TAIWANESE JOURNAL OF MATHEMATICS
Vol. 14, No. 3A, pp. 839-853, June 2010
This paper is available online at http://www.tjm.nsysu.edu.tw/

A METHOD FOR PROFILING THE DISTRIBUTION OF EIGENVALUES USING THE AS METHOD

Kenta Senzaki, Hiroto Tadano, Tetsuya Sakurai and Zhaojun Bai

Abstract. This paper is concerned with solving large-scale eigenvalue problems by algebraic sub-structuring and contour integral. We combine Algebraic Sub-structuring (AS) method and the Contour Integral Rayleigh-Ritz (CIRR) method. The AS method calculates approximate eigenpairs fast and has been shown to be efficient for vibration and acoustic analysis. However, the application areas of this method have been limited because its accuracy is usually lower than other methods. On the other hand, if the appropriate domains are chosen, the CIRR method produces accurate solutions. However, it is difficult to choose these domains without the information of eigenvalue distribution. We propose a combination of AS and CIRR such as the AS method is used as a method for profiling a distribution of eigenvalues, and the accurate solutions are produced by the CIRR method using the information of eigenvalue distribution provided by AS. We show our method is effective from the result of applying this method to the molecular orbital calculations.

1. Introduction

Large-scale eigenvalue problems appear in engineering computations such as vibration, structure, and acoustic analysis. A method for these problems has been developed by Benighof et al., known as Automated Multi-Level Sub-structuring (AMLS) method [1]. This method is a multi-level extension of a sub-structuring method called component mode synthesis (CMS) [3] originally developed in the 1960s for solving eigenvalue problems arising from structure analysis. The AMLS method has recently shown to be efficient for noise, vibration, and harshness (NVH) analysis, in particular, large-scale finite element models of automobile bodies [12]. The frequency response analysis performed in these studies requires several thousand eigenvalues and eigenvectors. It has been reported that the AMLS method is

Received August 27, 2008, accepted March 31, 2009.
2000 *Mathematics Subject Classification*: 65F15, 65F50.
Key words and phrases: Eigenvalue distribution, Profiling eigenvalues, Algebraic sub-structuring, CIRR.

significantly faster than the shift-invert Lanczos (SIL) method commonly used in structure engineering [11].

The term Algebraic Sub-structuring (AS) is used to refer to the process of applying matrix reordering and partitioning algorithm to divide the large-scale sparse matrix into smaller submatrices from which a subset of spectral components are extracted and combined to form an approximate solution to the original eigenvalue problem [10], and this term includes AMLS. Hence, we use the term AS in this paper.

It is important to note that the accuracy of approximate solutions produced by the AS method tends to be lower than the other methods because several submatrices are ignored in AS process for speed up. There are several ways to improve the accuracy of AS itself. These methods have been proposed in [6] to find other application of AS.

In this paper, we improve the accuracy of approximate solutions produced by the AS method using the Contour Integral Rayleigh-Ritz (CIRR) method, which is also referred to as the Sakurai-Sugiura method with Rayleigh-Ritz projection (SS-RR) [9, 18]. The CIRR method is based on a root-finding method for an analytic function [13]. This method finds eigenvalues and corresponding eigenvectors in a given domain. The combination of the CIRR method and the blocking method proposed in [8, 17] allows us to set the domain more flexibly with considerable accuracy.

If appropriate domains are determined, the CIRR method produces the highly accurate solutions. However, it is difficult to estimate such domains in advance, hence domains are determined empirically with knowledge of target problems in practice. These empirically-determined domains often produce the less-accurate solutions as a result of the CIRR method.

We show that a combination of the AS mehod and the CIRR method produces highly accurate solutions. We profile a distribution of eigenvalues using the AS method, and after that, the accurate solutions are calculated by the CIRR method using the information of eigenvalue distribution provided by the AS method. In the next section, we show a brief overview of the AS method. In section 3, we show a brief overview of the CIRR method and propose the estimation method of circular domains for the CIRR method. In section 4, we apply the proposed method to a generalized eigenvalue problem which appears in molecular orbital calculations, and show the effectiveness of the method from the results of some numerical experiments.

2. The AS Method

2.1. Single-Level Sub-structuring

We are concerned with the generalized eigenvalue problem

$$A\boldsymbol{x} = \lambda B\boldsymbol{x}, \tag{1}$$

where $A \in \mathcal{R}^{n\times n}$ is symmetric and $B \in \mathcal{R}^{n\times n}$ is symmetric positive definite. Let P be a permutation matrix obtained by applying a matrix reorder and partitioning algorithm such as the nested dissection (ND) algorithm [2] to the structure of the matrix $|A| + |B|$ (ignoring numerical cancellation), and let $\tilde{A}$ and $\tilde{B}$ are permuted matrices with P. The structures of $\tilde{A}$ and $\tilde{B}$ are followed.

$$\tilde{A}=P^{\mathrm{T}}AP= \begin{array}{c c} & \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} & \begin{bmatrix} A_{11} & & A_{13} \\ & A_{22} & A_{23} \\ A_{13}^{\mathrm{T}} & A_{23}^{\mathrm{T}} & A_{33} \end{bmatrix} \end{array}, \quad \tilde{B}=P^{\mathrm{T}}BP= \begin{array}{c c} & \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} & \begin{bmatrix} B_{11} & & B_{13} \\ & B_{22} & B_{23} \\ B_{13}^{\mathrm{T}} & B_{23}^{\mathrm{T}} & B_{33} \end{bmatrix} \end{array}.$$

The labels n_1, n_2, and n_3 indicate the dimensions of the submatrix blocks, and hold $n_1 + n_2 + n_3 = n$.

We apply a block factorization

$$\tilde{A} = LDL^{\mathrm{T}},$$

where

$$L = \begin{bmatrix} I_{n_1} & & \\ & I_{n_2} & \\ A_{13}^{\mathrm{T}}A_{11}^{-1} & A_{23}^{\mathrm{T}}A_{22}^{-1} & I_{n_3} \end{bmatrix}, \quad D = \begin{bmatrix} \hat{A}_{11} & & \\ & \hat{A}_{22} & \\ & & \hat{A}_{33} \end{bmatrix}.$$

I_{n_i} is a $n_i \times n_i$ identity matrix, $\hat{A}_{11} = A_{11}$, $\hat{A}_{22} = A_{22}$, and the last diagonal block of D, often known as *Schur complement,* is defined by

$$\hat{A}_{33} = A_{33} - A_{13}^{\mathrm{T}}A_{11}^{-1}A_{13} - A_{23}^{\mathrm{T}}A_{22}^{-1}A_{23}.$$

Let $\hat{A}$ and $\hat{B}$ be matrices applied a congruence transformation to matrices $\tilde{A}$ and $\tilde{B}$ with the inverse of the lower triangle matrix L. $\hat{A}$ and $\hat{B}$ are defined as

$$\hat{A} = L^{-1}\tilde{A}L^{-\mathrm{T}} = D, \quad \hat{B} = L^{-1}\tilde{B}L^{-\mathrm{T}} = \begin{bmatrix} \hat{B}_{11} & & \hat{B}_{13} \\ & \hat{B}_{22} & \hat{B}_{23} \\ \hat{B}_{13}^{\mathrm{T}} & \hat{B}_{23}^{\mathrm{T}} & \hat{B}_{33} \end{bmatrix},$$

where $\hat{B}_{11} = B_{11}$, $\hat{B}_{22} = B_{22}$, and the last diagonal block of $\hat{B}$ satisfies

$$\hat{B}_{33} = B_{33} - \sum_{i=1}^{2}(A_{i3}^{\mathrm{T}}A_{ii}^{-1}B_{i3} + B_{i3}^{\mathrm{T}}A_{ii}^{-1}A_{i3} - A_{i3}^{\mathrm{T}}A_{ii}^{-1}B_{ii}A_{ii}^{-1}A_{i3}),$$

and the off-diagonal blocks satisfy

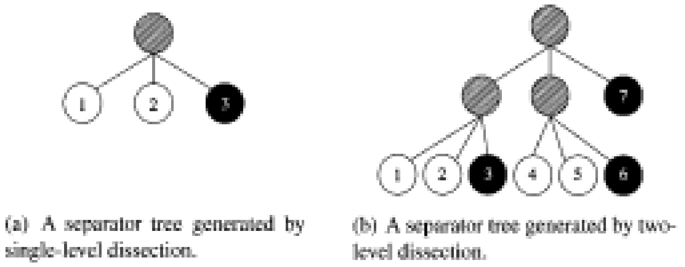
$$\hat{B}_{i3} = B_{i3} - B_{ii}A_{ii}^{-1}A_{i3}, \quad \text{for } i = 1, 2.$$

The eigenvalues of $(\hat{A}, \hat{B})$ are identical to those of (A, B), and corresponding eigenvectors $\hat{\boldsymbol{x}}$ are related to the eigenvectors of the original problem (1) through $\hat{\boldsymbol{x}} = L^{\mathrm{T}}\boldsymbol{x}$.

At the end phase of the AS algorithm, approximate eigenpairs are calculated from projected matrix. Let S be a $n \times p$ matrix in the form of

$$S = \begin{array}{c c} & \begin{array}{ccc} k_1 & k_2 & k_3 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} & \left[\begin{array}{ccc} S_1 & & \\ & S_2 & \\ & & S_3 \end{array} \right] \end{array},$$

where S_i is a matrix which consists of k_i selected eigenvectors of matrix pencil $(\hat{A}_{ii}, \hat{B}_{ii})$, and labels k_1, k_2, and k_3 hold $k_1 + k_2 + k_3 = p$. We assume $p \ll n$. The approximate eigenpairs are obtained by projecting the pencil $(\hat{A}, \hat{B})$ to the subspace spanned by S. The eigenvalues of the projected pencil $(S^{\mathrm{T}}AS, S^{\mathrm{T}}BS)$ are approximate to original eigenvalues, and corresponding eigenvectors $\boldsymbol{q}$ are related to the eigenvectors of the original problem (1) through $\boldsymbol{z} = L^{-\mathrm{T}}S\boldsymbol{q}$. Note that the method for decision of k_i have been proposed in [7, 10].



(a) A separator tree generated by single-level dissection.

(b) A separator tree generated by two-level dissection.

Fig. 1. Separator trees generated by the ND ordering.

The Single-Level Sub-structuring algorithm can be extended to a Multi-Level algorithm in a natural way using the recursive ND ordering. A matrix can be partitioned into three submatrices with ND ordering. Their relation can be illustrated by the graph in Figure 1(a). The stroked node shows the node before partitioning. The nodes marked $\{1, 2\}$ are independent of each other, and the node marked $\{3\}$ is a boundary part for node $\{1\}$ and node $\{2\}$.

We can divide a matrix into a number of smaller substructures applying the ND ordering recursively to the independent nodes such as $\{1, 2\}$. Figure 1(b) is the separator tree generated by two-level dissection. Multi-Level Sub-structuring method can be realized using the structure of the partitioned matrix.

3. Estimation of Circular Domains for the CIRR Method Using the Result of AS

3.1. The CIRR method

Contour Integral Rayleigh-Ritz method (CIRR) [9, 18] is a solver for large-scale generalized eigenvalue problems. This method finds several eigenvalues located inside given circles, and also calculates the corresponding eigenvectors. We show the brief of this method below.

In this method, the Rayleigh-Ritz subspace $Z \in \mathcal{R}^{n\times M}$ is provided by a contour integral. Let Γ be a circle with radius ρ and centered at γ, and let $\lambda_1, \lambda_2, \ldots, \lambda_m$ be m eigenvalues of the matrix pencil (A, B), which are supposed to be located inside Γ. For a nonzero vector $\boldsymbol{v} \in \mathcal{R}^n$, we define

$$\boldsymbol{s}_k := \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B\boldsymbol{v} \mathrm{d}z,\ k = 0, 1, \ldots, M-1, \tag{2}$$

with a complex parameter z. When $M \geq m$ and Z is the orthonormal basis of the space spanned by $\{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}\}$, then m Ritz values are $\lambda_1, \lambda_2, \ldots, \lambda_m$ [18]. This implies that the eigenvalues inside Γ can be obtained by the contour integral.

By approximating the contour integral via the N-point trapezoidal rule, we obtain the following approximation for $\boldsymbol{s}_k$:

$$\boldsymbol{s}_k \approx \hat{\boldsymbol{s}}_k := \frac{1}{N} \sum_{j=0}^{N-1} \left(\frac{\omega_j - \gamma}{\rho} \right)^{k+1} (\omega_j B - A)^{-1} B\boldsymbol{v},\ k = 0, 1, \ldots, M-1, \tag{3}$$

where

$$\omega_j := \gamma + \rho \mathrm{e}^{\frac{2\pi \mathrm{i}}{N}(j+\frac{1}{2})},\ j = 0, 1, \ldots, N-1. \tag{4}$$

Hence, computing $\hat{\boldsymbol{s}}_k$ is equivalent for solving N linear systems

$$(\omega_j B - A)\boldsymbol{y}_i = B\boldsymbol{v},\ j = 0, 1, \ldots, N-1. \tag{5}$$

Since $\hat{\boldsymbol{s}}_k$ suffer from the quadrature error which arises from eigenvalues located outside the circle, we take the size of the subspace larger than the exact number of the eigenvalues inside the circle. Thus we set, in practice,

$$Z \in \mathrm{span}\left(\hat{\boldsymbol{s}}_0, \hat{\boldsymbol{s}}_1, \ldots, \hat{\boldsymbol{s}}_{M-1}\right), \tag{6}$$

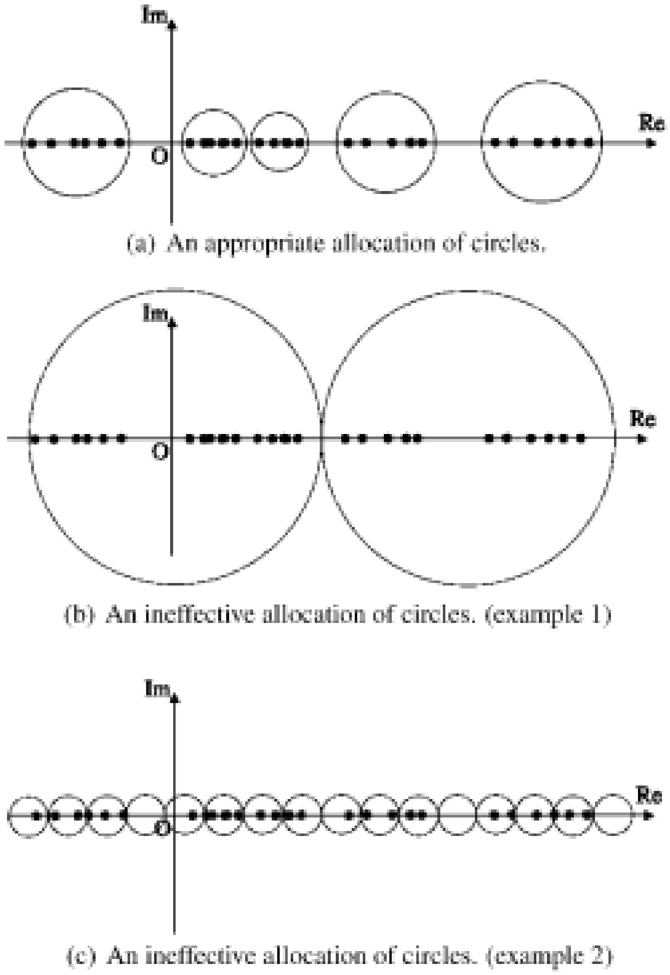
with M $(> m)$, and this approach is efficient to decrease the influence of the quadrature error.

A block variant of the method is proposed in [8, 17], which improves numerical accuracy. In this method, a matrix $V := [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L] \in \mathcal{R}^{n\times L}$ is used instead of $\boldsymbol{v}$

in (5), where $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L$ are linearly independent, and positive value L is a block size.

The CIRR method is appropriate for distributed computing environment because not only each circular domain can be computed in parallel, but also $\hat{\boldsymbol{s}}_k$ can be computed in parallel.

3.2. Initial guess of circular domains for the CIRR method



(a) An appropriate allocation of circles.

(b) An ineffective allocation of circles. (example 1)

(c) An ineffective allocation of circles. (example 2)

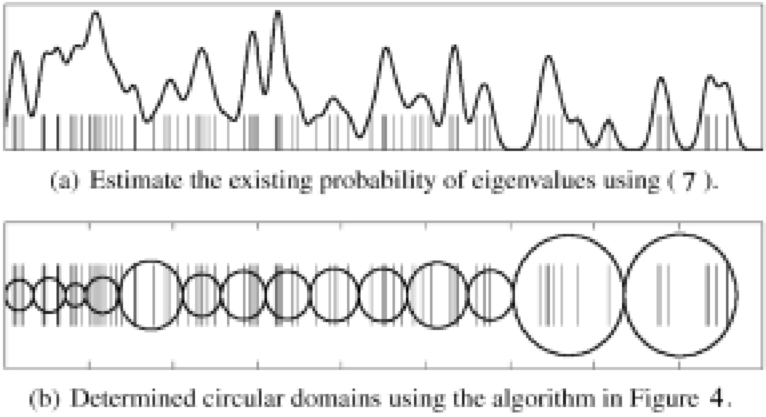
Fig. 2. Circular domains of the CIRR method. (bullet • on the real axis denote an eigenvalue).

The desirable circular domain for the CIRR method, such as Figure 2(a), is the domain which have following features: 1) The number of eigenvalues involved inside a domain is nearly equal in each domain. 2) Smaller circular domains are put in dense area of eigenvalues, and larger circular domains are put in spotty area of eigenvalues, considering proximity of adjacent eigenvalues. 3) The boundary of domain are kept away from eigenvalues, because eigenvalues outside a given circle have an effect on solutions inside a given circle [14, 19].

However, if we have no information for the target problem, we set circles unrelated to the actual distribution of eigenvalues. If many eigenvalues are involved in a circle such as Figure 2(b), the accuracy of the solution would be sacrificed. On the other hand, if the radius of circles is smaller such as Figure 2(c), the number of eigenvalues in a circle might be less and accuracy of the solutions can be high. However, the number of circles could become larger and the whole calculation amount might also become significantly more expensive.

Considering these features, we present the approach to determine circular domains for the CIRR method. Each eigenvalue obtained by the AS method tends to be less accurate itself, but the distribution of them, sparse or dense, appears to be similar to that of the exact values. We propose a method that sets circular domains for the CIRR method, estimating a distribution of eigenvalues from the result of the AS method.

3.3. Estimation of circular domains for the CIRR method


(a) Estimate the existing probability of eigenvalues using (7).

(b) Determined circular domains using the algorithm in Figure 4.

Fig. 3. Estimate the existing probability of eigenvalues and determine the circular domains.

Let θ_j be the jth eigenvalue calculated by the AS method. Suppose θ_j have been ordered so that $\theta_1 < \theta_2 < \cdots < \theta_p$, where p is the number of eigenvalues calculated by the AS method. The maximum (or minimum) number of eigenvalues involved in a circle is denoted by $N_{\max}$ (or $N_{\min}$). Considering the error of the AS method, the interval that CIRR circles will be located is denoted by $[\theta_1 - \varepsilon, \theta_p + \varepsilon]$, where ε is a small number, and this initial interval is denoted by I. The kth divided interval is denoted by I_k. The eigenvalues involved in the interval I_k are denoted by $\{\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_{p_k}^{(k)}\}$. N_k denotes the number of eigenvalues involved in the kth interval. The range of I_k is denoted by $[\Theta_{\mathrm{start}}^{(k)}, \Theta_{\mathrm{end}}^{(k)}]$.

We propose an approach for dividing intervals using a following Gauss function,

$$G_k(t) = \sum_{j=1}^{N_k} \exp\left\{ - \left(\frac{w}{|\Theta_{\mathrm{end}}^{(k)} - \Theta_{\mathrm{start}}^{(k)}|} \left(t - \theta_j^{(k)} \right) \right)^2 \right\}, \qquad (7)$$

$$\Theta_{\mathrm{start}}^{(k)} \le t < \Theta_{\mathrm{end}}^{(k)},$$

where w denotes weight. This function implies the existing probability of eigenvalues at t in the interval I_k. We divide the interval I_k at the cutting point $t_{\mathrm{cut}}^{(k)}$, where

$$t_{\mathrm{cut}}^{(k)} = \{ t | \min G_k(t) \} .$$

It means that we may divide the interval I_k at the sparsest point of eigenvalues distribution in I_k. The algorithm is shown in Figure 4. We can set the $N_{\max}$ and $N_{\min}$ empirically from the required accuracy of the CIRR method.

Algorithm: Estimation method for circular domains of CIRR

1. Set $N_{\max}$, $N_{\min}$ and weight w.
2. Repeat dividing an interval using Gauss function to be defined in (7) until all intervals involves eigenvalues less than $N_{\max}$.
3. Repeat applying the following process to I_k in ascending order of N_k. If $N_k < N_{\min}$, $I_{k'}$ denotes the interval which satisfies $\min(|\theta_{p_{k-1}}^{(k-1)} - \theta_1^{(k)}|, |\theta_1^{(k+1)} - \theta_{p_k}^{(k)}|)$, and another interval is denoted by $I_{k''}$. If $N_{k'} + N_k \le N_{\max}$, merge I_k and $I_{k'}$. If $N_{k'} + N_k > N_{\max}$, apply this process to $I_{k''}$. If $N_{k''} + N_k > N_{\max}$, the interval I_k is determined. If the interval I_k involves θ_1 (or θ_p), this process is applied to only I_{k+1} (or I_{k-1}).

Figure 4: Algorithm of estimation method for circular domains of CIRR.

4. Numerical Experiments

We present three numerical experiments in this section to illustrate the effectiveness of the combination of the AS method and the CIRR method. We also point out the issue of the AS method and propose the solution in second experiment. The test problem is a generalized eigenvalue problem $A\boldsymbol{x} = \lambda B\boldsymbol{x}$, which appears in computation of molecular orbital(MO). The eigenvector computed in MO calculation shows a molecular orbital, and the corresponding eigenvalue shows the energy level of this orbital. In MO calculation, analysis of two MOs around the frontier orbital is important to analyze the mechanism of various chemical reactions. These MOs are called *Highest Occupied MO*(*HOMO*) and *Lowest Unoccupied MO*(*LUMO*). We estimate the eigenvalue distribution using the AS method and calculate hundreds of eigenpairs around HOMO-LUMO by block CIRR method.

The all AS processes were performed on four AMD Opteron Processor 848 (2.2 GHz) with 16 GB of RAM. The external software packages were: LAPACK[4], METIS[5], and GotoBLAS. We compiled all the codes using GNU C Ver. 4.1.2 with `-O3` optimization flag.

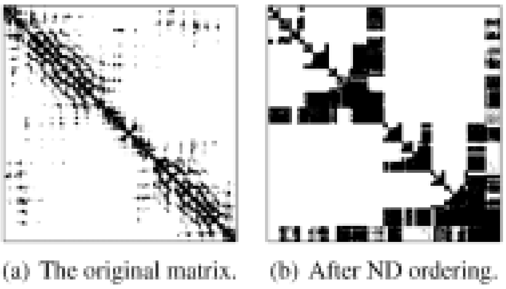

(a) The original matrix. (b) After ND ordering.

Fig. 5. The sparsity pattern of the matrix in Example 4.1.

Example 4.1. We execute the the proposed method to obtain the eigenpairs around HOMO-LUMO. The test matrices are derived from computation of the molecular orbitals of Epidermal Growth Factor Receptor (EGFR). The size of matrices is $n = 26,461$. The number of nonzero elements of matrix $C(= |A| + |B|)$ is $14,175,935$. The eigenvalue of HOMO is $\lambda_{\mathrm{HOMO}} = 0.087436432526632$, and the eigenvalue of LUMO is $\lambda_{\mathrm{LUMO}} = 0.098158257155242$. Figure 5(a) shows the sparsity patterns of matrix C, Figure (b) shows the sparsity patterns of matrix C after ND ordering.

At first, we profiled a distrubution of eigenvalues around HOMO-LUMO using the AS method. The conditions of the AS method were as follows. Eigenpairs of each diagonal submatrix were computed by LAPACK routine `DSYGVD`. The size of subspace for Rayleigh-Ritz projection was 5%. This subspace was provided by the selected eigenvectors which corresponding eigenvalues were close to HOMO-LUMO.

In Figure 5, the upper bars denote the eigenvalues calculated by CIRR with very small circles, and we assume that this distribution is accurate. The lower bars in Figure 5 denote eigenvalues calculated by the AS method. The parameter $N_{\max}$, $N_{\min}$ and w in Figure 4 were $N_{\max} = 48$, $N_{\min} = 24$ and $w = 30$. Ten circles, shown in Figure 5, for the CIRR method were put around HOMO-LUMO using the proposed method shown in Figure 4. This figure shows that the eigenvalue distribution computed by the AS method was similar to the actual distribution, and the eigenvalue distribution would have reflected in determination of the circular domain, smaller circles were put in dense area of eigenvalue distribution, larger circles were put in sparse area. Table 1 shows the number of eigenvalues in each circle shown in Figure 5. This table shows that circular domains which determined by the method shown in 5 included the close number of eigenvalues to the actual number.

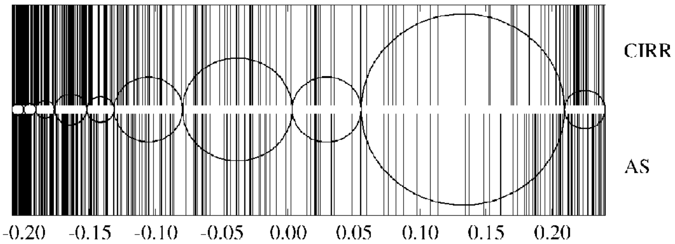


Fig. 6. Circles for the CIRR method in Example 4.1. (Upper bars: Eigenvalues calculated by CIRR with small circles, Lower bars: Eigenvalues calculated by AS).

Table 1. The number of eigenvalues in each domain shown in Figure 6

Domain	1	2	3	4	5	6	7	8	9	10	Total
CIRR	48	36	46	55	24	43	37	13	31	41	375
AS	41	32	46	46	26	45	38	13	42	42	371

We have shown that the AS method could profile the eigenvalue distribution, however, it tends to take long time to complete the AS method if we apply the AS method to the generalized eigenvalue problem arising from MO computation. The matrices which appear in MO calculation tend to have many nonzero elements, and in this case, it takes long time to complete AS process because the large submatrices appear after the ND ordering. We use the AS method to obtain the rough eigenvalue distribution, not to obtain the highly accurate solution. Hence, we apply "Cutoff" to the target problem in order to reduce the number of nonzero elements and to execute the AS method faster. Cutoff is the method to obtain the matrix M_c from the matrix M, which is defined as follows using small positive value δ,

$$M_{\mathrm{c}} = \{\tilde{m}_{i,j}\}\,,\ \tilde{m}_{i,j} = \begin{cases} m_{i,j} & |m_{i,j}| > \delta, \quad \text{for} \quad i \neq j, \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

In the next numerical example, we applied Cutoff to the matrices used in Example 4.1 in order to obtain the sparser matrices and to execute AS faster.

Example 4.2. We apply "Cutoff" to the target problem in order to reduce the nonzero elements and to execute the AS method faster. The test matrices are same as Example 4.1.

At first, we applied Cutoff to the original problem and obtained matrix A_c and B_c. Next, approximate eigenvalues of $(A_\mathrm{c}, B_\mathrm{c})$ were computed by AS method. The relation between the number of nonzero elements and computational time of AS in each Cutoff value δ is shown in Table 2. It took 233.87 seconds to complete AS with original problem ($\delta = 0$), which is the slowest example, while it took 39.14 seconds with $\delta = 5.0 \times 10^{-3}$, which is the fastest example. $\delta = 0$ means that the eigenvalues were calculated by the AS method without Cutoff. The eigenvalue distributions calculated by the AS method in several Cutoff values are shown in Figure **??**. In this figure, top bars show the distribution of eigenvalues calculated by the AS method without Cutoff, and lower bars show the distributions of eigenvalues calculated by the AS method with several Cutoff value δ. From the result of this numerical experiment, if Cutoff is applied with suitable δ, AS would be significantly faster without the heavy influence to eigenvalue distribution.

Table 2. Relation between the number of nonzero element and computational time of AS in several Cutoff values

Cutoff value δ	The number of nonzero elements	Computational time of AS
0	14,175,935	233.87
5.0×10^{-7}	9,794,715	177.46
1.0×10^{-6}	8,235,523	158.08
5.0×10^{-6}	5,426,771	118.28
1.0×10^{-5}	4,553,065	107.75
5.0×10^{-5}	3,112,715	78.15
1.0×10^{-4}	2,661,275	68.76
5.0×10^{-4}	1,872,181	52.96
1.0×10^{-3}	1,613,039	49.49
5.0×10^{-3}	1,111,515	39.14

Example 4.3. We execute the block CIRR method with domains determined in Example 4.1.

We executed the block CIRR method using these circular domains. The parameters of the block CIRR were as follows. The block size L was 16. The number of nodes per circle N was 24. The size of Rayleigh-Ritz subspace M was 16. The preconditioned COCG method [15] was used for iterative linear solver. The stopping criterion of liner systems for the relative residual was 1.0×10^{-12}. The preconditioner was constructed by applying a complete factorization for an approximate coefficient matrix which was obtained from drop-thresholding of the original matrix [20]. The drop-thresholding parameter was 1.0×10^{-4}. The complete factorization was performed by sparse direct solver, the PARDISO library [16]. Intel C and Fortran compiler 9.1 were used to compile the codes of the block CIRR with Intel Math Kernel Library. Computation was performed in double-precision arithmetic.

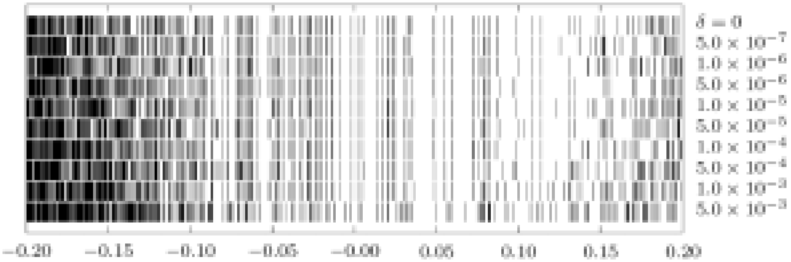


Fig. 7. Relation between the Cutoff value and the eigenvalue distribution calculated by the AS method.

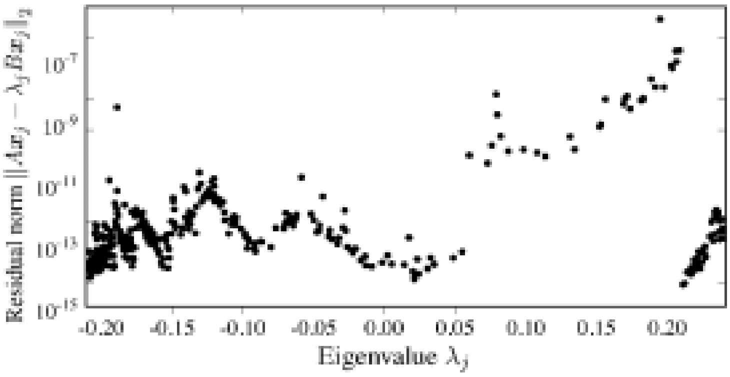


Fig. 8. Residual norm $\|A\boldsymbol{x}_j - \lambda_j B\boldsymbol{x}_j\|_2$ in Example 4.1.

In Figure 8, bullet • shows the residual $\|A\boldsymbol{x}_j - \lambda_j B\boldsymbol{x}_j\|_2$ for each approximate eigenpair calculated by the block CIRR method. It took 3524.00 seconds to find 375 eigenpairs in given 10 circular domains, 401.48 seconds to finish the slowest domain, 318.17 seconds to finish the fastest domain.

These eigenvalues and corresponding eigenvectors were accurate from practical viewpoint, however, several eigenpairs involved in the second domain from the right were less accurate than others. It was caused by the fact that this domain was relatively larger than others, hence vector $\boldsymbol{s}_k$ suffered from the quadrature error. In

Figure 9, bullet • shows the residual for each approximate eigenpair calculated by the block CIRR method in case of $N = 24$, and square □ shows the residual in case of $N = 48$. From this result, we find that if we could set the appropriate number of nodes for numerical integration, the solutions are improved.

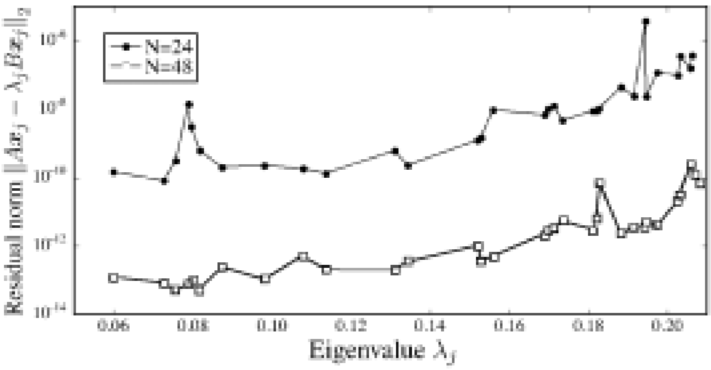


Fig. 9. Residual norm $\|A\boldsymbol{x}_j - \lambda_j B\boldsymbol{x}_j\|_2$ of each eigenpair included in the second domain from the right. N is the number of nodes for numerical integration in block CIRR process.

5. Concluding Remarks

We proposed an efficient combination of the AS method and the CIRR method to obtain accurate solution of the generalized eigenvalue problem. From the results of numerical experiments, an automated determination of circular domains for the CIRR method with AS is valuable to obtain accurate solutions. We also showed the effectivity of Cutoff to estimate the rough eigenvalue distribution faster.

The development of a criterion to estimate appropriate circles is a part of our future works. The determination of the appropriate parameters for block CIRR method using the profiling result of eigenvalue distribution is one of the future works. Both the analysis of perturbation from Cutoff and the determination of the suitable Cutoff value δ will be reported elsewhere.

References

1. J. K. Bennighof, An automated multi-level substructuring method for eigenspace computation in linear elastdynamics, *SIAM J. Sci. Comput.*, **25**, (2004), 2084-2106.

2. A. George, Nested Dissection of a Regular Finite Element Mesh, *SIAM J. Numer. Anal.*, **10(2)** (1973), 345-363.

3. W. C. Hurty, Vibrations of structure systems by component mode synthesis, *Journal of the Engineering Mechanics Division*, **86** (1960), 51-69.

4. *Lapack-Linear Algebra Package*, http://netlib.org/lapack.

5. *METIS - Family of Multilevel Partitioning Algorithms*, http://glaros.dtc.umn.edu/gkhome/views/metis.

6. K. Bekas and Y. Saad, Computation of smallest eigenvalues using spectral Schur complements, *SIAM J. Scientific Computing*, **27** (2005), 458-481.

7. K. Elsseland and H. Voss, An a priori bound for Automated Multi-Level Substructuring, *SIAM J. Matrix Anal. Appl.*, **28** (2006), 386-397.

8. T. Ikegami, T. Sakurai and U. Nagashima, Block Sakurai-Sugiura Method for Filter Diagonalization, in: *Abstract of Recent Advances in Numerical Methods for Eigenvalue Problems*, Hsinchu, 2008.

9. T. Sakurai and H. Sugiura, A projection method for generalized eigenvalue problems using numerical integration, *Jounal of Computational Applied Mathmatics*, **159** (2003), 119-128.

10. C. Yang, W. Gao, Z. Bai, X. S. Li, L. Lee, P. Husbands and E. Ng, An algebraic substructuring method for large-scale eigenvalue calculation, *SIAM J. Sci. Comput.*, **27** (2005), 873-892.

11. A. Kropp and D. Heiserer, Efficient broadband vibro-accoustic analysis of passenger car bodies using an FE-based component mode synthesis approach, *J. Computational Acoustics*, **2** (2003), 139-157.

12. M. F. Kaplan, *Implementation of Automated Multilevel Substructuring for Frequency Response Analysis of Structure*, University of Texas at Austin, 2001.

13. P. Kravanja, T. Sakurai and M. Van Barel, On locating clusters of zeros of analytic functions, *BIT*, **39** (1999), 646-682.

14. P. Kravanja, T. Sakurai, H. Sugiura and M. Van Barel, A perturbation result for generalized eigenvalue problems and its application to error estimation in a quadrature method for computing zeros of analytic functions, *J. Comput. Appl. Math.*, **161** (2003), 339-347.

15. H. A. van der Vorst and J. B. M. Melissen, A Petrov-Gelerkin type method for solving $A\boldsymbol{x} = \boldsymbol{b}$, where A is a symmetric complex matrix, *IEEE Trans. on Magnetics*, **26** (1990), 706-708.

16. O. Schenk and K. Gärtner, Solving unsymmetric sparse systems of linear equations with PARDISO, *Future Gen. Comput. Sys.*, **20** (2004), 457-587.

17. T. Sakurai, H. Tadano and U. Nagashima, A parallel eigensolver using contour integration for generalized eigenvalue problems in molecular simulation, in: *Abstract of Recent Advances in Numerical Methods for Eigenvalue Problems*, Hsinchu, 2008.

18. T. Sakurai and H. Tadano, CIRR: a Rayleigh-Ritz type method with contour integral for generalized eigenvalue problems, *Special Issue of Hokkaido Mathematical Journal*, **36** (2007), 745-757.

19. T. Sakurai, P. Kravanja, H. Sugiura and M. Van Barel, An error analysis of two related quadrature methods for computing zeros of analytic functions, *J. Comput. Appl. Math.*, **152** (2003), 467-480.

20. M. Okada, T. Sakurai and K. Teranishi, A preconditioner for Krylov subspace method using a sparse direct solver, in: *Abstract of 2007 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications*, Toulouse, Precond, 2007.

21. T. Sakurai, Y. Kodaki, H. Tadano, H. Umeda, Y. Inadomi, T. Watanabe and U. Nagashima, A master-worker type eigensolver for molecular orbital computation, *Lecture Notes in Computer Sciences*, **4699** (2007), 617-625.

Kenta Senzaki
Department of Computer Science,
Graduate School of Systems and Information Engineering,
University of Tsukuba,
Japan
E-mail: senzaki@mma.cs.tsukuba.ac.jp

Hiroto Tadano and Tetsuya Sakurai
Graduate School of Systems and Information Engineering,
University of Tsukuba,
Japan
E-mail: tadano@cs.tsukuba.ac.jp
sakurai@cs.tsukuba.ac.jp

Zhaojun Bai
Department of Computer Science,
University of California,
Davis, CA 95616,
U.S.A.
E-mail: bai@cs.ucdavis.edu