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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 is studied in terms of running time when 1–10 eigenpairs are sought for, the computational domain being discretized with 500–32 000-node 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 thermo-acoustic 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 an appropriate 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 (EVP) whose spectral

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elements are the pulsation ω and the pressure complex amplitude $\hat{p}$. The frequency f is obtained with the relation $\omega = 2\pi f$. Using a finite element method to discretize the flow domain leads to an algebraic 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 the EVP is 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* $c_0 Z \nabla \hat{p} \cdot \mathbf{n} - \mathrm{i}\omega \hat{p} = 0$, 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 EVP is quadratic [3, 4] and can be expressed as

$$\mathbf{AP} + \omega \mathbf{BP} + \omega^2 \mathbf{CP} = 0 \tag{1}$$

where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are sparse, square matrices of size close to the mesh size N. $\mathbf{A}$ is also symmetric, $\mathbf{B}$ and $\mathbf{C}$ are diagonal. $\mathbf{P}$ 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 EVP must be solved at each sub-iteration, seeking the most efficient method for solving quadratic EVPs is relevant to the non-linear thermo-acoustic problem.

2. NUMERICAL METHODS

2.1. Framework

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

- The matrix $\mathbf{C}$ 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

$$\mathbf{C}^{-1}\mathbf{AP} + \omega \mathbf{C}^{-1}\mathbf{BP} + \omega^2 \mathbf{P} = 0$$

- 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 $\mathbf{y} = \mathbf{C}^{-1}\mathbf{Ax}$, and $\mathbf{y} = \mathbf{C}^{-1}\mathbf{Bx}$, 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 thermo-acoustic instabilities. The objective of this paper is thus to assess the efficiency of matrix-free methods to compute a few frequencies and associated

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modes of quadratic EVPs. 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 AR [5]. AR constructs eigenvalue approximation for the standard EVP:

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

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

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

using the recurrence relation

$$\mathbf{A}\mathbf{Q}_k=\mathbf{Q}_k\mathbf{H}_k+h_{k+1,k}\mathbf{q}_{k+1}\mathbf{e}_k^{\mathrm{T}} \tag{2}$$

Here, $\mathbf{Q}_k=[\mathbf{q}_1\ \ \mathbf{q}_2\ \ \cdots\ \ \mathbf{q}_k]$ and $\mathbf{e}_k$ are the kth canonical basis vectors 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

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

Note that the matrix $\mathbf{H}_k$ is computed as a side result of the Arnoldi relation. The Ritz value θ is an approximation for the eigenvalue ω.

Unfortunately, quadratic EVPs cannot be handled directly by AR. We therefore first rewrite the quadratic problem into an equivalent standard EVP of size $2N$ [6], for example,

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

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

The exterior eigenvalues, which are the eigenvalues at the extremes of the spectrum, tend to 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

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

where σ is a shift near the eigenvalues of interest and $\mathbf{M}$ the block matrix in Equation (3). 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 such as GMRES. Unfortunately, these systems are very ill

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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 Lehoucq *et al.* [7], 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 JD [8] was originally proposed as a method for solving the standard EVP. It was quickly realized that JD could easily be extended for solving polynomial EVP [9]. The potential of the method for quadratic EVPs was shown in [10, 11].

The JD method is, similar to 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

$$\mathbf{r}=\mathbf{A}\mathbf{u}+\theta\mathbf{B}\mathbf{u}+\theta^2\mathbf{C}\mathbf{u} \tag{4}$$

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 to 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

$$\theta^2\mathbf{Q}^*\mathbf{C}\mathbf{Q}\mathbf{y}+\theta\mathbf{Q}^*\mathbf{B}\mathbf{Q}\mathbf{y}+\mathbf{Q}^*\mathbf{A}\mathbf{Q}\mathbf{y}=0 \tag{5}$$

This projected system is computed explicitly in JD; this is 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

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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.

3. NUMERICAL EXPERIMENTS

3.1. Test cases

The 2D and 3D 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 $L_z \longrightarrow \infty$ 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

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

for the 3D case ($n_z=0$ in 2D). All the computations discussed in this paper have been validated by comparing the computed eigenvalues with the theoretical values from these (implicit) dispersion relations. Note that the eigenvalues are complex valued. Uniform, finite element meshes with linear elements (triangles in 2D, tetrahedras in 3D) have been used to generate quadratic EVPs with 500, 2000, 8000 and 32 000 degrees of freedom. In the following we will refer to these EVPs as 2D-500, 2D-2000, ..., 3D-8000, 3D-32 000.

3.2. Results

The stopping criterion is imposed to make a fair comparison. For AR an eigenvalue is considered converged if $\|r_{\mathrm{AR}}\|<\mathrm{tol}\|\omega\|$ and if $\|r_{\mathrm{JD}}\|<\mathrm{tol}\|\omega\|\sqrt{1+\|\omega\|^2}$ for JD. 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 number of nodes 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 the quadratic problem directly while the linearized problem, Equation (3), is solved by AR. Note also that the running time increases faster for AR than for JD; for the 3D case, the central processing unit 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-node 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 are sought for. Eventually, Figure 3 displays the scaled running times as a function of the subspace dimension for the 8000-node meshes. The scaling factor corresponds to JD applied 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 both methods are insensitive to this parameter.

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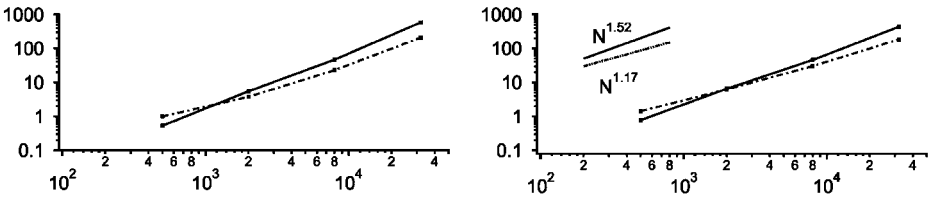

Figure 1. Scaled running times required by the AR (——) and JD (- - - -) methods as a function of the size of the EVP. Left: 2D case, Right: 3D case.

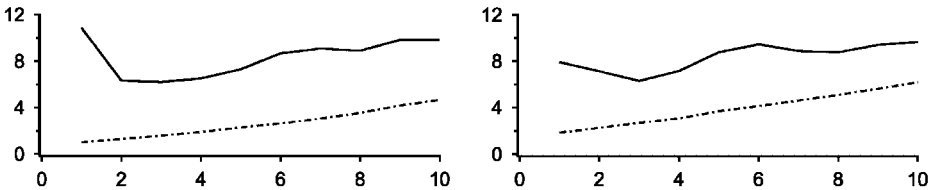

Figure 2. Scaled running times required by the AR (——) and JD (- - - -) methods as a function of the number of eigenpairs required. Left: 2D-8000 case, Right: 3D-8000 case.

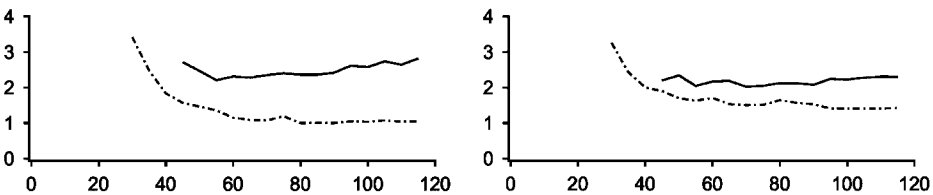

Figure 3. Scaled running times required by the AR (——) and JD (- - - -) methods as a function of the dimension of the search subspace. Left: 2D-8000 case, Right: 3D-8000 case.

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