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Comparison of Spectral Methods for Flows on Spheres

CHA-MEI TANG

Jaycor, Alexandria, Virginia 22304

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Aliasing in pseudospectral transform calculations was reported to be insignificant for two-dimensional flow in Cartesian geometry by Fox and Orszag [*J. Computational Physics* 11 (1973), 612]. In this paper, we show that aliasing is also unimportant in spherical geometry using surface-harmonics as the spectral expansion functions. We also comment on some technical properties associated with spectral methods for the primitive variable formulation of flow in spherical geometry. To maintain stability, a special truncation procedure for the modal coefficients has to be applied every time step. The truncation procedure is generalized to three-dimensional primitive variable formulations. The use of a vector pole condition, discussed by Orszag [*Monthly Weather Rev.* **102** (1974), 56], can simplify the implementation of the truncation procedure. With correct truncation, the full spectral method is an energy conservative scheme while the pseudospectral method is not.

1. INTRODUCTION

We will present results pertaining to spectral methods for numerical calculation of two-dimensional flows on the surface of a sphere using surface-harmonics as the expansion functions. In this paper, we focus on the primitive variable formulation of the flow equations, because these equations are easily generalizable to three-dimensions.

In Sec. 2, we define the equations of motion, and describe the calculation procedures. In Sec. 3, we discuss truncation problems and vector pole conditions. For the vorticity-streamfunction formulation of two-dimensional flow, simple truncation of spectral series at every time step presents no instabilities. However, for the primitive variable formulation, Orszag [2] pointed out the existence of the vector pole conditions relating the dependent variables. These pole conditions must be maintained by the numerical scheme in order to avoid numerical instabilities.

The truncation procedures suggested by the vector pole conditions are equally applicable to pseudospectral simulations. Energy conservation properties and aliasing errors of the pseudospectral calculations will be discussed in Sec. 4. The results of accuracy and timing tests of the pseudospectral method will be presented there.

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2. Equations of Motion and the Calculation Procedures

The equations of motion for an incompressible flow field, $\mathbf{u}$, in a rotating coordinate frame are

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{u} \times (\nabla \times \mathbf{u}) - 2\mathbf{\Omega} \times \mathbf{u} - \nabla P + \nu \nabla^2 \mathbf{u} \tag{1}$$

and

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

where Ω is the rate of angular rotation, ν is kinematic viscosity and P is the pressure head. For two-dimensional flow on the surface of a sphere, $\mathbf{u} = u_\theta(\theta, \phi)\, \hat{\imath}_\theta + u_\phi (\theta, \phi)\, \hat{\imath}_\phi$, where the angles θ and ϕ refer to latitude and longitude respectively. The flow field can also be described by the vorticity, $\zeta \hat{\imath}_r = (\nabla_{\theta,\phi} \times \mathbf{u})$, and streamfunction, ψ. The velocity field is expressible as $\nabla_{\theta,\phi} \times (-\psi \hat{\imath}_r)$.

The variables ζ, ψ and P are scalar variables, meaning that their values are independent of the coordinate frame. Scalars, such as ψ, are expanded as

$$\psi(\theta, \phi) = \sum_{|m|=0}^{N} \sum_{n=|m|}^{N} \psi_{nm} Y_n^m(\theta, \phi), \tag{3}$$

where Y_n^m is the surface-harmonic of degree n and order m. The surface harmonic Y_n^m is defined in terms of the associated Legendre polynomial, $P_n^m(\cos\theta)$, as

$$Y_n^m(\theta, \phi) = b_{nm} P_n^m(\cos\theta)\, e^{im\phi} \tag{4}$$

where $b_{nm} = [(2n + 1)(n - m)!]^{1/2}\, [4\pi(n + m)!]^{-1/2}$.

The vector components u_θ and u_ϕ change sign when the pole is crossed. They are expansible as

$$u_\theta = \frac{U}{\sin\theta} \quad \text{and} \quad u_\phi = \frac{V}{\sin\theta} \tag{5}$$

where U and V are scalars. We would like to write the equations of motion in terms of U and V. Substituting (5) into (2), the continuity equations becomes

$$-\frac{\partial U}{\partial \cos\theta} + \frac{1}{\sin^2\theta} \frac{\partial V}{\partial \phi} = 0. \tag{6}$$

Substituting (5) into (1), the momentum equations become

$$\frac{\partial U}{\partial t} = \sin^2\theta \frac{\partial P}{\partial \cos\theta} + V\zeta + 2\Omega \cos\theta V + \nu \nabla^2 U \tag{7}$$

and

$$\frac{\partial V}{\partial t} = -\frac{\partial P}{\partial \phi} - U\zeta - 2\Omega \cos\theta U + \nu[\nabla^2 V + 2\cos\theta\zeta] \tag{8}$$

where

$$\zeta = -\frac{\partial V}{\partial \cos\theta} - \frac{1}{\sin^2\theta}\frac{\partial U}{\partial \phi}.$$

Since U, V, P and ζ are scalars, they can all be expanded similar to Eq. 3 with u_{nm}, v_{nm}, p_{nm}, and ζ_{nm} as the coefficients of expansion respectively.

Transform methods to efficiently implement spectral methods for streamfunction formulation of the equations of motion are discussed by Orszag [2]. For the primitive variable equations, the transform method is nearly the same. U, V and ζ are obtained at the grid points, (θ_j, ϕ_k), from the coefficients of surface harmonics, u_{nm}, v_{nm} and ζ_{nm} respectively, using Legendre transform in θ and Fourier transform in ϕ. Let

$$U' = V\zeta + 2\Omega\cos\theta\zeta, \tag{9}$$

and

$$V' = -U\zeta - 2\Omega\cos\theta\zeta. \tag{10}$$

U' and V' are transformed into modal using Gaussian quadrature in θ and Fourier transform in ϕ. The pressure, P, conteracts any divergent flow produced by the convective and rotational terms. The calculation of P uses this fact. Substituting U' into (7) and V' into (8), ignoring the dissipative terms, and taking the divergence of the resultant equations, we get

$$\nabla^2 P = \frac{-\partial U'}{\partial \cos\theta} + \frac{1}{\sin^2\theta}\frac{\partial V'}{\partial \phi} \tag{11}$$

The solution of P in terms of surface harmonic coefficients, p_{nm}, can be solved. P is then substituted into (7) and (8). The equivalent forms of Eqs. (7) and (8), in terms of the surface harmonic coefficients with leapfrog time differencing as an example, are

$$\frac{u_{nm}^{t+\Delta t} - u_{nm}^{t-\Delta t}}{2\,\Delta t} = u'_{nm} + (n+2)(n+m+1)(2n+3)^{-1} p_{n+1,m} + (n-m)(1-n)(2n-1)^{-1} p_{n-1,m} - \nu n(+1)\, u_{nm}^{t} \tag{12}$$

$$\frac{v_{nm}^{t+\Delta t} - v_{nm}^{t-\Delta t}}{2\,\Delta t} = v'_{nm} - imp_{nm} - \nu n(n+1)\, v_{nm}^{t} + 2\nu\left[\frac{n-m}{2n+1}\zeta_{n-1,m}^{t} + \frac{n+m+1}{2n+3}\zeta_{n+1,m}^{t}\right], \tag{13a}$$

or

$$v_{nm}^{t+\Delta t} = \frac{1}{im}\left[B_{np}(n-1)\, u_{n-1,m}^{t+\Delta t} + B_{nm}(n+1)\, u_{n+1,m}^{t+\Delta t}\right], \tag{13b}$$

where

$$B_{np}(n) = -n(n-m+1)(2n+1)^{-1} \text{ and } B_{nm}(n) = (n+1)(n+m)(2n+1)^{-1}.$$

[The results, presented in Sec. 4, actually used the 3-cycle method of Lorentz [3].]

To summarize, the calculation procedure follows the steps outlined from Eqs. (9) to (13), along with the simplifying identity that $\zeta_{nm} = -in(n+1)\, m^{-1}\, u_{nm}$, which is obtained using $u = -(\partial\psi/\partial\phi)$ and $\zeta = \nabla^2\psi$. The integration for one time step is complete except for spectral truncation and the application of pole conditions.

3. Truncation and Pole Conditions

For a full spectral simulation of the vorticity-streamfunction equations, the modes to be retained are those with $|m| \leqslant n \leqslant N$. For the primitive variable formulation, setting $u_{nm} = v_{nm} = 0$ for $n > N$ and $m > N$ will lead to incorrect results because the condition $\nabla \cdot \mathbf{u} = 0$ is violated. The correct procedure is to set

$$\begin{aligned} u_{Nm} &= 0 \\ v_{N-1,m} &= -iB_{np}(N-2)\, m^{-1}\, u_{N-2,m} \\ v_{Nm} &= -iB_{np}(N-1)\, m^{-1}\, u_{N-1,m} \end{aligned} \tag{14a-c}$$

Note that the even (odd) n modes of u_{nm} are coupled to the odd (even) n modes of v_{nm}. This is true for all flows in spherical geometry. The details of the derivation of the relationship at the pole,

$$u_\theta{}^m \sim -i\, \mathrm{sign}(m) \cos\theta u_\phi{}^m \text{ at } \theta = 0 \text{ and } \pi \tag{15a, b}$$

is in Orszag [2]. The superscript m denotes the coefficient of mth mode of the variation in ϕ. The alternative forms of Eq. 15a, b in terms of the modal coefficients u_{nm} and v_{nm} are

$$\sum_{\substack{n=|m| \\ n \text{ even}}}^{N} u_{nm}\, g_{nm} = i \sum_{\substack{n=|m| \\ n \text{ odd}}}^{N} v_{nm}\, g_{nm} \tag{16a}$$

and

$$\sum_{\substack{n=|m| \\ n \text{ odd}}}^{N} u_{nm}\, g_{nm} = -i \sum_{\substack{n=|m| \\ n \text{ even}}}^{N} v_{nm}\, g_{nm} \tag{16b}$$

where

$$g_{nm} = b_{nm} P_n{}^m(\cos\theta) \sin^{-m}\theta 2^m m! \text{ at } \theta = 0.$$

Since a plynomial expression of $P_n{}^m(\cos\theta)$ is

$$P_n{}^m(\cos\theta) = \frac{\sin^m\theta}{2^m} \sum_{j=0}^{n-m} \frac{(n+m+j)!\,(-1)^j}{(n-m-j)!\,(m+j)!\,(j)!} \left(\frac{1-\cos\theta}{2}\right)^j \tag{17}$$

At $\theta = 0$,

$$\sin^{-m} \theta P_n^m(\cos \theta) = (n + m)! \, [2^m m!(n - m)!]^{-1} \tag{18}$$

Therefore, $g_{nm} = [(2n + 1)(n + m)!/(n - m)!]^{1/2}$. It can be shown that Eqs. (14a–c) satisfy the vector pole condition.

In three-dimensions, the velocity field can be described by a horizontally non-divergent component $\nabla_{\theta,\phi} \times (-\psi \hat{\imath}_r)$. a horizontally divergent component, $\nabla_{\theta,\phi} \alpha$, and a radial component, u_r, (Morse and Feshback [5]).

$$\mathbf{u} = u_r \hat{\imath}_r + \nabla_{\theta,\phi} \alpha + \nabla_{\theta,\phi} \times (-\psi \hat{\imath}_r) \tag{19}$$

where α, ψ and u_r are expansible as scalars. $\mathbf{u}$ automatically satisfies the vector pole condition. The use of the vector pole condition can simplify the truncation procedure.

Before truncation, the relationship between U and V are

$$\begin{aligned} u_{N-1,m} &= -im\psi_{N-1,m} - B_{np}(N-2)\,\alpha_{N-2,m} + \hat{u}_{N-1,m} \\ u_{N,m} &= -B_{np}(N-1)\,\alpha_{N-1,m} + \hat{u}_{N,m} \\ v_{N-1,m} &= im\alpha_{N-1,m} - B_{np}(N-2)\,\psi_{N-2,m} + \hat{v}_{N-1,m} \\ v_{N,m} &= -B_{np}(N-1)\,\psi_{N-1,m} + \hat{v}_{N,m} \end{aligned} \tag{20a–d}$$

The terms with "^" are not written out in detail because those terms will be dropped. Here $\alpha_{N-1,m}$ and $\alpha_{N-2,m}$ can be obtained by the method similar to those described by Eqs. (45)–(49) in Eliasen, Machenhauer and Rasmussen [4] or by

$$\left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 u_r\right)_{n,m} = (\nabla^2 \alpha)_{nm} = -n(n+1)\,\alpha_{nm} \tag{21}$$

The remaining unknowns, $\psi_{N-1,m}$ and $\psi_{N-2,m}$ can be obtained by calculating the vorticity or simply by applying Eqs. (15a–b).

Vector pole conditions can be also applied to the truncation of the shallow water equations. The results,

$$u_{Nm} = \frac{-1}{g_{Nm}} \left[\sum_{\substack{n=|m| \\ n \text{ odd}}}^{N-1} u_{nm} g_{nm} + i \sum_{\substack{n=|m| \\ n \text{ even}}}^{N-1} v_{nm} g_{nm} \right] \tag{22a}$$

and

$$v_{Nm} = \frac{1}{g_{Nm}} \left[-\sum_{\substack{n=|m| \\ n \text{ odd}}}^{N-1} v_{nm} g_{nm} + i \sum_{\substack{n=|m| \\ n \text{ even}}}^{N-1} u_{nm} g_{nm} \right] \tag{22b}$$

for odd N, are equivalent to Eqs. (36)–(37) of Eliasen, Machenhauer and Rasmussen [4].

4. Pseudospectral Method

Orszag [2] pointed out that $4N$ grid points in ϕ and $3N/2$ grid points in θ at chosen locations are needed for full spectral simulation. The minimum requirements are $2N$ points in ϕ and N points in θ. Thus, Legendre transforms and Gaussian quadrature for the pseudospectral method should cost only 1/3 as much as that for the full spectral method. The actual cost of the complete pseudospectral simulation is about 43 % of the cost of the full spectral simulation.

The increase in computational speed is a trade off for the appearance of a small amount of aliasing errors in the pseudospectral calculations. If the nonlinear interactions of a full spectral simulation generated a term of the form, $P_r{}^m(\cos\theta)\, e^{im\phi}$ for $0 < N < r < 2N$, or $P_n{}^r(\cos\theta)\, e^{ir\phi}$ for $0 < N < r < 2N$ and $m = r - 2N$, then this term will appear as

$$\sum_{n=|m|}^{N} a_{nm} P_n{}^m(\cos\theta) e^{im\phi} \tag{23}$$

in the pseudospectral calculations.

Aliasing errors, however, do not destroy the proper relationships between U and V, except in the last two modes of n for each m, if the pressure is implemented correctly, meaning that the velocity field at the end of one time step calculation remains solenoidal. Eqs. (14a–c) should also be used to truncate U and V for the pseudospectral calculations. For a given m, the terms of the surface harmonic expansions of U and V that are dropped during truncation are denoted by $\hat{U}^m$ and $\hat{V}^m$ respectively. Their expressions are

$$\hat{U}^m = \hat{u}_{Nm} b_{Nm} P_N{}^m \tag{24a}$$

and

$$\hat{V}^m = \hat{v}_{N-1,m} b_{N-1,m} P_{N-1}^m + \hat{v}_{Nm} b_{Nm} P_N{}^m \tag{24b}$$

Let us examine the energy conservation properties associated with the truncation procedure without dissipation.

$$u_\theta^{t+\Delta t} = u_\theta{}^t + \left((u_\phi\zeta)^t + \sin\theta \frac{\partial P}{\partial \cos\theta} - \hat{u}_\theta\right) \Delta t \tag{25}$$

$$u_\phi^{t+\Delta t} = u_\phi{}^t - \left((u_\theta\zeta)^t + \frac{1}{\sin\theta}\frac{\partial P}{\partial \phi} + \hat{u}_\phi\right) \Delta t \tag{26}$$

The scheme is called energy conservative if

$$\tfrac{1}{2}\int_0^{2\pi}\int_0^{\pi} (u_\theta{}^t \hat{u}_\theta + u_\phi{}^t \hat{u}_\phi) \sin\theta \, d\theta \, d\phi = \tfrac{1}{2} \sum_{|m|=0}^{N} \sum_{n=|m|}^{N} \psi_{nm}^t \hat{\zeta}_{nm} \tag{27}$$

is zero. At the beginning of each time step, $\psi_{nm}^t = 0$ for $n \geqslant N$ and $|m| \geqslant N$ and

$$\hat{\zeta}^m = -\frac{\partial \hat{V}^m}{\partial \cos\theta} - \frac{im}{\sin^2\theta} \hat{U}^m \tag{28}$$

For pseudospectral method with $(\hat{U}^m)$ and $(\hat{V}^m)$ described by Eqs. (24a, b), $\hat{\zeta}_{nm} \neq 0$ for some $|m| \leqslant n \leqslant N$ and $|m| \leqslant N$. Therefore, pseudospectral method is not an energy conservative scheme. On the other hand, $\hat{\zeta}_{nm}$ of the full spectral method is zero for $|m| \leqslant n \leqslant N$ and $|m| \leqslant N$, and is nonzero for $n > N$ and $|m| > N$. Thus, the full spectral method is an energy conservative scheme.

We have tested the accuracy of the pseudospectral method compared to the full spectral method in evolution from identical initial conditions. The energy spectrum of the initial flow is chosen to be

$$E(n) = (n/1.5)\exp(-n/1.5) \tag{29}$$

where

$$E(n) = 1/2 \sum_{|m|=0}^{n} n(n+1)\,|\psi_{nm}|^2.$$

The details of the initial flow are generated randomly. For each (n, m) a pair of random numbers between -1 and 1 is scaled by (29) and assigned to ψ_{nm}. The errors of the

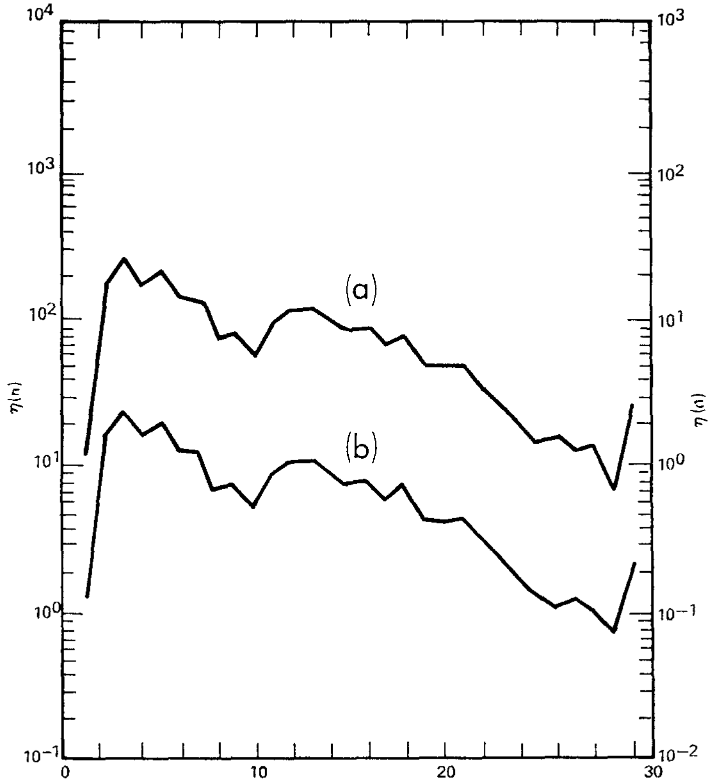

FIG. 1. Enstrophy dissipation spectra, $\eta(n)$, for (a) pseudospectral and (b) full spectral method at $t = 2.88$ for Rossby number $\epsilon = 1$, Ekman number $E = .005$ and rotation. The scales of (a) and (b) are on the right and left sides of the graph respectively.

calculations tend to show more clearly in high-order derivatives. The entropy dissipation rate, η, given by

$$\eta = 2\nu\langle|\nabla \times (\nabla \times \mathbf{u})|^2\rangle = \sum_{n=1}^{N} \eta(n) \tag{30}$$

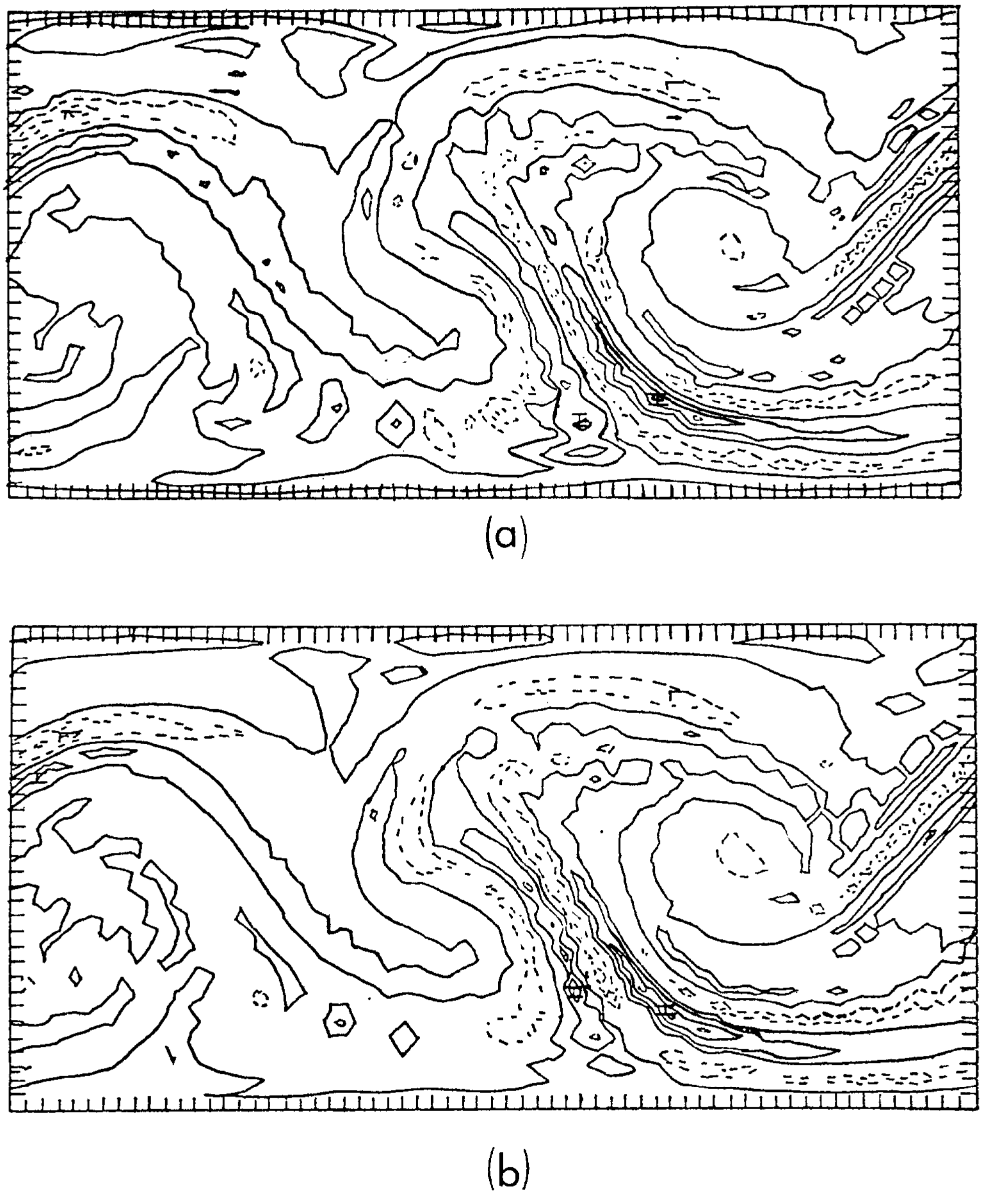

FIG. 2. (a) and (b) are the contour plots of $\nabla \times (\nabla \times \mathbf{u})$ for pseudospectral and full spectral method respectively.

where

$$\eta(n) = 2\nu n^2(n+1)^2 E(n),$$

is especially suitable for these comparisons.

Fig. 1 is the plot of $(2\nu)^{-1}\,\eta(n)$ for $\nu = .005$, $\Omega = 1$ and $N = 32$ at $t = 2.88$, when turbulence is well established. $(2\nu)^{-1}\,\eta(n)$ emphasizes the highest wave numbers. We do not notice any difference until $n = 24$. Figs. 2a, b are contour plots of $\nabla \times (\nabla \times \mathbf{u})$ at $t = 2.88$ for pseudospectral and full spectral method respectively. The differences are small. The pseudospectral method is as accurate as the full spectral method for these flows. This agrees with the results in Cartesian geometry with Fourier series expansion reported by Fox and Orzsag [1]. The results here does not imply that pseudospectral method with other types of expansions is always as accurate as the full spectral method.

4. Conclusion

We have studied the transform pseudospectral method for two-dimensional flow on the surface of a sphere. We found that the scheme is very accurate and fast despite the presence of aliasing errors and loss of energy conservation properties when using surface-harmonics as the spectral expansion function.

The appropriate truncation of modal coefficients of primitive variables for incompressible flow was discussed. The existence of the vector pole condition provide an efficient method for the implementation of the truncation procedure.

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