Application of the Jacobi–Davidson method to accurate analysis of singular linear hydrodynamic stability problems

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SUMMARY

The aim of this paper is to show that the Jacobi–Davidson (JD) method is an accurate and robust method for solving large generalized algebraic eigenvalue problems with a singular second matrix. Such problems are routinely encountered in linear hydrodynamic stability analysis of flows that arise in various areas of continuum mechanics. As we use the Chebyshev collocation as a discretization method, the first matrix in the pencil is nonsymmetric, full rank, and ill-conditioned. Because of the singularity of the second matrix, QZ and Arnoldi-type algorithms may produce spurious eigenvalues. As a systematic remedy of this situation, we use two JD methods, corresponding to real and complex situations, to compute specific parts of the spectrum of the eigenvalue problems. Both methods overcome potentially severe problems associated with spurious unstable eigenvalues and are fairly stable with respect to the order of discretization. The real JD outperforms the shift-and-invert Arnoldi method with respect to the CPU time for large discretizations. Three specific flows are analyzed to advocate our statements, namely a multicomponent convection–diffusion in a porous medium, a thermal convection in a variable gravity field, and the so-called Hadley flow.

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1. INTRODUCTION

In a linear hydrodynamic stability analysis, one first considers the linearization of the governing equations around a steady-state flow. The perturbation variables are described by a linear system of coupled partial differential equations supplied with a set of boundary conditions. The discretization of this system frequently leads to some *non-Hermitian generalized eigenvalue problems* with *singular second-order matrix in pencil* of the form

$$\mathbf{A}\cdot\mathbf{x}=\lambda\mathbf{B}\cdot\mathbf{x}, \tag{1}$$

where the matrices $\mathbf{A}$ and $\mathbf{B}$ satisfy $\mathrm{rank}\mathbf{B}<\mathrm{rank}\mathbf{A}$.

The singularity of $\mathbf{B}$ can have two different reasons. First reason can be physical, that is, in incompressible flows, this matrix is associated with the transition terms in governing equations, and then, the singularity comes from the fact that continuity equation for such flows does not have a time-dependent term. Second, the singularity comes from the numerical method of discretization. We are mainly interested in this second situation. This singularity is responsible for the so-called *spurious eigenvalues* or *eigenvalues at infinity*. They complicate the numerics because most iterative methods favor the eigenvalues with the largest modulus, not those with largest real part. However, there are

many examples of such problems. One of the first was obtained in [1] in connection with stability of convective motion in a variable gravity field. In [2], the authors analyze the stability of convective flows in porous media, and in [3–5], the authors consider various physical situations such as thermal convection in a box, a multicomponent convection–diffusion, and the so-called Hadley flow. All the previously quoted papers are connected with the name of B. Straughan. The same phenomenon is noticed in [6] for various incompressible flows. When the linear stability analysis of some two-phase flows and free-surface flows (in MHD) are considered, the presence of eigenvalue at infinity in solving problems of type (1) is observed in [7] and [8].

The level of discretization needed to describe accurately the perturbed fields gives rise to large matrices, that is, of order of thousands and larger. This large dimension of problems rules out the calculation of the entire spectrum: usually, only the leading eigenvalues (those with the largest or the smallest real part) are computed. In spite of this fact,up to our knowledge, the classical QZ method was used in quasitotality of such *singular generalized eigenvalue problems* encountered in linear hydrodynamic stability; see [9] for one of the first applications of QZ in this context. Our papers [10] and [11] are not an exception to this situation.

Unfortunately, the QZ method has two main drawbacks. First, its complexity is of order $O(n^3)$, and because of large CPU times required, it is hardly applicable to large problems. Second, because of the singularity of $\mathbf{B}$, it provides eigenvalues at infinity.

In [6], the authors carry out a short review of method available to eliminate nonphysical eigenvalues in such non-Hermitian singular problems. They observe that the most effective techniques are based on some form of preconditioning and Krylov subspace projection methods [12]. They also remark that such techniques are computationally expensive and, in fact, do not eliminate the eigenvalues at infinity from the spectrum because the dimension of the transformed problem is the same as the original one. The eigenvalues are only mapped to a part of spectrum of the transformed eigenproblem that will not be favored by the iterative methods. Eventually, in [6], some ad hoc methods, based essentially on the physics of the flow, were designed to eliminate these spurious eigenvalues.

To avoid any confusion, we have to underline that the classical Orr–Sommerfeld equation, when solved with spectral methods, generates regular generalized eigenvalue problems. When coupled with other equations, which implies nonstandard boundary conditions, just a few spurious eigenvalues could appear. Thus, in [13], the authors couple this equation with the Squire's equation (normal vorticity equation), discretize them by Chebyshev collocation, and then use a transformation that maps the spurious eigenvalues to an arbitrary location in the complex plane to remove them. In [14] and [15], for *spectral Galerkin* and *Chebyshev tau (Lanczos)*, respectively, the authors suggest practical tricks to remove the spurious modes in similar problems. The authors of [16] obtain reliable results for the rightmost eigenvalue of Orr–Sommerfeld equation provided that a scale resolution assumption is fulfilled, that is, the ratio between the Reynolds number and the square of the cut-off parameter is 'small'. The sequence of quotations could be much longer, but we restrict ourselves to these works and observe that, whenever the boundary conditions are exactly enforced, the eigenvalues at infinity can be avoided in such problems.

Hence, there is a need for a more specialized algorithm that computes only a few specific eigenvalues of such singular generalized algebraic eigenvalue problems. In the case of hydrodynamic stability problems considered hereafter, one is typically interested in the eigenvalues closest to zero. Consequently, in this paper, we propose to use (a real variant [17] of) the Jacobi–Davidson (JD) method [18] to solve the arising generalized eigenvalue problems. Advantages of the JD method are that it is applicable to large-scale eigenvalue problems and that it can deal with *spurious eigenvalues at infinity* [19]. Concerning the eigenvalues at infinity, in principle, JD can also be hampered by their presence. However, by clever selection strategies, this can be avoided. Furthermore, in the paper [19] on purification, it is described how shift-and-invert/Cayley transformation strategies can be employed to avoid convergence to eigenvalues at infinity.

However, we want to stress that, up to our knowledge, the JD method has not been applied previously to these singular hydrodynamic stability problems, and hence, it is a novelty of our paper.

On the other hand, we are thoroughly aware of the existence of several methods designed to compute a specified subset of eigenspectrum, such as Krylov-based methods (see the paper of Golub and van Loan [20] for the main research developments in the area). The reason we focus

on JD and Arnoldi is that, in our paper, we have to deal with pencils (**A**,**B**) with singular B, for which both JD and Arnoldi are reliable methods [17, 19]; JD may have an advantage over Arnoldi when the matrices become large because no direct solutions are required, as they are required for shift-and-invert Arnoldi.

A partially similar study with ours is that of Valdettaro *et al.* [21]. The authors solve a two-dimensional eigenvalue problem by spectral collocation on the basis of Legendre and Chebyshev polynomials. The generalized eigenvalue problem is solved by a Krylov subspace-type method (incomplete Arnoldi–Chebyshev). For this method, a detailed analysis of round-off error is provided. But whereas our study refers to *singular pencils*, Valdettaro *et al.* consider *regular pencils*.

The paper is organized as follows. In Section 2, we first introduce a linear hydrodynamic stability problem, comment on its weak and minimization formulations, and use the 'D^2' strategy from [10] to transform it into a second-order system supplied with Dirichlet boundary conditions. By Chebyshev collocation, the generalized algebraic eigenvalue problem is obtained. Then, second and third singular problems are discretized with the same strategy. In Section 3, the JD method is described. Numerical experiments are reported in Section 4 along with comments concerning the convergence and round-off errors involved. Conclusions are contained in Section 5.

2. THREE SPECIFIC SINGULAR LINEAR HYDRODYNAMIC STABILITY PROBLEMS

In [10], the following even-order eigenvalue problem was considered:

$$\begin{cases} (D^2-a^2)^2 W = R(1+\varepsilon h(z))a^2\Theta, \\ (D^2-a^2)\Theta = -RW, \end{cases} \tag{2}$$

$$W = D^2W = \Theta = 0 \quad \text{at } z = 0, 1. \tag{3}$$

In these equations, as well as in the following two problems, D stands for the derivative with respect to the variable z. $Ra := R^2$ is the Rayleigh number that represents the eigenparameter of the problem (2)-(3), a is the wavenumber, W and Θ are the amplitudes of the vertical velocity and temperature perturbation, and $\varepsilon h(z)$ signifies the gravity variation in the layer of fluid.

To reduce the order of differentiation in this problem, we introduce the new variable

$$\Psi := (D^2-a^2)W. \tag{4}$$

Consequently, the two-point boundary value problem (2)–(3) can be rewritten as a second-order system

$$\begin{cases} (D^2-a^2)W - \Psi = 0, \\ (D^2-a^2)\Psi - R(1+\varepsilon h(z))a^2\Theta = 0, \\ (D^2-a^2)\Theta + RW = 0, \end{cases} \tag{5}$$

supplied with the homogeneous Dirichlet boundary conditions

$$W = \Psi = \Theta = 0 \text{ at } z = 0, 1. \tag{6}$$

It is important to observe that problem (2)–(3) can also be formulated as a sixth-order differential equation

$$(D^2-a^2)^3 W = -Ra(1+\varepsilon h(z))a^2 W, \tag{7}$$

supplied with the hinged boundary conditions, namely

$$W = D^2W = D^4W = 0 \quad \text{at } z = 0, 1. \tag{8}$$

A weak formulation for the new problem (7)–(8) reads as follows: find $w \in K\backslash\{0\}$ and $Ra \in \mathbb{C}$ such that

$$\begin{aligned} &\int_0^1 D^3wD^3v\,\mathrm{d}z + 3a^2\int_0^1 D^2wD^2v\,\mathrm{d}z + 3a^4\int_0^1 DwDv\,\mathrm{d}z + a^6\int_0^1 wv\,\mathrm{d}z = \\ &\quad = a^2Ra\int_0^1 (1+\varepsilon h(z))wv\,\mathrm{d}z, \ \forall v \in K, \end{aligned} \tag{9}$$

where the set K is a closed subspace of $H^4(0,1)$ defined by

$$K := \left\{ v \in H^4(0,1) | v(0) = v(1) = D^2 v(0) = D^2 v(1) = D^4 v(0) = D^4 v(1) = 0 \right\}.$$

More than that, the critical Rayleigh number can be characterized by the following minimization problem

$$Ra = \min_{v \in K} \frac{\int_0^1 (D^3 v)^2 \mathrm{d}z + 3a^2 \int_0^1 (D^2 v)^2 \mathrm{d}z + 3a^4 \int_0^1 (Dv)^2 \mathrm{d}z + a^6 \int_0^1 v^2 \mathrm{d}z}{a^2 \int_0^1 (1 + \varepsilon h(z)) v^2 \mathrm{d}z}, \tag{10}$$

whenever the quantity $1 + \varepsilon h(z)$ remains positive. In fact, in all our experiments, this condition is fulfilled.

The 'D^2' strategy implemented with Chebyshev collocation method to solve problem (5)–(6) leads to a singular generalized eigenvalue problem of type (1), namely

$$\mathbf{A} \cdot \mathbf{x} = Ra \mathbf{B} \cdot \mathbf{x}, \tag{11}$$

where the matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$\mathbf{A} = \begin{pmatrix} 4\mathbf{D2} - \mathbf{a}^2\mathbf{I} & -\mathbf{I} & \mathbf{Z} \\ \mathbf{Z} & 4\mathbf{D2} - \mathbf{a}^2\mathbf{I} & \mathbf{Z} \\ \mathbf{Z} & \mathbf{Z} & 4\mathbf{D2} - \mathbf{a}^2\mathbf{I} \end{pmatrix}, \ \mathbf{B} = \begin{pmatrix} \mathbf{Z} & \mathbf{Z} & \mathbf{Z} \\ \mathbf{Z} & \mathbf{Z} & \mathbf{I} - \varepsilon\mathbf{Dx} \\ -\mathbf{I} & \mathbf{Z} & \mathbf{Z} \end{pmatrix}. \tag{12}$$

The submatrices **D2**, **I**, and **Z** stand respectively for the second-order differentiation matrix on the Chebyshev nodes of the second kind $\mathbf{x} := \{x_1, \ldots, x_{N-1}\}$, the unitary matrix of order $N-1$, and the matrix with all zero entries of order $N-1$, N being as usual the spectral (cut-off or resolution) parameter. They have the same significance in the forthcoming two problems. The matrix **Dx** signifies the diagonal matrix $\mathbf{diag}(h(\mathbf{x}))$. It is important to note that, in the differentiation matrix **D2**, the boundary conditions are enforced; thus, the rows and columns corresponding to the first node x_0 and the last node x_N are deleted. All the differentiation matrices we have used come from [22]. The matrix **B** is singular of rank $N-1$.

As a second test problem, we consider another representative singular hydrodynamic stability problem. In this case, we solve an eighth-order differential system that models multicomponent convection–diffusion in a porous medium. In defining a^2 to be the wavenumber and λ the eigenparameter, the nondimensional linear perturbation equations read [4]:

$$\begin{cases} (D^2 - a^2)W - 2(\zeta - z)a^2 S - a^2 \Psi^1 - a^2 \Psi^2 = 0, \\ (D^2 - a^2)S - RW = \lambda S, \\ (D^2 - a^2)\Psi^1 - R_1 W = \lambda P_1 \Psi^1, \\ (D^2 - a^2)\Psi^2 - R_2 W = \lambda P_2 \Psi^2, \ z \in (0,1), \end{cases} \tag{13}$$

supplied with the boundary conditions

$$W = S = \Psi^1 = \Psi^2 = 0, \ z = 0, 1. \tag{14}$$

In the system (13), W, S, Ψ^1, and Ψ^2 are the perturbations of velocity, temperature, and two solutes, R and R_β are thermal and solute Rayleigh numbers, respectively, and P_β are salt Prandtl numbers, $\beta = 1, 2$. Eventually, ζ signifies a quantity connected with the temperature of the upper boundary. The 'D^2' strategy casts this problem into a generalized eigenvalue one with the matrices $\mathbf{A}$ and $\mathbf{B}$ defined as follows:

$$\begin{aligned} \mathbf{A} &:= \begin{pmatrix} 4\mathbf{D2} - a^2\mathbf{I} & -2(\zeta - z)a^2\mathbf{I} & -a^2\mathbf{I} & -a^2\mathbf{I} \\ -R\mathbf{I} & 4\mathbf{D2} - a^2\mathbf{I} & \mathbf{Z} & \mathbf{Z} \\ -R_1\mathbf{I} & \mathbf{Z} & 4\mathbf{D2} - a^2\mathbf{I} & \mathbf{Z} \\ -R_2\mathbf{I} & \mathbf{Z} & \mathbf{Z} & 4\mathbf{D2} - a^2\mathbf{I} \end{pmatrix}, \\ \mathbf{B} &:= \begin{pmatrix} \mathbf{Z} & \mathbf{Z} & \mathbf{Z} & \mathbf{Z} \\ \mathbf{Z} & P\mathbf{I} & \mathbf{Z} & \mathbf{Z} \\ \mathbf{Z} & \mathbf{Z} & P_1\mathbf{I} & \mathbf{Z} \\ \mathbf{Z} & \mathbf{Z} & \mathbf{Z} & P_2\mathbf{I} \end{pmatrix}. \end{aligned} \tag{15}$$

As a third test problem, we consider the stability of the so-called Hadley flow. It refers to convection in a layer of porous medium where the basic temperature field varies in the vertical (i.e., z direction) as well as along one of the horizontal directions, which is defined as x direction. The nondimensional perturbation equations [4] are

$$\begin{cases} (D^2 - a^2)W + a^2 S = 0, \\ (D^2 - a^2 - i\sigma - ikU(z))S + ika^{-2} R_H DW - (DT)W = 0, \ z \in \left(-\frac{1}{2}, \frac{1}{2}\right), \end{cases} \tag{16}$$

supplied with boundary conditions

$$W = S = 0, \quad z = \pm\frac{1}{2}. \tag{17}$$

In (16), $W(z)$ and $S(z)$ are the third component of velocity and temperature field perturbations, respectively. The steady-state solutions have the form

$$\begin{aligned} U(z) &:= R_H z, \\ T(z) &:= -R_V z + \tfrac{1}{24} R_H^2 \left(z - 4z^3\right) - R_H x, \end{aligned}$$

where R_H and R_V are the horizontal and vertical Rayleigh numbers, respectively, $a^2 := k^2 + m^2$ with k and m being the x and y wavenumbers, and σ is the eigenparameter. The same strategy casts this problem into a generalized eigenvalue one with the matrices $\mathbf{A}$ and $\mathbf{B}$ defined as follows:

$$\begin{aligned} \mathbf{A} &:= \begin{pmatrix} \mathbf{4D2} - a^2\mathbf{I} & a^2\mathbf{I} \\ \left(-\frac{R_H^2}{24} + R_V\right)\mathbf{I} + \left(\frac{R_H^2}{2}\right)\mathbf{X} + \left(ik\frac{R_H^2}{a^2}\right)\mathbf{D1} & \mathbf{4D2} - a^2\mathbf{I} - ik \cdot \mathrm{diag}\left(\frac{R_H x}{2}\right) \end{pmatrix}, \\ \mathbf{B} &:= \begin{pmatrix} \mathbf{Z} & \mathbf{Z} \\ \mathbf{Z} & \mathbf{I} \end{pmatrix}, \end{aligned} \tag{18}$$

where $\mathbf{X} := \mathrm{diag}(x^2/4)$ and $\mathbf{D1}$ is the first-order differentiation matrix. We finish this section with the remark that problem (16)–(17) can be reduced to a fourth order one in W containing the leading term $\left(D^2 - a^2\right)^2$.

Our strategy is strongly motivated by the conditioning of the matrices $\mathbf{A}$, $(4\mathbf{D2} - \mathbf{a}^2\mathbf{I})$ and its second, third, and fourth powers. In Figure 1, the log of the condition numbers of these matrices is depicted. In logarithmic terms, this picture shows that conditioning of the fourth-order

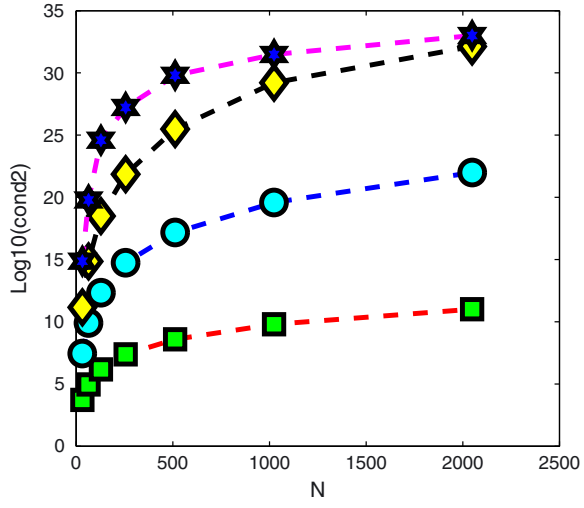

Figure 1. Log of the condition number of the matrices $\mathbf{D^2} - \mathbf{a}^2\mathbf{I}$, $(\mathbf{D^2} - \mathbf{a}^2\mathbf{I})^2$, $(\mathbf{D^2} - \mathbf{a}^2\mathbf{I})^3$, and $(\mathbf{D^2} - \mathbf{a}^2\mathbf{I})^4$ versus N in ascending order; $a = 4.92$.

differentiation matrix doubles, and that conditioning of the sixth-order differentiation matrix triples, the conditioning of second-order matrix. The conditioning of the eighth-order differentiation matrix is (roughly) only 3.43 times larger than that of the second-order differentiation matrix. It means powers two, three, or 3.43 of the conditioning of second-order differentiation matrix, for the conditioning of higher-order differentiation matrices, respectively. It is the main reason for which we did not apply directly collocation scheme to problem (7)–(8) or to its weak formulation (9) or even to its minimization formulation (10). A completely analogous remark holds for problems (13)–(14) and (16)–(17).

3. COMPUTING A FEW SPECIFIC EIGENVALUES

As mentioned in Section 1, the major drawback of full space methods such as the QR method (for ordinary eigenvalue problems) and the QZ method (for generalized eigenvalue problems) [23] is their computational complexity of $O(n^3)$, where n is the dimension of the problem. Consequently, for $n \gg 5000$, direct computation of the complete spectrum is no longer feasible using the QR or QZ method (see the uppermost curve in Figure 2).

On the other hand, for the application described in this paper (and for many other applications as well), one is not interested in the *complete* spectrum but in a *few specific* eigenvalues: the eigenvalues closest to zero. In fact, the eigenvalue closest to zero is the most important. Before describing the proposed algorithm, first, the requirements for an eigensolution method for the application of this paper are summarized:

1. Given the number k of wanted eigenvalues and a target (e.g., closest to zero), the methods must produce k eigenvalues closest to the target.
2. The method must be scalable with respect to the dimension of the eigenvalue problem.
3. The method must produce *real* approximate values for *real* eigenvalues and *complex* (conjugated pairs of) approximate values for *complex* eigenvalues.
4. The method must not be hampered by eigenvalues at infinity of the eigenvalue problems (11)–(12), (15), and (18).

In the following, we briefly describe the JD method [18], an iterative method for the computation of a few specific eigenvalues. We also show why this method satisfies the aforementioned requirements. For more details, see [17, 18, 24].

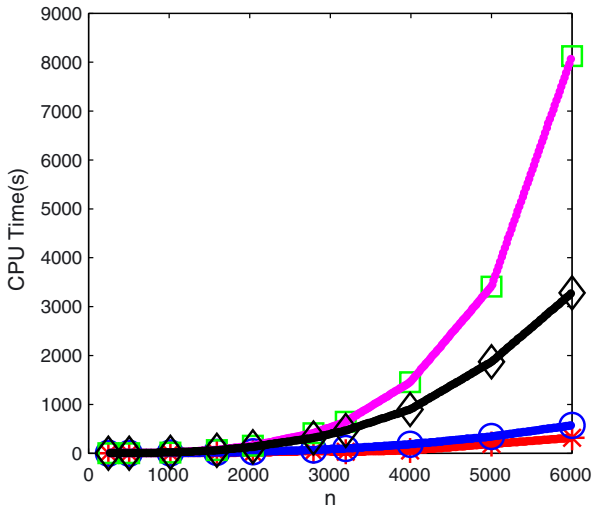

Figure 2. CPU time versus $n = (N-2) * 4$ for problem (15). Star line corresponds to rJDQZ, circle line to Arnoldi, diamond line to JDQZ, and square line to QZ.

3.1. The Jacobi–Davidson method

The JD method [18] combines two principles to compute eigenpairs of eigenvalue problems $A\mathbf{x} = \lambda\mathbf{x}$. The first (Davidson) principle is to apply the Ritz–Galerkin approach with respect to the search space spanned by the orthonormal columns of $V_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k] \in \mathbb{C}^{n\times k}$:

$$AV_k\mathbf{s} - \theta V_k\mathbf{s} \perp \{\mathbf{v}_1, \ldots, \mathbf{v}_k\},$$

which leads to k Ritz pairs $(\theta_i, \mathbf{q}_i = V_k\mathbf{s}_i)$, where $(\theta_i, \mathbf{s}_i)$ are eigenpairs of $V_k^* A V_k$ and star symbol stands for the hermitian conjugate or adjoint. The second (Jacobi) principle is to compute a correction $\mathbf{t}$ orthogonal to the selected eigenvector approximation $\mathbf{q}$ (e.g., corresponding to the largest Ritz value θ) from the JD correction equation

$$(I - \mathbf{q}\mathbf{q}^*)(A - \theta I)(I - \mathbf{q}\mathbf{q}^*)\mathbf{t} = -(A\mathbf{q} - \theta\mathbf{q}).$$

The search space is expanded with (an approximation of) $\mathbf{t}$. A Ritz pair is accepted if $\|\mathbf{r}\|_2 = \|A\mathbf{q} - \theta\mathbf{q}\|_2$ is smaller than a given tolerance. The basic JD method is shown in Algorithm 1. A variant for generalized eigenvalue problems is described in [24].

If the correction equations are solved exactly, JD is an exact Newton method [18, 25], but one of the powerful properties of JD is that it is often sufficient for convergence to solve the correction equation up to moderate accuracy only, using, for instance, a (preconditioned) linear solver such as the generalized minimal residual algorithm (GMRES) [26]. For our applications, however, the linear systems arising in the correction equation can be solved exactly in an efficient way. JDQR (QZ) methods, which compute partial (generalized) Schur forms for standard (generalized) eigenproblems, are described in [24, 25].

Reflecting on the requirements listed previously, the JD method is known to be able to satisfy requirements 1 and 2. In the following section, we describe how the other two can be dealt with.

Algorithm 1 The Jacobi-Davidson method

INPUT: $n \times n$ matrix A, initial vector $\mathbf{v}_1$, tolerance ϵ

OUTPUT: approximate eigenpair $(\theta, \mathbf{q})$ with $\|A\mathbf{q} - \theta\mathbf{q}\| < \epsilon$

$\mathbf{t} = \mathbf{v}_1$
$V_0 = W_0 = H_0 = []$
for $i = 1, 2, \ldots$ **do**
  $\mathbf{v}_i = \mathrm{MGS}(V_{i-1}, \mathbf{t})$ {Modified Gram-Schmidt [24]}
  $\mathbf{v}_i = \mathbf{v}_i / \|\mathbf{v}_i\|_2$
  $V_i = [V_{i-1}, \mathbf{v}_i]$
  $\mathbf{w}_i = A\mathbf{v}_i$
  $W_i = [W_{i-1}, \mathbf{w}_i]$
  $H_i = \begin{bmatrix} H_{i-1} & V_{i-1}^*\mathbf{w}_i \\ \mathbf{v}_i^* W_{i-1} & \mathbf{v}_i^*\mathbf{w}_i \end{bmatrix}$
  Select suitable eigenpair $(\theta, \mathbf{s})$ of H_i
  $\mathbf{q} = V_i\mathbf{s} / \|V_i\mathbf{s}\|_2$
  $\mathbf{r} = A\mathbf{q} - \theta\mathbf{q}$
  if $\|\mathbf{r}\|_2 \le \epsilon$ **then**
    Stop
  end if
  Solve (approximately) $\mathbf{t} \perp \mathbf{q}$ from correction equation

$$(I - \mathbf{q}\mathbf{q}^*)(A - \theta I)(I - \mathbf{q}\mathbf{q}^*)\mathbf{t} = -\mathbf{r}$$

end for

3.2. Computing a partial generalized real Schur form

The JDQZ [24] method for generalized eigenvalue problems computes a partial generalized Schur form [23]

$$AQ_kS_k = BZ_kT_k, \tag{19}$$

where $Q_k, Z_k \in \mathbb{C}^{n\times k}$ contain the generalized Schur vectors and $S_k, T_k \in \mathbb{C}^{k\times k}$ are upper triangular matrices whose generalized eigenvalues $\lambda(S_k, T_k)$ are approximations (called Petrov values) of eigenvalues of (A, B). Note that $k \ll n$.

Although the JDQZ method can be used for the problem described in this paper, there is one property that makes JDQZ in its current form less applicable: although matrices A and B are known to be real and, hence, have real or complex-conjugated pairs of eigenvalues, the produced partial Schur form is complex. In principle, this should not be an issue. However, JDQZ does not guarantee that approximations to *real* eigenvalues are *real*, which could lead to confusion when computing eigenvalues of large systems. In other words, because approximations of real eigenvalues might, in fact, be complex-conjugated pairs of eigenvalues (with negligible although nonzero imaginary part), this could lead to wrong conclusions in practice.

In [17], a variant of JDQZ, called rJDQZ, is proposed that computes partial generalized *real* Schur form for then pencil (A, B):

$$AQ_kS_k = BZ_kT_k, \tag{20}$$

where $Q_k, Z_k \in \mathbb{R}^{n\times k}$ contain the generalized Schur vectors, $S_k \in \mathbb{R}^{k\times k}$ is upper triangular, and $T_k \in \mathbb{R}^{k\times k}$ is quasi-upper triangular (i.e., the diagonal contains a 1×1 entry for real eigenvalues and a 2×2 block for complex-conjugated pairs of eigenvalues). The generalized eigenvalues $\lambda(S_k, T_k)$ are approximations (called Petrov values) of eigenvalues of (A, B). Note again that $k \ll n$.

The key difference between JDQZ and rJDQZ is that the latter uses only real search spaces, whereas JDQZ uses complex search spaces. Because rJDQZ uses real search spaces, the approximate eigenvalues are either real or appear in complex-conjugated pairs, which is in line with requirement 3. Apart from this, it was shown in [17] that because less complex arithmetic is used in rJDQZ, the method is also faster and more memory-efficient compared with JDQZ.

Finally, because we are interested in the eigenvalues closest to zero, we do not expect any numerical problems caused by eigenvalues at infinity (requirement 4), as also described in [19]. However, when one is interested in, for example, the rightmost *finite* eigenvalues, one might consider purification techniques described in [19, 27].

3.3. Alternatives

An alternative method to compute a few specific eigenvalues is the Arnoldi method [28]. Because the Arnoldi method was originally derived for ordinary eigenvalue problems of the form $Ax = \lambda x$, it is not directly applicable to problems of the form $Ax = \lambda Bx$ (cf. (11)). However, if it is possible to solve systems $Ay = b$, one can apply the Arnoldi method to the transformed problem $A^{-1}Bx = \mu x$, where $\lambda = 1/\mu$. Note that A is not inverted explicitly; during the Arnoldi process, systems $Ay = b$ are solved instead (for more details see, e.g., [29]). If solves with A can be done efficiently and accurately, the Arnoldi method may be an interesting alternative for the JD method (note that the JD method is still applicable if solves with A are not feasible).

For the problem at hand, the Arnoldi method is applicable because of the sparsity of matrix **B** and relatively cheap solves with A.

4. NUMERICAL RESULTS

In this section, we will report some representative numerical results obtained in solving the generalized algebraic eigenvalue problems defined by (11), (15), and (18). All numerical computations reported in [10] and [11] were carried out using the MATLAB code eig, which is an implementation of the QZ method. Alternatively, we use in this paper the JDQZ implementation

from *http://www.math.uu.nl/people/sleijpen/JD_software/JDQZ.html*, the rJDQZ implementation described in [17], and compare the results with those obtained using the MATLAB code eig for the QZ method (see also Table 3 in [10]), and the MATLAB code $eigs$ for the Arnoldi method. As far as we know and as the Matlab help shows, the eigs implementation relies on the implicitly restarted Arnoldi method from ARPACK library. All computations were carried out using MATLAB 2010a on an HP xw8400 workstation with clock speed of 3.2 Ghz.

The computed values of the first three eigenvalues, that is, $R_1, R_2, R_3, \lambda_1, \lambda_2, \lambda_3$, corresponding to problems (11) and (15), respectively, are displayed in Table I. The eigenvalues $\sigma_1, \sigma_2, \sigma_3$ corresponding to problem (18) are reported in Table II. The CPU times reported in these tables, as well as in Figure 2, measure the time required for the computation of the first six eigenvalues except QZ method, which computes the whole spectrum.

They are obtained for the following sets of fixed physical parameters: $a^2 = 21.344$, $\zeta = 0.14286$, $R = 228.009$, $R_1 = -291.066$, $R_2 = 261.066$, $P_1 = 4.5454$, $P_2 = 4.7619$, in case of problem (15); $\varepsilon = 0.03$ and $a = 4.92$ in case of problem (11); and $k = 0$, $m = 10$, $R_H = 114.2$, $R_V = 100$, in case of problem (18).

It is fairly clear from both tables that numerical approximations of the first three leading eigenvalues computed by all JDQZ, QZ, and Arnoldi are almost indistinguishable.

The CPU times required by the all four methods are depicted in Figure 2. It is important to observe that rJDQZ computed only the first two eigenvalues for spectral parameter N larger than 1000.

With respect to the memory usage, we have to mention that for all three methods Arnoldi, JD, and rJD, this is of order $O(kn)$, k being the maximal dimension of the search space, and $O(n^\alpha)$ with $1 < \alpha \leqslant 3$ for the system solves, where for sparse systems $\alpha < 2$ may be expected. For $\alpha > 2$, costs increase rapidly, and JD/rJD would be only alternative because inexact solves could be used (e.g., GMRES, of course of costs $O(mn)$, where m is the number of GMRES iterations).

However,the actual performance of JD relies on many factors, including the size of the search spaces, construction of projection spaces, shift selection (Ritz, Petrov, harmonic), and the accuracy of correction equation solves.

The real variant of JDQZ, rJDQZ, does produce real eigenvalues because it uses real search spaces, as explained in Section 3.2.

Both Arnoldi and the JD-based methods did not show any difficulties with spurious eigenvalues.

Table I. Numerical evaluations of the first three eigenvalues by using JDQZ, rJDQZ, and Matlab functions eig and eigs, for $N = 512$.

	JDQZ	rJDQZ	eig (QZ)	eigs (Arnoldi$A^{-1}B$)
R_1	25.8365	25.836514	25.836514	25.836514
R_2	134.387	134.386749	134.386750	134.386749
R_3	412.323	412.323554	412.323571	412.323571
CPU (s)	48.7	9.36	57.15	9.75
λ_1	−5.60913	−5.609129	−5.609129	−5.609129
λ_2	−8.96417	−8.964170	−8.964170	−8.964170
λ_3	−11.1226	−11.122552	−11.122552	−11.122552
CPU (s)	133.0	16.14	157.12	30.70

Table II. Numerical evaluations of the first three eigenvalues by using JDQZ, rJDQZ, and Matlab functions eig and eigs, for $N = 256$ ($n = 508$).

	JDQZ	rJDQZ	eig (QZ)	eigs (Arnoldi$A^{-1}B$)
σ_1	−0.293433	−0.293432	−0.293432	−0.293432
σ_2	−0.692455	−0.692454	−0.692454	−0.692454
σ_3	−329.278	−329.2778	−311.5122	−329.2778
CPU (s)	3.21	1.90	1.38	1.31

We also have to emphasize that, as far as we know, we have used the largest spectral order N in such eigenvalue computations. Comparatively, in [2] and [4], values of N attain 50, in [7] the authors work with N of order 100, in [6] the authors consider that $N = 602$ is fine enough to predict correctly the leading eigenvalues of the problem, and in [16] this order attains 1000. In older papers, the authors simply work with N much less than 100.

Some more comments on the convergence and round-off errors in rJDQZ and Arnoldi methods when singular generalized eigenvalue problems are solved are now in order. We define first the error of a method as the absolute value of the difference between the computed eigenvalue and the converged one, that is, obtained with the largest resolution. Then, we observe that the pseudospectra of our pencils (A, B) can be unbounded, that is, they extend to the whole complex plane for sufficiently large perturbations [30]. Thus, to obtain some information, we cut up from the whole spectrum the region surrounding the first two eigenvalues and observe that our computation is

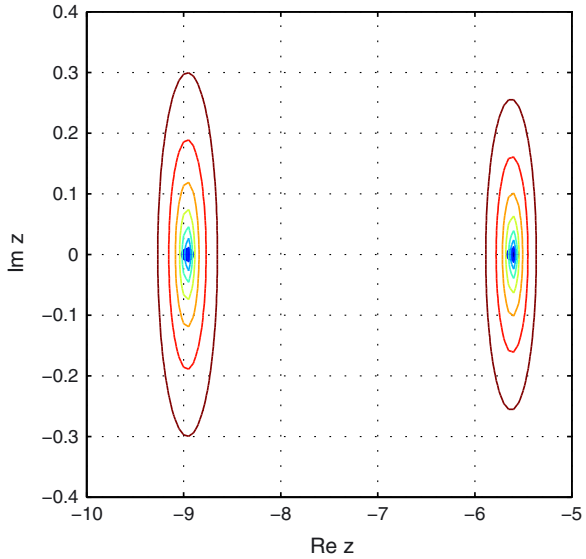

Figure 3. The part of pseudospectrum surrounding the first two eigenvalues of problem (15) obtained using rJDQZ. The largest contour line corresponds to an error of order $1{\cdot}10^{-01}$, and the nested contours correspond to errors decreasing successively with $1 \cdot 10^{-02}$.

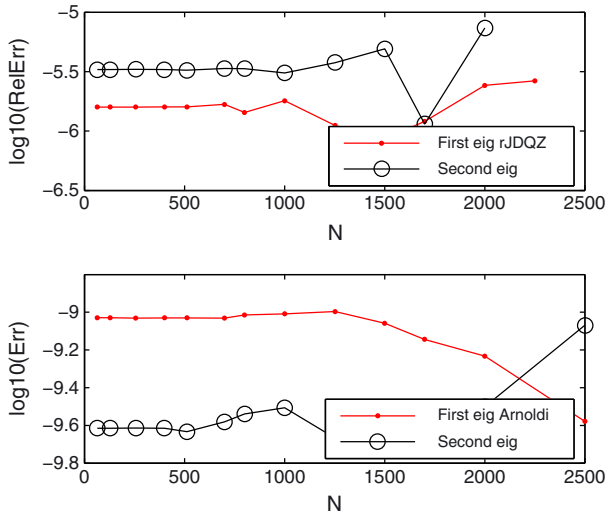

Figure 4. Semilog plot of error versus N for the first two eigenvalues computed with rJDQZ, respectively, Arnoldi.

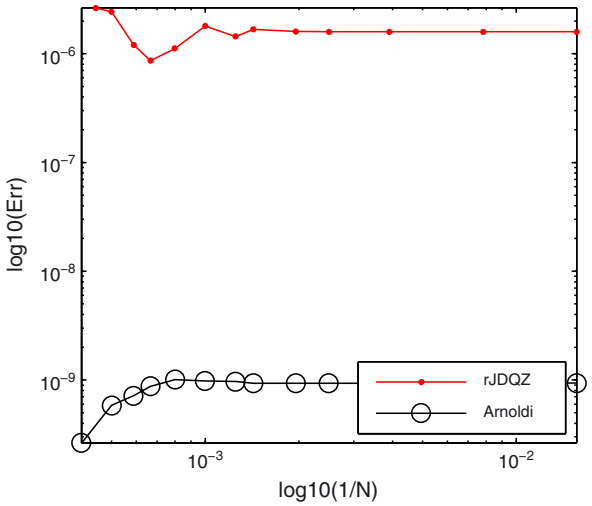

Figure 5. Loglog plot of error versus $1/N$ for the first eigenvalues computed with rJDQZ, respectively, Arnoldi.

backward stable in the sense that the line of level that equals the error encloses the computed eigenvalue. By using a resolution of 256, which implies a matrix of order $1 \cdot 10^{+03}$, the pseudospectrum is depicted in Figure 3. As the diameter of the enclosed area provides a hint of the largest possible relative error on the respective eigenvalue, we can infer a more sensitive second eigenvalue than the first one.

The errors of the first two computed eigenvalues, by rJDQZ and respectively Arnoldi, versus $1/N$, as usual in spectral methods, are depicted in Figure 4. For resolutions larger than 1500, this picture shows that the computation of the second eigenvalue becomes unstable in both methods. It is in accordance with the conclusion provided by the pseudospectrum. To observe the order of convergence of both methods, we depicted Figure 5. The rJDQZ method for resolutions inferior to 1700 has order of convergence that could attain unity, that is, Err is of order $(1/N)^p$, $0 < p \leqslant 1$. These resolutions are satisfactory in hydrodynamic stability problems. Arnoldi method behaves better. It has a comparable order of convergence but looks more accurate. The large but still acceptable error of rJDQZ can be explained by the fact that the convergence tolerance was set to $1 \cdot 10^{-6}$. Higher accuracy can be obtained for lower tolerances, at the cost of additional JD iterations. With respect to Arnoldi method, we have to observe that this method confirms its performances established in [21] also for generalized singular eigenvalue problems.

5. CONCLUDING REMARKS

In this paper, we have shown that the JD and Arnoldi methods can be successfully used to compute the smallest eigenvalues of large-scale matrix pencils arising in hydrodynamic stability problems.

Both methods are not hampered by eigenvalues at infinity. Because these methods are applicable to large-scale problems, they are preferred over the QZ method, which is only applicable to small eigenvalue problems. The variant of the JD method that uses only real search spaces, rJDQZ, takes advantage of using such search spaces resulting in real approximations of real eigenvalues. Consequently, it is the fastest method for solving such large and singular generalized eigenvalue problems. Moreover, this method is completely independent of the physical formulation of the problem at hand.

Eventually, we want to emphasize that the Chebyshev collocation (discretization) method proved again to be very implementable and feasible, for fairly large values of spectral parameter, provided that accurate differentiation matrices are used.

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REFERENCES

1. Straughan B. Convection in a variable gravity field. *Journal of Mathematical Analysis and Applications* 1989; **140**:467–475.
2. Straughan B, Walker DW. Two very accurate and efficient methods for computing eigenvalues and eigenfunctions in porous convection problems. *Journal of Computational Physics* 1996; **127**:128–141.
3. Dondarra JJ, Straughan B, Walker DK. Chebyshev tau-QZ algorithm methods for calculating spectra of hydrodynamic stability problems. *Applied Numerical Methods* 1996; **22**:399–434.
4. Hill AA, Straughan B. A Legendre spectral element method for eigenvalues in hydrodinamic stability. *Mathematical Methods in Applied Sciences* 2006; **29**:363–381.
5. Hill AA, Straughan B. Linear and nonlinear stability tresholds for thermal convection in a box. *Mathematical Methods in Applied Sciences* 2006; **29**:2123–2132.
6. Valerio JV, Carvalho MS, Tomei C. Filtering the eigenvalues at infinity from the linear stability analysis of incompressible flows. *Journal of Computational Physics* 2007; **227**:229–243.
7. Boomkamp PAM, Boersma BJ, Miesen RHM, Beijnon GVA. A Chebyshev collocation method for solving two-phase flow stability problems. *Journal of Computational Physics* 1997; **132**:191–200.
8. Giannakis D, Fischer PF, Rosner R. A spectral Galerkin method for the coupled Orr–Sommerfeld and induction equations for free surface MHD. *Journal of Computational Physics* 2009; **228**:1188–1233. DOI: 10.1016/j.jcp.2008.10.016.
9. Khorrami MR, Malik MR, Ash LR. Application of spectral collocation techniques to the stability of swirling flows. *Journal of Computational Physics* 1989; **81**:206–229.
10. Gheorghiu CI, Dragomirescu IF. Spectral methods in linear stability. Application to thermal convection with variable gravity field. *Applied Nunerical Mathematics* 2009; **59**:1290–1302. DOI: 10.1016/j.apnum.2008.07.004.
11. Dragomirescu IF, Gheorghiu CI. Analitical and numerical solutions to an electrohydrodynamic stability problem. *Applied Mathematics and Computation*; **2010**(216):3718–3727. DOI: 10.1016/j.acm.2010.05.028.
12. Saad Y. *Iterative Methods for Sparse Linear Systems*. PWS Publishing: NY, 1996.
13. Schmid PJ, Henningson DS. *Stability and Transition in Shear Flows*. Springer-Verlag: New York, 2001. 489.
14. Zebib A. Removal of spurious modes encountered in solving stability problems by spectral methods. *Journal of Computational Physics* 1987; **70**:521–525.
15. Lindsay KA, Ogden RR. A practical implementation of spectral methods resistant to the generation of spurious eigenvalues. *International Journal for Numerical Methods in Fluids* 1992; **15**:1277–1292.
16. Melenk JM, Kirchner NP, Schwab C. Spectral Galerkin discretization for hydrodynamic stability problems. *Computing* 2000; **65**:97–118.
17. van Noorden TL, Rommes J. Computing a partial generalized real Schur form using the Jacobi–Davidson method. *Numerical Linear Algebra with Applications* 2007; **14**:197–215.
18. Sleijpen GL, van der Vorst HAA. A Jacobi–Davidson iteration method for linear eigenvalue problems. *SIAM Journal of Matrix Analysis and Applications* 1996; **17**:401–425.
19. Rommes J. Arnoldi and Jacobi–Davidson methods for generalized eigenvalue problems $Ax = \lambda Bx$ with B singular. *Mathematics of Computation* 2008; **77**:995–1015.
20. Golub GH, Van der Vorst HA. Eigenvalue computation in the 20th century. *Journal of Computational and Applied Mathematics* 2000; **123**:35–65.
21. Valdettaro L, Rieutord M, Braconnier T, Frayssé V. Convergence and round-off errors in a two-dimensional eigenvalue problem using spectral methods and Arnoldi–Chebyshev algorithm. *Journal of Computational and Applied Mathematics* 2007; **205**:382–393.
22. Weideman JAC, Reddy SC. A MATLAB differentiation matrix suite. *ACM Transactions in Mathematical Software* 2000; **26**:465–519.
23. Golub GH, van Loan CF. *Matrix Computations*, third ed. The John Hopkins University Press: Baltimore, 1996.
24. Fokkema DR, Sleijpen GLG, van der Vorst HA. Jacobi–Davidson style QR and QZ algorithms for the reduction of matrix pencils. *SIAM Journal of Scientific Computing* 1998; **20**:94–125.
25. Sleijpen GLG, Booten JGL, Fokkema DR, van der Vorst HA. Jacobi–Davidson type methods for generalized eigenproblems and polynomial eigenproblems. *BIT* 1996; **36**:595–633.
26. Saad Y, Schultz MH. GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM Journal of Scientific and Statistic Computing* 1986; **7**:856–869.
27. Meerbergen K, Spence A. Implicitely restarted Arnoldi with purification for the shift-invert transformation. *Mathematics of Computation* 1997; **66**:667–689.
28. Arnoldi WE. The principle of minimized iteration in the solution of the matrix eigenproblem. *Quartely of Applied Mathematics* 1951; **9**:17–29.
29. Bai Z, Demmel J, Dongarra J, Ruhe A, van der Vorst HA. *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*. SIAM: Philadelphia, 2000.
30. van Dorsslaer JLM. Pseudospectra for matrix pencils and stability of equilibria. *BIT* 1997; **37**:833–845.