Multilevel Methods for Eigenspace Computations in Structural Dynamics

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Summary. Modal analysis of three-dimensional structures frequently involves finite element discretizations with millions of unknowns and requires computing hundreds or thousands of eigenpairs. We review in this paper methods based on domain decomposition for such eigenspace computations in structural dynamics. We distinguish approaches that solve the eigenproblem algebraically (with minimal connections to the underlying partial differential equation) from approaches that couple tightly the eigensolver with the partial differential equation.

1 Introduction

The goal of our paper is to provide a brief review of multilevel methods for eigenspace computations in structural dynamics. Our review is not meant to be exhaustive and so we apologize for relevant work not discussed. In particular, our interest is in multilevel algorithms for the numerical solution of the algebraic generalized eigenvalue problem arising from the finite element discretization of three-dimensional structures. Our interest is also restricted to methods that are scalable, both with respect to the mesh size and the number of processors of extremely large distributed-memory architectures. We start our paper by a formal discussion of the origin of the eigenvalue problem.

The dynamic analysis of a three-dimensional structure is modeled by the hyperbolic partial differential equation

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - \mathcal{E}(\mathbf{u}) = \mathbf{f}(t) \quad \text{in } \Omega \tag{1}$$

where $\mathbf{u}$ is the vector of displacements, $\mathcal{E}$ is a self-adjoint elliptic differential operator, ρ is the mass density, and $\mathbf{f}$ is a vector function for loading. We assume that appropriate homogeneous boundary and initial conditions are specified on the three-dimensional simply connected domain Ω.

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Structural dynamic analyses are usually divided into two categories: frequency response and transient simulation. In the former category, natural frequencies of the structure and their mode shapes are determined to verify their separation from frequencies of excitation or to compute the response from a given input force at a given location. In the second category, we study the motion of the structure and its time history under prescribed loads. For these dynamic response problems, several solution methods are available and we refer the reader to [16] and the references therein for an overview. Often, modal analysis is an effective solution method because, due to the orthogonality of the modes, modal superposition gives the solution. In addition, the frequency range of excitation is usually in the low end of the natural frequencies of the structure. Consequently, high frequency modes have a much lower participation in the response than lower modes and the contribution of high frequency modes can be neglected.

The vibration frequencies and mode shapes of the structure are solutions of the problem

$$-\mathcal{E}(\mathbf{u}) = \lambda\rho\mathbf{u} \quad \text{in } \Omega \tag{2}$$

with the same homogeneous boundary conditions as (1). The eigenvalue λ is the square of the natural frequency ω. A finite element discretization of the weak form of the vibrational problem (2) leads to the generalized eigenvalue problem

$$\mathbf{K}\mathbf{u}^h = \mathbf{M}\mathbf{u}^h\lambda^h \tag{3}$$

where $\mathbf{K}$ and $\mathbf{M}$ are the stiffness and mass matrices of order n respectively that represent the elastic and inertial properties of a structure. The parameter h is the characteristic mesh size. We assume a choice of boundary conditions such that both matrices are symmetric and positive definite.

Finite element discretizations of three-dimensional structures frequently involve well over one million unknowns and modal truncation requires often hundreds or thousands of eigenpairs. Consequently, computing these eigenpairs results in a challenging linear algebra problem. The remainder of our paper reviews two approaches that can be used to compute the needed modes. We will focus on techniques to compute eigenpairs in the low end of the spectrum for two reasons. First, the frequency range of excitation and the dominant modes for the structural response are in the low end of the natural frequencies. Secondly, standard results from finite element theory [3, 48] give the following *a priori* error estimates

$$\lambda \leq \lambda^h \leq \lambda(1 + Ch^2\lambda), \tag{4}$$

assuming sufficient regularity. These estimates imply that the finite element discretization represents more accurately the modes with small natural frequency.

Our paper is organized as follows. Section 2 describes algebraic approaches to solve the eigenvalue problem (3). Section 3 discusses variational methods tightly coupled to the partial differential operator $\mathcal{E}$.

2 Algebraic approach

A popular approach is to use a block Lanczos [26] code with a shift-invert transformation $(\mathbf{K} - \sigma\mathbf{M})^{-1}\mathbf{M}$. If σ is a real number, then the standard eigenvalue problem

$$(\mathbf{K}-\sigma\mathbf{M})^{-1}\mathbf{M}\mathbf{u}^h = \mathbf{u}^h\nu, \quad \left(\nu = \frac{1}{\lambda^h - \sigma}\right), \tag{5}$$

results by subtracting $\sigma\mathbf{M}$ from both sides of (3) followed by *cross-multiplication*. This standard eigenvalue problem is no longer symmetric. However, a careful choice of inner product renders the operator $(\mathbf{K}-\sigma\mathbf{M})^{-1}\mathbf{M}$ symmetric (for instance, the $\mathbf{M}$-inner product).

The Lanczos algorithm builds iteratively a basis for the Krylov subspace

$$\mathcal{K}_{m+1} = \text{span}\{\mathbf{x}_0, (\mathbf{K}-\sigma\mathbf{M})^{-1}\mathbf{M}\mathbf{x}_0, \cdots, [(\mathbf{K}-\sigma\mathbf{M})^{-1}\mathbf{M}]^m\mathbf{x}_0\} \tag{6}$$

to approximate the eigenpairs (see [20, 26, 34] for further details). At every Lanczos iteration, the action of $(\mathbf{K}-\sigma\mathbf{M})^{-1}$ on a vector or a block of vectors is required. Grimes et al. [26] solve the resulting set of linear equations by forward and backward substitution with the factors computed by a sparse direct factorization. However, performing sparse direct factorizations becomes prohibitively expensive when the dimension n is large or when the distributed-memory architecture has a large number of processors.

Other solutions are the following:

- replace the sparse direct method with a preconditioned iterative linear solver within the shift-invert Lanczos algorithm;
- replace the shift-invert Lanczos algorithm with a preconditioned eigenvalue algorithm.

These approaches are not new and we propose to review them.

For the first approach, most structural analysts choose a shift σ^*, $\sigma^* < \lambda_1^h$, so that the matrix $\mathbf{K}-\sigma^*\mathbf{M}$ is symmetric positive definite. This choice is motivated by the availability of scalable preconditioners for symmetric positive definite matrices. A scalable preconditioner for $\mathbf{K}-\sigma^*\mathbf{M}$ is desirable because the rate of convergence of the resulting preconditioned conjugate gradient iteration is independent of the mesh size and the number of processors. Recently, Farhat et al. [22] proposed a new iterative solver for symmetric indefinite matrices, *i.e.* allowing an arbitrary shift σ. Numerical experiments showed the scalability of the solver. However, to the best of our knowledge, their approach for symmetric indefinite matrices has not been coupled with a shift-invert Lanczos algorithm.

For a shift σ^* such that $\sigma^* < \lambda_1^h$, choices of scalable iterative linear solvers include FETI-DP [21], the conjugate gradient preconditioned by balanced domain-decompostion (BDDC) [19], or the conjugate gradient preconditioned by algebraic multigrid (AMG) [50, 49, 1]. No comparison is available to assess the quality of each combination. However, an efficient algorithm has been developed at Sandia National Laboratories.

Salinas [7, 8, 43] is a massively parallel implementation of finite element analysis for structural dynamics. This capability is required for high-fidelity validated models used in modal, vibrations, static, and shock analysis of weapons systems. A critical component of Salinas is scalable iterative linear algebra. The modal analysis is computed with a shift-invert Lanczos method (for a shift $\sigma^* < \lambda_1^h$) using parallel ARPACK [34, 37] and the FETI-DP iterative linear solver [23, 21]. Because the shift-invert Lanczos iteration used by ARPACK makes repeated calls to FETI-DP, the projected conjugate iteration used for computing the Lagrange multipliers retains a history of vectors computed during each FETI-DP invocation. After the first

FETI-DP call by ARPACK, the right-hand side in the projected conjugate iteration is first orthogonalized against this history of vectors. The number of projected conjugate iterations is therefore reduced as the number of Lanczos iterations needed by ARPACK increases. Besides the capability developed for Salinas, the authors are not aware of any multilevel-based modal analysis capabilities for use within a three-dimensional structural dynamics code.

Replacements for the shift-invert Lanczos algorithm include gradient schemes that attempt to minimize the Rayleigh quotient and Newton schemes that search for stationary points of the Rayleigh quotient. The gradient schemes include conjugate gradient algorithms [6, 24, 28, 31, 35, 40]. The Newton-based schemes include the Davidson-based methods [18] such as the Jacobi-Davidson algorithm [47].

All the algorithms perform a Rayleigh-Ritz analysis on a subspace $\mathcal{S}$ that is computed iteratively. At the $(m+1)$-th iteration, the current subspace $\mathcal{S}_{m+1}$ satisfies

$$\mathcal{S}_{m+1} \subset \text{span}(\mathcal{S}_m, \mathbf{N}^{-1}\mathbf{R}^{(m)}) \tag{7}$$

where $\mathbf{R}^{(m)}$ is the block vector of residuals

$$\mathbf{R}^{(m)} = \mathbf{K}\mathbf{X}^{(m)} - \mathbf{M}\mathbf{X}^{(m)}\Theta^{(m)}.$$

The current iterates $\mathbf{X}^{(m)}$ are the best eigenvector approximations for $(\mathbf{K}, \mathbf{M})$ in the subspace $\mathcal{S}_m$. The matrix $\Theta^{(m)}$ is diagonal and contains the Rayleigh quotients for the iterates $\mathbf{X}^{(m)}$.

The motivation for these preconditioned eigenvalue algorithms is to avoid the requirement for a linear solve so that a single application of a preconditioner per outer iteration can be used. So $\mathbf{N}$, applied in equation (7), is in general a preconditioner for the matrix $\mathbf{K}$ (the Jacobi-Davidson algorithm is one exception, see [47] for further details). Good preconditioners are a prerequisite for any of the preconditioned algorithms to perform satisfactorily. If a scalable preconditioner $\mathbf{N}$ is available for $\mathbf{K}$, then this preconditioner is a candidate for use within a preconditioned eigenvalue algorithm. Although less studied, preconditioned iterations for the eigenvalue problem should also be independent of the mesh size. The reader is referred to [30, 32] and [41, 42] for a review of the many issues involved and convergence theory, respectively. These papers also contain numerous citations to the engineering and numerical analysis literature.

Finally, little information is available that compares the merits of shift-invert Lanczos methods versus preconditioned eigensolvers when hundreds or thousands of eigenpairs are to be computed. In particular, practical experience with preconditioned algorithms for computing eigenpairs in an interval inside the spectrum is lacking. The paper [2] compares a number of preconditioned algorithms with the shift-invert Lanczos method (for a shift $\sigma^* < \lambda_1^h$) on several large-scale eigenvalue problems arising in structural dynamics when an algebraic multigrid preconditioner is available. For these particular engineering problems, the preconditioned algorithms were competitive when the preconditioner is applied in a block fashion and the block size is selected appropriately.

Ultimately, maintaining numerical orthogonality of the basis vectors is the dominant cost of the modal analysis as the number of eigenpairs requested increases. The cost is quadratic in the number of basis vectors. The cost of maintaining numerical orthogonality is a crucial limitation that motivates the next approach.

3 Variational approach

The previous section described schemes where knowledge of the partial differential equation is only required through the application of a linear solver or a preconditioner. In contrast, the approaches in this section make extensive use of the variational form of the equation.

The leading method in the automotive industry to compute hundreds or thousands of eigenpairs is the automated multilevel substructuring method (AMLS) [4, 5]. For example, in [33], the authors show how AMLS is more efficient than the shift-invert Lanczos method [26] coupled with a sparse direct solver to compute a large number of eigenpairs for two-dimensional problems. AMLS is a variation of a component mode synthesis technique (CMS). Component mode synthesis techniques [29, 17] originated in the aerospace engineering community . These schemes decompose a structure into numerous components (or substructures), determine component modes, and then synthesize these modes to approximate the eigenpairs of (3). Their goal is to generate approximations that aptly describe the low frequency modal subspace rather than to solve iteratively the eigenproblem. The reader is referred to [46] for a review of CMS methods from a structural dynamics perspective. The variational formulation and analysis of classical CMS techniques is due to Bourquin [9, 10, 11].

To make the process concrete, suppose that the structure Ω is divided into two subdomains Ω_1 and Ω_2 with the common interface Γ. We look for solutions of

$$-\mathcal{E}(\mathbf{u}) = \lambda\rho\mathbf{u} \quad \text{in } \Omega \tag{8a}$$

$$\mathbf{u} = \mathbf{0} \qquad \text{on } \partial\Omega. \tag{8b}$$

Let $(\mathbf{u}_j^1)_{1\le j\le m_1}$ (resp. $(\mathbf{u}_j^2)_{1\le j\le m_2}$) represent eigenvectors on Ω_1 (resp. Ω_2) for the same operator $\mathcal{E}$ with homogeneous Dirichlet boundary conditions on $\partial\Omega\cap\partial\Omega_1$ (resp. on $\partial\Omega\cap\partial\Omega_2$) and specific boundary conditions on Γ that will be discussed later. Component mode synthesis techniques compute approximations to eigenpairs of (8) via a Rayleigh-Ritz analysis on an appropriate subspace coupling the information spanned by the vectors $(\mathbf{u}_j^1)_{1\le j\le m_1}$ and $(\mathbf{u}_j^2)_{1\le j\le m_2}$. These techniques differ by the boundary conditions specified on Γ and by the definition of the *coupling* subspace. In practice, the eigenpairs on Ω_1 and Ω_2 are discretized by finite elements and are computed numerically.

The family of *fixed interface* CMS methods was introduced by Hurty [29] and improved by Craig and Bampton [17]. *Fixed interface* methods impose homogeneous Dirichlet boundary condition along the interface Γ. Coupling between the local sets of vectors $(\mathbf{u}_j^1)_{1\le j\le m_1}$ and $(\mathbf{u}_j^2)_{1\le j\le m_2}$ is achieved by adding a set of vectors defined on Γ harmonically extended into Ω. The definition of these coupling vectors distinguishes the various *fixed interface* CMS methods.

Other researchers proposed *free interface* methods where a homogeneous Neumann boundary condition is imposed on Γ. Continuity on Γ for the approximation of the eigenvectors of (3) is enforced so that constraints with Lagrange multipliers appear in a subspace [45] for the final Rayleigh-Ritz analysis. The recent paper by Rixen [44] reviews several CMS techniques and introduces a dual *fixed interface* method. For a one-dimensional model problem, Bourquin [9] showed that a *fixed interface* method better approximates the eigenspace than a *free interface* method. Consequently, we focus our discussion on *fixed interface* methods.

AMLS [5] is a *fixed interface* method where the coupling modes are harmonic extension of eigenmodes for the Steklov-Poincaré and the mass complement operators. After a finite element discretization, the mass and stiffness matrices are ordered as follows, for two subdomains,

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_{\Omega_1} & \mathbf{0} & \mathbf{M}_{\Omega_1,\Gamma} \\ \mathbf{0} & \mathbf{M}_{\Omega_2} & \mathbf{M}_{\Omega_2,\Gamma} \\ \mathbf{M}_{\Omega_1,\Gamma}^T & \mathbf{M}_{\Omega_2,\Gamma}^T & \mathbf{M}_{\Gamma} \end{bmatrix} \quad \text{and} \quad \mathbf{K} = \begin{bmatrix} \mathbf{K}_{\Omega_1} & \mathbf{0} & \mathbf{K}_{\Omega_1,\Gamma} \\ \mathbf{0} & \mathbf{K}_{\Omega_2} & \mathbf{K}_{\Omega_2,\Gamma} \\ \mathbf{K}_{\Omega_1,\Gamma}^T & \mathbf{K}_{\Omega_2,\Gamma}^T & \mathbf{K}_{\Gamma} \end{bmatrix}. \quad (9)$$

The coupling mode pencil is $(\tilde{\mathbf{K}}_\Gamma, \tilde{\mathbf{M}}_\Gamma)$, where

$$\tilde{\mathbf{K}}_\Gamma = \mathbf{K}_\Gamma - \sum_{i=1}^{2} \mathbf{K}_{\Omega_i,\Gamma}^T \mathbf{K}_{\Omega_i}^{-1} \mathbf{K}_{\Omega_i,\Gamma}$$

and $\tilde{\mathbf{M}}_\Gamma$,

$$\mathbf{M}_\Gamma - \sum_{i=1}^{2} \left(\mathbf{K}_{\Omega_i,\Gamma}^T \mathbf{K}_{\Omega_i}^{-1} \mathbf{M}_{\Omega_i,\Gamma} + \mathbf{M}_{\Omega_i,\Gamma}^T \mathbf{K}_{\Omega_i}^{-1} \mathbf{K}_{\Omega_i,\Gamma} - \mathbf{K}_{\Omega_i,\Gamma}^T \mathbf{K}_{\Omega_i}^{-1} \mathbf{M}_{\Omega_i} \mathbf{K}_{\Omega_i}^{-1} \mathbf{K}_{\Omega_i,\Gamma} \right),$$

are the Schur and mass complement matrices. The AMLS method forms these interface matrices and factors the Schur complement. For the case of two subdomains, AMLS is summarized in the following three steps

1. Compute local eigenvectors $(\mathbf{u}_j^1)_{1 \le j \le m_1}$ and $(\mathbf{u}_j^2)_{1 \le j \le m_2}$.
2. Compute coupling modes $(\mathbf{u}_j^\Gamma)_{1 \le j \le m_\Gamma}$ for the pencil $(\tilde{\mathbf{K}}_\Gamma, \tilde{\mathbf{M}}_\Gamma)$.
3. Perform a Rayleigh-Ritz analysis for the pencil $(\mathbf{K}, \mathbf{M})$ on the subspace

$$\text{span} \left\{ (\mathbf{u}_j^1)_{1 \le j \le m_1}, (\mathbf{u}_j^2)_{1 \le j \le m_2}, (E\mathbf{u}_j^\Gamma)_{1 \le j \le m_\Gamma} \right\}$$

where E denotes the harmonic extension.

For large structures, AMLS recursively divides the structure into thousands of substructures and associated interfaces. This nested decomposition results in a hierarchical tree of substructures and interfaces or, analytically, in a direct sum decomposition of $\left(H_0^1(\Omega)\right)^3$ into orthogonal subspaces. The paper [5] examines a mathematical basis for AMLS in the continuous variational setting and the resulting algebraic formulation. AMLS computes efficiently a large number of eigenpairs because the orthogonalizations of large scale vectors are eliminated. The orthogonality of the approximations is obtained by the final Rayleigh-Ritz analysis. Unfortunately, AMLS is not well suited to three-dimensional eigenvalue problems when solid elements are used. Indeed, AMLS supposes that the interface matrices are formed and, sometimes, factored. Consequently, the cost of AMLS is that of computing a sparse direct factorization for the stiffness matrix using multifrontal methods. As is well known, sparse direct methods are not scalable with respect to mesh or the number of processors.

An alternative to AMLS is to not form the Schur and mass complements. In this case, we do not subdivide the interface into a hierarchy but consider one interface. A preconditioner for the Schur complement, for instance BDDC [19], can be used within a preconditioned eigensolver for the interface eigenvalue problem. Although the interface problem is reduced in size over that of the order of (3), the application

of the mass and Schur complements matrices and of the Schur complement preconditioner remains expensive. Bourquin [10] and Namar [38] consider different pencils to compute the coupling interface modes. But defining the most efficient choice of pencil remains an open question.

Finally, we comment on the eigenspace error. Bourquin [9, 10, 11] derived asymptotic results for second order elliptic differential eigenvalue problems and their finite element discretization. The error in the eigenspace computed by a CMS technique depends upon the error due to modal truncation and discretization. The bounds of Bourquin also indicate that the number of coupling modes necessary may become small when the interface Γ is small. Similarly, when the subdomains are small, the number of local modes needed is small. For further details, we refer the reader to [9, 10, 11].

To conclude this section, we review overlapping techniques to compute approximations for the eigenproblem (3). Charpentier et al. [15] defined a component mode synthesis technique using overlapping subdomains. Their approach simplifies the definition of the *coupling* space as it just combines the local sets of vectors from each subdomain. But performing the final Rayleigh-Ritz analysis on this subspace is more complex because the decomposition of $\left(H_0^1(\Omega)\right)^3$ is not a direct sum and the local sets of vectors lack orthogonality properties.

In analogy to multiplicative Schwarz preconditioners, Chan and Sharapov [14] define a multilevel technique that minimizes the Rayleigh quotient

$$\min_{\mathbf{x}\neq\mathbf{0}} \frac{\mathbf{x}^T\mathbf{K}\mathbf{x}}{\mathbf{x}^T\mathbf{M}\mathbf{x}} \tag{10}$$

with a series of subspace and coarse grid corrections. When computing the smallest eigenvalue, they show that convergence is obtained independently of the mesh size and the number of overlapping subdomains. However, experience with large-scale engineering problems is lacking.

Finally, multigrid techniques have also been used to approximate eigenpairs of (3). Neymeyr [39] reviews multigrid eigensolvers for elliptic differential operators. The Rayleigh quotient minimization algorithm [36, 25] uses corrections from each geometric grid to compute eigenpairs. Cai et al. [13] have established grid independent convergence estimates. Other researchers [27, 12] have applied multigrid as a nonlinear solver for the eigenproblem. Unfortunately, practical experience with computing many modes using multigrid techniques is lacking. Furthermore, all of the existing algorithms make use of geometry to define their set of grids. The authors are investigating the use of algebraic multigrid to define their grids and minimize the Rayleigh quotient.

4 Conclusions

We have reviewed several multilevel algorithms to compute a large number of eigenpairs for large-scale three-dimensional structures. We can distinguish two major approaches to solve this problem.

The first approach consists in using an efficient algebraic eigensolver coupled with a multilevel preconditioner or linear solver. Many of the schemes discussed are efficient. It will be interesting to see how shift-invert Lanczos can benefit from a

scalable iterative solver for symmetric indefinite matrices. But, ultimately, maintaining numerical orthogonality of the basis vectors is the dominant cost of the modal analysis.

The second approach couples more tightly the eigensolver with the variational form of the partial differential equation. The corresponding schemes have the advantage of minimizing or eliminating the orthogonalization steps with large scale vectors and so are appealing. However, practical experience is needed in order to ascertain the efficiency of the resulting approach for three-dimensional problems.

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