COMPUTING ON THE SPHERE PART I: SCALAR HARMONIC ANALYSIS

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One of the fundamental differences between spectral analysis on the sphere and rectangle is that vectors on the sphere are discontinuous and require a fundamentally different spectral representation.

For that reason we separate scalar and vector harmonic transforms and begin with scalar transforms of functions such as temperature, pressure, divergence, and vorticity.

TOPICS

Sphere vs rectangle	Least squares representation
Assoc. Legendre fns.	Double Fourier series
Computing the ALFs	Integration formulas
ALFPACK	Gauss points and weights
Scalar harmonic analysis	Generalized harmonic analysis
Aliases and Aliasing	Harmonic projectors
Selecting a finite basis	

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COMPARE SPHERE WITH RECTANGLE

Harmonic analysis is used on a sphere like Fourier analysis on a rectangle but with important differences:

1. Fourier representations are interpolative whereas harmonic representations are approximate in the weighted least squares sense.
2. Discrete Fourier transforms are norm preserving whereas harmonic transforms can magnify.
3. Vector functions are discontinuous (multivalued) at the poles in spherical coordinates.
4. Fourier analysis can be used for both scalar and vector functions on the rectangle. Different analyses are required for scalar and vector functions on the sphere.
5. The FFT can be used for the Fourier transform but not for the Legendre transform.
6. Many terms (not just coefficients) are unbounded in PDEs posed in spherical coordinates.
7. Clustering of grid points near the poles leads to classic "pole problem".
8. $O(N)$ locations are required to store the trigonometric functions whereas $O(N^3)$ locations are required to store the associated Legendre functions $P_n^m(\theta)$ (with notable exceptions).

THE ASSOCIATED LEGENDRE FUNCTIONS

On the sphere, the trigonometric functions are replaced by the modes of the Helmholtz equation (spherical harmonics) $Y_n^m = P_n^m(\theta)e^{im\lambda}$ where θ is colatitude and λ is east longitude.

The $P_n^m(\theta)$ satisfy:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{dP_n^m}{d\theta}) + [n(n+1) - \frac{m^2}{\sin^2\theta}]P_n^m = 0 \qquad (1)$$

With solution given by Rodrigue's formula

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

where $x = \cos\theta$.

Rodrigue's formula does not provide a satisfactory method for computing the associated Legendre functions from the standpoint of either speed or accuracy.

The three term recurrence relations are also subject to error near the poles. Consider instead the Fourier method.

THE FOURIER METHOD FOR COMPUTING THE LEGENDRE FUNCTIONS

The Fourier method provides a stable method for computing the associated Legendre functions for any m, n without having to compute the functions for any other m, n.

The differential equation for P_n^m has a solution of the following form that depends on the parity of m and n.

$$P_n^m(\theta) = \sum_{k=0}^{n/2} a_{m,n,k} \cos 2k\theta \qquad n \text{ even}, \quad m \text{ even} \tag{3}$$

$$P_n^m(\theta) = \sum_{k=1}^{n/2} a_{m,n,k} \sin 2k\theta \qquad n \text{ even}, \quad m \text{ odd} \tag{4}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \cos(2k-1)\theta \qquad n \text{ odd}, \quad m \text{ even} \tag{5}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \sin(2k-1)\theta \qquad n \text{ odd}, \quad m \text{ odd} \tag{6}$$

THE FOURIER METHOD
(continued)

The Fourier representations for $P_n^m(\theta)$ satisfy the differential equation if the $a_{m,n,k}$ satisfy the tridiagonal equations

$$[(2k-1)(2k-2)-n(n+1)]a_{m,n,k-1}-2[4k^2-n(n+1)+2m^2]a_{m,n,k} \\ +\ [(2k+1)(2k+2)-n(n+1)]a_{m,n,k+1} \ = \ 0\ .$$

The coefficient of $a_{m,n,n/2}$ is zero and the resulting finite number of equations are singular for $m=0,\ldots,n$.

A unique solution is determined by computing $a_{m,n,n/2}$ from Rodrigue's formula and the remaining coefficients by back substitution.

The toughest part is computing $a_{m,n,n/2}$ - more on this later.

Once the $a_{m,n,k}$ are determined the $P_n^m(\theta_i)$ can be tabulated using the quarterwave FFTs from `SPHEREPACK`.

THE RECURRENCE METHOD FOR THE LEGENDRE FUNCTIONS

Using the symmetric FFTs in FFTPACK, the Fourier method requires $O(\log N)$ operations per $P_n^m(\theta_i)$.

However only 4 flops are required using the following four term recurrence relation that is initialized by either P_n^0 or P_n^1 using the Fourier method.

$$
\begin{aligned}
P_n^m(\theta) &= P_{n-2}^m(\theta) + (n+m-2)(n+m-3)P_{n-2}^{m-2}(\theta) \\
&- (n-m+1)(n-m+2)P_n^{m-2}(\theta)
\end{aligned}
$$

This recurrence is quite stable in the indicated direction. Indeed the recurrence corresponds to an orthonormal transformation.

P. N. Swarztrauber and W. F. Spotz, Generalized discrete spherical harmonic transforms, *J. Comp. Phys.*, **159**(2000), pp. 213-230.

It does not contain a functional dependence on θ and can therefore be used to compute derivatives, etc.

Because the indices are spaced by 2 the even or odd functions can be computed independently.

All the associated Legendre functions are linear combinations of either P_n^0 or P_n^1.

SOFTWARE FOR COMPUTING THE ASSOCIATED LEGENDRE FUNCTIONS (ALFPACK)

ALFPACK has thirteen user entry points for computing single and double precision, normalized associated Legendre functions of the first kind.

ALFPACK uses the recurrence to tabulate $P_n^m(\theta)$ as a function of either m or n.

ALFPACK contains codes for computing the Fourier coefficients in the trigonometric representations of the Legendre functions

ALFPACK uses the symmetric FFTs to tabulate as a function of θ

ALFPACK contains codes for either a single value of θ or a table of values.

(ACCESSING ALFPACK)

ALFPACK is available via anonymous ftp by executing the command

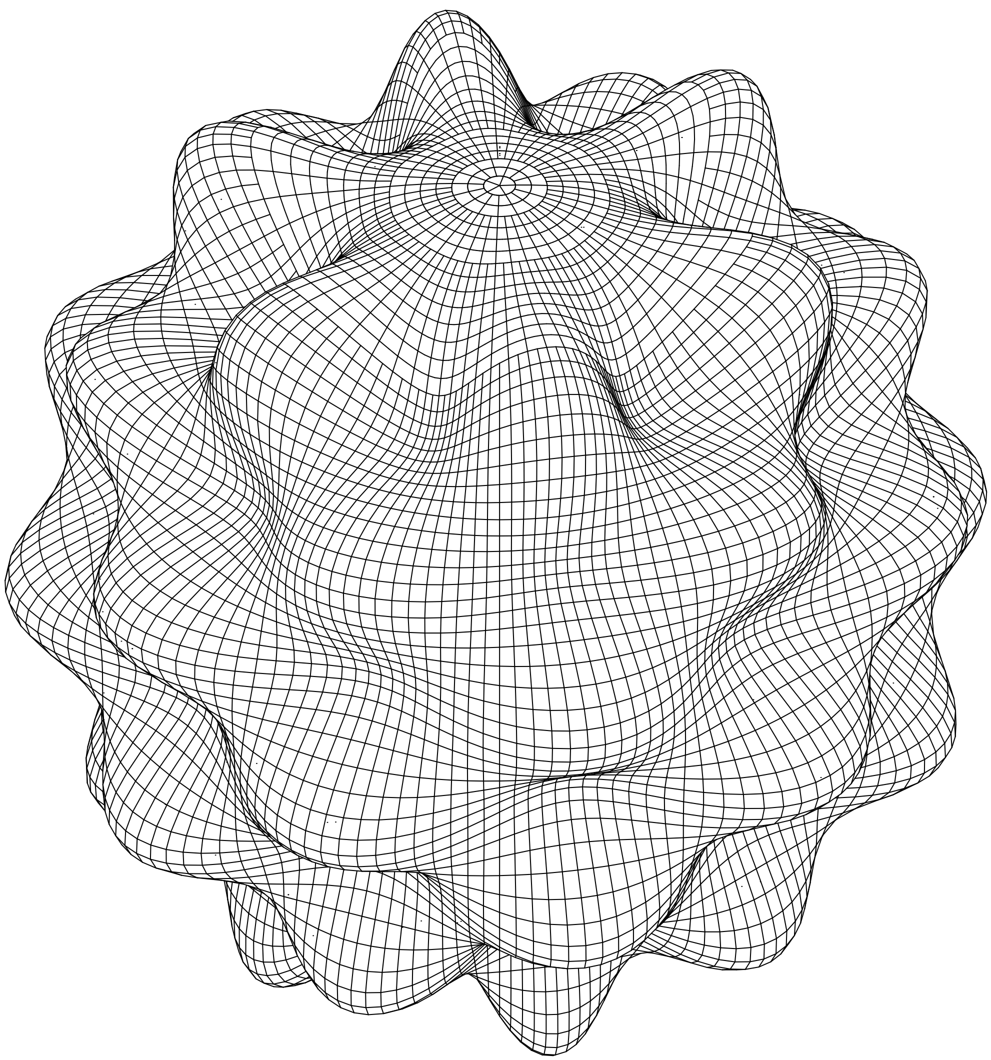
ftp ftp.ucar.edu

Then enter "anonymous" for your name, and your email address for the password. Then follow this session:

```
ftp> cd dsl/lib/alfpack
ftp> mget *
  .
  .  answer y to each question
  .
ftp> quit
```

Back on your host machine, you will have the source code for the entire ALFPACK library, including a makefile.

$\mathbf{Re}[\mathbf{Y}_{12}^{6}(\theta, \lambda)]$



Spherical harmonic, $n = 12, m = 6$ produced by subroutine `visequ` in `spherepack`.

SCALAR HARMONIC ANALYSIS

Given $f_{i,j} = f(\theta_i, \lambda_j)$ we wish to determine complex coefficients $c_{m,n}$ such that:

$$f_{i,j} = \sum_{n=0}^{N} \sum_{m=-n}^{n} c_{m,n} Y_n^m(\theta_i, \lambda_j) \tag{7}$$

where $Y_n^m(\theta_i, \lambda_j)$ are the spherical harmonics

$$Y_n^m(\theta_i, \lambda_j) \;=\; P_n^m(\theta_i) e^{im\lambda_j} \tag{8}$$

The interpolation problem on the sphere does not have a solution!

WHY NOT?

After all - $f_{i,j}$ can be interpolated with a doubly periodic trigonometric series representation .....

More on this later ...

ALIASES

There are only a finite number of e^{ikx} that can be distinguished on a set of points $x_n = n\frac{2\pi}{N}$

$$e^{ink\frac{2\pi}{N}} = e^{-imn2\pi}e^{in(k+mN)\frac{2\pi}{N}} = e^{in(k+mN)\frac{2\pi}{N}} \tag{9}$$

That is: For any k there exists $-N/2 < k_1 \leq N/2$ such that

$$e^{ikx_n} \;=\; e^{ik_1x_n} \tag{10}$$

Hence e^{ikx} and e^{ik_1x} cannot be distinguished on x_n.

They are alternate characterizations or "aliases" of one another.

Therefore we select the discrete Fourier basis as e^{ikx_n} with the smallest wave numbers $-N/2 < k_1 \leq N/2$.

ALIASING

But what happens if we attempt to interpolate a function with a series representation in terms of more wave numbers than exist in the discrete basis? e.g. assume $f(x)$ has $2N$ coefficients

$$f(x) \;=\; \sum_{k=-N}^{N} c_k \; e^{ikx} \tag{11}$$

On the points x_n the e^{ikx} for $|k| \;>\; N/2$ have aliases in the interval $|k| \;\leq\; N/2$ and

$$f(x_n) \;=\; \sum_{k=0}^{N/2-1} (c_k \;+\; c_{k-N}) \; e^{ink\frac{2\pi}{N}} \tag{12}$$

$$+ \sum_{k=-N/2}^{-1} (c_k \;+\; c_{k+N}) \; e^{ink\frac{2\pi}{N}} \tag{13}$$

Therefore, instead of the c_k a discrete analysis yields

$$c_k \;+\; c_{k-N} \quad \text{for} \quad 0 \;\leq\; k \;\leq\; N/2 \tag{14}$$

$$c_k \;+\; c_{k+N} \quad \text{for} \quad -N/2 \;\leq\; k \;\leq\; -1 \tag{15}$$

The high frequency components $|k| \;>\; N/2$ are said to **alias** onto the low frequency components $|k| \;\leq\; N/2$

We are unable to compute the higher coefficients AND those that we compute are in error.

SELECTING A FINITE DISCRETE BASIS ON THE SPHERE

Recall that $P_n^m(\theta)$ has the Fourier representation

$$P_n^m(\theta) \;=\; \sum_{k=0}^{n/2} a_{m,n,k} \cos 2k\theta \qquad n \text{ even}, \quad m \text{ even} \tag{16}$$

$P_n^m(\theta)$ is included in the discrete basis only if the individual terms in its representation do not have an alias with a smaller wave number. .

For grid with N latitudinal points n must therefore be less than or equal to N. By definition $m \leq n$, which then defines the discrete basis of harmonic functions.

This "triangular truncation" provides an analysis that is invariant under any rotation or translation of the spherical coordinate system. That is, the same harmonic representation is obtained no matter where the pole is placed.

LEAST SQUARES HARMONIC ANALYSIS

On a grid with $2N$ longitudes and N latitudes the discrete harmonic basis consists of the functions

$$\cos m\lambda P_n^m(\theta) \quad \text{and} \quad \sin m\lambda P_n^m(\theta) \tag{17}$$

for $m \le n$ and $n \le N$, which yields a total of N^2 basis functions

HOWEVER

this is half the number of grid points $2N^2$, which implies the interpolation problem on the sphere does not have a solution and

Spectral analysis on the sphere is given as the solution to a least squares problem.

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

A CONTRADICTION ?

Any function is doubly periodic on the sphere.

THEREFORE

$a_{m,n}$ can be found such that

$$f_{i,j} = \sum_{n=-N/2}^{N/2} \sum_{m=-N/2}^{N/2} a_{m,n} e^{i(m\theta_i + n\lambda_j)} \tag{18}$$

This would seem to solve the interpolation problem

HOWEVER

The complex exponentials do not provide a satisfactory basis since some are not smooth at the poles.

For example, $e^{i\lambda}$ is discontinuous (multivalued) at the poles and not suitable for the approximation of smooth functions on the sphere.

DOUBLE FOURIER SERIES AND AN IMPORTANT UNSOLVED PROBLEM

Although the double Fourier basis is discontinuous, a number of solvers and methods have been developed using them.... most with the possible exception of

W. F. Spotz, M. A. Taylor, and P. N. Swarztrauber, Fast shallow-water equation solvers in latitude-longitude coordinates, *J. Comp. Phys.*, **145**(1998) pp. 432-444.

The success of this paper is due to the use of a harmonic projection filter that consists of a harmonic analysis followed immediately by a harmonic synthesis.

However the projection slows the method and in some sense defeats the whole purpose of the double Fourier series approach.

Therefore it would be highly desirable to implement the harmonic projection using the double Fourier method.

And of course use the double Fourier method to implement the discrete harmonic transforms themselves.

LEAST SQUARES HARMONIC ANALYSIS
(properties)

Recall that spherical harmonics have representation in terms of homogeneous polynomials in x, y, and z.

Therefore functions are uniformly represented on the sphere independent of the variations in the grid spacing.

e.g. the tabulation $f_{i,j}$ is interpolated at the equator but the points in higher latitudes are progressively smoothed to a greater extent.

Therefore high frequencies that are artificially induced by the closeness of the points near the poles are eliminated.

Model time steps are limited by the distance between points on the equator rather than near the poles.

Unlike aliasing on the rectangle, harmonics of higher degree and order may or may not alias onto an individual harmonic in the discrete basis.

SCALAR HARMONIC ANALYSIS IN THE CONTINUUM

For a real function $f(\theta,\lambda)$ the harmonic analysis consists of determining coefficients $a_{m,n}$ and $b_{m,n}$ such that

$$f(\theta,\lambda) \;=\; \sum_{n=0}^{\infty}\sum_{m=0}^{n} P_n^m(\theta)(a_{m,n}\cos m\lambda \;+\; b_{m,n}\sin m\lambda) \qquad (19)$$

To that end $a_{m,n}$ and $b_{m,n}$ are given by

$$a_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}] \int_0^{2\pi} \int_0^{\pi} f(\theta,\lambda)P_n^m(\theta)\cos m\lambda \cos\theta d\theta d\lambda \qquad (20)$$

$$b_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}] \int_0^{2\pi} \int_0^{\pi} f(\theta,\lambda)P_n^m(\theta)\sin m\lambda \cos\theta d\theta d\lambda \qquad (21)$$

DISCRETE SCALAR HARMONIC ANALYSIS

The longitudinal integrals are approximated with the rectangle rule and computed efficiently using the FFT.

$$a_m(\theta) = \frac{2}{M} \sum_{j=0}^{M-1} f(\theta, \lambda_j) \cos m\lambda_j \tag{22}$$

$$b_m(\theta) = \frac{2}{M} \sum_{j=0}^{M-1} f(\theta, \lambda_j) \sin m\lambda_j \tag{23}$$

then

$$a_{m,n} = [\frac{2n+1}{2\pi} \frac{(n-m)!}{(n+m)!}] \int_0^{\pi} a_m(\theta) P_n^m(\theta) \cos\theta d\theta \tag{24}$$

$$b_{m,n} = [\frac{2n+1}{2\pi} \frac{(n-m)!}{(n+m)!}] \int_0^{\pi} b_m(\theta) P_n^m(\theta) \cos\theta d\theta \tag{25}$$

How are the latitudinal integrals computed?

LATITUDINAL QUADRATURES

Current weather/climate models use Gauss-Legendre quadrature with weights w_i and points θ_i

$$a_{m,n} \;=\; [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N-1} \; w_i P_n^m(\theta_i) a_m(\theta_i) \qquad (26)$$

$$b_{m,n} \;=\; [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N-1} \; w_i P_n^m(\theta_i) b_m(\theta_i) \qquad (27)$$

The Machenhauer-Daley (MD) quadrature provides the same accuracy on equally spaced points $\theta_i \;=\; i\pi/M$

$$a_{m,n} \;=\; [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N} \; Z_n^m(\theta_i) a_m(\theta_i) \qquad (28)$$

$$b_{m,n} \;=\; [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N} \; Z_n^m(\theta_i) b_m(\theta_i) \qquad (29)$$

LATITUDINAL QUADRATURES
(continued)

1. The $Z_n^m(\theta)$ are selected so the quadrature is exact for any $Y_n^m(\theta, \lambda)$ in the finite basis.

2. These seemingly different quadrature formulas will be unified and generalized to an arbitrary set θ_i on a later slide.

3. However, for now we note only that the $Z_n^m(\theta)$ have the same "form" in the forward transform as the $P_n^m(\theta)$ in the backward transform.

4. Although the Gauss and equally spaced quadratures provide the same accuracy, they alias differently...

5. Software is available in SPHEREPACK for both Gauss and equally spaced distribution of points.

REPRESENTING A VECTOR IN TERMS OF A GIVEN SET OF VECTORS

Given an arbitrary set of vectors $\mathbf{A}$ then

$$\mathbf{A}^{\mathrm{T}}(\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A} = \mathbf{I} \tag{30}$$

where for the moment we ignore the fact that the inverse may not exist.

If we define $\mathbf{W} = (\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1}$ then the vectors $\mathbf{A}$ are weighted orthogonal in the sense that $\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{A} = \mathbf{I}$.

Given an arbitrary vector $\mathbf{f}$ then $\mathbf{f} = \mathbf{A}\mathbf{a}$ where $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$, which provides the representation of $\mathbf{f}$ in terms of the vectors $\mathbf{A}$.

Now $\mathbf{W}^{-1} = \mathbf{A}\mathbf{A}^{\mathrm{T}}$ is symmetric positive semidefinite with decomposition $\mathbf{W}^{-1} = \mathbf{U}\mathbf{S}^2\mathbf{U}^{\mathrm{T}}$ where $\mathbf{U}$ is orthogonal (eigenvectors of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$) $\mathbf{S}^2$ is diagonal (eigenvalues of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$). Therefore

$$\mathbf{A}^{\mathrm{T}}\mathbf{U}\mathbf{S}^{-2}\mathbf{U}^{\mathrm{T}}\mathbf{A} = \mathbf{I}\ . \tag{31}$$

Therefore $\mathbf{V}^{\mathrm{T}} = \mathbf{S}^{-1}\mathbf{U}^{\mathrm{T}}\mathbf{A}$ is orthogonal and yields the singular value decomposition of an arbitrary matrix $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{T}}$.

REPRESENTING A FUNCTION IN TERMS OF OF A GIVEN SET OF FUNCTIONS

The vectors $\mathbf{A}$ on the previous slide were arbitrary and can therefore be tabulations of arbitrary functions on an arbitrary set of points. In this manner any tabulation $\mathbf{f}$ can be expressed in terms of the functions selected to determine $\mathbf{A}$ by $\hat{\mathbf{f}} = \mathbf{Aa}$ where

$$\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} \tag{32}$$

or in terms of the SVD

$$\mathbf{a} = \mathbf{V}\mathbf{S}^{-1}\mathbf{U}^{\mathrm{T}}\mathbf{f} \tag{33}$$

Note that

$$\mathbf{W} = (\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1} = \mathbf{U}\mathbf{S}^{-2}\mathbf{V}^{\mathrm{T}} \tag{34}$$

Therefore (33) would be preferred to (32) because of its superior conditioning.

However, for a large class of basis functions on a prescribed set of points one can often develop closed form representations for computing $\mathbf{a}$. e.g. Gauss and equally spaced point distributions.

This also provides formulas for computing the approximation of derivatives, integrals or a host of other derived quantities.

GENERALIZED LEGENDRE TRANSFORMS

We now turn to a specific example of the general theory developed above. Define $\mathbf{A}$ to be the Legendre polynomials tabulated on an arbitrary latitudes θ_i.

We now replace the arbitrary vectors $\mathbf{A}$ with the Legendre polynomials tabulated on an arbitrary set of latitudes θ_i.

$$\mathbf{A} = \begin{bmatrix} P_0(\theta_1) & \cdots & P_{N-1}(\theta_1) \\ \vdots & \ddots & \vdots \\ P_0(\theta_N) & \cdots & P_{N-1}(\theta_N) \end{bmatrix}, \tag{35}$$

The Christoffel-Darboux formula yields the following elements of $\mathbf{W}^{-1}$.

$$(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{i,j} = \frac{N}{\sqrt{4N^2-1}} \frac{P_N(\theta_i)P_{N-1}(\theta_j) - P_{N-1}(\theta_i)P_N(\theta_j)}{\cos\theta_i - \cos\theta_j}. \tag{36}$$

The diagonal elements can be computed directly from $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ or from l'Hôpital's rule.

$$(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{i,i} = \frac{N}{\sqrt{4N^2-1}\cos\theta_i}\left[P_{N-1}(\theta_i)\frac{d}{d\theta}P_N(\theta_i) - P_N(\theta_i)\frac{d}{d\theta}P_{N-1}(\theta_i)\right]. \tag{37}$$

GENERALIZED LEGENDRE TRANSFORMS
(continued)

In this manner the transform $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ generalizes the Legendre transform to an arbitrary set of latitudes and in the process, unifies Gauss and equally spaced latitudinal points θ_i.

If the θ_i are selected as the zeros of $P_N(\theta_i)$ then $\mathbf{W}$ is diagonal and the resulting θ_i are known as the Gaussian Legendre points and the $(\mathbf{W})_{i,i}$ are the Gaussian weights.

Note that this does not save compute time because the transform $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ still requires multiplication by $\mathbf{A}^{\mathrm{T}}$.

We turn now to the computation of the points and weights corresponding to Gauss-Legendre quadrature.

COMPUTING GAUSS-LEGENDRE POINTS

Recall that $P_n(\theta)$ has the Fourier representation

$$P_n(\theta) = \sum_{k=0}^{n} a_{n,k} \cos k\theta \, , \tag{38}$$

For $m = 0$ the tridiagonal equations for the coefficients $a_{m,n,k}$ reduce to the bidiagonal set of equations

$$[n(n+1)-k(k+1)]a_{n,k}+[(k+1)(k+2)-n(n+1)]a_{n,k+2} = 0. \tag{39}$$

The coefficient of $a_{n,n}$ is zero and therefore $a_{n,n}$ can be arbitrary. If we specify

$$a_{n,n} = \sqrt{\frac{2n+1}{2}} \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n-1} n!} = \sqrt{\frac{2n+1}{2}} \frac{\Gamma(2n+1)}{2^{2n-1} \Gamma^2(n+1)} \tag{40}$$

The resulting coefficients $a_{n,k}$ yield the normalized Legendre polynomials.

- $a_{n,n}$ can be difficult to compute because the Γ function will quickly overflow as a function of n.
- Instead we observe that $a_{n,n}$ is a smooth bounded function of $y = 1/n$ on the interval $[0, 1]$ that can be computed in 10 to 12 flops using a rational approximation.

COMPUTING GAUSS-LEGENDRE POINTS
(continued)

- Given its Fourier representation, the zeros of $P_n(\theta)$ or Gauss-Legendre points can now be computed using Newtons method.

- Near the equator the points are almost equally spaced. This provides a sufficiently accurate initial guess that only a single Newton iteration is required.

- Subsequent initial estimates are obtained by linear extrapolation of previous points. In practice, only a few of the points at the end of the interval require an additional Newton iteration.

  A method for computing the points and weights is presented in "Computing the points and weights for Gauss-Legendre quadrature", *SIAM J. Sci. Comput.*, **24**(2002) pp. 945-954.

COMPUTING GAUSS-LEGENDRE WEIGHTS

Using the three point recurrence satisfied by the Legendre polynomials and the fact that $P_n(\theta_i) = 0$ we obtain the following equivalent formulas for the Gauss-Legendre weights.

$$
\begin{aligned}
w_i^{(a)} &= -\frac{\sqrt{(2n-1)(2n+1)}\cos\theta_i}{n\bar{P}_{n-1}(\theta_i)\bar{P}_n'(\theta_i)} &\qquad w_i^{(b)} &= \frac{(2n-1)\cos^2\theta_i}{n^2\bar{P}_{n-1}^2(\theta_i)} \\
w_i^{(c)} &= \frac{\sqrt{(2n+1)(2n+3)}\cos\theta_i}{(n+1)\bar{P}_{n+1}(\theta_i)\bar{P}_n'(\theta_i)} &\qquad w_i^{(d)} &= \frac{(2n+3)\cos^2\theta_i}{(n+1)^2\bar{P}_{n+1}^2(\theta_i)} \\
w_i^{(e)} &= -\frac{\sqrt{(2n-1)(2n+3)}\cos^2(\theta_i)}{n(n+1)\bar{P}_{n-1}(\theta_i)\bar{P}_{n+1}(\theta_i)} &\qquad w_i^{(f)} &= \frac{2n+1}{\left[\bar{P}_n'(\theta_i)\right]^2}\,.
\end{aligned}
$$

- Although analytically identical - they differ computationally in the sense that only $w_i^{(f)}$ provides relative as well as absolute accuracy.
- The methods for computing Gauss points and weights have been implemented in subroutine `gaqd` in `spherepack` and tested to a million points in single precision.
- The points can be computed to machine precision for any n; however, the error growth in the weights is proportional to n.

GENERALIZED DISCRETE SPHERICAL HARMONIC TRANSFORMS

Here we summarize the results from Swarztrauber and Spotz, Generalized spherical harmonic transforms, *J. Comp. Phys.*, **159**(2000) pp. 213-230.

1. The Legendre transforms are generalized to an arbitrary latitudinal distribution of points thereby unifying the transforms based on Gauss and equally spaced distribution as well as providing new transforms for other grid distributions used to model geophysical processes.

2. Memory efficient alternative Legendre transforms are developed whose coefficients in spectral space are rotations of the traditional spectral coefficients. These transforms require $\mathcal{O}(N^2)$ memory compared to the traditional $\mathcal{O}(N^3)$.

3. Faster transforms are developed based on the alternative Legendre transforms and their orthogonal complement. A computational savings of up to 50% can be realized.

The speed and accuracy of several projection methods are given by Spotz and Swarztrauber in:

A performance comparison of associated Legendre projections, *J. Comp. Phys.*, **168**(2001) pp. 339-355.

SPHERICAL HARMONIC PROJECTORS

- Using the simplified notation developed earlier we define the forward transform into spectral space or harmonic analysis as $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ where $\mathbf{f}$ is the tabulation of some scalar function on the surface of the sphere. The transform back into physical space or harmonic synthesis is given by $\hat{\mathbf{f}} = \mathbf{A}\mathbf{a}$. Hence the projector is given by $\mathbf{P} = \mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}$.

- The forward followed by the backward transform can be subject to considerable error (or not exist) depending on the distribution of latitudinal points θ_i.

- This problem disappears if the projections are computed using the singular value decomposition $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{T}}$

$$\mathbf{W} = \mathbf{U}\mathbf{S}^{-2}\mathbf{U}^{\mathrm{T}} \quad \text{and} \quad \mathbf{P} = \mathbf{U}\mathbf{U}^{\mathrm{T}}. \tag{41}$$

- It is evident that $\mathbf{W}$ can be very ill conditioned (because of the factor $\mathbf{S}^{-2}$). However $\mathbf{P}$ is well conditioned (actually best possible) for any distribution of points θ_i.

- The attractive stability and accuracy of spectral transform method for weather and climate simulations result from the harmonic projectors that are explicit or implicit to these models.

SPHERICAL HARMONIC PROJECTORS

(Summary)

Here we summarize the results from Swarztrauber and Spotz, Spherical harmonic projectors, which will appear in *Math. Comp.*.

Variant spherical harmonic projections are defined with the following attributes.

1. The variant projection is norm preserving in the l_2 sense, unlike the traditional spherical harmonic projection.
2. On a Gaussian grid the singular values of the variant projectors are up to 10 percent less than the traditional analysis matrix.
3. The error associated with the variant projection is marginally less than the traditional projection on a Gauss distributed latitudinal grid but may be substantially less on an arbitrary grid.
4. The variant projections are symmetric and expressed as the outer product of orthonormal vectors from a single $N \times N$ matrix compared with traditional projections that require N such matrices.
5. The algorithm for computing the variant projections, as well as the projections themselves, are well conditioned for any latitudinal grid distribution.

LEAST SQUARES - IN WHAT NORM ?

Given $f_{i,j}$ both Gauss and MD quadratures determine $a_{m,n}$ and $b_{m,n}$ such that

$$\hat{f}_{i,j} \;=\; \sum_{n=0}^{N-1} \sum_{m=0}^{n} P_n^m(\theta_i)(a_{m,n} \cos m\lambda_j \;+\; b_{m,n} \sin m\lambda_j) \tag{42}$$

is a least squares approximation to $f_{i,j}$.

The continuous norm is:

$$||f(\theta,\lambda)||^2 \;=\; \frac{1}{2\pi} \int_0^{2\pi} \int_0^{\pi} f^2(\theta,\lambda) \cos\theta d\theta d\lambda \tag{43}$$

$$= \; \sum_{n=0}^{\infty} \sum_{m=0}^{n} a_{m,n}^2 \;=\; \mathbf{a}^{\mathrm{T}}\mathbf{a} \tag{44}$$

THE DISCRETE NORM

The continuous norm suggests the following discrete norm

$$\| \mathbf{f} \|_{\mathbf{W}} = \mathbf{a}^{\mathrm{T}}\mathbf{a} = \mathbf{f}^{\mathrm{T}}\mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} = \mathbf{f}^{\mathrm{T}}\mathbf{W}\mathbf{f} \tag{45}$$

1. This discrete norm with $\mathbf{W} = \mathbf{U}\mathbf{S}^{-2}\mathbf{V}^{\mathrm{T}}$ is exact for any Y_n^m in the discrete basis (otherwise a pseudo norm).

2. $\hat{f}_{i,j} = \mathbf{P}\mathbf{f} = \mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} = \mathbf{U}\mathbf{U}^{\mathrm{T}}\mathbf{f}$ is a weighted least squares approximation to $f_{i,j}$ in the $\mathbf{W}$ norm

3. $\hat{f}_{i,j}$ provides a uniform approximation to $f_{i,j}$ that is independent of the coordinate system and consequently eliminates the high frequencies that can be induced by the closeness of points near the poles.

COMPUTING ON THE SPHERE PART II: VECTOR HARMONIC ANALYSIS

Paul N. Swarztrauber*

June 26, 2003

As previously noted, vectors on the sphere are discontinuous (multiple valued at the poles) and therefore scalar spectral analysis cannot be applied to the individual components like Fourier analysis on the rectangle. Important examples for geophysical applications are the wind and the magnetic field.

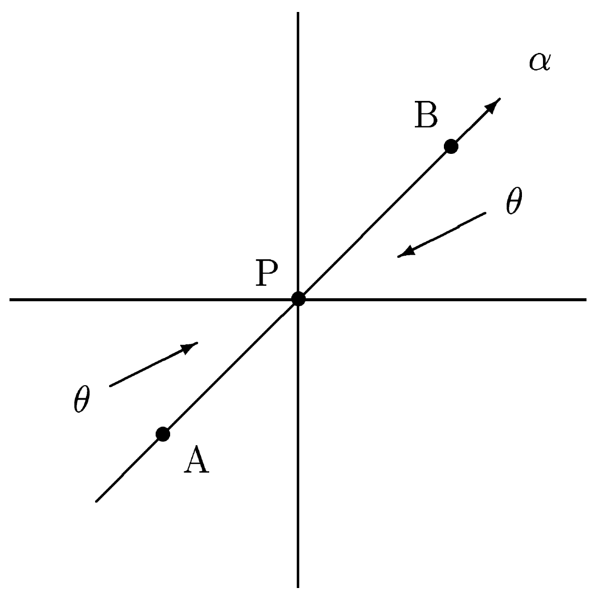
TOPICS

Discontinuous vectors	Vector Harmonic Analysis
Unbounded derivatives	Computing Vorticity, divergence, and gradients
Bounded differential expressions	Robert's variables U and V
Vector Harmonics	SPHEREPACK

*National Center for Atmospheric Research, which is supported by the National Science Foundation, P.O. Box 3000, Boulder, CO 80307

VECTOR FUNCTIONS ON THE SPHERE

The view of a polar neighborhood from above.



At point **A** the wind $(v_\theta\ , v_\lambda)$ is in the direction of increasing θ so $v_\theta(\mathbf{A}) \approx +\alpha$.

At point **B** the wind is in the direction of decreasing θ so $v_\theta(\mathbf{B}) \approx -\alpha$.

Therefore v_θ is discontinuous at the pole **P**. More specifically, as a function of λ, v_θ descends like a spiral staircase from **A** to **B** and then ascends back to **A**.

A DISCONTINUOUS VECTOR FUNCTION

Consider the velocity components of a sphere in solid rotation about an axis through the **equator**.

In Cartesian coordinates the velocity components are:

$$v_x = z \quad ; \quad v_y = 0 \quad , \quad v_z = -x \tag{1}$$

which are continuously differentiable everywhere.

However, in spherical coordinates

$$v_r = 0 \quad , \quad v_\theta = \cos\lambda \quad , \quad v_\lambda = -\sin\theta\sin\lambda \tag{2}$$

where both v_λ v_θ are discontinuous (multivalued) at the poles.

UNBOUNDED TERMS

The discontinuous vector functions produce unbounded terms in PDEs posed in spherical coordinates.

Consider the following term in the Navier-Stokes equations

$$E\mathbf{v} \;=\; \frac{1}{\cos^2\theta}\frac{\partial^2 v_\theta}{\partial\lambda^2} - \frac{2\sin\theta}{\cos^2\theta}\frac{\partial v_\lambda}{\partial\lambda} - \frac{v_\theta}{\cos^2\theta}\;. \tag{3}$$

For solid rotation with axis through the equator

$$E\mathbf{v} \;=\; -\frac{\cos\lambda}{\cos^2\theta} \;+\; 2\frac{\sin^2\theta\cos\lambda}{\cos^2\theta} - \frac{\cos\lambda}{\cos^2\theta} \;=\; -\,2\cos\lambda\;. \tag{4}$$

1. Although each term is unbounded - the total expression is bounded.
2. The terms (not just coefficients) are unbounded.
3. Unbounded terms are the rule rather than the exception.

UNBOUNDED DERIVATIVES

Consider the total time derivative of the velocity (v_λ, v_θ) of a sphere in solid rotation about an axis through the equator.

$$\frac{dv_\lambda}{dt} = \frac{\partial v_\lambda}{\partial t} + \frac{v_\lambda}{a\cos\theta}\frac{\partial v_\lambda}{\partial \lambda} + \frac{v_\theta}{a}\frac{\partial v_\lambda}{\partial \theta} \tag{5}$$

$$\frac{dv_\theta}{dt} = \frac{\partial v_\theta}{\partial t} + \frac{v_\lambda}{a\cos\theta}\frac{\partial v_\theta}{\partial \lambda} + \frac{v_\theta}{a}\frac{\partial v_\theta}{\partial \theta} \tag{6}$$

Substituting $v_\lambda = -\sin\theta\sin\lambda$ and $v_\theta = \cos\lambda$ we obtain

$$\frac{dv_\lambda}{dt} = \frac{\sin\lambda\cos\lambda}{\cos\theta} \tag{7}$$

$$\frac{dv_\theta}{dt} = \frac{\sin^2\lambda\sin\theta}{\cos\theta} \tag{8}$$

The total derivative of the velocity is unbounded at the poles and hence not equal to acceleration.

“Metric” terms are required to compute acceleration. Of course they are also unbounded.

UNBOUNDED DERIVATIVES
(continued)

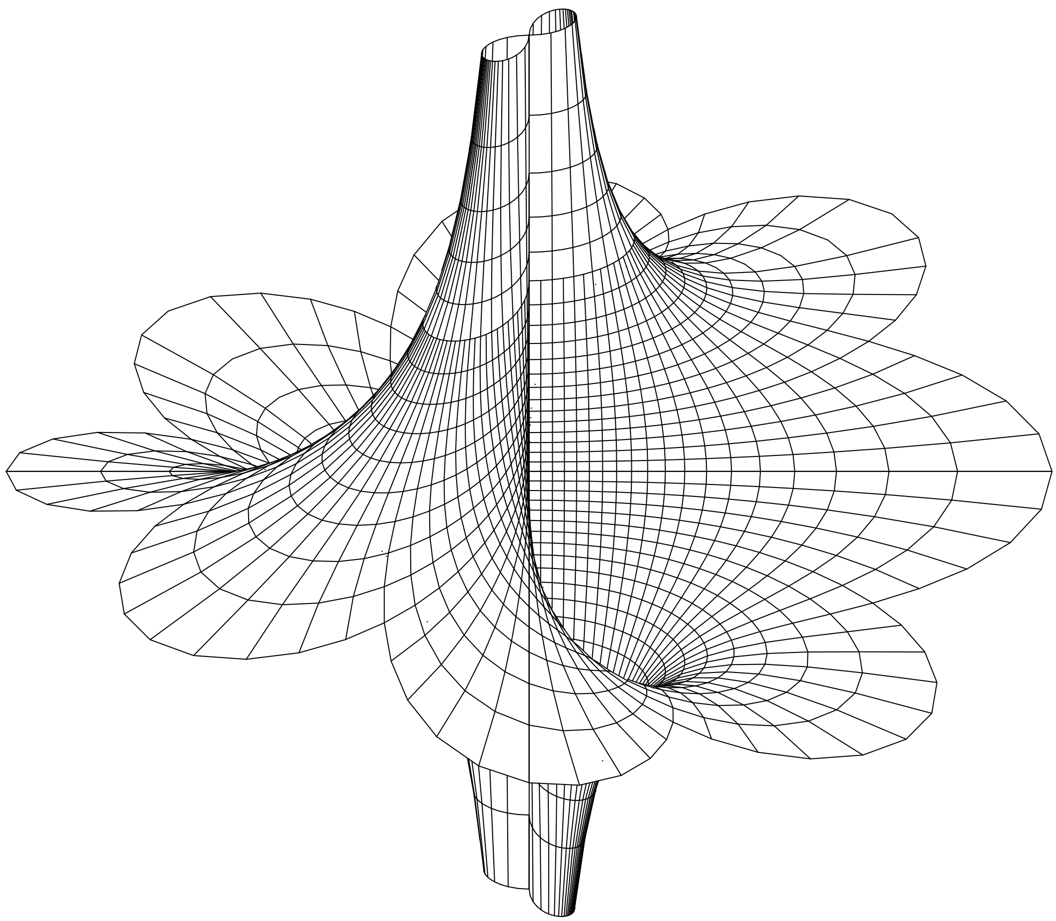


Figure 1: Total derivative of velocity in the neighborhood of the pole

VELOCITY TRANSFORMS

Any unbounded term in a partial differential equation can be combined with another or more to form a bounded differential expression because the dynamics of the modeled process is of course bounded.

The goal is to compute bounded expressions collectively because otherwise the cancellation between larger terms can result in a loss of accuracy and stability.

We therefore seek to identify the bounded differential expressions. To this end we begin with the transform of velocity between the Cartesian and spherical coordinate systems. If

$$\mathbf{Q} = \begin{bmatrix} -\sin\lambda & \cos\lambda & 0 \\ -\sin\theta\cos\lambda & -\sin\theta\sin\lambda & \cos\theta \\ \cos\theta\cos\lambda & \cos\theta\sin\lambda & \sin\theta \end{bmatrix} \tag{9}$$

then the Cartesian velocity components (v_x, v_y, v_z) and spherical components $(v_\lambda, v_\theta, v_r)$ are related by

$$\begin{bmatrix} v_\lambda \\ v_\theta \\ v_r \end{bmatrix} = \mathbf{Q} \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} . \tag{10}$$

BOUNDED DIFFERENTIAL EXPRESSIONS

If we define

$$\mathbf{C} = \begin{bmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} & \frac{\partial v_x}{\partial z} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} & \frac{\partial v_y}{\partial z} \\ \frac{\partial v_z}{\partial x} & \frac{\partial v_z}{\partial y} & \frac{\partial v_z}{\partial z} \end{bmatrix} \tag{11}$$

and

$$\mathbf{S} = \begin{bmatrix} \frac{1}{r\cos\theta}\frac{\partial v_\lambda}{\partial\lambda} - \frac{\sin\theta v_\theta}{r\cos\theta} + \frac{v_r}{r} & \frac{1}{r}\frac{\partial v_\lambda}{\partial\theta} & \frac{\partial v_\lambda}{\partial r} \\ \frac{1}{r\cos\theta}\frac{\partial v_\theta}{\partial\lambda} + \frac{\sin\theta v_\lambda}{r\cos\theta} & \frac{1}{r}\frac{\partial v_\theta}{\partial\theta} + \frac{v_r}{r} & \frac{\partial v_\theta}{\partial r} \\ \frac{1}{r\cos\theta}\frac{\partial v_r}{\partial\lambda} - \frac{v_\lambda}{r} & \frac{1}{r}\frac{\partial v_r}{\partial\theta} - \frac{v_\theta}{r} & \frac{\partial v_r}{\partial r} \end{bmatrix} \tag{12}$$

then it can be shown that

$$\mathbf{S} = \mathbf{Q}\mathbf{C}\mathbf{Q}^{\mathrm{T}} \,. \tag{13}$$

All the elements of **S** are bounded because **C** is bounded and **Q** is orthogonal and norm preserving.

BOUNDED DIFFERENTIAL EXPRESSIONS
(continued)

1. Since **Q** is orthogonal and norm preserving - the elements of **S** are also bounded.

2. The elements of **S** provide the bounded differential expressions into which the unbounded terms can be grouped.

3. All first order partial differential equations on the sphere can be written in terms of the elements of **S** just like all first order pde's on a rectangle can be written in terms of the elements of **C**.

4. All second order bounded differential expressions have also been identified: SIAM J. Numer. Analysis, 18(1981), pp. 191-210.

VECTOR SPHERICAL HARMONICS

We seek an alternate set of basis functions for vectors on the sphere because the spherical harmonics $Y_n^m(\theta, \lambda)$ do not provide a suitable basis for discontinuous functions.

Any surface vector function $(v_\lambda\ , v_\theta)$ can be written in terms of scalar functions Φ and Ψ using the Helmholtz relations:

$$v_\lambda = \frac{1}{\cos\theta}\frac{\partial\Phi}{\partial\lambda} - \frac{\partial\Psi}{\partial\theta} \tag{14}$$

$$v_\theta = \frac{\partial\Phi}{\partial\theta} + \frac{1}{\cos\theta}\frac{\partial\Psi}{\partial\lambda} \tag{15}$$

The vector spherical harmonic $\mathbf{B}_{m,n}$ is obtained from $\Phi = Y_n^m$ and $\Psi = 0$; $\mathbf{C}_{m,n}$ is obtained from $\Phi = 0, \Psi = Y_n^m$.

$$\mathbf{B}_{m,n} = \begin{bmatrix} iB_n^m \\ A_n^m \end{bmatrix} \frac{e^{im\lambda}}{\sqrt{n(n+1)}}\,, \quad \mathbf{C}_{m,n} = \begin{bmatrix} -A_n^m \\ iB_n^m \end{bmatrix} \frac{e^{im\lambda}}{\sqrt{n(n+1)}}\,, \tag{16}$$

where $A_n^m = \frac{dP_n^m}{d\theta} = \frac{1}{2}[(n+m)(n-m+1)P_n^{m-1} - P_n^{m+1}]$

and $B_n^m = \frac{m}{\cos\theta}P_n^m = \frac{1}{2}[(n+m)(n+m-1)P_{n-1}^{m-1} + P_{n-1}^{m+1}]$.

VECTOR HARMONIC ANALYSIS

The vector harmonics are complete on the surface of the sphere and therefore any vector function $\mathbf{v}$ that is smooth in Cartesian coordinates can be expressed as

$$\mathbf{v} \;=\; \sum_{n=0}^{\infty} \;\sum_{m=-n}^{n} (b_{m,n}\mathbf{B}_{m,n} \;+\; c_{m,n}\mathbf{C}_{m,n}). \tag{17}$$

where the analysis is classic, namely

$$b_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{B}_{m,n})^*\mathbf{v}\cos\theta d\theta d\lambda \tag{18}$$

$$c_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{C}_{m,n})^*\mathbf{v}\cos\theta d\theta d\lambda \tag{19}$$

The series converges even for discontinuous $\mathbf{v}$ at a rate that is determined by the smoothness of the vector function in Cartesian coordinates.

The discontinuities in the vector harmonics ”match” those in $\mathbf{v}$.

COMPUTING DIVERGENCE AND VORTICITY

A vector harmonic analysis of $\mathbf{v}$ yields coefficients $b_{m,n}$ and $c_{m,n}$ such that

$$\mathbf{v} \;=\; \sum_{n=0}^{N-1} \sum_{m=-n}^{n} (b_{m,n}\mathbf{B}_{m,n} \;+\; c_{m,n}\mathbf{C}_{m,n}). \tag{20}$$

From the identities

$$\nabla\cdot\mathbf{B}_{m,n}(\theta,\lambda) \;=\; \sqrt{n(n+1)}Y_n^m(\theta,\lambda) \;\;;\;\; \nabla\cdot\mathbf{C}_{m,n}(\theta,\lambda) \;=\; 0 \tag{21}$$

$$\nabla\times\mathbf{B}_{m,n}(\theta,\lambda) \;=\; 0 \;\;;\;\; \nabla\times\mathbf{C}_{m,n}(\theta,\lambda) \;=\; \sqrt{n(n+1)}Y_n^m(\theta,\lambda) \tag{22}$$

Note that an irrotational fluid can be modeled with only the $\mathbf{B}_{m,n}$ and will remain irrotational throughout time.

COMPUTING DIVERGENCE AND VORTICITY
(continued)

Therefore

$$\zeta \ = \ \nabla \times \mathbf{v} \ = \ \sum_{n=0}^{N-1} \sum_{m=-n}^{n} \sqrt{n(n+1)} c_{m,n} Y_n^m(\theta, \lambda) \tag{23}$$

$$\delta \ = \ \nabla \cdot \mathbf{v} \ = \ \sum_{n=0}^{N-1} \sum_{m=-n}^{n} \sqrt{n(n+1)} b_{m,n} Y_n^m(\theta, \lambda) \tag{24}$$

Hence vorticity ζ and divergence δ and can be computed from scalar harmonic syntheses.

Also, given both ζ and δ the vector harmonic analysis $b_{m,n}$ and $c_{m,n}$ can be computed from two scalar analyses.

Note that the mean divergence and vorticity of any vector function on the sphere are both zero.

COMPUTING THE GRADIENT

A scalar harmonic analysis of an arbitrary scalar function Φ yields $d_{m,n}$ such that

$$\Phi = \sum_{n=0}^{N-1} \sum_{m=-n}^{n} d_{m,n} Y_n^m(\theta, \lambda) \tag{25}$$

Using the identity

$$\nabla Y_n^m(\theta, \lambda) = \sqrt{n(n+1)} \mathbf{B}_{m,n}(\theta, \lambda) \tag{26}$$

We obtain

$$\nabla \Phi = \sum_{n=0}^{N-1} \sum_{m=-n}^{n} \sqrt{n(n+1)} d_{m,n} \mathbf{B}_{m,n} \tag{27}$$

Hence $\nabla\Phi = [(\cos\theta)^{-1}\Phi_\lambda, \Phi_\theta]/a$ can be computed from a vector harmonic synthesis.

The derivative of $\mathbf{v}$ with respect to θ is also computed as a vector synthesis but with $\mathbf{B}_{m,n}$ and $\mathbf{C}_{m,n}$ replaced with their derivatives with respect to θ.

ROBERT'S U,V VARIABLES

Although (v_λ, v_θ) is discontinuous at the poles, $(U,V) = (\cos\theta v_\lambda, \cos\theta v_\theta)$ is smooth. For example

$$\cos\theta \mathbf{B}_{m,n} = \cos\theta \begin{bmatrix} iB_n^m \\ A_n^m \end{bmatrix} \frac{e^{im\lambda}}{\sqrt{n(n+1)}}, = \begin{bmatrix} i\cos\theta \frac{m}{\cos\theta} P_n^m \\ \cos\theta \frac{dP_n^m}{d\theta} \end{bmatrix} \frac{e^{im\lambda}}{\sqrt{n(n+1)}} \tag{28}$$

or, using the identity

$$\cos\theta \frac{dP_n^m}{d\theta} = \frac{1}{2n+1}[(n+1)(n+m)P_{n-1}^m - n(n-m+1)P_{n+1}^m] \tag{29}$$

we obtain

$$\cos\theta \mathbf{B}_{m,n} = \begin{bmatrix} imY_n^m \\ \frac{(n+1)(n+m)}{2n+1} Y_{n-1}^m - \frac{n(n-m+1)}{2n+1} Y_{n+1}^m] \end{bmatrix} . \tag{30}$$

Therefore the individual components of $\cos\theta \mathbf{B}_n^m$ are smooth at the poles and have a series representation in terms of the scalar harmonics Y_n^m. However, given U and V the reconstructions $v_\lambda = U/\cos\theta$ and $v_\theta = V/\cos\theta$ are subject to error near the poles.

SPHEREPACK

A software package that assists the modeling of geophysical processes.

1. Codes for both Gauss and equally spaced latitudes
2. Computations can be performed on a single hemisphere
3. The $P_n^m(\theta)$ and $Z_n^m(\theta)$ can be stored or recomputed with the usual tradeoffs between speed and storage.
4. Multiple analysis or synthesis can be performed.

ACCESS

FFTPACK and SPHEREPACK programs are available online at NCAR or a copy of SPHEREPACK can be downloaded from:

http://www.scd.ucar.edu/css/software/spherepack/

SPHEREPACK CONTENTS

SPHEREPACK CONTENTS
(continued)

- GRID TRANSFERS
- GEOPHYSICAL/MATHEMATICAL SPHERICAL COORDINATE CONVERSIONS
- SCALAR SPHERICAL HARMONIC ANALYSIS
- SCALAR SPHERICAL HARMONIC SYNTHESIS
- SCALAR PROJECTIONS
- VECTOR SPHERICAL HARMONIC ANALYSIS
- VECTOR SPHERICAL HARMONIC SYNTHESIS
- ASSOCIATED LEGENDRE FUNCTIONS
- COMPUTE THE ICOSAHEDRAL GEODESIC
- MULTIPLE FFTS
- GAUSS POINTS AND WEIGHTS
- GRAPHICS ON THE SPHERE

COMPUTING ON THE SPHERE PART III: SPECTRAL TRANSFORM METHODS

Paul N. Swarztrauber*

June 26, 2003

TOPICS

Shallow water equations	Shallow water equations with bounded terms
Ritchie's U, V model (ECMWF)	Vector harmonic method and attributes
Vorticity and divergence (NCAR model)	VHM results

*National Center for Atmospheric Research, which is supported by the National Science Foundation, P.O. Box 3000, Boulder, CO 80307

COMPUTING ON THE SPHERE PART III: SPECTRAL TRANSFORM METHODS

Here we describe the spectral transform method for modeling geophysical fluids. Three models of shallow water flow on the sphere are presented that are representative of the nine that are compared in:

Swarztrauber, P. N., Spectral transform methods for solving the shallow water equations on the sphere, *Mon. Wea. Rev.*, **124**(1996) pp. 730-744.

Also see:

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

SHALLOW WATER EQUATIONS

Let ϕ be the geopotential, λ be east longitude, θ be latitude, and u, v be the velocity components respectively. Let a be the radius of the earth, Ω its rotational rate, and $f = 2\Omega \sin\theta$ the Coriolis parameter. Then

$$\frac{\partial u}{\partial t} = -\frac{u}{a\cos\theta}\frac{\partial u}{\partial \lambda} - \frac{v}{a}\frac{\partial u}{\partial \theta} + (f + \frac{u}{a}\tan\theta)v - \frac{1}{a\cos\theta}\frac{\partial \phi}{\partial \lambda} \, , \qquad (1)$$

$$\frac{\partial v}{\partial t} = -\frac{u}{a\cos\theta}\frac{\partial v}{\partial \lambda} - \frac{v}{a}\frac{\partial v}{\partial \theta} - (f + \frac{u}{a}\tan\theta)u - \frac{1}{a}\frac{\partial \phi}{\partial \theta} \, , \qquad (2)$$

$$\frac{\partial \phi}{\partial t} = -\frac{u}{a\cos\theta}\frac{\partial \phi}{\partial \lambda} - \frac{v}{a}\frac{\partial \phi}{\partial \theta} - \frac{\phi}{a\cos\theta}[\frac{\partial u}{\partial \lambda} + \frac{\partial}{\partial \theta}(\cos\theta v)] \, . \qquad (3)$$

This is one of nine (9) forms that are displayed in:

"Spectral transform methods for solving the shallow water equations on the sphere", *Mon. Wea. Rev.*, **124**(1996) pp. 730-744.

Many terms, not just coefficients, are unbounded at the poles.

RITCHIE'S FORMULATION OF THE SWE IN TERMS OF U and V

This formulation of the shallow water equations is based on the variables $U = \cos\theta u$ and $V = \cos\theta v$ (Robert 1966) rather than u and v. Unlike u and v, the variables U and V are smooth at the poles. Although the coefficients are unbounded, the terms themselves are bounded near the poles. The model is posed on a Gauss distributed latitudinal grid. The shallow water equations are written as

$$\frac{\partial U}{\partial t} = -\frac{1}{a\cos^2\theta}(U\frac{\partial U}{\partial \lambda} + V\cos\theta\frac{\partial U}{\partial \theta}) + fV - \frac{1}{a}\frac{\partial \phi}{\partial \lambda}, \quad (4)$$

$$\frac{\partial V}{\partial t} = -\frac{1}{a\cos^2\theta}[U\frac{\partial V}{\partial \lambda} + V\cos\theta\frac{\partial V}{\partial \theta} + \sin\theta(U^2+V^2)] - fU - \frac{\cos\theta}{a}\frac{\partial \phi}{\partial \theta}, \quad (5)$$

$$\frac{\partial \phi}{\partial t} = -\phi\delta - \frac{1}{a\cos^2\theta}(U\frac{\partial \phi}{\partial \lambda} + V\cos\theta\frac{\partial \phi}{\partial \theta}). \quad (6)$$

H. Ritchie, Application of the semi-Lagrangian method to a spectral model of the shallow water equations. *Mon. Wea. Rev.*, **116**(1988) pp. 1587-1598.

RITCHIE'S FORMULATION
(continued)

Recall the vector harmonic analysis has the form

$$b_{m,n} = [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{B}_{m,n})^*\mathbf{v}\cos\theta d\theta d\lambda \qquad (7)$$

$$c_{m,n} = [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{C}_{m,n})^*\mathbf{v}\cos\theta d\theta d\lambda\ . \qquad (8)$$

In terms of Robert's variables $\mathbf{V} = (U, V)$

$$b_{m,n} = [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{B}_{m,n})^*\mathbf{V} d\theta d\lambda \qquad (9)$$

$$c_{m,n} = [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}]\int_0^{2\pi}\int_{-\pi/2}^{\pi/2}(\mathbf{C}_{m,n})^*\mathbf{V} d\theta d\lambda\ . \qquad (10)$$

Vorticity and divergence in terms of U and V are given by

$$\zeta = \frac{1}{a\cos^2\theta}(\frac{\partial V}{\partial\lambda} - \cos\theta\frac{\partial U}{\partial\theta}) \qquad (11)$$

$$\delta = \frac{1}{a\cos^2\theta}(\cos\theta\frac{\partial V}{\partial\theta} + \frac{\partial U}{\partial\lambda})\ . \qquad (12)$$

RITCHIE'S FORMULATION
(continued)

Temperton (1991) gives the following procedure.

1. Compute the longitudinal derivatives of U, V and ϕ by the formal differentiation of their Fourier representation in the longitudinal direction.

2. With its Fourier representation, proceed to compute the scalar harmonic representation of ϕ and differentiate to compute $\partial\phi/\partial\theta$.

3. Analyze U and V by computing the coefficients $b_{m,n}$, and $c_{m,n}$ using a variant of the vector harmonic analysis. Then immediately resynthesize U, V, and ϕ with truncated spectral coefficients.

4. Use $b_{m,n}$ and $c_{m,n}$ to compute vorticity and divergence with scalar backward transforms. Finally compute $\cos\theta\partial U/\partial\theta$ and $\cos\theta\partial V/\partial\theta$ by "backward" application of the formulas for vorticity and divergence.

Following these steps, the time derivatives are computed from the spatial derivatives and the solution is advanced to the next time level.

Clive Temperton, On scalar and vector transform methods for global spectral models, *Mon. Wea. Rev.* **119**(1991) pp.1303-1307.

THE VORTICITY AND DIVERGENCE FORMULATION OF THE SWE

This formulation also uses the U, V variables. The equations are rewritten with the prognostic variables of vorticity and divergence. Most of the individual terms are unbounded in the neighborhood of the poles. The model is posed on Gauss distributed latitudinal points.

$$\frac{\partial \zeta}{\partial t} = -\frac{1}{a \cos^2 \theta}\{\frac{\partial}{\partial \lambda}[(\zeta + f)U] + \cos\theta \frac{\partial}{\partial \theta}[(\zeta + f)V]\} \ , \qquad (13)$$

$$\frac{\partial \delta}{\partial t} = \frac{1}{a \cos^2 \theta}\{\frac{\partial}{\partial \lambda}[(\zeta+f)V] - \cos\theta \frac{\partial}{\partial \theta}[(\zeta+f)U]\} - \nabla^2[\phi + \frac{(U^2+V^2)}{2\cos^2\theta}] \qquad (14)$$

$$\frac{\partial \phi}{\partial t} = -\frac{1}{a \cos^2 \theta}[\frac{\partial(\phi U)}{\partial \lambda} + \cos\theta \frac{\partial(\phi V)}{\partial \theta}] \qquad (15)$$

Although greatly simplified here, this formulation is at the dynamical core of the NCAR weather/climate model.

Hack, J.J. and R. Jakob, 1992: Description of a global shallow water model based on the spectral transform method. NCAR/TN-343+STR, National Center for Atmospheric Research, Boulder, CO 80307, 39p.

THE VORTICITY AND DIVERGENCE FORMULATION OF THE SWE

(continued)

A time step begins with vorticity, divergence, and geopotential specified at some time level.

1. Analyze the vorticity ζ and divergence δ and truncate the resulting spectral coefficients to $2N/3$ modes.

2. Divide the spectral coefficients of ζ by $\sqrt{n(n+1)}$ and the coefficients of δ by $-\sqrt{n(n+1)}$ to obtain the vector harmonic analysis and synthesize U, V using a variant of the vector harmonic synthesis multiplied by $\cos\theta$.

3. Analyze the vector $\mathbf{g}^{\mathrm{T}} = [(\zeta+f)V, -(\zeta+f)U]$ and truncate the resulting coefficients to $2N/3$ modes. Compute the divergence and vorticity of $\mathbf{g}$, which provides the first terms on the right side of the vorticity and divergence equations.

4. Analyze the vector $\mathbf{h}^{\mathrm{T}} = (\phi U, \phi V)$ and truncate the coefficients to $2N/3$ modes. Compute the divergence of $\mathbf{h}$, which provides the right side of the geopotential equation.

5. Analyze $\phi + \frac{1}{2}(U^2 + V^2)/\cos^2\theta$ and truncate to $2N/3$ modes and multiply by $-n(n+1)$. The Laplacian is then obtained from a scalar synthesis.

Following these steps, the spatial derivatives are substituted into the right side of the SWE and the resulting time derivatives are used to advance the solution to the next time level.

VECTOR HARMONIC SPECTRAL TRANSFORM METHOD

1. Rewrite the differential equations in terms of bounded differential expressions.

2. Analyze all vector and scalar functions to obtain their spectral representations.

3. Evaluate the bounded differential expressions as applied to the spectral representations.

4. Evaluate the time derivatives from the bounded differential expressions.

5. Use (say) ”leapfrog” to integrate in time.

Swarztrauber, P. N., The Vector Harmonic Transform Method for Solving Partial Differential Equations in Spherical Geometry, *Mon. Wea. Rev.*, **121**(1993), pp. 3415-3437

SHALLOW WATER EQUATIONS WITH BOUNDED TERMS

Given vorticity and divergence

$$\zeta = \frac{1}{a\cos\theta}[\frac{\partial v}{\partial\lambda} - \frac{\partial}{\partial\theta}(\cos\theta u)] \, . \tag{16}$$

$$\delta = \frac{1}{a\cos\theta}[\frac{\partial u}{\partial\lambda} + \frac{\partial}{\partial\theta}(\cos\theta v)] \, , \tag{17}$$

the SWE can be written

$$\frac{\partial u}{\partial t} = -u\delta - \frac{v}{a}\frac{\partial u}{\partial\theta} + \frac{u}{a}\frac{\partial v}{\partial\theta} + fv - \frac{1}{a\cos\theta}\frac{\partial\phi}{\partial\lambda} \, , \tag{18}$$

$$\frac{\partial v}{\partial t} = -u\zeta - \frac{u}{a}\frac{\partial u}{\partial\theta} - \frac{v}{a}\frac{\partial v}{\partial\theta} - fu - \frac{1}{a}\frac{\partial\phi}{\partial\theta} \, , \tag{19}$$

$$\frac{\partial\phi}{\partial t} = -\phi\delta - \frac{u}{a\cos\theta}\frac{\partial\phi}{\partial\lambda} - \frac{v}{a}\frac{\partial\phi}{\partial\theta} \tag{20}$$

VECTOR HARMONIC SPECTRAL TRANSFORM METHOD FOR THE SWE

These equations are integrated numerically using the steps given below. The subroutines are readily accessible from `spherepack`.

1. Compute the coefficients in the scalar spectral representation of ϕ using subroutine `shags`.
2. Use these coefficients to compute the gradient $(\frac{1}{a\cos\theta}\frac{\partial\phi}{\partial\lambda}, \frac{\partial\phi}{\partial\theta})$ using the method outlined earlier, which is implemented in subroutine `gradgs`.
3. Compute the coefficients in the vector spectral representation of u, v using subroutine `vhags`.
4. Use these coefficients to compute the vorticity ζ and divergence δ using subroutine `divgs` and `vrtgs`.
5. Compute the derivative with respect to θ of u and v using subroutine `vtsgs`.

Following these steps, the spatial derivatives are substituted into the right side of the SWE and the resulting time derivatives are used to advance the solution to the next time level. Leap frog time differencing is used for the computational experiments reported in:

"Shallow water flow on the sphere", submitted to the *Mon. Wea. Rev.*.

ATTRIBUTES OF THE VECTOR TRANSFORM METHOD

1. Vector functions are transformed directly without introducing scalar functions.

2. The differential equation is rewritten in terms of bounded differential expressions without raising the order of the equations.

3. The method can be implemented on either a Gauss or equally spaced grid with a point at the pole since there are no divisions by $\cos\theta$

4. Strictly divergent (or rotational) fluids can be modeled with half the computing resource and remain strictly divergent or rotational.

5. The mean vorticity and divergence remain identically zero.

6. The method is accurate and stable without the traditional time and space filters or 2/3rds truncation.

SW FLOW INDUCED BY GEOPOTENTIAL HIGH ON STATIONARY SPHERE

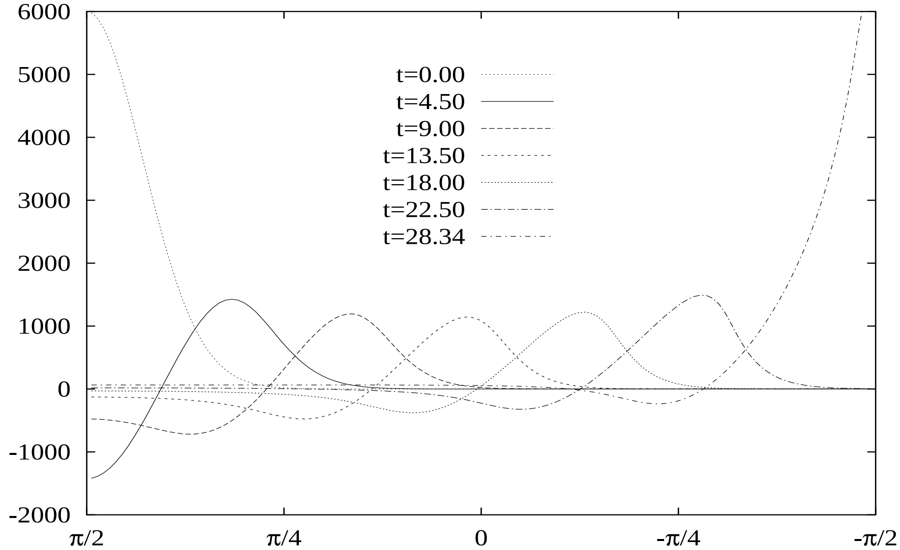


Figure 1: Left to right: Geopotential ϕ from $t = 0.0$ to $t = 28.34$ hours

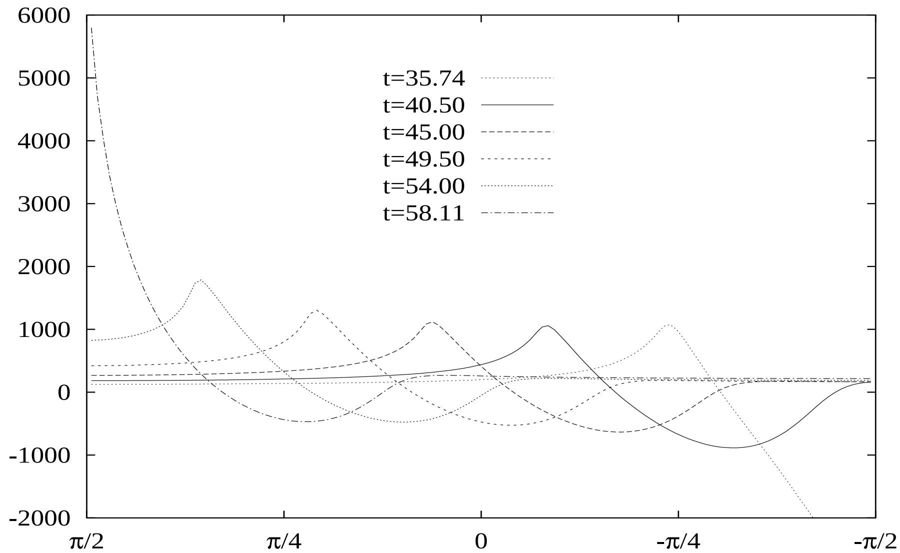


Figure 2: Right to left: Geopotential ϕ from $t = 35.74$ to $t = 58.11$ hours

SW FLOW INDUCED BY GEOPOTENTIAL HIGH ON STATIONARY SPHERE
(continued)

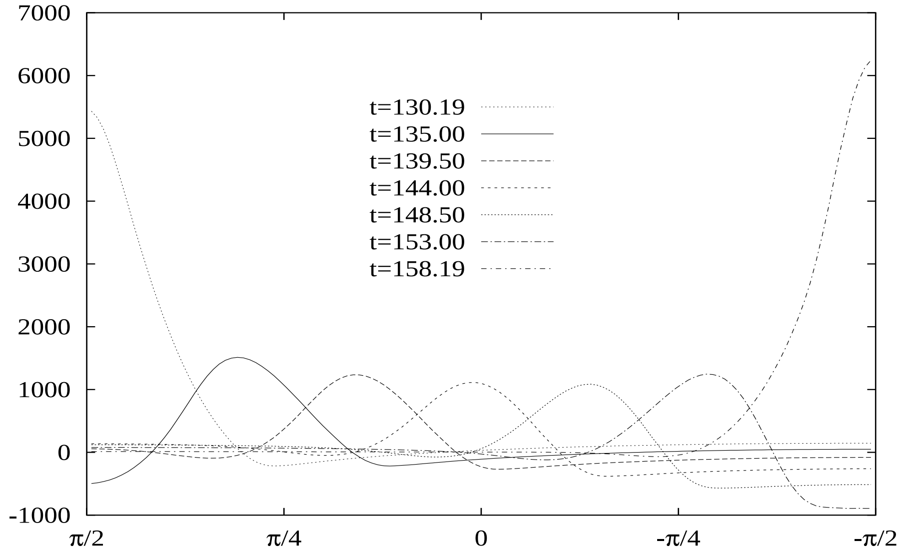


Figure 3: Left to right: Geopotential ϕ from $t = 130.19$, to $t = 158.19$ hours

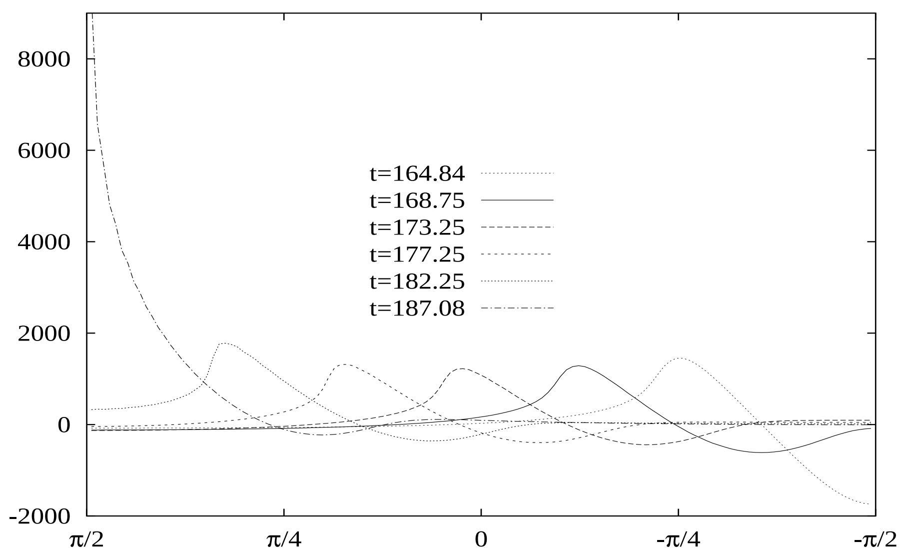


Figure 4: Right to Left: Geopotential ϕ from $t = 164.84$, to $t = 187.08$ hours

SW FLOW INDUCED BY GEOPOTENTIAL HIGH ON STATIONARY SPHERE

(continued)

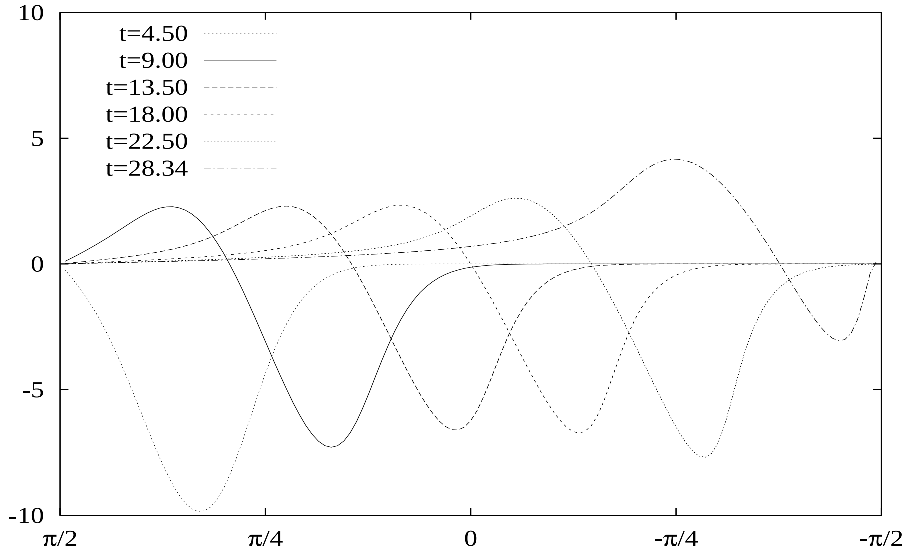


Figure 5: Left to right: Velocity v from $t = 4.50$, to $t = 28.34$ hours

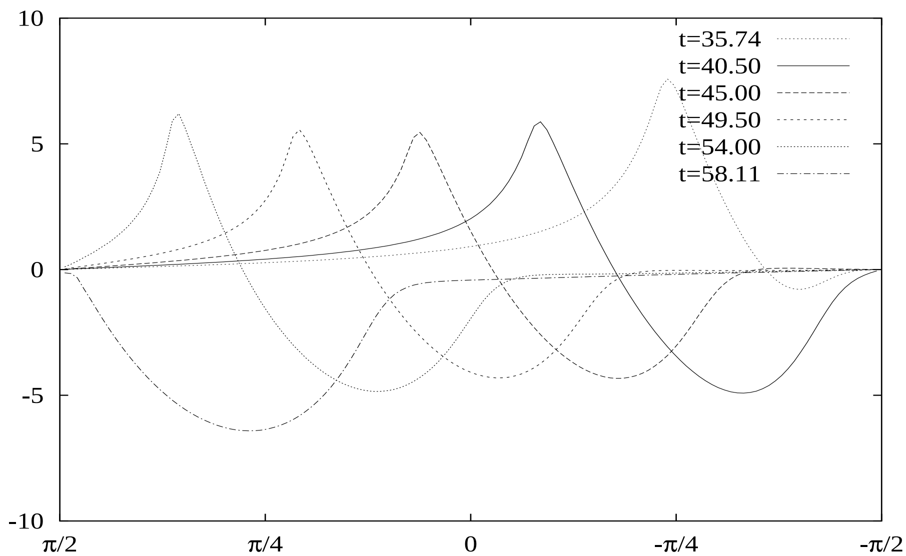


Figure 6: Right to Left: Velocity v from $t = 35.74$, to $t = 58.11$ hours

SW FLOW INDUCED BY GEOPOTENTIAL HIGH ON STATIONARY SPHERE

(continued)

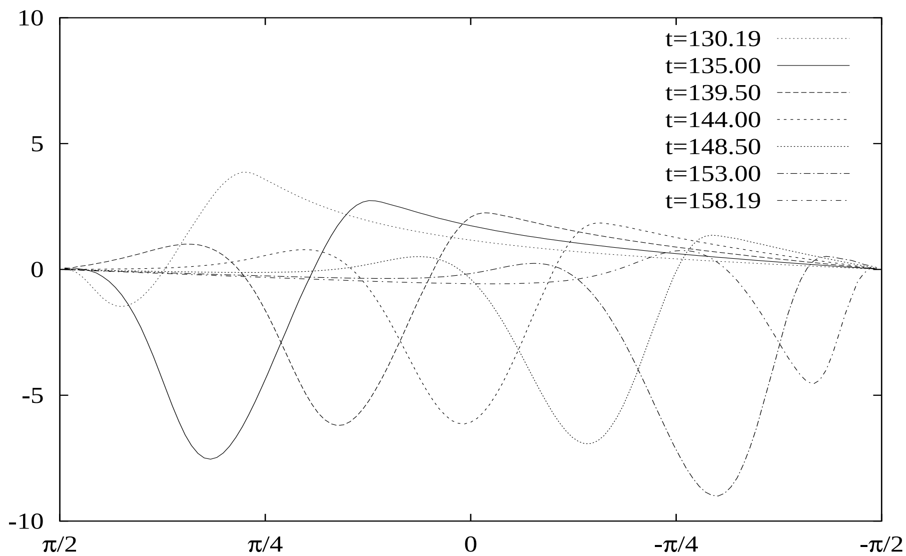


Figure 7: Left to right: Velocity v from $t = 130.19$, to $t = 158.19$ hours

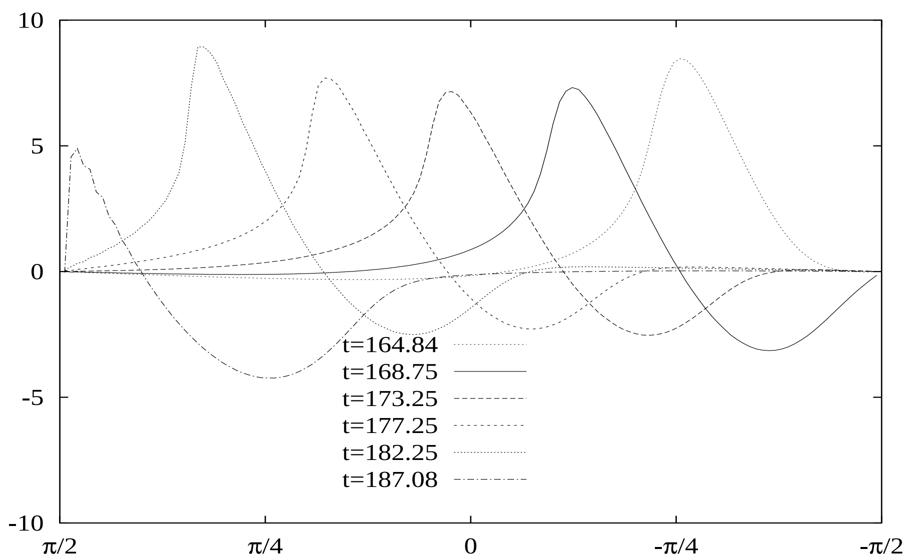


Figure 8: Right to Left: Velocity v from $t = 164.84$, to $t = 187.08$ hours

SW FLOW INDUCED BY VORTEX MOUND ON STATIONARY SPHERE

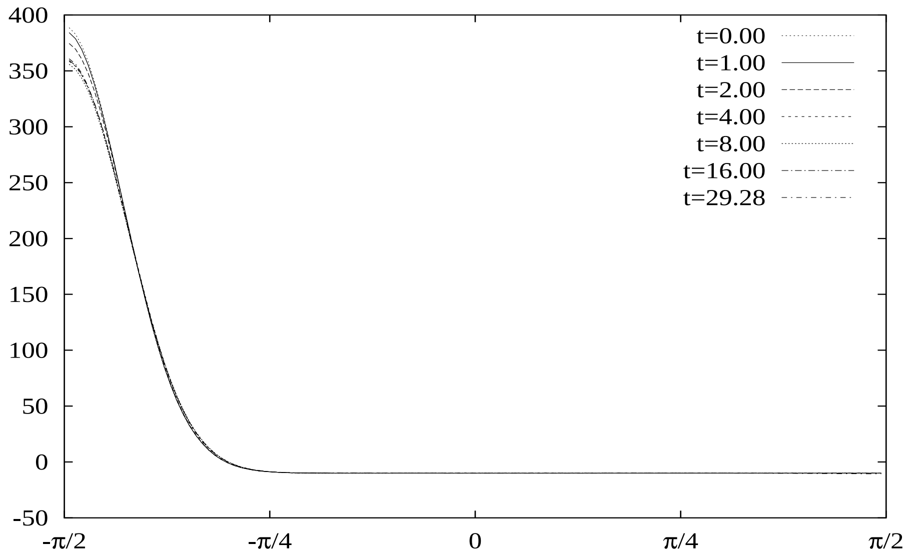


Figure 9: Vorticity ζ from $t = 0$ to $t = 29.28$ hours

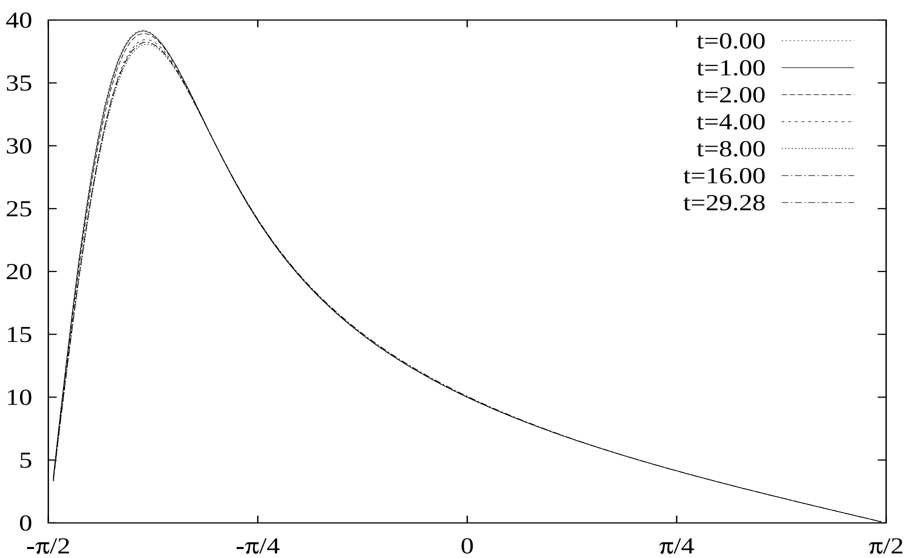


Figure 10: Longitudinal velocity u from $t = 0$ to $t = 29.28$ hours

SW FLOW INDUCED BY GEOPOTENTIAL HIGH ON A ROTATING SPHERE

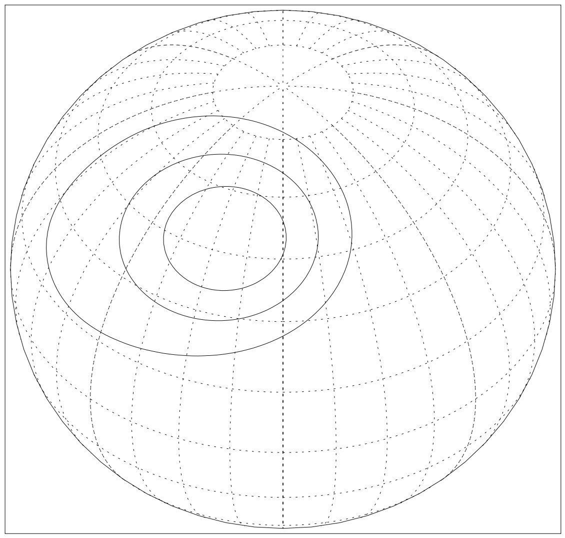


Figure 11: Geopotential ϕ at $t = 28.34$, viewed from $\lambda = 0$ and $\theta = \pi/4$.

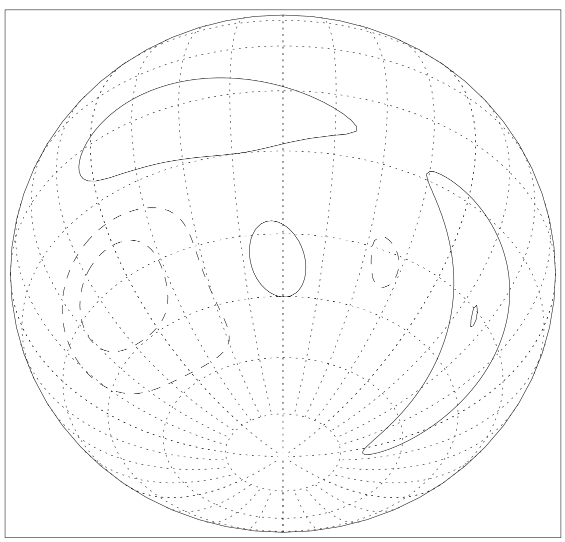


Figure 12: Geopotential ϕ at $t = 28.34$, viewed from $\lambda = \pi$ and $\theta = -\pi/4$.

SW FLOW INDUCED BY GEOPOTENTIAL LOW ON A ROTATING SPHERE

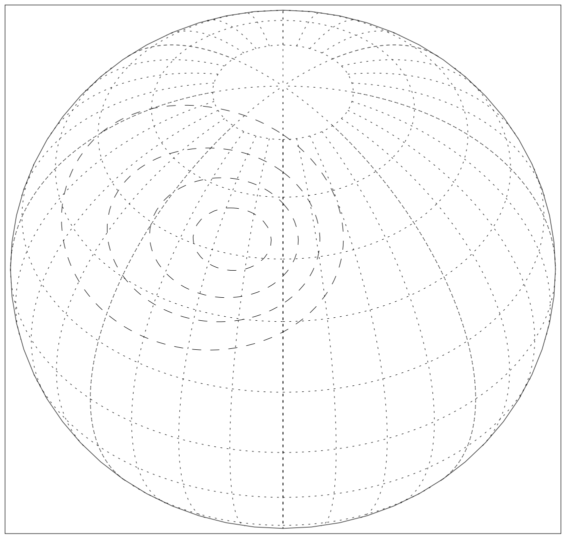


Figure 13: Geopotential ϕ at $t = 34.17$, viewed from $\lambda = 0$ and $\theta = \pi/4$.

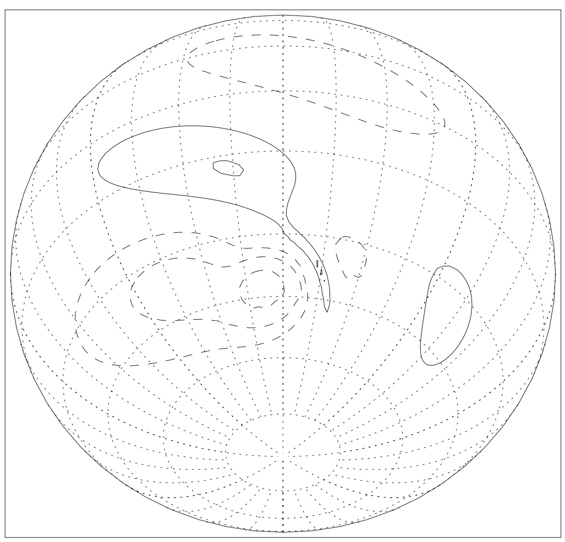


Figure 14: Geopotential ϕ at $t = 34.17$, viewed from $\lambda = \pi$ and $\theta = -\pi/4$.

SHALLOW WATER FLOW ON THE SPHERE: A SUMMARY

- Model development is facilitated by SPHEREPACK, which provides the programs for computing vector harmonic analysis, synthesis, divergence, vorticity, geopotential gradient, and the latitudinal derivatives of the velocity field.
- Leapfrog explicit integration is initialized with an implicit first time step that is computed using fixed point iteration.
- A Gaussian vortex remains almost stationary on a nonrotating sphere.
- The computations are quite stable without the traditional methods of smoothing including diffusion, 2/3rds rule, space or time filtering.
- Mass and energy are conserved to 6 decimal digits through an integration time of about 7 days. Computations were performed in 64 bit arithmetic.

SHALLOW WATER FLOW ON THE SPHERE: A SUMMARY
(continued)

- The quadratic error associated with the leapfrog time differencing dominated the spectral error and consequently convergence of mass and energy was quadratic.
- However convergence in the maximum norm is slower, which is symptomatic of nonuniform convergence due to the presence of singular or near singular solutions.
- The results for the rotating sphere are quite different from the stationary sphere. Instead of refocusing at the antipole, the geopotential defracts into a relatively smooth pattern of highs and lows.
- The original geopotential high (or low) is sustained relative to the solution on a stationary sphere where it disipates.
- It is likely that singular solutions to the shallow water equations exist on a stationary sphere. It seems less likely that they exist on a rotating sphere.

SOME GENERAL THOUGHTS ON SPECTRAL TRANSFORM METHODS

The three methods that were briefly reviewed here are presented in considerable detail (with six others) in

Spectral transform methods for solving the shallow water equations on the sphere, *Mon. Wea. Rev.*, **124**(1996) pp. 730-744.

- The computations were performed in both 32- and 64-bit arithmetic. Also, the effect of truncation and resynthesis was examined.
- All nine methods were compared on a rotated zonal steady wind given as one of the test problems in
- 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**(1992) pp. 211-224.
- With resynthesis, all nine methods provide satisfactory accuracy for a five-day, steady-state, zonal flow integration of the shallow water equations. Three- and six-decimal digits are provided with T21 and T42 truncations respectively.
- Stability and accuracy depend on resynthesis as well as classical numerical stability analysis. Satisfying the CFL criteria does not in itself guarantee stability.

A FEW QUESTIONS

- Does shallow water flow on the sphere admit singular solutions?
- If so what is the nature of the singularity or singularities?
- Does shallow water flow on the sphere admit multivalued solutions?
- Is shallow water flow on the sphere chaotic?

Models to help answer these questions can be easily developed using SPHEREPACK.

A MODEL TEST BED

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

THE SEMI-LAGRANGIAN METHOD

Implementation of the Semi-Lagrangian Method in a High-Resolution Version of the ECMWF Forecast Model, Harold Ritchie, Clive Temperton, Adrian Simmons, Mariano Hortal, Terry Davies, David Dent, and Mats Hamrud, *Mon. Wea. Rev.*, **123**(1995), pp. 489-514.

MOST REFERENCES AT:

http://www.scd.ucar.edu/css/staff/pauls/papers/index.html

LECTURE NOTES AT:

http://www.scd.ucar.edu/css/whatsnew/whatsnew.htm