Computation of Smallest Eigenvalues using Spectral Schur Complements *

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Abstract

The Automated Multilevel Substructing method (AMLS) was recently presented as an alternative to well-established methods for computing eigenvalues of large matrices in the context of structural engineering. This technique is based on exploiting a high level of dimensional reduction via domain decomposition and projection methods. This paper takes a purely algebraic look at the method and explains that it can be viewed as a technique based on a first order approximation to a nonlinear eigenvalue problem. A 'corrective projection' viewpoint leads us to explore variants of the method which use Krylov subspaces instead of eigenbasis to construct subspaces of approximants. The nonlinear eigenvalue problem viewpoint yields a second order approximation as an enhancement to the first order technique inherent to AMLS. Numerical experiments are presented to validate the approaches presented.

1 Introduction

The numerical solution of large sparse symmetric eigenvalue problems continues to be at the forefront of current research in scientifi c computing. In the last few decades, projection methods such as the Lanczos algorithm and its variants, have dominated the scene. For example, a block version of this method combined with shift-and-invert [7], whereby the problem $Ku = \lambda Mu$ is replaced by $(K - \sigma M)u = (\lambda - \sigma)Mu$, is used in major commercial structural engineering packages such as MCS.NASTRAN [10]. ARPACK [12], a package based on an implicitly restarted Arnoldi/Lanczos process, is currently the best known public-domain eigenvalue package for large eigenvalue problems.

The Lanczos process scales poorly with the number of eigenvalues to be computed, because of the need to orthogonalize large Krylov bases. In recent years, an alternative approach has emerged in structural engineering which has been reported to be superior to the standard shift-and-invert Lanczos approach. The algorithm, called Automated Multilevel Substructuring method (AMLS) is rooted in a domain decomposition framework. It has been reported as being capable of computing thousands of the smallest normal modes of dynamic structures on commodity workstations and of being orders of magnitude faster than the standard approach [11].

The paper [3] presents a theoretical framework for the algorithm from the point of domain decomposition, using adequate functional spaces and operators on them. The goal of our paper is to present a different, yet complementary viewpoint, which is entirely algebraic. AMLS is essentially a Schur complement method. Schur complement techniques are well understood for solving linear systems and play a major role in Domain Decomposition techniques [15, 16]. Relatively speaking, the formulation of this method for eigenvalue problems has been essentially neglected so far. One could of course extend the approach used for linear systems in order to compute eigenvalues, by formulating a Schur complement problem for each different eigenvalue, (e.g., by solving the eigenvalue problem as a sequence of linear systems through shift-and-invert). A more complete framework was suggested in early work by Abramov [1, 2] and Chichov [5].

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These authors presented what may termed a spectral Schur complement method. It can easily be verified that a scalar λ is an eigenvalue of a matrix A partitioned as

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix}$$

if and only if it is an eigenvalue of $S(\lambda) = C - E(B - \lambda I)^{-1}F$ (this is clearly restricted to those λ's that are not in the spectrum of B). This nonlinear eigenvalue problem may be solved by a Newton-type approach. Alternatively, one can also devise special iterative schemes based on the above observation. An approach of this type is clearly limited by the fact that a Schur complement (or several consecutive ones in an iterative process) is required for each different eigenvalue. It can, however, work well for computing one, or a few, eigenvalues or in some other special situations. For example, this nonlinear viewpoint led to the development of effective shifts of origin for the QR algorithm for tridiagonal matrices [14] (see also Parlett [13]).

The fundamental premise of AMLS, and its attraction, is that it is capable of extracting very good approximations *with only one Schur complement*. To achieve this, AMLS relies heavily on projection techniques. It builds good bases from one Schur complement, and expands them in an effective way to bigger and bigger domains.

This paper will begin with a brief overview of AMLS and an introduction of the notation. It will then introduce spectral (or nonlinear) Schur complements, and explore their relations to AMLS. With this relation established, two enhancements of the basic AMLS scheme are presented. The first introduces Krylov subspaces to the technique, and the second considers a more accurate (second order instead of first order) scheme.

2 The AMLS approach

Let $A \in \mathbb{C}^{n\times n}$ be a Hermitian matrix,

$$A = \begin{pmatrix} B & E \\ E^* & C \end{pmatrix}, \tag{1}$$

such that $B \in \mathbb{C}^{(n-p)\times(n-p)}$, $C \in \mathbb{C}^{p\times p}$ and $E \in \mathbb{C}^{(n-p)\times p}$. Consider the linear eigenvalue problem $A\tilde{u} = \lambda\tilde{u}$, which can be written as,

$$\begin{pmatrix} B & E \\ E^* & C \end{pmatrix} \begin{pmatrix} \tilde{u}^B \\ \tilde{u}^S \end{pmatrix} = \lambda \begin{pmatrix} \tilde{u}^B \\ \tilde{u}^S \end{pmatrix}, \tag{2}$$

where $\tilde{u}^B \in \mathbb{C}^{n-p}$ and $\tilde{u}^S \in \mathbb{C}^p$. Component Mode Synthesis (CMS) is a classical technique in structural dynamics for the computation of the smallest normal modes of a structure [6, 8]. In CMS, a structure is typically approximated by a discrete domain Ω which is then decomposed into several substructures separated by an interface Γ. Each of the substructures is approximated by a sumdomain $\Omega_i \subset \Omega$. Notice that the subdomains Ω_i can either overlap or not. In this paper we consider only the latter case. Thus, the unknowns in the interior of each subdomain Ω_i are completely decoupled from the unknowns in all other subdomains. Coupling among substructures is represented by the unknowns on the interface Γ and the unknowns in each Ω_i that are adjacent to Γ. Figure 1 provides a graphical illustration in the simplest case of two subdomains.

Consider now the simple model problem:

$$-\nabla^2\tilde{u} = \lambda\tilde{u} \tag{3}$$

on a rectangular domain Ω. If we employ a standard 5-point stencil centered differences discretization of (3) and count the unknowns in the subdomains Ω_i first and the unknowns on Γ last, then (2) is the algebraic eigenvalue problem that arises from the discretization of (3). Notice that matrix B contains the unknowns

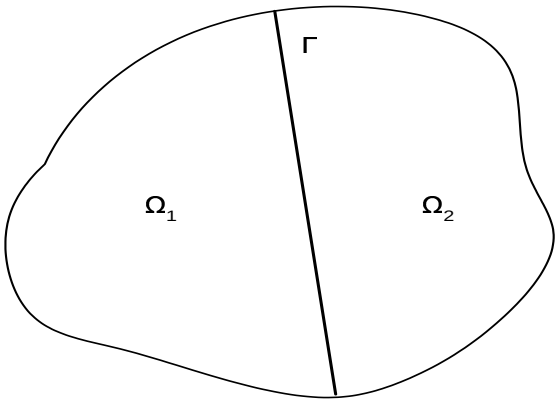

Figure 1: The simple case of two subdomains Ω_1, Ω_2 and an interface Γ.

across the domains Ω_i, C contains the unknowns on the interface Γ and E contains the coupling between the unknowns in B and C. Furthermore, since the unknowns in the domains Ω_i are decoupled, B will be block diagonal.

The idea of CMS is to begin by solving the problem $Bv = \mu v$. Since B is block diagonal, this is equivalent to solving each of the decoupled smaller eigenvalue problems corresponding to each subdomain Ω_i (in parallel). Then, CMS injects additional vectors to account for the coupling among subdomains. This is done invoking a carefully selected operator for the interface nodes.

Recently, Bennighof and Lehoucq [3], have presented an automated multilevel substructuring method (AMLS), that extends the basic framework of CMS in a multilevel method, capable of computing thousands of the smallest normal modes of structures on commodity workstations. AMLS was reported to be orders of magnitude faster than competitive commercial software based on the traditional shift-and-invert Lanczos approach [11].

Consider the matrix

$$U = \begin{pmatrix} I & -B^{-1}E \\ 0 & I \end{pmatrix}, \tag{4}$$

which is a block Gaussian eliminator for matrix (1), selected so that

$$U^*AU = \begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix},$$

where S is the Schur complement

$$S = C - E^*B^{-1}E. \tag{5}$$

We now consider the application of AMLS for only a single level of subdivision. The original problem (2) is replaced by the equivalent generalized eigenvalue problem $U^*AUu = \lambda U^*Uu$, which can be written as

$$\begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} u^B \\ u^S \end{pmatrix} = \lambda \begin{pmatrix} I & -B^{-1}E \\ -E^*B^{-1} & M_S \end{pmatrix} \begin{pmatrix} u^B \\ u^S \end{pmatrix}, \tag{6}$$

where $M_S = I + E^*B^{-2}E$. AMLS computes approximations to the eigenvalues and eigenvectors of the original problem by means of a projection method applied to the generalized problem (6). The subspace of

approximants is constructed from eigenvectors of a version of (6) in which the coupling in the right-hand side matrix (i.e., U^*U) is ignored. This gives the two decoupled eigenvalue problems:

$$Bv = \mu\, v \tag{7}$$
$$Sw = \eta\, M_S w. \tag{8}$$

Once the desirable eigenpairs have been obtained from (7–8), they are utilized in a projection method (Rayleigh-Ritz) applied to the original problem (6). The basis used for this projection is of the form

$$\left\{ \hat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad i = 1, \ldots, m_B; \qquad \hat{w}_j = \begin{pmatrix} 0 \\ w_j \end{pmatrix} \quad j = 1, \ldots, m_S \right\},$$

where $m_B < (n-p)$ and $m_S < p$. It is important to note that the projection is applied to (6) rather than to the original problem (2). There is an inherent change of basis between the two and, for reasons that will become clear later, the basis $\{\hat{v}_i\}_i, \{\hat{w}_j\}_j$, is well suited for the transformed problem rather than the original one.

The essence of AMLS is to "solve the problem (6) without the coupling and then use some eigenvectors obtained to solve the problem with its coupling". It is interesting to note that a very similar idea is utilized with great success in structural engineering: to solve a problem related to a dynamical system, one first obtains the modes of the problem without damping, then uses these modes to define a subspace in which the full problem (with damping) is solved. We refer to Algorithm 2.1 for an algorithmic description of AMLS for one level of subdivisions (SPD stands for symmetric positive definite matrices). In the multilevel case, this algorithmic step is applied recursively for every subdomain of the original domain. Observe that in practice the block Gaussian eliminator matrix U (line 4) is not formed. Instead, Gaussian elimination is applied to compute the Schur complement S and the matrix M_S, since

$$U^*U = \begin{pmatrix} I & -B^{-1}E \\ E^*B^{-1} & M_S \end{pmatrix}.$$

In this paper we are interested in an analysis of the basic approximation mechanism of AMLS. This analysis will serve to devise a few improvements to the basic method. For simplicity, our study will be restricted to the single level of subdomains.

ALGORITHM **2.1** AMLS **for a single level of subdomains**

Input: SPD matrix $A \in \mathbb{C}^{n\times n}$, integers $n_B < n$, $m_S < n$
and n_e (number of eigenvalues sought)
Output: The n_e smallest eigenvalues of A

1. *Define* $\mathtt{B} = \mathtt{A}(1:\mathtt{n_B}, 1:\mathtt{n_B})$, $\mathtt{C} = \mathtt{A}(\mathtt{n_B}+1:\mathtt{end}, \mathtt{n_B}+1:\mathtt{end})$
   and $\mathtt{E} = \mathtt{A}(1:\mathtt{n_B}, \mathtt{n_B}+1:\mathtt{end})$
2. *Compute Cholesky factorization $R^*R = B$*
3. *Compute Schur complement $S = C - E^*B^{-1}E$ (using the factor R)*
4. *Define $U = [I, -B^{-1}E; 0, I]$*
5. *Compute $M_S = I + (E^*B^{-1})(B^{-1}E)$ (using the factor R)*
6. *Compute m_S smallest eigenvalues of $Su_j^S = M_S u_j^S$*
   and set $U_S = [u_1^S, \ldots, u_{m_S}^S]$
7. *Compute m_B smallest eigenvalues and corresponding eigenvectors V_B of B*
7. *Define the matrix $Z = [V_B, 0; 0, U_S]$*
8. *Compute the n_e smallest eigenvalues of $(Z^*U^*AUZ)x = (Z^*U^*UZ)x$*

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3 Spectral Schur complements

The following equations result from (6)

$$\begin{aligned} Bu^B &= \lambda(u^B - B^{-1}Eu^S), \quad (9)\\ Su^S &= \lambda(-E^*B^{-1}u^B + M_S u^S). \quad (10)\end{aligned}$$

Assuming that λ is not an eigenvalue of B we can substitute (9) into (10) to obtain

$$Su^S = \lambda\left(\lambda E^*B^{-1}(B-\lambda I)^{-1}B^{-1}Eu^S + M_s u^S\right),$$

which results in the equivalent nonlinear eigenvalue problem

$$\left[S - \lambda\left(E^*B^{-2}E\right) - \lambda^2 E^*B^{-1}(B-\lambda I)^{-1}B^{-1}E\right]\ u^S \ = \ \lambda u^S. \quad (11)$$

Rewriting the above problem in an expanded notation we obtain the following nonlinear eigenvalue problem

$$\left[C - E^*B^{-1}(B + \lambda I + \lambda^2(B-\lambda I)^{-1})B^{-1}E\right]u^S = \lambda u^S. \quad (12)$$

We can show that the above problem is equivalent to a nonlinear eigenvalue problem involving the spectral Schur complement

$$S(\lambda) = C - E^*(B-\lambda I)^{-1}E. \quad (13)$$

The first resolvent equality (see [9]),

$$(B-\lambda I)^{-1} - B^{-1} = \lambda(B-\lambda I)^{-1}B^{-1}$$

can be substituted in the expression of the left hand matrix in (12) which we denote by $\hat{S}(\lambda)$,

$$\begin{aligned} \hat{S}(\lambda) &= C - E^*B^{-1}\left(I + \lambda B^{-1} + \lambda(B-\lambda I)^{-1} - \lambda B^{-1}\right)E\\ &= C - E^*\left(B^{-1} + \lambda B^{-1}(B-\lambda I)^{-1}\right)E\\ &= C - E^*\left(B^{-1} - B^{-1} + (B-\lambda I)^{-1}\right)E\\ &= C - E^*(B-\lambda I)^{-1}E\\ &= S(\lambda).\end{aligned}$$

In fact, the Schur complement S can be viewed as the first term of the Taylor series expansion of $S(\lambda)$ with respect to λ around $\lambda = 0$. The standard expansion of the resolvent (see [9])

$$(B-\lambda I)^{-1} = B^{-1}\sum_{k=0}^{\infty}(\lambda B^{-1})^k = \sum_{k=0}^{\infty}\lambda^k B^{-k-1}, \quad (14)$$

leads to the following series for $S(\lambda)$

$$\begin{aligned} S(\lambda) &= C - E^*\sum_{k=0}^{\infty}(\lambda^k B^{-k-1})E\\ &= C - E^*\left(B^{-1} + \lambda B^{-2} + \lambda^2 B^{-3} + \ldots\right)E. \quad (15)\end{aligned}$$

In AMLS the nonlinear eigenvalue problem (12) is approximated by the generalized eigenvalue problem

$$Su^S = \lambda M_S u^S, \quad (16)$$

which, after some algebraic manipulation, leads to the equations

$$\left(C - E^*(B^{-1} + \lambda B^{-2})E\right) u^S = \lambda u^S. \tag{17}$$

This can be considered as a truncated version of the original nonlinear problem (12), where we ignore the terms $\lambda^k B^{-k-1}$ for $k \geq 2$ in the expansion of the resolvent $(B - \lambda I)^{-1}$. This observation immediately leads to some possible suggestions on how to improve the approximation by including additional terms of the infinite expansion. Section 5 will describe a second order approximation to (12) obtained by adding the term $\lambda^2 B^{-3}$. We begin by analyzing how AMLS expands the approximation of the lower part u^S to an approximation $[u^B; u^S]^*$ of an eigenvector of the complete problem (6).

4 The projection view-point

Consider again the nonlinear Schur complement (13). The eigenvalues of the original problem, which do not belong to the spectrum of B, can be obtained from those of the nonlinear eigenvalue problem

$$S(\lambda)x = \lambda x.$$

Proposition 4.1 *Let λ, u^S be an eigenpair of the nonlinear eigenvalue problem (11), i.e., such that:*

$$S(\lambda)u^S = \lambda u^S$$

Then, λ is an eigenvalue of (2) with associated eigenvector:

$$\begin{pmatrix} -(B - \lambda I)^{-1} E u^S \\ u^S \end{pmatrix} \tag{18}$$

Proof. The proof consists of a simple verification. ■

Now assume that we have a good approximation to the nonlinear Schur complement problem, i.e., to a solution λ and u^S of the nonlinear problem (11). It is clear that the best we can do to retrieve the corresponding eigenvector of (2) is to use substitution, i.e., to compute the top part of (18):

$$u^B = -(B - \lambda I)^{-1} E u^S, \tag{19}$$

which will give us the top part of the exact eigenvector. This entails factoring the matrix $(B - \lambda I)$ for each different eigenvalue λ, which is not practical. As was seen in the previous section, AMLS extracts an approximation to the nonlinear problem (11) by solving the generalized eigenvalue problem (17) and then it replaces the substitution step (19) by a projection step. Specifically, once an approximate pair λ, u^S is obtained, AMLS computes approximate eigenvectors to the original problem by a projection process using the space spanned by the family of vectors:

$$\left\{ \begin{pmatrix} v_i^B \\ 0 \end{pmatrix} \right\}, \qquad \left\{ \begin{pmatrix} -B^{-1} E u_j^S \\ u_j^S \end{pmatrix} \right\}, \tag{20}$$

in which v_i^B are eigenvectors of B associated with its smallest eigenvalues. Note that these two sets of vectors are of the form $U \begin{pmatrix} v_i^B \\ 0 \end{pmatrix}$, for the first, and $U \begin{pmatrix} 0 \\ u_j^S \end{pmatrix}$ for the second, where U was defined earlier by Equation (4). The question is: why is this a good way to replace the substitution step (19)? Another issue is the quality we might expect from this process.

Ideally, the prolongation matrix U should be replaced by one which depends on the eigenvalue λ, namely

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

Indeed, if we were to use the prolongator $U(\lambda)$ instead of U, then $U(\lambda)\begin{pmatrix} 0 \\ u_j^S \end{pmatrix}$ would be an exact eigenvector. Of course, it is not practical to use a different prolongator $U(\lambda)$ for each different eigenvalue λ. What is interesting and important to note is that $U(\lambda)$ and U are likely to be close to each other for small (in modulus) eigenvalues λ. Furthermore, *the difference between the two consists mostly of components related to eigenvectors of B which are associated with eigenvalues close to λ*. It is helpful to examine this difference

$$\begin{aligned}[U(\lambda) - U]\begin{pmatrix} 0 \\ u^S \end{pmatrix} &= \begin{pmatrix} 0 & -((B-\lambda I)^{-1} - B^{-1})E \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ u^S \end{pmatrix} \\ &= \begin{pmatrix} -\lambda\,(B-\lambda I)^{-1}B^{-1}Eu^S \\ 0 \end{pmatrix}.\end{aligned}$$

In order to compensate for this difference, it is natural to add to the subspace eigenvectors of B in which this difference will have large components, i.e., those closest to zero. This is at the heart of the approximation exploited by AMLS which incorporates the first set in (20). Let us assume that we have the expansion in the eigenbasis of B

$$Eu^S = \sum_k^{N_B} \alpha_k v_k, \tag{21}$$

where $N_B = n - p$ is the dimension of B. Let $\hat{u}^B$ be the B-part of the approximation provided by AMLS. Then

$$u^B - \hat{u}^B = -\lambda\,(B-\lambda I)^{-1}B^{-1}\,Eu^S = \sum_k^{N_B} \frac{\lambda\alpha_k}{(\mu_k - \lambda)\mu_k} v_k.$$

As expected, when $\lambda = 0$, the projection process will yield exact eigenvectors. The error in the eigenvector of (2) will be of the order of the distance between the above vector and the space spanned by the added eigenvectors of B. If we call X^B the restriction to the B-part of the space of approximants, then

$$\begin{aligned} dist(u^B, X^B) &= \min_{v \in \mathtt{span}\,(v_1,\ldots,v_{m_B})} \|u^B - \hat{u}^B - v\|_2 \\ &= |\lambda| \left(\sum_{k>m_B}^{N_B} \frac{|\alpha_k|^2}{|\mu_k - \lambda|^2\,|\mu_k|^2} \right)^{1/2}, \end{aligned}$$

and therefore

$$dist(u^B, X^B) \leq \max_{k>m_B} \frac{|\lambda|}{|\mu_k - \lambda||\mu_k|} \|Eu^S\|_2. \tag{22}$$

Under the mild assumption that $\lambda < \mu_{m_B}$, it is clear that

$$dist(u^B, X^B) \leq \frac{|\lambda|}{|\mu_{m_B} - \lambda||\mu_{m_B}|} \|Eu^S\|_2. \tag{23}$$

Note that for $\lambda \ll \mu_{M_B}$, we will have $dist(u^B, X^B) \approx O(|\lambda/\mu_{M_B}^2|)$.

5 Higher degree approximations

In Section 3 it was explained that AMLS approximates the nonlinear eigenvalue problem (12) by the generalized eigenvalue problem (16). In particular, this problem can be seen as a truncated, first order approximation of (12). Let us now consider a second order approximation obtained by solving the quadratic eigenvalue problem

$$\left[\lambda^2 E^* B^{-3} E + \lambda\left(I + E^* B^{-2} E\right) - S\right] u^S \;=\; 0. \tag{24}$$

This problem can be solved by a linearization which leads to an equivalent generalized eigenvalue problem (see for example [17])

$$\begin{pmatrix} 0 & I \\ S & -K \end{pmatrix} \begin{pmatrix} u^S \\ \lambda u^S \end{pmatrix} = \lambda \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix} \begin{pmatrix} u^S \\ \lambda u^S \end{pmatrix}, \tag{25}$$

where $K = I + E^*B^{-2}E$ and $R = E^*B^{-3}E$.

In Section 4 we showed that adding eigenvectors of B to the space of approximants can improve the basic approximation provided by the nonlinear Schur complement. In order for the eigenvectors provided by this approximation to fit in well with the projection step, we need to modify this step so that the terms $-(B - \lambda I)^{-1}Eu^S$ are well approximated. One way to achieve this is to add more eigenvectors of B. However, a more relevant alternative in this case is to add a third set of vectors to the basis of approximants (20), namely the set:

$$\left\{ \begin{pmatrix} -B^{-2}Eu_j^S \\ u_j^S \end{pmatrix} \right\}.$$

To this end, we construct the matrix

$$Z = \begin{pmatrix} V_B & -B^{-1}EU_S & -B^{-2}EU_S \\ 0 & U_S & 0 \end{pmatrix}, \tag{26}$$

where V_B is a matrix of eigenvectors corresponding to the smallest eigenvalues of B and U_S is a matrix of eigenvectors associated with the smallest eigenvalues of (25), in modulus. We then solve the projected generalized eigenvalue problem

$$Z^* \begin{pmatrix} B & E \\ E^* & C \end{pmatrix} Z x = \lambda Z^* Z x. \tag{27}$$

Algorithm 5.1 illustrates a second order version of AMLS, based on this approach.

ALGORITHM **5.1 Second order** AMLS

Input: *SPD matrix $A \in \mathbb{C}^{n \times n}$, integers $n_B < n$, $m_S < n$ and n_e (number of eigenvalues sought)*

Output: *n_e of the smallest eigenvalues of A*

1. *Define* $\mathtt{B} = \mathtt{A}(1 : \mathtt{n_B}, 1 : \mathtt{n_B})$, $\mathtt{C} = \mathtt{A}(\mathtt{n_B} + 1 : \mathtt{end}, \mathtt{n_B} + 1 : \mathtt{end})$ *and* $\mathtt{E} = \mathtt{A}(1 : \mathtt{n_B}, \mathtt{n_B} + 1 : \mathtt{end})$
2. *Compute Cholesky factorization $R^*R = B$*
3. *Compute Schur complement $S = C - E^*B^{-1}E$ (using the factor R)*
4. *Compute $K = I + (E^*B^{-1})(B^{-1}E)$ and $R = (E^*B^{-1})B^{-1}(B^{-1}E)$ (using the factor R)*
5. *Compute m_S smallest in modulus eigenvalues and eigenvectors U_S of (24) by solving (25)*
6. *Compute m_B smallest eigenvalues and eigenvectors V_B of B*
7. *Define the matrix Z as in (26)*
8. *Compute the n_e smallest eigenvalues of $(Z^*AZ)x = (Z^*Z)x$*

Consider now the effect of this addition. We are looking again at the distance between u^B and the closest vector from the space of approximants X^B. Consider the vector $u^{(2)} = -B^{-2}Eu^S$. Assuming that the expansion (21) is available, then

$$u^B - \tilde{u}^B - \lambda u^{(2)} = -\lambda^2 \left(B - \lambda I\right)^{-1} B^{-2} \, Eu^S = \sum_k^{N_B} \frac{\lambda^2 \alpha_k}{(\mu_k - \lambda)\mu_k^2} v_k.$$

Therefore, the distance of u^B from the space of approximants X^B is such that

$$\begin{aligned} dist(u^B, X^B) &= \min_{v \in \mathtt{span}\{V_B\}} \|u^B - \tilde{u}^B - \lambda u^{(2)} - v\|_2 \\ &= |\lambda|^2 \left(\sum_{k>m_B}^{N_B} \frac{|\alpha_k|^2}{|\mu_k - \lambda|^2 \, |\mu_k|^4} \right)^{1/2} \end{aligned}$$

and therefore,

$$dist(u^B, X^B) \leq \max_{k>m_B} \frac{|\lambda|^2}{|\mu_k - \lambda||\mu_k|^2} \|Eu^S\|_2. \tag{28}$$

Under the mild assumption that $\lambda < \mu_{m_B}$, we have the bound

$$dist(u^B, X^B) \leq \frac{|\lambda|^2}{|\mu_{m_B} - \lambda||\mu_{m_B}|^2} \|Eu^S\|_2. \tag{29}$$

A comparison with the bound (23) for the first order approximation, indicates that one may expect a good improvement. Numerical experiments in Section 7 will verify this prediction.

6 Expanding the projection space with Krylov subspaces

Section 4 described AMLS as a projection technique which uses expanded subspaces of the form (20) to extract Ritz values and vectors. We denote by $\mathcal{V}_S$ the subspace

$$\mathcal{V}_S = \mathtt{span} \left\{ \begin{pmatrix} -B^{-1}Eu_j^S \\ u_j^S \end{pmatrix} \right\}, \tag{30}$$

where u_j^S are eigenvectors of the generalized eigenvalue problem (10). In this section we propose a different approach that is based, however, on similar reasoning. Observe that, ideally, the top part of $\mathcal{V}_S$ should be $-(B - \lambda I)^{-1} E u_j^S$. Therefore, instead of attempting to compensate for the difference $(B - \lambda I)^{-1} - B^{-1}$, we can approximate the resolvent $(B - \lambda I)^{-1}$ itself. The key is to expand the subspace $\mathcal{V}_S$ with the vectors $[V_\mathcal{K}; 0]$, where $V_\mathcal{K}$ is an orthonormal basis for the Krylov subspace $\mathcal{K}_m(B^{-1}, EU_S)$ and U_S is a matrix of approximate eigenvectors of (10). Algorithm 6.1 is a description of a method based on this approach, which will be subsequently called Krylov AMLS. Observe, that as in standard AMLS the block Gaussian eliminator matrix U (line 4) is never formed. Instead, a Gaussian elimination process is applied directly on its matrix arguments.

ALGORITHM **6.1 Krylov** AMLS

Input: SPD matrix $A \in \mathbb{C}^{n \times n}$, integers $n_B < n$, $m_S < n$, m_K and n_e (number of eigenvalues sought)

Output: n_e of the smallest eigenvalues of A

1. *Define* $\mathtt{B} = \mathtt{A}(1 : \mathtt{n_B}, 1 : \mathtt{n_B})$, $\mathtt{C} = \mathtt{A}(\mathtt{n_B} + 1 : \mathtt{end}, \mathtt{n_B} + 1 : \mathtt{end})$ *and* $\mathtt{E} = \mathtt{A}(1 : \mathtt{n_B}, \mathtt{n_B} + 1 : \mathtt{end})$
2. *Compute Cholesky factorization* $R^*R = B$
3. *Compute Schur complement* $S = C - E^*B^{-1}E$ *(using the factor R)*
4. *Define* $U = [I, -B^{-1}E; 0, I]$
5. *Compute* $M_S = I + (E^*B^{-1})(B^{-1}E)$ *(using the factor R)*
6. *Compute m_S smallest eigenvalues of* $Su_j^S = M_S u_j^S$ *and set* $U_S = [u_1^S, \ldots, u_{m_S}^S]$
7. *Compute orthogonal basis V_K for the Krylov subspace* $\mathcal{K}_{m_K}(B^{-1}, EU_S)$
8. *Define the basis:* $Z_K = [V_K, 0; 0, U_S]$
9. *Compute the n_e smallest eigenvalues of* $(Z_K^* U^* A U Z_K)x = (Z_K^* U^* U Z_K)x$

For simplicity, we examine the case where U_S has just one column. Observe that since $B^{-1}Eu_j^S \in \mathcal{K}_m(B^{-1}, Eu_j^S)$, the error in the eigenvector of (2) will be of the order of the distance

$$\|(B-\lambda I)^{-1}Eu_j^S - u\|, \quad \text{where} \quad u \in \mathcal{K}_m(B^{-1}, Eu_j^S).$$

Note that $u = P_m(B^{-1})Eu_j^S$ for a certain polynomial P_m of degree $m-1$. If X^B denotes again the restriction to the B-part of the space of approximants, then expanding the resolvent $(B-\lambda I)^{-1}$ yields,

$$dist(u^B, X^B) = \min_{\xi_k} \left\| (\sum_{k=0}^{\infty} \lambda^k B^{-k-1} - \sum_{k=0}^{m-1} \xi_k B^{-k}) Eu_j^S \right\| .$$

Thus if $\mu_{\min}$ is the smallest eigenvalue of B

$$dist(u^B, X^B) \leq \frac{1}{\mu_{\min} - \lambda} \left(\frac{\lambda}{\mu_{\min}} \right)^{m-1} \|Eu_j^S\|. \tag{31}$$

Therefore, if the ratio $\lambda/\mu_{\min}$ is small, then we can expect a very small distance $\|(B-\lambda I)^{-1}Eu^S - \mathcal{K}_m(B^{-1}, Eu_j^S)\|$. However, in practice we only have approximations to the eigenvalues and eigenvectors of the generalized eigenvalue problem (10) (our spectral Schur complement). Using a sufficiently large dimension m for the Krylov subspace $\mathcal{K}_m(B^{-1}, E\hat{u}_j^S)$ it is possible to extract good approximations to u_j^B.

The bound (31) justifies the use of the block Krylov subspace $\mathcal{K}_m(B^{-1}, EU_S)$, where U_S is a matrix of eigenvectors u_j^S of (10). Numerical experiments in Section 7 will confirm that using block Krylov subspaces will result in significantly improved approximations relative to the approximations of standard AMLS.

7 Numerical Experiments

The goal of the numerical tests described in this section is to verify the theoretical predictions of Sections 4, 5, and 6.

7.1 AMLS and Krylov AMLS

Bounds (23) and (31) suggest that if the smallest eigenvalue $\mu_{\min}$ of B is much larger than the smallest eigenvalue λ of matrix A, then the Krylov subspace framework in AMLS will yield better results than standard AMLS. We tested this prediction in the following experiment. The test matrix is BCSSTK11 from the Harwell-Boeing collection (availale from the matrix market, see [4]). This is a symmetric positive definite matrix of size $n = 1,473$, which has nnz=34241) nonzero entries. The matrix was symmetrically reordered using the nested dissection graph partitioning algorithm so that the matrix B will have block diagonal structure with two blocks (corresponding to two subdomains).

Figure 2 illustrates the non-zero structure of the matrix before (left) and after the partitioning (right). The sizes of the resulting two blocks of B are $n_1 = 696$ and $n_2 = 683$. The smallest eigenvalue of the matrix is $\lambda \approx 2.9641$ and the smallest eigenvalue of B is $\mu_{\min} \approx 40.3973$, so that $\lambda/\mu_{\min} \approx 0.0734$. We computed the five smallest eigenvalues and respective eigenvectors u_j^S, $j = 1, \ldots, 5$ of the generalized Schur eigenvalue problem (8). We then computed the $k = 10, 20, 30$ and 40, smallest eigenvalues and corresponding eigenvectors of the block diagonal simple eigenvalue problem (7). For the Krylov subspace framework in AMLS, we computed a basis for the block Krylov subspace $\mathcal{K}_m(B^{-1}, EU_S)$, where the columns of U_S are the eigenvectors u_j^S, for $m = 2, 4, \ldots, 8$. Figure 3 illustrates the absolute relative error obtained for the 5 smallest eigenvalues of the matrix for the selected values of k and m. We selected the values of m and k so that the dimension of the projection space will be equal in all cases. Observe that Krylov AMLS outperforms standard AMLS in all cases except when the dimension of the Krylov subspace is

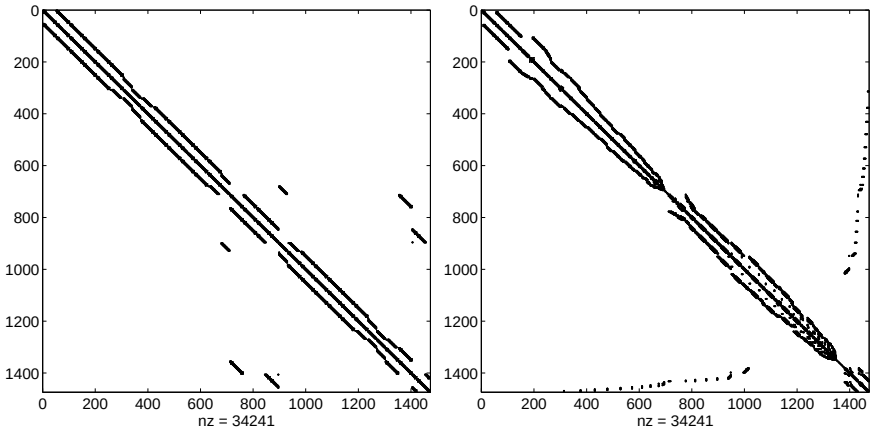

Figure 2: The non-zero structure of matrix BCSSTK11 before (left) and after (right) the nested dissection partitioning.

very small. It is interesting to note that Krylov AMLS for $m = 4$ (20 added vectors to the subspace $\mathcal{V}_S$ (30)) clearly outperforms standard AMLS for $k = 40$ (40 added eigenvectors of B).

We now consider the case where the ratio $\lambda/\mu_{\min}$ is close to 1. Observe that from interlacing properties of eigenvalues of Hermitian matrices, this ratio cannot be larger than 1. For this reason, we now omit to perform the nested dissection partitioning of the original matrix. As in the previous case we select the size of B to be $n_B = n_1 + n_2 = 1,379$. In this case $\mu_{\min} \approx 3.3975$ and thus $\lambda/\mu_{\min} \approx 0.8724$. Figure 4 illustrates the absolute relative error obtained for the 5 smallest eigenvalues of the matrix for the same span of values of k and m as in the previous experiments. It is clear that in this case the gains of the Krylov AMLS framework compared to standard AMLS are not as compelling as when the ratio $\lambda/\mu_{\min}$ is much smaller than 1.

7.2 Experiments with second order AMLS

To test the second order AMLS which was described in Section 5, we used matrix BCSSTK11, reordered as in the previous experiment. The second order polynomial eigenvalue problem (24) is solved via the linearized problem (25). We first show that we are able to retrieve improved approximations to the smallest eigenvalues of the nonlinear Schur eigenvalue problem (13) by means of the second order method. Figure 5 illustrates the absolute relative error for the approximations of the five smallest eigenvalues of (13), which correspond to the five smallest eigenvalues of the original matrix. It is clear that the second order approximation produces improved approximations. We now use these approximations, and the corresponding eigenvectors, in the Rayleigh-Ritz projection with the basis (26).

For standard AMLS we used an increasing number m_B of added eigenvectors of B: $m_B = 20, 40, 60$ and 100. On the other hand, for the second order AMLS we used $m_B = 10$ eigenvectors of B and $m_S = 2 \times 10$ additional vectors: 10 for $B^{-1}EU_S$ and another 10 for $B^{-2}EU_S$. Thus, in all cases matrix U_S had 10 columns which are eigenvectors corresponding to the smallest eigenvalues (in modulus) of the quadratic eigenvalue problem (24). Figure 6 illustrates the results. The accuracies achieved by the second order method are significantly better than the standard method. Notice that even when we used $m_B = 100$ eigenvectors of B for standard AMLS, the error of the second order AMLS method was still in the order of the square of the error of standard AMLS.

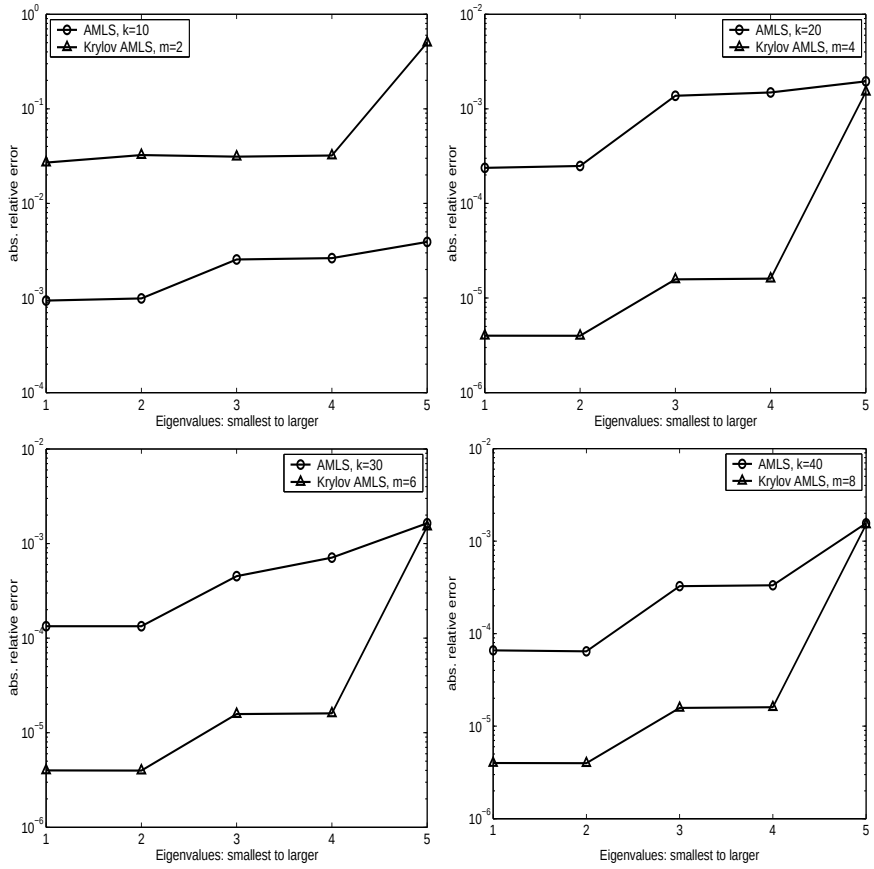

Figure 3: Relative errors for the five smallest eigenvalues of matrix BCSSTK11 computed, after a nested dissection reordering, by AMLS and Krylov AMLS for dimension of projection space equal to $k = 10, 20, ..., 40$.

7.3 Combining second order AMLS with Krylov subspaces

We now experiment with the combinations of second order AMLS with Krylov subspaces. Note that this entails computing a block Krylov subspace with B^{-1} rather than a set of eigenvectors of B (c.f. the algorithmic description in Algorithm 5.1). The test matrix we use results from a 5-point stencil discretization of the simple model problem (3) on the unit square, with $n_x = n_y = 30$ internal mesh nodes in each direction, so that the matrix size is $n = 900$. The matrix is reordered in order for the principal submatrix B to be block diagonal with two blocks and size $n_B = 840$. Initially, we are interested in the two smallest eigenvalues. We use five vectors in U_S, corresponding to the five smallest in modulus eigenvalues of (24). For second order AMLS we use ten eigenvectors of B, corresponding to its ten smallest eigenvalues, while in the block Krylov version we use $E[u_1^S, u_2^S]$ as starting vectors, where $u_j^S, j = 1, 2$ correspond to the two smallest in modulo eigenvalues of (24). We then compute a basis of length ten. Figure 7 (left) illustrates the results. It is clear that introducing Krylov basis vectors, instead of eigenvectors of B, yields improved results which are especially pronounced for the smallest eigenvalues. For larger eigenvalues however, the situation is reversed. This is due to the fact that the starting vectors of the block Krylov subspace are poor in directions towards $Eu_j^S, j = 3, \ldots$.

We then used five eigenvectors from (24) and computed a Krylov subspace of length twenty five. For comparison, we also augmented the eigenbasis in second order AMLS to a total of 25 eigenvectors. Figure 7 (right) illustrates the results. It is clear that in this case the additional starting vectors in the block Krylov

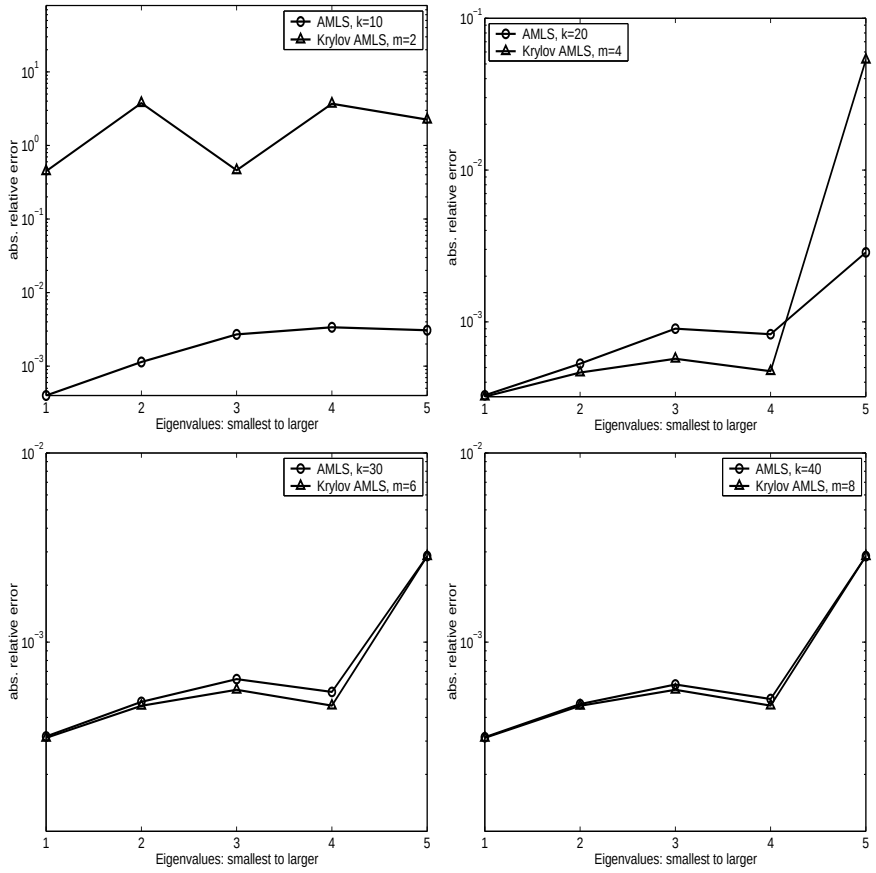

Figure 4: Relative errors for the five smallest eigenvalues of matrix BCSSTK11 computed, without a nested dissection reordering, by AMLS and Krylov AMLS for dimension of projection space equal to $k = 10, 20, ..., 40$.

subspace have a positive effect in improving the error for the corresponding largest eigenvalues, while the approximations for the two smallest eigenvalues remain practically unchanged. Compared to using eigenvectors of B, we observe that for the two smallest eigenvalues the block Krylov subspace approach remains superior, though the difference is not as pronounced as in the previous case. This is due to the increased length of the projection basis. On the other hand, for the larger eigenvalues we witness similar approximation for both approaches.

7.4 Combining AMLS and Krylov AMLS

An alternative type of combination occurs when in Krylov AMLS we augment the approximation subspace with eigenvectors of B that correspond to its smallest eigenvalues. The reasoning for such a combination is based on the fact that in order for the block Krylov subspace $\mathcal{K}_m(B^{-1}, EU_S)$ to adequately approximate the resolvent $(B - \lambda I)^{-1}$ for several different eigenvalues λ, without significantly increasing the Krylov steps m, we need to include many eigenvectors in the starting vectors matrix U_S. In an attempt to avoid this we can insert eigenvectors of B in the subspace as in standard AMLS. Thus, the projection matrix is

$$Z = \begin{pmatrix} V_B & V_K & 0 \\ 0 & 0 & U_S \end{pmatrix}, \tag{32}$$

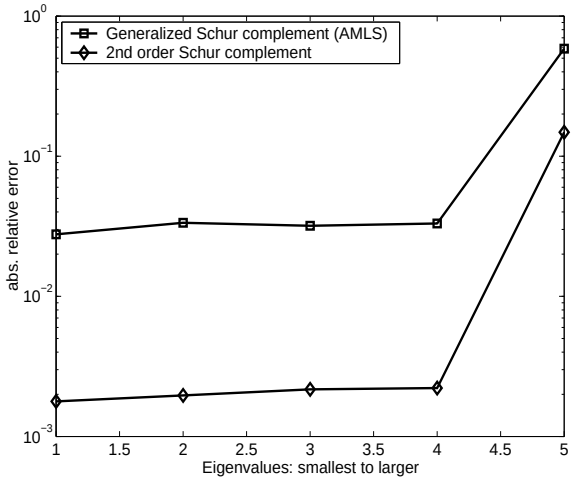

Figure 5: Absolute relative errors for the five smallest eigenvalues of matrix BCSSTK11 as they were approximated by the five smallest eigenvalues of (16) and by the five smallest, in modulus, eigenvalues of (25).

where V_B is a matrix of eigenvectors of B and V_K is an orthonormal basis for the block Krylov subspace. The projected eigenproblem is $(Z^*U^*AUZ)x = (Z^*U^*UZ)x$, where Z is as defined above and U is the block Gaussian eliminator matrix (4). In Figure (4) (top-right) we observe that it is possible that for the larger eigenvalues of the matrix, Krylov AMLS may be inferior to standard AMLS.

This is now explored further. We experimented with the same matrix as in the previous section (discretization of the model problem (3). Let again U_S contain eigenvectors corresponding to the five smallest eigenvalues of (16) and $V_\mathcal{K}$ be an orthonormal basis for $\mathcal{K}_m(B^{-1}, E[u_1^S, u_2^S])$ with $m = 5$. Thus $V_\mathcal{K}$ has ten columns. Let now V_B contain eigenvectors that correspond to the ten smallest eigenvalues of B. Figure 8 (left) illustrates the absolute relative errors for the approximations of the ten smallest eigenvalues of the original matrix as they were computed by standard AMLS and Krylov AMLS. In both cases the dimension of the projection space is equal to twenty. It is evident that for larger eigenvalues Krylov AMLS is inferior. This is due to the fact that the starting matrix $E[u_1^S, u_2^S]$ is very poor in directions corresponding to larger eigenvalues. We then added to Krylov AMLS ten eigenvectors of B, that correspond to its smallest eigenvalues. For comparison, in standard AMLS we use twenty eigenvectors of B, so that the dimension of the projection spaces would be equal to thirty in both cases. In the right plot of Figure 8 we illustrate the results. It is clear that we are able to obtain errors similar to standard AMLS for the larger eigenvalues, while we still obtain much better results for the smallest eigenvalues.

The practical application of the above hybrid will depend on the particular situation. A large block of initial vectors in Krylov AMLS will give very good accuracy, however with the analogous increase to the computational cost. Thus, adding eigenvectors of B may help keep this added cost moderate.

8 Conclusion

The AMLS algorithm can be viewed as a method which exploits a first order approximation to a nonlinear eigenvalue problem to extract a good subspace for a Rayleigh-Ritz projection process. This technique leads to approximations from a single Schur complement derived from a domain decomposition of the physical problem. Exploiting this observation, we have shown several possible enhancements to the original scheme. It is hoped that further improvements will be possible by exploiting similar approaches. For example, it would be interesting to explore the feasibility of an iterative scheme based on AMLS. Currently, AMLS is a one-shot algorithm in the sense that certain approximate eigenvectors are build from the last level up to

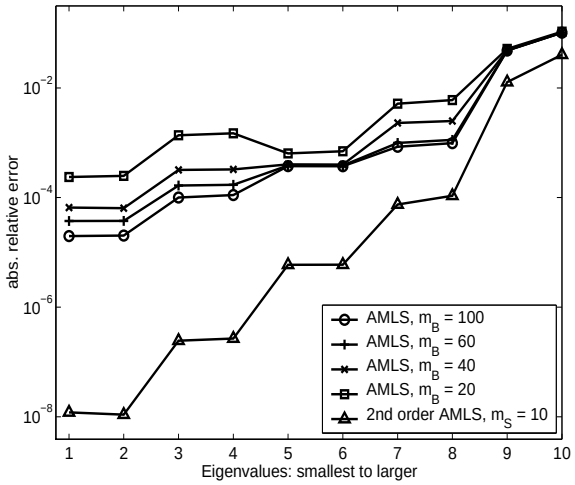

Figure 6: Absolute relative errors for the 10 smallest eigenvalues of matrix `BCSSTK11` computed by standard `AMLS` $(-\mathtt{o}-)$ and 2nd order `AMLS` $(-\triangle-)$.

the highest level and no further refinements are made. The current framework does not permit to iteratively refine these approximations. Yet, an analogy with the solution of linear systems tells us that this should be possible. This is important since the eigenvalues obtained in this manner do not always yield the high accuracy demanded in certain application areas.

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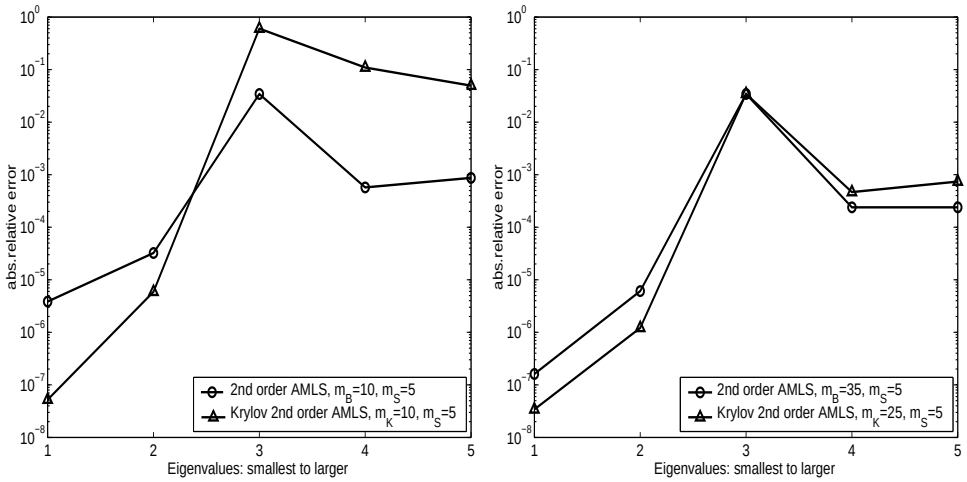

Figure 7: Absolute relative errors for the 5 smallest eigenvalues of (3) computed by second order AMLS (−o−) and 2nd order AMLS with block Krylov subspace (−△−).

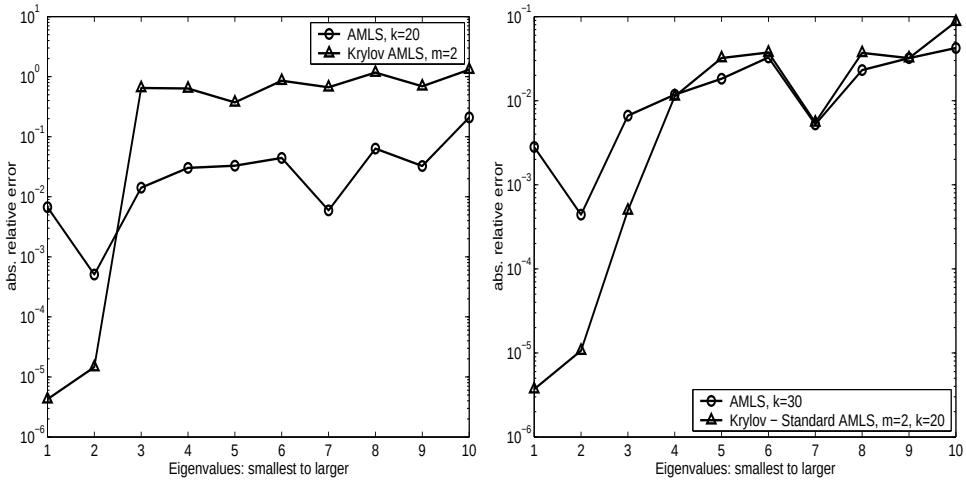

Figure 8: Left: Krylov AMLS (-△-) v.s. standard AMLS (-o-) for the model problem (3). Right: Combination of Krylov AMLS and AMLS (-△-) v.s. standard AMLS (-o-) for the model problem (3).

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