

A comparison of solvers for quadratic eigenvalue problems from combustion

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SUMMARY

Two iterative subspace methods (Arnoldi and Jacobi-Davidson) are compared for solving typical quadratic eigenvalue problems arising when studying combustion instabilities. An academic, representative test case is presented with associated analytical solution. The efficiency of the iterative methods are studied in terms of running time when 1 to 10 eigenpairs are sought for, the computational domain being discretized with 500 to 32000-nodes finite element meshes. The sensitivity of the methods to the dimension of the search subspace is also investigated. Copyright © 2007 John Wiley & Sons, Ltd.

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1. INTRODUCTION

One of the difficulties in the development of low emission aircraft engines is the occurrence of thermoacoustic instabilities that are caused by the coupling between the flame and the acoustic wave [1]. The linear acoustic wave equation for the pressure fluctuations written for a non isothermal reacting flow is the proper framework to study this phenomenon [2]. Assuming harmonic variations, it leads to a generalized Helmholtz equation with the unsteady heat release $\hat{\Omega}_T$ as a source term. Under the assumption that $\hat{\Omega}_T$ is a linear function of the acoustic pressure, the Helmholtz equation is nothing but a functional eigenvalue problem whose spectral elements are the pulsation ω and the pressure complex amplitude \hat{p} . Using a finite element method to discretise the flow domain leads to an algebraic eigenvalue problem (EVP) whose size is close to N , the number of nodes in the mesh [3]. Usually, a time delay between the acoustic field and the unsteady heat release is introduced so that $\hat{\Omega}_T$ depends exponentially on ω and

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the EVP non-linear in the eigenvalues. Even in the absence of flame-acoustic coupling ($\hat{\Omega}_T=0$), the EVP remains non-linear in the general case. Indeed, the boundary conditions imposed for the pressure fluctuation \hat{p} are usually chosen in order to prescribe an appropriate reduced boundary impedance Z . This means imposing a Robin condition to the pressure fluctuations, viz. $c_0 Z \nabla \hat{p} \cdot \mathbf{n} - i\omega \hat{p} = 0$, where \mathbf{n} is the unit outward vector normal to the boundary and c_0 the speed of sound. In the case where the boundary condition is given by a constant, complex valued impedance ($Z = Z_0$), the eigenvalue problem is quadratic [3, 4] and can be written as:

$$\mathbf{A}\mathbf{P} + \omega\mathbf{B}\mathbf{P} + \omega^2\mathbf{C}\mathbf{P} = 0 \quad (1)$$

where \mathbf{A} , \mathbf{B} and \mathbf{C} are square matrices of size close to the mesh size N and \mathbf{P} contains the nodal values of the complex pressure amplitude.

Since the extra non linearity arising from the acoustic flame coupling can be handled efficiently by using an iterative algorithm [3] where a quadratic eigenvalue problem must be solved at each sub iteration, seeking for the most efficient method for solving quadratic EVPs is relevant to the nonlinear thermo-acoustic problem.

2. NUMERICAL METHODS

2.1. Framework

The finite element method is used as a discretisation technique to derive the quadratic eigenvalue problem. In the discretisation, two important choices have been made that are of direct consequence for the solution methods:

- The matrix C corresponds to a *lumped* mass matrix, and hence is diagonal. This implies that operations both with \mathbf{C} and its inverse \mathbf{C}^{-1} are trivial to perform, and already in the discretization phase the general quadratic eigenvalue is reduced to the more simple problem

$$\mathbf{C}^{-1}\mathbf{A}\mathbf{P} + \omega\mathbf{C}^{-1}\mathbf{B}\mathbf{P} + \omega^2\mathbf{P} = 0 .$$

- The target problems are extremely large, and hence explicit computation and storage of the global matrices is avoided. Instead, the implementation of the problem is matrix-free, which means that only routines are supplied for performing the matrix-vector multiplications $\mathbf{y} = \mathbf{C}^{-1}\mathbf{A}\mathbf{x}$, and $\mathbf{y} = \mathbf{C}^{-1}\mathbf{B}\mathbf{x}$, and the matrices \mathbf{A} , \mathbf{B} , and \mathbf{C} are not explicitly available.

Clearly, the solution methods should satisfy the restrictions imposed by the above choices, which implies that the solution methods should only address the matrices for performing matrix-vector multiplications. This means, for example, that methods based on the QR decomposition are not appropriate for solving these large scale problems. Moreover, only the first modes with the smallest frequencies are of interest in the context of thermoacoustic instabilities. The objective of this paper is thus to assess the efficiency of matrix-free methods to solve quadratic eigenvalue problems. In this context, iterative subspace methods are the appropriate methods to consider. We will consider two of these methods.

2.2. The Arnoldi method - AR

The first method that we consider is the Arnoldi method [5]. AR constructs eigenvalue approximation for the standard eigenvalue problem

$$\mathbf{A}\mathbf{x} = \omega\mathbf{x}$$

by computing an orthonormal set of basis vectors $\mathbf{q}_1 \mathbf{q}_2 \cdots \mathbf{q}_k$ for the Krylov subspace

$$K_k(\mathbf{A}; \mathbf{q}_1) = \text{span}\{\mathbf{q}_1, \mathbf{A}\mathbf{q}_1, \mathbf{A}^2\mathbf{q}_1, \dots, \mathbf{A}^{k-1}\mathbf{q}_1\}$$

using the recurrence relation

$$\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_k\mathbf{H}_k + h_{k+1,k}\mathbf{q}_{k+1}\mathbf{e}_k^T. \quad (2)$$

Here, $\mathbf{Q}_k = [\mathbf{q}_1 \mathbf{q}_2 \cdots \mathbf{q}_k]$ and \mathbf{e}_k is the k -th canonical basis vector in \mathbb{R}^k . Approximate eigenvectors \mathbf{u} are constructed as linear combinations of the vectors \mathbf{q}_j ,

$$\mathbf{u} = \mathbf{Q}_k\mathbf{y},$$

and the weights \mathbf{y} in this linear combination are computed by imposing the Galerkin condition

$$\mathbf{Q}_k^* \mathbf{A} \mathbf{Q}_k \mathbf{y} = \theta \mathbf{y} \Leftrightarrow \mathbf{H}_k \mathbf{y} = \theta \mathbf{y}.$$

Note that the matrix \mathbf{H}_k does not have to be computed explicitly, it is computed as a side result of the Arnoldi relation. The Ritz value θ is an approximation for the eigenvalue ω .

Unfortunately, quadratic eigenvalue problems can not be handled directly by AR. We therefore first rewrite the quadratic problem into an equivalent standard eigenvalue problem of size $2N$ [7], for example

$$\begin{bmatrix} 0 & -\mathbf{I} \\ \mathbf{C}^{-1}\mathbf{A} & \mathbf{C}^{-1}\mathbf{B} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \mathbf{P}_\omega \end{bmatrix} + \omega \begin{bmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \mathbf{P}_\omega \end{bmatrix} = 0, \quad (3)$$

where \mathbf{I} is the unit matrix of size N and $\mathbf{P}_\omega = \omega\mathbf{P}$. We can then solve this system with the AR algorithm.

The exterior eigenvalues, which are the eigenvalues at the extremes of the spectrum, converge fastest and are generally speaking easiest to find with AR. Unfortunately, the eigenvalues we are interested, the ones close to zero, are interior eigenvalues of 3. A standard technique to find interior eigenvalues is to apply AR to the shifted and inverted problem

$$(\mathbf{A} - \sigma\mathbf{I})^{-1}\mathbf{x} = \mu\mathbf{x}$$

where σ is a shift near the eigenvalues of interest. The eigenvalues ω of the original problem can then be computed by $\omega = \sigma + 1/\mu$. The ω near the shift are mapped to exterior eigenvalues μ of the shifted and inverted problem and convergence to them is often fast. Unfortunately, in a matrix-free context it is hard to apply this technique, since the matrix \mathbf{A} is not explicitly available. Solving the shift-and-invert systems can therefore only be performed with an iterative technique like GMRES. Unfortunately these systems are very ill conditioned if the shift is close to an eigenvalue, which results in extremely slow convergence of GMRES. Moreover, it is not clear how to construct a good preconditioner to speed-up the convergence of GMRES if \mathbf{A} is not explicitly known. Finally, the shift-and-invert systems should be solved to a high enough accuracy not to disturb the Arnoldi relation (2), which would result in inaccurate eigenvalue approximations. In view of these drawbacks we have chosen to apply the standard AR-method, without shift-and-invert technique. We use the state-of-the-art ARPACK code of Sorensen and Lehoucq [6], which implements Arnoldi with implicit restarts to limit memory requirements and to compress the information of the desired eigenvectors into a small subspace.

2.3. The Jacobi-Davidson method -JD

The Jacobi-Davidson method [8] was originally proposed as a method for solving the standard eigenvalue problem. It was quickly realized that JD could easily be extended for solving polynomial eigenvalue problems [9]. The potential of the method for quadratic eigenvalue problems was shown in [11, 10].

The JD-method is, like AR, a subspace method. Hence the same two key ingredients can be recognized: the construction of a suitable expansion vector for the basis of the subspace (or search space), and the computation of eigenvalue approximations. JD computes basis vectors for the subspace by solving the so called correction equation, which is given by

$$\left(\mathbf{I} - \frac{\mathbf{w} \mathbf{u}^*}{\mathbf{u}^* \mathbf{w}}\right) (\mathbf{A} + \theta \mathbf{B} + \theta^2 \mathbf{C}) (\mathbf{I} - \mathbf{u} \mathbf{u}^*) \mathbf{t} = -\mathbf{r} .$$

In this equation \mathbf{u} is the latest approximation to the desired eigenvector, θ the corresponding eigenvalue approximation and the vector \mathbf{w} is given by

$$\mathbf{w} = \mathbf{B}\mathbf{u} + 2\theta\mathbf{C}\mathbf{u} .$$

The residual \mathbf{r} is given by

$$\mathbf{r} = \mathbf{A}\mathbf{u} + \theta\mathbf{B}\mathbf{u} + \theta^2\mathbf{C}\mathbf{u} . \quad (4)$$

The solution \mathbf{t} of the correction equation is orthogonalized with respect to the basis vectors of the search space which gives a new basis vector \mathbf{q}_k , where k denotes the iteration number. As in AR all basis vectors of the subspace are collected in a matrix $\mathbf{Q}_k = [\mathbf{q}_1 \ \mathbf{q}_2 \ \cdots \ \mathbf{q}_k]$, and approximate eigenvectors are constructed as linear combinations of the basis vectors $\mathbf{u} = \mathbf{Q}_k \mathbf{y}$. The idea behind solving the correction equation in JD is analogous the shift-and-invert idea in AR: to find expansions to the subspace that contain a large component in the direction of the wanted eigenvector. However, in JD solutions of the correction equation are sought in the space orthogonal to the latest eigenvector approximation which means that if the corresponding eigenvalue approximation θ is close to a real eigenvalue, the system is still well conditioned.

New eigenvalue approximations are computed by imposing the Galerkin condition that the residual has to be orthogonal to the search space, which yields

$$\theta^2 \mathbf{Q}^* \mathbf{C} \mathbf{Q} \mathbf{y} + \theta \mathbf{Q}^* \mathbf{B} \mathbf{Q} \mathbf{y} + \mathbf{Q}^* \mathbf{A} \mathbf{Q} \mathbf{y} = 0 . \quad (5)$$

This projected system is computed explicitly in JD, this in contrast to AR where the projected matrix \mathbf{H} is a by-product of the Arnoldi relation (2). The disadvantage of the JD approach is that the computation of the projected system is more costly. The advantage, on the other hand is that no matter what \mathbf{Q} is, the above relation is always consistent with (4), and hence only low-accurate solutions to the correction equations can be used as basis vectors for the search space. In practice, approximate solutions of the correction equation are computed by performing a few GMRES iterations.

It can be shown that JD is closely related to Newton's method, and if the correction equation is solved sufficiently accurately, convergence to the eigenpairs is quadratic.

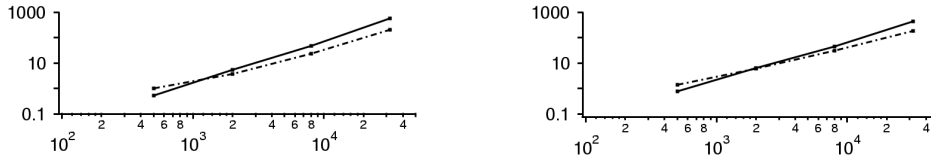


Figure 1. Scaled running times required by the AR (—) and JD (---) methods as a function of the size of the EVP. **left:** 2D case, **right:** 3D case.

3. NUMERICAL EXPERIMENTS

3.1. Test cases

Two and three dimensional model problems of increasing size are considered to compare the efficiency of the different methods. Both 2D and 3D cavities (corresponding to the domain $0 < x < L_x$, $0 < y < L_y$ and $0 < z < L_z$ for the 3D case, with $L_z \rightarrow \infty$ in 2D), acoustically open at the boundary $x = L_x$ are considered in this section. For numerical applications, $L_x = 1$, $L_y = 0.2$, $L_z = 0.1$ and the impedance is set to $Z_0 = -1.6 - 1.2j$.

Using a method of separation of variables, the analytical solution can be obtained and the corresponding dispersion relation in $k = \omega/c_0$ is

$$e^{2jk_x L_x} \left(k_x - \frac{k}{Z_0}\right) - \left(k_x + \frac{k}{Z_0}\right) = 0, \quad k_x = \sqrt{k^2 - \left(\frac{n_y \pi}{L_y}\right)^2 - \left(\frac{n_z \pi}{L_z}\right)^2}, \quad (n_y, n_z) \in \mathbb{N}^2$$

for the 3D case ($n_z = 0$ in 2D). All the computations discussed in this paper have been validated by comparing the computed eigenvalues to the theoretical values from these (implicit) dispersion relations. Note that the eigenvalues are complex valued. Uniform, finite element meshes with linear elements (triangle in 2D, tetraedra in 3D) have been used to generate quadratic EVPs with 500, 2000, 8000 and 32000 degrees of freedom. In the following we will refer to these EVPs as 2D-500, 2D-2000, ..., 3D-8000, 3D-32000.

3.2. Results

In all results presented in this section an eigenvalue is considered as converged if $\|\text{residual}(\text{ritzvalue})\| < \text{tol} \times \|\text{ritzvalue}\|$, the tolerance is set to $\text{tol} = 10^{-5}$ and the number of GMRES iterations for JD is 20.

The running times required by the AR and JD methods to obtain the 10 smallest eigenvalues are plotted in figure 1 as a function of N , the size of the finite element mesh used to discretize the EVP. The running time is scaled by the amount of time required by the JD algorithm for the case 2D-500, viz. 1.3 s. The JD method is more efficient than AR, certainly because it solves directly the quadratic problem while the linearised problem, eq. 3, is solved by AR. Note also the running time increases faster for AR than for JD; for the 3D case, the CPU time increasing roughly as $N^{1.52}$ for AR and only $N^{1.17}$ for JD. Figure 2 displays the scaled running times as a function of the number of eigenpairs required for the 8000-nodes cases. The scaling factor is the computing time required by the JD method to compute 1 eigenpair of the 2D-8000 case, viz. 6.41 s with the processor used. As for figure 1, JD is globally more efficient than AR, especially when a small number of eigenpairs is sought for. Eventually, figure 3 displays the scaled running times as a function of the subspace dimension for the 8000-nodes meshes. The scaling factor corresponds to JD applied

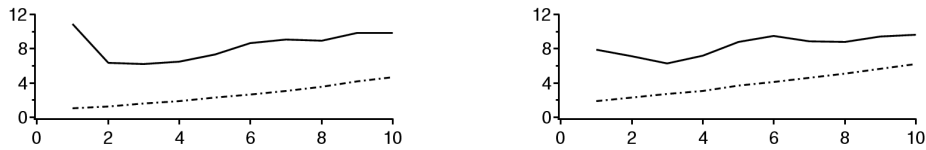


Figure 2. Scaled running times required by the AR (—) and JD (----) methods as a function of the number of eigenpairs required. **left:** 2D-8000 case, **right:** 3D-8000 case.

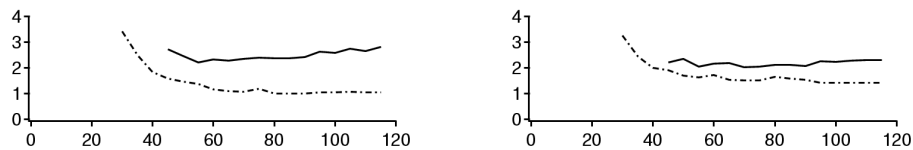


Figure 3. Scaled running times required by the AR (—) and JD (----) methods as a function of the dimension of the search subspace. **left:** 2D-8000 case, **right:** 3D-8000 case.

to the 2D case with a subspace dimension equal to 90 and for computing 10 eigenpairs, viz. 27.78 s. A nice result is that none of the methods is much sensitive to this parameter.

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