Numerical results of DSTEIN and DSTEIN-cWY on Computer 1.

$n$	1050	2100	3150	4200	5250	6300	7350	8400	9450	10500
$t$ [sec.]	2	9	25	55	106	178	276	400	560	758
$t_{cwy}$ [sec.]	1	2	5	10	16	25	37	57	81	113
$t/t_{cwy}$	2.00	4.50	5.00	5.50	6.63	7.12	7.46	7.02	6.91	6.71

**Table 4** Numerical results of DSTEIN and DSTEIN-cWY on Computer 2.

$n$	1050	2100	3150	4200	5250	6300	7350	8400	9450	10500
$t$ [sec.]	1	3	8	19	37	67	109	159	225	309
$t_{cwy}$ [sec.]	1	1	3	6	13	25	45	73	107	152
$t/t_{cwy}$	1.00	3.00	2.67	3.16	2.84	2.68	2.42	2.17	2.10	2.03



**Fig. 5** Dimension  $n$  of the glued-Wilkinson matrix and the computation time by DSTEIN and DSTEIN-cWY. the left graph corresponds to Computer1 and the right Computer 2.

It is noted that DSTEIN-cWY is faster than DSTEIN. We see that the change from MGS to the compact WY orthogonalization on the DSTEIN code in parallel computing results in a significant reduction in computation time. We introduce a barometer  $t/t_{cwy}$  of the reduction effect by using the program DSTEIN-cWY which depends on  $n$ , the dimension of  $W_g^\dagger$ . On Computer 1, the maximum value of  $t/t_{cwy}$  is 7.46 for  $n = 7,350$  and  $t/t_{cwy} = 6.71$  for  $n = 10,500$ . On Computer 2, the maximum value of  $t/t_{cwy}$  is 3.16 for  $n = 4,200$  and  $t/t_{cwy} = 2.03$  for  $n = 10,500$ . Considering these facts, even if the dimension of  $W_g^\dagger$  is larger than that in these examples, we cannot expect that the computation time can be further shortened by using DSTEIN-cWY.

### 5.3 Discussion on numerical experiments

It is shown that DSTEIN-cWY is faster than DSTEIN for any dimension  $n$  of

the glued-Wilkinson matrix both on Computers 1 and 2. As mentioned earlier, according to the theoretical background in section 3.3, this result shows that the compact WY orthogonalization is an effective algorithm in parallel computing.

The cause of this is related to the time required for floating-point arithmetic and for synchronization in parallel computing. The floating-point computation time increases with increasing  $n$  because the elements of the computation increase. In comparison, the synchronization cost does not change significantly even if  $n$  becomes larger. Therefore, in parallel computing, DSTEIN, which contains MGS (for which the number of synchronizations is large), creates a huge bottleneck for the synchronization cost when  $n$  is small. This bottleneck gradually becomes less when  $n$  is larger. However, DSTEIN-cWY has a smaller bottleneck for the synchronization cost because the compact WY orthogonalization requires less synchronization, and the floating-point computation time increases to a value greater than that of DSTEIN. This reduction effect is seen in Table 3 and 4.

## 6. Conclusions

In this study, we present a new inverse iteration algorithm for computing all the eigenvectors of a real symmetric tridiagonal matrix. The new algorithm is equipped with the compact WY algorithm in the orthogonalization process. We have performed numerical experiments for computing eigenvectors of certain real symmetric tridiagonal matrices that have many clusters with several thousand dimensions by using two types of inverse iteration algorithms on parallel computers. The results show that the compact WY inverse iteration is more efficient than the classical one owing to the reduction in computation time.

The main reason for this outcome is the parallelization efficiency with respect to computation time. This efficiency of the compact WY orthogonalization is greater than that of MGS where the classical inverse iteration is used. As the number of cores of the CPU increases, the parallelization efficiency increases.

In future studies, we will try to apply the new inverse iteration algorithms to other types of matrix eigenvector problem, such as eigenvectors of a real symmetric banded matrix, or singular vectors of a bidiagonal matrix.

**Acknowledgments** The authors thank Professor Yusaku Yamamoto of Kobe University for providing several helpful suggestions.

## References

- 1) J. W. Demmel, L. Grigori, M. Hoemmen and J. Langou, *Communication-optimal parallel and sequential QR and LU factorizations*, LAPACK Working Notes, No.204, 2008.
- 2) J. W. Demmel, O. A. Marques, B. N. Parlett, and C. Vömel, *Performance and accuracy of LAPACK's symmetric tridiagonal eigensolvers*, SIAM J. Sci. Comput., Vol. 30, No. 3, pp. 1508-1526, 2008.
- 3) I. S. Dhillon, *A new  $O(n^2)$  algorithm for the symmetric tridiagonal eigenvalue/eigenvector problem*, Ph.D. thesis, Computer Science Division, University of California, Berkeley, California, available as UC Berkeley Technical Report UCB//CSD-97-971, 1997.
- 4) I. S. Dhillon, B. N. Parlett, and C. Vömel, *Glued matrices and the MRRR algorithm*, SIAM J. Sci. Comput., Vol. 27, No. 2, pp. 496-510, 2005.
- 5) GotoBLAS2, <http://www.tacc.utexas.edu/tacc-projects/gotoblas2/>.
- 6) LAPACK, <http://www.netlib.org/lapack/>.
- 7) G. Peters and J. Wilkinson, *The calculation of specified eigenvectors by inverse iteration*, contribution II/18, in Linear Algebra, Handbook for Automatic Computation, Vol. II, Springer-Verlag, Berlin, pp. 418-439, 1971.
- 8) R. Schreiber and C. van Loan, *A storage-efficient WY representation for products of Householder transformations*, SIAM J. Sci. Stat. Comput., Vol. 10, No. 1, pp. 53-57, 1988.
- 9) H. Walker, *Implementation of the GMRES method using Householder transformations*, SIAM J. Sci. Stat. Comput., Vol. 9, No. 1, pp. 152-163, 1988.
- 10) Y. Yamamoto, *Parallelization of orthogonalization in Arnoldi process based on the compact WY representation*, Proceedings of the Annual Conference of JSIAM, pp. 39-40, 2010 (in Japanese).