On estimation of truncation errors using the −3 law for kinetic energy

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ABSTRACT

The truncation errors associated with the estimation of horizontal vorticity advection on a numerical grid are evaluated using Wiin-Nielsen's (1967) kinetic energy spectrum. It is found that previous estimates made by Chouinard & Robert (1972) are too low. The possible effect of aliasing errors on the initial estimation of horizontal vorticity advection are investigated and found to be serious.

1. Introduction

One of the most important areas of activity connected with GARP has been to determine the resolution requirements of numerical models so that numerical errors may be reduced sufficiently so as to be unimportant. This activity has led to studies of the sensitivity of general circulation models to variation in resolution (Miyakoda et al., 1971; Wellck et al., 1972) as well as studies of truncation error associated with the vorticity equation (Chouinard & Robert, 1972), hereafter referred to as CR. Of particular interest is the latter study, whereby the authors derived a formula for the truncation error associated with the advection of vorticity based on statistical estimates of the values of the derivatives of the geopotential height field derived from Gandin's space autocorrelation function (Gandin, 1965). However Gandin's autocorrelation function does not properly account for short wavelengths ($\lesssim 1\,500$ km) nor is it completely consistent with a kinetic energy spectrum which follows a -3 law, which appears to be the case for the atmosphere (Wiin-Nielsen, 1967). The purpose of this study is to estimate horizontal truncation errors associated with the computation of vorticity advection using various grid sizes and computational schemes. We use the observed kinetic energy spectrum and compare these results with those in CR. Further we formulate the problem in such a way as to include the possible effects of aliasing in the definition of the state of the atmosphere and indicate the role that this effect can play in the estimation of dynamical quantities.

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2. Formulation of the problem

Consider a scalar dynamical variable ψ which is 2π periodic in longitude and which we assume has a spectrum of variance defined by $\psi(k)$ such that

$$\Psi(\lambda) = \sum_{k=-K}^{+K} \psi(k)\, e^{ik\lambda} \tag{1}$$

While K should in fact be infinitely large so that the description of Ψ be complete, we shall assume that for $|k| \geqslant K$ there is very little variance.

Suppose now we defined an *observational* grid in λ in the domain $0 \leqslant \lambda \leqslant 2\pi$ such that,

$$\lambda_n = n\frac{2\pi}{N}, \quad n = 1, 2, 3, \ldots, N \tag{2}$$

then it follows that the observations of Ψ_0 at the grid points λ_n can be expressed as

$$\Psi_0(\lambda_n) = \sum_{+L}^{l=-L} \psi_A(l)\, e^{il\lambda_n} \tag{3}$$

where

$$\psi_A(l) = \frac{1}{N} \sum_{n=1}^{N} \Psi(\lambda_n)\, e^{-il\lambda_n} \tag{4}$$

and $N = 2L + 1$. $\psi_A(l)$ is then an estimate of $\psi(l)$ which may be contaminated by aliasing if $L < K$ and is also subject to errors of various kinds (random or biases). In what follows we shall assume that there are no observational errors associated with the values $\Psi(\lambda_n)$ but there may be aliasing errors associated with the sampling of the field $\Psi(\lambda)$.

The observations $\Psi_0(\lambda_n)$ should not simply be thought of as point values drawn from the spectrum of values $\Psi(\lambda)$, but rather the values should be thought of as representative of an interval of space near the grid point. One way to represent such an average would be to define $\Psi_0(\lambda_n)$ as an average over space of the sampled variable $\Psi(\lambda)$. Therefore let us define

$$\Psi_0(\lambda_n) = \overline{\Psi(\lambda)} \tag{5}$$

where the bar indicates some sort of average over space of the "true" variable. This average may in fact be accomplished to a considerable degree by the instrument or method of observation. In any case, if $R_0(k)$ represent the response of the averaging operator, then $\psi_A(k)$ is related to $\psi(k)$ by

$$\psi_A(k) = R_0(k)\, \psi(k) + \sum_{m \neq 0} R_0(k + mN)\, \psi(k + mN) \qquad \text{for } |k| \leqslant L \tag{6}$$

where the second term represents the aliasing contribution. If the bar operator was simply an integral average of perfect observations in a neighborhood $\pm \Delta\lambda/2$ then

$$R_0(k) = \frac{\sin k\Delta\lambda/2}{k\Delta\lambda/2}$$

Once we have obtained the estimate $\psi_A(k)$ on the observational grid, we may in fact define a *computational* grid (on which we wish to compute derivatives, say) which will be considerably more dense than the observational grid. In using this computational grid we would not add any further variance to the estimated spectrum $\psi_A(k)$, but rather use the expression (3) to calculate values at the intermediate points on the computational grid.

Let us then suppose that we define a *computational* grid as

$$\lambda_s = \frac{2\pi s}{S} \qquad s = 1, 2, \ldots, S \tag{7}$$

then it follows that

$$\Psi_0(\lambda_s) = \sum_{k=-L}^{L} \psi_A(k)\, e^{ik\lambda_s} \tag{8}$$

and any further operations would be performed on the expanded set of values $\Psi_0(\lambda_s)$.

3. The advection of relative vorticity as a measure of error

In the process of forecasting the large scale flow in mid-latitudes, the quantity which is normally sampled is the geopotential height field or more or less equivalently, the stream function. In lower latitudes, this process is no longer useful, and we rather sample the wind field. Nevertheless even in low latitudes it has been found convenient to use the wind observations to define a stream function before proceeding with a forecast and therefore we shall consider that the basic variable we deal with is a stream function. Further since it was shown in CR that a large part of the difference between integrations of the barotropic vorticity equation performed on different size grids can be accounted for in terms of linear truncation error, we choose to use a linear form of the advection of relative vorticity as a gauge by which we may evaluate different size computational grids and/or finite difference schemes. We shall work in only one dimension, but this will not affect the results since we assume that the atmospheric spectrum is isotropic and further we will use a relative measure of error.

Thus we shall investigate the quantity

$$\varepsilon = \left\langle \left[(\delta_3 \lambda)_A - \frac{\partial^3 \psi}{\partial \lambda^3} \right]^2 \right\rangle \Big/ \left\langle \left(\frac{\partial^3 \psi}{\partial \lambda^3} \right)^2 \right\rangle \tag{9}$$

where $(\delta_3\psi)_A$ is the numerical approximation to $\partial^3\psi/\partial\lambda^3$ taken on a grid defined by (7) using the data defined by (8); $\partial^3\psi/\partial\lambda^3$ is obtained using the assumed atmospheric spectrum but includes only those spectral components which have meaning on the observational grid; and $\langle\ \rangle$ indicates an average over longitude. The reason for including only a limited number of spectral components in the definition of the "true" third derivative is that we wish to evaluate grids, etc. with respect to the scale of observations we have. Naturally, because we ignore the variance in scales smaller than the observations, and because there is interaction between scales we may in fact not have sufficient observational resolution to perform a useful forecast. However, that is another question.

If we now denote the response of the numerical operator δ_3 by R_3 then

$$\varepsilon = E/T \tag{10}$$

where

$$E = 2\sum_{l=1}^{L} l^6 \{\psi_A(l)\,R_3(l) - \psi(l)\}^2 \tag{11}$$

$$T = 2\sum_{l=1}^{L} l^6\,\psi(l)^2 \tag{12}$$

where $R_3(l)$ depends on the size of the computational grid, measured by S, and $\psi_A(l)$ is related to $\psi(l)$ by (6). Then in view of (6) we obtain

$$\varepsilon = \frac{\sum_{l=1}^{L} l^6\{[\psi(l)\,R_0(l) + \sum_{m\neq 0} R_0(l+mN)\,\psi(l+mN)] \times R_3(l) - \psi(l)\}^2}{\sum_{l=1}^{L} l^6\psi(l)^2} \tag{13}$$

We note that if $R_0(l)$ was a perfect low pass filter and we used a numerical operator whose response was unity, then $\varepsilon = 0$.

4. Application to large scale atmospheric flow

As our purpose is to determine the relative merits of various grid sizes and numerical operators for large scale simulations it is clear that we should interpret (13) in a statistical sense. That is, we should evaluate ε in terms of the known statistics of large scale flow. Since there may be correlations between components of the flow, then there is no unique expression for the statistical value of ε that can be derived without a knowledge of these correlations. Therefore we shall evaluate ε assuming that the components are perfectly correlated in a positive sense and thus we define an upper bound for ε. Therefore we redefine

$$\varepsilon = \frac{\sum_{l=1}^{L} l^6[\,|\psi(l)|\,|R_0(l)\,R_3(l) - 1| + \sum_{m\neq 0} |R_0(l+mN) \times R_3(l)\,\psi(l+mN)|\,]^2}{\sum_{l=1}^{L} l^7\,|\psi(l)|^2} \tag{14}$$

where the vertical bars indicate the absolute values and further we shall evaluate $|\psi(l)|$ from an estimate of the average energy spectrum of large scale atmospheric flow.

To determine $|\psi(l)|$ we use the analytical representation of Wiin-Nielsen's (1967) kinetic energy spectrum which was suggested by Leith and Kraichnan (1972), namely

$$E_1(l) = \frac{A^2\pi}{L_0^2}\,\frac{\sin\theta/2}{(l^4 + L_0^4)^{1/4}} \tag{15}$$

where $\theta = \tan^{-1}(L_0/l)^2$, $A = 0.863$ day^{-1} and $L_0 = 7.1$ rad^{-1} (1 rad = 4 810 km). When distance is measured in these units, the possible values of l are integers corresponding to the number of waves around a latitude circle at 40° N. Further, since we may show that

$$2l^2\,|\psi(l)|^2 = \int_{l-1/2}^{l+1/2} E_1(l)\,dl \tag{16}$$

then it follows that

$$|\psi(l)| = \frac{1}{l}\left[\frac{E_1(l)}{2}\right]^{1/2} \tag{17}$$

where $\psi(l)$ is measured in units of rad^2 day^{-1}.

The spectrum as defined by (15) approximates a -3 power law as l becomes large compared to L_0. It is not clear from observations or theory just how far down the spectrum this -3 law should apply. We shall assume for this study that it applies down to $l=200$ which corresponds to a limiting wavelength of approximately 150 km.

There are a couple of choices to be made before we can proceed to calculate ε for different computational grids, etc., namely what scale should we choose for an observational grid, and what assumptions should we make as to the sort of filtering that has been applied to the raw data. The first choice is relevant because of the nature of the atmospheric spectrum. Since the kinetic energy is roughly distributed within the -3 power law, the largest contributions to vorticity advection come from the smallest scales. The second choice is important because aliasing can significantly contaminate the results unless we have good observational filtering.

5. Estimation of horizontal truncation errors

If we consider that we have a perfect low pass observational filter, then R_0 will be zero for wavelengths shorter than that defined by the observational grid and R_0 will be unity for those wavelengths defined on the observational grid. In this case then we are simply estimating truncation errors associated with approximating derivatives on a computational grid in analogy with CR. For this purpose we choose to study two observational grid sizes $N=61$ and $N=121$ corresponding to grid lengths of 495 km and 250 km at 40° N respectively. These grid lengths correspond roughly to the scale of observations anticipated for the First GARP Global Experiment. The results are presented in Figs. 1 and 2 where we have plotted the square root of ε expressed as a percentage (corresponding to the rms error in the computation of vorticity advection) versus the number of computational grid points we use to estimate vorticity advection. We have performed the calculation using a second-order scheme and a fourth-order scheme. For comparison we have also plotted the results obtained in CR. We note that for both observational resolutions, our curves are higher than those of CR but exhibit the -2 and -4 power dependence for second and fourth order finite difference schemes at the higher resolutions. The reason our curves are higher than those of CR is because

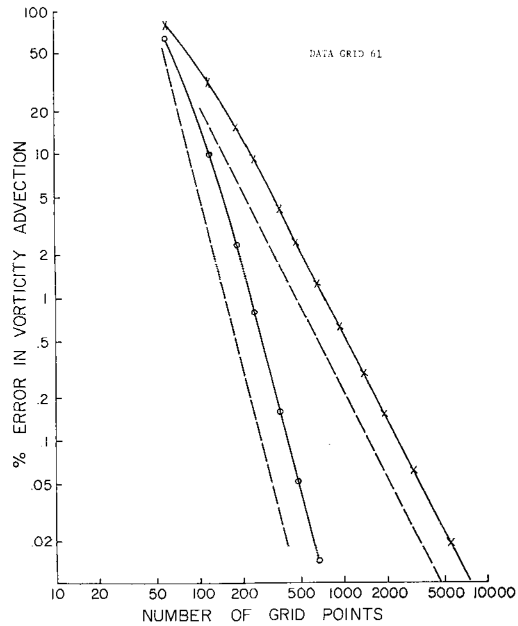

Fig. 1. The relative error in estimating the advection of relative vorticity on a data grid of 61 points as a function of the number of grid points used for the computation. The grid points are assumed to be equally-spaced on a latitude circle at 40° N. The solid lines are estimates made using Wiin-Nielsen's energy spectrum; with the 4th order scheme marked by open circles, the 2nd order is marked by crosses. The corresponding estimates given by Chouinard & Robert are given as dashed lines which are parallel but below the estimates made here.

we have considered higher resolutions in the observational grid. In fact we find that the curves of CR correspond to an observational grid of approximately 41 points in our terminology.

Because the main contribution to the error in vorticity advection comes from a small number of wavelengths (those that are the smallest on the observational grid) then we find that if we scale the computation grid in terms of the observational grid, then the variation of error with grid size is approximately independent of observational grid size. These curves are shown in Fig. 3 for the second and fourth order scheme.

We note that from these curves that if we wish to reduce the errors in vorticity advection to less than 1% we should use about 4 times as many grids on the computation grid as the observational grid using a fourth order scheme,

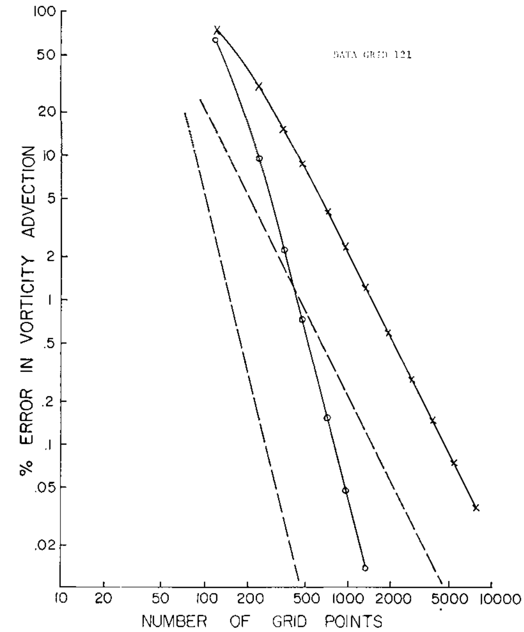

Fig. 2. Same as Fig. 1 except for a data grid of 121 points.

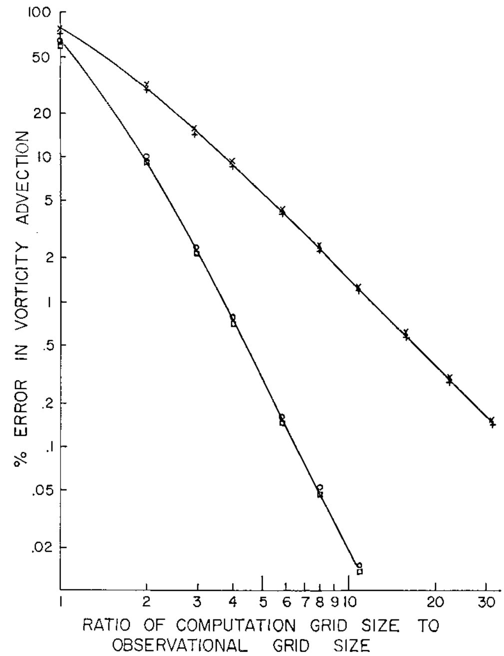

Fig. 3. The relative error in estimating the advection of relative vorticity as function of the ratio of computation grid size to observational grid size. (×, + corresponds to 2nd order for data grid 61, 121 respectively; ○, □ to 4th order for data grid 61, 121.)

and about 12 times for a second order scheme. If we use 2 times as many computational grid points as observational grid points (as is suggested by Smagorinsky & Bretherton, 1973) then we expect that the errors in vorticity advection will be about 10% using a fourth order scheme and 40% using a second order scheme.

From all these curves we note that the estimates of truncation follows power laws for higher computational resolutions. Further, the higher the observational grid resolution, the more the curves shift to higher computational grid resolution. Then if we wish to express the relative error in the estimation of vorticity advection by formulae of the following type

$$E_2 = C_2(\Delta x)^2 \tag{18}$$

$$E_4 = C_4(\Delta x)^4 \tag{19}$$

for second and fourth order schemes, then C_2 and C_4 will depend on the observational resolution. In Figs. 4 and 5 we present computations of the constant C_2 and C_4 for a range of observational grid sizes from 1 000 to 100 km. We note that the values quoted in CR correspond roughly to an observational grid of 800 km. As might be anticipated from the normalized curves given in Fig. 3, these curves have slopes of $+2$ and $+4$ for second and fourth order schemes respectively. Thus we are led to construct a more general formula than given by (18) and (19) where we take into account the observational grid size as well. Thus,

$$E_2 = A_2\left(\frac{\Delta x_c}{\Delta x_0}\right)^2 \tag{20}$$

$$E_4 = A_4\left(\frac{\Delta x_c}{\Delta x_0}\right)^4 \tag{21}$$

where Δx_c is the computational grid size, Δx_0 is the observational grid size and $A_2 = 147$, $A_4 = 200$, and E_2, E_4 are the percentage error in the computation of vorticity advection. The above formulae represent the computations shown in Figs. 1 to 5 to within about 5% as long as $\Delta x_c/\Delta x_0 < 0.5$, but are a significant overestimate when $\Delta x_c/\Delta x_0 > 0.5$.

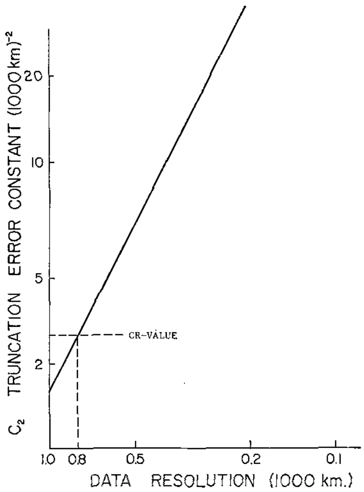

Fig. 4. The constant C_2 appearing in the asymptotic error formula for truncation error in the estimate of relative vorticity advection using a second order scheme. The dotted lines indicate value obtained by Chouinard & Robert.

6. Some effects of aliasing

In the previous section we considered only the contribution of numerical approximation to the error in the estimate of vorticity advection. In this section we present calculations which illustrate the effects of aliasing.

Firstly, let us consider a case where we assume that there is no filtering applied to the

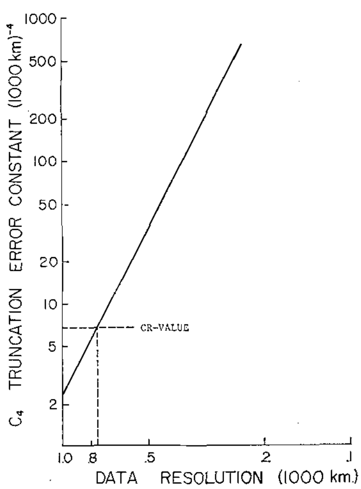

Fig. 5. Same as Fig. 4 except for C_4, fourth order.

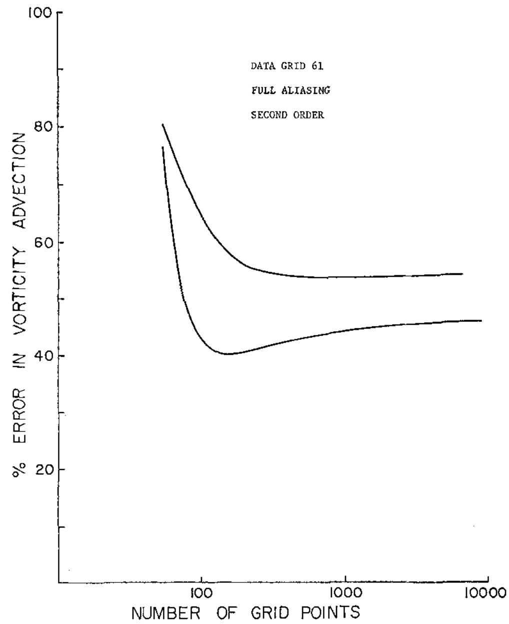

Fig. 6. The relative error in the estimation of the advection of relative vorticity on a data grid of 61 points using a second order scheme and including aliasing at full strength, as a function of the number of computational grid points. The upper curve assumes a component and its aliases are perfectly correlated, the lower corresponds to a zero correlation.

observations and therefore $R_0(l) \equiv 1$. As stated before we perform this calculation assuming that the observations are drawn from a spectrum whose kinetic energy follows a -3 law down to $l = 200$, and afterwards is zero. In Fig. 6 we present the results of this computation as a function of the number of computational grid points. The upper curve (1) corresponds to a perfect positive correlation between the principal components and its aliases, the lower curve (2) corresponds to a zero correlation. We note that these curves asymptote at high resolution to errors of approximately 54% and 45% respectively. We also note that curve 2 has a weak minimum, which indicates that it does not always pay to have a finer grid, since we may then incorporate aliasing errors at full strength. If we repeat this calculation but assume that the energy is zero when $l > 100$, the asymptotic error in the uncorrelated case is 44%, which indicates that the aliasing error is *not* dominated by aliases in the very short wavelengths.

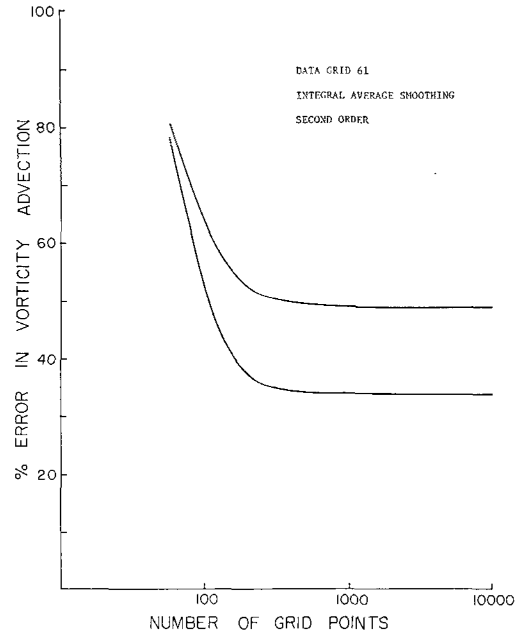

Fig. 7. Same as Fig. 6 except data are assumed to be filtered using an integral average.

These results are quite striking; but they are somewhat unrealistic since in fact an observation at a grid point is not really a point value, but should represent some sort of average value, which is representative of the area surrounding the grid point. Thus if we presume that the raw observations have been filtered by applying a space average in the neighborhood of the grid point, then

$$R_0(l) = \frac{\sin l\Delta\lambda/2}{l\Delta\lambda/2}$$

and if we repeat the calculation using this filter, we find that the asymptotic error levels have been reduced but are still in the 35–50% range (see Fig. 7).

These latter results serve to indicate that the aliasing errors are dominated by the wavelengths close to but less than the grid resolution. This fact requires that the observational filter must be much more sophisticated than that used here, and possess a much sharper cutoff, if we are to avoid these large errors in the initial evaluation of vorticity advection.

Thus far we have considered only the total, relative rms error in vorticity advection and not its distribution over the different scales.

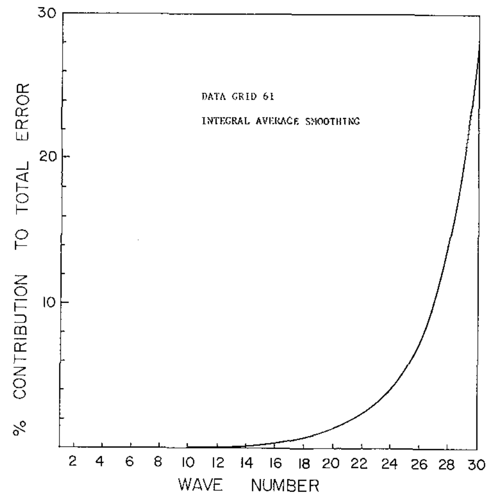

Fig. 8. The relative contribution of individual wave number components to the total error in the estimation of relative vorticity advection assuming a very high resolution computational grid. The data are assumed to be filtered according to an integral average.

In Fig. 8 we present the relative contribution of the different wavelengths to the total mean square error in vorticity advection for a very fine computational grid. As we might expect, the largest contributions came from the shortest wavelengths. This is tied into the fact that the spectrum of vorticity advection is an increasing function of wave number, presuming that the kinetic energy follows a −3 law.

7. Conclusions

The main body of this paper is devoted to a reexamination of the estimate of numerical errors associated with computation of vorticity advection, based upon the kinetic energy spectrum observed by Wiin-Nielsen (loc. cit.). It was found that Chouinard & Robert's results considerably underestimate the errors associated with different grid sizes because they used an energy spectrum (Gandin's) which does not account properly for wavelengths less than 1 500 km, because it cuts off more sharply than the −3 law.

Finally, we have performed some simple calculations which illustrate that in the initial estimation of vorticity advection, the effects of observational aliasing can be very large, and we urge further, more realistic study of the problem.

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ОЦЕНКА ОШИБОК АППРОКСИМАЦИИ С ИСПОЛЬЗОВАНИЕМ ЗАКОНА « – 3» ДЛЯ КИНЕТИЧЕСКОЙ ЭНЕРГИИ

Ошибки аппроксимации, связанные с представлением горизонтальной адвекции вихря на численной сетке, оцениваются путем использования спектра кинетической энергии Вин–Нильсена (1967). Найдено, что предыдущие оценки, проделанные Чуинардом и Робертом (1972), слишком занижены. Возможный эффект ошибки ложного взаимодействия на начальную оценку горизонтальной адвекции вихря исследован и найден весьма значительным.