

# Spectral Algorithms for Vector Elliptic Equations in a Spherical Gap

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This paper is devoted to the numerical solution of three-dimensional elliptic equations of a vector field in the region contained between two concentric spheres. The method of truncated series expansion in orthogonal functions is considered using Chebyshev polynomials and vector spherical harmonics. Spectral algorithms are described for solving two-point boundary-value problems of the vector modes of the Poisson, Helmholtz, and biharmonic equations supplemented by boundary conditions typical of fluid dynamical applications. The accuracy of the algorithms is illustrated by computing some analytical single-mode examples. The proposed algorithms when combined with efficient transform techniques can be used to solve multi-mode nonlinear problems. © 1985 Academic Press, Inc.

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## INTRODUCTION

Numerical methods for solving partial differential equations in regions of spherical shape or contained between two spheres are of a great interest for many problems in fluid dynamics, astrophysics, and geophysics. In analytical as well as computational models describing phenomena in a spherical geometry, it is very common to assume the rotational invariance with respect to a fixed axis passing through the centre—the so-called axisymmetry. In this case a double simplification of the mathematical problem is attained since, on the one hand, the number of the independent (spatial) variables is reduced resulting in a two-dimensional problem

and, on the other hand, the dependent variables for vector problems can be expressed simply in terms of scalar quantities such as the vorticity and stream function of a solenoidal velocity field. Although the assumption of axisymmetry is applicable to many important physical problems, there are also situations of great interest in which fully three-dimensional effects are significant. A few of them include the onset of instability of an incompressible flow past a sphere, the non-axisymmetric mode(s) of the viscous fluid motion in a narrow spherical gap between rotating spheres, natural convection patterns in fluid spherical mantles, hydro-magnetic coupling within a fluid sphere, etc.

The aim of the present paper is to develop numerical methods for the solution of fully three-dimensional equations of a vector field in a region within two concentric spheres. The analysis will be limited to linear equations of elliptic type, such as the Poisson, Helmholtz, and biharmonic equations. Actually, most of the problems of physical interest are such that convection or advection effects are very important, if not dominant, and therefore the main need is for numerical methods for nonlinear equations. In many instances, however, methods based on the direct solution of the linear, second-order part of the equation have proved adequate to calculate solutions of moderately nonlinear problems by means of proper iterative schemes. For such a reason, the discussion will concentrate on algorithms for the direct inversion of the mentioned elliptic equations, to be considered as the algorithmic kernel for the iterative solution of truly nonlinear equations.

The differential equations will be solved approximately by means of the method of truncated series expansion or spectral method using Chebyshev polynomials to represent the radial dependence and vector spherical harmonics to represent the angular dependence over the sphere (Sect. 1). Of the two bases of vector harmonics available to date, we have chosen the basis consisting of purely radial and tangential fields, since it is more convenient to impose the gauge condition for a vector potential on the spheres (Sect. 2) and to impose the integral conditions required by the solution of the biharmonic equation as a system of two second-order equations (Sect. 4). In this basis the Laplace operator couples each radial vector component to one of the two tangential components. The original partial differential equation is thus reduced to a system of ordinary differential equations (two-point boundary-value problems) for the coefficients of the expansion which are coupled in pairs or uncoupled. After introducing a simple mapping of the radial variable, the radial part of the Laplace operator is transformed into a constant coefficient operator containing second-order and first-order derivatives; the transformed equations are then approximated using Chebyshev polynomials which provide very accurate solutions to boundary-value problems (Sect. 5). The Chebyshev approximation to the integral conditions for the biharmonic equation is also considered (Sect. 6). In the case of the Poisson equation, a method for solving the Chebyshev equations efficiently by reducing the matrix of coefficients to a quasi-pentadiagonal profile is proposed (Sect. 7). The spectral algorithms are employed in the solution of some analytical examples to assess the accuracy and convergence of the proposed method (Sect. 8).

## 1. POISSON EQUATION AND VECTOR SPHERICAL HARMONICS

Let us consider the vector Poisson equation

$$-\nabla^2 \mathbf{A} = \mathbf{F} \quad (1.1)$$

to be solved in the three-dimensional space between two concentric spheres of radii  $r_1$  and  $r_2$  ( $> r_1$ ). In a spherical coordinate system  $(r, \theta, \varphi)$  with the origin at the centre of the spheres, the Laplace operator in Eq. (1.1) assumes the well-known form

$$\nabla^2 \equiv \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \quad (1.2)$$

and the spatial dependence of the vector fields  $\mathbf{A}$  and  $\mathbf{F}$  is expressed as  $\mathbf{A} = \mathbf{A}(r, \theta, \varphi)$  and  $\mathbf{F} = \mathbf{F}(r, \theta, \varphi)$ . The unknown vector field  $\mathbf{A}(r, \theta, \varphi)$ , as well as the source field  $\mathbf{F}(r, \theta, \varphi)$ , can be expanded as a series of vector spherical harmonic  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  [1] with coefficients depending on the radial coordinate  $r$ . Thus we may write

$$\mathbf{A}(r, \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{l^*} \sum_{m=-l}^l A_{ll^*m}(r) \mathbf{Y}_{ll^*m}(\theta, \varphi) \quad (1.3)$$

where  $l^*$  takes on the values  $l+1, l$ , and  $l-1$ . The vector spherical harmonic  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  are defined in terms of the (scalar) spherical harmonics  $Y_{lm}(\theta, \varphi)$  through the relationships

$$\mathbf{Y}_{l, l+1, m}(\theta, \varphi) = \frac{1}{[(l+1)(2l+1)]^{1/2}} [r \nabla Y_{lm}(\theta, \varphi) - \hat{\mathbf{r}}(l+1) Y_{lm}(\theta, \varphi)], \quad (1.4a)$$

$$\mathbf{Y}_{llm}(\theta, \varphi) = \frac{1}{[l(l+1)]^{1/2}} \nabla \times [r \mathbf{Y}_{lm}(\theta, \varphi)], \quad (1.4b)$$

$$\mathbf{Y}_{l, l-1, m}(\theta, \varphi) = \frac{1}{[l(2l+1)]^{1/2}} [r \nabla Y_{lm}(\theta, \varphi) + \hat{\mathbf{r}}l Y_{lm}(\theta, \varphi)], \quad (1.4c)$$

where  $\hat{\mathbf{r}} \equiv \mathbf{r}/r$  denotes the radial unit vector. The scalar spherical harmonics are the orthonormalized eigenfunctions of the angular part of  $\nabla^2$ , i.e.,

$$-\left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] Y_{lm} = l(l+1) Y_{lm}. \quad (1.5)$$

From the orthonormality of the basis of the scalar functions  $Y_{lm}(\theta, \varphi)$ , there follow the orthonormality of the basis of the vector functions  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  over the unit sphere, namely, if the bar denotes the complex conjugate,

$$\int \bar{\mathbf{Y}}_{ll^*m}(\theta, \varphi) \cdot \mathbf{Y}_{l'l'^*m'}(\theta, \varphi) \sin \theta \, d\theta \, d\varphi = \delta_{ll'} \delta_{l^*l'^*} \delta_{mm'}. \quad (1.6)$$

The vector basis defined by Eqs. (1.4) is well suited for solving the vector Poisson equation (1.1) since each vector field  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  is a vector eigenfunction of the angular part of the Laplace operator. In other words, each vector spherical harmonic  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  constitutes an invariant subspace insofar as, by virtue of Olsson's expressions [1, pp. 84–85], we have, for any function  $A(r)$ ,

$$\nabla^2[A(r) \mathbf{Y}_{ll^*m}(\theta, \varphi)] = [\mathcal{D}_l A(r)] \mathbf{Y}_{ll^*m}(\theta, \varphi), \quad (1.7)$$

where  $\mathcal{D}_l$  is the usual radial part of  $\nabla^2$  in spherical coordinates, i.e.,

$$\mathcal{D}_l \equiv \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2}, \quad l=0, 1, \dots \quad (1.8)$$

Therefore, by means of this basis, the vector Poisson (or Helmholtz) equation is reduced to a system of uncoupled, linear, second-order ODEs for the scalar coefficients  $A_{ll^*m}(r)$ , supplemented by suitable conditions, at  $r=r_1$  and  $r=r_2$  (two-point boundary-value problems). However, the foregoing approach has the drawback that the spherical harmonics  $\mathbf{Y}_{ll^*m}(\theta, \varphi)$  have a mixed radial-tangential character. In fact, a direct inspection of Eqs. (1.4) shows that  $\mathbf{Y}_{llm}$  is purely tangential whereas  $\mathbf{Y}_{ll\pm 1m}$  have both radial and tangential components. Such a circumstance can cause difficulties in the treatment of the boundary conditions on the spheres and in the physical interpretation of results for problems of practical significance.

A different basis of vector spherical harmonics which is orthonormal over the unit sphere and, in addition, has purely radial and tangential fields, is that considered by Morse and Feshbach [2], namely,

$$\mathbf{P}_{lm}(\theta, \varphi) = \hat{\mathbf{r}} Y_{lm}(\theta, \varphi), \quad l \geq 0, \quad (1.9a)$$

$$\mathbf{B}_{lm}(\theta, \varphi) = \frac{1}{[l(l+1)]^{1/2}} r \nabla Y_{lm}(\theta, \varphi), \quad l > 0, \quad (1.9b)$$

$$\mathbf{C}_{lm}(\theta, \varphi) = \frac{1}{[l(l+1)]^{1/2}} \nabla \times [\mathbf{r} Y_{lm}(\theta, \varphi)], \quad l > 0, \quad (1.9c)$$

and  $\mathbf{B}_{00} = \mathbf{C}_{00} = 0$ , by definition. Notice that  $\hat{\mathbf{r}} \times \mathbf{C}_{lm}(\theta, \varphi) = \mathbf{B}_{lm}(\theta, \varphi)$  and  $\hat{\mathbf{r}} \times \mathbf{B}_{lm}(\theta, \varphi) = -\mathbf{C}_{lm}(\theta, \varphi)$  so that, at any point  $(\theta, \varphi)$ ,  $\mathbf{B}_{lm}(\theta, \varphi) \cdot \mathbf{C}_{lm}(\theta, \varphi) = 0$ . However, in this basis the (angular part of the) Laplace operator is not fully diagonal, i.e., some invariant subspaces are multidimensional. In order to demonstrate this result, it is convenient to derive the relationships for the curl and the divergence of the vector spherical harmonics defined by Eqs. (1.9). By simple calculations we obtain

$$\nabla \times [A(r) \mathbf{P}_{lm}(\theta, \varphi)] = [l(l+1)]^{1/2} \frac{A(r)}{r} \mathbf{C}_{lm}(\theta, \varphi), \quad (1.10a)$$

$$\nabla \times [A(r) \mathbf{B}_{lm}(\theta, \varphi)] = -\left(\frac{d}{dr} + \frac{1}{r}\right) A(r) \mathbf{C}_{lm}(\theta, \varphi), \quad (1.10b)$$

$$\nabla \times [A(r) \mathbf{C}_{lm}(\theta, \varphi)] = [l(l+1)]^{1/2} \frac{A(r)}{r} \mathbf{P}_{lm}(\theta, \varphi) + \left( \frac{d}{dr} + \frac{1}{r} \right) A(r) \mathbf{B}_{lm}(\theta, \varphi), \quad (1.10c)$$

$$\nabla \cdot [A(r) \mathbf{P}_{lm}(\theta, \varphi)] = \left( \frac{d}{dr} + \frac{2}{r} \right) A(r) Y_{lm}(\theta, \varphi), \quad (1.11a)$$

$$\nabla \cdot [A(r) \mathbf{B}_{lm}(\theta, \varphi)] = -[l(l+1)]^{1/2} \frac{A(r)}{r} Y_{lm}(\theta, \varphi), \quad (1.11b)$$

$$\nabla \cdot [A(r) \mathbf{C}_{lm}(\theta, \varphi)] = 0, \quad (1.11c)$$

for any scalar function  $A(r)$ . By means of these expressions, it is not difficult to obtain

$$\begin{aligned} \nabla^2 [A^1(r) \mathbf{P}_{lm}(\theta, \varphi) + A^2(r) \mathbf{B}_{lm}(\theta, \varphi) + A^3(r) \mathbf{C}_{lm}(\theta, \varphi)] \\ = (\mathbf{P}_{lm}(\theta, \varphi), \mathbf{B}_{lm}(\theta, \varphi), \mathbf{C}_{lm}(\theta, \varphi)) \cdot \mathbb{D}_l \mathbf{A}(r), \end{aligned} \quad (1.12)$$

where the dot denotes the scalar product between vectors,  $\mathbf{A}(r) = (A^1(r), A^2(r), A^3(r))$  and  $\mathbb{D}_l$  is the matricial differential operator

$$\mathbb{D}_l \equiv \begin{bmatrix} \mathcal{D}_l - \frac{2}{r^2} & \frac{2[l(l+1)]^{1/2}}{r^2} & 0 \\ \frac{2[l(l+1)]^{1/2}}{r^2} & \mathcal{D}_l & 0 \\ 0 & 0 & \mathcal{D}_l \end{bmatrix} \quad (1.13)$$

acting on vector functions of the single variable  $r$ . For each value of the pair  $(l, m)$  ( $l > 0, |m| \leq l$ ) there are two invariant subspaces: the first subspace is spanned by the normal spherical harmonic  $\mathbf{P}_{lm}(\theta, \varphi)$  and the tangential spherical harmonic  $\mathbf{B}_{lm}(\theta, \varphi)$ , which are coupled by the operator  $\nabla^2$ ; the second space is spanned instead by the single tangential spherical harmonic  $\mathbf{C}_{lm}(\theta, \varphi)$ . In the present work the basis defined by Eqs. (1.9) is preferred due to its advantages in the treatment of the boundary conditions in problems of physical interest.

The unknown  $\mathbf{A}(r, \theta, \varphi)$  of Eq. (1.1) is expanded as

$$\begin{aligned} \mathbf{A}(r, \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l [A_{lm}^1(r) \mathbf{P}_{lm}(\theta, \varphi) \\ + A_{lm}^2(r) \mathbf{B}_{lm}(\theta, \varphi) + A_{lm}^3(r) \mathbf{C}_{lm}(\theta, \varphi)] \end{aligned} \quad (1.14)$$

and similarly the source term  $\mathbf{F}(r, \theta, \varphi)$ . For each pair  $(l, m)$  the vector  $\mathbf{A}_{lm}(r) \equiv (A_{lm}^1(r), A_{lm}^2(r), A_{lm}^3(r))$  will be referred to as a *vector mode* of the representation

given by Eq. (1.14). Using such an expansion, for each vector mode Eq. (1.1) provides the ordinary differential problem

$$-\mathbb{D}_r \mathbf{A}_{lm}(r) = \mathbf{F}_{lm}(r), \quad (1.15)$$

i.e., a system of two coupled second-order equations plus a single second-order equation uncoupled from the others. These equations are supplemented by boundary conditions at  $r = r_1$  and  $r = r_2$  which will be discussed in the next section.

## 2. BOUNDARY CONDITIONS

Two types of boundary conditions for the vector Poisson equation (1.1) are considered:

- (i) Dirichlet conditions for the three components of  $\mathbf{A}$ ;
- (ii) a combination of two Dirichlet conditions for the tangential components with a mixed condition stemming from the gauge condition  $\nabla \cdot \mathbf{A} = 0$ .

In the first case, using spherical coordinates, the boundary conditions read

$$\mathbf{A}(r, \theta, \varphi)|_S = \mathbf{a}(\theta, \varphi), \quad (2.1)$$

where  $S$  indicates both spherical surfaces  $r = r_1$  and  $r = r_2$  and  $\mathbf{a}(\theta, \varphi)$  denotes the vector field prescribed on  $S$ . (There are two such a boundary data, one for each sphere, but we use only one symbol for notational simplicity.) By expanding  $\mathbf{a}(\theta, \varphi)$  in vector spherical harmonics

$$\mathbf{a}(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l [a_{lm}^1 \mathbf{P}_{lm}(\theta, \varphi) + a_{lm}^2 \mathbf{B}_{lm}(\theta, \varphi) + a_{lm}^3 \mathbf{C}_{lm}(\theta, \varphi)], \quad (2.2)$$

we immediately obtain the boundary conditions for the differential equation (1.15) given by

$$\mathbf{A}_{lm}(r)|_S = \mathbf{a}_{lm}. \quad (2.3)$$

When the field  $\mathbf{A}$  is a vector potential, it is very common to require that  $\mathbf{A}$  satisfy the gauge condition  $\nabla \cdot \mathbf{A} = 0$ . In this case, we must impose the boundary condition expressed by

$$\nabla \cdot \mathbf{A}|_S = 0. \quad (2.4)$$

Using the expansion (1.14) and Eqs. (1.11), we obtain, for each vector mode, the Robin-type boundary condition

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) A_{lm}^1(r) - \frac{[l(l+1)]^{1/2}}{r} A_{lm}^2(r) \right] \Big|_s = 0 \quad (2.5a)$$

which couples the first and the second components of the vector mode. The other two conditions are typically Dirichlet conditions for the tangential components of the mode, namely

$$A_{lm}^2(r)|_s = a_{lm}^2 \quad \text{and} \quad A_{lm}^3(r)|_s = a_{lm}^3. \quad (2.5b)$$

It is noteworthy that the boundary conditions (2.5) have the same block structure as the differential system (1.15).

In the particular case  $l=m=0$ , the first equation of (1.15) and the Robin condition (2.5a) become

$$-\left( \mathcal{D}_0 - \frac{2}{r^2} \right) A_{00}^1(r) = F_{00}^1(r), \quad (2.6a)$$

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) A_{00}^1(r) \right] \Big|_s = 0, \quad (2.6b)$$

respectively. However, the problem defined by Eqs. (2.6) is indeterminate. In fact, we immediately see that

$$\left( \mathcal{D}_0 - \frac{2}{r^2} \right) = \frac{1}{r} \left( \frac{d}{dr} - \frac{1}{r} \right) r \left( \frac{d}{dr} + \frac{2}{r} \right),$$

so that, due to boundary condition (2.6b),  $A_{00}^1(r)$  is determined up to an additive term  $(r/r_0)^{-2}$ , with arbitrary  $r_0$ . In order to fix the solution uniquely, the value of  $A_{00}^1(r)$  at, say  $r=r_1$ , must be specified. Therefore for  $l=m=0$ , condition (2.6b) at  $r=r_1$  is replaced by the Dirichlet specification

$$A_{00}^1(r)|_{r=r_1} = 0. \quad (2.6b')$$

### 3. HELMHOLTZ EQUATION

Another elliptic equation, very often encountered in the solution of physical problems, is the Helmholtz equation

$$(-\nabla^2 + \gamma) \mathbf{A} = \mathbf{F}, \quad (3.1)$$

$\gamma$  being a positive constant. Helmholtz equations are typically obtained when parabolic equations for transient problems are discretized in time using the finite difference method; in such a case  $\gamma$  is a quantity proportional to the reciprocal of

the time step. The corresponding equations for the coefficients of the expansion in vector spherical harmonics are

$$(-\mathbb{D}_l + \gamma \mathbb{I}) \mathbf{A}_{lm}(r) = \mathbf{F}_{lm}(r), \quad (3.2)$$

where  $\mathbb{I}$  is the  $3 \times 3$  identity matrix. The boundary conditions more frequently associated with Eq. (3.2) are the Dirichlet conditions given by Eq. (2.3).

#### 4. BIHARMONIC EQUATION

##### 4.1. Biharmonic Equation in Factorized Form

A third elliptic equation of interest in fluid dynamical problems is the biharmonic equation

$$\nabla^4 \mathbf{A} \equiv (-\nabla^2)(-\nabla^2) \mathbf{A} = \mathbf{F}. \quad (4.1)$$

In view of its application to time-dependent problems of an incompressible viscous fluid (e.g., see [3]), we consider the slightly more general equation

$$(-\nabla^2 + \gamma)(-\nabla^2) \mathbf{A} = \mathbf{F}, \quad (4.2)$$

where  $\gamma$  is a constant. Instead of solving Eq. (4.2) as a single fourth-order equation, we prefer to split or factorize it into a system of two second-order equations by introducing an intermediate variable  $\zeta$ ; i.e., we write

$$(-\nabla^2 + \gamma) \zeta = \mathbf{F}, \quad (4.3a)$$

$$(-\nabla^2) \mathbf{A} = \zeta. \quad (4.3b)$$

In a fluid dynamical context,  $\mathbf{A}$  is the vector potential of the solenoidal velocity field  $\mathbf{u}$  so that  $\mathbf{u} = \nabla \times \mathbf{A}$  and  $\zeta = \nabla \times \mathbf{u}$  is the vector vorticity. The boundary conditions which supplement Eq. (4.2) and henceforth Eqs. (4.3) are more complex than those relative to second-order elliptic equations and will be discussed in the following with reference to fluid dynamical applications.

##### 4.2. Boundary Conditions

Let us now derive the complete set of boundary conditions when the velocity field  $\mathbf{u}$  is prescribed on the two spheres, i.e.,  $\mathbf{u}|_S = \mathbf{b}$  with  $\mathbf{b}$  a prescribed vector. Under the assumption that  $\nabla \cdot \mathbf{F} = 0$ , the solenoidal character of the vorticity field will be assured by imposing the boundary condition

$$\nabla \cdot \zeta|_S = 0. \quad (4.4a)$$



Since the tangential components of  $\mathbf{u} = \nabla \times \mathbf{A}$  on  $S$  are prescribed, the vector potential  $\mathbf{A}$  must satisfy the derivative conditions

$$(\nabla \times \mathbf{A})_{\theta}|_S = b_{\theta} \quad \text{and} \quad (\nabla \times \mathbf{A})_{\varphi}|_S = b_{\varphi}. \quad (4.4b)$$

The radial component of  $\mathbf{u}$  on  $S$  is also prescribed and therefore  $(\nabla \times \mathbf{A})_r|_S = b_r$ . It is possible to show [4] that this condition can be translated into equivalent conditions for the tangential component of  $\mathbf{A}$ , according to the relationships

$$A_{\theta}|_S = a_{\theta} \quad \text{and} \quad A_{\varphi}|_S = a_{\varphi}, \quad (4.4c)$$

where  $a_{\theta}$  and  $a_{\varphi}$  are to be determined in terms of the boundary datum  $b_r$ . Finally, from the gauge condition  $\nabla \cdot \mathbf{A} = 0$  which has been implicitly assumed when writing  $-\nabla^2 \mathbf{A} = \zeta$  in place of  $\nabla \times \nabla \times \mathbf{A} = \zeta$ , we find the boundary condition

$$\nabla \cdot \mathbf{A}|_S = 0. \quad (4.4d)$$

By expanding the fields  $\mathbf{F}$ ,  $\zeta$ ,  $\mathbf{A}$  as well as the boundary data  $\mathbf{b}$ ,  $\mathbf{a}$  in vector spherical harmonics, the system of differential equations and boundary conditions governing the two vector modes  $\zeta_{lm}(r)$  and  $\mathbf{A}_{lm}(r)$  is obtained. By omitting the subscript indices  $l$  and  $m$ , for simplicity, the differential equations are

$$(-\mathbb{D}_l + \gamma \mathbb{I}) \zeta = \mathbf{F}, \quad (4.5a)$$

$$-\mathbb{D}_l \mathbf{A} = \zeta, \quad (4.5b)$$

whereas the boundary conditions (4.4) become, by virtue of Eqs. (1.10) and (1.11),

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) \zeta^1 - \frac{[l(l+1)]^{1/2}}{r} \zeta^2 \right] \Big|_S = 0 \quad (4.5c)$$

$$\left[ \frac{[l(l+1)]^{1/2}}{r} A^1 - \left( \frac{d}{dr} + \frac{1}{r} \right) A^2 \right] \Big|_S = b^3 \quad \text{and} \quad \left[ \left( \frac{d}{dr} + \frac{1}{r} \right) A^3 \right] \Big|_S = b^2, \quad (4.5d)$$

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) A^1 - \frac{[l(l+1)]^{1/2}}{r} A^2 \right] \Big|_S = 0, \quad (4.5e)$$

$$A^2|_S = a^2 \quad \text{and} \quad A^3|_S = a^3. \quad (4.5f)$$

The form of the boundary conditions (4.5c-f) is such that an independent solution of the equations for  $\zeta$  and  $\mathbf{A}$  is not possible. In fact, the boundary conditions for the two tangential components of  $\zeta$  are missing, whereas there are two redundant boundary conditions for  $\mathbf{A}$ , i.e., conditions (4.5d), which couple the

equations for  $\zeta$  and  $\mathbf{A}$ . It is remarkable, however, that this coupling has the same block structure as the operator  $\mathbb{D}_l$  since the first condition of (4.5d) couples  $A^1$  and  $A^2$  whereas the second condition leaves the component  $A^3$  uncoupled.

### 4.3. Integral Conditions

The equations for  $\zeta$  and  $\mathbf{A}$  can be split by introducing conditions of an integral character for the variable  $\zeta$  much in the same manner as in the case of the scalar variables vorticity and stream function for two-dimensional problems [5]. The integral conditions for the vector variable  $\zeta$  come from an application of the Green's identity for the operator  $\mathbb{D}_l$ , namely,

$$\int_{r_1}^{r_2} r^2 (\mathbf{B} \cdot \mathbb{D}_l \mathbf{A} - \mathbf{A} \cdot \mathbb{D}_l \mathbf{B}) dr = \left[ r^2 \left( \mathbf{B} \cdot \frac{d\mathbf{A}}{dr} - \mathbf{A} \cdot \frac{d\mathbf{B}}{dr} \right) \right]_{r_1}^{r_2}, \quad (4.6)$$

where  $\mathbf{A} = \mathbf{A}(r)$  and  $\mathbf{B} = \mathbf{B}(r)$  are arbitrary vector functions. Identity (4.6) is a straightforward consequence of the corresponding identity for the operator  $\mathcal{D}_l$  (see, e.g., [6, 7]). By taking  $\mathbf{B} \equiv \boldsymbol{\eta}$  with  $\mathbb{D}_l \boldsymbol{\eta} = 0$  and  $-\mathbb{D}_l \mathbf{A} = \zeta$ , identity (4.6) provides

$$\int_{r_1}^{r_2} \zeta \cdot \boldsymbol{\eta} r^2 dr = - \left[ r^2 \left( \boldsymbol{\eta} \cdot \frac{d\mathbf{A}}{dr} - \mathbf{A} \cdot \frac{d\boldsymbol{\eta}}{dr} \right) \right]_{r_1}^{r_2}. \quad (4.7)$$

By a suitable choice of the boundary conditions for  $\boldsymbol{\eta}$ , the boundary values of  $\mathbf{A}$  and  $d\mathbf{A}/dr$  in the right-hand side of Eq. (4.7) can be expressed in terms of the boundary data. Let  $\boldsymbol{\eta}$  be any solution of the problem

$$\mathbb{D}_l \boldsymbol{\eta} = 0, \quad (4.8a)$$

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) \boldsymbol{\eta}^1 - \frac{[l(l+1)]^{1/2}}{r} \boldsymbol{\eta}^2 \right] \Big|_s = 0, \quad \boldsymbol{\eta}^2|_s \neq 0, \quad \boldsymbol{\eta}^3|_s \neq 0. \quad (4.8b)$$

By using the boundary conditions (4.5d) and (4.5e) to eliminate  $d\mathbf{A}/dr$  in favor of  $\mathbf{A}$  and then employing the boundary conditions (4.5f), Eq. (4.7) provides the integral conditions

$$\int_{r_1}^{r_2} (\zeta^1 \boldsymbol{\eta}^1 + \zeta^2 \boldsymbol{\eta}^2) r^2 dr = \left[ r^2 \left\{ b^3 \boldsymbol{\eta}^2 + a^2 \left[ \left( \frac{d}{dr} + \frac{1}{r} \right) \boldsymbol{\eta}^2 - \frac{[l(l+1)]^{1/2}}{r} \boldsymbol{\eta}^1 \right] \right\} \right]_{r_1}^{r_2}, \quad (4.9')$$

$$\int_{r_1}^{r_2} \zeta^3 \boldsymbol{\eta}^3 r^2 dr = \left[ r^2 \left\{ -b^2 \boldsymbol{\eta}^3 + a^3 \left( \frac{d}{dr} + \frac{1}{r} \right) \boldsymbol{\eta}^3 \right\} \right]_{r_1}^{r_2}. \quad (4.9'')$$

It is noteworthy that two expressions are obtained from the single equation (4.7) since the nonhomogeneous boundary conditions for  $\boldsymbol{\eta}^2$  and  $\boldsymbol{\eta}^3$  in problem (4.8) can

be specified independently and the block structure of  $\mathbb{D}_l$  leaves  $\eta^3$  uncoupled from the components  $\eta^1$  and  $\eta^2$ . By virtue of the integral conditions (4.9), the problem defined by Eqs. (4.5) can be restated in the split form

$$(-\mathbb{D}_l + \gamma \mathbb{I}) \zeta = \mathbf{F}, \quad (4.10a)$$

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) \zeta^1 - \frac{[l(l+1)]^{1/2}}{r} \zeta^2 \right] \Big|_S = 0 \quad (4.10b)$$

$$\int_{r_1}^{r_2} (\zeta^1 \eta^1 + \zeta^2 \eta^2) r^2 dr = \left[ r^2 \left\{ b^3 \eta^2 + a^2 \left[ \left( \frac{d}{dr} + \frac{1}{r} \right) \eta^2 - \frac{[l(l+1)]^{1/2}}{r} \eta^1 \right] \right\} \right]_{r_1}^{r_2}, \quad (4.10c)$$

$$\int_{r_1}^{r_2} \zeta^3 \eta^3 r^2 dr = \left[ r^2 \left\{ -b^2 \eta^3 + a^3 \left( \frac{d}{dr} + \frac{1}{r} \right) \eta^3 \right\} \right]_{r_1}^{r_2}; \quad (4.10d)$$

$$-\mathbb{D}_l \mathbf{A} = \zeta, \quad (4.11a)$$

$$\left[ \left( \frac{d}{dr} + \frac{2}{r} \right) A^1 - \frac{[l(l+1)]^{1/2}}{r} A^2 \right] \Big|_S = 0, \quad (4.11b)$$

$$A^2|_S = a^2, \quad (4.11c)$$

$$A^3|_S = a^3. \quad (4.11d)$$

It is remarkable that the integral conditions (4.10c) and (4.10d) have the same block structure as the differential operator  $\mathbb{D}_l$ . Also notice that two linearly independent solutions to problem (4.8) need to be considered in each expression (4.10c) and (4.10d).

In order to impose the integral conditions directly, the analytical solutions of Eqs. (4.8) have to be determined. Another method for making such conditions satisfied, although in an indirect manner, is provided by the influence matrix method. This method has been employed in the solution of the equations for incompressible viscous flows to determine the lacking boundary values of the pressure [8, 9] and to impose the integral conditions of the scalar vorticity [5]. The influence matrix method avoids the explicit determination of the solutions  $\boldsymbol{\eta}(r)$  but requires the solution of a double number of equations with respect to the method based on the direct use of the integral conditions. Therefore, in the present work the direct method has been preferred.

When applied to the calculation of incompressible viscous flows, the scheme based on Eqs. (4.10) and (4.11) is alternative to the method using poloidal and toroidal scalar potentials for the representation of a solenoidal vector field in a spherical region [6, 7].

5. DISCRETIZATION OF THE RADIAL DEPENDENCE  
BY CHEBYSHEV POLYNOMIALS

The Chebyshev polynomials are now employed to obtain approximate solutions to the two-point boundary-value problems formulated in the previous sections [10]. In order to obtain constant coefficient differential equations in the radial direction, a logarithmic variable  $x$  is introduced by means of the transformation

$$x = 2 \frac{\ln(r/r_1)}{\ln(r_2/r_1)} - 1 \quad (5.1)$$

which maps the interval  $r_1 \leq r \leq r_2$  on the interval  $-1 \leq x \leq 1$ . In the new variable, the system of equations (1.15) for the Poisson problem assumes the form

$$-\mathbb{D}_l^{(x)} \mathbf{A}(x) = r_1^2 \exp[2(x+1)/\alpha] \mathbf{F}(x), \quad (5.2)$$

where  $\alpha = 2/\ln(r_2/r_1)$  and the differential operators

$$\mathbb{D}_l^{(x)} \equiv \begin{bmatrix} \mathcal{D}_l^{(x)} - 2 & 2[l(l+1)]^{1/2} & 0 \\ 2[l(l+1)]^{1/2} & \mathcal{D}_l^{(x)} & 0 \\ 0 & 0 & \mathcal{D}_l^{(x)} \end{bmatrix} \quad (5.3)$$

and

$$\mathcal{D}_l^{(x)} \equiv \alpha^2 \frac{d^2}{dx^2} + \alpha \frac{d}{dx} - l(l+1) \quad (5.4)$$

have constant coefficients. Let us first consider the scalar equation for the uncoupled component  $A^3$  and write  $A^3 = A$ , for simplicity. The differential equation supplemented by Dirichlet boundary conditions can be written in the form

$$-\mathcal{D}_l^{(x)} A(x) = r_1^2 \exp[2(x+1)/\alpha] F(x) \quad (5.5a)$$

$$A(\pm 1) = a^\pm, \quad (5.5b)$$

where  $a^- = a(r_1)$  and  $a^+ = a(r_2)$ . Let us then expand  $A(x)$  and  $F(x)$  as a truncated series of Chebyshev polynomials  $T_n(x) \equiv \cos[n \cos^{-1}(x)]$  [11–13], to obtain

$$A(x) = \sum_{n=0}^N A_n T_n(x) \quad \text{and} \quad F(x) = \sum_{n=0}^N F_n T_n(x). \quad (5.6)$$

The discrete form of the problem defined by Eqs. (5.5) is provided by the tau method [11, 13] as

$$-\alpha^2 A_n^{(2)} - \alpha A_n^{(1)} + l(l+1) A_n = \sum_{n'=0}^N E_{nn'} F_{n'}, \quad 0 \leq n \leq N-2 \quad (5.7a)$$

$$\sum_{n=0}^N (\pm 1)^n A_n = a^\pm, \quad (5.7b)$$

where the notation  $\psi_n^{(i)}$  indicates the coefficients of the  $i$ th derivative of a Chebyshev series with coefficients  $\psi_n$ . The matrix  $E_{nn'}$  in Eq. (5.7a) is defined by

$$E_{nn'} = \left( \frac{\pi}{2} c_n \right)^{-1} r_1^2 \int_{-1}^{+1} \frac{\exp[2(x+1)/\alpha] T_n(x) T_{n'}(x) dx}{(1-x^2)^{1/2}}, \quad (5.8)$$

where  $c_0 = 2$  and  $c_n = 1$  for  $n > 0$ . If instead of the Dirichlet condition one considers the Robin condition for the uncoupled component  $A^3$ , for instance, the second boundary condition of Eqs. (4.5d), Eqs. (5.5b) and (5.7b) would be replaced by the equations

$$\left( \alpha \frac{d}{dx} + 1 \right) A(\pm 1) = \exp[(\pm 1 + 1)/\alpha] b^\pm \quad (5.5b')$$

and

$$\sum_{n=0}^N (-\alpha n^2 + 1)(\pm 1)^n A_n = \exp[(\pm 1 + 1)/\alpha] b^\pm \quad (5.7b')$$

respectively, where  $b^- = b(r_1)$  and  $b^+ = b(r_2)$ .

The system of two coupled equations for  $A^1(x)$  and  $A^2(x)$  can be handled in a quite similar way. Using the ordering  $A_0^1, A_0^2, A_1^1, A_1^2, \dots, A_N^1, A_N^2$  of the unknowns, the linear system of algebraic equations has the same structure as the linear system for  $A_0^3, A_1^3, \dots, A_N^3$  with scalar coefficient replaced by two-by-two matrices. Both systems can be solved efficiently by means of the algorithm for inverting the operator  $\mathcal{D}_l^{(x)}$  to be presented in Section 7.

In the case of the Helmholtz equation, the transformed equations are more difficult to solve due to the presence of a variable coefficient term. In fact, after the change of variable, Eq. (3.2) reads

$$[-\mathbb{D}_l^{(x)} + \gamma r_1^2 \exp[2(x+1)/\alpha] \mathbb{I}] \mathbf{A}(x) = r_1^2 \exp[2(x+1)/\alpha] \mathbf{F}(x). \quad (5.9)$$

For instance, the Chebyshev equations for the third component  $A^3 = A$  are

$$-\alpha^2 A_n^{(2)} - \alpha A_n^{(1)} + l(l+1) A_n + \gamma \sum_{n'=0}^N E_{nn'} A_{n'} = \sum_{n'=0}^N E_{nn'} F_{n'}, \quad (5.10a)$$

$$\sum_{n=0}^N (\pm 1)^n A_n = a^\pm. \quad (5.10b)$$

The presence of the full matrix  $E_{nn'}$  on the left-hand side of Eq. (5.10a) prevents use of the efficient algorithm which deals with the constant coefficient equations. In the numerical examples to be discussed, the full matrix system for Helmholtz problems is solved by a direct UL factorization without pivoting. The efficient iterative method developed by Orszag [14] for solving equations with variable coefficients could also be employed for the Helmholtz equations considered.

## 6. CHEBYSHEV APPROXIMATION TO THE INTEGRAL CONDITIONS

As far as the integral conditions (4.10c) and (4.10d) are concerned, after transformation (5.1) they can be written as

$$\begin{aligned} & \frac{r_1^3}{\alpha} \int_{-1}^{+1} (\zeta^1 \eta^1 + \zeta^2 \eta^2) \exp[3(x+1)/\alpha] dx \\ &= \left[ r^2 \left\{ b^3 \eta^2 + \frac{a^2}{r} \left[ \left( \alpha \frac{d}{dx} + 1 \right) \eta^2 - [l(l+1)]^{1/2} \eta^1 \right] \right\} \right]_{-1}^{+1}, \end{aligned} \quad (6.1)$$

$$\begin{aligned} & \frac{r_1^3}{\alpha} \int_{-1}^{+1} \zeta^3 \eta^3 \exp[3(x+1)/\alpha] dx \\ &= \left[ r^2 \left\{ -b^2 \eta^3 + \frac{a^3}{r} \left( \alpha \frac{d}{dx} + 1 \right) \eta^3 \right\} \right]_{-1}^{+1}. \end{aligned} \quad (6.2)$$

where  $r = r(x) = r_1 \exp[(x+1)/\alpha]$ . The functions  $\boldsymbol{\eta}(x) \equiv (\eta^1(x), \eta^2(x), \eta^3(x))$  to be used in Eqs. (6.1) and (6.2) are the linearly independent solutions of the system

$$\begin{aligned} \mathbb{D}_l^{(x)} \boldsymbol{\eta} = 0, \quad & \left[ \left( \alpha \frac{d}{dx} + 2 \right) \eta^1 - [l(l+1)]^{1/2} \eta^2 \right] \Big|_s = 0, \\ & \eta^2|_s \neq 0, \eta^3|_s \neq 0. \end{aligned} \quad (6.3)$$

They can be chosen as the functions  $(\eta^1, \eta^2, 0)^\pm$  which satisfy the Robin-type boundary condition in Eq. (6.3) together with the boundary conditions for the second component given by

$$\begin{aligned} \eta^{2-}(-1) &= 1, & \eta^{2-}(+1) &= 0; \\ \eta^{2+}(-1) &= 0, & \eta^{2+}(+1) &= 1; \end{aligned}$$

and as the functions  $(0, 0, \eta^3)^\pm$  which satisfy the boundary conditions

$$\begin{aligned} \eta^{3-}(-1) &= 1, & \eta^{3-}(+1) &= 0; \\ \eta^{3+}(-1) &= 0, & \eta^{3+}(+1) &= 1. \end{aligned}$$

The analytical solutions  $(\eta^1, \eta^2, 0)^\pm$  are easily found to be, for any  $l > 0$ ,

$$\begin{aligned} \eta^{1\pm}(x) &= \frac{\pm 1}{2 \sinh[(2l+1)/\alpha]} \left\{ \left( \frac{l}{l+1} \right)^{1/2} \exp[(\pm(l+2) + (l-1)x)/\alpha] \right. \\ & \quad \left. + \left( \frac{l+1}{l} \right)^{1/2} \exp[(\mp(l-1) - (l+2)x)/\alpha] \right\}, \end{aligned} \quad (6.4a)$$

$$\eta^{2\pm}(x) = \frac{\pm 1}{2 \sinh[(2l+1)/\alpha]} \left\{ \exp[(\pm(l+2) + (l-1)x)/\alpha] - \exp[(\mp(l-1) - (l+2)x)/\alpha] \right\}, \quad (6.4b)$$

whereas the solutions  $(0, 0, \eta^3)^\pm$  are found to be

$$\eta^{3\pm}(x) = \frac{\pm 1}{2 \sinh[(2l+1)/\alpha]} \left\{ \exp[(\pm(l+1) + lx)/\alpha] - \exp[(\mp l - (l+1)x)/\alpha] \right\}. \quad (6.5)$$

Considering the uncoupled component  $\zeta^3 = \zeta$ , for simplicity, the integral conditions (6.2) become in the Chebyshev representation

$$\sum_{n=0}^N h_n^\pm \zeta_n = \left[ r^2 \left\{ -b\eta^\pm + \frac{a^3}{r} \left( \alpha \frac{d}{dx} + 1 \right) \eta^\pm \right\} \right]_{-1}^{+1}, \quad (6.6)$$

where  $\eta^\pm$  stands for  $\eta^{3\pm}$  and the coefficients  $h_n^\pm$  are defined by the integrals

$$h_n^\pm = \frac{r^3}{\alpha} \int_{-1}^{+1} \eta^\pm(x) \exp[3(x+1)/\alpha] T_n(x) dx. \quad (6.7)$$

Since Chebyshev functions  $T_n(x)$  are polynomials in  $x$ , the integrals in expression (6.7) can be evaluated analytically. Equations (6.6) for the integral conditions on  $\zeta = \zeta^3$  supplement the Chebyshev equations approximating the Helmholtz equation for  $\zeta^3$ .

## 7. REDUCTION OF CHEBYSHEV EQUATIONS TO QUASI-PENTADIAGONAL FORM

A well-known disadvantage of spectral methods with respect to finite differences or elements is that spectral approximations lead to full matrices. In the linear system (5.7), for instance, all coefficients in the upper triangle are different from zero. In the particular case of constant coefficient equations, the matrix coefficients are, however, distributed according to a regular pattern which can be exploited to recast the matrix in a banded form. The matrix corresponding to the Chebyshev approximation to the operator  $(d^2/dx^2 - k)$  can be made pentadiagonal, but for the boundary condition equations, by the elimination scheme recently suggested in [15] (see also [13], pp. 119-120), although already considered in the older reference [16] pointed out by a reviewer. With minor modifications, this scheme can also be applied with the first derivative, as described below. Let us rewrite the

ordinary differential problem (5.5) with constant coefficients in the slightly more general form

$$tA'' + uA' + vA = G, \quad (7.1a)$$

$$A(\pm 1) = a^\pm, \quad (7.1b)$$

where  $t$ ,  $u$ , and  $v$  are known constants and the prime denotes the derivative with respect to  $x$ . The corresponding Chebyshev equations provided by the tau method [13] are

$$t \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^N p(p^2 - n^2) A_p + 2u \sum_{\substack{p=n+1 \\ p+n \text{ odd}}}^N pA_p + vc_n A_n = c_n G_n, \quad 0 \leq n \leq N-2, \quad (7.2a)$$

$$\sum_{n=0}^N (\pm 1)^n A_n = a^\pm. \quad (7.2b)$$

For  $2 \leq n \leq N-4$  (we assume  $N \geq 6$ ) we can consider a linear combination of Eqs. (7.2a) in the form

$$\text{Eq}(n-2)/[4n(n-1)] - \text{Eq}(n)/[2(n^2-1)] + \text{Eq}(n+2)/[4n(n+1)],$$

where  $\text{Eq}(n')$  means Eq. (7.2a) for  $n = n'$ . By means of simple calculations we obtain

$$\begin{aligned} & \frac{vc_{n-2}}{4n(n-1)} A_{n-2} + \frac{u}{2n} A_{n-1} + \left[ t - \frac{v}{2(n^2-1)} \right] A_n - \frac{u}{2n} A_{n+1} + \frac{v}{4n(n+1)} A_{n+2} \\ & = \frac{c_{n-2}}{4n(n-1)} G_{n-2} - \frac{1}{2(n^2-1)} G_n + \frac{1}{4n(n+1)} G_{n+2}, \quad 2 \leq n \leq N-4. \end{aligned} \quad (7.3)$$

The linear system (7.2) is thus replaced by the equivalent one composed by Eqs. (7.2b), corresponding to the boundary conditions, Eqs. (7.3) for  $2 \leq n \leq N-4$ , and, finally Eqs. (7.2a) for  $N-5 \leq n \leq N-2$ . In total we have  $2 + (N-5) + 4 = N+1$  equations for the  $N+1$  coefficients  $\{A_n\}$ . The structure of the resulting matrix is shown in Fig. 1, where it appears to be basically pentadiagonal except for the first two rows, whose elements are all different from zero, and the fourth row from the end, which contains an extra nonzero element. It is important that the first two equations of the linear system be Eqs. (7.2b) for the boundary conditions when the system is solved without pivoting. In fact, if the system is ordered with the boundary condition equations placed at the bottom, as  $N$  increases the relative error of the solution does not decrease to the machine accuracy level and then level out, as it should. On the contrary, after a certain value of  $N$  it starts increasing. Convergence to machine accuracy is obtained instead without requiring the use of a pivot if the first two rows of the matrix correspond to the boundary conditions (7.2b). An apparent disadvantage of such an ordering is that the LU factorization fills the zero coefficients in the upper triangle with nonzero values; this incon-



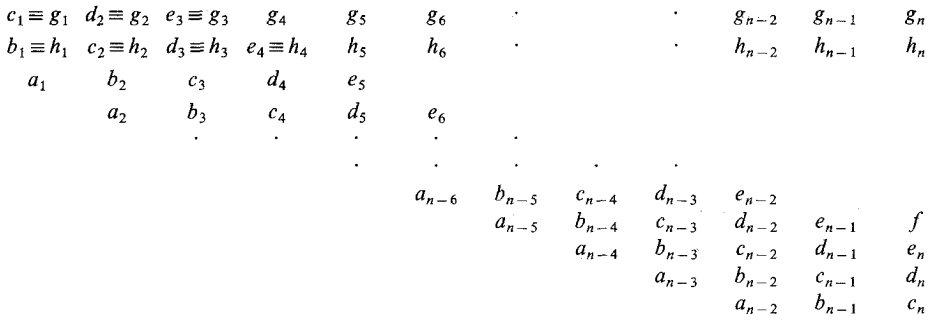


FIGURE 1.

venience can be however eliminated by resorting to a UL factorization, as suggested by Zang [17]. The Appendix contains the algorithm for performing the UL fac-

The operation count of the proposed quasi-pentadiagonal algorithm is  $O(N)$  so that the rate-determining step of the solution of Eqs. (5.7) is the formation of the right-hand side of Eqs. (5.7a) which requires  $O(N^2)$  operations. In order to actually exploit the efficiency of the algorithm the right-hand side of Eqs. (5.7a) can be formed by first evaluating  $r_1^2 \exp[2(x + 1)/\alpha] F(x)$  at the Chebyshev points and then applying the Fast Fourier Transform to the vector of the gridpoint values of this function. If  $F(x)$  is known only by means of its Chebyshev coefficients, an additional anti-transform step is required to obtain the gridpoint values of  $F(x)$ . The above transform method, however, has not been employed in the numerical examples to be shown in the next section.

### 8. NUMERICAL EXAMPLES

In order to compare the Chebyshev approximations with the exact analytical solution we proceed as follows. The assumed exact solution  $A_e(x)$  is differentiated analytically to obtain the exact source term  $F_e(x)$ . A Chebyshev approximation  $F(x)$  to the latter is obtained from the truncated series

$$F(x) = \sum_{n=0}^N F_n T_n(x), \tag{8.1}$$

with the coefficients  $F_n$  evaluated by the expressions

$$F_n = \frac{1}{\bar{c}_n} \frac{2}{N} \sum_{j=0}^N \frac{1}{\bar{c}_j} F_e(x_j) \cos(nj\pi/N), \quad 0 \leq n \leq N, \tag{8.2}$$

where  $x_j = \cos(j\pi/N)$ ,  $0 \leq j \leq N$ ,  $\bar{c}_0 = 2$ ,  $\bar{c}_j = 1$  for  $1 \leq j \leq N-1$  and  $\bar{c}_N = 2$ . From the computed coefficients  $A_n$  of the approximate solution  $A(x)$ , point values  $A(x_j)$  are determined by means of the expansion

$$A(x_j) = \sum_{n=0}^N A_n \cos(nj\pi/N), \quad 0 \leq j \leq N. \quad (8.3)$$

The relative  $L_2$  error of the Chebyshev approximation is then defined in the standard way by the equation

$$E[A] \equiv \|A - A_e\| / \|A_e\|, \quad (8.4)$$

where  $\|A\|^2 = (A, A) = \int_{-1}^{+1} [A(x)]^2 (1-x^2)^{-1/2} dx$ . The weighted integral is evaluated according to the quadrature formula [18]

$$\int_{-1}^{+1} \frac{F(x) dx}{(1-x^2)^{1/2}} = \frac{\pi}{N+1} \sum_{j=0}^N F(x_j). \quad (8.5)$$

The first example considered here is the solution of the  $l=2$  vector mode of the Poisson equation supplemented with Dirichlet boundary conditions. The relative errors of  $A_1$ ,  $A_2$ , and  $A_3$  for different values of  $N$  are given in Table I, where the convergence rate of infinite order typical of spectral approximations is clearly seen. Although the present example pertains to a narrow gap, the methods proposed in this paper can also be applied to problems with an up to infinite region around a sphere, by truncating the infinite domain at a large but finite radius [19]. If the asymptotic behaviour of the solution as  $r \rightarrow \infty$  is known, an optimum domain size for a fixed number of Chebyshev polynomials can be estimated [20].

The use of different boundary conditions of purely Dirichlet type, Eq. (2.3), or combined Robin and Dirichlet type, Eqs. (2.5), for the Poisson equation has then

TABLE I  
Poisson Equation with Dirichlet Boundary Conditions

N	Relative error		
	$A_1$	$A_2$	$A_3$
10	0.27(-3)	0.13(-2)	0.36(-2)
14	0.37(-6)	0.22(-5)	0.76(-5)
18	0.15(-9)	0.10(-8)	0.44(-8)
22	0.16(-13)	0.13(-12)	0.61(-12)
26	0.91(-16)	0.74(-16)	0.23(-15)
30	0.94(-16)	0.75(-16)	0.12(-15)

Note.  $1 \leq r \leq 1.1$ ;  $l=2$ ;  $\mathbf{A}(r) = (\cos 90r, \sin 100r, \cos 100r)$ .

TABLE II  
Comparison of Different Boundary Conditions for the Poisson Equation

N	Relative error					
	Dirichlet conditions			Robin and Dirichlet conditions		
	$A_1$	$A_2$	$A_3$	$A_1$	$A_2$	$A_3$
8	0.50(-3)	0.50(-3)	0.49(-3)	0.72(-3)	0.50(-3)	0.49(-3)
16	0.10(-8)	0.10(-8)	0.10(-8)	0.15(-8)	0.10(-8)	0.10(-8)
24	0.42(-15)	0.42(-15)	0.42(-15)	0.63(-15)	0.42(-15)	0.42(-15)
32	0.19(-16)	0.19(-16)	0.34(-16)	0.48(-16)	0.29(-16)	0.33(-16)

Note.  $1 \leq r \leq 2$ ;  $l = 5$ ;  $\mathbf{A}(r) = (e^{5r}, e^{5r}, e^{5r})$ .

been addressed and the respective errors have been given in Table II. Since the analytical solution  $\mathbf{A}(r) = (e^{5r}, e^{5r}, e^{5r})$  does not satisfy the homogeneous condition (2.5a) an appropriate source term has been appended to the right-hand side. From the results it appears that the Robin condition deteriorates the accuracy of the component  $A_1$  only marginally (with respect to the use of Dirichlet conditions) whereas it does not affect at all that of the component  $A_2$  which is coupled to  $A_1$  for  $l = 5 > 0$ . The solution of a vector mode of the Helmholtz equation with  $\gamma = 1$  has also been considered and the results are shown in Table III. The numerical errors are found to be identical to those (not reported in Table III) of the corresponding Poisson equation ( $\gamma = 0$ ). In other words, the accuracy of the algorithm is not strongly dependent on the term  $\gamma \mathbf{A}$  for  $\gamma = O(1)$ .

Three examples dealing with the fourth-order equations in factorized form have then been considered. In all cases the integral conditions for  $\zeta$  have been imposed directly according to the method described in Section 6. Table IV shows the rate of convergence of  $\zeta$  and  $\mathbf{A}$  in the case of the biharmonic equation. For comparison we give in Table V the errors for the same problem solved with the aid of the influence

TABLE III  
Helmholtz Equation with Dirichlet Boundary Conditions

N	Relative error		
	$A_1$	$A_2$	$A_3$
8	0.23(-1)	0.41(-1)	0.12(0)
12	0.15(-3)	0.37(-3)	0.39(-2)
16	0.60(-6)	0.27(-5)	0.46(-4)
20	0.22(-8)	0.17(-7)	0.55(-6)

Note.  $\frac{1}{2} \leq r \leq \frac{3}{2}$ ;  $\gamma = 1$ ;  $l = 5$ ;  $\mathbf{A}(r) = (\cos 8r, \sin 10r, \cos 12r)$ .

TABLE IV  
Biharmonic (Poisson–Poisson) Equation

Relative error						
$N$	$\zeta_1$	$\zeta_2$	$\zeta_3$	$A_1$	$A_2$	$A_3$
6	0.34(-2)	0.73(-2)	0.14(-1)	0.34(-2)	0.53(-2)	0.10(-1)
8	0.14(-3)	0.44(-3)	0.11(-2)	0.12(-3)	0.34(-3)	0.87(-3)
10	0.58(-5)	0.23(-4)	0.72(-4)	0.55(-5)	0.18(-4)	0.57(-4)
12	0.22(-6)	0.11(-5)	0.42(-5)	0.21(-6)	0.91(-6)	0.34(-5)
14	0.85(-8)	0.51(-7)	0.32(-6)	0.80(-8)	0.41(-7)	0.18(-6)
16	0.30(-9)	0.21(-8)	0.17(-7)	0.28(-9)	0.17(-8)	0.91(-8)

Note.  $\frac{1}{2} \leq r \leq 2$ ;  $\gamma = 0$ ;  $l = 3$ ;  $\mathbf{A}(r) = (e^{(3/2)r}, e^{2r}, e^{(5/2)r})$ .

TABLE V  
Biharmonic (Poisson–Poisson) Equation. Influence Matrix Method

Relative error						
$N$	$\zeta_1$	$\zeta_2$	$\zeta_3$	$A_1$	$A_2$	$A_3$
6	0.14(-1)	0.10(0)	0.11(0)	0.87(-2)	0.70(-2)	0.13(-1)
8	0.83(-3)	0.52(-2)	0.69(-2)	0.43(-3)	0.39(-3)	0.97(-3)
10	0.41(-4)	0.25(-3)	0.40(-3)	0.20(-4)	0.20(-4)	0.61(-4)
12	0.20(-5)	0.12(-4)	0.23(-4)	0.98(-6)	0.10(-5)	0.36(-5)
14	0.94(-7)	0.56(-6)	0.12(-5)	0.45(-7)	0.45(-7)	0.19(-6)
16	0.41(-8)	0.24(-7)	0.62(-7)	0.19(-8)	0.19(-8)	0.97(-8)

Note.  $\frac{1}{2} \leq r \leq 2$ ;  $\gamma = 0$ ;  $l = 3$ ;  $\mathbf{A}(r) = (e^{(3/2)r}, e^{2r}, e^{(5/2)r})$ .

TABLE VI  
Biharmonic (Helmholtz–Poisson) Equation

Relative error						
$l$	$\zeta_1$	$\zeta_2$	$\zeta_3$	$A_1$	$A_2$	$A_3$
0	0.17(-9)	—	—	0.21(-9)	—	—
1	0.19(-9)	0.13(-8)	0.81(-8)	0.72(-9)	0.17(-8)	0.94(-8)
2	0.23(-9)	0.16(-8)	0.92(-8)	0.32(-9)	0.17(-8)	0.93(-8)
3	0.30(-9)	0.21(-8)	0.11(-7)	0.28(-9)	0.17(-8)	0.93(-8)
4	0.31(-9)	0.24(-8)	0.14(-7)	0.25(-9)	0.17(-8)	0.92(-8)
5	0.24(-9)	0.12(-8)	0.14(-7)	0.25(-9)	0.17(-8)	0.92(-8)

Note.  $\frac{1}{2} \leq r \leq 2$ ;  $\gamma = 1$ ;  $\mathbf{A}(r) = (e^{(3/2)r}, e^{2r}, e^{(5/2)r})$ ;  $N = 16$ .

TABLE VII  
 Comparison of Integral and Dirichlet Conditions  
 in the Solution of the Factorized Biharmonic Equation

	Dirichlet conditions	Integral conditions
$\zeta_1$	0.2421(-9)	0.2420(-9)
$\zeta_2$	0.1280(-8)	0.1280(-8)
$\zeta_3$	0.1475(-7)	0.1475(-7)
$A_1$	0.2560(-9)	0.2552(-9)
$A_2$	0.1724(-8)	0.1724(-8)
$A_3$	0.9212(-8)	0.9213(-8)

Note.  $\frac{1}{2} \leq r \leq 2$ ;  $\gamma = 1$ ;  $l = 5$ ;  $\mathbf{A}(r) = (e^{(3/2)r}, e^{2r}, e^{(5/2)r})$ ;  $N = 16$ .

matrix method [5]. The proposed direct method, which is more efficient, turns out to be also more accurate than the influence matrix approach. In Table VI we show the relative errors of the modes with  $l = 0, 1, \dots, 5$  for the case of the general fourth-order equation (4.2), i.e., the Helmholtz–Poisson factorized equation. The errors are only weakly sensitive to the value of  $l$  in the range considered. Table VII compares the accuracy resulting from the use of the integral conditions for  $\zeta$  with the accuracy obtainable if the boundary values of  $\zeta_2$  and  $\zeta_3$  were available. In the example considered the relative errors are found to be almost identical.

All calculations have been performed using double precision arithmetic on a UNIVAC 1100/81 computer.

## 9. CONCLUSION

This paper provides a method for solving elliptic equations of a vector field in spherical regions, spectrally. The numerical results of some test calculations indicate that spectral convergence in the approximation of the radial dependence can be achieved for the three cases of Laplace, Helmholtz, and biharmonic equations and for all types of boundary conditions considered. The most relevant result is that, for the case of the vector biharmonic equation in factorized form, as the vorticity-vector potential equations for incompressible viscous flows, the use of integral conditions for the vector modes produces a splitting of the vorticity equations with the same structure of the matrix differential operator. In this respect, the paper contains the first application of the concept of vorticity integral conditions in a fully vectorial context.

In order to make effective the analysis and the algorithms of this paper in the solution of multi-mode and nonlinear problems, efficient methods for evaluating transform and anti-transform as well as the nonlinear terms in spherical coordinates are required. Owing to the 3D and vector character of the quantities to be evaluated, the calculation of nonlinear terms via the interaction coefficients [21–23]

seems prohibitive in terms of both memory requirements and execution speed. Such terms can however be calculated efficiently by means of transform techniques. The Chebyshev truncated expansion being a cosine series, the well-established FFT algorithm can be employed [24], whereas efficient transform techniques for spherical harmonics are less standard and still under investigations (see, e.g., for the scalar case [25–28] and for an extension to the vector case [29]). Furthermore, and very importantly, the transformation algorithm most convenient to perform efficient calculations depends on the type of the computer, a sequential or parallel machine, and on the availability of vector or array processors. Since the solution of the equations of the single vector modes is an aspect of the problem independent from the transform choices, we have limited our analysis to the specific examination of the single-mode equations, leaving the complete study of multi-mode equations for a future investigation.

## APPENDIX:

### UL FACTORIZATION OF A QUASI-PENTADIAGONAL MATRIX

This Appendix contains the algorithm to perform the UL factorization and the backward and forward substitutions of a  $n \times n$  matrix with the structure shown in Fig. 1.

#### *UL Factorization and Substitutions of a Quasi-Pentadiagonal Matrix*

##### Factorization

```

 $a_{n-1}, a_n, b_n := 0;$ 
do  $i := n$  step  $-1$  until  $3$ 
   $c_i := c_i - d_{i+1}b_i - e_{i+2}a_i;$ 
  if  $i > 3$  then  $d_i := d_i - e_{i+1}b_i;$ 
  if  $i = n - 1$  then  $e_i := e_i - fb_i;$ 
  if  $i = n - 2$  then  $d_i := d_i - fa_i;$ 
   $h_i := h_i - h_{i+1}b_i - h_{i+2}a_i;$ 
   $g_i := g_i - g_{i+1}b_i - g_{i+2}a_i;$ 
   $b_{i-1} := (b_{i-1} - d_{i+1}a_{i-1})/c_i;$ 
   $a_{i-2} := a_{i-2}/c_i;$ 
end

 $e_4 := h_4; d_3 := h_3; e_3 := g_3;$ 

 $i := 2;$ 
 $c_i, h_i := h_i - h_{i+1}b_i - h_{i+2}a_i;$ 
 $d_i, g_i := g_i - g_{i+1}b_i - g_{i+2}a_i;$ 
 $h_{i-1}, b_{i-1} := (b_{i-1} - d_{i+1}a_{i-1})/c_i;$ 

 $i := 1;$ 
 $c_i, g_i := g_i - g_{i+1}b_i - g_{i+2}a_i;$ 

```

## Substitutions

Backward substitution for the upper triangular matrix

$$x_n := x_n/c_n;$$

$$x_{n-1} := (x_{n-1} - d_n x_n)/c_n;$$

**do**  $i := n - 2$  **step**  $-1$  **until**  $3$

$$\quad \text{if } i = n - 3 \text{ then } x_i := x_i - f x_{i+3};$$

$$\quad x_i := (x_i - d_{i+1} x_{i+1} - e_{i+2} x_{i+2})/c_i;$$

**end**

$$x := x_2; \text{ do } j := 3 \text{ step } 1 \text{ until } n \text{ } x := x - h_j x_j \text{ end}; x_2 := x/c_2;$$

$$x := x_1; \text{ do } j := 2 \text{ step } 1 \text{ until } n \text{ } x := x - g_j x_j \text{ end}; x_1 := x/c_1;$$

Forward substitution for the lower triangular matrix

$$x_2 := x_2 - b_1 x_1;$$

**do**  $i := 3$  **step**  $1$  **until**  $n$

$$\quad x_i := x_i - b_{i-1} x_{i-1} - a_{i-2} x_{i-2};$$

**end**

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