

Efficient Solution of a Generalized Eigenvalue Problem Arising in a Thermoconvective Instability

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Received 9 January 2007; Accepted (in revised version) 25 March 2007

Available online 27 September 2007

Abstract. The aim of this paper is to develop an efficient numerical method to compute the eigenvalues of the stability analysis of a problem describing the motion of a fluid within a cylindrical container heated non-homogeneously from below. An axisymmetric stationary motion settles in, at certain values of the external parameters appearing in the set of partial differential equations modeling the problem. This basic solution is computed by discretizing the equations with a Chebyshev collocation method. Its linear stability is formulated with a generalized eigenvalue problem. The numerical approach (generalized Arnoldi method) uses the idea of preconditioning the eigenvalue problem with a modified Cayley transformation before applying the Arnoldi method. Previous works have dealt with transformations requiring regularity to one of the submatrices. In this article we extend those results to the case in which that submatrix is singular. This method allows a fast computation of the critical eigenvalues which determine whether the steady flow is stable or unstable. The algorithm based on this method is compared to the QZ method and is found to be computationally more efficient. The reliability of the computed eigenvalues in terms of stability is confirmed via pseudospectra calculations.

AMS subject classifications: 65F15, 35Q35

Key words: Rayleigh-Bénard convection, Chebyshev collocation, preconditioners, Arnoldi method, Hopf bifurcation.

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1 Introduction

The problem of thermoconvective instabilities in fluid layers driven by a temperature gradient has become a classical subject in fluid mechanics [1, 21]. It is well known that two different effects are responsible for the onset of motion when the temperature difference becomes larger than a certain threshold: gravity and capillary forces. The numerical resolution of these hydrodynamical problems has been widely studied [8, 10, 12]. In [13] the linear stability analysis of some convection problems is solved with a Chebyshev collocation method in the primitive variable formulation taking appropriate boundary conditions for pressure. In [15, 16] the method is applied to study a laterally heated fluid within an annulus. In this work we focus on a physical set-up that has been thoroughly studied in [20]. It consists of a fluid filling a cylindrical container. The upper surface is open to the air and the fluid is heated from below with a Gaussian temperature profile. The stationary and axisymmetric solution that appears at certain values of the external parameters, referred to as the basic state, is computed by using a Chebyshev collocation method as detailed in [20]. The linear stability analysis of these solutions is also formulated in its discrete version with a Chebyshev collocation method. The associated generalized eigenvalue problem has a novel matrix structure. The aim of this paper consists of describing an efficient numerical technique to compute the eigenvalues in this case. Pseudospectra are also calculated.

Many applications require the computation of eigenvalues in generalized eigenvalue problems. In particular these arise in the numerical study of linear stability of partial differential equations. There exist several methods to compute eigenvalues. For low dimensional matrices such as those appearing when collocation methods are used, the QZ algorithm is the standard method [11]. As this technique requires the computation of the whole set of eigenvalues, it is computationally very demanding. A more appropriate choice to treat these and even larger problems, are the selective algorithms which only compute the eigenvalues with largest real part, i.e., those closer to the instability threshold. The Jacobi-Davidson QZ method has been used in this context [26], but the most common algorithm of these is the Implicitly Restarted Arnoldi Method [17, 18, 24]. The application of this method to specific block structured matrices is treated in Ref. [5]. See [3, 22] for more recent exploration and application of these methods for finite elements in this context. The numerical approach implemented in this work uses the idea of preconditioning the eigenvalue problem with a modified Cayley transformation before applying the Arnoldi method. This idea has already been used in [5, 23], but some results need to be proved before it can be extended to the resulting block structured matrices that appear with our collocation discretization. In particular if we express the problem as $Aw = \lambda Bw$, where

$$A = \begin{bmatrix} K & C \\ \widehat{C}^T & 0 \end{bmatrix}, \quad B = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}, \quad w = \begin{bmatrix} v \\ p \end{bmatrix}, \quad (1.1)$$

the matrix M is singular whereas in the context of finite element approximation con-

sidered in Ref. [5] the matrix M is positive definite. We prove that the modified Cayley transformation can still be used to compute the critical eigenvalues which determine whether the steady flow is stable or unstable. A comparison of the computing time between the standard QZ and the preconditioned Arnoldi method shows that the latter is much more efficient as might be expected. Note that the matrix blocks that arise are dense. Pseudospectra computations confirm the reliability of the eigenvalues and bifurcation thresholds.

The article is organized as follows. In Section 2 an overview of the physical problem behind the generalized eigenvalue problem is provided. The numerical approach to compute critical eigenvalues using the Cayley transformation and the Arnoldi method are explained in Section 3. Details of the algorithm, a comparison of its efficiency with respect to the QZ method and pseudospectra computations are given in Section 4. In Section 5 conclusions are summarized.

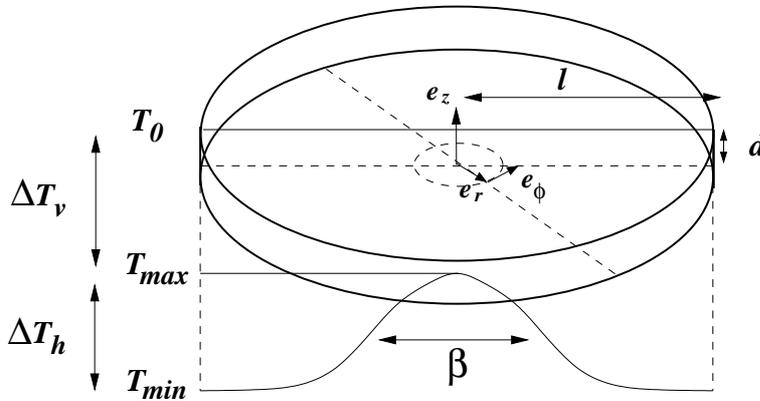


Figure 1: Problem set-up.

2 Formulation of the problem

The physical set up considered (see Fig. 1) is that studied in [20]. It consists of a horizontal fluid layer in a cylindrical container of radius l (r coordinate) and depth d (z coordinate). The upper surface is open to the atmosphere which is at temperature T_0 , and the rigid bottom plate is heated with a Gaussian temperature profile. The imposed temperature is T_{\max} at $r=0$ and T_{\min} at the outer part ($r=l$). We define $\Delta T_v = T_{\max} - T_0$, $\Delta T_h = T_{\max} - T_{\min}$ and $\delta = \Delta T_h / \Delta T_v$.

2.1 Equations and boundary conditions

The system evolves according to the momentum and mass balance equations and to the energy conservation principle. The governing dimensionless equations [20] are the con-

tinuity equation,

$$\nabla \cdot \mathbf{u} = 0, \quad (2.1)$$

the energy balance equation,

$$\partial_t \Theta + \mathbf{u} \cdot \nabla \Theta = \nabla^2 \Theta, \quad (2.2)$$

and the Navier-Stokes equations,

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = Pr (-\nabla p + \nabla^2 \mathbf{u} + R\Theta e_z), \quad (2.3)$$

where $\mathbf{u} = (u_r, u_z, u_\phi)$ is the velocity field, Θ is the temperature and p is the pressure. The dimensionless numbers are Pr which is the Prandtl number and R which is the Rayleigh number. The unit vector in the vertical direction is e_z .

The boundary conditions are as follows. The upper surface is flat and free slip, which implies the following conditions on the velocity,

$$u_z = \partial_z u_r = \partial_z u_\phi = 0 \quad \text{on} \quad z = 1. \quad (2.4)$$

The lateral and bottom walls are rigid, so

$$u_r = u_\phi = u_z = 0 \quad \text{on} \quad z = 0, \quad (2.5)$$

$$u_r = u_\phi = u_z = 0 \quad \text{on} \quad r = \Gamma, \quad (2.6)$$

where $\Gamma = l/d$.

As far as the temperature is concerned, we consider the dimensionless form of Newton's law for heat exchange at the surface,

$$\partial_z \Theta = -B\Theta \quad \text{on} \quad z = 1, \quad (2.7)$$

where B is the Biot number. At the bottom a Gaussian profile is imposed,

$$\Theta = 1 - \delta(e^{b^{-2}} - e^{(1-(\frac{r}{\Gamma})^2)^2 b^{-2}}) / (e^{b^{-2}} - 1) \quad \text{on} \quad z = 0, \quad (2.8)$$

where b is a measure of the width of the profile. The lateral wall is insulated,

$$\partial_r \Theta = 0 \quad \text{on} \quad r = \Gamma. \quad (2.9)$$

The use of cylindrical coordinates, which are singular at $r = 0$, requires regularity conditions on velocity, pressure and temperature fields which are expressed as follows [13, 20]

$$\frac{\partial(u_r e_r + u_\phi e_\phi)}{\partial \phi} = \partial_\phi u_z = \partial_\phi p = \partial_\phi \Theta = 0 \quad \text{on} \quad r = 0, \quad (2.10)$$

where e_r and e_ϕ are the unit vectors in the r and ϕ directions respectively. The fact that the pressure is retained in the equations means that additional boundary conditions are required. These conditions were obtained using the continuity equation at $z = 0$ and the normal component of the momentum equations on $r = \Gamma$ and $r = 0$ [13, 14, 20].

2.2 Basic state

The horizontal temperature gradient at the bottom (i.e., $\delta \neq 0$) leads to a stationary motion called the basic state: this is a time independent solution to the stationary problem obtained from equations (2.1)-(2.3). The basic state is axisymmetric, therefore it only depends on the r - z coordinates (i.e., all derivatives with respect to ϕ are zero). The velocity field of the basic flow is restricted to $u = (u_r, u_\phi = 0, u_z)$. For computational convenience the domain $[0, \Gamma] \times [0, 1]$ is transformed into $\Omega = [-1, 1] \times [-1, 1]$. This change of coordinates introduces scaling factors in equations and boundary conditions which are not explicitly given here. The new version of equations (2.1)-(2.3) together with the boundary and regularity conditions, are solved by treating the nonlinearity with an iterative Newton method (see [20]). Each step in the iterative scheme is solved with a Chebyshev collocation method. The unknown fields are expanded in a truncated series of Chebyshev polynomials

$$u_r = \sum_{l=0}^n \sum_{s=0}^m a_{ls}^{u_r} T_l(r) T_s(z), \quad (2.11)$$

and similarly for the rest of the fields. These expansions are introduced into the equations and boundary conditions and evaluated at the Chebyshev-Gauss-Lobatto points (r_j, z_i) ,

$$r_j = -\cos(j\pi/n), \quad \forall j=0, \dots, n, \quad (2.12)$$

$$z_i = -\cos(i\pi/m), \quad \forall i=0, \dots, m, \quad (2.13)$$

following evaluation rules that are detailed in [20]. Two types of numerical solutions are found for different parameter values, linear flows and return flows which are formed by one or several co-rotating rolls (see [20]). Fig. 2 displays temperature and velocity fields for the linear flow type solutions.

2.3 Linear stability analysis

The stability of the basic state is studied by perturbing it with a vector field depending on the r, ϕ and z coordinates, in a fully 3D analysis, for instance:

$$u_r(r, \phi, z) = u_r^b(r, z) + \bar{u}_r(r, z) \exp(ik\phi + \lambda t), \quad (2.14)$$

and similarly for u_ϕ , u_z , Θ and p . Here the superscript b indicates the corresponding quantity in the basic state and the bar refers to the perturbation. Fourier modes along the angular coordinate ϕ , satisfy the periodic boundary conditions as long as k is an integer. Expression (2.14) and similar expressions for the rest of the fields are substituted into the basic equations (2.1)-(2.3) and boundary and regularity conditions. The resulting system is linearized and an eigenvalue problem in λ is obtained.

The eigenvalue problem is discretized following the method of [13] by expanding perturbations \bar{u}_r , \bar{u}_ϕ , \bar{u}_z , $\bar{\Theta}$ and \bar{p} in a truncated series of orthonormal Chebyshev poly-

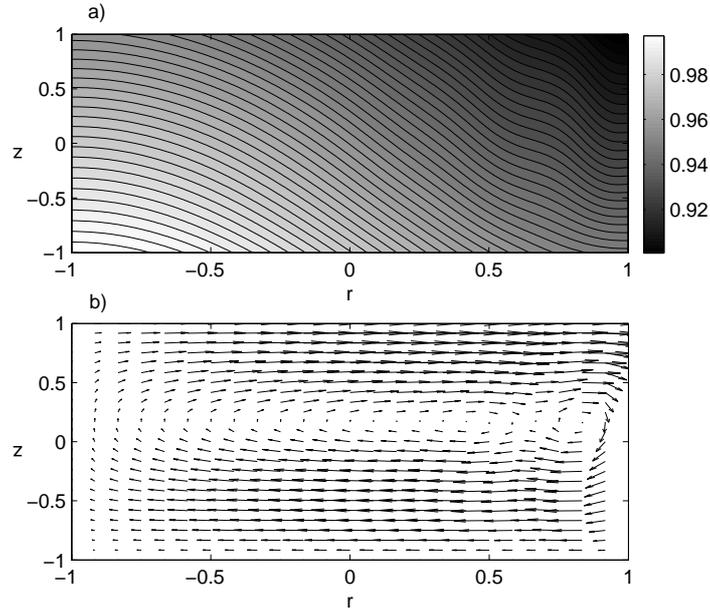


Figure 2: A basic linear flow, a) isotherms; b) velocity field. The parameters are $Pr=0.4$, $\Gamma=10$, $B=0.05$, $\delta=0.05$, $b=5$ and $R=1.9 \cdot 10^4$.

nomials as done for the basic state, i.e.,

$$\bar{u}_r = \sum_{l=0}^n \sum_{s=0}^m a_{ls}^{\bar{u}_r} T_l(r) T_s(z), \tag{2.15}$$

and similarly for \bar{u}_ϕ , \bar{u}_z , $\bar{\Theta}$ and \bar{p} . There are $P=5 \times (n+1) \times (m+1)$ unknowns which are determined by a collocation method. In particular, expansions (2.15) are substituted into the eigenvalue problem and those are evaluated at the Gauss-Lobatto collocation points (r_j, z_i) according to the following evaluation rules: the conveniently linearized Eqs. (2.1)-(2.3) are evaluated at nodes $i=1, \dots, m-1, j=1, \dots, n-1$; the boundary conditions at $z=-1$, (2.5) and (2.8) at $i=0, j=1, \dots, n-1$; the boundary conditions at $z=1$, (2.4) and (2.7) at $i=m, j=1, \dots, n-1$; the regularity conditions at $r=-1$, namely (2.10), take different expressions depending on the wavenumber k (see [13]). For $k=0$ and $k>1$ they are evaluated at $i=0, \dots, m, j=0$. Although the conditions for the case $k=1$ are evaluated at the same nodes, they are not sufficient and therefore the expansion of \bar{u}_ϕ is reduced as detailed in [13]; finally the boundaries at $r=1$, (2.6) and (2.9) at $i=0, \dots, m, j=n$.

The system of equations is completed with additional boundary conditions that eliminates any spurious modes for pressure. At $z=-1$, Eq. (2.1) is evaluated at nodes $i=0, j=1, \dots, n-1$; at $z=1$ the second component of Eq. (2.3) is evaluated at nodes $i=m, j=1, \dots, n$; at $r=1$ the third component of Eq. (2.3) is evaluated at $i=0, \dots, m-1, j=n$. With these rules the matrix associated to the linear algebraic system is singular due to the fact that pressure is defined up to an additive constant. To fix this constant the boundary condi-

tion (2.3) in node $i=m-2, j=n$ is replaced by a Dirichlet condition for pressure (i.e., $p=0$ at $i=m-2, j=n$). The eigenvalue problem is then transformed into its discrete form

$$Aw = \lambda Bw, \quad (2.16)$$

where w is a vector which contains P unknowns and A and B are $P \times P$ matrices. The discrete eigenvalue problem (2.16) has a finite number of eigenvalues $\lambda_i, i=1, \dots, P$.

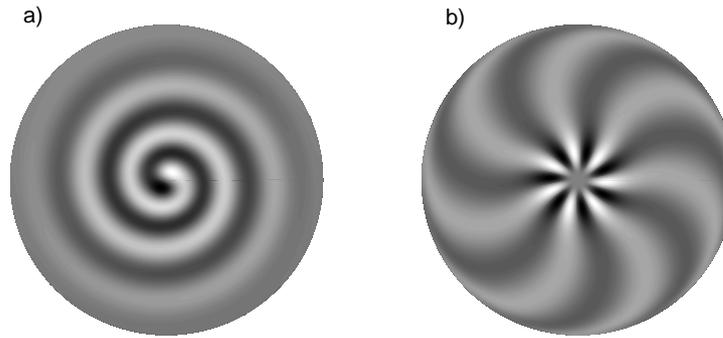


Figure 3: a) Isotherms on the horizontal plane at $z=1$ of the growing perturbation at an oscillatory instability threshold $R_c = 1.71 \cdot 10^4$, ($\delta = -0.03$, $b = 1.1$); b) isotherms on the horizontal plane at $z=1$ of the growing perturbation at a stationary instability threshold $R_c = 7.77 \cdot 10^4$, ($\delta = 1$, $b = 1$). The rest of the parameters are $Pr = 0.4$, $\Gamma = 10$ and $B = 0.05$.

The stability condition for the discrete problem depends on λ_{\max} , where $\lambda_{\max} = \max \text{Re}(\lambda_i)$. A bifurcation occurs when $\lambda_{\max}(R)$ changes from a negative value to a positive one as R varies. The value of R_c for which $\lambda_{\max}(R_c) = 0$ is the critical value. $\lambda_{\max}(R_c)$ is a function of the wave number k . The eigenvalue with maximum real part corresponds to $k = k_c$ that is the critical wave number. If this eigenvalue is complex the bifurcation is oscillatory, and if it is real the instability is stationary. Depending on the parameters, different instabilities are obtained: either stationary or oscillatory with different growing modes. In Fig. 3, two different bifurcating structures are shown, a spiral wave with critical wave number $k_c = 1$ or a stationary structure with $k_c = 7$. The aim of this article is to develop an algorithm which efficiently solves this eigenvalue problem as explained in Section 3.

2.4 Numerical convergence

A test on the convergence of the method has been performed by increasing the order of the expansion truncation. Table 1 shows the critical R_c values for different truncations in the case in which $\beta = 5$ and $\delta = 0.05$. Under the same conditions Fig. 4a) shows relative differences between consecutive truncations:

$$\varepsilon(n \times m) = \frac{|R_c^{n \times m} - R_c^{(n-2) \times (m-2)}|}{R_c^{n \times m}}.$$

Table 1: Critical R_c for different successive truncations of the expansions in Chebyshev polynomials. The set of external parameters are: $Pr=0.4$, $\Gamma=10$, $B=0.05$, $\delta=0.05$ and $b=5$.

	$m=9$	$m=11$	$m=13$	$m=15$	$m=17$
$n=29$	19065	19066	19066	19066	19066
$n=31$	19063	19063	19063	19063	19063
$n=33$	19063	19064	19064	19064	19064
$n=35$	19063	19064	19064	19064	19064
$n=37$	19063	19064	19064	19064	19064

As the order increases the differences tend to zero. Fig. 4b) contains a logarithmic representation of the same figure, the gradient which is nearly 5, represents the order of the method.

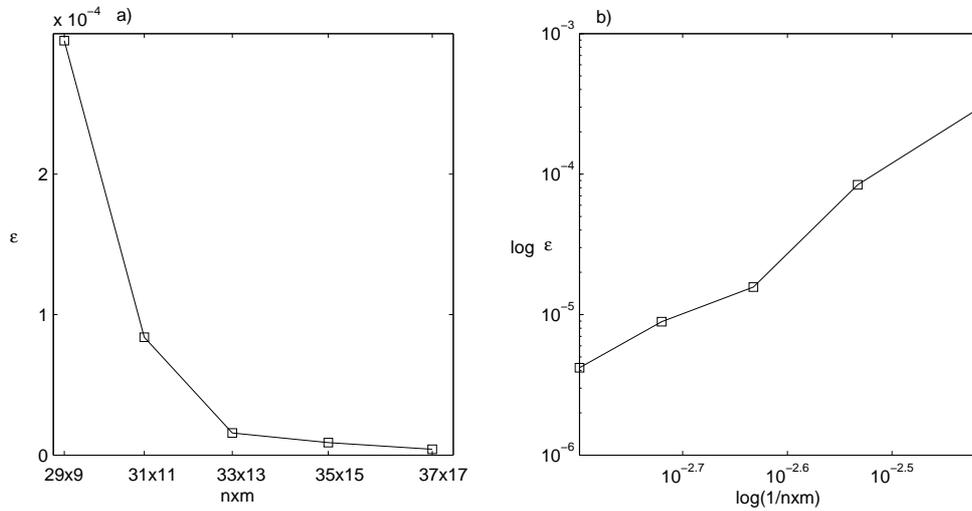


Figure 4: a) Relative differences ϵ between successive expansions as a function of the number of polynomials; b) a logarithmic representation of a). The set of external parameters are $Pr=0.4$, $\Gamma=10$, $B=0.05$, $\delta=0.05$ and $b=5$.

3 Generalized Arnoldi method

In the eigenvalue problem (2.16), A , B and w have the block form described in the introduction:

$$A = \begin{bmatrix} K & C \\ \widehat{C}^T & 0 \end{bmatrix}, \quad B = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}, \quad w = \begin{bmatrix} v \\ p \end{bmatrix}, \quad (3.1)$$

with $\bar{n} \times \bar{n}$ matrices K and M , and $\bar{n} \times \bar{m}$ matrices C and \widehat{C} ($\bar{n} > \bar{m}$). The values of \bar{n} and \bar{m} are $\bar{n} = 4(n+1)(m+1)$ and $\bar{m} = (n+1)(m+1)$.

In [5, 6], a straightforward analysis of (2.16) and (3.1) is shown in the case when M is positive definite and $C = \widehat{C}$ is of full rank. In our case, the matrix M does not have these properties and it is not even of full rank. Moreover, we deal with the case $C \neq \widehat{C}$ but both matrices have full rank. The fact that M has not full rank is due to the boundary conditions we are considering, which are necessary to preserve pressure stability in the context of the given approximation method. Another difference to the finite element approach is that the matrix M is nonsymmetric. The fact that $C \neq \widehat{C}$ is due to the discretization based on a spectral method [7]. However, here we will show that a similar result to the one obtained in [5] is possible.

In order to clarify our contribution in the case when M is singular we recall also some results of Cliffe et al. [5]. We say that λ is a *finite eigenvalue* of (2.16) if $\lambda \in \mathbb{C}$ is a solution of $\det(A - \lambda B) = 0$, although we usually omit the adjective 'finite'.

For generalized eigenvalue problems with singular B (as in our case) it is standard to consider the concept of an '*infinite*' eigenvalue. If (2.16) is rewritten as $(1/\lambda)Aw = Bw$, then roughly speaking an '*infinite*' eigenvalue is associated with w being a null vector of B . Clearly, the eigenvalue computation in the presence of infinite eigenvalues presents difficulties.

The first step in the study of the eigenvalue problem is to find the number of finite eigenvalues of (2.16) with (3.1).

First we note that since C has full rank, the QR factorization of C has the form

$$C = QR = [Q_1 \quad Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \quad (= Q_1 R_1),$$

where R is $\bar{n} \times \bar{m}$, R_1 is $\bar{m} \times \bar{m}$ nonsingular and upper triangular, Q is $\bar{n} \times \bar{n}$ orthogonal, Q_1 is $\bar{n} \times \bar{m}$ and provides an orthonormal basis for $\text{range}(C)$, and Q_2 is $\bar{n} \times (\bar{n} - \bar{m})$ and provides an orthonormal basis for C^\perp . Analogously, for the matrix \widehat{C} we have

$$\widehat{C} = \widehat{Q}\widehat{R} = [\widehat{Q}_1 \quad \widehat{Q}_2] \begin{bmatrix} \widehat{R}_1 \\ 0 \end{bmatrix} \quad (= \widehat{Q}_1 \widehat{R}_1).$$

Before giving the results regarding to the number of finite eigenvalues of (2.16)-(3.1) we will establish the structure of matrices C and M .

Remark 3.1. The structure of the matrix C is as follows:

$$C = (C_1 \quad \tilde{O}_1 \quad C_2 \quad \tilde{O}_2 \quad C_3 \quad \tilde{O}_3 \quad C_4 \quad \tilde{O}_4 \quad C_5 \quad \tilde{O}_5)^T. \quad (3.2)$$

The size of the submatrices in C is $(n-1)(m-1) \times \bar{m}$ for $C_i, i=1,2$, C_3 is $(m+1) \times \bar{m}$, C_4 is $m \times \bar{m}$ and C_5 is $n \times \bar{m}$. The matrices \tilde{O}_i are filled with zeros and they have the following sizes:

$$\begin{aligned} &(n-1)(m-1) \times \bar{m} \text{ for } \tilde{O}_1, \quad ((n-1)(m-1) + 4(m+1)) \times \bar{m} \text{ for } \tilde{O}_2, \\ &3(m+1) \times \bar{m} \text{ for } \tilde{O}_3, \quad 4(n-1) \times \bar{m} \text{ for } \tilde{O}_4, \quad (3n-m-4) \times \bar{m} \text{ for } \tilde{O}_5. \end{aligned}$$

In Fig. 5a) the shape of this matrix is displayed for $n=7$ and $m=5$.

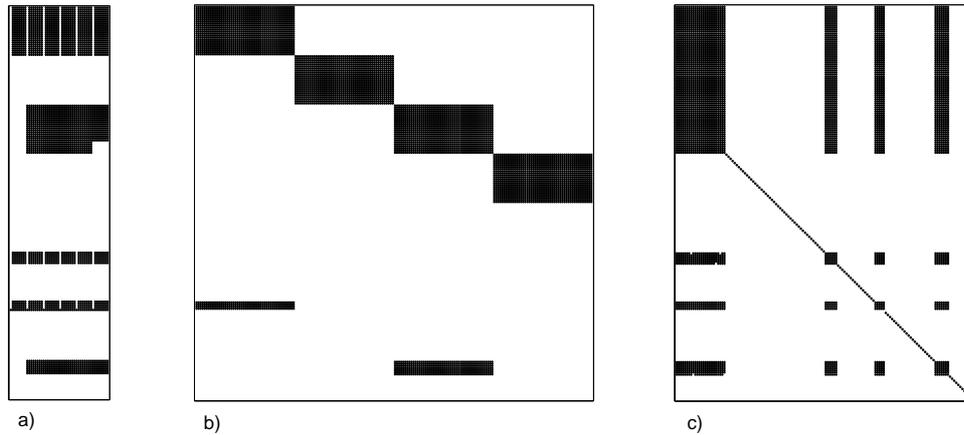


Figure 5: a) Structure of the matrix C ; b) structure of the matrix M ; c) structure of the matrix Q_2 . The values of n and m used are $n=7$ and $m=5$.

Remark 3.2. The structure of the matrix M is as follows:

$$M = \begin{pmatrix} M_1 & O_1 & O_1 & O_1 \\ O_1 & M_2 & O_1 & O_1 \\ O_1 & O_1 & M_3 & O_1 \\ O_1 & O_1 & O_1 & M_4 \\ O_2 & O_2 & O_2 & O_2 \\ M_5 & O_3 & O_3 & O_3 \\ O_4 & O_4 & O_4 & O_4 \\ O_5 & O_5 & M_6 & O_5 \\ O_6 & O_6 & O_6 & O_6 \end{pmatrix}. \tag{3.3}$$

The size of the submatrices in M is $(n-1)(m-1) \times (n+1)(m+1)$ for $M_i, i=1,2,3,4$, M_5 is $(m-1) \times (n+1)(m+1)$ and M_6 is $n \times (n+1)(m+1)$. The matrices O_i are filled with zeros and they have the following sizes:

$$\begin{aligned} &(n-1)(m-1) \times (n+1)(m+1) \text{ for } O_1, \quad 8(m+1) \times (n+1)(m+1) \text{ for } O_2, \\ &(m-1) \times (n+1)(m+1) \text{ for } O_3, \quad (4n-3) \times (n+1)(m+1) \text{ for } O_4, \\ &n \times (n+1)(m+1) \text{ for } O_5, \quad (3n-m-4) \times (n+1)(m+1) \text{ for } O_6. \end{aligned}$$

In Fig. 5b) the shape of this matrix is displayed for $n=7$ and $m=5$.

Lemma 3.1. The matrix Q_2 resulting from the QR factorization has the following form:

$$Q_2 = (Q_{21} \ D_{21} \ Q_{22} \ D_{22} \ Q_{23} \ D_{23} \ Q_{24} \ D_{24}), \tag{3.4}$$

where Q_{21} is $\bar{n} \times (3(n-1)(m-1) - \bar{m})$, Q_{22} is $\bar{n} \times (m+1)$, Q_{23} is $\bar{n} \times m$ and Q_{24} is $\bar{n} \times n$. The matrices D_{2i} have the following sizes:

$$\begin{aligned} &\bar{n} \times ((n-1)(m-1) + 4(m+1)) \text{ for } D_{21}, \quad \bar{n} \times 3(m+1) \text{ for } D_{22}, \\ &\bar{n} \times 4(n-1) \text{ for } D_{23}, \quad \bar{n} \times (3n-m-4) \text{ for } D_{24}, \end{aligned}$$

and all of them are null matrices with the exception of a diagonal block, I_{21} in D_{21} of size $((n-1)(m-1)+4(m+1))^2$ beginning at $3(n-1)(m-1)+1$, I_{22} in D_{22} of size $(3(m+1))^2$ beginning at $4(n-1)(m-1)+5(m+1)+1$, I_{23} in D_{23} of size $(4(n-1))^2$ beginning at $4(n-1)(m-1)+9(m+1)$ and I_{24} in D_{24} of size $(3n-m-4)^2$ beginning at $4(n-1)(m-1)+9(m+1)+4(n-1)+n$.

Proof. Let $\vec{u}_1, \dots, \vec{u}_{\bar{m}}$ be the columns of the matrix C . By applying the Gram-Schmidt method to these vectors we get the following orthogonal vectors

$$\begin{aligned} \vec{v}_1 &= \vec{u}_1, \\ \vec{v}_2 &= \vec{u}_2 - \frac{\vec{u}_2 \circ \vec{v}_1}{\vec{v}_1 \circ \vec{v}_1} \vec{v}_1, \\ \vec{v}_3 &= \vec{u}_3 - \frac{\vec{u}_3 \circ \vec{v}_1}{\vec{v}_1 \circ \vec{v}_1} \vec{v}_1 - \frac{\vec{u}_3 \circ \vec{v}_2}{\vec{v}_2 \circ \vec{v}_2} \vec{v}_2, \\ &\vdots \\ \vec{v}_{\bar{m}} &= \vec{u}_{\bar{m}} - \frac{\vec{u}_{\bar{m}} \circ \vec{v}_1}{\vec{v}_1 \circ \vec{v}_1} \vec{v}_1 - \dots - \frac{\vec{u}_{\bar{m}} \circ \vec{v}_{\bar{m}-1}}{\vec{v}_{\bar{m}-1} \circ \vec{v}_{\bar{m}-1}} \vec{v}_{\bar{m}-1}. \end{aligned}$$

All these vectors have zeros in the parts corresponding to \tilde{O}_i $i = 2, \dots, 5$. Denoting by h_i the norm of \vec{v}_i , $i = 1, \dots, \bar{m}$, vectors $\vec{w}_i = \vec{v}_i/h_i$, $i = 1, \dots, \bar{m}$ give us the columns of matrix Q_1 in the QR factorization. Let $\{\vec{e}_{\bar{m}+1}, \dots, \vec{e}_{\bar{n}}\}$ be the last $\bar{n} - \bar{m}$ vectors of the canonical basis of $\mathbb{R}^{\bar{n}}$ and consider

$$\begin{aligned} \vec{v}_{\bar{m}+1} &= \vec{e}_{\bar{m}+1} - \frac{\vec{e}_{\bar{m}+1} \circ \vec{v}_1}{\vec{v}_1 \circ \vec{v}_1} \vec{v}_1 - \dots - \frac{\vec{e}_{\bar{m}+1} \circ \vec{v}_{\bar{m}}}{\vec{v}_{\bar{m}} \circ \vec{v}_{\bar{m}}} \vec{v}_{\bar{m}}, \\ &\vdots \\ \vec{v}_{\bar{n}} &= \vec{e}_{\bar{n}} - \frac{\vec{e}_{\bar{n}} \circ \vec{v}_1}{\vec{v}_1 \circ \vec{v}_1} \vec{v}_1 - \dots - \frac{\vec{e}_{\bar{n}} \circ \vec{v}_{\bar{n}-1}}{\vec{v}_{\bar{n}-1} \circ \vec{v}_{\bar{n}-1}} \vec{v}_{\bar{n}-1}. \end{aligned}$$

It is clear that

$$\begin{aligned} \vec{v}_{3(n-1)(m-1)+1} &= \vec{e}_{3(n-1)(m-1)+1}, \quad \dots, \\ \vec{v}_{4(n-1)(m-1)+4(m+1)+1} &= \vec{e}_{4(n-1)(m-1)+4(m+1)+1} \end{aligned}$$

because \vec{v}_i , $i = 1, \dots, 3(n-1)(m-1)$, have the zeros corresponding to the block \tilde{O}_2 . Analogously,

$$\begin{aligned} \vec{v}_{4(n-1)(m-1)+5(m+1)+1} &= \vec{e}_{4(n-1)(m-1)+5(m+1)+1}, \quad \dots, \\ \vec{v}_{4(n-1)(m-1)+8(m+1)} &= \vec{e}_{4(n-1)(m-1)+8(m+1)} \end{aligned}$$

because of \tilde{O}_3 and the same for the vectors corresponding to the blocks \tilde{O}_4 and \tilde{O}_5 . Vectors $\{\vec{w}_i\}_{i=\bar{m}+1}^{\bar{n}}$ are the columns of Q_2 . So Q_2 has the structure given in (3.4) (see also Fig. 5c). This completes the proof of this lemma. \square

Theorem 3.1. *If M singular has the form given in (3.3), the number of finite eigenvalues of the eigenvalue problem (2.16) with (3.1) is $\bar{r} \leq (n-1)(3m-4) < \bar{n} - \bar{m}$.*

Proof. In [5], it is proven that the eigenvalue problem (2.16) and (3.1) has the same finite eigenvalues as the ‘reduced’ eigenvalue problem of dimension $\bar{n} - \bar{m}$

$$Q_2^T(K - \lambda M)\hat{Q}_2 z = 0. \tag{3.5}$$

It is straightforward to prove that the structure of product $\tilde{M} = Q_2^T M$ is

$$\tilde{M} = (\tilde{M}_1 \quad \hat{O}_1 \quad \tilde{M}_2 \quad \hat{O}_2 \quad \tilde{M}_3 \quad \hat{O}_3 \quad \tilde{M}_4 \quad \hat{O}_4)^T,$$

where $\tilde{M}_i, i = 1, \dots, 4$ are different from zero, \tilde{M}_1 is $(4(n-1)(m-1) - \bar{m}) \times \bar{n}$, \tilde{M}_2 is $(m+1) \times \bar{n}$, \tilde{M}_3 is $m \times \bar{n}$ and \tilde{M}_4 is $n \times \bar{n}$; $\hat{O}_i, i = 1, \dots, 4$ are null matrices of the following sizes: \hat{O}_1 is $4(m+1) \times \bar{n}$, \hat{O}_2 is $3(m+1) \times \bar{n}$, \hat{O}_3 is $4(n-1) \times \bar{n}$ and \hat{O}_4 is $(3n-m-4) \times \bar{n}$.

Problem (3.5) can be rewritten as $Q_2^T K \hat{Q}_2 z = \lambda Q_2^T M \hat{Q}_2 z$. The number of finite eigenvalues of (3.5) is

$$\begin{aligned} \bar{r} &\leq \text{rank}(Q_2^T M \hat{Q}_2) \leq \min\{\text{rank}(\tilde{M}), \text{rank}(\hat{Q}_2)\} \\ &= \text{rank}(\tilde{M}) \leq \text{number of non null rows of } \tilde{M} \\ &= 4(n-1)(m-1) - \bar{m} + (m+1) + m + n = (n-1)(3m-4). \end{aligned}$$

This completes the proof of this theorem. \square

Conjecture 1. In fact if M has the form given in (3.3), the number of finite eigenvalues of (2.16)-(3.1) is $\bar{r} = (n-1)(3m-4)$. For all the numerical examples we have used this is satisfied.

3.1 Cayley transform

The idea to calculate the eigenvalues of the problem $Aw = \lambda Bw$, which admits infinite eigenvalues, is to transform it into another one with all its eigenvalues finite. This transformation must be done in such a way that an infinite eigenvalue of the original problem corresponds to a concrete and known finite eigenvalue for the new eigenvalue problem. Also it must transform the finite eigenvalues of the original problem into the remaining finite eigenvalues of the new problem in such a way that applying the Arnoldi method to the transformed problem will give the eigenvalue for the original eigenvalue problem with largest real part under inverse transformation.

Denote by $\lambda_i, i = 1, \dots, \bar{r}$, the \bar{r} finite eigenvalues of (2.16) with (3.1) and by $\sigma(A, B)$ the set of these eigenvalues. We consider next the direct extension of the Cayley transform [5] for the eigenvalue problem (2.16) with (3.1):

For $\alpha_1, \alpha_2 \in \mathbb{R}$ with $\alpha_2 < \alpha_1 < 0$ and $\alpha_1 \notin \sigma(A, B)$, consider the problem

$$(A - \alpha_2 B)w = \mu(A - \alpha_1 B)w. \tag{3.6}$$

It is not difficult to show that the eigenvalues of problem (3.6) are given by

$$\begin{aligned}\mu_i &= (\lambda_i - \alpha_2) / (\lambda_i - \alpha_1), & i = 1, \dots, \bar{r}, \\ \mu_i &= 1, & i = \bar{r} + 1, \dots, \bar{n} + \bar{m}.\end{aligned}$$

Here, the eigenvalue equal to 1 of multiplicity $\bar{n} + \bar{m} - \bar{r}$ arises from the infinite eigenvalue of (2.16) with (3.1).

Let α_1 and α_2 be as above. For a general $\lambda \in \mathbb{C}$, the equation

$$\mu = C(\lambda) = (\lambda - \alpha_2) / (\lambda - \alpha_1) \quad (3.7)$$

represents a conformal transformation between the λ and μ planes. The transformation $C(\lambda)$ has the very useful property that the values of λ lying to the right (left) of the line $Re(\lambda) = \frac{1}{2}(\alpha_1 + \alpha_2)$ are mapped to $C(\lambda)$ lying outside (inside) the unit circle:

$$Re(\lambda) \geq (\leq) \frac{1}{2}(\alpha_1 + \alpha_2) \Leftrightarrow |\mu| \geq (\leq) 1. \quad (3.8)$$

Following the idea of [9], if α_1 and α_2 are as above and $\mu = C(\lambda)$, $\lambda \in \mathbb{C}$, is given by (3.7), then

$$\begin{aligned}Re(\lambda) \in (-\infty, \alpha_2) &\Leftrightarrow \mu \in B\left(\frac{1}{2}, \frac{1}{2}\right), \\ Re(\lambda) \in \left(\alpha_2, \frac{1}{2}(\alpha_1 + \alpha_2)\right) &\Leftrightarrow \mu \in \left\{ B(0, 1) - B\left(\frac{1}{2}, \frac{1}{2}\right) \right\}, \\ Re(\lambda) \in \left(\frac{1}{2}(\alpha_1 + \alpha_2), \alpha_1\right) &\Leftrightarrow \mu \in \left\{ \{z \in \mathbb{C} : Re(z) \leq 1\} - B(0, 1) \right\}, \\ Re(\lambda) \in (\alpha_1, 0) &\Leftrightarrow \mu \in \left\{ \{z \in \mathbb{C} : Re(z) > 1\} - B\left(\frac{\alpha_1 + \alpha_2}{2\alpha_1}, \frac{\alpha_2 - \alpha_1}{2\alpha_1}\right) \right\}, \\ Re(\lambda) \in (0, \infty) &\Leftrightarrow \mu \in B\left(\frac{\alpha_1 + \alpha_2}{2\alpha_1}, \frac{\alpha_2 - \alpha_1}{2\alpha_1}\right).\end{aligned}$$

The λ and μ planes are therefore divided into corresponding regions which are illustrated in Fig. 6. The vertical line $Re(\lambda) = \alpha_1$ in the λ plane is transformed into the line $Re(\mu) = 1$ in the μ plane. The remaining vertical lines on the right and on the left of $Re(\lambda) = \alpha_1$ are transformed into circles which have the common point $\mu = 1$. It is verified in each case that

$$\lim_{Im(\lambda) \rightarrow \pm\infty} C(\lambda) = 1,$$

i.e., points in the λ plane with very large imaginary part are transformed into points nearer to $\mu = 1$.

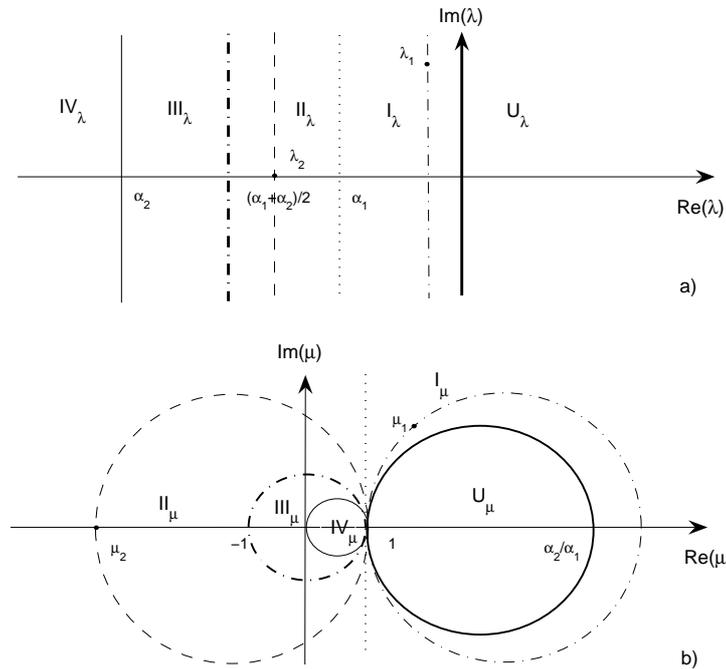


Figure 6: Graphical description of the relationship of the regions in the μ and λ plane as given in Section 2. Under $\mu=C(\lambda)$, region I_λ is mapped to region I_μ , etc. a) Original λ plane. b) Transformed μ plane.

3.2 Cliffe, Garratt & Spence (CGS) transform

As pointed out in [5] we could have some problems if the critical eigenvalue λ we are looking for has the property that its transformed value, μ , satisfies $|\mu| \approx 1$. This problem can be solved if we can move the eigenvalue 1 where it does not cause difficulties. This can be done with a simple modification of the Cayley transform as shown in [5]; it is however required there that M has full rank. Here, a theorem for the case that M is singular will be proven.

We introduce the following eigenvalue problem

$$\begin{bmatrix} K - \alpha_2 M & \alpha_3 C \\ \alpha_3 \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \beta \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix}. \tag{3.9}$$

Theorem 3.2. Assume $\alpha_2 < \alpha_1$, $\alpha_1 \notin \{\lambda_i\}_1^{\bar{r}}$, $\alpha_3 \notin \{C(\lambda_i)\}_1^{\bar{r}}$ and M is singular. Then (3.9) has eigenvalues satisfying

$$\beta_i = C(\lambda_i) = (\lambda_i - \alpha_2) / (\lambda_i - \alpha_1), \quad i = 1, \dots, \bar{r}, \tag{3.10a}$$

$$\beta_i = 1, \quad i = \bar{r} + 1, \dots, \bar{n} - \bar{m}, \tag{3.10b}$$

$$\beta_i = \alpha_3, \quad i = \bar{n} - \bar{m} + 1, \dots, \bar{n} + \bar{m}. \tag{3.10c}$$

Proof. It is easy to prove that if $\mu_i = C(\lambda_i) = (\lambda_i - \alpha_2) / (\lambda_i - \alpha_1)$, $i = 1, \dots, \bar{r}$ is an eigenvalue of (3.6), then it is an eigenvalue of (3.9).

If $\mu_i = C(\lambda_i) = (\lambda_i - \alpha_2) / (\lambda_i - \alpha_1)$, $i = 1, \dots, \bar{r}$ is an eigenvalue of (3.6), then there exists $[v_i, p_i]^T \neq 0 \in \mathbb{R}^{\bar{n} + \bar{m}}$ such that

$$\begin{bmatrix} K - \alpha_2 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v_i \\ p_i \end{bmatrix} = \mu_i \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v_i \\ p_i \end{bmatrix}.$$

In particular, $\widehat{C}^T v_i = 0$. If we take $\tilde{v}_i = v_i$ and $\tilde{p}_i = (1 - \mu_i) / (\alpha_3 - \mu_i) p_i$, then we have

$$\begin{bmatrix} K - \alpha_2 M & \alpha_3 C \\ \alpha_3 \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} \tilde{v}_i \\ \tilde{p}_i \end{bmatrix} = \mu_i \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} \tilde{v}_i \\ \tilde{p}_i \end{bmatrix},$$

so $\beta_i = C(\lambda_i) = (\lambda_i - \alpha_2) / (\lambda_i - \alpha_1)$, $i = 1, \dots, \bar{r}$ is an eigenvalue of (3.9).

We show now that $\beta = 1$ is an eigenvalue of multiplicity $\bar{n} - \bar{m} - \bar{r}$. Consider the problem

$$Q_2^T ((\alpha_1 - \alpha_2) M) \widehat{Q}_2 z = 0 \tag{3.11}$$

As $rank(Q_2^T M \widehat{Q}_2 z) = \bar{r}$, (3.11) has an eigenvalue 0 of multiplicity $\bar{n} - \bar{m} - \bar{r}$. If 0 is an eigenvalue of (3.11) then $\exists z \neq 0 \in \mathbb{R}^{\bar{n} - \bar{m}}$ such as $Q_2^T ((\alpha_1 - \alpha_2) M) \widehat{Q}_2 z = 0$. Let us take $v = \widehat{Q}_2 z$ (note that then $\widehat{C}^T v = 0$) and $p = 0$. We have

$$\begin{bmatrix} K - \alpha_2 M & \alpha_3 C \\ \alpha_3 \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix},$$

which indicates that $\beta = 1$ is an eigenvalue of (3.9).

We will finally prove that $\beta = \alpha_3$ is an eigenvalue of multiplicity $2\bar{m}$. Denote

$$\tilde{A} = \begin{bmatrix} K - \alpha_2 M & \alpha_3 C \\ \alpha_3 \widehat{C}^T & 0 \end{bmatrix}, \quad \tilde{B} = \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix}.$$

Problem (3.9) is rewritten as $\tilde{A}w = \beta \tilde{B}w$. Consider the problem $(\tilde{A} - \alpha_3 \tilde{B})w = \tilde{\beta} \tilde{B}w$, where $\tilde{\beta} = (\beta - \alpha_3)$. In an extended form it is

$$\begin{bmatrix} (1 - \alpha_3)K - (\alpha_2 - \alpha_1 \alpha_3)M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \tilde{\beta} \begin{bmatrix} K - \alpha_1 M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix}. \tag{3.12}$$

Consider also the problem

$$\begin{bmatrix} (1 - \alpha_3)K - (\alpha_2 - \alpha_1 \alpha_3)M & C \\ \widehat{C}^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \sigma \begin{bmatrix} K - \alpha_1 M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix}. \tag{3.13}$$

It is clear that (3.13) has $\bar{n} - \bar{m}$ finite eigenvalues because $rank(K - \alpha_1 M) = \bar{n}$ and all of the eigenvalues are different from zero because the matrix on the left hand side is not singular [5]. It can be easily proved that every finite eigenvalue of (3.13) is an eigenvalue

Table 2: Eigenvalues $C(\lambda_{max})$ and λ_{max} obtained for different values of the number of iterations (it) in the Arnoldi method. The values of the parameters are: $Pr=1$, $\Gamma=10$, $B=0.05$, $\delta=1$, $b=1$, $k=7$ and $R=5.9 \cdot 10^4$. The values for α_1 and α_2 are -0.1 and -18 , respectively.

	$C(\lambda_{max})$	λ_{max}
$it=5$	-1.294	-7.902
$it=12$	-1.294	-7.902
$it=13$	$0.999 \pm 0.320i$	$-0.114 \pm 55.913i$
$it=55$	$0.999 \pm 0.320i$	$-0.114 \pm 55.913i$
$it=95$	$0.999 \pm 0.320i$	$-0.114 \pm 55.913i$

of (3.12) and vice versa. As (3.12) has only finite eigenvalues because the matrix on the right hand side is not singular, it has the eigenvalue $\tilde{\beta}=0$ of multiplicity $2\bar{m}$. So $\beta=\alpha_3$ is an eigenvalue of (3.9) of multiplicity $2\bar{m}$. \square

We show this distribution of eigenvalues in an example. For $n=7$ and $m=5$ ($\bar{n}=192$, $\bar{m}=48$, $\bar{r}=66$) and after applying the Cayley transform, 174 eigenvalues are 1. With the second transformation (3.9) for $\alpha_3=0$, $78(=\bar{n}-\bar{m}-\bar{r})$ eigenvalues stay as 1 and $96(=2\bar{m})$ eigenvalues become 0. However, the remaining eigenvalues $\lambda=1$ could give some problems and some sensitive cases could take place. A sensitive case occurs when finite eigenvalues with large imaginary parts appear. They are transformed via the Cayley application to values of μ such that $|\mu|$ is close to 1. In this case the convergence of the Arnoldi method becomes slower, but these cases become clear when enough iterations of the Arnoldi method are performed. In Table 2 an example of this situation is shown. An incorrect (non-extreme) value for the eigenvalue $\lambda_2=-7.902$ is obtained with 12 iterations or less, however the correct value $\lambda_1=-0.114 \pm 55.913i$ is obtained after 13 iterations. We have fixed the number of iterations at 15 in the following.

4 Numerical implementation

Another difficulty is introduced by the sensitive cases. The situation can be observed in Figs. 6a) and 6b). In Fig. 6a) if we consider an eigenvalue λ_1 belonging to region I_λ with a large imaginary part and another eigenvalue $\lambda_2 \in II_\lambda$, $\lambda_2 = (\alpha_1 + \alpha_2)/2$ with $Re(\lambda_2) < Re(\lambda_1)$, λ_1 is transformed into μ_1 in Fig. 6b) with $|\mu_1|$ close to 1 and λ_2 is transformed into μ_2 in Fig. 6b). For the Arnoldi method, $|\mu_2| > |\mu_1|$, therefore if the method has to choose between them, μ_2 will be chosen and μ_1 will be left out. In [19], the problem is solved by moving the parameter α_2 to the right and increasing the number of eigenvalues s calculated at each step of the Arnoldi method. In this way there are less eigenvalues in regions I_λ and II_λ , more eigenvalues are calculated and therefore there is more chance to capture all of them. However, an increase in CPU time is introduced by the increase in the number of eigenvalues. We proceed differently. We fix the number of eigenvalues s at 20, for instance, and we increase the value of α_2 till at least one of the eigenvalues

calculated by the Arnoldi method μ_p becomes inside III_μ or IV_μ , i.e., as $|\mu_p| < 1$: we are then sure that all the rest of the important eigenvalues have norm greater than $|\mu_p|$, and no eigenvalue in the regions I_μ , II_μ or U_μ is lost. Therefore the corresponding λ are in I_λ , II_λ or U_λ and no important eigenvalue is left out. This means that $C(\lambda_{\max})$ is one of the eigenvalues caught and λ_{\max} can be easily obtained using $\mu = C(\lambda)$. The proposed algorithm follows this strategy as it is detailed next.

4.1 Algorithm

Input: The matrices K , M , C and \hat{C} of the eigenvalue problem $Aw = \mu Bw$. s , number of eigenvalues to be computed; it , number of iterations in Arnoldi method; α_1 , α_2 and α_3 , parameters for the transforms ($\alpha_3 = 0$ and the starting values of α_2 and α_1 are $\alpha_2 = -6$ and $\alpha_1 = -0.1$).

Output: $(\lambda_{\max}, v_{\max})$ eigenvalue with the largest real part and the corresponding eigenvector.

Algorithm 4.1:

-
1. Define matrices \hat{A} and \hat{B} using the parameters α_1 , α_2 and α_3 .
 2. Compute $D = \hat{B} \setminus \hat{A}$.
 3. Compute using Arnoldi method the s eigenvalues of D with the largest magnitude: μ_i , $i = 1, \dots, s$ with the Matlab function `eigs`.
 4. Calculate in : the number of these eigenvalues with $|\mu| < 1$.
 5. **while** $in = 0$
 - (a) Increase α_2 , $\alpha_2 = \alpha_2 \cdot factor$ where $factor < 1$.
 - (b) If $\alpha_2 > \alpha_1$ exchange the values of α_1 and α_2 between them.
 - (c) Define matrices \hat{A} and \hat{B} using the new values of α_1 and α_2 .
 - (d) Compute the new $D = \hat{B} \setminus \hat{A}$.
 - (e) Compute the new s eigenvalues of D via Arnoldi method.
 - end**
 6. Calculate the λ_i , $i = 1, \dots, s$ finite eigenvalues using $\mu = C(\lambda) = (\lambda - \alpha_2) / (\lambda - \alpha_1)$.
 7. Get λ_{\max} eigenvalue with the largest real part in \mathcal{G} , and its corresponding eigenvector v_{\max} .
-

4.2 Efficiency

Efficiency is an important property of the new algorithm. Typically collocation methods and in particular our Chebyshev collocation method discretize the problem produc-

Table 3: Computing time for the Arnoldi generalized (AG) algorithm and the Matlab command eig (QZ method) for different values of m and n . The values of the parameters are the same as in Table 2.

$n \times m$	23×7	27×9	31×11
AG	16.62 s	32.82 s	65.86 s
QZ	231.84 s	432.51 s	2073.4 s

Table 4: Eigenvalues $C(\lambda_{max})$ and λ_{max} obtained for $Pr=1$, $\Gamma=14.70$, $B=0.05$, $\delta=0.03$, $b=5$ and $k=0$.

Stable case ($R=1.49 \cdot 10^4$)	Unstable case ($R=1.53 \cdot 10^4$)
$\mu = 1.767 \pm 10.065i$	$\mu = 3.797 \pm 9.006i$
$\lambda = -0.055 \pm 0.583i$	$\lambda = 0.085 \pm 0.597i$

Table 5: Eigenvalues $C(\lambda_{max})$ and λ_{max} obtained for $Pr=1$, $\Gamma=14.70$, $B=0.05$, $\delta=0.03$, $b=0.4$ and $k=19$.

Stable case ($R=1.465 \cdot 10^4$)	Unstable case ($R=1.49 \cdot 10^4$)
$\mu = 67.314$	$\mu = 33.99$
$\lambda = -0.010$	$\lambda = 0.079$

ing matrices with many non-zero entries and moderate dimension (in our problem the maximum is $\bar{n} + \bar{m} = 1700$). Table 3 compares the computing time required to find the eigenvalue with the largest real part using the algorithm developed in this work with the standard Matlab eig command, which uses the QZ method. For matrices of small size, the difference in the computational time required by these algorithms reaches order ten. As the size of the matrix increases the factor grows almost exponentially, and in the largest case of those tested it rises up to a factor 40. This is due to the fact that the QZ method requires the computation of the whole set of eigenvalues. In practice, applications such as computing bifurcations and instabilities of partial differential equations do not need this computational effort. In fact the efficiency of the generalized Arnoldi method becomes of great interest in studies such as that of Ref. [20] where an intensive study of the solution bifurcations is performed depending on several external physical parameters. If the time invested to compute one eigenvalue is multiplied by the number of eigenvalue calculations required in the thermoconvective instability problems we are dealing with, the new algorithm leads to a huge reduction of the overall computing time.

4.3 Detection of the bifurcations

Here, we show how this algorithm detects both Hopf and stationary bifurcations when increasing the Rayleigh number R , the control parameter in this case. The eigenvalue with maximum norm in the μ -plane obtained with the Arnoldi method corresponds to the eigenvalue with largest real part in the λ -plane. A bifurcation occurs in the λ -plane when, increasing the control parameter, an eigenvalue crosses the imaginary axis

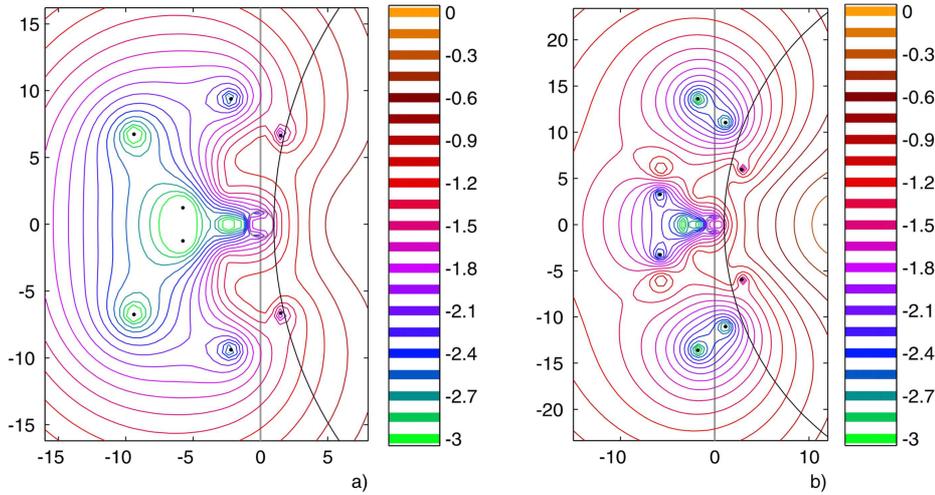


Figure 7: a) Eigenvalues and pseudospectra for the stable case of an oscillatory bifurcation at $R=1.49 \cdot 10^4$. b) Eigenvalues and pseudospectra for the unstable case of oscillatory bifurcation at $R=1.53 \cdot 10^4$. In both cases the rest of the parameters are $Pr=1$, $\Gamma=14.70$, $B=0.05$, $\delta=0.03$, $b=5$ and $k=0$.

($Re(\lambda) = 0$). In the μ -plane the corresponding eigenvalue crosses the U_λ circle boundary:

$$||z - (\alpha_1 + \alpha_2)/2\alpha_1|| = (\alpha_1 - \alpha_2)/2\alpha_1$$

(see Fig. 6). In Table 4, the value of the right-most eigenvalue λ_{\max} and its transform $\mu = C(\lambda_{\max})$ are given for a wavenumber $k=0$ at $R=1.49 \cdot 10^4$ before an oscillatory bifurcation takes place (left column), and at $R=1.53 \cdot 10^4$ once the state has become unstable (right column). In Fig. 7 we have displayed both states, stable (Fig. 7a) and unstable (Fig. 7b) in the μ plane. The eigenvalues are plotted as black dots. We have plotted only eight eigenvalues. It is clear from Fig. 7a) that the eigenvalue $C(\lambda_{\max})$ is outside the circular unstable region and in Fig. 7b) that it is inside it.

The same situation, but in the case of a stationary bifurcation, is presented in Table 5 for $k=19$ at $R=1.46 \cdot 10^4$ before the stationary bifurcation takes place and at $R=1.49 \cdot 10^4$, after the bifurcation has occurred. In Fig. 8 the stable case is shown. Fig. 8b) is a magnification of Fig. 8a) and shows clearly how the eigenvalue $C(\lambda_{\max})$ is outside the unstable region. In Fig. 9 the unstable case is presented. Fig. 9b) shows a zoom of Fig. 9a) where we can see how the eigenvalue $C(\lambda_{\max})$ is inside the unstable region.

In order to test the reliability of the eigenvalue calculations it is important to study the sensitivity of the eigenvalues to small perturbations, i.e., to study the pseudospectra. Suppose we have a square n -by- n complex matrix, $D \in \mathbb{C}^{n \times n}$. The eigenvalues of D satisfy the following definition:

$$\begin{aligned} \sigma(D) &= \{z \in \mathbb{C} : \det(zI - D) = 0\} \\ &= \left\{ \text{points where } (zI - D)^{-1} \text{ is undefined} \right\}. \end{aligned}$$

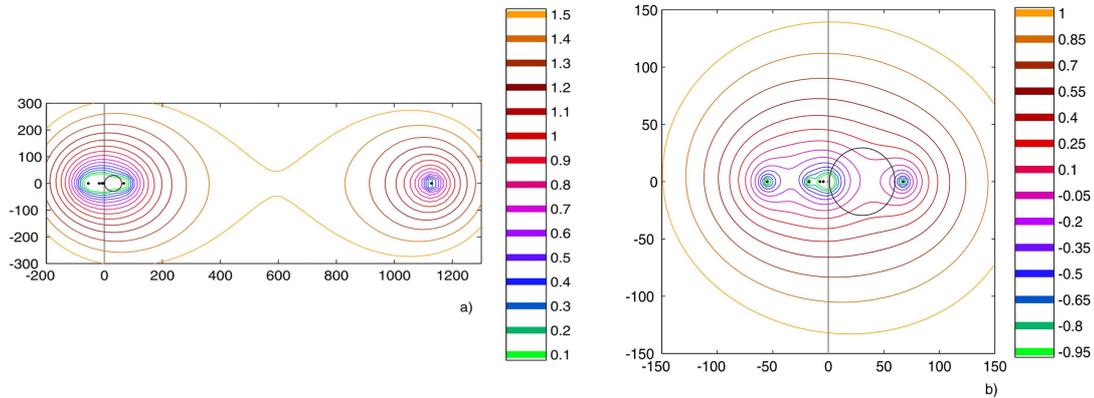


Figure 8: a) Eigenvalues and pseudospectrum for the stable case of a stationary bifurcation. b) Detail of Fig. 8a). The rest of the parameters are $Pr=1$, $\Gamma=14.70$, $B=0.05$, $\delta=0.03$, $b=0.4$ $k=19$ and $R=1.465 \cdot 10^4$.

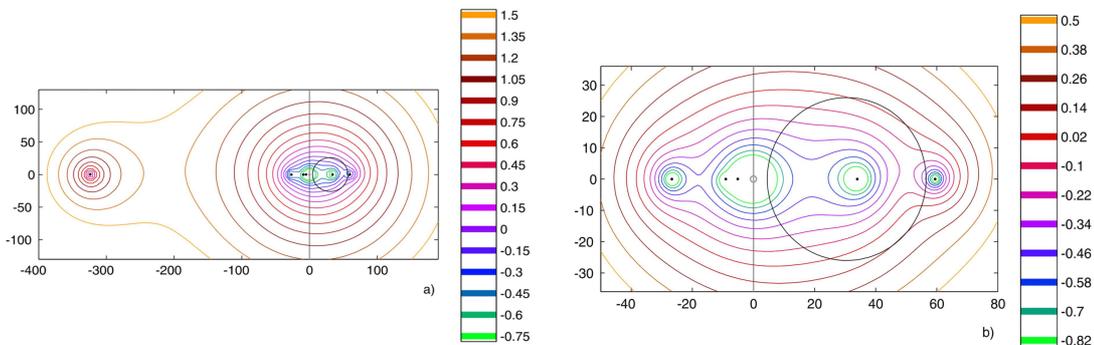


Figure 9: a) Eigenvalues and pseudospectra for the unstable case of a stationary bifurcation. b) Detail of Fig. 9a). The rest of the parameters are $Pr=1$, $\Gamma=14.70$, $B=0.05$, $\delta=0.03$, $b=0.4$ $k=19$ and $R=1.465 \cdot 10^4$.

If z is an eigenvalue of D , then by convention the norm of $(zI - D)^{-1}$ can be defined as infinity [25, 27, 28]. If $\|(zI - D)^{-1}\|$ is finite but very large z should be close to an eigenvalue. This description leads to the definition of the ϵ -pseudospectrum of D :

$$\Lambda_\epsilon(D) = \left\{ z \in \mathbb{C} : \|(zI - D)^{-1}\| \geq \epsilon^{-1} \right\}.$$

Further details of the ϵ -pseudospectrum may be found in [25, 27, 28]. In Figs. 7, 8 and 9 pseudospectra plots are shown. The eigenvalues are plotted as black dots in the complex plane μ and colored lines mark the boundaries of various pseudospectra. The color bar on the right indicates the \log_{10} of each boundary, so in Fig. 7 we draw the boundaries of the ϵ -pseudospectra for $\log_\epsilon \epsilon$ from -3 to 0 with steps of 0.3 . In Figs. 8a) and 9a) $\log_\epsilon \epsilon$ goes from -1 to $3/2$. Note that for small values of ϵ , the pseudospectrum is connected and very near to the calculated eigenvalues. This means the eigenvalue results and the bifurcation detection are highly reliable.

5 Conclusions

We have developed an efficient numerical method for computing the eigenvalues of the generalized eigenvalue problem arising in the description of instabilities developed in a fluid heated non-homogeneously from below. The partial differential equations modeling this problem are discretized with a Chebyshev collocation method. After numerically computing the steady states at certain values of the external parameters, its linear stability is formulated in terms of a generalized eigenvalue problem. This eigenvalue problem presents an original block matrix structure such that one of the submatrices is singular. The preconditioning of the eigenvalue problem with a modified Cayley transformation and the use of a second transformation for the 'infinite' eigenvalues allows the application of the Arnoldi method. However some care is necessary as not all the infinite eigenvalues disappear. We have designed an easy to use algorithm from which the critical eigenvalues determining whether the steady flow is stable or unstable and the bifurcation points are obtained. Both stationary and oscillatory bifurcations are detected. A comparison of the computing time between the standard QZ and the generalized Arnoldi method shows that the latter is significantly more efficient. Pseudospectra calculations confirm the reliability of the eigenvalues and bifurcations. The computational advantage of the generalized Arnoldi method becomes of great interest in studies such as that of Ref. [20] where an intensive study of the solution bifurcations is performed depending on several external physical parameters.

Acknowledgments

MCN and HH are partially supported by the Research Grants MCYT (Spanish Government) MTM2006-14843-C02-01 and CCYT (JC Castilla-La Mancha) PAC-05-005, which include FEDER funds. AMM thanks support by Grants from CSIC (PI-200650I224), Comunidad de Madrid (SIMUMAT S-0505-ESP-0158) and Junta de Castilla-La Mancha (PAC-05-005-2).

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