Computers & Fluids 39 (2010) 215-224

Contents lists available at ScienceDirect

# **Computers & Fluids**

journal homepage: www.elsevier.com/locate/compfluid

## An efficient spectral code for incompressible flows in cylindrical geometries

### I. Mercader \*, O. Batiste, A. Alonso

Universitat Politècnica de Catalunya, Dep. Fisica Aplicada, Jordi Girona 1-3, 08034 Barcelona, Spain

#### ARTICLE INFO

Article history: Received 17 November 2008 Received in revised form 12 June 2009 Accepted 25 August 2009 Available online 1 September 2009

#### ABSTRACT

An efficient and accurate numerical scheme is proposed to solve the incompressible Navier–Stokes equations in a bounded cylinder. The scheme is based on a projection method formulated in primitive variables to maintain the incompressibility constraint, with a second-order semi-implicit scheme for the time integration, and a pseudospectral approximation for the space variables. The Chebyshev-collocation method applied in the radial and axial directions, and the Fourier–Galerkin approximation used in the azimuthal direction lead to a sequence of two-dimensional Helmholtz and Poisson equations for every azimuthal coefficient that are solved by a diagonalization technique. Radial expansions are considered in the diameter of the cell in order to avoid clustering about the axis, and the number of points are selected to ensure that r = 0 is not a collocation point. A minimal number of regularity conditions are timposed implicitly at the origin by forcing the proper parity of the Fourier expansions in the radial direction. The method has been tested on analytical solutions and compared with other reliable three-dimensional results. The improvements introduced in the treatment of the spatial discretization reduce significantly the difficulty of implementation of the code, and facilitate the use of high resolutions. Different boundary conditions can also be easily implemented.

© 2009 Elsevier Ltd. All rights reserved.

#### 1. Introduction

In this paper, we present an efficient and accurate spectral scheme to solve time-dependent three-dimensional thermal convection of an incompressible fluid contained in an enclosed cylinder. The code uses a projection method formulated in primitive variables, and takes into account the odd-even radial parity of the Fourier coefficients. Stationary solutions and rotating waves are also efficiently computed, so branch-following algorithms can be easily applied. To develop the code, we have taken advantage of our previous experience with fractional step techniques applied to spectral collocation methods in different geometries. In addition, we have made some improvements in the spatial treatment of the equations in order to increase efficiency as compared with other available cylindrical codes. The main characteristics of the resulting code are: (i) simplicity of implementation; a minimum prepossessing is required; (ii) accuracy; spectral methods provide much better resolution properties and accuracy than finite difference/volume methods; (iii) efficiency in large-scale simulations; there are no severe time-step restrictions even in the simulation of complex flows when using large resolutions, due to the absence of clustering at the origin; and (iv) flexibility; different boundary conditions can easily be implemented.

Different methods can be applied to fulfil numerically the divergence-free condition required in incompressible fluid dynamics. Below we detail our choice for the projection scheme and for the spatial discretization by comparison with different alternatives found in the literature. In a first group of methods, the velocity field is written in terms of scalar potentials such that the divergence-free condition is satisfied by construction. The streamfunction-vorticity formulation in two-dimensional problems, and the velocity decomposition into toroidal and poloidal potentials [1] in the three-dimensional case are well-known examples of this group. The method is attractive because pressure is not present in the equations; however, in bounded systems it leads to systems of partial differential equations of higher order whose boundary conditions are coupled. Marqués et al. [2] used this formulation to perform a linear stability analysis of cylindrical Rayleigh-Bénard convection. The resulting system was solved, but a slight deviation in the boundary conditions was present in the numerical implementation. Recently, Boronski and Tuckerman [3] solved the high-order magnetohydrodynamic equations exactly by separating the system, with the influence matrix technique, into a sequence of problems of lower order, each with its own boundary conditions. However, this procedure has large memory requirements and the complexity of the numerical code is considerable. Slightly different velocity potentials were introduced in [4] to prevent the coupling of the potentials in the boundary conditions. Rüdiger and Feudel used this formulation in the simulation of thermal convection in a cylinder [5], but resolution in this implementation was strongly limited due to the resulting coupled equations. Petrov-Galerkin





<sup>\*</sup> Corresponding author. Tel.: +34 934016891; fax: +34 934016090. *E-mail addresses:* isabel@fa.upc.edu (I. Mercader), oriol@fa.upc.edu (O. Batiste), arantxa@fa.upc.edu (A. Alonso).

<sup>0045-7930/\$ -</sup> see front matter  $\odot$  2009 Elsevier Ltd. All rights reserved. doi:10.1016/j.compfluid.2009.08.003

methods and solenoidal Galerkin formulations are also based on building up a solenoidal velocity field through the construction of bases of trial functions that satisfy the incompressibility condition identically [6]. As far as the authors know, these methods have been successfully used in the computation of axially periodic flows in cylindrical and annular geometries [7], but they have not been implemented in bounded three-dimensional domains.

In a second group of methods, a primitive variable formulation of the equations is adopted. In this case, projection methods provide an interesting solution to overcome the velocity-pressure coupling problem, since they have the advantage that only one sequence of decoupled elliptic equations needs to be solved (see [8] for a recent overview of projection methods for incompressible flows). Examples of these methods are: the spectral code developed by López et al. for the Navier–Stokes equations in cylindrical coordinates [9], and the code developed by Serre and Pulicani [10] for thermal convection. The code we present here is based on a time-stepping method. In particular, we have implemented the improved projection scheme proposed in [11] (we used this method for the first time in the simulation of binary mixture convection in rectangular domains [12]), though any other time-splitting method could also be used, such as that proposed in [13].

The spatial discretization of the equations we have implemented deals with the main difficulties that arise in cylindrical geometry, without introducing additional complexity in the implementation of the code. Some key aspects of the spectral scheme under consideration (Chebyshev-collocation in the radial and vertical directions, Fourier-Galerkin in the azimuthal direction) should be emphasized. First, the radial expansions are considered in the diameter of the cell  $r \in [-R, R]$  rather than in its radius. In this way, excessive clustering of points near the center is avoided [14]. Second, the problem of singularity at the origin is avoided by ensuring that r = 0 is not a collocation point, and by taking into account the appropriate radial parity of the Fourier coefficients of the variables. This procedure forces the minimal number of regularity conditions at the origin that ensure the well-posedness of the formulation, and has the additional advantage that the size of the matrices is substantially reduced, while spatial resolution can be increased. This approach is known as unshifted Chebyshev polynomials of appropriate parity in [15]. Clustering is also avoided in the method followed in [9], where a suitable basis of Legendre polynomials is built up to perform a Galerkin technique in the radial direction, although the implementation of the code becomes more complex. In [10], the Chebyshev-collocation method is used, with Gauss-Lobatto points distributed over the radius of the cylinder. With spectral methods, the axis can also be avoided by using Gauss-Radau nodes [16]. Finally, the change of variables combining the radial and azimuthal components of the velocity field we use to obtain a predictor velocity yields Helmholtz equations, which can be straightforwardly diagonalized.

Spectral element methods for the space discretization of the equations have also been used for Navier–Stokes equations in cylindrical geometries [17], although the greater sophistication of these methods makes them more suitable for complex geometries. In fact, some care should be taken when applying these methods to study the bifurcation structure of a system. Assemat et al. [18] have recently reported some subtle numerical effects of the grid on the bifurcation diagrams when studying the patterns arising in Marangoni convection in circular and near circular domains. The difference in symmetry between the grid and the container can cause an artificial split in the bifurcation maps.

This paper is structured as follows. After introducing the physical problem in Section 2, the projection scheme and the time discretization of the equations are described in Section 3, while details of the spatial discretization are presented in Section 4. The procedure for computing steady solutions and rotating waves is described in Section 5. The numerical performance of the code is analyzed in Section 6, which also includes an extensive comparison with other numerical results. Some concluding remarks are given in Section 7.

#### 2. The physical problem

We consider Rayleigh–Bénard convection in a vertical cylinder of height *d* and radius *R*. The radial aspect ratio of the cylinder is defined as  $\Gamma = R/d$ . The cylinder is heated from below in the presence of a vertical gravitational force  $\mathbf{g} = -g\hat{\mathbf{e}}_z$ ,  $\Delta T$  being the temperature difference between the lids. By scaling length with the height of the layer *d*; time with the vertical thermal diffusion time  $d^2/\kappa$ , where  $\kappa$  is the thermal diffusivity, and temperature with  $\Delta T$ , then the non-dimensional equations that describe the evolution of the velocity field  $\mathbf{u} = (u, v, w)$  in cylindrical coordinates  $(r, \theta, z)$  and the deviation of the temperature  $\Theta$  from the linear profile in the Boussinesq approximation, are

$$\nabla \cdot \mathbf{u} = \mathbf{0},\tag{1a}$$

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \sigma \nabla^2 \mathbf{u} + Ra\sigma \Theta \hat{\mathbf{e}}_z + \mathbf{F}, \tag{1b}$$

$$\partial_t \Theta + (\mathbf{u} \cdot \nabla)\Theta = \mathbf{w} + \nabla^2 \Theta, \tag{1c}$$

where **F** is an externally imposed force. The two dimensionless parameters describing thermal convection are the Rayleigh number Ra, and the Prandtl number  $\sigma$ , defined as

$$Ra = \frac{\alpha \Delta Tgd^3}{\kappa v}, \quad \sigma = \frac{v}{\kappa}, \tag{2}$$

where  $\alpha$  is the thermal expansion coefficient and v is the kinematic viscosity. The Rayleigh number is the control parameter of the system and measures the strength of the imposed temperature gradient, while the Prandtl number relates momentum diffusion to thermal diffusion. If the cylinder is rotating around the axis at a constant rotation rate  $\omega$ , the same system of Eqs. (1) can be used to describe the evolution of the fields **u** and  $\Theta$  in the rotating frame by including the non-inertial Coriolis and centrifugal terms

$$2\sigma\Omega \mathbf{u} \times \hat{\mathbf{e}}_z - \frac{\sigma F r R a}{\Gamma} (1 - z + \Theta) r \hat{\mathbf{e}}_r$$
(3)

in **F**. Two additional non-dimensional parameters appear in this case, the Coriolis number  $\Omega$  and the Froude number *Fr*:

$$\Omega = \frac{\omega d^2}{v}, \quad Fr = \frac{\omega^2 R}{g}.$$

Finally, it is assumed that conditions consistent with the incompressibility of the fluid are imposed on the boundaries. However, the introduction of new variables combining the radial and azimuthal components of the velocity field, as detailed in the next section, requires that u and v satisfy boundary conditions of the same type, i.e.

$$au + b\partial_n u = h_u$$
,  $av + b\partial_n v = h_v$ .

This requirement is satisfied when Dirichlet boundary conditions are specified at the lateral boundary, which besides rigid walls is indeed the case in many interesting situations in fluid dynamics, such as the flow in a cylinder with a rotating or sliding wall, or when fluid is injected across the boundary. The only limitation consists in specifying different kinds of boundary conditions for the azimuthal and radial components of the velocity, as is the case with stress-free boundary condition in the cylinder wall, but this will only arise in some idealized geophysical problems and is unlikely to occur in a laboratory situation. I. Mercader et al./Computers & Fluids 39 (2010) 215-224

#### 3. The temporal discretization and the projection scheme

For the time discretization, a second order stiffly-stable scheme is used [13], which leads to the following system:

$$\nabla \cdot \mathbf{u}^{n+1} = \mathbf{0},\tag{4a}$$

$$\frac{3\mathbf{u}^{n+1} - 4\mathbf{u}^n + \mathbf{u}^{n-1}}{2\Delta t} = -2NL(\mathbf{u}^n) + NL(\mathbf{u}^{n-1}) - \nabla p^{n+1} + \sigma \nabla^2 \mathbf{u}^{n+1} + Ra\sigma \Theta^{n+1} \hat{\mathbf{e}}_z + \mathbf{F}_1^{n+1} + 2\mathbf{F}_2^n - \mathbf{F}_2^{n-1}, \qquad (4b)$$

$$\frac{3\Theta^{n+1} - 4\Theta^n + \Theta^{n-1}}{2\Delta t} = -2NL(\mathbf{u}^n, \Theta^n) + NL\left(\mathbf{u}^{n-1}, \Theta^{n-1}\right) + 2w^n - w^{n-1} + \nabla^2 \Theta^{n+1}, \qquad (4c)$$

where we have split **F** into two parts:  $F_1$  is independent of the velocity field whereas  $F_2$  depends on it. Thus, the centrifugal force is treated implicitly, while the Coriolis force is treated explicitly.

This time-stepping method, hereafter referred to as IPS, was proposed by Hugues and Randriamampianina [11] and constitutes an improvement on the projection scheme proposed by Goda [19] and implemented by Gresho [20] in finite element approximations. The fractional steps consist of a predictor for the pressure, directly derived from the Navier–Stokes equations with the Neumann boundary condition [13]; a predictor for an intermediate velocity field from the momentum equation, which takes into account the predicted pressure obtained from the previous time level, and finally a projection step with an explicit evaluation of the final divergence-free velocity field. We previously used this method to analyze two-dimensional oscillatory pure and binary fluid convection, both in large aspect ratio containers heated from below [12,21,22] and in laterally heated cavities [23,24].

In this section, we detail the fractional steps of the second order splitting method when the improved projection scheme (IPS) proposed in [11] is used.

•  $\Theta^{n+1}$  is obtained from the Helmholtz-type problem

$$\left(\nabla^{2} - \frac{3}{2\Delta t}\right)\Theta^{n+1} = 2NL(\mathbf{u}^{n},\Theta^{n}) - NL\left(\mathbf{u}^{n-1},\Theta^{n-1}\right) - 2w^{n} + w^{n-1} - \frac{4\Theta^{n} - \Theta^{n-1}}{\Delta t},$$
(5)

• A preliminary pressure field is obtained from the Navier–Stokes and continuity equations

$$\nabla^{2} \bar{p}^{n+1} = \nabla \cdot \left\{ -2NL(\mathbf{u}^{n}) + NL(\mathbf{u}^{n-1}) + Ra\sigma \Theta^{n+1} \hat{\mathbf{e}}_{z} + \mathbf{F}_{1}^{n+1} + 2\mathbf{F}_{2}^{n} - \mathbf{F}_{2}^{n-1} + \frac{4\mathbf{u}^{n} - \mathbf{u}^{n-1}}{2\Delta t} \right\},$$
(6)

with a boundary condition for the pressure obtained from the semi-discrete equation (4b), where the viscous linear term is rewritten as a solenoidal part approximated by an explicit scheme and an irrotational part approximated by an implicit scheme of appropriate order.

• A predictor velocity field  $\mathbf{u}^* = (u^*, v^*, w^*)$  is calculated from the Navier–Stokes equation by including the predictor pressure  $\bar{p}$  with the actual boundary conditions

$$\left( \nabla^2 - \frac{3}{2\sigma\Delta t} \right) \mathbf{u}^* = \sigma^{-1} \nabla \bar{p}^{n+1} + \sigma^{-1} \left[ 2NL(\mathbf{u}^n) - NL(\mathbf{u}^{n-1}) - \mathbf{F_1^{n+1}} - 2\mathbf{F_2^n} + \mathbf{F_2^{n-1}} - \frac{4\mathbf{u}^n - \mathbf{u}^{n-1}}{2\Delta t} \right] - Ra\Theta^{n+1} \hat{\mathbf{e}}_z.$$
(7)

Since the velocity components (u, v) are coupled in the linear viscous term,

$$\left(\nabla^2 \mathbf{u}^*\right)_r = \nabla^2 u^* - \frac{2}{r^2} \frac{\partial v^*}{\partial \theta} - \frac{u^*}{r^2}, \quad \left(\nabla^2 \mathbf{u}^*\right)_{\theta} = \nabla^2 v^* + \frac{2}{r^2} \frac{\partial u^*}{\partial \theta} - \frac{v^*}{r^2},$$

it is convenient to introduce a new set of complex functions following [25]

$$u_{+}^{*} = u^{*} + iv^{*}, \quad u_{-}^{*} = u^{*} - iv^{*}.$$

Under the new unknowns, system (7) gives rise to decoupled equations for  $(u_+^*, u_-^*, w^*)$ .

• In the correction step, the system

$$\frac{3(\mathbf{u}^{n+1} - \mathbf{u}^*)}{2\Delta t} = -\nabla(p^{n+1} - \bar{p}^{n+1}),$$
(8a)  
 $\nabla \cdot \mathbf{u}^{n+1} = 0.$ 
(8b)

is solved with the first equation satisfied in the interior as well as in the boundary, with the correct boundary condition for the normal component of the velocity field. This system gives rise to a Poisson equation for variable  $\Phi = 2/3\Delta t(p^{n+1} - \bar{p}^{n+1})$ , with Neumann boundary condition  $\partial \Phi / \partial n = 0$ . Finally, the corrected pressure and velocity fields,  $p^{n+1}$  and  $\mathbf{u}^{n+1}$ , are calculated from the value of  $\Phi$ 

$$p^{n+1} = \bar{p}^{n+1} + \frac{3\Phi}{2\Delta t},\tag{9a}$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \nabla \Phi. \tag{9b}$$

#### 4. Spatial discretization

The cylindrical components of the velocity field and temperature are functions of the cylindrical coordinates  $(r, \theta, z)$ . The azimuthal dependence is solved by using Fourier expansions. For u, w,  $\Theta$  the expansions are of the type:

$$\Phi(r,\theta,z) = \sum_{k=-n_{0}/2}^{n_{0}/2-1} F_{k}(r,z) e^{ik\theta},$$
(10)

where the complex functions  $F_k(r, z)$  satisfy

$$\begin{split} F_0(r,z) &= f_0(r,z), \\ F_{-n_{\theta}/2}(r,z) &= f_{n_{\theta}-1}, \\ F_k(r,z) &= f_{2k-1}(r,z) + \mathrm{i} f_{2k}(r,z), \quad \text{for } k = 1: n_{\theta}/2 - 1 \\ F_{-k}(r,z) &= \overline{F}_k(r,z), \quad \text{for } k = 1: n_{\theta}/2 - 1, \end{split}$$

and where the over bar means complex conjugate. This gives  $n_{\theta}$  independent real-valued functions  $f_i$ , with l = 0:  $n_{\theta} - 1$  (l = 2k - 1 for the real part and l = 2k for the imaginary part), for fixed values of (r, z).

It is convenient to choose a different expansion for the azimuthal velocity v

$$\nu(r,\theta,z) = i \sum_{k=-n_{\theta}/2}^{n_{\theta}/2-1} F_k(r,z) e^{ik\theta},$$
(11)

where the complex functions  $F_k(r, z)$  now satisfy

$$\begin{split} F_0(r,z) &= \mathrm{i} f_0(r,z), \\ F_{-n_\theta/2}(r,z) &= \mathrm{i} f_{n_\theta-1}, \\ F_k(r,z) &= f_{2k-1}(r,z) + \mathrm{i} f_{2k}(r,z), \quad \text{for } k = 1: n_\theta/2 - 1, \\ F_{-k}(r,z) &= -\overline{F}_k(r,z) \quad \text{for } k = 1: n_\theta/2 - 1. \end{split}$$

Different expansions of the components u, w and v are used so that only purely real or purely imaginary parts of the unknowns appear in the equations. For example, the divergence free equation for the Fourier mode k splits into two equations,

$$r^{-1}\partial_r(ru_{2k-1}(r,z)) + \partial_z(w_{2k-1}(r,z)) - kr^{-1}v_{2k-1}(r,z) = 0,$$
  
$$r^{-1}\partial_r(ru_{2k}(r,z)) + \partial_z(w_{2k}(r,z)) - kr^{-1}v_{2k}(r,z) = 0.$$

In the same manner, the real (imaginary) part of the complex *k*-Fourier mode of  $u_{\pm}^*$ ,  $(U_{\pm}^*)_k(r, z)$ , involves only the real (imaginary) parts of the *k*-Fourier modes of  $u^*$  and  $v^*$ . Thus,

$$(U_{\pm}^{*})_{k}(r,z) = (u_{2k-1}^{*}(r,z) \mp v_{2k-1}^{*}(r,z)) + i(u_{2k}^{*}(r,z) \mp v_{2k}^{*}(r,z))$$

With respect to the radial dependence, a scalar function *f* on a disk is known to be analytic at the origin if the following regularity conditions of the Fourier coefficients are satisfied:  $F_k(r) = r^{|k|}p(r^2)$ , where *p* is a polynomial [15,9]. These conditions arise as a consequence of the singularity of the cylindrical coordinates at r = 0. An overview of the different options for dealing with the apparent singularity using spectral methods can be seen in [15]. The regularity conditions can be imposed for all azimuthal modes by using expansions in appropriate special functions [26,27], although the practical implementation is far from simple. Other approaches impose the regularity conditions only for some of the most dangerous modes [28]. In our approach, named unshifted Chebyshev polynomials of appropriate parity in [15], only the minimal set of regularity conditions on the axis needed for the well-posedness of our weak formulation of Navier-Stokes equations is imposed; the appropriate parity of the Fourier coefficients is forced, and clustering at the origin is avoided. Furthermore, the implementation is very simple.

Chebyshev expansions in *r* and *z* are assumed for the radial and vertical dependence of the variables, where the unknowns are the values of the azimuthal coefficients at the collocation points  $r_j, z_l$ . Following the method described in [29] in the formulation proposed by [14], the radial expansions are considered in  $r \in [-R, R]$ , and the appropriate parity at the origin is forced. It is important to notice that  $(r, \theta + \pi, z)$  represents the same point as  $(-r, \theta, z)$ , so any scalar function satisfies  $F(r, \theta + \pi, z) = F(-r, \theta, z)$ . More care is needed for vector quantities, since the radial and azimuthal basis vectors are reversed,  $\hat{r}(r, \theta + \pi, z) = -\hat{r}(-r, \theta, z)$  and  $\hat{\theta}(r, \theta + \pi, z) = -\hat{\theta}(-r, \theta, z)$ . As a result, the complex Fourier coefficients  $F_k(r, z)$  of variables *u* and *v* must have the same parity as k + 1 and those of variables *w* and  $\Theta$  the same parity as *k*.

Assuming a radial-Chebyshev expansion in  $2n_r + 2$  polynomials (from  $j = 0 : 2n_r + 1$ ), equations are written in  $r_j = R \cos(\pi j)/(2n_r + 1)$  with  $j = 0 : n_r$ . By ensuring that the origin is never a collocation point, the problem of singularity at r = 0 is avoided. Additionally, the points are not clustered in the radial direction near the pole. The radial derivatives of the functions are calculated using a matrix multiplication method. Instead of using a single  $(2n_r + 2) \times (2n_r + 2)$  Chebyshev differentiation matrix, two different matrices of dimension  $(n_r + 1) \times (n_r + 1)$  are built, one for odd parity functions (even Fourier coefficients of u and v, and even Fourier coefficients of w and  $\Theta$ ).

As a result of the splitting, several Helmholtz and Poisson equations must be solved. For the real and imaginary parts of every Fourier mode k of temperature, of the vertical component of the velocity field and of pressure, these equations are written as

$$\partial_{rr}f + 1/r\partial_r f - k^2/r^2 f + \partial_{zz}f + af = h, \qquad (12a)$$

whereas for the real and imaginary parts of the Fourier mode k for variables  $u_{\pm}^*$  they are

$$\partial_{rr}g + 1/r\partial_{r}g - (k\pm 1)^{2}/r^{2}g + \partial_{zz}g + ag = h.$$
(12b)

To solve these equations, some regularity conditions need to be imposed at the origin. By expanding the  $1/r^m$  terms in Taylor series for f(r) and g(r), the regularity conditions reduce to

$$f'(0) = 0$$
, if  $k = 0$ ;  $g'(0) = 0$ , if  $|k \pm 1| = 0$ , (13a)

$$f(0) = 0$$
, if  $|k| = 1$ ;  $g(0) = 0$ , if  $|k \pm 1| = 1$ , (13b)

$$f(0) = f'(0) = 0$$
, if  $|k| > 1$ ;  $g(0) = g'(0) = 0$ , if  $|k \pm 1| > 1$ .  
(13c)

As stated in [30], it suffices to consider only one of the last two regularity conditions, since any regular solution of Helmholtz and Poisson differential equations will satisfy both. Thus, if one condition is imposed and a regular solution is obtained, it will necessarily satisfy both regularity conditions. It is important to notice that although pole conditions are not written explicitly in the code, the parity of the Fourier coefficients of the functions ensures that conditions (13a) and (13b) and one of the conditions (13c) are satisfied. The Helmholtz and Poisson equations for every Fourier mode k are solved using a diagonalization technique in the two coordinates r and z [31]. Unlike in the cylindrical code of Serre and Pulicani [10], where the predictor velocity step for the combined variables  $u_{\perp}^*$  is not solved, all the eigenvalues of the matrix involving the radial part in the differential equation (12) are real, and the diagonalization technique is straightforward to apply. Notice that due to the coupling between the radial and azimuthal part, for every Fourier mode k we need to calculate the eigenvalues, the eigenvectors and the inversion of the corresponding matrix of the radial part. This preprocessing step is done once and the results stored before starting the time integration. Accuracy in the computation of these eigenvalues and eigenvectors, obtained with the pole conditions commented above, is essential to ensure the correct treatment of the origin.

#### 5. Computing steady solutions and rotating waves

An efficient method for the computation of steady states of the Navier–Stokes equations was recently introduced by Tuckerman and collaborators [32–34]. The method uses a first order semi-implicit time scheme for the calculation of a Stokes preconditioner, which allows a matrix-free inversion of the preconditioned Jacobian. This idea can be straightforwardly applied to the computation of rotating waves, provided that the new terms arising from the change in the frame of reference are properly treated in the time-stepping algorithm. The method is based on solving in a very efficient manner the system resulting from each Newton iteration

$$(\mathbf{L} + \mathbf{N}_{\mathbf{X}})\,\boldsymbol{\delta}\mathbf{X} = (\mathbf{L} + \mathbf{N})\mathbf{X},\tag{14a}$$

$$\mathbf{X} \leftarrow \mathbf{X} - \boldsymbol{\delta} \mathbf{X}. \tag{14b}$$

Here, **X** represents the spatially discretized fields,  $\delta X$  the correction fields in every Newton iteration; **L** and **N** the spatially discretized linear and non-linear operators, respectively, and **N**<sub>X</sub> the Jacobian of the non-linear term evaluated at **X**.

Notice that the first order semi-implicit time scheme

$$\frac{\mathbf{X}^{n+1} - \mathbf{X}^n}{\Delta t} = \mathbf{L}\mathbf{X}^{n+1} + \mathbf{N}\mathbf{X}^n,\tag{15}$$

where *n* determines the time instant,  $t_{n+1} = t_n + \Delta t$ , can be rewritten as

$$\frac{\mathbf{X}^{n+1} - \mathbf{X}^n}{\Delta t} = (\mathbf{I} - \Delta t \mathbf{L})^{-1} (\mathbf{L} + \mathbf{N}) \mathbf{X}^n.$$
(16)

If  $\mathbf{P} = (\mathbf{I} - \Delta t \mathbf{L})^{-1}$ , with a large value of  $\Delta t$ , is used as a preconditioner of system (14a) in every Newton iteration

$$(\mathbf{I} - \Delta t\mathbf{L})^{-1}(\mathbf{L} + \mathbf{N}_{\mathbf{X}})\,\delta\mathbf{X} = (\mathbf{I} - \Delta t\mathbf{L})^{-1}(\mathbf{L} + \mathbf{N})\mathbf{X},\tag{17}$$

and relationship (16) is taken into account, then the right-hand-side of (17) can be obtained by carrying out a time step evolution, and the left-hand-side by carrying out a linearized time step. In this way, the linear system (17) can be solved by using a matrix-free method [35], and neither the building of the Jacobian matrix  $(\mathbf{L} + \mathbf{N}_{\mathbf{X}})$  nor its storage are needed.

I. Mercader et al. / Computers & Fluids 39 (2010) 215-224

To calculate rotating waves, we propose the method described in our recent work [36]. Since the dependence of any variable  $\chi$ in a rotating wave on coordinate  $\theta$  and time *t* is of the form  $\chi_{\rm RW}(x,y,z,t) = \chi_{\rm RW}(\theta - \omega' t,y,z)$ , by letting  $\tilde{\theta} = \theta - \omega' t$  in the governing equations, the time derivative of  $\chi$  in the associated evolution equation becomes  $-\omega' \partial_{\bar{\theta}} \chi$ . Thus, we obtain a steady system of equations in the new spatial coordinates  $\tilde{\theta}$ , y, and z. The unknown angular velocity  $\omega'$  can be determined by adding an equation to fix the phase of the solution. To do this, we typically force the real or imaginary part of a Fourier azimuthal coefficient at a fixed point (r, z) to be zero. Special care must be taken in the selection of the coefficient and point in order to prevent the value of the coefficient at that point from being previously fixed by any of the symmetries of the solution. Once we have converted the evolution equations into a steady system, we can apply the standard procedures to solve these new equations. We propose that this new term receive the same numerical treatment as the advective non-linear terms  $\mathbf{u} \cdot \nabla \boldsymbol{\gamma}$ , both in the Navier–Stokes equations and in the rest of conservation equations.

We have used this method to calculate and follow by continuation both steady solutions and travelling waves in several two dimensional problems [23,37–40]. It has very recently been used to analyze three dimensional steady convection in a vertical cylinder [41].

#### 6. Numerical tests

In this section, we present some tests performed with the cylindrical code in order to check the accuracy of the solutions and to prove the spectral convergence obtained with the full time dependent code. We also present some numerical tests in which a comparison with recent reported results, both in purely hydrodynamic problems and in thermo-convective problems, has been made.

#### 6.1. Accuracy and spectral convergence

In order to check the accuracy of the solutions obtained with the numerical code, we first show the convergence properties of the Poisson and Helmholtz solvers, on which the splitting scheme is based. We show results for the maximum error as a function of the radial and vertical number of points displaying the expected spectral convergence; the same behaviour is also obtained in the azimuthal direction. The test problem used is  $\nabla^2 u = f$ , with  $u = \sin^4(r) \exp(2z) \sin 2\theta$ . We compare u with the numerical solution obtained by solving the problem numerically using f calculated analytically. The results are presented in Tables 1 and 2 and displayed in Fig. 1, where the expected spectral convergence can be seen.

In order to show that the scheme also retains the spectral accuracy when applied to a fully non-linear solution, we have chosen a solution obtained with our code in a Rayleigh–Bénard configuration. This solution, described in Section 6.2, can be seen in Fig. 6a and corresponds to a pattern of seven straight rolls. The total kinetic energy associated to every azimuthal mode can be seen in Fig. 2a, while in Fig. 2b we show the spectral Chebyshev amplitudes for the dominant azimuthal mode of the kinetic energy, for

**Table 1** Maximum error for different  $n_r$  with  $n_{\theta} = 20$  and  $n_z = 20$ .

		-	
n <sub>r</sub>	max(E)	n <sub>r</sub>	max(E)
3	4.423723	11	$2.831639 \times 10^{-5}$
5	1.553011	13	$1.131021 \times 10^{-10}$
7	$1.43994  imes 10^{-1}$	15	$2.478102 \times 10^{-13}$
9	$3.304688 \times 10^{-3}$		

Maximum error for different  $n_z$  with  $n_{\theta} = 20$  and  $n_r = 21$ .

n <sub>z</sub>	max(E)	nz	max(E)
8	0.1590711	16	$1.564922 \times 10^{-8}$
10	0.004306517	18	$1.482476 \times 10^{-10}$
12	$8.471913 \times 10^{-5}$	20	$1.432454 \times 10^{-11}$
14	$1.288486 \times 10^{-6}$		

radial coefficients (crosses), and for axial coefficients (circles). These figures show clearly the expected exponential decay characteristic of spectral accuracy. The same solution is also used to show how the code treats flows having non-zero radial velocity components along the axis, as is the case for the central roll of this solution. The correct treatment of these flows is manifest in Fig. 3, where the projection of the velocity field is plotted on a plane perpendicular to the axis of the cylinder.

Finally, in order to show the computational performance of the present method, we give an example of the time required for a typical computation (see Table 3). Let us say that this time should be of the same order of magnitude as similar codes using similar semi-implicit splitting schemes together with diagonalization techniques for the solution of the diffusive operators. The main advantage of our method is the combination of this high efficiency with the prevention of clustering at the axis, as well as the easy and flexible implementation of different boundary conditions.

#### 6.2. Comparison with reported results

In this section, we present the results corresponding to several numerical tests in which a comparison with recent reported results, both in purely hydrodynamic problems and in thermo-convective problems, has been made. In the interests of brevity, we hereafter refer to a solution which is invariant under a rotation of  $2\pi/m$  as an *m* solution.

We start with the problem analyzed in [42,9], where the flow in an enclosed right-circular cylinder is driven by the rotation of one of its endwalls. The authors use a semi-implicit second-order projection scheme and a Fourier expansion in the azimuthal direction, while the axial and vertical directions are discretized with a Legendre expansion [9]. The Poisson-like equations are solved using a spectral-Galerkin method [43]. The flow for a fixed aspect ratio  $\Gamma = 1/3$  is computed at several Reynolds numbers *Re*, with  $Re = \omega_b R^2 / v$ , where  $\omega_b$  is the angular velocity of the bottom lid. Starting from the basic steady non-trivial axisymmetric flow, there is a supercritical Hopf bifurcation to an m = 4 rotating wave (RW) at Re = 2730. This mode can only be observed inside and around the strong jet close to the wall. By increasing the Reynolds number to Re = 2900, a secondary bifurcation takes place. It is a supercritical Neimark-Sacker bifurcation to a 2-torus; a modulated rotating wave (MRW). A second frequency appears, associated with the presence of the azimuthal mode m = 1, which becomes apparent in and near the axis. In our numerical test we reproduce the resecondary bifurcation. grid ported Using of а  $(n_r, n_\theta, n_z) = (64, 42, 64)$ , our results show that this instability occurs at  $Re \approx 3000$ , this value being obtained from the linear fitting of the values of the mean kinetic energy of the m = 1 mode near the bifurcation. Fig. 4 shows contours of the perturbation of axial velocity w (the azimuthal m = 0 Fourier mode has been subtracted) for the m = 4 rotating wave at Re = 2850 and for the modulated wave at Re = 3030, both obtained with our numerical code. Following the procedure in [43], the discontinuous boundary condition for the azimuthal velocity at the bottom corner is avoided by using a boundary layer function that provides a reasonable representation of the experimental gap.

I. Mercader et al. / Computers & Fluids 39 (2010) 215-224



Fig. 1. Accuracy of the Helmholtz solver. Maximum error in the solution of a test problem. (a) Dependence on radial resolution and (b) dependence on vertical resolution.



**Fig. 2.** Mode amplitudes of the kinetic energy corresponding to the steady solution shown in Fig. 6a ( $\Gamma$  = 4), insulating sidewalls,  $\sigma$  = 1, Ra = 1805.44 (in [5]). (a) Fourierazimuthal modes of the kinetic energy, and (b) Chebyshev amplitudes of the kinetic energy of the dominant Fourier component for the radial (crosses) and axial (circles) directions.



**Fig. 3.** (a) Representation of the horizontal component of the velocity field at  $z = 0.9 \Gamma$  for a steady convection solution with  $\Gamma$  = 4, insulating sidewalls,  $\sigma$  = 1, Ra = 1805.44 (in [5]). (b) Detail region marked with a dashed square in (a).

Table 3
Example of computation time for various resolutions using an Intel Pentium 4 CPU at
3.20 GHz with 1024K L2 cache.

n <sub>r</sub>	$n_{ heta}$	nz	$\Delta t$	Time	Computation time
32	80	32	$5 \times 10^{-3} t_d$	100t <sub>d</sub>	98 min 7.860 s
32	60	32	$5 \times 10^{-3} t_d$	100t <sub>d</sub>	69 min 28.834 s
32	40	32	$5 \times 10^{-3} t_d$	100 <i>t</i> <sub>d</sub>	45 min 49.918 s
24	80	24	$5 \times 10^{-3} t_d$	100 <i>t</i> <sub>d</sub>	68 min 10.420 s
16	80	16	$5 \times 10^{-3} t_d$	$100t_d$	46 min 4.195 s

The second problem we consider is the flow in an enclosed cylinder rotating at rate  $\omega$ , in which motions are driven by a contact top lid that differentially rotates at rate  $\omega_t$  (or which rotates in the inertial frame of reference at rate  $\omega^* = \omega + \omega_t$ ). We focus on the reference work [44], in which the counter-rotation of the top end-wall is investigated both numerically and experimentally. The authors used the same numerical method as in the previous problem [9]. The Reynolds number  $Re = \omega R^2 / v$  and aspect ratio  $\Gamma = R/d$  are held fixed (Re = 1000,  $\Gamma = 2$ ), and the rotation rate of the top lid, quantified through the non-dimensional parameter  $S = -\omega^* / \omega$ , is allowed to vary. A retrograde driving situation with  $\omega_t < -\omega$  is considered, so that *S* is positive. The numerical results in this paper show that the axisymmetric basic state undergoes a Hopf bifurcation as S is increased beyond 0.408, leading to an m = 4 rotating wave state (RW<sub>4</sub>). By continuing this branch to

220

I. Mercader et al./Computers & Fluids 39 (2010) 215-224



**Fig. 4.** Contour plots of the perturbation of the axial velocity (obtained by subtracting the m = 0 azimuthal mode) at z = 0.8d for (a) the rotating wave at Re = 2850 and (b) the modulated rotating wave at Re = 3030. (Numerical test related with results published in [42].)

larger values of S, the authors obtain a supercritical Neimark-Sacker bifurcation leading to a stable 2-torus at S = 0.441. The new solution is a modulated wave in which, among the new arising modes, the maximum kinetic energy corresponds to m = 5. As S is further increased, the modulated wave undergoes a reverse Neimark–Sacker bifurcation at  $S \approx 0.462$ , where the rotating wave RW<sub>4</sub> is re-stabilized. Although these bifurcations are numerically robust, the modulated wave could not be detected experimentally. In the numerical tests with our code, we are able to locate the bifurcation of the basic state to the m = 4 rotating wave, reproducing exactly the values of the RW4 wave frequencies included in Fig. 17 in [44], and identifying the two Neimark-Sacker bifurcations, which destabilize and re-stabilize the RW<sub>4</sub>. By using two different grids, (46,80,48) and (34,80,36), the Hopf bifurcation is obtained at S = 0.406. With regard to the Neimark–Sacker bifurca– tions, in Fig. 5a we plot the mean kinetic energies associated to modes m = 4 and m = 5 of the modulated wave as a function of the *S* parameter in the zone where the modulated wave appears. The range of S values where the modulated wave exists is almost the same as that reported in the aforementioned paper (see Fig. 11 in [44]). As an indication of the correct treatment of the origin, in Fig. 5b we plot the vertical vorticity at z = 0.6d of a modulated wave for S = 0.455. As can be observed, contour plots of vertical vorticity do not exhibit any oscillation around the origin.

In a second group of tests, we reproduce some of the states arising in thermal convection in a cylinder, which have been obtained by several authors using different numerical codes. We first show in Fig. 6a the pattern consisting of *seven straight rolls* obtained by Rüdiger and Feudel [5] in a cylinder of aspect ratio  $\Gamma$  = 4 and insulating sidewalls, at a Rayleigh number  $Ra \approx 1805.44$  for a fluid of Prandtl number  $\sigma$  = 1. Following [1,4], the authors solve the equations and boundary conditions using a spectral collocation code in a formulation based on the decomposition of the velocity field into its axisymmetric and non-axisymmetric parts, each of them expressed as a function of two potential functions

$$\mathbf{u} = \nabla \times \left( \chi(r,\theta,z) \, \mathbf{e}_{\mathbf{r}} + \psi(r,\theta,z) \, \mathbf{e}_{\mathbf{z}} + \frac{1}{r} f(r,z) \, \mathbf{e}_{\theta} \right) + \tilde{\nu}(r,z) \, \mathbf{e}_{\theta}.$$

The four potential functions and temperature are decomposed into Fourier functions in the azimuthal direction and Chebyshev polynomials in the r and z direction. The proper parity of the potentials and temperature with respect to r = 0 is forced in the decomposition.

The pattern in Fig. 6b corresponds to the so-called *star pattern*, obtained in a cylinder of aspect ratio  $\Gamma$  = 2 and perfectly conducting sidewalls for a fluid of Prandtl number  $\sigma$  = 6.7 by Boronska [45]. In order to reproduce the experimental results reported in [46], where the coexistence of several stable states for one configuration of control parameters was observed, the authors performed a sequence of simulations varying the initial state and the Rayleigh number. The six-armed star pattern was obtained when using an arbitrary perturbation as initial condition at *Ra* = 25,000. The code



**Fig. 5.** (a) Mean kinetic energy associated to azimuthal modes m = 4 (circles) and m = 5 (squares) of the modulated rotating wave as a function of the parameter *S*, which measures the counter-rotation of the top endwall. (b) Vertical vorticity of a modulated wave for S = 0.455. (Numerical test related with results published in [44].)

I. Mercader et al. / Computers & Fluids 39 (2010) 215-224



**Fig. 6.** Contour plots of the perturbation of the temperature at  $z = 0.5\Gamma$  for different convection patterns. (a) Steady solution,  $\Gamma = 4$ , insulating sidewalls,  $\sigma = 1$ , Ra = 1805.44 (in [5]), (b) steady solution,  $\Gamma = 2$ , perfectly conducting sidewalls,  $\sigma = 6.7$ , Ra = 25,000 (in [45]), (c) rotating wave (m = 2),  $\Gamma = 1$ , insulating sidewalls,  $\sigma = 6.8$ , Ra = 30,000,  $\Omega = 30$  (in [48]), and (d) rotating wave (m = 21),  $\Gamma = 5$ , insulating sidewalls,  $\sigma = 6.4$ , Ra = 21,380,  $\Omega = 274$  (in [49]).

used in that work is based on a spectral Tau method for the spatial discretization, where the deviation of temperature and the velocity components are expanded in Chebyshev polynomials in the radial and vertical directions, and in Fourier series in the azimuthal direction. In these expansions, the parity and the regularity conditions described in [47] are taken into account. For the time discretization, a semi-implicit second order scheme with an Adams–Bashforth explicit formula for the non-linear terms and buoyancy term and an implicit Crank–Nicholson scheme for the linear term were used. Incompressibility was ensured by using a influence matrix technique.

The pattern in Fig. 6c was obtained by Rüdiger and Knobloch [48] in a rotating cylinder with insulating walls, aspect ratio  $\Gamma$  = 1, Coriolis number  $\Omega$  = 30 and for a fluid of Prandtl number  $\sigma$  = 6.8. Centrifugal effects were neglected. The solution corresponds to the so-called '2 + 0' rotating wave, obtained at Ra = 30,000. This solution is only invariant under a rotation by  $\pi$ . The other symmetry of the m = 2 solution that bifurcates from the conductive state, a rotation through an angle  $\pi/2$  followed by a midplane reflection, is broken at  $Ra \approx$  4000. The numerical code used by these authors is the same as that used in [5] to obtain the solution in Fig. 6a.

The solution shown in Fig. 6c is also a rotating wave, an m = 21 wall mode obtained recently by Sánchez-Alvarez et al. [49] at Ra = 21,380, in a cylinder of aspect ratio  $\Gamma = 5$  with insulating sidewalls, rotating at a Coriolis number  $\Omega = 274$ , filled with a fluid of Prandtl number  $\sigma = 6.4$ . The spectral projection method used by the authors is described in [10]. A collocation-Chebyshev expansion is used both in the radial and axial directions, and a Fourier–Galerkin method is used for the azimuthal dependence. The

projection scheme employed to maintain the incompressibility constraint is the same as that in our code [11]. The main differences with our method concern the spatial treatment. In [10], the radial dependence of the functions was approximated by a Chebyshev expansion  $[0, \Gamma] \rightarrow [-1, +1]$  on a Gauss–Lobatto distribution of points, which generates a cluster of points near the axis. Additionally, a change of dependent variables was used to enforce a boundary condition at the axis for the m = 1 Fourier mode. This change of variables entails dealing with complex eigenvalues when the diagonalization technique is applied. Furthermore, the use of a predictor velocity for the radial and azimuthal velocity components, as opposed to the coupled variables  $u_{+}^*, u_{-}^*$  proposed in our code, forces a different time evaluation (implicit/explicit) in two parts of the radial diffusion term (see Appendix A in [10]).

Finally, as a test of the method for calculating and following steady solutions using continuation techniques, in Fig. 7 we show the bifurcation diagram giving the location and connection with the basic conductive state of the solution in Fig. 6a. In this figure, where we plot the value of the zero azimuthal mode of the temperature deviation at a fixed point (r, z) as a function of the Rayleigh number, three branches of steady solutions can be observed. This figure shows only the branches involved in the connection with the basic state, although additional branches of steady solutions not shown in this figure do exist for this range of parameter values. Since the steady solutions of every branch possess different symmetries, it is convenient to begin the description of the dynamics with a brief discussion of the symmetries of the system (non-rotating cylinder with insulating sidewalls). Equations and boundary conditions are equivariant under the group of symmetries  $\mathbf{O}(\mathbf{2}) \times \mathbf{Z}_{\mathbf{2}}$ , where  $\mathbf{O}(\mathbf{2})$  is generated by proper rotations  $R_{\alpha}$  and I. Mercader et al./Computers & Fluids 39 (2010) 215-224



**Fig. 7.** Bifurcation diagram for a non-rotating cylinder of  $\Gamma$  = 4, insulating sidewalls, and  $\sigma$  = 1. The steady solutions of the different branches possess different symmetries. Insets are contour plots of the deviation of temperature at mid height.

reflections  $\kappa$  with respect to vertical planes containing the axis, while **Z**<sub>2</sub> accounts for the reflections with respect to the midplane  $\gamma$ . These symmetries act on the fields *u*, *v*, *w*,  $\Theta$  as follows:

$$R_{\alpha}: (r, \theta, z) \to (r, \theta + \alpha, z), \quad (u, v, w, \Theta) \to (u, v, w, \Theta),$$
(18)

$$\kappa : (\mathbf{r}, \theta, \mathbf{z}) \to (\mathbf{r}, -\theta, \mathbf{z}), \quad (\mathbf{u}, \mathbf{v}, \mathbf{w}, \mathbf{\Theta}) \to (\mathbf{u}, -\mathbf{v}, \mathbf{w}, \mathbf{\Theta}),$$
(19)

$$\gamma: (r, \theta, z) \to (r, \theta, -z), \quad (u, v, w, \Theta) \to (u, v, -w, -\Theta).$$
(20)

Notice that this system is equivariant under the same group of symmetries as the two dimensional thermal convection in periodic channels is. Thus, the classification of the primary solution bifurcations, extensively studied in the 2D channel [50,51], can be directly applied to the cylinder.

The primary solution for this system (solid line), which appears in a supercritical pitchfork bifurcation of the conductive state at Ra = 1739.2, is an m = 1 solution invariant under the following transformations: reflections with respect to an appropriate vertical plane  $\kappa$ ; the midplane reflection combined with a rotation  $\gamma R_{\pi}$ , and the combination of both transformations  $\kappa \gamma R_{\pi}$ . Fig. 7 includes the contour plot of temperature deviation for a solution of the primary branch near the onset. This solution manifests the exponential dependence in  $\theta$  expected from the *m* = 1 modal dependence. Notice that, due to the  $\kappa \gamma R_{\pi}$  symmetry, the temperature deviation at mid height verifies  $\Theta(r, \theta, 0) = -\Theta(r, \theta + \pi, 0)$ . The primary solution loses stability at Ra = 1755.7 in a slightly subcritical bifurcation where symmetries  $\gamma R_{\pi}$  and  $\kappa \gamma R_{\pi}$  are broken and symmetry  $\kappa$  is maintained. The secondary branch (dot-dashed line) ends as a bifurcation at Ra = 1787.7, where stability is transferred to a new branch of solutions (dashed line), which are again invariant under  $\kappa$ ,  $\gamma R_{\pi}$  and  $\kappa \gamma R_{\pi}$ . By increasing the Rayleigh number from this bifurcation, we obtain the stable solution of seven straight rolls plotted in Fig. 6a.

A bifurcation diagram incorporating branches of several *m*-solutions bifurcating from the conductive state and their stability has recently been obtained in this system [41]. The aim of this work was to analyze the multiplicity of steady states in a cylinder of aspect ratio  $\Gamma$  = 2 and Prandtl number  $\sigma$  = 6.7, which corresponds to the physical setting of the experiment in [46]. As in the method presented in this paper, the authors use a first-order time-stepping formulation to calculate steady solutions. However, the formulation employed is based on an improved version of the algorithm

proposed in [52,53], with a central difference method on a staggered grid for the spatial discretization.

#### 7. Concluding remarks

In this paper, we present a spectral-projection method for solving the three-dimensional Navier-Stokes equations in an enclosed cylinder. The use of a projection scheme to fulfil the incompressibility constraint, and a pseudospectral approximation in combination with a diagonalization technique to solve the sequence of Helmholtz and Poisson equations resulting from the splitting, lead to an accurate and efficient code for computing unsteady 3D incompressible flows. Special emphasis is placed on keeping the development of the code simple, since a minimum preprocessing is required. The spatial discretization proposed in the scheme overcomes the difficulties arising from the presence of the pole singularity in cylindrical geometry without introducing additional complexity of implementation. Moreover, stationary solutions and rotating waves can also be efficiently computed, and branch following techniques can be applied straightforwardly. The code maintains spectral accuracy and gives a correct treatment of flows having a non-zero radial velocity. An excellent agreement is obtained when comparing our code with earlier studies in non-rotating and rotating cylindrical cavities in which flows are driven by a rotating lid or by a thermal gradient.

Finally, it is worth emphasizing that the flexibility of the code allows different boundary conditions to be implemented and new fields to be introduced in a simple way. Indeed, several groups are currently using the code in different problems with success. For instance, López et al. [54] have analyzed the role of the Eckhaus-Benjamin-Feir instability in the dynamics of the wall modes arising in convection in a regime dominated by the Coriolis force. Furthermore, the study of the role of centrifugal effects in rotating convection has been addressed in the work of Marqués et al. [40], and time-dependent boundary conditions have been implemented by Rubio et al. [55] in order to study the axisymmetric patterns arising in modulated rotating Rayleigh-Bénard convection. The complex spatiotemporal dynamics near the threshold of convection in binary fluid convection, which requires the introduction of a concentration field, has also been analyzed in a very recent work [56].

#### Acknowledgements

This work was supported by DGICYT under Grant FIS2006-08954 and by AGAUR under Grant 2005SGR-0024. We are grateful to F. Marqués and A. Meseguer for useful discussions.

#### References

- Marqués F. On boundary conditions for velocity potentials in confined flows: application to Couette flow. Phys Fluids A 1990;2:729–37.
- [2] Marqués F, Net M, Massaguer JM, Mercader I. Thermal convection in vertical cylinders. A method based on potentials. Comput Meth Appl Mech Eng 1993;110:157–69.
- [3] Boronski P, Tuckerman L. Poloidal-toroidal decomposition in a finite cylinder. I. Influence matrices for the magnetohydrodynamic equations. J Comput Phys 2007;227:1523–43.
- [4] Goldstein HF, Knobloch E, Mercader I, Net M. Convection in a rotating cylinder. Part 1. Linear theory for moderate Prandtl numbers. J Fluid Mech 1993;248: 583–604.
- [5] Rüdiger S, Feudel F. Pattern formation in Rayleigh-Bénard convection in a cylindrical container. Phys Rev E 2000;62:4927–31.
- [6] Canuto C, Hussaini MY, Quarteroni A, Zhang TA. Sectral methods in fluid dynamics. Berlin: Springer; 1988.
- [7] Meseguer A, Avila M, Mellibovsky F, Marqués F. Solenoidal spectral formulations for the computation of secondary flows in cylindrical and annular geometries. Eur Phys J Special Top 2007;146:249–59.
- [8] Guermond JL, Minev P, Shen J. An overview of projection methods for incompressible flows. Comput Meth Appl Mech Eng 2006;195:6011–45.

## Author's personal copy

224

#### I. Mercader et al. / Computers & Fluids 39 (2010) 215-224

- [9] López JM, Marqués F, Shen J. An efficient spectral-projection method for the Navier-Stokes equations in cylindrical geometries. II. Three dimensional cases. | Comput Phys 2002;176:384-401.
- [10] Serre E, Pulicani JP. A three-dimensional pseudospectral method for rotating flows in a cylinder. Comput Fluids 2001:30, 491-519.
- [11] Hugues S, Randriamampianina A. An improved projection scheme applied to pseudospectral methods for the incompressible Navier-Stokes equations. Int J Numer Methods Fluids 1998:28:501-21.
- [12] Batiste O, Net M, Mercader I, Knobloch E. Oscillatory binary fluid convection in large aspect-ratio containers. Phys Rev Lett 2001;81(11):2309-12.
- [13] Karniadakis GE, Israeli M, Orszag SA. High order splitting methods for the incompressible Navier-Stokes equations. J Comput Phys 1991;97:414-43.
- [14] Fornberg B. A practical guide to pseudospectral methods. Cambridge: Cambridge University Press; 1998. [15] Boyd J. Chebyshev and fourier spectral methods. New York: Dover; 2001.
- [16] Millour E, Labrosse G. Sensitivity of binary liquid thermal convection to confinement. Phys Fluids 2003;15:2791-802.
- [17] Blackburn HM, López JM. Symmetry breaking of the flow in a cylinder driven by a rotating endwall. Phys Fluids 2000;12(11):2698-701.
- [18] Assemat P, Bergeon A, Knobloch E. Nonlinear Marangoni convection in circular and elliptical cylinders. Phys Fluids 2007;19:104101. [19] Goda K. A multistep technique with implicit difference schemes for calculating
- two- and three-dimensional cavity flows. J Comput Phys 1979;30:76-95.
- [20] Gresho P. On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly consistent mass matrix. Part I. Theory. Int J Numer Meth Fluids 1990;11:587-620.
- [21] Alonso A, Batiste O, Meseguer A, Mercader I. Complex dynamical states in binary mixture convection with weak negative Soret coupling. Phys Rev E 2007;75:026310-1-026310-15.
- [22] Alonso A, Batiste O, Mercader I. Numerical simulations of binary fluid convection in large aspect ratio annular containers. Eur Phys J Special Top 2007:146:261-77.
- [23] Meca E, Mercader I, Batiste O, Ramírez-Piscina L. Blue sky catastrophe in double-diffusive convection. Phys Rev Lett 2004;93(23):450-1-4.
- [24] Mercader I, Batiste O, Ramírez de la Piscina L, Ruíz X, Rüdiger S, Casademunt J. Bifurcations and chaos in single-roll natural convection with low Prandtl number. Phys Fluids 2005;17:104108-1-104108-13
- [25] Orszag SA, Patera AT. Secondary instability of wall-bounded shear flows. J Fluid Mech 1983;128:347–85.
- [26] Matsushima T, Marcus PS. A spectral method for polar coordinates. J Comput Phys 1995;120:365-74.
- [27] Boronski P, Tuckerman L. Poloidal-toroidal decomposition in a finite cylinder. II. Discretization, regularization and validation. J Comput Phys 2007;227: 1544-66.
- [28] Prymak VG, Miyazaki T. Accurate Navier-Stokes investigation of transitional and turbulent flows in a circular pipe. I Comput Phys 1998:142:370-411
- [29] Trefethen LN. Spectral methods in Matlab. Philadelphia (PA): SIAM; 2000. [30] Mercader I, Net M, Falqués A. Spectral methods for high order equations.
- Comput Meth Appl Mech Eng 1991;91:1245–51.
- [31] Zaho S, Yedlin MJ. A new iterative Chebyshev spectral method for solving the
- elliptic equation ∇ (σ∇u) = f. J Comput Phys 1995;113:215–23.
  [32] Mamun CK, Tuckerman LS. Asymmetry and Hopf bifurcation in spherical Couette flow. Phys Fluids 1995;7:80–91.
- [33] Tuckerman LS, Barkley D. Bifurcation analysis for timesteppers. In: Doedel E, Tuckerman LS, editors. Numerical methods for bifurcation problems and largescale dynamical systems. Berlin: Springer; 2000. p. 453-66.

- [34] Bergeon A, Henry D, BenHadid H, Tuckerman L. Natural doubly diffusive convection in binary mixtures with Soret effect. J Fluid Mech 1998;375:143-77.
- [35] Frayssé V, Giraud L, Gratton S, Langou J. A set of GMRES routines for real and complex arithmetics on high performance computers. Technical Report TR/PA/ 03/3, CERFACS; 2003. Public domain software available on: www.cerfacs/ algor/Softs.
- [36] Mercader I, Batiste O, Alonso A. Continuation of travelling-wave solutions of the Navier-Stokes equations. Int J Numer Meth Fluids 2006:52:707-21.
- [37] Meca E, Mercader I, Batiste O, Ramírez-Piscina L. Complex dynamics in doublediffusive convection. Theoret Comput Fluid Dyn 2004;18:231-8.
- [38] Mercader I, Alonso A, Batiste O. Numerical analysis of the Eckhaus instability in travelling-wave convection in binary mixtures. Eur Phys J E 2004;15:311-8.
- [39] Batiste O, Knobloch E, Alonso A, Mercader I. Spatially localized binary-fluid convection. J Fluid Mech 2006;560:149–58.
- [40] Marqués F, Mercader I, Batiste O, López J. Centrifugal effects in rotating convection: axisymmetric states and three-dimensional instabilities. J Fluid Mech 2007;580:303-18.
- [41] Ma DJ, Sun DJ, Yin XY. Multiplicity of steady states in cylindrical Rayleigh-Bénard convection. Phys Rev E 2006;74:037302-1-2-4.
- [42] Marqués F, López JM. Precessing vortex breakdown mode in an enclosed cylinder flow. Phys Fluids 2001;13(6):,1679–1682.
- [43] López JM, Shen J. An efficient spectral-projection method for the Navier-Stokes equations in cylindrical geometries. I. Axisymmetric cases. J Comput Phys 1998;139:308-26.
- [44] López JM, Hart JE, Marqués F, Kittelman S, Shen J. Instability and mode interactions in a differentially driven rotating cylinder. J Fluid Mech 2002:462(6):383-409.
- [45] Boronska K. Three-dimensional patterns in cylindrical Rayleigh-Bénard convection. Ph.D. thesis, Paris Sud University; 2005.
- [46] Hof B, Lucas GJ, Mullin T. Flow state multiplicity in convection. Phys Fluids 1999;11:2815-[47] Tuckerman L. Divergence-free velocity fields in nonperiodic geometries. I
- Comput Phys 1989;80:403-41. [48] Rüdiger S, Knobloch E. Mode interaction in rotating Rayleigh-Bénard
- convection. Fluid Dyn Res 2003;33:477-92. [49] Sánchez-Alvarez JJ, Serre E, Crespo del Arco E, Busse FH. Square patterns in
- rotating Rayleigh–Bénard convection. Phys Rev E 2005;72:036307
- [50] Prat J, Massaguer JM, Mercader I. Large-scale flows and resonances in 2-D thermal convection. Phys Fluids 1995;7:121–34. [51] Prat J, Mercader I, Knobloch E. Resonant mode interactions in Rayleigh-Bénard
- convection. Phys Rev E 1998;58(3):3145-56. [52] Verzicco R, Orlandi P. A finite difference scheme for three-dimensional incompressible flows in cylindrical coordinates. Comput 1996:123:402-14.
- [53] Ma DJ, Henry D, Ben Hadid H. Three-dimensional numerical study of natural convection in vertical cylinders partially heated from the side. Phys Fluids 2005;17:124101.
- [54] López J, Marqués F, Mercader I, Batiste O. Onset of convection in a moderate aspect-ratio rotating cylinder: Eckhaus-Benjamin-Feir instability. J Fluid Mech 2007;590:187-208.
- [55] Rubio A, López JM, Marqués F. Modulated rotating convection: radially traveling concentric rolls. J Fluid Mech 2008;608:357-78.
- [56] Mercader I, Alonso A, Batiste O. Spatiotemporal dynamics near the onset of convection for binary mixtures in cylindrical containers. Phys Rev E 2008;77:036313.