The Vector Harmonic Transform Method for Solving Partial Differential Equations in Spherical Geometry

by

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ABSTRACT

The development of computational methods for solving partial differential equations in spherical geometry is complicated by problems induced by the spherical coordinate system itself. Even though the solution is smooth in Cartesian coordinates, in spherical coordinates the components of vector fields such as the wind are multi-valued at the poles and the differential equations have unbounded terms. For example, the total derivative of the velocity is unbounded at the poles. Here we present the vector harmonic transform method for the effective treatment of these problems. Vector fields such as the wind are expanded in terms of vector harmonics and scalar fields such as pressure and temperature are expanded in terms of scalar harmonics. Unbounded terms in the differential equation are grouped into bounded expressions that are evaluated by their formal application to the spectral expansions. The method can be applied to any differential equation without introducing scalar dependent variables, such as divergence or vorticity, or without raising the order of the differential equations. The method can be implemented on either a Gauss or equally spaced latitudinal grid with points located at the poles because the method does not contain any divisions by the cosine of the latitude. The computational requirements are comparable to traditional spectral methods.

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1. Introduction

In this paper we are concerned with solving either steady or time dependent partial differential equations that are posed in spherical coordinates. We introduce the vector harmonic transform method of solution which belongs to the category of spectral transform methods. The choice of spherical coordinates is made largely for the convenience associated with the prescription of the boundary and boundary conditions. However, this choice leads to a number of both theoretical and computational problems that have for the most part been resolved both here and elsewhere in the literature on this subject. We will review these problems briefly by first considering several fundamental differences between problem solving on the sphere in spherical coordinates and on the rectangle in Cartesian coordinates.

1. On the rectangle and with a uniform grid, the discrete basis for the spectral method consists of those trigonometric functions that do not alias on the grid. Similarly, on the sphere, the discrete basis consists of those harmonics that do not alias on the grid. However, the number of harmonic basis functions is half the number of trigonometric functions which leads to the following fundamental difference between approximations on the sphere and the rectangle.
2. Fourier representations on the rectangle are interpolative whereas harmonic representations are least squares but not in the l_2 norm. This is a computational aspect that is associated with the discrete approximation of functions that are tabulated on the surface of the sphere. The least squares approximation of functions on the sphere and the discrete norm are discussed in Swarztrauber (1979).
3. Vector functions such as the wind are continuously differentiable everywhere in Cartesian coordinates but they are discontinuous at the poles in spherical coordinates. Indeed vector functions are multi-valued at the poles because the derivatives of the spherical coordinate system with respect to the Cartesian coordinate system are multi-valued at the poles. An example is given later in this section.
4. The individual terms in a partial differential equation in Cartesian coordinates are bounded whereas many terms in the same equation posed in spherical coordinates are unbounded at the poles. In addition, the clustering of points in a spherical grid system leads to accuracy and stability problems. These and other computational problems induced by the spherical coordinate system are collectively referred to the "pole problem."

5. Fourier analysis can be used for both scalar and vector functions on the rectangle. However different analyses are required for scalar and vector functions on the sphere. Vector harmonics provide a suitable basis for the discontinuous vector functions and scalar harmonics provide a suitable basis for scalar functions such as pressure and temperature that are smooth at the poles.
6. On the rectangle the fast Fourier transform (FFT) can be used in both the x and y directions to speed the Fourier transform. On the sphere the harmonic transform consists of the Fourier transform in the longitudinal direction and the Legendre transform in the latitudinal direction. The FFT can only be used to speed the Fourier transform and hence the computational time required for the harmonic transform is, to first order, determined by the Legendre transform which at present remains a slow transform.

The development of computational methods for solving partial differential equations on the surface of the sphere is complicated by problems induced by the spherical coordinate system itself. The horizontal velocity components are discontinuous at the poles in spherical coordinates even though they are continuous in Cartesian coordinates. For example, a sphere in solid rotation but with the axis of rotation perpendicular to the coordinate axis, i.e. the axis of rotation passes through the equator of the spherical coordinate system. If Ω is the rotational rate, then in Cartesian coordinates the velocity components are $X = \Omega z$, $Y = 0$, and $Z = -\Omega x$ which are continuous everywhere. However, if we let a be the radius of the sphere, λ be east longitude, θ be latitude, and let u and v be the corresponding velocity components, then $u = -\Omega a \sin\theta \sin\lambda$ and $v = -\Omega a \cos\lambda$. Both components are multi-valued and hence discontinuous at the poles $\theta = \pm\pi/2$. Indeed any nonzero vector field at the poles is discontinuous.

These discontinuities create a fundamental problem associated with solving differential equations on the surface of the sphere; namely, they induce unbounded terms in the differential equations in the neighborhood of the poles (Swarztrauber, 1981, 1984). Indeed, the total derivative of the velocity with respect to time is unbounded. Since $u = a \cos\theta \, d\lambda/dt$ and $v = a \, d\theta/dt$, the total derivative is

$$\frac{dv}{dt} = \frac{\partial v}{\partial t} + \frac{u}{a\cos\theta}\frac{\partial v}{\partial \lambda} + \frac{v}{a}\frac{\partial v}{\partial \theta} \tag{1.1}$$

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{u}{a\cos\theta}\frac{\partial u}{\partial \lambda} + \frac{v}{a}\frac{\partial u}{\partial \theta} \,. \tag{1.2}$$

If the velocity components given above are substituted into these equations, then the total derivative of the velocity of a sphere in solid rotation about an axis through the equator is

$$\frac{dv}{dt} = -\Omega^2 a \frac{\sin^2\lambda \sin\theta}{\cos\theta} \ , \tag{1.3}$$

$$\frac{du}{dt} = \Omega^2 a \frac{\sin\lambda \cos\lambda}{\cos\theta} \ . \tag{1.4}$$

Since $\cos\theta$ vanishes at the poles the total derivative of the velocity is unbounded. A view of du/dt is given in Figure 1 which shows two lobes extending to plus infinity that are adjacent to two lobes that extend to minus infinity. The view includes only a very small neighborhood of the pole which corresponds to the single vertical line that extends from $-\infty$ to $+\infty$. Although these terms are unbounded they always combine with other unbounded terms to form bounded differential expressions. For example, the total derivative of the velocity combines with the metric terms to obtain the fluid acceleration. Discontinuous velocities and unbounded terms create computational problems both at and in the vicinity of the poles. Traditional finite-difference or spectral methods cannot be used to evaluate unbounded terms since convergence would be slow and the lack of cancellation between unbounded terms would introduce substantial error. The problems have led researchers to reformulate the equations in terms of scalar dependent variables (Bacus, 1967).

Spectral methods were first used by Silberman (1954), who solved the nondivergent barotropic vorticity equation using an interaction coefficient method to calculate the nonlinear terms. This method was not competitive with finite-difference methods because of the extensive computation required to evaluate the nonlinear terms. Robert (1966) solved the problem of discontinuous velocity components by transforming the vector functions (velocity) to scalar functions (pseudo-scalars) by multiplying the velocity components by the cosine of the latitude. The resulting functions are continuously differentiable, both in Cartesian and spherical coordinates and, therefore, a spectral representation in terms of surface spherical harmonics has the desired convergence properties.

When the transform method was introduced (Eliassen et al., 1970; Orszag, 1970), spectral techniques became competitive with finite-difference methods in terms of the computation required to obtain a given accuracy. A well known transform method is based on scalar spherical harmonic functions (Bourke, 1972; Bourke et.al., 1977; Machenhauer and Rasmussen, 1972; Machenhauer and Daley, 1972; Machenhauer, 1979). The vector momentum equations are replaced by scalar equations with vorticity and divergence as dependent variables. All of the terms in the equations are bounded and all of the dependent variables are smooth at the poles and, hence, expandable in terms of the scalar spherical harmonics. The severe restriction on the time step for a finite-difference method using spherical coordinates is removed since the highest wave number is determined by the grid spacing at the equator, rather than the spacing next to the pole. This is discussed in detail by Orszag (1974). This approach is currently in wide use throughout the weather and climate modeling community (e.g., Baede et al., 1979; Boer et al., 1984; Williamson et al., 1987).

In this paper we describe the vector harmonic transform method in which the velocity is expanded in terms of vector harmonics. It has been shown (Swarztrauber, 1981) that the convergence properties of this representation are determined by the smoothness of the vector function in Cartesian coordinates. The series representation in terms of vector harmonics will converge uniformly to a vector whose components are smooth in Cartesian coordinates even though they are discontinuous in spherical coordinates. The unbounded terms can be grouped into bounded differential expressions that can be evaluated using the vector harmonic transform method presented here. Like the traditional spectral methods the time step for the method is based on the largest grid spacing at the equator rather than the smallest at the poles. The equations are treated in their original form without raising their differential order. These as well as other attributes of the method are listed below.

1. All dependent variables, including the velocity, are represented directly as spectral expansions without introducing scalar dependent variables or raising the differential order of the equations.
2. Unbounded terms in each differential equation are grouped into bounded differential expressions that can be evaluated by formal application to the spectral expansions. This reformulation can be applied to any vector differential equation and is not restricted to the example given in Section 3 for the shallow water equations.
3. The method can be implemented on either a Gauss or equally spaced latitudinal grid with points located at the poles because the method does not contain any

divisions by cos θ. The experimental results presented in Browning, et.al. (1989), were computed on a equally spaced grid and compared with the scalar transform on a Gaussian grid.

4. The velocity components are carried as dependent variables and expanded in terms of vector harmonics. The transform is norm preserving and, hence, does not contribute to the error growth that results from the repeated transforms between physical and spectral space.
5. The vector harmonics separate naturally into nondivergent and irrotational sets that form a complete basis for nondivergent and irrotational vector functions respectively. Therefore, if appropriate, nondivergence can be maintained throughout the period of integration by representing the vector function in terms of the nondivergent basis. This approach also halves the amount of computation.
6. The computational requirements of the vector harmonic transform method are the same as the traditional spectral method. To first order, the computational time required by the model dynamics, is determined by the number of Legendre and Legendre-type transforms. In Section 3 it is shown that the shallow water equations can be solved with nine (9) Legendre-type transforms per time step which is the same as the traditional spectral transform method (Temperton, 1991).
7. The method provides a modular approach to model development. Once modules are provided for computing the analysis and synthesis of vector and scalar functions, together with modules for computing the spatial derivatives, geophysical models can be developed quickly and conveniently.

Although vector and related harmonics have been used for solving vector partial differential equations (James, 1976), for the most part they have been used in electromagnetic applications including particle and astrophysics. Exceptions include Bjorklund (1973), Jones (1970, 1971), Moses (1974), Yakimiw (1976), Swarztrauber (1984), and a modal analysis of the Laplace tidal equations in Swarztrauber and Kasahara (1985). The vector harmonic transform method was compared with the finite-difference composite-mesh and traditional spectral method in Browning, et.al. (1989). The computational and storage requirements for a five day integration were compared for both two and four digits of accuracy and the requirements for the two spectral methods were found to be comparable. These experiments provide considerable information on the relative performance of the vector harmonic transform method and hence, this paper does not contain any computational experiments. However, operation counts in terms of Legendre and Legendre-type transforms are presented in Section 3. Although the method is outlined in Browning, et.al. (1989), the details of the vector harmonic method together with reference materials and recent computational improvements are included in this paper. A set of benchmarks for the testing and comparing models is given in Williamson et.al. (1992).

With the exception of Browning, et.al. (1989), papers that use vector harmonics generally focus on theory and do not provide the details that are necessary for a computer implementation. Although this paper contains a theoretical development of the vector harmonic transform method, it also focuses on the computational details that are necessary for a practical implementation of the method. For example, the efficient computation of Gauss and equally spaced transforms are presented in Section 4 together with efficient methods for computing the associated Legendre functions. Hence, this paper is a self-contained reference source for both the theory and implementation of the vector harmonic transform method.

The vector spherical harmonics are developed in the next section together with the analysis and synthesis of an arbitrary vector field on the surface of the sphere. The analysis and synthesis of scalar fields are also reviewed. In practice most scalar and vector fields are real and therefore, real versions of the usual complex transforms are provided. The real versions offer a savings of two over the complex transforms. Additional savings can be realized by using two algorithmic variants that are presented in the second half of Section 2. Each variant halves the computation and both can be implemented which reduces the computation by a factor of four.

The vector harmonic transform method is applicable to any vector differential equation on the sphere; however, for purposes of exposition in Section 3, it is implemented in the simplified context of the shallow water equations. The shallow water equations are of interest since a large fraction of the energy in the atmosphere is contained in the modes supported by these equations. The method is developed for two different forms of the shallow water equations and focuses on the computation of the spatial derivatives that appear on the right side of the equations. Section 3 contains the computation of the bounded differential expressions that are most frequently required to implement the method. The spectral method is used to compute the divergence, vorticity, vector Laplacian of a vector field, and the gradient and Laplacian of a scalar field. The inverse operators are also implemented. For example, given the vorticity and divergence then the vector spectral method provides a straightforward way to determine the corresponding vector field. Although the focus is on the shallow water equations, the section ends with two methods that provide all the differential expressions that are required to solve the general partial differential equation.

The key computational elements of the vector harmonic transform method are presented in Section 4. Efficient methods are presented for the computation of the associated Legendre functions and other related functions that are used in the computation of the spherical harmonic transforms. This section provides the fundamental link between theory and the computer implementation of the transforms and the vector harmonic transform method. The section also includes efficient and accurate discrete transforms for both Gauss and equally spaced latitudinal grid points. A uniform longitudinal grid is assumed throughout.

The vector harmonic transform method relies extensively on identities that are satisfied both by the scalar and vector harmonics. For example, to compute the divergence of a vector field it is necessary to use the identity that expresses the divergence of the vector harmonics in terms of the scalar harmonics. A large number of identities both for scalar and vector harmonics are presented in Section 5. Most of the identities used in this paper are assembled in Section 5. However, additional identities are included as a reference for model development activities that are not explicitly presented in this paper. Section 5 also includes the development of the surface vector Laplacian together with the identities that are necessary to facilitate its computation. The surface vector Laplacian provides a natural dissipation term for fluid computations that are posed on the sphere. Section 5 also contains a review of the differential geometry of the spherical coordinate system that is used to develop the transform method given in Section 3 for the general differential equation. In addition to their use in the other sections, Sections 4 and 5 provide reference material for the development of other models that are based on the vector harmonic transform method.

2. Scalar and vector spherical harmonic analysis and synthesis

From the introduction it is evident that the spectral representation of scalar and vector functions must be quite different. Since the scalar harmonics can be expressed as polynomials in the Cartesian coordinates x, y, and z, they provide a suitable basis for scalar functions such as divergence and vorticity which are also smooth at the poles. However, since vector functions such as the velocity are multi-valued and, hence, discontinuous at the poles, the scalar harmonics do not provide a suitable set of basis functions since convergence to a discontinuous function would be prohibitively slow. On the other hand, the vector spherical harmonics have discontinuities that "match" the discontinuities in vector functions that are induced by the spherical coordinate system. As a result, the convergence of a vector harmonic spectral representation is uniform even for discontinuous vector functions as long as the vector function is smooth in Cartesian coordinates.

In this section we develop the vector spherical harmonics. We also provide both the complex and real forms of both the scalar and vector harmonic transforms. The real transforms require half the computation required by the complex forms. The second half of the section includes two algorithmic variants, each of which halve the the amount of computation in both the analysis and synthesis. If both variants are implemented then the computation is reduced by a factor of four. At first reading the second half of this section can be omitted without loss of continuity.

We begin with the scalar spherical harmonics. With latitude θ and $x = \sin\theta$ the associated Legendre functions are given by

$$P_n^m(\theta) = \frac{1}{2^n n!}(-\cos\theta)^m \frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n \ . \tag{2.1}$$

These functions are defined as solutions of the ordinary differential equation

$$\frac{1}{\cos\theta}\frac{d}{d\theta}\left[\cos\theta\frac{dP_n^m(\theta)}{d\theta}\right] + [n(n+1) - \frac{m^2}{\cos^2\theta}]P_n^m(\theta) = 0 \ . \tag{2.2}$$

With λ defined as longitude the scalar spherical harmonics are given by

$$Y_n^m(\lambda,\theta) = P_n^m(\theta)e^{im\lambda} \ . \tag{2.3}$$

It is known that any smooth function $\phi(\lambda,\theta)$ has a uniformly convergent series representation in terms of the scalar spherical harmonics

$$\phi(\lambda,\theta) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{m,n} Y_n^m(\lambda,\theta) \ . \tag{2.4}$$

If we define the inner product of two functions $f(\lambda,\theta)$ and $g(\lambda,\theta)$ as

$$(f, g) = \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} \overline{f}(\lambda,\theta)\, g(\lambda,\theta) \cos\theta \, d\theta \, d\lambda \ , \tag{2.5}$$

then the scalar spherical harmonics satisfy the orthogonality relations

$$(Y_n^m, Y_k^j) = \begin{cases} \dfrac{4\pi}{2n+1} \dfrac{(n+m)!}{(n-m)!} & \text{if } m=j \text{ and } n=k \\ 0 & \text{if } m \neq j \text{ or } n \neq k \end{cases} . \tag{2.6}$$

The scalar harmonic analysis of $\phi(\lambda,\theta)$ consists of computing the coefficients $a_{m,n}$ in (2.4). Multiplying both sides of (2.4) by $Y_n^{\overline{m}}$ and integrating over the sphere we obtain

$$a_{m,n} = \frac{\alpha_{m,n}}{2} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} Y_n^{\overline{m}} \phi(\lambda,\theta) \cos\theta \, d\theta \, d\lambda \tag{2.7}$$

where

$$\alpha_{n,m} = \frac{2n+1}{2\pi} \frac{(n-m)!}{(n+m)!} \ . \tag{2.8}$$

This completes the development of the scalar harmonic transforms for any complex scalar function $\phi(\lambda,\theta)$. Consider now the development of the vector harmonic transforms.

In Cartesian coordinates the Fourier representation can be used for both scalar and vector functions on the rectangle. While it is true that the scalar harmonic transform can be used for the vertical (or radial) component of a vector it can not be used for the horizontal components. This is because the radial component is smooth at the poles whereas the horizontal components are discontinuous as discussed in the introduction. Therefore, attention is directed to the spectral representation of the horizontal components of a vector in spherical geometry. Let $\mathbf{v}^T = [u(\lambda,\theta), v(\lambda,\theta)]$ be a two dimensional vector that is tangent to the surface of the sphere and whose first component $u(\lambda,\theta)$ corresponds to east longitude and the second component $v(\lambda,\theta)$ corresponds to latitude.

The selection of a suitable set of basis functions for $\mathbf{v}$ begins with the Helmholtz relations. Any vector function on the surface of the sphere can be expressed in terms of the stream function Ψ and velocity potential χ by the Helmholtz relations

$$u = \frac{1}{a\cos\theta}\frac{\partial\chi}{\partial\lambda} - \frac{1}{a}\frac{\partial\Psi}{\partial\theta} \tag{2.9}$$

and

$$v = \frac{1}{a\cos\theta}\frac{\partial\Psi}{\partial\lambda} + \frac{1}{a}\frac{\partial\chi}{\partial\theta}. \tag{2.10}$$

Since Ψ and χ are scalar functions, they can be represented in terms of the surface harmonics Y_n^m. Indeed, it is possible to generate a sequence of vector functions by substituting the scalar spherical harmonics for Ψ and χ in the right side of (2.9) and (2.10). In particular, as a possible basis for vector functions, it is reasonable to consider the set of vector functions that is obtained by first setting $\Psi=0$, $\chi = aY_n^m/\sqrt{n(n+1)}$ and then setting $\Psi = aY_n^m/\sqrt{n(n+1)}$, $\chi = 0$. In doing so we obtain the horizontal structure of the vector spherical harmonics (Morse and Feshbach, 1953), namely

$$\mathbf{B}_n^m = \begin{bmatrix} iW_n^m \\ V_n^m \end{bmatrix} e^{im\lambda} \quad \text{and} \quad \mathbf{C}_n^m = \begin{bmatrix} -V_n^m \\ iW_n^m \end{bmatrix} e^{im\lambda} \tag{2.11}$$

where V_n^m and W_n^m are functions of latitude only given by

$$\sqrt{n(n+1)}V_n^m(\theta) = \frac{dP_n^m}{d\theta} = ½[P_n^{m+1} - (n+m)(n-m+1)P_n^{m-1}] \tag{2.12}$$

and

$$\sqrt{n(n+1)}W_n^m(\theta) = \frac{m}{\cos\theta}P_n^m = ½[P_{n-1}^{m+1} + (n+m)(n+m-1)P_{n-1}^{m-1}]. \tag{2.13}$$

The vector spherical harmonics form a complete orthogonal set of basis functions for the spectral representation of vector functions on the sphere. Any vector function **v** that is smooth in Cartesian coordinates has the uniformly convergent series representation

$$\mathbf{v} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} b_{m,n} \mathbf{B}_n^m + c_{m,n} \mathbf{C}_n^m \tag{2.14}$$

even though **v** is discontinuous at the poles. This is because $\mathbf{B}_n^m$ and $\mathbf{C}_n^m$ have discontinuities that "match" those of **v** induced by the spherical coordinate system. The computation of the coefficients $b_{m,n}$ and $c_{m,n}$ in (2.14) is straightforward using the orthogonality relations for $\mathbf{B}_n^m$ and $\mathbf{C}_n^m$ that are given below. The vector inner product of two arbitrary vector functions $\mathbf{u}(\lambda,\theta)$ and $\mathbf{v}(\lambda,\theta)$ is

$$(\mathbf{u}, \mathbf{v}) = \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} \mathbf{u}^* \ \mathbf{v} \cos\theta \, d\theta \, d\lambda \tag{2.15}$$

where * denotes the conjugate transpose. The orthogonality relations for the vector spherical harmonics are

$$(\mathbf{B}_n^m, \mathbf{C}_k^j) = 0 \tag{2.16}$$

and

$$(\mathbf{B}_n^m, \mathbf{B}_k^j) = (\mathbf{C}_n^m, \mathbf{C}_k^j) = \begin{cases} \dfrac{4\pi}{2n+1} \dfrac{(n+m)!}{(n-m)!} & \text{if } m=j \text{ and } n=k \\ 0 & \text{if } m \neq j \text{ or } n \neq k \end{cases} . \tag{2.17}$$

The computation of $b_{m,n}$ and $c_{m,n}$ or the vector harmonic analysis can now be computed. Multiplying (2.14) by either $(\mathbf{B}_n^m)^*$ or $(\mathbf{C}_n^m)^*$ and integrating over the sphere we obtain

$$b_{m,n} = \frac{\alpha_{m,n}}{2} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} (\mathbf{B}_n^m)^* \ \mathbf{v} \cos\theta \, d\theta \, d\lambda \tag{2.18}$$

$$c_{m,n} = \frac{\alpha_{m,n}}{2} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} (\mathbf{C}_n^m)^* \ \mathbf{v} \cos\theta \, d\theta \, d\lambda \ . \tag{2.19}$$

To this point the analyses and syntheses have been developed for complex functions. However, in practice one is more likely to encounter real valued functions and hence, we now develop the real forms of the harmonic transforms. These forms are about twice as efficient as the complex transforms and hence represent the preferred transforms for real functions. We begin with the development of the synthesis of a real scalar function. Equation (2.4) can be written

$$\phi(\lambda,\theta) = \sum_{n=0}^{\infty}\left(a_{0,n}P_n^0 + \sum_{m=1}^{n} a_{-m,n}Y_n^{-m} + \sum_{m=1}^{n} a_{m,n}Y_n^m\right) . \tag{2.20}$$

From (5.23) $Y_n^{-m} = (-1)^m \dfrac{(n-m)!}{(n+m)!}\overline{Y_n^m}$ which when substituted into (2.7) yields $a_{-m,n} = (-1)^m \dfrac{(n+m)!}{(n-m)!}\overline{a_{m,n}}$. Substituting these results into (2.20) we obtain

$$\phi(\lambda,\theta) = \sum_{n=0}^{\infty}\left[a_{0,n}P_n^0 + \sum_{m=1}^{n} 2\mathrm{Re}(a_{m,n}Y_n^m)\right] . \tag{2.21}$$

If we define $a_{m,n} = \frac{1}{2}(ar_{m,n} - i\ ai_{m,n})$ then the real form of the scalar harmonic synthesis is

$$\phi(\lambda,\theta) = \sum_{m=0}^{\infty}{}' \sum_{n=m}^{\infty} P_n^m(ar_{m,n}\cos m\lambda + ai_{m,n}\sin m\lambda) . \tag{2.22}$$

The prime notation on the sum indicates that the first term corresponding to $m = 0$ is multiplied by ½. The real form of the scalar harmonic analysis can be obtained from the real and imaginary parts of (2.7), namely

$$ar_{m,n} = \alpha_{m,n}\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}\phi(\lambda,\theta)P_n^m(\theta)\cos m\lambda\cos\theta\, d\theta\, d\lambda \tag{2.23}$$

and

$$ai_{m,n} = \alpha_{m,n}\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}\phi(\lambda,\theta)P_n^m(\theta)\sin m\lambda\cos\theta\, d\theta\, d\lambda. \tag{2.24}$$

Proceeding in a similar manner we can develop the following real forms for the vector harmonic transforms. If we define $b_{m,n} = \frac{1}{2}(br_{m,n} - i\ bi_{m,n})$ and $c_{m,n} = \frac{1}{2}(-cr_{m,n} + i\ ci_{m,n})$ then the real form of vector harmonic synthesis (2.14) is

$$u(\lambda,\theta) = \sum_{m=0}^{\infty}{}' \sum_{n=m}^{\infty} [W_n^m (bi_{m,n} \cos m\lambda - br_{m,n} \sin m\lambda)$$

$$+ V_n^m (cr_{m,n} \cos m\lambda + ci_{m,n} \sin m\lambda)] \qquad (2.25)$$

$$v(\lambda,\theta) = \sum_{m=0}^{\infty}{}' \sum_{n=m}^{\infty} [V_n^m (br_{m,n} \cos m\lambda + bi_{m,n} \sin m\lambda)$$

$$+ W_n^m (-ci_{m,n} \cos m\lambda + cr_{m,n} \sin m\lambda)] \, . \qquad (2.26)$$

The prime notation on the sum indicates that the first term corresponding to $m = 0$ is multiplied by ½. The real form of vector harmonic analysis (2.18) and (2.19) is

$$br_{m,n} = \alpha_{m,n} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} [v V_n^m \cos m\lambda - u W_n^m \sin m\lambda] \cos\theta \, d\theta \, d\lambda \qquad (2.27)$$

$$bi_{m,n} = \alpha_{m,n} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} [u W_n^m \cos m\lambda + v V_n^m \sin m\lambda] \cos\theta \, d\theta \, d\lambda \qquad (2.28)$$

$$cr_{m,n} = \alpha_{m,n} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} [u V_n^m \cos m\lambda + v W_n^m \sin m\lambda] \cos\theta \, d\theta \, d\lambda \qquad (2.29)$$

$$ci_{m,n} = \alpha_{m,n} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} [-v W_n^m \cos m\lambda + u V_n^m \sin m\lambda] \cos\theta \, d\theta \, d\lambda \, . \qquad (2.30)$$

This completes the development of the real scalar and vector harmonic transforms.

The second half of this section will now be devoted to the development of two variants of the harmonic transforms presented above. These variants can reduce the computation by up to a factor of four and will likely be of interest to those who will implement the vector harmonic transform method. The reader who is interested only in the development of the method can omit the remainder of this section without a loss in continuity.

The vector harmonic transforms defined in Section 2 require about four times the computational effort required by the scalar harmonic transforms. In the remainder of this section we will develop two variants, each of which can be used to halve the computation. If both variants are implemented the computation can be reduced by a factor of four. We begin with a technique that has been used to speed the transforms used in the traditional spectral transform method (Temperton, 1991). The approach is to express the V_n^m in terms of the W_n^m which is then used to halve the computation and storage requirements. It is known (5.19) that the associated Legendre polynomials satisfy the identity

$$\cos\theta \frac{dP_n^m}{d\theta} = \frac{(n+1)(n+m)}{2n+1} P_{n-1}^m - \frac{n(n-m+1)}{2n+1} P_{n+1}^m \ . \qquad (2.31)$$

Dividing by cosθ and using the definitions (2.12) and (2.13), we obtain

$$V_n^m = \mathrm{c1}_{m,n} W_{n-1}^m - \mathrm{c2}_{m,n} W_{n+1}^m \qquad (2.32)$$

where

$$\mathrm{c1}_{m,n} = \frac{(n+m)\sqrt{(n-1)(n+1)}}{m(2n+1)} \quad \text{and} \quad \mathrm{c2}_{m,n} = \frac{(n-m+1)\sqrt{n(n+2)}}{m(2n+1)} \ . \qquad (2.33)$$

Since $W_n^0 = 0$ the right side of (2.32) is indeterminate for $m = 0$. Therefore, (2.32) is used only for $m > 0$ and V_n^0 must be retained for the transforms. V_n^0 can occupy the locations reserved for W_n^0. Substituting (2.32) into (2.27) we obtain

$$br_{m,n} = \alpha_{m,n} \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} [v(\lambda,\theta)(\mathrm{c1}_{m,n} W_{n-1}^m - \mathrm{c2}_{m,n} W_{n+1}^m)\cos m\lambda$$

$$- u(\lambda,\theta) W_n^m \sin m\lambda]\cos\theta d\theta d\lambda \ . \qquad (2.34)$$

If we compute $a_{m,n}$, $b_{m,n}$, $c_{m,n}$, and $d_{m,n}$ from (2.39) through (2.48) below, then (2.49) is obtained from (2.34). A similar development can be obtained for $bi_{m,n}$, $cr_{m,n}$, and $ci_{m,n}$ resulting in the vector harmonic analysis as presented in (2.39) through (2.52) below.

The vector harmonic synthesis is given in (2.53) through (2.64) below. Its derivation begins with the substitution of (2.32) into (2.25)

$$u(\lambda,\theta) = \tfrac{1}{2} \sum_{n=1}^{\infty} cr_{0,n} V_n^0 + \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} [W_n^m (bi_{m,n} \cos m\lambda - br_{m,n} \sin m\lambda)$$

$$+ (c1_{m,n} W_{n-1}^{m} - c2_{m,n} W_{n+1}^{m})(cr_{m,n} \cos m\lambda + ci_{m,n} \sin m\lambda)] , \qquad (2.35)$$

or

$$u(\lambda,\theta) = \tfrac{1}{2} \sum_{n=1}^{\infty} cr_{0,n} V_n^0 + \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} W_n^m (bi_{m,n} \cos m\lambda - br_{m,n} \sin m\lambda)$$

$$+ \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} c1_{m,n+1} W_n^m (cr_{m,n+1} \cos m\lambda + ci_{m,n+1} \sin m\lambda) \qquad (2.36)$$

$$- \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} c2_{m,n-1} W_n^m (cr_{m,n-1} \cos m\lambda + ci_{m,n-1} \sin m\lambda) ,$$

or

$$u(\lambda,\theta) = \sum_{n=1}^{\infty} \tfrac{1}{2} cr_{0,n} V_n^0$$

$$+ \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} W_n^m [(-c2_{m,n-1} cr_{m,n-1} + c1_{m,n+1} cr_{m,n+1} + bi_{m,n}) \cos m\lambda \qquad (2.37)$$

$$+ (-c2_{m,n-1} ci_{m,n-1} + c1_{m,n+1} ci_{m,n+1} - br_{m,n}) \sin m\lambda] .$$

Once the coefficients $a_{m,n}$ and $b_{m,n}$ are computed from (2.53) and (2.54), then (2.37) takes the form

$$u(\lambda,\theta) = \tfrac{1}{2} \sum_{n=1}^{\infty} cr_{0,n} V_n^0 + \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} W_n^m (a_{m,n} \cos m\lambda + b_{m,n} \sin\lambda) \qquad (2.38)$$

which requires half the computation required by the synthesis (2.25) or the same computational effort as a scalar synthesis using (2.22). A similar result can be obtained for $v(\lambda,\theta)$ thereby halving the computation required for a vector synthesis using (2.25) and (2.26). The algorithmic details of the efficient vector harmonic analysis and synthesis are presented below without derivation. We begin with the analysis.

Given the vector function $\mathbf{v}^T = [u(\lambda,\theta), v(\lambda,\theta)]$ with east longitude and latitude components respectively then the vector harmonic analysis can be computed in the following three steps.

1. For $m = 0$ up to some maximum wave number $m = N$, compute the Fourier transforms:

$$au_m(\theta) = \int_0^{2\pi} u(\lambda,\theta) \cos m\lambda \, d\lambda \qquad (2.39)$$

$$bu_m(\theta) = \int_0^{2\pi} u(\lambda,\theta)\sin m\lambda \, d\lambda \tag{2.40}$$

$$av_m(\theta) = \int_0^{2\pi} v(\lambda,\theta)\cos m\lambda \, d\lambda \tag{2.41}$$

$$bv_m(\theta) = \int_0^{2\pi} v(\lambda,\theta)\sin m\lambda \, d\lambda \tag{2.42}$$

These integrals can be computed rapidly using the rectangle rule and the fast Fourier transform. The rectangle rule corresponds to a Gauss quadrature for periodic functions and is therefore quite accurate. Efficient FFT methods on both vector and parallel computers are presented in Swarztrauber (1987).

2. For $m = 0$ and $n = m,...,N$ compute the Legendre-type transforms in the latitudinal direction. The coefficients for $m = 0$ must be computed from (2.27) and (2.29) since the identity (2.32) is not valid for $m=0$. Note that $bi_{0,n}$ and $ci_{0,n}$ are both zero since W_n^0 is zero. Equation (2.8) contains the definition of $\alpha_{m,n}$.

$$br_{0,n} = \alpha_{m,n} \int_{-\pi/2}^{\pi/2} av_0(\theta) V_n^0(\theta)\cos\theta \, d\theta \tag{2.43}$$

and

$$cr_{0,n} = \alpha_{m,n} \int_{-\pi/2}^{\pi/2} au_0(\theta) V_n^0(\theta)\cos\theta \, d\theta \ . \tag{2.44}$$

For $m = 1,...,N$ and $n = m,...,N$ compute the Legendre-type transforms in the latitudinal direction.

$$a_{m,n} = \int_{-\pi/2}^{\pi/2} au_m(\theta) W_n^m(\theta)\cos\theta \, d\theta \tag{2.45}$$

$$b_{m,n} = \int_{-\pi/2}^{\pi/2} bu_m(\theta) W_n^m(\theta)\cos\theta \, d\theta \tag{2.46}$$

$$c_{m,n} = \int_{-\pi/2}^{\pi/2} av_m(\theta) W_n^m(\theta)\cos\theta \, d\theta \tag{2.47}$$

$$d_{m,n} = \int_{-\pi/2}^{\pi/2} bv_m(\theta) W_n^m(\theta)\cos\theta \, d\theta \ . \tag{2.48}$$

These integrals can be computed accurately on an equally spaced latitudinal grid using the discrete transform presented in Machenhauer and Daley (1972) and described in Swarztrauber (1979). Traditionally, these integrals have been evaluated on an unequally spaced grid using Gauss quadrature. Both of these methods are discussed in Section 4.

3. For $m=1,...,N$ and $n=m,...,N$ we can now compute the coefficients in the vector harmonic spectral representation (2.14) or (2.25) and (2.26). The coefficients $\mathrm{c1}_{m,n}$ and $\mathrm{c2}_{m,n}$ are defined in (2.33).

$$br_{m,n} = \alpha_{m,n}(\mathrm{c1}_{m,n}\, c_{m,n-1} - \mathrm{c2}_{m,n}\, c_{m,n+1} - b_{m,n}) \tag{2.49}$$

$$bi_{m,n} = \alpha_{m,n}(\mathrm{c1}_{m,n}\, d_{m,n-1} - \mathrm{c2}_{m,n}\, d_{m,n+1} + a_{m,n}) \tag{2.50}$$

$$cr_{m,n} = \alpha_{m,n}(\mathrm{c1}_{m,n}\, a_{m,n-1} - \mathrm{c2}_{m,n}\, a_{m,n+1} + d_{m,n}) \tag{2.51}$$

$$ci_{m,n} = \alpha_{m,n}(\mathrm{c1}_{m,n}\, b_{m,n-1} - \mathrm{c2}_{m,n}\, b_{m,n+1} - c_{m,n})\ . \tag{2.52}$$

This completes the analysis of a vector function on the sphere. We now describe the synthesis of a vector function. Given the coefficients $br_{m,n}$, $bi_{m,n}$, $cr_{m,n}$, and $ci_{m,n}$ the synthesis can be computed in the following three steps.

1. For $m=1,...,N$ and $n=m,...,N$ compute

$$a_{m,n} = -\mathrm{c2}_{m,n-1} cr_{m,n-1} + \mathrm{c1}_{m,n+1} cr_{m,n+1} + bi_{m,n}\ , \tag{2.53}$$

$$b_{m,n} = -\mathrm{c2}_{m,n-1} ci_{m,n-1} + \mathrm{c1}_{m,n+1} ci_{m,n+1} - br_{m,n}\ , \tag{2.54}$$

$$c_{m,n} = -\mathrm{c2}_{m,n-1} br_{m,n-1} + \mathrm{c1}_{m,n+1} br_{m,n+1} - ci_{m,n}\ , \tag{2.55}$$

$$d_{m,n} = -\mathrm{c2}_{m,n-1} bi_{m,n-1} + \mathrm{c1}_{m,n+1} bi_{m,n+1} + cr_{m,n}\ . \tag{2.56}$$

2. For $m=0$ we first compute

$$A_0(\theta) = \tfrac{1}{2}\sum_{n=1}^{N} a_{0,n} V_n^0(\theta) \tag{2.57}$$

$$C_0(\theta) = \tfrac{1}{2}\sum_{n=1}^{N} c_{0,n} V_n^0(\theta)\ . \tag{2.58}$$

Next, for $m = 1,...,N$ compute the following Legendre-type transformations

$$A_m(\theta) = \sum_{n=m}^{N} a_{m,n} W_n^m(\theta) \tag{2.59}$$

$$B_m(\theta) = \sum_{n=m}^{N} b_{m,n} W_n^m(\theta) \tag{2.60}$$

$$C_m(\theta) = \sum_{n=m}^{N} c_{m,n} W_n^m(\theta) \tag{2.61}$$

$$D_m(\theta) = \sum_{n=m}^{N} d_{m,n} W_n^m(\theta) \ . \tag{2.62}$$

3. The vector harmonic synthesis is completed with the following Fourier syntheses in the longitudinal direction

$$u(\lambda,\theta) = \sum_{m=0}^{N} [A_m(\theta)\cos m\lambda + B_m(\theta)\sin m\lambda] \tag{2.63}$$

$$v(\lambda,\theta) = \sum_{m=0}^{N} [C_m(\theta)\cos m\lambda + D_m(\theta)\sin m\lambda] \ . \tag{2.64}$$

This completes the variant of the vector harmonic transforms based on the replacement of V_n^m by W_n^m using (2.32). This variant resulted in a savings of two in computational time. It is important to note that the accuracy of this variant has yet to be investigated.

Consider now a second somewhat more traditional variant that can halve the computational requirements of both the vector and scalar harmonic transforms. Beginning with the vector analysis we first rewrite equation (2.45) as

$$a_{m,n} = \int_0^{\pi/2} [au_m(\theta)W_n^m(\theta) - au_m(-\theta)W_n^m(-\theta)]\cos\theta \, d\theta \tag{2.65}$$

or

$$a_{m,n} = \int_0^{\pi/2} [au_m(\theta) \pm au_m(-\theta)]W_n^m(\theta)]\cos\theta \, d\theta \tag{2.66}$$

where ± is chosen + if $W_n^m(\theta)$ is odd about the equator or − if $W_n^m(\theta)$ is even. From (2.13) and (4.1) through (4.4) it can be determined that ± is set to + if $n-m$ is even and − if $n-m$ is odd.

The savings of two is now evident since the functions $au_m(\theta) \pm au_m(-\theta)$ can be computed in advance of (2.66) in a time that is negligible compared to (2.66). Then equation (2.66) can be computed in half the time compared with (2.45) since the interval of integration has been halved.

A similar savings can be obtained for the harmonic syntheses. From (2.59) we obtain

$$A_m(\theta) + A_m(-\theta) = \sum_{n=m}^{N} a_{m,n}[W_n^m(\theta) + W_n^m(-\theta)] \tag{2.67}$$

$$A_m(\theta) - A_m(-\theta) = \sum_{n=m}^{N} a_{m,n}[W_n^m(\theta) - W_n^m(-\theta)] \ . \tag{2.68}$$

Since $W_n^m(\theta)$ is either even or odd, every other term in the sums on the right of (2.67) and (2.68) are zero. Hence, both can be computed in the same time as the single sum on the right side of (2.59). In addition, θ ranges from 0 to $\pi/2$ in (2.67) and (2.68) compared with $-\pi/2$ to $\pi/2$ in (2.59). The saving is now evident since the time required by (2.67) and (2.68) for a single θ is the same as (2.59), however (2.67) and (2.68) are tabulated at only half the points required by (2.59). Once (2.67) and (2.68) are tabulated then $A_m(\theta)$ can be reconstructed from their sum and difference in a time that is negligible compared with (2.67) and (2.68). This variant is better known than the first variant and currently used to speed most scalar spherical harmonic transform codes.

3. Solving partial differential equations

In this section we present four methods for solving vector partial differential equations on the sphere. The first two are presented in the context of two different formulations of the shallow water equations. The remaining two methods are applicable to any system of first order partial differential equations. However, they require more computing resource than the first two when applied to the shallow water equations. The underlying task that is common to all of the methods is the computation of the horizontal spatial derivatives. A task that is complicated by the difficulties that were discussed in the introduction.

In a previous paper (Browning, et.al., 1989) three different methods for solving partial differential equations on the sphere were compared. In particular the composite-mesh finite-difference, traditional spectral, and vector harmonic transform methods were compared. The methods were compared in the context of the shallow water equations. They were implemented on the Cray XMP and compared in terms of the computing resource required to obtain a specific level of accuracy for a five-day integration The computing requirements for the vector harmonic transform method were found to be comparable to the traditional spectral method. Here we compare the vector harmonic transform method applied to two different formulations of the shallow water equations as well as two different methods for the general partial differential equation. They are compared in terms of the number of Legendre-type transforms required per time step to implement the formulation. In this regard we follow Temperton (1991) who used the number of Legendre-type transforms as a measure of the computing resource required by the dynamics portion of the computations. This is an appropriate measure since these transforms dominate the computing time. Computational experiments are not presented here since the vector harmonic transform method is compared with the traditional spectral method and the composite-grid finite-difference method in Browning, et.al. (1989).

In the course of solving the shallow water equations we will describe modules for computing and inverting several common differential operators. Given a vector function we will show how to compute the scalar functions of divergence and vorticity. This computation can be inverted. That is, given divergence and vorticity, then the corresponding vector function can be determined in a straightforward manner. We also show how to compute the vector function corresponding to the gradient of a vector field. In addition both the scalar and vector Laplacians are evaluated and inverted. The vector Laplacian provides a way to include dissipation in the model equations.

Model development for vector partial differential equations on the sphere could be significantly simplified if these modules were available in a software package.

We will first review the vector transform method as it was applied to the $u-v$ formulation of the shallow water equations as given in (3.1), (3.2) and (3.3) below. Next we outline the steps required for the vector harmonic transform method as applied to the $\nabla \frac{1}{2} \mathbf{v}^T \mathbf{v}$ variant of the shallow water equations given in (3.8), (3.9), and (3.10) below. The shallow water equations can be written in several different forms. Unlike the $u-v$ and $\nabla \frac{1}{2} \mathbf{v}^T \mathbf{v}$ formulations, most partial differential equations contain unbounded terms. In Swarztrauber (1981) it is shown that u_θ, v_θ, $(\cos\theta)^{-1} (\partial v / \partial \lambda + \sin\theta u)$, and $(\cos\theta)^{-1} (\partial u / \partial \lambda - \sin\theta v)$ are bounded differential expressions on the sphere even though the individual terms in the last two expressions are unbounded. It is also shown that any bounded first order differential equation can be written in terms of these expressions in the same way that any bounded first order differential equation in Cartesian coordinates can be written in terms of $\partial u / \partial x$, $\partial u / \partial y$, $\partial v / \partial x$, and $\partial v / \partial y$.

However, the set given above for spherical coordinates is not unique. For example, any first order differential equation on the sphere can also be written in terms of $\partial u / \partial \theta$, $\partial v / \partial \theta$, δ, and ζ, where δ is divergence and ζ is vorticity defined in (5.3) and (5.4) respectively. This result is immediate since the two sets can be written in terms of each other. In the $u-v$ formulation the shallow water equations are written in terms of $\partial u / \partial \theta$, $\partial v / \partial \theta$, δ, and ζ which, as will be shown, can be readily determined from the analyses of u, v, and ϕ. The $u-v$ formulation of the shallow water equations is

$$\frac{\partial u}{\partial t} = -\frac{u}{a}\delta - \frac{v}{a}\frac{\partial u}{\partial \theta} + \frac{u}{a}\frac{\partial v}{\partial \theta} + fv - \frac{1}{a\cos\theta}\frac{\partial \phi}{\partial \lambda}, \tag{3.1}$$

$$\frac{\partial v}{\partial t} = -\frac{u}{a}\zeta - \frac{u}{a}\frac{\partial u}{\partial \theta} - \frac{v}{a}\frac{\partial v}{\partial \theta} - fu - \frac{1}{a}\frac{\partial \phi}{\partial \theta}, \tag{3.2}$$

$$\frac{\partial \phi}{\partial t} = -\frac{\phi}{a}\delta - \frac{v}{a}\frac{\partial \phi}{\partial \theta} - \frac{u}{a\cos\theta}\frac{\partial \phi}{\partial \lambda}, \tag{3.3}$$

where ϕ is the geopotential. These equations can be numerically integrated using the vector harmonic transform method that is defined in the following four steps.

1. Analyze $u(\lambda,\theta)$ and $v(\lambda,\theta)$ by computing the coefficients $br_{m,n}$, $bi_{m,n}$, $cr_{m,n}$, and $ci_{m,n}$ from (2.27) through (2.30) or the variant (2.39) through (2.52). Also analyze $\phi(\lambda,\theta)$ by computing the coefficients $ar_{m,n}$ and $ai_{m,n}$ from (2.23) and (2.24).
2. Use the spectral representations (2.22), (2.25), and (2.26) to compute the spatial derivatives that occur on the right side of the shallow water equations (3.1), (3.2), and (3.3). The details are presented below.
3. Substitute the spatial derivatives into the right side of equations (3.1), (3.2), and (3.3) to compute the time derivatives $\partial u/\partial t$, $\partial v/\partial t$, and $\partial\phi/\partial t$.
4. Use "leap frog" time differencing to advance u, v, and ϕ to the next time level. Note that the high-order spatial accuracy may justify the use of a high-order time integrator such as the Runge-Kutta scheme (Fulton and Schubert, 1987).

Some computational considerations that are related to aliasing and spectral truncation are discussed at the end of Section 4. Step 2 above requires further discussion.

2a) From (5.3), (2.2), (2.12), (2.13), (2.25), and (2.26), it can be shown that

$$\delta = -\sum_{m=0}^{N}{}' \sum_{n=m}^{N} \sqrt{n(n+1)}P_n^m(\theta)(br_{n,m}\cos m\lambda + bi_{n,m}\sin m\lambda) \tag{3.4}$$

which has the same form as (2.22) and therefore the divergence can be computed by setting $ar_{m,n} = -\sqrt{n(n+1)}br_{m,n}$ and $ai_{m,n} = -\sqrt{n(n+1)}bi_{m,n}$ and performing a single scalar spherical harmonic synthesis. This result can be obtained in complex form using (5.8).

2b) From (5.4), (2.2), (2.12), (2.13), (2.25), and (2.26), it can be shown that

$$\zeta = \sum_{m=0}^{N}{}' \sum_{n=m}^{N} \sqrt{n(n+1)}P_n^m(\theta)(cr_{n,m}\cos m\lambda + ci_{n,m}\sin m\lambda) \tag{3.5}$$

which also has the same form as (2.22) and hence the vorticity can be computed by setting $ar_{m,n} = \sqrt{n(n+1)}cr_{m,n}$ and $ai_{m,n} = \sqrt{n(n+1)}ci_{m,n}$ and performing a second scalar spherical harmonic synthesis. This result can be obtained in complex form using (5.9). Steps 2a and 2b are invertible either individually or together. That is, given the divergence and vorticity then a unique vector function can be determined or if only one or the other is given then the corresponding solenoidal or rotational vector function can be reconstructed.

2c) The derivatives $\partial u/\partial\theta$ and $\partial v/\partial\theta$ can be computed from a vector synthesis like (2.25) and (2.26) but with $V(\theta)$ and $W(\theta)$ replaced with $\frac{d}{d\theta} V_n^m(\theta)$ and $\frac{d}{d\theta} W_n^m(\theta)$ respectively. These derivatives also satisfy the recurrence (5.14) and can therefore be computed in a manner similar to that given for the $P_n^m(\theta)$ in Section 4. This step requires the same computing time as a vector synthesis or two scalar syntheses.

2d) From (2.12), (2.13), and (2.22)

$$\frac{1}{\cos\theta}\frac{\partial\phi}{\partial\lambda} = \sum_{m=0}^{M}{}' \sum_{n=m}^{M} \sqrt{n(n+1)}W_n^m(\theta)(ai_{m,n}\cos m\lambda - ar_{m,n}\sin m\lambda) \tag{3.6}$$

$$\frac{\partial\phi}{\partial\theta} = \sum_{m=0}^{M}{}' \sum_{n=m}^{M} \sqrt{n(n+1)}V_n^m(\theta)(ar_{m,n}\cos m\lambda + ai_{m,n}\sin m\lambda) \tag{3.7}$$

which has the form of a vector synthesis (2.25) and (2.26) but with $cr_{m,n} = ci_{m,n} = 0$. Therefore the gradient of $\phi(\lambda,\theta)$ can be computed as a vector synthesis by setting $br_{m,n} = \sqrt{n(n+1)}ar_{m,n}$, $bi_{m,n} = \sqrt{n(n+1)}ai_{m,n}$, and $cr_{m,n} = ci_{m,n} = 0$. This result can be obtained in complex form using (5.10). It is also invertible thus providing the capability to reconstruct any scalar field from its gradient. This step requires the same time as a vector synthesis or two scalar syntheses.

2e) If dissipation were included in the equations (3.1) and (3.2) then the vector Laplacian (5.7) can be computed from the vector analysis by multiplying the coefficients $br_{m,n}$, $bi_{m,n}$, $cr_{m,n}$, and $ci_{m,n}$ by $-n(n+1)$ and performing a vector synthesis. The vector Laplacian can also be inverted. The cost of this step is a vector synthesis which requires the same amount of computation as two scalar syntheses.

The cost in terms of Legendre transforms of the vector harmonic transform method applied to the $u-v$ formulation of the shallow water equations is: three for the analyses in step 1, one for step 2a, one for step 2b, two for step 2c, and two for step 2d. Hence the total number of Legendre-type transforms is nine which is the same as the number reported by Temperton (1991) for the traditional spectral method. These counts, as well as Temperton's, require the use of the transform variants given in Section 2. This completes the $u-v$ formulation of the shallow water equations.

Consider now the $\nabla \frac{1}{2} \mathbf{v}^T \mathbf{v}$ formulation of the shallow water equations. This formulation is motivated by a desire to eliminate the computation of the θ derivatives of the velocity components in step 2c above. Equations (3.1) through (3.3) can be rewritten:

$$\frac{\partial u}{\partial t} = (\zeta + f)v - \frac{1}{a\cos\theta}\frac{\partial}{\partial\lambda}[\phi + \tfrac{1}{2}(u^2+v^2)] , \tag{3.8}$$

$$\frac{\partial v}{\partial t} = -(\zeta + f)u + \frac{1}{a}\frac{\partial}{\partial\theta}[\phi + \tfrac{1}{2}(u^2+v^2)] , \tag{3.9}$$

$$\frac{\partial \phi}{\partial t} = -\nabla_s \cdot (\phi \mathbf{v}) . \tag{3.10}$$

The solution of equations (3.8), (3.9), and (3.10) proceeds as follows.

1. Analyze $u(\lambda,\theta)$ and $v(\lambda,\theta)$ by computing the coefficients $br_{m,n}$, $bi_{m,n}$, $cr_{m,n}$, and $ci_{m,n}$ from (2.27) through (2.30) or the variant (2.39) through (2.52).
2. Use step 2b above to compute the vorticity ζ.
3. Analyze the scalar function $\phi + \frac{1}{2}(u^2+v^2)$ using (2.23) and (2.24).
4. Compute $\nabla_s [\phi + \frac{1}{2}(u^2+v^2)]$ in a manner similar to step 2d above.
5. Analyze the vector function $\phi\mathbf{v}$ in a manner similar to step 1.
6. Compute the divergence $\nabla_s \cdot (\phi\mathbf{v})$ using a procedure like that in step 2a above.

Following these steps all quantities on the right side of equations (3.8), (3.9), and (3.10) are available and hence, the time derivatives can be computed and the solution advanced to the next time step.

The number of Legendre transforms for the $\nabla \frac{1}{2} \mathbf{v}^T \mathbf{v}$ formulation of the shallow water equations is: two for the analysis in step 1, one for step 2, one for step 3, two for step 4, two for step 5, and one for step 6. Therefore, the total number of Legendre-type transforms is nine which is the same as the number for the $u-v$ formulation. However, as mentioned above, the $\nabla \frac{1}{2} \mathbf{v}^T \mathbf{v}$ formulation does not require the computation of the θ derivatives of $\mathbf{v}$.

Although the techniques used above for the shallow water equations will apply to most differential equations, we will complete this section with the computation of all first order partial derivatives on the surface of the sphere. As mentioned in the introduction, certain terms in a differential equation on the sphere are unbounded an therefore not suited for evaluation using a spectral representation. However, first each unbounded term can be assembled together with other unbounded terms into a bounded differential expression. Any first-order differential equation can then be written in terms of these bounded differential expressions. One such set is given by the elements of the matrix **S** defined below at (3.12). The proof that these elements are bounded can be derived from the relation that **S** has to the Jacobian of the velocity $\mathbf{v}_c^T = [X(x,y,z), Y(x,y,z), Z(x,y,z)]$ in Cartesian coordinates which is given by

$$\mathbf{C} = \begin{bmatrix} \frac{\partial X}{\partial x} & \frac{\partial X}{\partial y} & \frac{\partial X}{\partial z} \\ \frac{\partial Y}{\partial x} & \frac{\partial Y}{\partial y} & \frac{\partial Y}{\partial z} \\ \frac{\partial Z}{\partial x} & \frac{\partial Z}{\partial y} & \frac{\partial Z}{\partial z} \end{bmatrix} . \tag{3.11}$$

In Section 5 it is shown that C is similar to

$$\mathbf{S} = \begin{bmatrix} \frac{1}{a\cos\theta}\frac{\partial u}{\partial\lambda} - \frac{v\sin\theta}{a\cos\theta} + \frac{w}{a} & \frac{1}{a}\frac{\partial u}{\partial\theta} & \frac{\partial u}{\partial r} \\ \frac{1}{a\cos\theta}\frac{\partial v}{\partial\lambda} + \frac{u\sin\theta}{a\cos\theta} & \frac{1}{a}\frac{\partial v}{\partial\theta} + \frac{w}{a} & \frac{\partial v}{\partial r} \\ \frac{1}{a\cos\theta}\frac{\partial w}{\partial\lambda} - \frac{u}{a} & \frac{1}{a}\frac{\partial w}{\partial\theta} - \frac{v}{a} & \frac{\partial w}{\partial r} \end{bmatrix} . \tag{3.12}$$

That is,

$$\mathbf{S} = \mathbf{Q}\ \mathbf{C}\ \mathbf{Q}^T \tag{3.13}$$

where **Q** is defined in (5.44). It is orthonormal and transforms a Cartesian vector to spherical coordinates as demonstrated in (5.49). Since **Q** is norm preserving and the elements in **C** are assumed bounded, the elements in **S** must also be bounded. In addition, any first-order partial differential in spherical coordinates can be expressed in terms of the elements in **S** in the same manner that any first-order partial differential equation in Cartesian coordinates can be expressed in terms of the elements of **C**. It remains, therefore, to evaluate the terms in **S** for a given velocity field **v** specified on the surface of the sphere. In what follows we will present two methods for computing the elements of **S**. The first method computes the elements of **C** and subsequently the elements of **S** from (3.13). The second method computes the elements directly using the vector spherical harmonic representations of **v**.

Given the vector $\mathbf{v}_s^T = (u, v, w)$ in spherical coordinates and defined on the surface of the sphere then **C** can be computed as follows.

1. Compute the Cartesian velocity components $\mathbf{v}_c^T = (X, Y, Z)$ using $\mathbf{v}_c = \mathbf{Q}\,\mathbf{v}_s$ where **Q** is defined in (5.44).
2. Since the Cartesian components X, Y, and Z are smooth they can expanded in terms of the scalar spherical harmonics. In this step we analyze these components. For example, we compute coefficients $x_{m,n}$ such that

$$X = \sum_{n=0}^{N} \sum_{m=-n}^{n} x_{m,n} Y_n^m(\lambda,\theta) . \tag{3.14}$$

3. The three dimensional Cartesian derivatives in the Jacobian **C** require the extension of the components X, Y, and Z off the surface of the sphere into three space. This is achieved by multiplying $Y_n^m(\lambda,\theta)$ by r^n. The resulting functions are exterior solutions of Laplaces equation and defined for all x, y, and z. For example,

$$X = \sum_{n=0}^{N} \sum_{m=-n}^{n} x_{m,n} r^n Y_n^m(\lambda,\theta) . \tag{3.15}$$

   This step is conceptual only and does not require computation.
4. The Cartesian derivatives can now be computed using the identities at the end of Section 5. For example, using (5.65) we obtain

$$\frac{\partial X}{\partial y} = \sum_{n=0}^{N} \frac{i}{2} \sum_{m=-n}^{n} [(n+m+2)(n+m+1)x_{m+1,n+1} + x_{m-1,n+1}] Y_n^m(\lambda,\theta) . \tag{3.16}$$

   Hence, $\partial X/\partial y$ can be computed from a scalar spherical harmonic analysis. The remaining derivatives in the Jacobian **C** can be computed in a similar manner.

5. Once **C** has been computed then **S** can be computed from $\mathbf{S} = \mathbf{Q}\ \mathbf{C}\ \mathbf{Q}^T$.

The elements of **S** then provide the bounded differential expressions that occur in any first-order system of differential equations that are posed on the surface of the sphere. Indeed all of the derived expressions such as divergence and vorticity that were computed earlier in this section can also be computed from the elements of **S**. For example, if $s_{i,j}$ denotes the element in the ith row and jth column, then the divergence (5.3) is given by $\delta = s_{1,1} + s_{2,2}$.

Although this approach can be used to solve the general first-order equation it is somewhat more costly than the methods given earlier for the shallow water equations. Three scalar analyses are required for X, Y, and Z in step 2 and nine scalar syntheses are required to compute the Cartesian derivatives in step 4. Therefore, a total of twelve Legendre-type transforms are required to compute the spatial derivatives of the velocity. This does not include the computations that are required for the geopotential if this approach is used to solve the shallow water equations.

The fourth and last method computes the elements of **S** directly by application to the vector harmonic representation of the velocity field. Let $s_{i,j}(\mathbf{v})$ denote the term of **S** corresponding to row i and column j evaluated for the vector **v**. From (2.14)

$$s_{i,j}(\mathbf{v}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} b_{m,n}\, s_{i,j}(\mathbf{B}_n^m) + c_{m,n}\, s_{i,j}(\mathbf{C}_n^m)\ . \qquad (3.17)$$

Hence, the terms in **S** can be evaluated for **v** once the terms have been evaluated for the vector spherical harmonics. In what follows we evaluate the terms in **S** as applied to the vector harmonics. Evaluations are given only for the elements that correspond to the 2×2 matrix in the upper left corner of **S** since the evaluation of the other elements is straightforward. We begin with the element $s_{1,1}$ in the upper left-hand corner applied to the spherical vector harmonic $\mathbf{B}_n^m$. From (2.11) and (3.12) we obtain

$$s_{1,1}(\mathbf{B}_n^m) = \frac{iW_n^m}{a\cos\theta} ime^{im\lambda} - \frac{\sin\theta}{a\cos\theta} V_n^m e^{im\lambda} \qquad (3.18)$$

or

$$s_{1,1}(\mathbf{B}_n^m) = -\frac{e^{im\lambda}}{\sqrt{n(n+1)}} \left(\frac{m^2}{a\cos^2\theta} P_n^m + \frac{\sin\theta}{a\cos\theta} \frac{\partial P_n^m}{\partial\theta} \right)\ . \qquad (3.19)$$

From (5.27) we obtain

$$s_{1,1}(\mathbf{B}_n^m) = -\frac{e^{im\lambda}}{4a\sqrt{n(n+1)}}[P_n^{m+2} + 2(n^2+m^2+n)P_n^m$$

$$+ (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] \ . \qquad (3.20)$$

Proceeding in a similar manner and using (5.25) we obtain

$$s_{1,2}(\mathbf{B}_n^m) = \frac{ie^{im\lambda}}{4a\sqrt{n(n+1)}}[P_{n-1}^{m+2} + 2m(n+m)P_{n-1}^m$$

$$- (n+m)(n-m+1)(n+m-1)(n+m-2)P_{n-1}^{m-2}] \ . \qquad (3.21)$$

Similarly,

$$s_{2,1}(\mathbf{B}_n^m) = \frac{ie^{im\lambda}}{4a\sqrt{n(n+1)}}[P_{n-1}^{m+2} + 2m(n+m)P_{n-1}^m$$

$$- (n+m)(n-m+1)(n+m-1)(n+m-2)P_{n-1}^{m-2}] \ . \qquad (3.22)$$

Next

$$s_{2,2}(\mathbf{B}_n^m) = \frac{1}{a}\frac{\partial V_n^m}{\partial\theta}e^{im\lambda} = \frac{e^{im\lambda}}{a\sqrt{n(n+1)}}\frac{d^2P_n^m}{d\theta^2} \ . \qquad (3.23)$$

Using (5.18)

$$s_{2,2}(\mathbf{B}_n^m) = \frac{e^{im\lambda}}{4a\sqrt{n(n+1)}}[P_n^{m+2} - 2(n^2-m^2+n)P_n^m$$

$$+ (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] \ . \qquad (3.24)$$

Consider now the application of the terms to the vector spherical harmonics $\mathbf{C}_n^m$. Proceeding in a manner similar to that above we obtain:

$$s_{1,1}(\mathbf{C}_n^m) = -\frac{ie^{im\lambda}}{4a\sqrt{n(n+1)}}[P_{n-1}^{m+2} + 2m(n+m)P_{n-1}^m$$

$$- (n+m)(n-m+1)(n+m-1)(n+m-2)P_{n-1}^{m-2}] \qquad (3.25)$$

$$s_{1,2}(\mathbf{C}_n^m) = -\frac{e^{im\lambda}}{4a\sqrt{n(n+1)}}[P_n^{m+2} - 2(n^2-m^2+n)P_n^m$$

$$+ (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] \tag{3.26}$$

$$s_{2,1}(\mathbf{C}_n^m) = -\frac{e^{im\lambda}}{4a\sqrt{n(n+1)}}[P_n^{m+2} + 2(n^2+m^2+n)P_n^m$$
$$+ (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] \tag{3.27}$$

$$s_{2,2}(\mathbf{C}_n^m) = \frac{ie^{im\lambda}}{4a\sqrt{n(n+1)}}[P_{n-1}^{m+2} + 2m(n+m)P_{n-1}^m$$
$$- (n+m)(n-m+1)(n+m-1)(n+m-2)P_{n-1}^{m-2}]\ . \tag{3.28}$$

The terms in any first-order partial differential equation on the sphere can be expressed in terms of the elements of **S** given in (3.12). Although this approach can be used for any partial differential equation it is not as efficient as the approaches defined in the early part of this section. The evaluation of $s_{1,1}$, $s_{1,2}$, $s_{2,1}$, and $s_{2,2}$ using (3.17) requires six Legendre-type transforms rather than eight because $s_{1,1}(\mathbf{C}_n^m) = -s_{2,2}(\mathbf{C}_n^m)$ and $s_{1,2}(\mathbf{B}_n^m) = -s_{2,1}(\mathbf{B}_n^m)$. Note that the Legendre-type transforms require a synthesis in terms of linear combinations of P_n^m defined in (3.20) through (3.28). Forming these linear combinations may increase the computing time unless they are precomputed and subsequently used for repeated transformations. It may be possible to further reduce the number of syntheses because the four elements in the upper left of (3.12) are not independent since only two fields, such as the divergence and vorticity, are required to completely specify the vector function.

This approach may be more efficient than computing **C** in (3.11) and then **S** from (3.13). However, it is more expensive than the two approaches given for the shallow water equations at the beginning of this section.

4. Computational methods

In this section we will describe efficient and accurate methods for computing $P_n^m(\theta)$, $V_n^m(\theta)$, and $W_n^m(\theta)$. We will also describe the computation of the integrals in the harmonic analyses both on a Gauss and equally distributed latitudinal grid. Several comments on spectral truncation and aliasing are included at the end of the section. The purpose of this section is to provide the numerical techniques that are central to the computer implementation of the harmonic transforms and thereby provide the means to implement the theoretical developments that were presented in the previous sections. Two methods for computing the associated Legendre functions are presented. The first is the Fourier method which can be used to tabulate the $P_n^m(\theta)$ as a function of θ for any m and n independent of any other m and n. The second method uses the recurrence relation (5.14) and is more efficient when the complete set of $P_n^m(\theta)$ for $m < n < N$ are required.

We begin now with a description of the Fourier method. If a real trigonometric series is substituted into (2.2) then it can be determined that the $P_n^m(\theta)$ have one of the following trigonometric forms depending on the parity of m and n.

$$P_n^m(\theta) = \sum_{k=0}^{n/2} a_{m,n,k} \cos 2k\theta \qquad n \text{ even} \ ; \ m \text{ even} \tag{4.1}$$

$$P_n^m(\theta) = \sum_{k=1}^{n/2} a_{m,n,k} \sin 2k\theta \qquad n \text{ even} \ ; \ m \text{ odd} \tag{4.2}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \sin(2k-1)\theta \qquad n \text{ odd} \ ; \ m \text{ even} \tag{4.3}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \cos(2k-1)\theta \qquad n \text{ odd} \ ; \ m \text{ odd} . \tag{4.4}$$

The coefficients $a_{m,n,k}$ can be determined from the following three term recurrence relations that result when (4.1) through (4.4) are substituted into (2.2). If n is even, then

$$[(2k-1)(2k-2)-n(n+1)]a_{m,n,k-1} + 2[4k^2-n(n+1)+2m^2]a_{m,n,k}$$

$$+ [(2k+1)(2k+2)-n(n+1)]a_{m,n,k+1} = 0\ . \tag{4.5}$$

And if n is odd, then

$$[(2k-2)(2k-3)-n(n+1)]a_{m,n,k-1} + 2[(2k-1)^2-n(n+1)+2m^2]a_{m,n,k}$$
$$+ [2k(2k+1)-n(n+1)]a_{m,n,k+1} = 0\ . \tag{4.6}$$

Although these relations define an infinite set of tridiagonal equations they have a solution with a finite number of non zero $a_{m,n,k}$ For example, in (4.5) the coefficient of $a_{m,n,k-1}$ is zero for $k=n/2+1$ and the coefficient of $a_{m,n,k+1}$ is zero for $k=-n/2-1$. The resulting set of equations corresponding to $k=-n/2$ to $k=n/2$ is singular with a nonzero solution $a_{m,n,k}$. Furthermore, it can be shown that $a_{m,n,-k} = \pm a_{m,n,k}$ depending on the parity of m and n which can be used to halve the number of equations and simplify their solution.

A nontrivial solution to the resulting singular system of equations can be determined by inverse iteration or by the following method that also produces the correct scaling. The coefficient $a_{m,n,n}$ is first computed from Rodrigue's formula, and the remaining coefficients $a_{m,n,k}$ are determined by a backward recurrence of either (4.5) or (4.6). A backward recurrence can preserve the relative accuracy of the $a_{m,n,k}$ for large values of k, even though they may be much smaller than machine epsilon times the maximum $a_{m,n,k}$. This permits one to formally differentiate the trigonometric series and obtain an accurate value of the derivative of $P_n^m(\theta)$ which is necessary for $V_n^m(\theta)$.

Consider now the computation of $a_{m,n,n}$ from Rodrigue's formula (2.1). Expanding the highest power of both sinθ and cosθ, we obtain the coefficient of the trigonometric term with the highest wave number n.

$$P_n^m(\theta) = \frac{1}{2^n n!}\left[\frac{(-1)^{\frac{n-m}{2}}}{2^{n-1}}\frac{(2n)!}{(n-m)!}\cos n\theta + \cdots\right] \tag{4.7}$$

for $n-m$ even, and

$$P_n^m(\theta) = \frac{1}{2^n n!}\left[\frac{(-1)^{\frac{n-m-1}{2}}}{2^{n-1}}\frac{(2n)!}{(n-m)!}\sin n\theta + \cdots\right] \tag{4.8}$$

for $n-m$ odd. Therefore,

$$a_{m,n,n} = \frac{(-1)^{\frac{n-m}{2}}}{2^{2n-1}n!}\frac{(2n)!}{(n-m)!} \qquad n-m \text{ even} \tag{4.9}$$

$$a_{m,n,n} = \frac{(-1)^{\frac{n-m-1}{2}}}{2^{2n-1} n!} \frac{(2n)!}{(n-m)!} \qquad n-m \text{ odd} . \qquad (4.10)$$

As previously mentioned, the remaining $a_{n,n,k}$ are determined by the backward recurrence of either (4.5) or (4.6). Although the Fourier method can be used to compute any $P_n^m(\theta)$, it is not as efficient as using a recurrence relation that relates $P_n^m(\theta)$ with adjacent m and n.

The Fourier method is an efficient way of computing $P_n^m(\theta)$ when only a few functions must be computed, particularly for large values of m and n. However, the harmonic transforms require a complete set of the functions that are computed efficiently using the four-point recurrence relation (5.14). This recurrence can be initialized by computing $P_n^0(\theta)$ and $P_n^1(\theta)$ using the Fourier method. It can also be used to compute $P_n^m(\theta)$ for $m=n$ and $m=n-1$ by setting $P_n^m(\theta)=0$ for $n<m$. This recurrence has the following characteristics.

1. The values of m and n form a square with stride two in m,n space. Therefore, it can be used to compute values of m and n such that $n-m$ is even (odd) without computing values of m and n such that $n-m$ is odd (even). This can be used to halve the amount of computation for solutions that are symmetric or antisymmetric about the equator. The recurrence can be used to compute $P_n^m(\theta)$ that are even about the equator without computing odd $P_n^m(\theta)$ and vice versa. When symmetries permit, this enables models to be formulated on the hemisphere which halves the computation.

2. Unlike other recurrence relations for $P_n^m(\theta)$, the coefficients in (5.14) do not have a functional dependence on latitude θ. Hence, the derivative of $P_n^m(\theta)$ also satisfies (5.14). From (2.12)

$$V_n^m(\theta) = \sqrt{\frac{(n-2)(n-1)}{n(n+1)}}\left[V_{n-2}^m(\theta) + (n+m-2)(n+m-3)V_{n-2}^{m-2}(\theta)\right] - (n-m+1)(n-m+2)V_n^{m-2}(\theta) . \qquad (4.11)$$

This recurrence can be initialized from $V_n^0(\theta)$ and $V_n^1(\theta)$ which can be obtained by differentiating the trigonometric series for $P_n^0(\theta)$ and $P_n^1(\theta)$. A recurrence relation for $W_n^m(\theta)$ can also be obtained by substituting $P_n^m(\theta) = m^{-1}\cos\theta W_n^m(\theta)$ into (5.14).

$$W_n^m(\theta) = \sqrt{\frac{(n-2)(n-1)}{n(n+1)}}[W_{n-2}^m(\theta) + \frac{m(n+m-2)(n+m-3)}{m-2}W_{n-2}^{m-2}(\theta)]$$
$$- \frac{m(n-m+1)(n-m+2)}{m-2}W_n^{m-2}(\theta) . \tag{4.12}$$

Since $W_n^0(\theta) = 0$, (4.12) must be initialized with $W_n^1(\theta)$ and $W_n^2(\theta)$. Both can be computed from a trigonometric series that is obtained from the trigonometric series for $P_n^1(\theta)$ and $P_n^2(\theta)$. This completes our discussion of the computation of the associated Legendre and related functions.

Consider now the approximation of the integrals in the harmonic analyses. We begin with the approximation of the integrals on an equally spaced latitude grid. Machenhauer and Daley (1972) developed a discrete transform for equally spaced latitudinal points that are as accurate as Gauss quadrature. An outline of their development will be presented here however, a detailed description can also be found in Swarztrauber (1979). An analysis using Gauss quadrature with N points is exact for any function with a finite expansion.

$$\phi(\lambda,\theta) = \sum_{n=0}^{N} \sum_{m=0}^{n}{}' P_n^m(\theta)(a_{m,n}\cos m\lambda + b_{m,n}\sin m\lambda). \tag{4.13}$$

However, an exact analysis of (4.13) can also be developed on an equally spaced grid $\theta_i = -\pi/2 + i\pi/N$ for $i = 0, \ldots, N$. From (2.23) we obtain

$$ar_{m,n} = \alpha_{m,n} \int_{-\pi/2}^{\pi/2} a_m(\theta) P_n^m(\theta)\cos\theta \, d\theta \tag{4.14}$$

where

$$a_m(\theta) = \int_0^{2\pi} \phi(\lambda,\theta)\cos m\lambda \, d\lambda . \tag{4.15}$$

For even m it can be shown that $P_n^m(\theta)$ and hence $a_m(\theta)$ have a cosine expansion in terms of colatitude $\pi/2-\theta$ with wave numbers that are less than or equal to N since $\phi(\lambda,\theta)$ has the finite expansion (4.13). Hence, $a_m(\theta)$ is given exactly by

$$a_m(\theta) = \frac{2}{N} \sum_{k=0}^{N}{}'' [\sum_{i=0}^{N}{}'' a_m(\theta_i)\cos k(\pi/2-\theta_i)]\cos k(\pi/2-\theta) . \tag{4.16}$$

The double prime notation on the sum indicates that the first and last terms are multiplied by ½. Substituting (4.16) into (4.14) we obtain the desired formula

$$ar_{m,n} = \sum_{i=0}^{N} Z_n^m(\theta_i) a_m(\theta_i) \tag{4.17}$$

where

$$Z_n^m(\theta_i) = \frac{2}{N} \sum_{k=0}^{N}{}'' \cos k(\pi/2 - \theta_i) \int_{-\pi/2}^{\pi/2} \cos k(\pi/2 - \theta) P_n^m(\theta) \sin\theta d\theta \ . \tag{4.18}$$

A similar development for odd m yields formulas like (4.17), but with $i=1,...,N-1$ and

$$Z_n^m(\theta_i) = \frac{2}{N} \sum_{k=0}^{N}{}'' \sin k(\pi/2 - \theta_i) \int_{-\pi/2}^{\pi/2} \sin k(\pi/2 - \theta) P_n^m(\theta) \sin\theta d\theta \ . \tag{4.19}$$

The main difference between the equally spaced and Gauss analysis is that the weights $Z_n^m(\theta_i)$ are functions of the three index variables i, m, and n. Nevertheless, use of the $Z_n^m(\theta_i)$ in the analysis is consistent with the use of $P_n^m(\theta_i)$ in the synthesis and requires the same computational effort.

The finite representation (4.13) is called a triangular truncation because the the values of m and n that correspond to nonzero $a_{m,n}$ and $b_{m,n}$ lie in a triangle in (m,n) space. A triangular truncation is preferred since the analysis of $\phi(\lambda,\theta)$ will be exact for any orientation of the spherical coordinate system. That is, the analysis is exact no matter where the poles are located.

Just as (5.14) was used to compute both $V_n^m(\theta)$ and $W_n^m(\theta)$, it can also be used to compute $Z_n^m(\theta)$. If the operator on the right side of (4.18) is applied to the recurrence (5.14) then $Z_n^m(\theta)$ is seen to also satisfy (5.14). Therefore, $Z_n^m(\theta)$ can be computed in the same manner as $P_n^m(\theta)$, namely:

1. The integrals in (4.18) and (4.19) are computed exactly by substituting one of the exact forms (4.1) through (4.4) for $P_n^m(\theta)$ formally integrating. These integrals then constitute the Fourier coefficients in a trigonometric series which in turn yield trigonometric expansions for $Z_n^m(\theta)$ similar to (4.1) through (4.4). A noteworthy difference is that the range of summation in the trigonometric expansion is equal to the number of latitudes, rather than n/2 or (n+1)/2, as in the case

of the $P_n^m(\theta)$. The fast Fourier transform can then be used to tabulate $Z_n^m(\theta_i)$.

2. Like the computation of $P_n^m(\theta)$, one could use the Fourier expansion of $Z_n^m(\theta)$ to compute $Z_n^m(\theta)$ for any n and m. However, since all $Z_n^m(\theta)$ are required for a synthesis, it is more efficient to compute $Z_n^0(\theta)$ and $Z_n^1(\theta)$ using the Fourier expansion and the remaining $Z_n^m(\theta)$ using (5.14) with $P_n^m(\theta)$ replaced by $Z_n^m(\theta)$. This completes the discussion of the discrete transform for equally spaced latitudinal points.

Consider now the computation of the Gauss Legendre quadrature. Gauss quadrature also provides an accurate approximation to the latitudinal integrals required for both the scalar and vector harmonic transforms. Here we will briefly review an effective method (Golub and Welsch, 1969) for computing the Gauss latitude points $x_j = \sin\theta_j$ and weights w_j. for $j = 1, \ldots, N$.

For reasons that will become evident, we will use the normalized associated Legendre functions

$$\overline{P_n^m}(\theta) = (-1)^m \left[\frac{2n+1}{2}\frac{(n-m)!}{(n+m)!}\right]^{1/2} P_n^m(\theta) \tag{4.20}$$

and the normalized Legendre polynomials $\overline{P_N}(x) = \overline{P_N^0}(\theta)$ where $x = \sin\theta$. It is known that the Gauss points x_i are given as the zeros of $\overline{P_N}(x)$. If we define $\overline{P_{-1}}(x) = 0$, and use $\overline{P_0}(x) = 1/\sqrt{2}$, then the remaining $\overline{P_n}(x)$ can be computed from the recurrence

$$x\overline{P_n}(x) = \frac{n}{\sqrt{(2n+1)(2n-1)}}\overline{P_{n-1}}(x) + \frac{n+1}{\sqrt{(2n+1)(2n+3)}}\overline{P_{n+1}}(x) . \tag{4.21}$$

Define the vectors $\mathbf{p}^T(x) = [\overline{P_0}(x), \ldots, \overline{P_{N-1}}(x)]$ and $\mathbf{p}_j = \mathbf{p}(x_j)$. Golub and Welsch (1969), credit Wilf with the following formula for the Gauss weights

$$w_j = [\mathbf{p}_j^T \mathbf{p}_j]^{-1} . \tag{4.22}$$

Therefore, the zeros x_j of $\overline{P_N}(x)$ provide the Gauss points and they can also be used to compute the weights using (4.22). We show now that the Gauss points x_j and weights w_j can be computed from the eigenvalues and eigenvectors of a symmetric tridiagonal matrix. The QR algorithm can then be used to compute the eigensystem and hence the Gauss Legendre quadrature.

Define $\mathbf{T}$ as the symmetric tridiagonal matrix with zero diagonal and elements $a_n = n/\sqrt{(2n-1)(2n+1)}$ below the diagonal for $n = 1, \ldots, N-1$. Also define $\mathbf{e}_N$ as an N-vector with zero elements except for the last element which is 1. From (4.21)

$$\mathbf{T}\mathbf{p}(x) = x\,\mathbf{p}(x) + \frac{N}{\sqrt{(2N-1)(2n+1)}}\overline{P}_N(x)\,\mathbf{e}_N \,. \tag{4.23}$$

$\mathbf{T}$ is symmetric since (4.21) is written in terms of the normalized associated Legendre polynomials. If x_j is a zero of $\overline{P}_N(x)$ then $\mathbf{p}_j = \mathbf{p}(\mathbf{x}_j)$ is an eigenvector of $\mathbf{T}$ and hence the Gauss points are given as the eigenvalues of $\mathbf{T}$. Let $\mathbf{q}^{T_j} = (q_{1,j}, \ldots, q_{N,j})$ be a normalized eigenvector of $\mathbf{T}$, i.e. $\mathbf{q}_j^T\mathbf{q}_j = 1$. Since $\mathbf{p}_j$ is also an eigenvector of $\mathbf{T}$ it differs from $\mathbf{q}_j$ only by a multiplicative constant, i.e., $\mathbf{q}_j = c\,\mathbf{p}_j$. However, from (4.22)

$$w_j\,\mathbf{p}_j^T\mathbf{p}_j = 1 = \mathbf{q}_j^T\mathbf{q}_j = c^2\mathbf{p}_j^T\mathbf{p}_j \,. \tag{4.24}$$

Therefore, $c = \sqrt{w_j}$ and hence $q_{1,j} = \sqrt{w_j}\,\overline{P}_0(x_j) = \sqrt{w_j}/\sqrt{2}$ which implies

$$w_j = 2\,q_{1,j}^2 \,. \tag{4.25}$$

This provides a convenient way to compute the weights for the Gauss Legendre quadrature. The Gauss points are given as the eigenvalues of the symmetric matrix $\mathbf{T}$ and the Gauss weights w_j can be computed from the first element of the jth eigenvector using (4.25). Both the eigenvalues and eigenvectors can be computed efficiently using the QR algorithm that is available in EISPACK (Smith, et.al., 1976). The Gauss points on the sphere are given by $\theta_j = \arcsin(x_j)$. The weights w_i on the sphere are symmetric about the equator.

We close this section with a brief discussion about spectral truncation and aliasing that will also point out a somewhat subtle difference between the Gauss quadrature and the discrete transform on an equally spaced latitudinal grid. Consider now the implementation of the vector harmonic transform method as defined in steps 1 through 4 following equations (3.1) through (3.3). Because of the quadratic terms in these equations, the number of coefficients in the exact spectral series are unbounded. Hence it is necessary to truncate these series on the computer. There are three sources of error; namely, series truncation, aliasing and roundoff. Of these three, aliasing can be eliminated by the following variant of step 1. First, a spectral truncation limit N is chosen and applied to all the coefficients computed in step 1. Next, the truncated coefficients are resynthesizing to produce filtered u, v, and ϕ. Then steps 2. through 4. proceed without aliasing on a Gauss grid with $(3N+1)/2$ points or on a equally spaced grid with $2N+1$ points. The spectral truncation is restored by subsequent truncations and resynthesizations that occur in step 1. The resynthesization in step 1 adds about 33% to the computation for which one obtains a completely unaliased model in which the only sources of error are roundoff and the truncation of the spectral series. Indeed the truncation in step 1. can be accumulated and provides a measure of the accuracy of the method.

Note that one third more grid points are required if aliasing is to be avoided on an equally spaced grid. However, in Browning, et.al. (1989) the vector harmonic transform method on a equally spaced grid was implemented with $(3N + 1)/2$ points, and the accuracy was comparable to the traditional spectral method that was also implemented on $(3N + 1)/2$ points. This is not surprising since the equally spaced discrete transform and Gauss quadrature have the same accuracy, even though they have different aliasing properties.

5. Differential and algebraic identities

In this section the identities are categorized into three groups. The first group contains differential identities that permit the evaluation of differential operators applied to the spectral representation of either scalar or vector functions. Identities are provided that assist in the evaluation of divergence and vorticity or permit the reconstruction of a vector function from its divergence and vorticity fields. Identities are also given that provide for the computation of the gradient of a scalar field. This computation can also be inverted, e.g., a scalar field can be reconstructed from its gradient. Finally the vector surface Laplacian is defined with eigenvalues $-n(n+1)$ and eigenvectors equal to the vector spherical harmonics. This facilitates the straightforward computation of the vector Laplacian and its inverse. The vector Laplacian corresponds to a diffusion operator which provides a convenient way to include dissipation in fluid models on the sphere.

The second group consists of selected identities that are satisfied by the associated Legendre functions. These basic identities have been used elsewhere in this paper and can be used to verify the new identities for the vector spherical harmonics that are presented in this section. Proofs of the new identities are not presented, since they are lengthy and in some instances they were developed using the a symbolic programming system.

The third group consists of polynomial identities. The vector spherical harmonic with a coefficient x, y, or z is expressed as a linear combination of vector spherical harmonics. The purpose of these identities is to expand the class of applications to vector differential equations that have polynomial coefficients. Most of the identities in this section are used elsewhere in this paper. The remaining identities, such as those in the third group, provide a reference to assist in the development of fluid models on the sphere. The section closes with a review of the differential geometry of the spherical coordinate system and a proof of equation (3.13).

We will now develop several differential identities and show that the vector spherical harmonics are the eigensolutions of a second-order vector differential operator. This result permits the inclusion and evaluation of a vector surface diffusion operator into fluid models on the sphere. Let $\mathbf{v}^T = [u(\lambda,\theta), v(\lambda,\theta)]$ and $\phi(\lambda,\theta)$ be an arbitrary vector and scalar functions defined on the surface of the sphere. We wish to evaluate the following differential operators

$$\nabla_s \phi = \begin{bmatrix} \dfrac{1}{\cos\theta} \dfrac{\partial \phi}{\partial \lambda} \\ \dfrac{\partial \phi}{\partial \theta} \end{bmatrix}, \tag{5.1}$$

$$\mathbf{k}\times\nabla_s\phi = \begin{bmatrix} -\dfrac{\partial\phi}{\partial\theta} \\ \dfrac{1}{\cos\theta}\dfrac{\partial\phi}{\partial\lambda} \end{bmatrix}, \tag{5.2}$$

$$\delta = \nabla_s\cdot\mathbf{v} = \frac{1}{\cos\theta}\left[\frac{\partial}{\partial\theta}(\cos\theta v) + \frac{\partial u}{\partial\lambda}\right], \tag{5.3}$$

and

$$\zeta = \mathbf{k}\cdot\nabla_s\times\mathbf{v} = \frac{1}{\cos\theta}\left[\frac{\partial v}{\partial\lambda} - \frac{\partial}{\partial\theta}(\cos\theta u)\right]. \tag{5.4}$$

Next we define the second-order differential operators:

$$\nabla_s^2\phi = \frac{1}{\cos\theta}\frac{\partial}{\partial\theta}(\cos\theta\frac{\partial\phi}{\partial\theta}) + \frac{1}{\cos^2\theta}\frac{\partial^2\phi}{\partial\lambda^2}, \tag{5.5}$$

and

$$\mathbf{L}_D\mathbf{v} = \nabla_s(\nabla_s\cdot\mathbf{v}), \text{ and } \mathbf{L}_C\mathbf{v} = \nabla_s\times(\mathbf{k}\cdot\nabla_s\times\mathbf{v}). \tag{5.6}$$

Finally, we define the differential operator that is central to the vector spherical harmonics, namely

$$\mathbf{L}\mathbf{v} = \mathbf{L}_D\mathbf{v} + \mathbf{L}_C\mathbf{v} = \begin{bmatrix} \nabla_s^2 u - \dfrac{2\sin\theta}{\cos^2\theta}\dfrac{\partial v}{\partial\lambda} - \dfrac{u}{\cos^2\theta} \\ \nabla_s^2 v + \dfrac{2\sin\theta}{\cos^2\theta}\dfrac{\partial u}{\partial\lambda} - \dfrac{v}{\cos^2\theta} \end{bmatrix}. \tag{5.7}$$

If we substitute the vector spherical harmonics (2.11) into (5.3) and (5.4) and use (2.2) we obtain

$$\nabla_s\cdot\mathbf{B}_n^m = -\sqrt{n(n+1)}Y_n^m \;;\; \nabla_s\cdot\mathbf{C}_n^m = 0, \tag{5.8}$$

and

$$\mathbf{k}\cdot\nabla_s\times\mathbf{B}_n^m = 0 \;;\; \mathbf{k}\cdot\nabla_s\times\mathbf{C}_n^m = -\sqrt{n(n+1)}Y_n^m. \tag{5.9}$$

Furthermore if we substitute (2.3) into (5.1) and (5.2) and use (2.11) through (2.13) we obtain

$$\nabla_s Y_n^m = \sqrt{n(n+1)}\mathbf{B}_n^m \;;\; \mathbf{k}\times\nabla_s Y_n^m = \sqrt{n(n+1)}\mathbf{C}_n^m. \tag{5.10}$$

From (5.8) and (5.9) it is evident that a vector field can be analyzed in terms of its rotational and solenoidal parts following its analysis in terms of the vector spherical harmonics. From these identities we obtain

$$\mathbf{L}_D \mathbf{B}_n^m = -n(n+1)\mathbf{B}_n^m \, , \quad \mathbf{L}_D \mathbf{C}_n^m = 0 \, , \tag{5.11}$$

$$\mathbf{L}_C \mathbf{B}_n^m = 0 \, , \quad \mathbf{L}_C \mathbf{C}_n^m = -n(n+1)\mathbf{C}_n^m \, . \tag{5.12}$$

Therefore,

$$\mathbf{L}\mathbf{B}_n^m = -n(n+1)\mathbf{B}_n^m \quad \text{and} \quad \mathbf{L}\mathbf{C}_n^m = -n(n+1)\mathbf{C}_n^m \, . \tag{5.13}$$

Hence, the vector spherical harmonics are eigenfunctions of the second-order differential operator $\mathbf{Lv}$ corresponding to the eigenvalues $-n(n+1)$. This completes the differential identities. Consider now the following identities that are satisfied by the associated Legendre functions. The first identity is used extensively for computing the associated Legendre functions as described in Section 4.

$$(n+m)(n+m-1)P_{n-1}^{m-1} - (n-m+1)(n-m+2)P_{n+1}^{m-1} + P_{n-1}^{m+1} - P_{n+1}^{m+1} = 0 \, . \tag{5.14}$$

This identity demonstrates that all P_n^{2m} can be written as a linear combination of P_n^0 and all P_n^{2m+1} can be written as a linear combination of P_n^1. Hence, the associated Legendre functions comprise a linearly dependent set of functions that satisfy the following algebraic identities.

$$\frac{m}{\cos\theta} P_n^m = ½[(n+m)(n+m-1)P_{n-1}^{m-1} + P_{n-1}^{m+1}] \, , \tag{5.15}$$

$$\frac{m}{\cos\theta} P_n^m = ½[(n-m+1)(n-m+2)P_{n+1}^{m-1} + P_{n+1}^{m+1}] \, , \tag{5.16}$$

$$m \frac{\sin\theta}{\cos\theta} P_n^m = ½[(n+m)(n-m+1)P_n^{m-1} + P_n^{m+1}] \, , \tag{5.17}$$

$$\frac{dP_n^m}{d\theta} = ½[P_n^{m+1} - (n+m)(n-m+1)P_n^{m-1}] \, , \tag{5.18}$$

$$\cos\theta \frac{dP_n^m}{d\theta} = \frac{1}{2n+1}[(n+1)(n+m)P_{n-1}^m - n(n-m+1)P_{n+1}^m] , \qquad (5.19)$$

$$\cos\theta P_n^m = \frac{1}{2n+1}(P_{n+1}^{m+1} - P_{n-1}^{m+1}) , \qquad (5.20)$$

$$\cos\theta P_n^m = \frac{1}{2n+1}[(n+m)(n+m-1)P_{n-1}^{m-1} - (n-m+1)(n-m+2)P_{n+1}^{m-1}] , \qquad (5.21)$$

and

$$\sin\theta P_n^m = \frac{1}{2n+1}[(n+m)P_{n-1}^m + (n-m+1)P_{n+1}^m] . \qquad (5.22)$$

These identities are valid for all m and n if we define

$$P_n^{-m} = \begin{cases} (-1)^m \dfrac{(n-m)!}{(n+m)!} P_n^m & \text{if } |m| \le n \\ 0 & \text{if } |m| > n \end{cases} . \qquad (5.23)$$

The following identities can be derived from those given above and used to evaluate the bounded differential expressions applied to the vector spherical harmonics.

$$m\frac{\sin\theta}{\cos\theta}\frac{dP_n^m}{d\theta} + \frac{m}{\cos^2\theta}P_n^m = \frac{1}{4}[P_n^{m+2} + 2mP_n^m$$
$$- (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] , \qquad (5.24)$$

$$\frac{m}{\cos\theta}\frac{dP_n^m}{d\theta} + m\frac{\sin\theta}{\cos^2\theta}P_n^m = \frac{1}{4}[P_{n-1}^{m+2} + 2m(n+m)P_{n-1}^m$$
$$- (n+m)(n-m+1)(n+m-1)(n+m-2)P_{n-1}^{m-2}] , \qquad (5.25)$$

$$\frac{1}{\cos\theta}\frac{dP_n^m}{d\theta} + m^2\frac{\sin\theta}{\cos^2\theta}P_n^m = \frac{1}{4}[P_{n-1}^{m+2} + 2(n+1)(n+m)P_{n-1}^m$$
$$+ (n+m)(n-m+1)(n+m-2)(n+m-1)P_{n-1}^{m-2}] , \qquad (5.26)$$

and

$$\frac{\sin\theta}{\cos\theta}\frac{dP_n^m}{d\theta} + \frac{m^2}{\cos^2\theta}P_n^m = \frac{1}{4}[P_n^{m+2} + 2(n^2+m^2+n)P_n^m$$

$$+ (n+m)(n-m+1)(n+m-1)(n-m+2)P_n^{m-2}] \; . \qquad (5.27)$$

The next category of identities is for scalar and vector spherical harmonics with polynomial coefficients; namely, for $x = \cos\theta\cos\lambda$, $y = \cos\theta\sin\lambda$, and $z = \sin\theta$ times the spherical harmonics. We begin with identities for the scalar harmonics.

$$\sin\theta Y_n^m = \frac{n+m}{2n+1} \; Y_{n-1}^m + \frac{n-m+1}{2n+1} \; Y_{n+1}^m \; , \qquad (5.28)$$

$$\cos\theta e^{i\lambda} Y_n^m = \frac{1}{2n+1}(Y_{n+1}^{m+1} - Y_{n-1}^{m+1}) \; , \qquad (5.29)$$

$$\cos\theta e^{-i\lambda} \; Y_n^m = \frac{(n+m)(n+m-1)}{2n+1} Y_{n-1}^{m-1} - \frac{(n-m+1)(n-m+2)}{2n+1} \; Y_{n+1}^{m-1} \; . \qquad (5.30)$$

We continue with identities for the vector spherical harmonics.

$$\sin\theta \; \mathbf{B}_n^m = \frac{\sqrt{(n-1)(n+1)}}{n} \; \frac{n+m}{2n+1} \; \mathbf{B}_{n-1}^m + \frac{\sqrt{n(n+2)}}{n+1} \; \frac{n-m+1}{2n+1} \; \mathbf{B}_{n+1}^m - \frac{im}{n(n+1)} \; \mathbf{C}_n^m \; , \qquad (5.31)$$

$$\cos\theta e^{i\lambda} \mathbf{B}_n^m = -\frac{\sqrt{(n-1)(n+1)}}{n(2n+1)} \; \mathbf{B}_{n-1}^{m+1} + \frac{\sqrt{n(n+2)}}{(n+1)(2n+1)} \; \mathbf{B}_{n+1}^{m+1} + \frac{i}{n(n+1)} \; \mathbf{C}_n^{m+1} \; , \qquad (5.32)$$

$$\cos\theta e^{-i\lambda} \mathbf{B}_n^m = \frac{\sqrt{(n-1)(n+1)}}{n} \; \frac{(n+m-1)(n+m)}{2n+1} \; \mathbf{B}_{n-1}^{m-1} - \frac{\sqrt{n(n+2)}}{n+1} \; \frac{(n-m+1)(n-m+2)}{2n+1} \; \mathbf{B}_{n+1}^{m-1} + \frac{i(n+m)(n-m+1)}{n(n+1)} \; \mathbf{C}_n^{m-1} \; , \qquad (5.33)$$

$$\sin\theta \mathbf{C}_n^m = \frac{\sqrt{(n-1)(n+1)}}{n} \frac{(n+m)}{2n+1} \mathbf{C}_{n-1}^m + \frac{\sqrt{n(n+2)}}{n+1} \frac{(n-m+1)}{2n+1} \mathbf{C}_{n+1}^m + \frac{im}{n(n+1)} \mathbf{B}_n^m , \tag{5.34}$$

$$\cos\theta e^{i\lambda} \mathbf{C}_n^m = -\frac{\sqrt{(n-1)(n+1)}}{n(2n+1)} \mathbf{C}_{n-1}^{m+1} + \frac{\sqrt{n(n+2)}}{(n+1)(2n+1)} \mathbf{C}_{n+1}^{m+1} - \frac{i}{n(n+1)} \mathbf{B}_n^{m+1} , \tag{5.35}$$

$$\cos\theta e^{-i\lambda} \mathbf{C}_n^m = \frac{\sqrt{(n-1)(n+1)}}{n} \frac{(n+m-1)(n+m)}{2n+1} \mathbf{C}_{n-1}^{m-1} - \frac{\sqrt{n(n+2)}}{n+1} \frac{(n-m+1)(n-m+2)}{2n+1} \mathbf{C}_{n+1}^{m-1} - \frac{i(n+m)(n-m+1)}{n(n+1)} \mathbf{B}_n^{m-1} . \tag{5.36}$$

These identities are valid for all m and n if we define

$$\mathbf{B}_n^{-m} = \begin{cases} (-1)^m \dfrac{(n-m)!}{(n+m)!} \mathbf{B}_n^{\overline{m}} & \text{if } |m| \le n \\ 0 & \text{if } |m| > n \end{cases} , \tag{5.37}$$

and

$$\mathbf{C}_n^{-m} = \begin{cases} (-1)^m \dfrac{(n-m)!}{(n+m)!} \mathbf{C}_n^{\overline{m}} & \text{if } |m| \le n \\ 0 & \text{if } |m| > n \end{cases} . \tag{5.38}$$

The rest of this section contains a proof of equation (3.13) in Section 3. We begin with a review of the differential geometry of the spherical coordinate system.

$$x = r \cos\theta \cos\lambda \; ; \; y = r \cos\theta \sin\lambda \;\text{ and }\; z = r \sin\theta \tag{5.39}$$

has the modified Jacobian

$$\mathbf{J} = \begin{bmatrix} \dfrac{1}{a \cos\theta} \dfrac{\partial x}{\partial \lambda} & \dfrac{1}{a} \dfrac{\partial x}{\partial \theta} & \dfrac{\partial x}{\partial r} \\ \dfrac{1}{a \cos\theta} \dfrac{\partial y}{\partial \lambda} & \dfrac{1}{a} \dfrac{\partial y}{\partial \theta} & \dfrac{\partial y}{\partial r} \\ \dfrac{1}{a \cos\theta} \dfrac{\partial z}{\partial \lambda} & \dfrac{1}{a} \dfrac{\partial z}{\partial \theta} & \dfrac{\partial z}{\partial r} \end{bmatrix} . \tag{5.40}$$

Define

$$\mathbf{K} = \begin{bmatrix} a\ \cos\theta\ \dfrac{\partial\lambda}{\partial x} & a\ \cos\theta\ \dfrac{\partial\lambda}{\partial y} & \cos\theta\ \dfrac{\partial\lambda}{\partial z} \\ a\ \dfrac{\partial\theta}{\partial x} & a\ \dfrac{\partial\theta}{\partial y} & a\ \dfrac{\partial\theta}{\partial z} \\ \dfrac{\partial r}{\partial x} & \dfrac{\partial r}{\partial y} & \dfrac{\partial r}{\partial z} \end{bmatrix}, \qquad (5.41)$$

then

$$\mathbf{JK} = \begin{bmatrix} \dfrac{\partial x}{\partial x} & \dfrac{\partial x}{\partial y} & \dfrac{\partial x}{\partial z} \\ \dfrac{\partial y}{\partial x} & \dfrac{\partial y}{\partial y} & \dfrac{\partial y}{\partial z} \\ \dfrac{\partial z}{\partial x} & \dfrac{\partial z}{\partial y} & \dfrac{\partial z}{\partial z} \end{bmatrix} = \mathbf{I}. \qquad (5.42)$$

From (5.39) and (5.40)

$$\mathbf{J} = \mathbf{Q}^T = \begin{bmatrix} -\sin\lambda & -\sin\theta\cos\lambda & \cos\theta\cos\lambda \\ \cos\lambda & -\sin\theta\sin\lambda & \cos\theta\sin\lambda \\ 0 & \cos\theta & \sin\theta \end{bmatrix} \qquad (5.43)$$

which is orthogonal and hence from (5.42)

$$\mathbf{K} = \mathbf{Q} = \begin{bmatrix} -\sin\lambda & \cos\lambda & 0 \\ -\sin\theta\cos\lambda & -\sin\theta\sin\lambda & \cos\theta \\ \cos\theta\cos\lambda & \cos\theta\sin\lambda & \sin\theta \end{bmatrix}. \qquad (5.44)$$

Equations (5.43) and (5.44) provide closed forms for the derivatives in (5.40) and (5.41). From (5.39) through (5.44) we obtain:

$$\frac{dx}{dt} = -\sin\lambda\ a\ \cos\theta\ \frac{d\lambda}{dt} - \sin\theta\cos\lambda\ a\ \frac{d\theta}{dt} + \cos\theta\cos\lambda\ \frac{dr}{dt} \qquad (5.45)$$

$$\frac{dy}{dt} = \cos\lambda\ a\ \cos\theta\ \frac{d\lambda}{dt} - \sin\theta\sin\lambda\ a\ \frac{d\theta}{dt} + \cos\theta\sin\lambda\ \frac{dr}{dt} \qquad (5.46)$$

$$\frac{dz}{dt} = \cos\theta\ a\ \frac{d\theta}{dt} + \sin\theta\ \frac{dr}{dt}. \qquad (5.47)$$

Since $u = a \cos\theta \, d\lambda/dt$, $v = a \, d\theta/dt$, $w = dr/dt$, $X = dx/dt$, $Y = dy/dt$, and $Z = dz/dt$, then (5.45), (5.46), and (5.47) have matrix form:

$$\mathbf{v}_c = \mathbf{Q}^T \mathbf{v}_s \tag{5.48}$$

or

$$\mathbf{v}_s = \mathbf{Q} \, \mathbf{v}_c \tag{5.49}$$

where

$$\mathbf{v}_s = (u, v, w) \text{ and } \mathbf{v}_c = (X, Y, Z). \tag{5.50}$$

At this point we begin the proof of (3.13). Since

$$\mathbf{Q} \frac{\partial \mathbf{v}_c}{\partial x} = \mathbf{Q} \left[a \cos\theta \frac{\partial \lambda}{\partial x} \frac{1}{a \cos\theta} \frac{\partial \mathbf{v}_c}{\partial \lambda} + a \frac{\partial \theta}{\partial x} \frac{1}{a} \frac{\partial \mathbf{v}_c}{\partial \theta} + \frac{\partial r}{\partial x} \frac{\partial \mathbf{v}_c}{\partial r} \right], \tag{5.51}$$

from (5.41) and (5.44) we obtain

$$\mathbf{Q} \frac{\partial \mathbf{v}_c}{\partial x} = -\sin\lambda \, \mathbf{Q} \frac{1}{a \cos\theta} \frac{\partial \mathbf{v}_c}{\partial \lambda} - \sin\theta \cos\lambda \, \mathbf{Q} \frac{1}{a} \frac{\partial \mathbf{v}_c}{\partial \theta} + \cos\theta \cos\lambda \, \mathbf{Q} \frac{\partial \mathbf{v}_c}{\partial r} \tag{5.52}$$

From (5.49)

$$\mathbf{Q} \frac{\partial \mathbf{v}_c}{\partial r} = \frac{\partial \mathbf{v}_s}{\partial r} = \begin{bmatrix} \frac{\partial u}{\partial r} \\ \frac{\partial v}{\partial r} \\ \frac{\partial w}{\partial r} \end{bmatrix}. \tag{5.53}$$

From (5.48)

$$\mathbf{Q} \frac{1}{a} \frac{\partial \mathbf{v}_c}{\partial \theta} = \frac{1}{a} \mathbf{Q} \frac{\partial \mathbf{Q}^T}{\partial \theta} \mathbf{v}_s + \frac{1}{a} \frac{\partial \mathbf{v}_s}{\partial \theta}, \tag{5.54}$$

or

$$\mathbf{Q} \frac{1}{a} \frac{\partial \mathbf{v}_c}{\partial \theta} = \frac{1}{a} \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} + \frac{1}{a} \frac{\partial \mathbf{v}_s}{\partial \theta}, \tag{5.55}$$

or

$$\mathbf{Q}\ \frac{1}{a}\ \frac{\partial \mathbf{v}_c}{\partial \theta} = \begin{bmatrix} \dfrac{1}{a}\ \dfrac{\partial u}{\partial \theta} \\ \dfrac{1}{a}\ \dfrac{\partial v}{\partial \theta} + \dfrac{w}{a} \\ \dfrac{1}{a}\ \dfrac{\partial w}{\partial \theta} - \dfrac{v}{a} \end{bmatrix}. \tag{5.56}$$

Also from (5.48)

$$\mathbf{Q}\ \frac{1}{a\ \cos\theta}\ \frac{\partial \mathbf{v}_c}{\partial \lambda} = \frac{1}{a\ \cos\theta}\left[\mathbf{Q}\ \frac{\partial \mathbf{Q}^T}{\partial \lambda}\ \mathbf{v}_s + \frac{\partial \mathbf{v}_s}{\partial \lambda}\right], \tag{5.57}$$

or

$$\mathbf{Q}\ \frac{1}{a\ \cos\theta}\ \frac{\partial \mathbf{v}_c}{\partial \lambda} = \frac{1}{a\ \cos\theta}\ \begin{bmatrix} -\cos\theta & 0 & 0 \\ \sin\theta & 0 & 0 \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} + \frac{1}{a\ \cos\theta}\ \frac{\partial \mathbf{v}_s}{\partial \lambda}, \tag{5.58}$$

or

$$\mathbf{Q}\ \frac{1}{a\ \cos\theta}\ \frac{\partial \mathbf{v}_c}{\partial \lambda} = \begin{bmatrix} \dfrac{1}{a\ \cos\theta}\dfrac{\partial u}{\partial \lambda} - \dfrac{v\ \sin\theta}{a\ \cos\theta} + \dfrac{w}{a} \\ \dfrac{1}{a\ \cos\theta}\dfrac{\partial v}{\partial \lambda} + \dfrac{u\ \sin\theta}{a\ \cos\theta} \\ \dfrac{1}{a\ \cos\theta}\dfrac{\partial w}{\partial \lambda} - \dfrac{u}{a} \end{bmatrix}. \tag{5.59}$$

Substituting (5.53), (5.56) and (5.59) into (5.52), we obtain

$$\mathbf{Q}\ \frac{\partial \mathbf{v}_c}{\partial x} = \mathbf{S}\ \mathbf{x} \tag{5.60}$$

where $\mathbf{x}^T = (x, y, z)$ is the first column of $\mathbf{Q}$ and

$$\mathbf{S} = \begin{bmatrix} \dfrac{1}{a\ \cos\theta}\ \dfrac{\partial u}{\partial \lambda} - \dfrac{v\ \sin\theta}{a\ \cos\theta} + \dfrac{w}{a} & \dfrac{1}{a}\ \dfrac{\partial u}{\partial \theta} & \dfrac{\partial u}{\partial r} \\ \dfrac{1}{a\ \cos\theta}\ \dfrac{\partial v}{\partial \lambda} + \dfrac{u\ \sin\theta}{a\ \cos\theta} & \dfrac{1}{a}\ \dfrac{\partial v}{\partial \theta} + \dfrac{w}{a} & \dfrac{\partial v}{\partial r} \end{bmatrix}. \tag{5.61}$$

Proceeding in a similar manner for $\partial \mathbf{v}_c / \partial y$ and $\partial \mathbf{v}_c / \partial z$, we obtain

$$\mathbf{Q}\ \mathbf{C} = \mathbf{S}\ \mathbf{Q} \quad \text{or} \quad \mathbf{C} = \mathbf{Q}^T\ \mathbf{S}\ \mathbf{Q} \tag{5.62}$$

where

$$\mathbf{C} = \begin{bmatrix} \frac{\partial X}{\partial x} & \frac{\partial X}{\partial y} & \frac{\partial X}{\partial z} \\ \frac{\partial Y}{\partial x} & \frac{\partial Y}{\partial y} & \frac{\partial Y}{\partial z} \\ \frac{\partial Z}{\partial x} & \frac{\partial Z}{\partial y} & \frac{\partial Z}{\partial z} \end{bmatrix} \tag{5.63}$$

which completes the proof of (3.13).

In Section 3 we develop a method for computing the bounded differential expressions in (5.61) that is based on (5.62) and the Cartesian derivatives in (5.63). However, the Cartesian derivatives cannot be computed for a function that is defined solely on the surface of the sphere. One possible approach is to continue the solution on the surface to a solution of Laplaces equation above the surface. Since the Cartesian velocity components X, Y, and Z are smooth, they can be expanded in terms of the scalar harmonics Y_n^m. The continuation is then obtained by multiplying each harmonic by either r^n or $r^{-(n+1)}$ depending on whether the solution is continued as an interior or exterior solution of the three dimensional Laplace equation. The Cartesian derivatives can then be determined by applying one of the following two sets of three identities (Swarztrauber, 1981).

$$\frac{\partial r^n Y_n^m}{\partial x} = \frac{r^{n-1}}{2}[(n+m)(n+m-1)Y_{n-1}^{m-1} - Y_{n-1}^{m+1}]\ , \tag{5.64}$$

$$\frac{\partial r^n Y_n^m}{\partial y} = i\frac{r^{n-1}}{2}[(n+m)(n+m-1)Y_{n-1}^{m-1} + Y_{n-1}^{m+1}]\ , \tag{5.65}$$

and

$$\frac{\partial r^n Y_n^m}{\partial z} = r^{n-1}(n+m)Y_{n-1}^m\ , \tag{5.66}$$

or

$$\frac{\partial r^{-(n+1)} Y_n^m}{\partial x} = \frac{r^{-(n+2)}}{2} [(n-m+1)(n-m+2) Y_{n+1}^{m-1} - Y_{n+1}^{m+1}] \ , \tag{5.67}$$

$$\frac{\partial r^{-(n+1)} Y_n^m}{\partial y} = i \frac{r^{-(n+2)}}{2} [(n-m+1)(n-m+2) Y_{n+1}^{m-1} + Y_{n+1}^{m+1}] \ , \tag{5.68}$$

and

$$\frac{\partial r^{-(n+1)} Y_n^m}{\partial z} = -r^{-(n+2)} (n-m+1) Y_{n+1}^m \ . \tag{5.69}$$

The identities in this section have been drawn from several sources including Swarztrauber (1979, 1981), Morse and Feshbach (1953), Hobson (1955), and Abramowitz and Stegun (1964). In addition Hill (1954) contains a discussion of the vector spherical harmonics as well as several identities.

6. Summary and conclusions

In this paper we have developed the vector harmonic method for solving partial differential equations in spherical geometry. A numerical implementation was described with the objective to maximize performance while at the same time providing a reasonable balance between the utilization of main storage and minimizing the total operation count. In previous work (Browning et.al., 1989) it was determined that the operation count for the vector harmonic method is about 30% lower than the conventional spectral transform method. This appears to be an artifact of the implementations since the results in this paper, together with those published by Temperton (1991) imply that the vector and traditional transform methods should require the same computing time.

The attributes of the vector harmonic transform method are listed in the introduction. Perhaps the most important attribute is associated with accuracy of the method. All transforms are norm preserving and there are no divisions by the cosine of the latitude. This latter point permits the inclusion of the poles as grid points but more importantly it reduces roundoff error in the vicinity of the poles. This concept has not been that important in the past. However, it is likely to become more important as model resolution increases, particularly for models running on powerful workstations with half-precision (32-bit) arithmetic.

We close with an observation about spectral and finite-difference methods. The difficulty in comparing spectral and finite-difference methods can be illustrated by the following simple analysis. A spectral method with N modes requires $O(N^3)$ operations per time step compared with $O(M^2)$ operations for the finite-difference method on an $M \times M$ grid. However, the accuracy of the spectral method is $O(e^{-N})$ compared with $O(M^{-6})$ for the sixth-order finite-difference method. Hence, for comparable accuracy, $N = 6 \ln M + C$ for some constant C. This implies that the operation counts for the finite-difference and spectral methods are $O(M^2)$ and $O[(\ln M)^3]$ respectively. Therefore, in the limit, the spectral method will require fewer operations to achieve an accuracy that is comparable to the finite-difference method.

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REFERENCES

Abramowitz, M., and L.A. Stegun, 1964: Handbook of Mathematical Functions. National Bureau of Standards, Applied Mathematics Series, *U.S. Government Printing Office*, Washington, DC.

Backus, G.E., 1967: Converting vector and tensor equations to scalar equations in spherical coordinates. *Geophys. J. Roy. Astro. Soc.,* **13,** 71-101.

Baede, A. P. M., M. Jarraud, and U. Cubasch, 1979: Adiabatic formulation and organization of ECMWF's model. ECMWF Tech. Rep. No. 15, 40 pp. [Available from ECMWF, Shinfield Park, Reading, Berkshire, RG2 9AX, England.]

Bjorklund, S., H. Markarian, N. Pleszkoch, and J. Rivero, 1973: A brief review of the application of vector spherical harmonics to global weather prediction. IBM Report, Federal Systems Division, Gaithersburg, Maryland.

Boer, G. J., N. A. McFarlane, R. Laprise, J. D. Henderson, and J.-P. Blanchet, 1984: The Canadian Climate Centre spectral atmospheric general circulation model. *Atmos.-Ocean,* **22,** 226-243.

Bourke, W., 1972: An efficient, one-level, primitive-equation spectral model. *Mon. Wea. Rev.,* **100,** 683-698.

Bourke, W., B. McAvaney, K. Puri, and R. Thurling, 1977: Global modeling of atmospheric flow by spectral methods. *General Circulation Models of the Atmosphere, Methods of Computational Physics.* Academic Press, New York.

Browning, G. L., J. J. Hack, and P. N. Swarztrauber, 1989: A comparison of three numerical methods for solving differential equations on the sphere. *Mon. Wea. Rev.,* **117,** 1058-1075.

Eliasen, E., B. Machenhauer, and E. Rasmussen, 1970: On a numerical method for integration of the hydrodynamical equations with a spectral representation of the horizontal fields. Rep. No. 2, Institut for Teoretisk Meteorologi, Kobenhavns Universitet, Denmark.

Fulton, S. R., and W. H. Schubert, 1987: Chebyshev spectral methods for limited-area models. Part I: Model problem analysis. *Mon. Wea. Rev.,* **115,** 1940-1953.

Golub G. H., and J. H. Welsch, 1969: Calculation of Gauss quadrature rules. *Math. Comp.,* **23,** 221-230.

Hill, E. L., 1954: The theory of vector spherical harmonics, *Amer. J. Phys.,* **22,** 211-214.

Hobson, E. W., 1955: Spherical and Ellipsoidal Harmonics, *Chelsea,* New York, NY.

James, R. W., 1976: New tensor spherical harmonics, for application to the partial differential equations of physics. *Phil. Trans. R. Soc. Lond.,* **A 281,** 195-221.

Jones, M. N., 1970: Atmospheric Oscillations-I. *Planet. Space Sci.,* **18,** 1393-1416.

---------------, 1971: Atmospheric Oscillations-II. *Planet. Space Sci.,* **19,** 609-634.

Machenhauer, B., and E. Rasmussen, 1972: On the integration of the spectral hydrodynamical equations by a transform method. Rep. No. 3, Institut for Teoretisk Meteorologi, Kobenhavns Universitet, Denmark.

Machenhauer, B. and R. Daley, 1972: A baroclinic primitive equation model with spectral representation in three dimensions. Rep. No. 4, Institut for Teoretisk Meteorologi, Kobenhavns Universitet, Denmark.

Machenhauer, B., 1979: The spectral method. Numerical Methods Used in Atmospheric Models, GARP Publication Series **17,** 121-275, World Meteorological Organization, Geneva, Switzerland.

Morse, P. M., and H. Feshbach, 1953: *Methods of Theoretical Physics.* McGraw-Hill, New York.

Moses, H. E., 1974: Use of vector spherical harmonics in global meteorology and aeronomy. *J. Atmos. Sci.,* **31,** 1490-1499.

Orzag, S. A., 1970: Transform method for calculation of vector coupled sums: Application to the spectral form of the vorticity equation. *J. Atmos. Sci.,* **27,** 890-895.

Orzag, S. A., 1974: Fourier series on spheres. *Mon. Wea. Rev.,* **102,** 56-75.

Phillips, N., 1957: A map projection system suitable for large-scale numerical weather prediction. *J. Met. Soc. of Japan,* **75,** 262-267.

Robert, A. J., 1966: The integration of a low order spectral form of the primitive meteorological equations. *J. Meteor. Soc. Japan,* **44,** 237-245.

Silberman, I., 1954: Planetary waves in the atmosphere. *J. Meteor.,* **11,** 27-34.

Smith, B. T., J. M. Boyle, J. J. Dongarra, B. S. Garbow, Y. Ikebe, V. C. Klema, and C. B. Moler, 1976: Matrix Eigensystem Routines - EISPACK Guide, 2nd edition, Lecture Notes in Computer Science, no. 6, *Springer-Verlag,* New York, NY.

Swarztrauber, P. N., 1979: On the spectral approximation of discrete scalar and vector functions on the sphere. *SIAM J. Numer. Anal.,* **16,** 934-949.

Swarztrauber, P. N., 1981: The approximation of vector functions and their derivatives on the sphere. *SIAM J. Numer. Anal.,* **18,** 191-210.

Swarztrauber, P. N., 1984: On the spectral analysis of vector differential equations on the sphere. *Proc. Conference on Computer methods for Partial Differential Equations, Fifth IMACS Int. Symp.,* R. Vichnevetsky and R.S. Stepleman, Eds., Lehigh University, Bethlehem, PA.

Swarztrauber, P. N., and A. Kasahara, 1985: The vector harmonic analysis of Laplace's tidal equations. *SIAM J. Sci. Stat. Comput.,* **6,** 464-491.

Swarztrauber, P. N., 1987: Multiprocessor FFTs. *Parallel Computing.* **5,** 197-210.

Temperton, C., 1991: On scalar and vector transform methods for global spectral models. *Mon. Wea. Rev.* **119,** 1303-1307.

Williamson, D. L., J. T. Kiehl, V. Ramanathan, R. E. Dickinson, and J. J. Hack, 1987: Description of NCAR Community Climate Model (CCM1), NCAR Tech. Rep. TN-285+STR, June 1987, National Center for Atmospheric Research, Boulder, CO.

Williamson, D. L., J. B. Drake, J. J. Hack, R. Jakob, and P. N. Swarztrauber, 1992: A Standard test set for numerical approximations to the shallow water equations in spherical geometry. *J. Comp. Phys.*, **102,** 211-224.

Yakimiw, E., 1976: On the symmetry properties of the spherical "interaction coefficients." Notes Scientifiques et Techniques, no. 2, Atmospheric Environment Service, Recherche en Prévision Numérique, Montreal.