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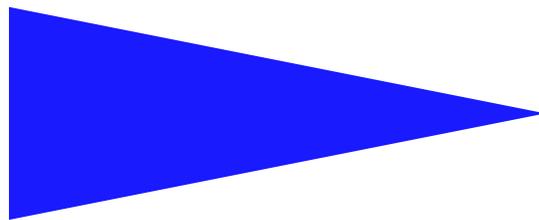
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ON CORRECTION EQUATIONS AND DOMAIN  
DECOMPOSITION FOR COMPUTING INVARIANT  
SUBSPACES

BERNARD PHILIPPE AND YOUSEF SAAD



## On correction equations and domain decomposition for computing invariant subspaces

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**Abstract:** This paper considers a number of schemes for computing an approximate invariant subspace associated with the smallest eigenvalues of a sparse symmetric (real) matrix. The approach taken is that of the so-called “correction equation” which leads to such standard schemes as the Jacobi-Davidson method or Olsen’s method. We consider the situation of block corrections and discuss two algorithms. The application of the viewpoint that is developed is then explored for Domain Decomposition methods.

**Key-words:** eigenvalues, invariant subspace, correction, Jacobi-Davidson, Olsen, block algorithms, domain decomposition

*(Résumé : tsvp)*

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## **Equations de correction et décomposition de domaine dans le calcul de sous-espaces invariants**

**Résumé :** Dans ce papier, sont étudiés plusieurs schémas pour le calcul des plus petites valeurs propres d'une matrice creuse symétrique réelle. L'approche choisie consiste à utiliser une équation dite de "correction" qui peut aboutir à des schémas connus du type des méthodes de Jacobi-Davidson ou d'Olsen. Nous considérons le cas de corrections par blocs en comparant deux algorithmes. Ce point de vue est ensuite appliqué au cas des méthodes de décomposition de domaines.

**Mots clés :** valeurs propres, espaces invariants, correction, Jacobi-Davidson, Olsen, algorithmes par blocs, décomposition de domaine

## 1 Introduction

A number of schemes have been developed in recent years for enhancing the convergence of subspace-based methods for computing eigenvalues and eigenvectors of large matrices. These approaches essentially take the viewpoint that the eigenvalue problem is a nonlinear system of equations and attempt to find a good way to correct a given approximate eigenpair  $\tilde{\lambda}, \tilde{u}$ , by introducing to the most recent subspace of approximants, an information that is not redundant with this subspace. In practice, this means that we need to solve the correction equation, i.e., the equation which updates the current approximate eigenvector, in a subspace that is orthogonal to the most current approximate eigenvectors.

Several methods can be mentioned including the Trace Minimization method [12, 11], the Davidson method [4, 9] and the Jacobi-Davidson approach [14, 13, 16]. Most of these methods update an existing approximation by a step of Newton's method and this was illustrated in a number of papers, see, e.g., [8], and in [17].

One can think of the problem as that of solving  $(A - \lambda I)u = 0$ , but since there are  $n + 1$  unknowns, a constraint must be added, for example,  $\|u\|_2 = 1$ . If the current approximate eigenpair is  $(\tilde{\lambda}, \tilde{u})$ , it is assumed that  $\|\tilde{u}\|_2 = 1$ , and that  $\tilde{\lambda}$  is the Rayleigh quotient of  $\tilde{u}$ . We define the residual  $r = A\tilde{u} - \tilde{\lambda}\tilde{u}$ . If a correction  $\delta, z$  to  $\tilde{\lambda}, \tilde{u}$  is sought, then we write the equations to be satisfied as

$$\begin{aligned} [(A - \tilde{\lambda}I) - \delta I](\tilde{u} + z) &= 0 \\ (\tilde{u} + z)^T(\tilde{u} + z) &= 1. \end{aligned}$$

Ignoring second order terms, this yields the system of equations,

$$(A - \tilde{\lambda}I)z - \tilde{u} \delta = -r \quad (1)$$

$$-\tilde{u}^T z = 0. \quad (2)$$

The above equations can be solved in a number of ways, for example as an  $(n + 1) \times (n + 1)$  linear system. A simpler solution is to invoke the orthogonal projector  $P = I - \tilde{u}\tilde{u}^T$ . Multiplying the first equation by  $P$ , and observing that  $P\tilde{u} = 0, Pr = r$ , yields,

$$P(A - \tilde{\lambda}I)z = -r. \quad (3)$$

Note that this system is degenerate - i.e., it has an infinite number of solutions  $z$ . Among all the solutions of this system, we require one that is orthogonal to  $\tilde{u}$ , i.e., one such that  $Pz = z$ . This can be enforced by solving  $P(A - \tilde{\lambda}I)Pz_0 = -r$ , for  $z_0$ , and defining the solution to be  $z = Pz_0$  (instead of  $z_0$ ). This  $z$  will satisfy the equation (1). Indeed,

$$(A - \tilde{\lambda}I)z = P(A - \tilde{\lambda}I)z + (I - P)(A - \tilde{\lambda}I)z = -r + \tilde{u}\tilde{u}^T(A - \tilde{\lambda}I)z = -r + \tilde{u}r^T z$$

and therefore, (1) is satisfied with  $\delta = r^T z$ . In addition (2) is trivially satisfied because  $z = Pz_0$ . Note that the correction  $\delta$  to  $\tilde{\lambda}$  can be ignored since the new approximate eigenvalue will just be defined as the new Rayleigh quotient. So we are left with the equation,

$$P(A - \tilde{\lambda}I)Pz = -r. \quad (4)$$

The Jacobi-Davidson scheme, the Trace Minimization method and a number of related algorithms are based on the above development. In other methods, the projection is not considered since the matrix  $A$  is not used exactly. Instead,  $A$  is replaced by a “preconditioner” when solving the system  $(M - \tilde{\lambda}I)z = -r$  in place of the system (3). This viewpoint is most useful in a Davidson approach to build a subspace for a projection technique [17].

The Newton-type framework just described determines one vector at a time and it is interesting to explore situations where a block of vectors must be corrected. This is important in many practical applications. We will explore a few block correction schemes which are derived in a manner that is similar to what was done above for the one-dimensional case.

One of the possible applications of these schemes lies in domain decomposition methods. In these methods, one can consider the invariant subspaces obtained from subdomains as approximately invariant for the global operator. Such an approximation can be very rough and one may be tempted to correct them in some way. This technique is taken to the limit and exploited in a quite effective way in the Automated Multi-Level Substructuring (AMLS) algorithm [2, 7]. In AMLS, the subspaces are corrected by adding correction terms from the interface variables.

## 2 Block correction

This section examines a few schemes for “correcting” a given approximate invariant subspace. We are given a subspace in the form of a certain basis  $U = [u_1, u_2, \dots, u_m]$  and would like to find a correction  $W$  of the same dimensions as  $U$ , such that  $U + W$  is a better invariant subspace than  $U$ . Schemes of this type are well-known for the case when  $m = 1$ , and they lead to the standard Olsen’s method or Jacobi-Davidson scheme.

### 2.1 Correction of an orthonormal basis

Let us assume that  $U \in \mathbb{R}^{n \times m}$  is an orthonormal basis of an approximate invariant subspace of  $A \in \mathbb{R}^{n \times n}$ . In particular,  $U^T U = I$ . Let  $D = U^T A U$  the interaction matrix whose eigenvalues are approximations of eigenvalues of  $A$ . The residual of the corresponding subspace is :

$$R = AU - UD \quad (5)$$

$$= (I - UU^T)AU. \quad (6)$$

The last expression shows that  $R$  lies in a space that is orthogonal to  $U$ , i.e.,

$$U^T R = 0. \quad (7)$$

The goal is to obtain  $(W, \Delta) \in \mathbb{R}^{n \times m}, \mathbb{R}^{m \times m}$  respectively, which will correct  $(U, D)$  so that the perturbed pair of matrices  $(U + W, D + \Delta)$  satisfy the (nonlinear) equation :

$$A(U + W) = (U + W)(D + \Delta). \quad (8)$$

This equation involves  $mn$  equations and  $mn + m^2$  unknowns. In order to close the system,  $m^2$  equations must be added. We consider the additional constraint :

$$U^T W = 0. \quad (9)$$

The above constraint may seem arbitrary but it can be interpreted as follows. It can be viewed as a means of restricting the information that is being added to the current system ( $W$ ) to being non redundant. Another condition we could have imposed is that the new system  $U + W$  should be orthonormal. This would have  $m^2$  constraints as desired, but these constraints are nonlinear. However, up to second order approximation these constraints will imply the requirement (9). Indeed,

$$(U + W)^T (U + W) = I \quad \rightarrow \quad U^T W + W^T U + W^T W = 0.$$

Neglecting second order terms from the system of equations (8) and (9), yields the equations:

$$\begin{cases} AW - WD - U\Delta = -R \\ U^T W = 0. \end{cases} \quad (10)$$

By multiplying the first equation on the left side by  $U^T$ , and using relation (7) we obtain the following expression for  $\Delta$ ,

$$\Delta = U^T AW. \quad (11)$$

Therefore, system (10) is equivalent to solving

$$(I - UU^T)AW - WD = -R \quad (12)$$

and then computing  $\Delta = U^T AW$ . It can be easily shown that the obtained solution  $W$  satisfies  $U^T W = 0$  as required.

## 2.2 Non orthonormal systems and the projection viewpoint

We now adapt what was developed above to the correction of a non orthonormal basis  $X \in \mathbb{R}^{n \times m}$  of an approximation of an invariant subspace. Along with  $X$  is a certain representation of  $A$  in the subspace in the form of a matrix  $D \in \mathbb{R}^{m \times m}$  such that  $A$ ,  $X$ , and  $D$  satisfy the relation

$$AX = XD + R,$$

where  $R$  is a certain residual matrix. The only requirement on  $X$ ,  $D$ , and  $R$  is that  $X^T R = 0$ . This implies in particular that  $D = (X^T X)^{-1} (X^T AX)$ .

We seek  $(W, \Delta) \in \mathbb{R}^{n \times m} \times \mathbb{R}^{m \times m}$  such that  $X^T W = 0$  and

$$A(X + W) = (X + W)(D + \Delta). \quad (13)$$

When the above equations are satisfied, then  $(X + W)$  spans an invariant subspace of  $A$  and the eigenvalues of  $(D + \Delta)$  are eigenvalues of  $A$ . By neglecting the second order terms, the equation becomes :

$$AW - WD - X\Delta = -R, \quad (14)$$

which implies that  $\Delta = (X^T X)^{-1} (X^T AW)$ . Let  $P = X(X^T X)^{-1} X^T$  be the orthogonal projection onto  $X$ . The final equation which generalizes equation (12) is :

$$(I - P)AW - WD = -R \quad (15)$$

with  $(I - P)W = W$ .

It is clear that if  $X$  and an orthonormal system  $U$  span the same subspace, then the resulting subspace obtained by the above process should be identical with the one resulting from the treatment of Section 2.1. In other words the matrices  $W, \tilde{W}$  obtained in both cases are related by a nonsingular  $p \times p$  transformation  $S$ , i.e.,  $W = \tilde{W}S$ .

### 2.3 Nonlinear correction

Clearly the original correction equation is nonlinear and its exact solution will yield an exactly invariant subspace. It is possible to solve the nonlinear equations iteratively and this section explores this possibility. In this section we go back to the case when  $U$  is orthonormal. Equation (8) is expanded as

$$AW - WD = -R + U\Delta + W\Delta \quad (16)$$

We still need to impose  $m^2$  constraints in the form of (9). Multiplying both sides of (16) by  $U^T$  yields the same expression for  $\Delta$ , i.e.,  $\Delta$  is again given by (11). This means that we have again removed the unknown  $\Delta$  from the system (8) and we can write:

$$AW - WD = -R + (U + W)U^T AW \quad (17)$$

Grouping like terms leads to the nonlinear system,

$$(I - UU^T)AW - W(D + U^T AW) + R = 0. \quad (18)$$

This system can be solved with some form of iteration and then  $\Delta$  can be obtained from  $\Delta = U^T AW$ . The solution  $W$  obtained also satisfies  $U^T W = 0$  as required.

It is interesting to examine a Newton approach for solving (18). Newton's method is equivalent to starting from a certain  $W_0$  (for example  $W_0 = 0$ ) and then iterating as  $W_{k+1} = W_k + Z_k$  where  $W_k + Z_k$  is made to satisfy (18) for up to first order terms in  $Z_k$ . This yields after a little calculation,

$$(I - (U + W_k)U^T)AZ_k - Z_k(D + U^T AW_k) = -R - (I - UU^T)AW_k + W_k(D + U^T AW_k) \quad (19)$$

The above system is a Sylvester equation in  $Z_k$  and with the notation  $U_k = U + W_k = U_{k-1} + Z_{k-1}$  and  $D_k = D + U^T AW_k$  it becomes

$$(I - U_k U_k^T)AZ_k - Z_k D_k = -R_k \quad (20)$$

where  $R_k$  is the right-hand side seen above

A few observations will provide some insight. The matrix  $D_k = D + U^T AW_k$  is the right-corrected projection matrix since  $D_k = D + U^T AW_k = U^T A(U + W_k)$ . There is some loss of symmetry in this process. In the end the Newton scheme would be as follows:

0. Select  $W_0$  (e.g.,  $W_0 = 0$ )
1. For  $k = 0, \dots$ , until convergence Do:
  2. Set  $D_k = D + U^T AW_k$ ;  $R_k = (I - UU^T)AW_k - W_k D_k + R$
  3. Solve (for  $Z_k$ ):  $(I - (U + W_k)U^T)AZ_k - Z_k D_k = -R_k$
  4. Set  $W_{k+1} = W_k + Z_k$
5. EndDo

Observe that when  $W_0 = 0$ , then the first step corresponds simply to the previous linearized scheme and this is expected. If we define  $U_k = U + W_k$ ,  $D_k = D + U^T AW_k = U^T AU_k$  the

iteration can be rewritten in terms of  $U_k$ . Note first that the expression for  $R_k$  can be simplified :

$$\begin{aligned}
R_k &= (I - UU^T)AW_k - W_kD_k + R \\
&= (I - UU^T)A(U_k - U) - (U_k - U)D_k + R \\
&= (I - UU^T)AU_k - (I - UU^T)AU - U_kD_k + UD_k + R \\
&= AU_k - U(U^T AU_k) - R - U_kD_k + UD_k + R \\
&= AU_k - UD_k - U_kD_k + UD_k \\
&= AU_k - U_kD_k
\end{aligned}$$

This gives the following alternative expression of the previous algorithm

**ALGORITHM 2.1** *Newton-Sylvester iteration*

0. Select  $U_0$  s.t.  $U_0^T U = I$  (e.g.,  $U_0 = U$ )
1. For  $k = 0, \dots$ , until convergence Do:
2. Compute  $D_k = U^T AU_k$ , and  $R_k = AU_k - U_kD_k$
3. Solve (for  $Z_k$ ):  $(I - U_kU^T)AZ_k - Z_kD_k = -R_k$
4. Set  $U_{k+1} = U_k + Z_k$
5. EndDo

An important note here concerns the solution of the Sylvester equation in Line 3. Since we would like to solve the correction equation with the constraint that  $W_k^T U =$ , we would like the relation  $Z_k^T U = 0$  should be satisfied in general. The relation it is trivially satisfied for  $k = 0$  a consequence of the choice made in Line 0. For a general  $k$ , the relation  $Z_k^T U = 0$  is equivalent to  $U_k^T U = I$ . We can use a little induction argument. Assume that the relation is satisfied for  $k$ . Then multiplying the equation by  $U^T$  yields  $U^T Z_k D_k = 0$ . This will imply that  $U^T Z_k = 0$  when  $D_k$  is nonsingular, which may be true under certain assumptions. However, in order to avoid difficulties, *we will always assume that the system (20) is solved for a  $Z$  that is orthogonal to  $U$* . When  $D_k$  is nonsingular, then as was seen,  $U^T Z_k = 0$  is automatically satisfied. When  $D_k$  is singular, we can for example shift both  $A$  and  $D_k$  by the same shift  $\sigma$  so that  $D_k - \sigma I$  is nonsingular. Then we solve, instead of (20), its shifted variant:

$$(I - U_kU^T)(A - \sigma I)Z_k - Z_k(D_k - \sigma I) = -R_k \quad (21)$$

Now since  $D_k - \sigma I$  is nonsingular,  $Z_k^T U = 0$  and this  $Z_k$  is also solution of (20). In practice this issue does not arise.

When convergence takes place it is quadratic at the limit, a characteristic of Newton's method. A relation which will establish this fact independently can also be proved.

**Lemma 2.1** *At each step of the Newton-Sylvester iteration the following relations hold:*

$$U_k^T U = I \quad (22)$$

$$R_k = (I - U_kU^T)AU_k \quad (23)$$

$$U^T R_k = 0 \quad (24)$$

$$R_{k+1} = -Z_kU^T AZ_k \quad (25)$$

**Proof.** The first relation was discussed in detail above. It comes from the fact that at each step  $U^T Z_k = 0$ . The second relation follows immediately from the definition of  $D_k$  and the 3rd is obtained by multiplying the second by  $U^T$  to the left and making use of (22). For the 4th relation we write,

$$\begin{aligned} R_{k+1} &= A(U_k + Z_k) - (U_k + Z_k)(D_k + U^T A Z_k) \\ &= AU_k + AZ_k - U_k D_k - Z_k D_k - U_k U^T A Z_k - Z_k U^T A Z_k \\ &= \underbrace{R_k + (I - U_k U^T) A Z U_k - Z_k D_k - Z_k U^T A Z_k}_{=0} = -Z_k U^T A Z_k \end{aligned}$$

■

Equations (22) and (23) show that the method is equivalent to finding a block  $U_*$  such that  $(I - U_* U_*^T) A U_* = 0$  subject to the condition that the system  $U_*, U$  be bi-orthogonal. Note that from (23), we can easily infer that  $\|R_k\| = O(\|U_k - U_*\|)$  where  $U_*$  is the limit. Indeed, using the fact  $(I - U_* U_*^T) A U_* = 0$

$$\begin{aligned} R_k &= (I - U_k U^T) A U_k - (I - U_* U_*^T) A U_* \\ &= (I - U_k U^T) A U_k - (I - U_k U^T) A U_* + (I - U_k U^T) A U_* - (I - U_* U_*^T) A U_* \\ &= (I - U_k U^T) A (U_k - U_*) - (U_k - U_*) U^T A U_* \end{aligned}$$

The following relationship will confirm this and provide some additional insight:

$$R_{k+1} = -Z_k U^T A Z_k$$

In the case when  $m = 1$  we get the following iteration for  $k = 0, 1, \dots$ , starting with  $u_0 = u$ :

$$\begin{cases} d_k &= u^T A u_k \\ r_k &= A u_k - d_k u_k \\ (I - u_k u^T) A z_k - d_k z_k &= -r_k \\ u_{k+1} &= u_k + z_k \end{cases}$$

Note that the scalar  $d_k$  is an approximate eigenvalue. Indeed,  $u_k^T u = (u + w_k)^T u = u^T u = 1$  and therefore  $d_k = (u^T A u_k) / (u^T u_k)$ . When (and if)  $u_k$  converges to an eigenvector, then  $d_k$  will converge to the corresponding eigenvalue.

The residual system in the 3rd line of the above algorithm can be transformed. The system is

$$(I - u_k u^T) A z_k - z_k d_k = -r_k \quad \rightarrow \quad (A - d_k I) z_k - u_k u^T A z_k = -r_k$$

and it can be solved in block form by setting  $\xi_k = -u^T A z_k$  and putting the unknowns  $u_k, \xi_k$  in one vector:

$$\begin{pmatrix} A - d_k I & u_k \\ u^T A & 1 \end{pmatrix} \begin{pmatrix} z_k \\ \xi_k \end{pmatrix} = \begin{pmatrix} -r_k \\ 0 \end{pmatrix}$$

The advantage of writing the system in this form is that we can better exploit any sparsity in  $A$ . In contrast the matrix  $(I - u_k u^T) A - d_k I$  is generally not sparse, though the Sherman-Morrison formula can also be invoked with a similar result.

A more traditional way of invoking the Newton approach is for the case  $m = 1$ , by solving directly the equation  $Au - u(u^T Au) = 0$ , with the constraint  $\|u\|_2 = 1$ . Extending this to the  $m$  dimensional case is doable but the constraint that  $U$  be unitary yields a more complicated iteration. The scheme shown above avoids the problem of orthogonalization - but it yields an iteration that is somewhat nonsymmetric.

So far symmetry has not been exploited. When  $A$  is symmetric, the term  $U^T AZ_k$  in the above expression is the transpose of  $Z_k^T AU = Z_k^T (AU - UD) = Z_k^T R_0$  so that

$$A = A^T \quad \rightarrow \quad R_{k+1} = -Z_k^T R_0^T Z_k .$$

with  $R_0 = R$ . If only one step is performed then  $R_1 = -Z_1 R_0^T Z_1$ . So, if one step is performed, and the process restarted (i.e.,  $U_1$  is orthogonalized and  $U$  is set to  $U_1$ , etc.) then one should expect a cubic convergence according to this formula. This is explored next.

## 2.4 Iterative correction

In this section, we consider the following modification of the Newton-Sylvester scheme discussed in the previous section.

**ALGORITHM 2.2** *Iterative correction*

0. Select  $U_0$  (e.g.,  $U_0 = U$ )
1. For  $k = 0, \dots$ , until convergence Do:
2. Compute  $D_k = U_k^T A U_k$ , and  $R_k = A U_k - U_k D_k$
3. Solve (for  $W_k$ ):  $(I - U_k U_k^T) A W_k - W_k D_k = -R_k$
4. Orthogonalize :  $[U_{k+1}, S_k] = \text{qr}(U_k + W_k)$ .
5. EndDo

In line 4, Matlab notation is used so that  $U_{k+1}$  is the result or orthonormalizing  $U_k + W_k$ .

**Theorem 2.1** *When the process converges, it exhibits a cubic convergence at the limit, as expressed by the following relation :*

$$R_{k+1} = -W_k R_k^T W_k S_k^{-1} + O(\|W_k\|^4). \quad (26)$$

**Proof.** We first remark that  $(U_k + W_k)^T (U_k + W_k) = S_k^T S_k = I + W_k^T W_k$ .

Let us denote  $\overline{D}_k = (U_k + W_k)^T A (U_k + W_k)$  and  $\overline{R}_k = R_{k+1} S_k = A (U_k + W_k) - (U_k + W_k) (S_k^T S_k)^{-1} \overline{D}_k$ .

Therefore, with  $\Delta_k = U_k^T A W_k$ , the correction implies that

$$A (U_k + W_k) - (U_k + W_k) (D_k + \Delta_k) = -W_k \Delta_k, \quad (27)$$

and remembering that  $U_k^T W_k = 0$ ,

$$\overline{D}_k - (I + W_k^T W_k) (D_k + \Delta_k) = -W_k^T W_k \Delta_k,$$

which can be rewritten as

$$\overline{D}_k = D_k + \Delta_k + W_k^T W_k D_k. \quad (28)$$

For the residual, we estimate

$$\begin{aligned} \overline{R}_k &= A(U_k + W_k) - (U_k + W_k)(I - W_k^T W_k)\overline{D}_k + O(\|W_k\|^4), \\ &= A(U_k + W_k) - (U_k + W_k)\overline{D}_k + (U_k + W_k)W_k^T W_k \overline{D}_k + O(\|W_k\|^4), \\ &= -W_k \Delta_k - (U_k + W_k)W_k^T W_k D_k + (U_k + W_k)W_k^T W_k (D_k + \Delta_k) + O(\|W_k\|^4), \\ &= -W_k \Delta_k - (U_k + W_k)W_k^T W_k \Delta_k + O(\|W_k\|^4), \\ &= (-W_k - U_k W_k^T W_k)\Delta_k + O(\|W_k\|^4), \\ &= (-W_k - U_k W_k^T W_k)U_k^T A W_k + O(\|W_k\|^4), \\ &= (-W_k - U_k W_k^T W_k)(R_k^T W_k + D_k U_k^T W_k) + O(\|W_k\|^4), \\ &= -W_k R_k^T W_k + O(\|W_k\|^4). \end{aligned}$$

Since, clearly  $\|W_k\| = O(\|R_k\|)$ , this ends the proof.  $\blacksquare$

## 2.5 Inverse iteration and RQI

The above developments lead to Olsen's scheme and the Jacobi-Davidson approach, see, e.g., [17]. A simpler scheme is often used in practice which consists of ignoring the projection step. In the situation of a single vector iteration, this scheme is simply the inverse iteration algorithm, which computes a new direction by solving

$$(A - \mu I)u_{new} = u \quad (29)$$

in which  $\mu$  is typically a fixed shift close to an eigenvalue. Note that the right-hand side is an approximate eigenvector instead of a residual. A block generalization can be written from the scheme (12) by using a different right-hand side, namely, we solve

$$AU_{new} - U_{new}D = U.$$

If  $R \equiv AU - UD$ , and  $U_{new} = U + W$  then the above condition, can be rewritten as  $AW - WD = U - R$ . Note that now  $D$  is no longer defined as  $D = U^T AU$  but can be a diagonal matrix of shifts. Also a normalization must be added to the basic step mentioned above, in the form of a QR factorization of  $U_{new}$ .

In Rayleigh quotient iteration, the shift  $\mu$  in (29) is changed to the Rayleigh quotient at each step. This, however is not practical as it requires an expensive re-factorization of the matrix at each step. Of course the same is true of Algorithm 2.1, where a change in the matrix  $D_k$  would require expensive refactoring in the method used to solve the Sylvester equation.

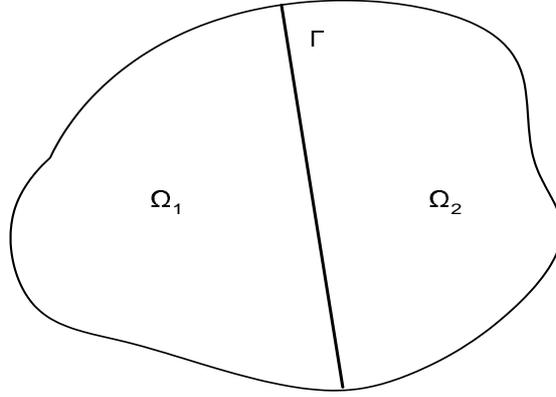


Figure 1: The simple case of two subdomains  $\Omega_1, \Omega_2$  and an interface  $\Gamma$ .

### 3 Domain decomposition: CMS and AMLS

Let  $A \in \mathbb{R}^{n \times n}$  be a symmetric real matrix, partitioned as

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix}, \quad (30)$$

where  $B \in \mathbb{R}^{(n-p) \times (n-p)}$ ,  $C \in \mathbb{R}^{p \times p}$  and  $E \in \mathbb{R}^{(n-p) \times p}$ . Assume that the above matrix arises from the discretization of a certain self-adjoint operator (e.g., a Laplacean) on a domain  $\Omega$  which is then partitioned into several subdomains separated by an interface  $\Gamma$ , see Figure 1 for the simplest case of two subdomains. The subdomains, which may overlap, are separated by an interface  $\Gamma$ . The unknowns in the interior of each subdomain  $\Omega_i$  are completely decoupled from the unknowns of all other subdomains. Coupling among subdomains is through the unknowns of the interface  $\Gamma$  and the unknowns in each  $\Omega_i$  that are adjacent to  $\Gamma$ . With the situation just described, the matrix  $B$  is block diagonal, consisting of two diagonal blocks corresponding to the unknowns that are interior to each subdomains. The  $C$  block corresponds to the variables on the interface.

The eigenvalue problem  $Au = \lambda u$ , can be written as,

$$\begin{pmatrix} B & E \\ E^T & C \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \lambda \begin{pmatrix} u \\ y \end{pmatrix}, \quad (31)$$

where  $u \in \mathbb{C}^{n-p}$  and  $y \in \mathbb{C}^p$ . A method for computing eigenvalues of matrices partitioned in this manner was introduced in structural dynamics by [6, 7]. Referred to as the method of Component Mode Synthesis (CMS), this method begins by solving the problem  $Bv = \mu v$ . This amounts to solving each of the decoupled smaller eigenvalue problems corresponding to each subdomain  $\Omega_i$  separately. The method then injects additional vectors to account for the coupling among subdomains. This is done by invoking a carefully selected operator for the interface nodes. AMLS is a multilevel approach which exploits recursivity by continuing this approach into lower levels recursively, see e.g., [2, 1] for details.

In the following, the main steps of CMS - i.e., one level of AMLS, will be reviewed. Consider the matrix

$$U = \begin{pmatrix} I & -B^{-1}E \\ 0 & I \end{pmatrix}. \quad (32)$$

This is a block Gaussian eliminator for matrix (30), which is selected so that

$$U^T A U = \begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix},$$

where  $S$  is the Schur complement

$$S = C - E^T B^{-1} E. \quad (33)$$

The original problem (31) is equivalent to the generalized eigenvalue problem  $U^T A U u = \lambda U^T U u$ , which becomes

$$\begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \lambda \begin{pmatrix} I & -B^{-1}E \\ -E^T B^{-1} & M_S \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix}, \quad (34)$$

where  $M_S = I + E^T B^{-2} E$ . The next step of CMS is to neglect the coupling matrices (blocks in positions (1,2) and (2,1)) in the right-hand side matrix of (34). This yields the uncoupled problem

$$Bv = \mu v \quad (35)$$

$$Ss = \eta M_S s. \quad (36)$$

Once the desirable eigenpairs have been obtained from (35–36), they are utilized in a projection method (Rayleigh-Ritz) applied to the original problem (34). The basis used for this projection is of the form

$$\left\{ \hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad i = 1, \dots, m_B; \quad \hat{s}_j = \begin{pmatrix} 0 \\ s_j \end{pmatrix} \quad j = 1, \dots, m_S \right\}, \quad (37)$$

where  $m_B < (n - p)$  and  $m_S < p$ .

It is important to note that the projection is applied to (34) rather than to the original problem (31). There is an inherent change of basis between the two and, for reasons that will become clear shortly, the basis  $\{\hat{v}_i\}_i, \{\hat{s}_j\}_j$ , is well suited for the transformed problem rather than the original one. In fact let us consider this point in detail. We could also think of using the transformed basis

$$\left\{ \hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad i = 1, \dots, m_B; \quad \hat{u}_j = \begin{pmatrix} -B^{-1} E s_j \\ s_j \end{pmatrix} \quad j = 1, \dots, m_S \right\}, \quad (38)$$

for solving the original problem (31). instead of basis (37). As can be easily seen, these two options are mathematically equivalent.

**Lemma 3.1** *The Rayleigh-Ritz process using the basis (37) for problem (34) is mathematically equivalent to the Rayleigh-Ritz process using the basis (38) for problem (31).*

**Proof.** For a given matrix  $A$ , and a given basis (not necessarily orthogonal) consisting of the columns of a certain matrix  $Z$ , the Rayleigh Ritz process can be written as

$$Z^T AZ \underline{v} = \underline{\lambda} Z^T Z \underline{v}$$

If  $Z$  is the basis (37) then the basis (38) is nothing but  $UZ$ . Comparing the two projection processes gives the result. ■

In the rest of the paper we will use the basis (38) on the original problem (31) for describing the CMS projection.

### 3.1 Links with the correction equation

One of the purposes of this paper is to present CMS/AMLS from the angle of the correction equation. Notice at first that CMS does implement a correction: it corrects the eigenvectors of  $B$  to try to obtain better approximations to the eigenvectors of the whole matrix  $A$ . This is done by using the Schur complement matrix and constructing a good (improved) basis to perform the Rayleigh Ritz projection. This viewpoint (correction) is important because there are many variants for correcting eigenvectors and some are better than others.

Consider eigenvectors of  $B$  associated with smallest eigenvalues.

$$Bv_i = \mu_i v_i .$$

One can consider the vectors

$$\hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix}$$

as approximate eigenvectors of  $A$ . The eigenvectors obtained in this manner amount to neglecting all the couplings and are likely to yield very crude approximations. We can now think of correcting these eigenvectors via a *correction equation* as is usually done in the previous sections.

An interesting observation is that the residuals  $r_i = (A - \mu I)\hat{v}_i$  have components only on the interface variables, i.e., they have the shape:

$$r_i = \begin{pmatrix} 0 \\ z_i \end{pmatrix} \tag{39}$$

where the partitioning corresponds to the one above and where  $z_i = E^T v_i$ .

Consider a single vector inverse iteration correction. In this case, for each approximate eigenvector  $v_i$  we would seek a new approximation  $u_i$  by solving an equation of the type (29),  $(A - \mu I)u_i = v_i$  . where  $\mu$  is a certain shift. In a typical inverse iteration correction,  $\mu$  is constant to reduce cost of factorization.

The matrix  $A - \mu I$  can be factored as

$$(A - \mu I) = \begin{pmatrix} I & 0 \\ E^T(B - \mu I)^{-1} & I \end{pmatrix} \begin{pmatrix} B - \mu I & E \\ 0 & S(\mu) \end{pmatrix} \quad (40)$$

where  $S(\mu)$  is the Schur complement

$$S(\mu) = C - \mu I - E^T(B - \mu I)^{-1}E$$

Taking the particular structure of  $v_i$  into account we find that

$$u_i = (A - \mu I)^{-1} \begin{pmatrix} v_i \\ 0 \end{pmatrix} = \begin{pmatrix} [I + (B - \mu I)^{-1}ES(\mu)^{-1}E^T](B - \mu I)^{-1}v_i \\ -S(\mu)^{-1}E^T(B - \mu I)^{-1}v_i \end{pmatrix}$$

In other words,

$$u_i = \begin{pmatrix} z_i + (B - \mu I)^{-1}Es_i \\ s_i \end{pmatrix} \quad \text{with} \quad z_i = (B - \mu I)^{-1}v_i \quad \text{and} \quad s_i = S(\mu)^{-1}z_i$$

There is a strong similarity between the result of this correction and that obtained from CMS. This can be seen from the nature of the basis (38) which consists of the vectors

$$\begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad \begin{pmatrix} -B^{-1}Es_j \\ s_j \end{pmatrix} \quad (41)$$

where the  $s_i$ 's are eigenvectors of a Schur complement, and the  $v_i$ 's are eigenvectors of the  $B$  block.

### 3.2 Correction equations and Domain Decomposition

Consider now the application of the correction equation (12) to the Domain Decomposition framework discussed above. Specifically, we consider the Newton approach discussed in Section 2.3 and we will apply one step of the Newton-Sylvester algorithm, i.e., Algorithm (2.1). Note that since we are only considering one step of the process, there is no difference between this algorithm and Algorithm 2.2. The index  $k$  is removed for simplicity and  $U_{k+1}$  in Line 4 is denoted by  $U^{new}$ . We denote by  $V_1 \in \mathbb{R}^{p \times m}$  ( $1 \leq m \leq p < n$ ) an orthogonal basis of an invariant subspace of  $B$ , so that  $BV_1 = V_1D$ , where  $D = \text{diag}(\mu_1, \dots, \mu_m)$  and we let  $U = \begin{pmatrix} V_1 \\ 0 \end{pmatrix} \in \mathbb{R}^{n \times m}$ . To simplify notation we will denote by  $P_1$  the orthogonal projector  $P_1 \equiv I - V_1V_1^T$ , so that

$$I - UU^T = \begin{pmatrix} I - V_1V_1^T & 0 \\ 0 & I \end{pmatrix} \equiv \begin{pmatrix} P_1 & 0 \\ 0 & I \end{pmatrix} \quad (42)$$

In addition, the matrix  $D_k$  in Line 2 of Algorithm 2.1 is simply the diagonal matrix  $D$ :

$$U^T AU = [V_1^T \quad 0]A \begin{pmatrix} V_1 \\ 0 \end{pmatrix} = V_1^T BV_1 = D.$$

Similarly, the residual matrix  $R_k$  has a simple structure due to (39):

$$R = AU - UD = \begin{pmatrix} 0 \\ E^T V_1 \end{pmatrix}$$

Now the Sylvester system in Line 3 of Algorithm 2.1 can be written  $(I - UU^T)AZ - ZD = -R$ . Since  $D$  is diagonal this system decouples into the  $p$  distinct linear systems,

$$(I - UU^T)Az_i - \mu_i z_i = -r_i = - \begin{pmatrix} 0 \\ E^T v_i \end{pmatrix}. \quad (43)$$

Writing  $z_i = \begin{pmatrix} y_i \\ s_i \end{pmatrix}$  the system (43) translates to:

$$\begin{aligned} P_1 B y_i + P_1 E s_i - \mu_i y_i &= 0 \\ E^T y_i + (C - \mu_i I) s_i &= -E^T v_i \end{aligned}$$

Note that the first equation is equivalent to  $P_1(B - \mu_i I)y_i + P_1 E s_i = 0$  the solution of which is

$$y_i = -[P_1(B - \mu_i I)]^\dagger P_1 E s_i.$$

Substituting this solution in the second equation results in:

$$-E^T P_1 (B - \mu_i I)^\dagger P_1 E s_i + (C - \mu_i I) s_i = -E^T v_i$$

which gives the following equation to solve for  $s_i$ :

$$[C - \mu_i I - E^T P_1 (B - \mu_i I)^\dagger P_1 E] s_i = -E^T v_i \quad (44)$$

This leads to a natural definition of a *projected Schur complement*,

$$S_*(\mu_i) = C - \mu_i I - E^T P_1 (B - \mu_i I)^\dagger P_1 E$$

from which the solution is readily expressible. In what follows it is assumed that  $S_*(\mu_i)$  is not singular (A less restrictive assumption is that  $S_*(\mu_i)$  is not singular in the range of  $E^T$ .)

In the end the column-vectors of the new matrix  $U^{new}$  are given by

$$u_i^{new} = u_i + z_i = \begin{pmatrix} v_i - P_1 (B - \mu_i I)^\dagger P_1 E s_i \\ s_i \end{pmatrix} \quad \text{with} \quad s_i = -S_*(\mu_i)^{-1} E^T v_i \quad (45)$$

An interesting property which can be shown is that

$$(A - \mu_i I) u_i^{new} = \begin{pmatrix} -V_1 V_1^T E s_i \\ 0 \end{pmatrix}.$$

It is, of course possible to apply additional steps of this correction process. However, these additional steps will require expensive Sylvester-like equations to be solved at each step with different shifts.

Instead of considering these we can instead gain insight from the AMLS procedure and try to define good subspaces for a projection process. Specifically, the question is: *which subspace should be added to  $\text{span}V_1$  if the goal is to obtain a good approximation to the original eigenspace?*

A comparison between (45) and the basis (41) used by CMS suggests that we replace  $\mu_i$  by zero in (45) and that we enrich the basis  $V_1$  by the vectors

$$\begin{pmatrix} -P_1 B^{-1} P_1 E s_i \\ s_i \end{pmatrix} \quad \text{with} \quad s_i = -S_*(0)^{-1} E^T v_i.$$

Note that  $P_1 B^{-1} P_1 = P_1 B^{-1} = B^{-1} P_1$ . In other words we can consider performing a Rayleigh-Ritz process on the original problem (31) with the basis

$$\left\{ \hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix}; \hat{u}_i = \begin{pmatrix} -P_1 B^{-1} E s_i \\ s_i \end{pmatrix} \quad i = 1, \dots, m \right\}, \quad \text{with} \quad s_i = -S_*(0)^{-1} E^T v_i. \quad (46)$$

The differences with the basis used by CMS are (1) the way in which the  $s_i$ 's are defined and (2) the presence of the projector  $P_1$  in the definition of  $\hat{u}_i$ . We can also define a simplified basis, which we will refer to as the Newton-CMS basis, in which the projectors are removed:

$$\left\{ \hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix}; \hat{u}_i = \begin{pmatrix} -B^{-1} E s_i \\ s_i \end{pmatrix} \quad i = 1, \dots, m \right\}, \quad \text{with} \quad s_i = -S^{-1} E^T v_i. \quad (47)$$

Note that  $S_*(0)$  has been replaced by the standard Schur complement  $S = C - E^T B^{-1} E$ . Experiments indicated that at least for a one level AMLS (i.e., for a CMS algorithm), there is no difference between the two bases (46) and (47). The following will provide a partial explanation for this question which is still being investigated.

Assume for a moment that the vector  $s_i$ s are the same in both (46) and (47). Then the two bases would be the same. Indeed, the added vectors  $\hat{u}_i$  in (47) can be written

$$\hat{u}_i = \begin{pmatrix} -B^{-1} E s_i \\ s_i \end{pmatrix} = \begin{pmatrix} -P_1 B^{-1} E s_i \\ s_i \end{pmatrix} + \begin{pmatrix} -(I - P_1) B^{-1} E s_i \\ 0 \end{pmatrix}$$

However, the second component in the decomposition is a subset of the span of  $\{\hat{v}_i\}$ , i.e., the first part of (46). So in this situation the two bases would actually generate the same space. Though the  $s_i$  in both bases (46) and (47) are not the same, what is observed experimentally for the two domain case, is that they span the space. In other words, the subspaces spanned by  $S^{-1} E^T V_1$  and  $S_*(0)^{-1} E^T V_1$  are the same. If this is the case then it is easy to see that the two methods will give the subspaces overall and therefore the same approximations.

One of the main weaknesses of AMLS is that it is a one-shot algorithm, in the sense that it just provides one set of approximations that cannot (at least with the classical algorithm definition) be improved. Because of the close relationship between the AMLS algorithm and the correction equation, we can think of using more steps of the correction algorithms described earlier to fill the gap. The biggest appeal of AMLS is that it is essentially a method which performs one factorization (direct) only to extract a large number of eigenvectors. In the numerical experiments we will test the

following adaptation of Algorithm 2.2 in which  $U_0$  corresponds to the initial set of CMS which is the first part of the basis (38). For this reason it is important to set  $D_k$  to zero throughout. In addition, following the spirit of CMS, the correction in Line 4 of Algorithm 2.2 is replaced by a projection step using the sets given by  $U_k$  and  $Z_k$ . This gives following iterative, or corrected, variant of CMS.

**ALGORITHM 3.1** *Iterative CMS*

0. Select  $U_0$  s.t.  $U_0^T U_0 = I$  from eigenvectors in each subdomain.
1. For  $k = 0, \dots$ , until convergence Do:
2.     Compute  $R_k = AU_k - U_k(U_k^T AU_k)$
3.     Solve (for  $Z_k$ ):  $(I - U_k U_k^T)AZ_k = -R_k$
4.     Set  $V = [U_k, Z_k]$
5.     Compute  $U_{k+1}$  from a Rayleigh-Ritz projection on  $A$  using the basis  $V$ .
6.     EndDo

This algorithm will be tested for a 2-domain case in the next section.

## 4 Numerical Examples

All the tests are run in the MATLAB environment.

### 4.1 Quadratic and Cubic convergence

The first test considers a matrix of small order ( $n = 238$ ). This matrix is the classical matrix obtained by the discretization of the 2D Laplacean by finite differences on a  $14 \times 17$  rectangular mesh. The twenty smallest eigenvalues are sought. The two principal diagonal blocks of order 112, the leading one and the trailing one, are separated by a block of dimension 14. When adequately permuted, the matrix profile is shown in Figure 2 (a). The evolution of the residual norms are displayed in Figure 2 (b) for the Newton-Sylvester iteration, and in Figure 2(c) for the Iterative Correction. The quadratic and cubic convergences are well illustrated by the curves. During the first iterations, the two methods stagnate as long as they have not yet determined a good approximation of an invariant subspace. The computed eigenvalues are not the 20 smallest ones : there are some missing eigenvalues. For Algorithm 2.1, the 12 smallest eigenvalues are computed and the last 8 computed eigenvalues correspond to eigenvalues ranking between the 14th and the 25th eigenvalue of the matrix. For Algorithm 2.2, the result is almost equivalent although a bit worse: the first 10 eigenvalues are computed and the last 10 computed eigenvalues range between the 12th and the 26th eigenvalue.

### 4.2 Computing inner eigenvalues

In this section, we consider as test matrix  $A_0$ , the matrix PLAT1919 from the test suite Matrix Market [3]. The matrix is of order 1919 and its sparsity pattern is shown in Figure 3 (a). By applying a symmetric reordering  $P$  obtained from the Symmetric Reverse Cuthill-McKee algorithm, the matrix  $A_P = P^T A P$  has a smaller bandwidth. Considering the permuted matrix  $A_P$ , two diagonal blocks are defined by the intervals of indices  $I_1 = [1 : 1040]$  and  $I_2 = [1081 : 1919]$ . The interval  $J = [1041 : 1080]$  is the separator. By renumbering symmetrically rows and columns of  $A_P$ , with the numbering defined by  $Q = [I_1, I_2, J]$ , one gets the test matrix  $A$  whose is displayed in Figure 3 (b).

The full spectrum of PLAT1919, computed by the QR method, is displayed in Figure 4. The goal of the tests is to analyze the behavior of the two algorithms 2.1 and 2.2 for computing a basis of an invariant subspace corresponding to six eigenvalues in a neighborhood of  $\sigma = 0.995$ .

The same initial guess  $U_0 \in \mathbb{R}^{1919 \times 6}$  of a basis of the sought invariant subspace is considered for the two methods. It is built, consistently with Section 3.2, by the following : for each of the two blocks, the three eigenvectors corresponding to the eigenvalues which are the closest to  $\sigma$  are computed ; in that way, two orthonormal blocks  $U^{(1)} \in \mathbb{R}^{1040 \times 3}$  and  $U^{(2)} \in \mathbb{R}^{849 \times 3}$  are obtained and  $U_0$  is then defined by

$$U_0 = \begin{pmatrix} U^{(1)} & 0 \\ 0 & U^{(2)} \\ 0 & 0 \end{pmatrix}. \quad (48)$$

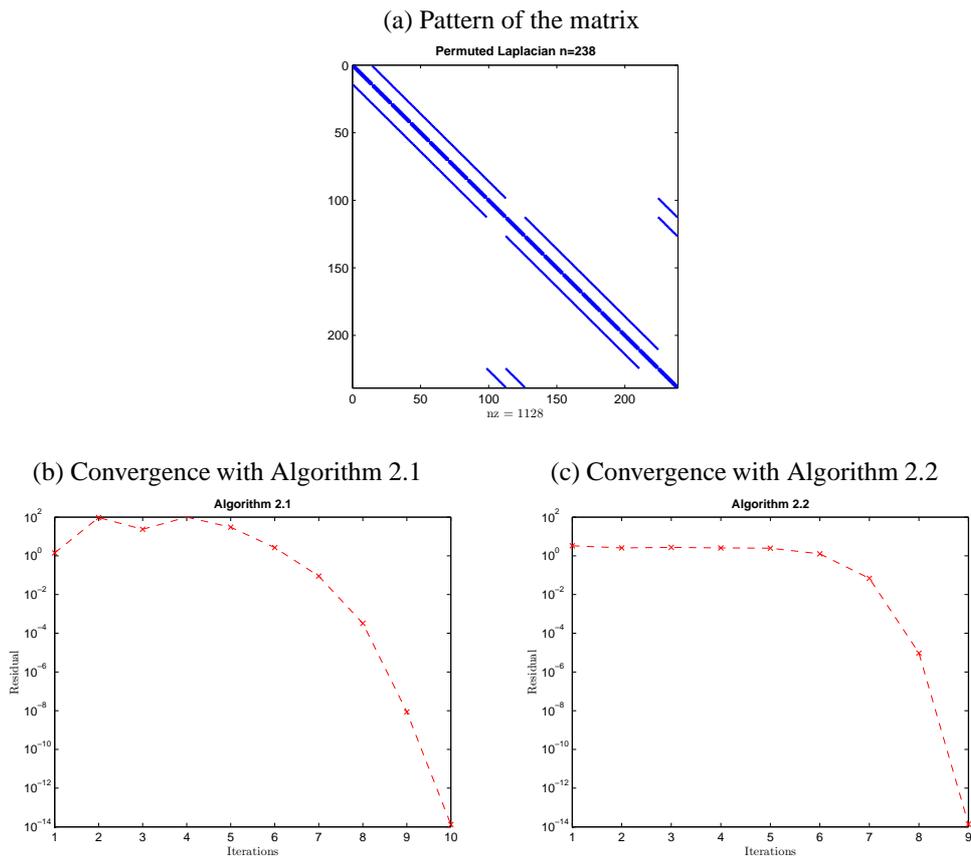


Figure 2: Test with the Laplacean

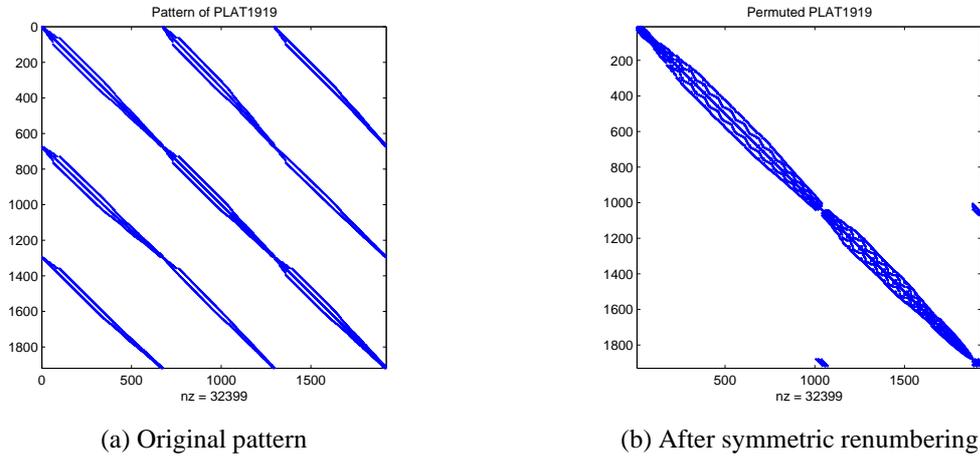


Figure 3: Sparsity patterns of PLAT1919

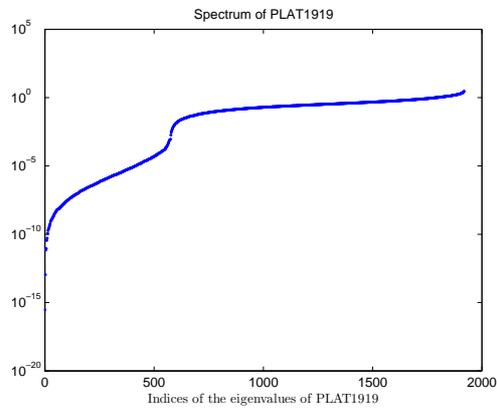


Figure 4: Spectrum of Matrix PLAT1919

Table 1 shows, for each of the two methods, the computed eigenvalues, corresponding to the invariant subspace defined by the last computed basis  $U_k$ . In each case, the eigenvalues of  $D_k$  are given, along with their respective index in the spectrum of the matrix, and their absolute error. The eigenvalues are labeled in ascending order. In Figure 5, the computed eigenvalues are located in the whole

<b>Algorithm 2.1</b> After $k = 10$ iterations Residual : $5 \times 10^{-2}$			<b>Algorithm 2.2</b> After $k = 6$ iterations Residual : $3 \times 10^{-11}$		
eigenvalue	index	error	eigenvalue	index	error
0.91576	1771	$4 \times 10^{-3}$	0.96497	1782	$1 \times 10^{-15}$
0.97367	1785	$2 \times 10^{-3}$	0.99000	1786	$1 \times 10^{-15}$
0.98842	1786	$2 \times 10^{-3}$	0.99359	1788	$2 \times 10^{-15}$
0.99213	1788	$1 \times 10^{-3}$	0.99515	1791	$2 \times 10^{-15}$
0.99964	1791	$4 \times 10^{-3}$	1.0053	1793	$4 \times 10^{-15}$
1.0866	1812	$2 \times 10^{-3}$	1.0113	1794	$2 \times 10^{-15}$

Table 1: Computed eigenvalues of PLAT1919 near  $\sigma = 0.995$

spectrum of matrix PLAT1919. On this example, the superiority of Algorithm 2.2 over Algorithm

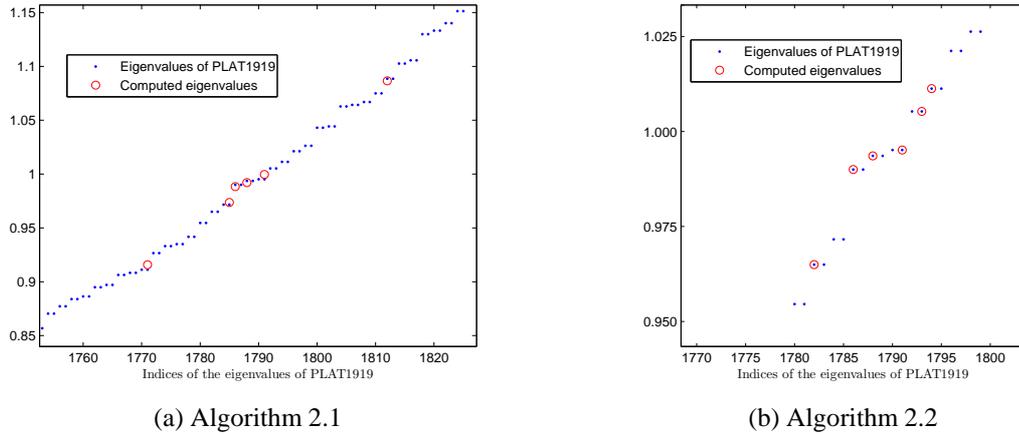


Figure 5: Location of the computed eigenvalues in the spectrum

2.1 is clear : the eigenvalues computed by the former are closer to the reference number  $\sigma$  and they are much more precise. Actually, the run of Algorithm 2.1 showed a lack of convergence. We rerun Algorithm 2.1 with  $U$  equal to the Q-factor in the QR factorization of the last estimate  $U_k$  of the first run. After 10 additional iterations, the residual reached  $10^{-6}$  and the computed eigenvalues were corresponding to eigenvalues of PLAT1919 with indices from 1771 to 1815, with a precision higher than  $10^{-12}$ . It appears that, this algorithm needs a better initial estimate than its counterpart.

A drawback of Algorithm 2.1 lies in its Step 3 which corresponds to a non symmetric Sylvester equation. However, complex computation can be avoided since it can be proved that, although non symmetric, Matrix  $Dk$  is similar to a symmetric matrix.

### 4.3 Tests with domain decomposition

We consider a Schrödinger operator (a Hamiltonian) of the form

$$H = -\Delta + V$$

on a rectangular domain in 2 dimensions. Here the potential  $V$  is the Gaussian

$$V(x, y) = -\beta e^{-(x-x_c)^2 - (y-y_c)^2}$$

in which  $(x_c, y_c)$  is the center of the domain. We selected  $\beta = 100$ , and discretized the domain uniformly using centered finite differences and applied Dirichlet boundary conditions. The domain is a rectangle of dimension  $(n_x + 1) \times h = 1$  and  $(n_y + 1) \times h$ , where  $n_x, n_y$  are the number of discrete points on the  $x$  and  $y$  directions, respectively, excluding boundary points. The domain is then split in two horizontally, in the middle of the domain. The matrix is reordered by putting the interface variables at the end as is usually done to illustrate DD orderings. The resulting matrix is shown on the left side of Figure 6.

The first experiments is only for demonstrating the power of the CMS algorithm and its variants. For We found in general very little difference between the different variants of the same idea. Figure 6 compares the following 4 methods for computing the smallest  $nev$  eigenvalues. In the test  $nev = 8$ .

**No correction** This performs a Rayleigh Ritz procedure with eigenvectors from the two domains. The process takes  $nev$  eigenvectors from each domain which will form the column vectors of two matrices  $U_1, U_2$  then gathers them in a basis  $W = [U_1, U_2]$  and then proceeds to a Rayleigh Ritz projection on  $A$  with the  $nev$  vectors in  $W$ .

**CMS** This approach consists of a the CMS projection, which takes the same  $W$  from above and augments it with the set  $Z$  obtained as

$$Z = \begin{pmatrix} -B^{-1}G \\ G \end{pmatrix}$$

in which  $G$  is matrix of eigenvectors of  $S$  associated with the smallest  $nev$  eigenvalues.

**Newton-CMS** This is similar with the previous method, but the  $G$  matrix is replaced by the matrix  $E^T W$ . Note that this matrix has  $2nev$  columns instead of  $nev$  for CMS.

**Newton-CMS with projection** The only difference between this and the previous process is that the projector  $P_1 = I - WW^T$  is used. The inverse of  $B$  is replaced by  $P_1 B^{-1}$  when defining  $S$  and the  $Z$  matrix above.

Figure 6 shows an illustration for a case when  $n_x = 35, n_y = 33$  which yields a matrix of size  $n = 1,155$ . As it turns out it is very difficult for this example to find cases where the last 3 methods yield (significantly) different results. Because  $n_x$  is relatively small, the subspace spanned by the matrices  $G$  involved above is the same or very close and this leads to the same approximations. In all cases we tested for this example, Methods 3 and 4 seemed to be exactly identical. This means that the  $G$  matrices generate the same subspace in both cases. What is remarkable is the quality of the approximation obtained from CMS-type approaches. The accuracy obtained by using eigenvectors from subdomains alone (no correction) is already quite good, considering the simplicity of this approach.

In the next test we consider the iterative CMS, Algorithm 3.1, discussed earlier. Only two correction steps (corresponding to the  $k$  loop in the algorithm) are taken. In this test we take  $n_x = 45, n_y = 43$  which leads to a bigger matrix of size  $n = 1,935$ . Figure 7 shows the result of computing the 20 lowest eigenvalues with the three methods: Newton-CMS, 1st step of Iterative CMS, and 2nd step of Iterative CMS. The results are much improved, especially for the lowest 10 eigenvalues. Note also, that the biggest improvement is achieved by the first corrective step. What is important to emphasize here is that the improvements achieved by the two corrections are obtained without any additional factorizations of the matrix  $A$ . The system  $(I - UU^T)AZ = -R$  can be solved, for example, by setting  $T = U^T AZ$  and then solving

$$\begin{pmatrix} A & -U \\ U^T A & -I \end{pmatrix} \begin{pmatrix} Z \\ T \end{pmatrix} = \begin{pmatrix} -R \\ 0 \end{pmatrix}.$$

Since  $U$  is typically of low rank, the above system can be easily solved with one factorization of  $A$ .

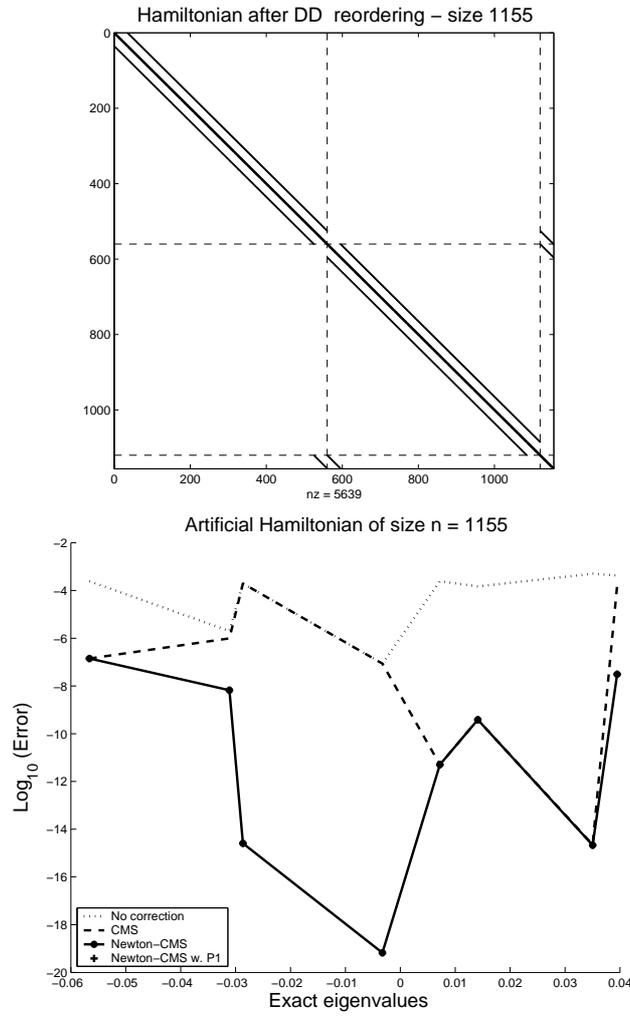


Figure 6: Left: Pattern of the Hamiltonian matrix after reordering. Right: Performance of 4 techniques for computing its 8 smallest eigenvalues

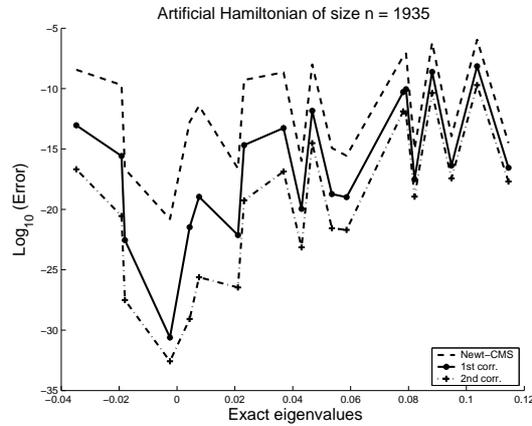


Figure 7: Performance of Newton-CMS and two the results of two corrective steps of Algorithm 3.1. The 20 lowest eigenvalues are computed.

## 5 Summary and Conclusion

We have discussed a few variants of certain algorithms based on the correction equation for solving eigenvalue problems and we showed how they can be adapted in a domain decomposition framework. In particular, block variants of the correction equation were derived by viewing the eigenvalue problem as a system of nonlinear equations. The resulting algorithms converge cubically or quadratically but they require the solution of a different Sylvester equation at each step. In the case of CMS, experiments show that it is possible to obtain good improvements by versions of these algorithms which do not require to refactor the matrix at each step.

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