A SIMPLE ATMOSPHERIC MODEL ON INFINITE DOMAINS

by

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ABSTRACT

The study of many atmospheric phenomena calls for models in which one of the spatial coordinates, for example the vertical coordinate, extends to infinity. The possibility of modeling infinite-domain systems via spectral techniques is investigated. It is found that the infinite domain can be handled under certain circumstances: most importantly, when the propagation is linear or only weakly nonlinear at large distances. A linear barotropic shallow water model on a domain with one infinite (horizontal) coordinate was formulated. The numerical simulation successfully mimics the expected behaviour.
L'étude de plusieurs phénomènes atmosphériques requiert l'usage de modèles dans lesquels une des coordonnées spatiales (par exemple la coordonnée verticale) s'étend à l'infini. La possibilité de modélisation des systèmes à domaine infini par le biais de techniques spectrales est étudiée. Nous avons trouvé que dans certaines circonstances, principalement lorsque la propagation est linéaire ou quasi-linéaire à de grandes distances, il est possible de traiter un domaine infini. Un modèle barotrope linéaire basé sur les équations de Saint Venant, dont le domaine a une coordonnée horizontale infinie, a été développé. La simulation numérique reproduit avec succès le comportement escompté.
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CHAPTER I: INTRODUCTION

1.1 The Numerical Treatment of Space Dependence in Atmospheric Models

Atmospheric models concerned with large-scale weather patterns and their motions are often global or hemispheric in areal extent. In this case, the largest horizontal length scales are on the order of $10^7$ meters. When this is compared to an often-used vertical length scale of 9 km, the scale height of an isothermal atmosphere, the tendency is to think of the domain as essentially two-dimensional. From the point of view of phenomena of meteorological interest this perception is, to some extent, justified. As a result, as numerical weather prediction (NWP) and general circulation (GCM) models have become increasingly more sophisticated, the subdivision of the vertical domain has evolved from one to something of the order of 15 points. The horizontal domain is, on the other hand, represented by many more points.

Vertical variations in the actual atmosphere are influenced by the continuous decrease in density with increasing height. There is no specified "top" to the atmosphere and the appropriate mathematical formulation evidently involves a semi-infinite domain.
The advantages of treating variations in the horizontal via the spectral method are well known: by expanding the dependent variables into sums involving coefficients dependent on time and an appropriately chosen set of orthogonal space-dependent basis functions, substituting these sums into the governing equations and then making use of the orthogonality relations, one can convert a system of partial differential equations into a set of ordinary differential equations involving the spectral coefficients (Haltiner and Williams 1980). The actual physical parameters can then be determined by a simple summation. The geometry in the horizontal, being finite, is particularly well-suited to this type of procedure. However, due to the difficulties involved and the prevailing two-dimensional view of the atmosphere such spectral methods are not usually generalized to include variations in the vertical. Spectral NWP and GCM models are only truly "spectral" in the horizontal. They use a discrete set of from one to something on the order of 15 levels to calculate derivatives in the vertical. The word "levels" can refer to levels of constant height, pressure or sigma, \( \sigma \), which is defined as the pressure divided by the surface pressure. Although the three formulations have quite different properties, they must inevitably break down since they cannot effectively model the semi-infinite domain appropriate to the problem.
1.1.1. The Upper Boundary Condition

The real-space representation of the vertical dimension requires a boundary condition to be imposed as the height, z, goes to infinity. The governing equations have solutions involving different types of wave phenomena. The mathematically appropriate upper boundary condition depends on the nature of the model. For a nonlinear system it is not well-understood. For a linear model the possibilities can be summarized as follows: a) For a time-dependent inviscid model with energy initially confined to the low levels, the energy of the wave disturbances must vanish as z goes to infinity. b) For a steady-state inviscid model the disturbances have had time to reach infinite heights. In this case one must require that the energy be propagating upwards as z goes to infinity. In the case of a model with viscosity, both the viscous term and the wave amplitude increase in importance as z gets large due to the low density. The result may be that the disturbances are completely destroyed at large heights. In the real atmosphere, the question is more complicated since continuum mechanics itself ceases to apply at the highest levels.

In a numerical, time-dependent model using height (or pressure) as the independent variable, the boundary condition described in a) above is arbitrarily replaced by
the requirement that the vertical velocity be zero at the highest level (or that the top surface, \( p = 0 \), behaves as a free surface). This is effectively equivalent to placing a lid on the atmosphere (Lindzen et al. 1968) and the model is seen to differ markedly from the physical system. As a result, wave energy incident upon the top surface is reflected back into the domain, eventually contaminating the numerical solution at even the lowest levels.

A number of numerical techniques designed to reduce or eliminate these spurious modes have been devised. They can be grouped into the three categories discussed below.

1.1.2. Previous Attempts to Remove Spurious Motions

1.1.2.1. Vertical Coordinate Transformations

In these procedures the infinite domain is simply mapped onto a finite one. The governing equations can then be expressed in terms of the new coordinate and the upper boundary condition can be applied at a finite value of the new coordinate. In meteorological models "\( \sigma \)" is often used. In this case the semi-infinite domain corresponds to \( \sigma \) varying between zero and one.

Grosch and Orszag (1976) have investigated the effect
of various algebraic and exponential mappings of infinite regions on equations of fluid-dynamical interest. They pointed out that mappings, in general, are only helpful if the solution has a simple behaviour at infinity. For the particular problem of meteorological waves propagating in the vertical this may, in fact, be true. They investigated the problem using the wave equation:

$$\frac{\partial^2 \psi(z, t)}{\partial t^2} - \gamma^2 \frac{\partial^2 \psi(z, t)}{\partial z^2} = 0$$

Numerical accuracy was maintained for a certain period of time after which reflections from large values of the coordinate, $z$, were observed to contaminate the solution. The length of time over which accuracy was maintained depended on the particular mapping used. These results are similar to what one would obtain by simply truncating the domain by assuming that the wave amplitude is zero for $z$ larger than some large finite value.

It can be seen that, although mappings may provide accurate calculations for longer periods of time than simple domain truncation, they will eventually produce non-physical results due to reflections from large values of $z$.

If the real space coordinate, $z$, is mapped onto the new coordinate, $\xi$, such that $z = 0$ corresponds to $\xi = \xi_0$.
and \( z = \infty \) corresponds to a finite \( \sigma = \sqrt{\infty} \), then the problem lies in the fact that as the mapping coordinate, \( \sigma \), approaches \( \sqrt{\infty} \), the real space resolution gets progressively poorer. This is a manifestation of the fact that the transformed governing equations are singular at \( \sqrt{\infty} \) as a consequence of the map. Eventually a propagating wave of wavelength \( \lambda \) enters a region where the resolution is such that \( \lambda \) is of the order of the grid length. This is due to the fact that for weakly non-linear solutions in uniform media, \( \lambda \) is a constant when measured in terms of the real coordinate, \( z \), but gets progressively smaller as \( \sigma \) approaches \( \sqrt{\infty} \) when measured in terms of the mapping coordinate, \( \sigma \). Stated another way, the distance \( \Delta z \) between successive levels of constant \( \sigma \) approaches infinity as \( \sigma \) approaches \( \sqrt{\infty} \). The result is that resolution of small features in the solution becomes impossible near \( \sqrt{\infty} \). The consequence must be numerical error which evidently manifests itself in terms of reflections back towards \( z = 0 \).

The height at which the reflections occur depends on the wavelength. A pulse-like feature involving many wavelengths will not maintain its shape as it propagates. It will suffer continuous partial reflections as it approaches \( \sqrt{\infty} \). In this way the shortest wavelengths will be affected first and the shape of the pulse will become increasingly distorted until all of the energy is

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propagating in the wrong direction. In this respect the numerical solution obtained through a coordinate transformation is unlike that found via a domain truncation. In the latter case, if the domain is truncated at \( z = z_c \), the pulse will be completely reflected at that point maintaining its shape.

One should note that there may be situations in which spurious reflections are not present in both truncated domain and coordinate transform models. The first possibility can be realized if there is a natural internal mechanism which reflects waves in the region \( z < z_c \). The coordinate transformation can also work if the medium is such that the wavelength increases as \( z \) gets large. In this case the singularity introduced into the governing equations by the map is a removable one. However, barring these special circumstances, the essential feature of both procedures is that they lead to reflections of energy back into the region of interest. This has been demonstrated for atmospheric pressure coordinate models using the boundary condition \( \frac{d\mathbf{p}}{dt} = 0 \) at \( p = 0 \) by Lindzen et al (1968).
1.1.2.2. Viscous Layers

Assuming an accurate numerical solution of a model is required only below some height, \( z_0 \), then one can, in principle, avoid the problem of large amplitude reflections by introducing a monotonically increasing viscosity above \( z_0 \). The result is a so-called "sponge layer" whose role is to dissipate all incoming energy. By adjusting the viscosity gradient the bulk of the energy dissipation can be confined to large heights.

The problem with this technique lies in the fact that spatial variations in viscosity can also lead to reflections. In order to minimize these reflections, the viscosity must be allowed to vary only over distances greater than a few characteristic wavelengths of the flow. This requires the computation of a set of virtually meaningless fields over a sizeable domain (all points above \( z_0 \)). The associated computational effort may be prohibitively expensive.

1.1.2.3. Radiation Boundary Conditions

Atmospheric models are usually, like the atmosphere, nonlinear. Their governing equations can be linearized in order to describe small perturbations about some basic
state solution to the nonlinear equations. The solutions
to these linearized equations may accurately describe
regions of the atmosphere which are nearly linear. If the
upper atmosphere is such a region, and if, further, it has
no spatial variation in the mean flow and is initially
devoid of disturbances, then the linear equations can be
solved. The solutions will involve both upward and
downward propagating modes. If \( z_0 \) is the lower boundary of
the linear region, then all wave solutions must be
propagating upwards at \( z_0 \), and throughout the region
\( z > z_0 \).

Typically the solutions will be dispersive waves of
the form:

\[
\psi = A(x, t) e^{i(kz - \sigma(k)t)}
\]

where \( \sigma(k) = \hat{f}(k) \pm g(k) \)

The upward propagating modes are those for which the group
velocity \( C_g(k) \) is positive. This implies upward
propagation of energy and will rule out one of the branches
of \( \sigma(k) \). Then the following approximate condition is
applied at \( z_0 \):

\[
\frac{\partial \psi(z_0, t)}{\partial t} + C_p(k) \frac{\partial \psi(z_0, t)}{\partial z} = 0
\]
where $C_p(k)$ is the phase velocity associated with the branch yielding positive group velocity.

Below $z_0$ the model behaviour is assumed to be fully nonlinear. It is therefore solved numerically on a discrete grid and the solution is subjected to the above constraint at the top of the computational domain, $z_0$. In this way it is hoped that upward travelling waves pass through $z_0$ freely while the numerical solution contains no downward propagating modes at $z_0$.

For dispersive waves it is necessary to determine the appropriate wavenumber, $k$, at which the phase velocity, $C_p(k)$, is calculated. Pearson (1974) made the assumption that the source is active only at small times and at small values of the coordinate, $z$. Since the speed of energy propagation is given by the group velocity, $C_g(k)$, then at large $z$ and $t$:

$$C_g(k) \sim \frac{z_0}{t}$$

where $z_0$ is the height of the computational domain. This equation is used to determine the relevant $k$ at which the above boundary condition is applied. Waves excited after the initial switch-on can never be treated correctly and the approximation requires $z_0$ to be large. The condition can be made valid for all frequencies and wavelengths by introducing Fourier and Laplace transforms (Bennet 1976,
Béland and Warn 1975). However, this requires the storage of the entire history of the parameter values at the computational boundary. Thus the reduction of domain size is achieved at the expense of storing the fields over many time steps.

In order for any of these procedures to be valid, one must linearize the equations about a basic state which accurately describes the physical system above the computational boundary. If this is not possible, for example if nonlinearity were important in the upper atmosphere, then the real system may well have downward propagating waves at the top of the model and the radiation boundary condition would be totally inappropriate. In this case the problem is impossible to resolve and all techniques would fail.

1.2. The Infinite Domain Spectral Representation

In principle the solution to the model equations on a semi-infinite domain can be represented via Fourier methods in wavenumber space. This may also require an infinite region in this new space. However, truncation of the wavenumber is not equivalent to truncation of the real space domain, but rather a limitation on the smallest
scales in the real space solution. An atmospheric model, so truncated, is still useful in predicting the large scale features of the flow. In this case, an infinite domain in real space can be modeled by a finite region in wavenumber space.

There are two important aspects to the representation of functions on an infinite domain in real or spectral space. They are the resolution and the size of the region over which the function (or its spectrum) differs significantly from zero. In real space, adequate resolution can be achieved with a relatively coarse grid spacing if the flow is dominated by the larger scales. However, as time increases the size of the region over which the solution differs significantly from zero increases without bound. In order to describe the function accurately, new grid points must be continuously added to the computational domain. In the spectral representation, the situation is reversed. In general, the expansion is of the form:

\[
\psi(x,t) = \sum_{k=-\infty}^{\infty} a_k(t) f_k(x) + \int_{-\infty}^{\infty} a(k,t) \tilde{f}(k,x) dk \tag{1-1}
\]

where the a's refer to spectral coefficients and the f's are basis functions. The effect of the boundary condition is to modify the nature of the spectrum. If the real-space domain is truncated, the spectrum will be discrete and
\( a(k,t) = 0 \). If the domain is infinite and the model equation coefficients are constant, then the spectrum is continuous and \( a_n(t) = 0 \). Finally, if the domain is infinite and the coefficients are variable then the spectrum will involve both contributions.

The discrete spectrum can easily be dealt with numerically. For example, this is the situation in the horizontal. The added complication due to the infinite-domain formulation is the integration over a continuous spectrum of eigenvalues:

\[
\int_{-\infty}^{\infty} a(k,t) f(k,x) \, dk.
\]

If the solutions involve wavelike phenomena, then the function \( a(k,t) \) will oscillate in time. Typically, a solution of the form:

\[ a(k,t) = a(k,0) e^{\sigma(k)t} \]

where \( a(k,0) \) is a smooth function of \( k \), can be isolated. Such a solution also oscillates in \( k \) with the "frequency" \( \frac{d\sigma(k)}{dt} \). Therefore, as time increases the size of the \( k \)-space domain, where \( a(k,t) \) differs significantly from zero, remains the same. However, the oscillations in \( k \) produce an increasingly smaller-scale structure in the function \( a(k,t) \). As a result, a finer \( k \)-spacing is
eventually required. It will also be noted that if the integrand is discretized in wavenumber space and represented by \( N \) points, ie:

\[
\int_{-\infty}^{\infty} a(k, t) f(k, x) \, dk \approx \sum_{k=1}^{N} b_k a(k, t) f(k, x)
\]

where the \( b_k \) are the weights of one of the elementary quadrature formulae, then the numerical evaluation may be similar to real space domain truncation. This is reflected by the fact that the sum appears to be composed of a set of discrete normal modes. The "phase mixing" implied by the integration is lost. This problem is discussed in more detail in section 2.1.2. It can, in fact, be avoided through the use of special quadrature schemes.

The solutions to a primitive equations atmospheric model can be divided into two groups: 1) highly nonlinear Rossby and low-frequency gravity waves called "slow modes" and 2) weakly nonlinear high-frequency gravity waves known as "fast modes". The slow modes are observed to have measurable amplitudes in the atmosphere and are therefore an important part of the model. The fast modes are often generated by the model but usually have small amplitudes in the real atmosphere.

Consider an inviscid time-dependent model with no initial disturbances above some height, \( z_o \). As time
increases, the height, \( z_s \geq z_o \), to which the slow modes have propagated increases slowly due to their small vertical group velocities. On the other hand, the height of significant fast mode activity, \( z_f \geq z_o \), increases more rapidly. As a result, the problems referred to in section 1.1.2 are encountered sooner. If the nearly linear fast modes can be described by spectral techniques on an infinite domain, then the height, \( z_c \), of the computational domain can be lowered from \( z_c > z_f \) to \( z_c > z_s \). If the slow mode behaviour is linear above a certain level, then \( z_c \) may be lowered still further. Even if this is not the case, the time for which the model forecast would remain valid would increase significantly given the same height, \( z_c \), of the computational domain.

The objective of this work is to consider whether wave propagation on a semi-infinite domain in a dispersive, multidimensional, nonlinear primitive equations atmospheric model can be effectively modeled numerically in spectral space. If this is possible only for the fast modes the length of time over which such a model remains valid could be improved.

In chapter 2 these ideas are applied to a simple non-dispersive, one-dimensional system. The properties required of the quadrature schemes are then discussed. In section 2.2 dispersion is introduced along with a
consequential generalization of the numerical techniques. The forced problem is treated in section 2.3. The spectral techniques are applied to a shallow water equations model with an infinite horizontal domain in chapter 3. Numerical experiments with a linear model and some aspects of the nonlinear model are discussed in sections 3.2.2.2 and 3.2.3 respectively. The conclusions are found in chapter 4.
CHAPTER 2 : EXPERIMENTS IN ONE DIMENSION

It is convenient to begin with by considering wave propagation on an infinite domain for a simple one-dimensional system. The numerical techniques developed will then be used to deal with the more complex multidimensional atmospheric problem.

2.1. Non-Dispersive Waves

2.1.1. The Formulation of the Problem

Consider the one-dimensional non-dispersive system:

\[
\frac{\partial^2 \phi(x,t)}{\partial t^2} - c^2 \frac{\partial^2 \phi(x,t)}{\partial x^2} = 0
\]

where \( 0 \leq x < \infty \), \( \phi(0,t) = 0 \) and \( \phi(x,t) \rightarrow 0 \) as \( x \rightarrow \infty \). The initial conditions are:

\[
\phi(x,0) = \eta(x) , \quad \frac{\partial \phi(x,0)}{\partial t} = \lambda(x)
\]

By applying a Fourier sine transform or equivalently, by separation of variables one obtains:
\[
\varphi(x, t) = \sqrt{\frac{2}{\pi}} \int_0^\infty a_1(k) \cos ck t \sin kx \, dk \\
+ \sqrt{\frac{2}{\pi}} \int_0^\infty a_2(k) \sin ck t \sin kx \, dk, \tag{2-1}
\]

where
\[
a_1(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty q(x) \sin kx \, dx \\
a_2(k) = \frac{1}{ck} \sqrt{\frac{2}{\pi}} \int_0^\infty h(x) \sin kx \, dx.
\]

2.1.2. Numerical Quadrature and Aliasing

The problem to be addressed now is the numerical evaluation of the integral (2-1). If the assumption is made that \(a_1(k)\) and \(a_2(k)\) are smooth functions of \(k\) then the integrand involves the products of two oscillating functions of \(k\) whose frequencies depend on time and \(x\). Most quadrature schemes require specifying the integrand on a uniformly distributed mesh. An accurate discrete representation in the present case would require high resolution, particularly for large \(t\) and \(x\), since then the integrand is rapidly oscillating.

In an atmospheric model one is concerned primarily with the solution close to the origin. However, \(t\) must be allowed to attain high values. If the integrand in (2-1) becomes too rapidly oscillatory for the \(k\)-space resolution, \(\Delta k\), then aliasing will occur. In this case a relatively high-frequency oscillation will be incorrectly interpreted
as having a lower frequency.

In a simple polynomial approximation quadrature scheme such as Simpson's rule or the trapezoidal rule, the integral is expressed as a linear combination of the grid point values of the integrand.

$$\int_{a}^{b} f(s) \, ds \approx \sum_{k=1}^{N} b_{k} f_{k}$$

For the integrals in (2-1) this would correspond to:

$$\hat{\varphi}(x,t) = \frac{i}{\pi} \sum_{k=1}^{N} b_{k} a_{k}(\pi \Delta k) \cos(c \pi \Delta k) \sinh(x \pi \Delta k)$$

$$+ \frac{i}{\pi} \sum_{k=1}^{N} b_{k} a_{k}(\pi \Delta k) \sin(c \pi \Delta k) \sinh(x \pi \Delta k),$$

where $\hat{\varphi}(x,t)$ represents the numerical evaluation of $\varphi(x,t)$. The frequencies being commensurate, all terms in this sum are periodic over a distance $\frac{2\pi}{\Delta k}$ and over a time period $\frac{2\pi}{c \Delta k}$. Therefore the numerical solution $\hat{\varphi}(x,t)$ will be periodic in both space and time. If a pulse of wave energy is propagating outwards from small $x$ at $t = 0$, it will eventually "bounce off" of the periodic extension of the boundary condition at $x = 0$. Since $\varphi(x,t)$ is described by a sine transform, both $\varphi(x,t)$ and $\hat{\varphi}(x,t)$ are asymmetric about the origin. Therefore on the way back to the origin, the pulse will be displaced toward the other side of the line $\varphi(x,t) = 0$. Such reflections will occur
ad infinitum. In this respect the behaviour is qualitatively similar to the case where the domain has simply been truncated in real space and the spectral formulation is of no advantage whatsoever. It is true that the length over which the numerical solution is periodic can be increased by increasing the resolution in $k$-space but this is no improvement over simply extending the domain in real space.

Filon (1929) developed a quadrature scheme specifically designed for integrands which could be written as the product of a slowly varying function and a sinusoidal oscillation. Essentially, the procedure is to fit the slowly varying function to parabolic arcs (as in Simpson's rule) and then carry out the integration over each subinterval analytically. If

$$ I(\omega) = \int_{a}^{b} f(s) \sin \omega s \, ds, $$

where $\omega \neq \omega(s)$, then the Filon approximation is:

$$ \hat{I}(\omega) = \Delta s \left\{ a \left[ f(a) \omega a - f(b) \cos \omega b \right] + b \right\} , \quad (2-2) $$

$$ + \beta S_{2n} + \gamma S_{2n-1} \} , $$
where $\Delta s$ is the grid point spacing in $s$. If the parameter $\theta$ is defined as $\theta = \omega \Delta s$ then the functions $a$, $b$ and $\gamma$ are given by

\[
O^3 \alpha = \theta^2 + \theta \sin \theta \cos \theta - 2 \sin^2 \theta
\]
\[
O^3 \beta = 2 \left[ \theta (1 + \cos^2 \theta) - 2 \sin \theta \cos \theta \right]
\]
\[
O^3 \gamma = 4 \left( \sin \theta - \theta \cos \theta \right)
\]

Also

\[
S_{2n} = \frac{1}{2} \left[ f(a) \sin \omega a + f(b) \sin \omega b \right] + f(a + 2\Delta s) \sin \omega (a + 2\Delta s)
\]
\[+ f(a + 4\Delta s) \sin \omega (a + 4\Delta s) + \ldots + f(b - 2\Delta s) \sin \omega (b - 2\Delta s) \]

and

\[
S_{2n-1} = f(a + \Delta s) \sin \omega (a + \Delta s) + f(a + 3\Delta s) \sin \omega (a + 3\Delta s)
\]
\[+ \ldots + f(b - \Delta s) \sin \omega (b - \Delta s) .
\]

The same procedure can be applied to the integral

\[
I(\omega) = \int_a^b f(s) \cos \omega s \, ds
\]

by replacing the cosines by negative sines in the boundary term and by replacing the sines by cosines in the two sums $S_{2n}$ and $S_{2n-1}$.

The advantage of this technique is that with a given
resolution one can handle higher frequency oscillations with Filon quadrature than with Simpson's rule. In fact, if the integration
\[ \int_a^b f(s) \, ds \]
can be performed accurately, then one might expect that
\[ I(\omega) = \int_a^b f(s) \sin \omega s \, ds \]
can be found for any value of \( \omega \) since the oscillatory part of the integration is carried out analytically. Numerical experiments show that this statement must be qualified. The integral \( I(\omega) \) is seen to approach zero as \( \omega \to \infty \) via the Riemann-Lebesque lemma. Its numerical approximation also approaches zero. However, it does so at a different rate. As a result, the absolute error \( I(\omega) - \hat{I}(\omega) \) approaches zero, while the relative error \( (I(\omega) - \hat{I}(\omega))/I(\omega) \) may grow, decay or remain constant depending on \( f(s) \). In this sense the numerical approximation may not be good for extremely large values of \( \omega \).

To understand the inaccuracies associated with Filon quadrature consider a comparison between the following two schemes. One is the simplest form of polynomial approximation: the value of the integrand at the grid point is used to approximate the function over the subinterval.
The other scheme will have Filon's separation of the integrand into a slowly varying part, approximated as above, and a rapid sinusoidal oscillation treated, in some sense, analytically. If

$$I(\omega) = \int_a^b f(s) \sin \omega s \, ds,$$

then the polynomial approximation can be written;

$$\hat{I}_p(\omega) = \Delta s \sum_{n=1}^{N} f(n\Delta s) \sin (\omega n\Delta s)$$

(2-3)

and the crude form of Filon quadrature will be given by:

$$\hat{I}_F(\omega) = \sum_{n=1}^{N} f(n\Delta s) \int_{(n-1)\Delta s}^{(n+1)\Delta s} \sin \omega s \, ds$$

$$= \frac{2 \sin \left( \frac{1}{2} \omega \Delta s \right)}{\omega \Delta s} \hat{I}_p(\omega)$$

The complication arising from the separation of the integrand into rapidly and slowly oscillating parts has served to modify the corresponding polynomial approximation by a factor which is itself a function of \( \omega \). One can clearly see that whereas \( \hat{I}_p(\omega) \) is periodic in \( \omega \), \( \hat{I}_F(\omega) \to 0 \) as \( \omega \to \infty \). This is precisely the property required to obtain non-periodic numerical solutions to the wave equation where \( \omega \) plays the role of the coordinates x or ct and s is replaced by the wavenumber, k.
Since Filon-type quadrature schemes were used throughout this work to evaluate Fourier integrals, it is appropriate to investigate their applicability within this context. Given a transform pair:

\[ I(\omega) = \frac{\sqrt{\frac{2}{\pi}}} \int_{0}^{\infty} \mathcal{J}(s) \sin \omega s \, ds \]

\[ \mathcal{J}(s) = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} I(\omega) \sin \omega s \, d\omega \]

one can calculate the simplified-Filon numerical equivalent:

\[ \hat{I}_F(\omega) = 2 \frac{\sqrt{\frac{2}{\pi}}} \int_{0}^{\infty} \frac{\sin \left( \frac{1}{2} \omega \Delta s \right)}{\omega} \sum_{n=0}^{N} \mathcal{J}(n\Delta s) \sin \left( \omega n\Delta s \right) \]

Using (2-4) one can obtain an expression for \( \mathcal{J}(n\Delta s) \) in (2-5). Interchanging the order of summation and integration one obtains:

\[ \hat{I}_F(\omega) = \int_{0}^{\infty} I(\omega') \hat{W}_F(\omega, \omega') \, d\omega' \]

where

\[ \hat{W}_F(\omega, \omega') = \frac{4}{\pi} \frac{\sin \left( \frac{1}{2} \omega \Delta s \right)}{\omega} \sum_{n=0}^{N} \sin \left( \omega' n\Delta s \right) \sin \left( \omega n\Delta s \right) \]

Note that if use were made of the simple polynomial approximation, (2-6) could still be written with a different weighting function.
\[ W_p(\omega, \omega') = \frac{2}{\pi} \Delta s \sum_{k=1}^{N} \sin(\omega' \pi s_k) \sin(\omega \pi s_k). \]

In this case the function is periodic in both arguments:

1) \[ W_p(\omega, \omega' \pm \frac{2\pi f}{\Delta s}) = W_p(\omega, \omega'), \quad f = 0, 1, 2, \ldots \]

2) \[ W_p(\omega \pm \frac{2\pi f}{\Delta s}, \omega') = W_p(\omega, \omega') \]

Property 1) states that when calculating the function \( \hat{I}(\omega) \), the weighting function, \( W_p(\omega, \omega') \) weights the value of the analytic \( I(\omega \pm \frac{2\pi f}{\Delta s}) \) as heavily as the value \( I(\omega) \). This is simply the statement that high frequencies are aliased in the standard sense. Property 2) implies that when the numerical approximation is calculated at \( \omega \pm \frac{2\pi f}{\Delta s} \), the same value is obtained i.e.

\[ \hat{I}_p(\omega \pm \frac{2\pi f}{\Delta s}) = \hat{I}_p(\omega) \]

That is to say that the "spectrum" is periodic.

Although 1) and 2) were derived using the simplest form of polynomial approximation, they are also valid for the trapezoidal rule, Simpson's rule and the discrete Fourier transform. The reason is that all of these schemes approximate the integral as:
\[ \hat{I}(\omega) = \sum_{k=1}^{N} b_k \delta(n \Delta s) \sin(\omega n \Delta s) \]  

(2-7)

where the \( b_n \)'s, although they become increasingly more complicated with the sophistication of the scheme, are not functions of \( \omega \).

In the case of the simplified-Filon scheme one can see that 1) still holds. However, 2) is no longer true since

\[ W_F(\omega, \omega') = \frac{2 \sin\left(\frac{\omega \Delta s}{2}\right)}{\omega \Delta s} W_F(\omega, \omega') \]  

(2-8)

In other words, the coefficients of (2-7) are now functions of \( \omega \). Although the spectrum is still aliased, it is no longer periodic. In fact it approaches zero as \( \omega \) approaches infinity. From the form of (2-6) and (2-8) it follows that:

\[ \hat{I}_F(\omega + \frac{2\pi}{\Delta s}) = \int_{0}^{\infty} W_F(\omega + \frac{2\pi}{\Delta s}, \omega') I(\omega') \, d\omega' \]

\[ = -\frac{\omega}{(\omega + \frac{2\pi}{\Delta s})} \hat{I}_F(\omega) \]  

(2-9)

Therefore given the value of the function at \( \omega \), its value at \( \omega + \frac{2\pi}{\Delta s} \) is determined uniquely by the quadrature scheme. This is to be expected since given the original function, \( \chi(s) \), at the grid points, \( n \Delta s \), one cannot determine the spectrum for wavelengths less than \( 2\Delta s \) (Hamming 1962). However, for a reasonably smooth function which does not
oscillate wildly between grid points one would expect the spectrum to go to zero at large \( \omega \). This explains why the Filon "spectrum" is observed to tend to zero as \( \omega \) increases but at a different rate than the analytic spectrum. In this sense the relative error may become large only in that portion of the spectrum where the energy is small. Figure 1 shows the spectrum of \( e^{-10|s|} \):

\[
|F_n|^2 = \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-10|s|} \cos ns ds \right|^2
\approx \frac{1}{\pi^2 (10\theta + \gamma^2)^2}
\]

This is over a finite interval. Therefore \( n \) is only allowed to take on integer values. \( |F_n|^2 \) is plotted versus \( n \) for the analytic solution, Filon quadrature, Simpson's rule and the discrete Fourier transform. As has been explained above, the behaviour of the different spectra at large \( n \) is quite different from one to another. It will be noted that the polynomial or Fourier approximations give spectra in the region \( \frac{\pi}{\Delta s} < n < \frac{2\pi}{\Delta s} \) which are mirror images of the values in the region \( 0 < n < \frac{\pi}{\Delta s} \). The frequency of oscillation \( \pi/\Delta s \), called the Nyquist (or folding) frequency, corresponds to a wavelength of 2 grid lengths. It is the frequency beyond which high-frequency oscillations are aliased and all quadrature schemes break down (Hamming 1962). The Filon and analytical spectra on the other hand, are observed to approach zero at large \( n \).
Figure 1: The spectrum $|F|^2$ versus $N$ using various quadrature schemes.
2.1.3. Numerical Results

The problem at hand is to evaluate the integrals (2-1) numerically. The initial conditions used were:

\[ \phi(x, 0) = \psi \left\{ e^{\chi \rho \left[ \frac{-(x-x_0)^2}{\alpha} \right]} - e^{\chi \rho \left[ -\frac{(x+x_0)^2}{\alpha} \right]} \right\} \]

\[ \frac{\partial \phi(x, 0)}{\partial t} = -2\chi \rho \left\{ (x+x_0) e^{\chi \rho \left[ \frac{-(x-x_0)^2}{\alpha} \right]} + (x-x_0) e^{\chi \rho \left[ -\frac{(x+x_0)^2}{\alpha} \right]} \right\} \]

Restricting the domain to \( x \geq 0 \), this represents a Gaussian-shaped pulse of e-folding width \( \alpha \) initially centred at \( x_0 \) and propagating towards \( x = 0 \). If \( \alpha \) is used as the length unit, then the values used were: \( \psi = 0.25 \alpha \) and \( x_0 = 5\alpha \). The integral was computed for \( 0 \leq x \leq 20\alpha \) at intervals of \( 0.8\alpha \). The k-space resolution, \( \Delta k \), was \( 0.15\alpha^{-1} \). Twenty-one points were used in k-space covering the range \( 0 \leq k \leq 3\alpha^{-1} \). With the above set of parameters, the Nyquist, or folding, frequency is \( 21\alpha \). This is close to the largest value of \( x \) for which the integral was calculated.

Given the initial conditions the real space displacement can be calculated by evaluating:
Since the integrals are of a simple form, the analytic function can also be calculated:

\[
\varphi(x, t) = \int_0^\infty \frac{2\pi}{\sqrt{\pi}} e^{-\frac{k^2 \alpha^2}{4}} \sin k x_0 \sin k x \cos ct k \, dk
\]

\[
- \int_0^\infty \frac{2\pi}{\sqrt{\pi}} e^{-\frac{k^2 \alpha^2}{4}} \cos k x_0 \sin k x \sin ct k \, dk
\]

It is shown in figure 2a).

In figure 2b) Simpson's rule was used to evaluate \( \varphi \). The result will be called \( \hat{\varphi} \). The numerical solution is, as was explained above, periodic in both space and time. The pulse is seen to reflect off of the point \( x = T/\Delta k \) as is to be expected. It will also be noted that a secondary pulse is artificially created at large \( x \). This is due to the aliasing involved in the evaluation of the factor \( \sin k x \).
Figure 2: Non-dispersive wave propagation in 1-dimension

a) analytical solution,

b) Simpson's rule approximation,
Figure 3 shows the results using Filon quadrature. In this case it is necessary to specify the part of the integral that was treated analytically. Since both integrals are of the same form, only one will be considered:

\[ \int_{0}^{k_{max}} \left[ e^{-k^{2}k_{x}^{2}/4} \sin kx_{0} \sin kx \right] \cos ctk \, dk \]

In figure 3a) the cos ctk term was treated analytically. The result is \( \hat{p}_{r1}(x,t) \). This implies that the rest of the integral must be relatively slowly varying. In order for this to be true both \( x_{0} \) and \( x \) must be small. If \( x_{0} \) is small enough, this procedure should produce a valid description of the spectrum near the origin for all times. However, since the variation in \( x \) is represented by only 21 waves whose frequencies are commensurate, the resulting numerical solution is periodic in \( x \). It also shows the secondary pulse at large \( x \) as in Simpson's rule. The spatial periodicity implies that the pulse will bounce off of the point \( x = \pi/\Delta k \). However, the numerical solution must remain valid for small \( x \) for all time. This can only be accomplished by decreasing the pulse amplitude so that by the time the reflected pulse reaches the region near the origin, its amplitude is negligible. This behaviour can be seen in figure 3a).
Figure 3: Non-dispersive wave propagation in 1-dimension using Filon quadrature with:

a) time treated analytically,

b) time and space treated analytically,
\( \varphi(x,t) \) can of course be rewritten via some trigonometric identities as:

\[
\varphi(x,t) = \frac{\psi_2}{\pi} \int_{0}^{k_{\text{max}}} \cos k \left( x-x_0 + ct \right) dk
\]

\[
- \frac{\psi_2}{\pi} \int_{0}^{k_{\text{max}}} \cos k \left( x+x_0 - ct \right) dk
\]

In this case the Gaussian function is treated as the slowly varying part approximated by parabolic arcs, while the cosine factor is treated analytically. The advantage of this formulation is clear: now both space and time are treated analytically and the slowly varying function never becomes oscillatory in \( k \). This is due to the fact that \( (x \pm x_0 \pm ct) \) are the characteristic coordinates of the system. As discussed above, the relative error in the quadrature formula will be large for large values of \( |x \pm x_0 \pm ct| \). This is the case far from the pulse maximum where the amplitude goes to zero. Since the numerical and analytical solutions both go to zero, the absolute error is small. Figure 3b) shows the results of this formulation, \( \hat{\varphi}_2(x,t) \). It can be seen that the numerical solution shows no reflections and is, for most purposes, identical to the analytical solution. It also involves fewer operations and requires about 20 per cent less computational effort.

Although the most accurate quadrature is \( \hat{\varphi}_2(x,t) \) it
is clear that this type of formulation will not be possible for the set of spectral equations governing an atmospheric model. However, if one seeks solutions of the form

\[ a(k,t) = \lambda(k) e^{i\omega t} \]

one can then treat at least these modes as above. If the basis functions on the infinite domain are \( f(k)e^{ix} \), then the real space parameters will be calculated by evaluating an integral of the form:

\[
\int_{-\infty}^{\infty} \lambda(k)f(k)e^{i(kx-\omega t)} \, dk
\]

where both space and time are contained in the rapidly oscillating function that is treated "analytically" in the sense that it is integrated over a continuous spectrum of wavenumbers, \( k \).

2.2. Dispersive Waves

Since both gravity and Rossby waves are dispersive, a quadrature scheme capable of producing an accurate representation for dispersive waves is essential.
2.2.1. Generalization of the Quadrature Schemes

The integrals to be calculated are now of the form:

\[
\int_0^{k=\infty} f(k) e^{i (kx - \sigma(k)t)} \, dk.
\]

One possible scheme for evaluating such an integral based on Filon's separation into slowly and rapidly varying parts was proposed by Levin (1982). Filon quadrature over a double subinterval is based on the expansion:

\[
\int_{-\Delta s}^{\Delta s} f(s) e^{i\omega s} \, ds = \sum_{h=1}^{3} a_h \int_{-\Delta s}^{\Delta s} \Phi_h(s) e^{i\omega s} \, ds,
\]

where \( \Phi_h(s) = s^{-1} \). Levin performed the same expansion for the more complicated case where \( \omega s = q(s) \):

\[
\int_{a}^{b} f(s) e^{i q(s)} \, ds = \sum_{h=1}^{M} \Delta_h \int_{a}^{b} \Phi_h(s) e^{i q(s)} \, ds. \tag{2-10}
\]

The integrals on the right hand side are easily performed if the \( \Phi_h(s) \) can be expressed in terms of another set of functions \( u_n(s) \) via:

\[
\Phi_h(s) = u_n(s) + \frac{q'(s)}{q(s)} u_n(s)
\]

In this case:

\[
\int_{a}^{b} \Phi_h(s) e^{i q(s)} \, ds = \int_{a}^{b} \frac{d}{ds} \left[ u_n(s) e^{i q(s)} \right] \, ds.
\]
From the expansion of the function $f(s)$

$$f(s) \sim \sum_{k=1}^{N} a_k \phi_k(s)$$

$$= \sum_{k=1}^{N} a_k \left[ u_k'(s) + i q'(s) u_k(s) \right].$$

One can now determine the $N$ coefficients, $a_n$, by considering $N$ points in $s$ and $N$ corresponding values of $f(s_j)$. This involves specifying a suitable set of basis functions, $u_n(s)$, such as $u_n(s) = s^{n-1}$ for example. The problem now becomes

$$\sum_{k=1}^{N} a_k \left[ u_k'(s_j) + i q'(s_j) u_k(s_j) \right] = f(s_j)$$

or

$$\sum_{k=1}^{N} \beta_{jk} a_n = f_j$$

Once the matrix $\beta_{jk}$ has been inverted, the coefficients, $a_n$, are determined and the integral in (2-10) can be calculated.

Although this scheme works for arbitrary dispersion relations, it is costly to perform. The use of 10 points in $k$-space would require the inversion of a 10 by 10 matrix for every calculation of the displacement in $x$-$k$ space. The use of 10 points also implies the fitting of a 9th order polynomial to $f(s)$ over the interval $a$ to $b$. Often fitting high-order polynomials to noisy data gives disastrous results.
Due to the matrix inversion, the calculation of the integral requires order $N^2$ operations, whereas Filon quadrature requires order $N$ operations. An effective order $N$ operation generalization of Filon quadrature can be developed by expanding the phase function. The integration can be performed accurately, with relative ease, up to second order in $s$. If the range of integration is broken up into subintervals of width $2\Delta s$, then:

$$\int_{-\Delta s}^{\Delta s} f(s) e^{iq(s)} ds = \frac{3}{\Delta s} \Delta s \int_{-\Delta s}^{\Delta s} \phi_k(s) e^{iq(s)} ds, \quad (2-11)$$

where \( \phi_k(s) = s^{k-1} \) and if

$$q(s) \approx q(i) + \frac{dq}{ds} \bigg|_{s=i} + \frac{1}{2} \frac{d^2q}{ds^2} \bigg|_{s=i} s^2,$$

then the integrals on the right hand side of (2-11) can be expressed as the difference between two complex error functions. The functions need only be calculated and tabulated once. The details of this scheme are found in appendix A.

2.2.2. Numerical Results

The initial conditions used described a Gaussian modulated oscillation of wavenumber $k_0$ with no initial transverse velocity propagating through an infinite domain:
The first experiment involves the dispersion relation

\[ \sigma(k) = A_0 + A_2 k^2 \]

for which the phase function expansion is exact. The transform is given by

\[
\alpha(k, \omega) = \frac{\chi}{Z \sqrt{2}} \left[ \exp \left( -\frac{\alpha^2}{4} (k-k_0)^2 \right) \right.
\]

\[ + \exp \left( -\frac{\alpha^2}{4} (k+k_0)^2 \right) \] \hspace{1cm} (2-12)

For the purpose of the subsequent numerical evaluations, the leftward propagating wave packet described by the second term was dropped. Therefore the integral to be calculated was

\[
\Phi(x, \omega) = \frac{\chi}{4 \sqrt{\pi}} \text{Re} \int_{-\infty}^{\infty} e^{\frac{\alpha^2}{4} (k-k_0)^2} \times e^{i (kx - \sigma(k) t)} \, dk \hspace{1cm} (2-13)
\]

The analytical solution is
\begin{equation}
\psi(x,t) = \sum_{k} \text{Re} \left[ \exp \left( -\frac{(x - 2A_{z}k_{0}t)^{2}}{\Delta k^{2}(1 + i\gamma A_{z}t/\Delta k)} \right) \exp \left( i \left( k_{0}x - (A_{0} + A_{z}k_{0})t \right) \right) \right] \left( 1 + \frac{i\gamma A_{z}t}{\Delta k^{2}} \right)^{1/2}
\end{equation}

The analytical solution is shown in figure 4a). Figure 4b) shows the numerical solution calculated with Levin's quadrature formula involving matrix inversion and figure 4c) displays the same calculation done using the generalized Filon scheme developed in appendix A. The values used, in terms of \( \Delta k \), were: \( \gamma = 2\Delta \), \( k_{0} = 12\Delta^{-1} \), \(-3\Delta^{-1} \leq k-k_{0} \leq 3\Delta^{-1} \), \( \Delta k = 0.6\Delta^{-1} \). Eleven points were used in \( k \)-space and the real space result was calculated for \( 0 \leq x \leq 5\Delta \) at intervals of \( \Delta t \) where \( C_{g}(k_{0})\Delta t = 0.48\Delta \). The constants in the dispersion relation, \( \sigma(k) = A_{0} + A_{z}k^{2} \), were both set equal to one.

The generalized Filon scheme produces an acceptably accurate result. It is also non-periodic and requires 23% less computational effort for an eleven point quadrature and 61% less for a twenty-one point quadrature when compared to Levin's matrix inversion scheme.
Figure 4: The propagation of dispersive waves with

a) The analytical solution (equation (2-20))

b) Levin's quadrature scheme

c) generalized-Filon scheme
Since the dispersion relation tested above is only second order in $k$, the expansion of the phase function in the generalized-Filon scheme was exact. A more rigorous test is provided by the Klein-Gordon equation:

$$\frac{\partial^2 \varphi(x,t)}{\partial t^2} - c^2 \frac{\partial^2 \varphi(x,t)}{\partial x^2} = -\chi \varphi(x,t)$$

The dispersion relation is:

$$\sqrt{k} = \pm \left(c^2 k^2 + \chi\right)^{1/2}$$

As above, only the rightward propagating term was calculated and the values of $c$ and $\chi$ were set to one and $144\lambda^{-2}$ respectively. The time interval at which the calculations were made was adjusted to give $Cg(k_0)\Delta t = 0.42\lambda$. Otherwise, all parameters remain the same. The results are displayed in figure 5. The conclusion is as above: the generalized-Filon scheme gives the same result as the much more expensive scheme proposed by Levin (1982).
Figure 5: The propagation of dispersive waves with

a) Levin's quadrature scheme

b) generalized-Filon scheme
2.3. Forced Waves

It will be seen to be relevant from the point of view of an atmospheric model to consider spectral equations of the form.

$$\frac{\partial a(k,t)}{\partial t} + c \sigma(k) a(k,t) = d(k,t) \quad (2-15)$$

where $d(k,t)$ is a time-dependent forcing at wavenumber, $k$. The description of one-dimensional wave propagation in section 2.2 refers only to the conversion from spectral space to real space. The applicability of the numerical techniques depends on whether or not a meaningful solution of the form

$$a(k,t) = \lambda(k) e^{-\gamma(k)t}$$

can be isolated. This part of the solution can be treated as above and will yield a useful result even at large times. However, it will not, in general, be the total solution. If the solution to (2-15) can be written in terms of a forced part and a free oscillation, then:

$$a(k,t) = \lambda(k) e^{-\gamma(k)t} + \xi(k,t) \quad (2-16)$$

Substituting this into (2-15) yields:
\[ \frac{\partial \beta (k,t)}{\partial t} + i \sigma(k) \beta (k,t) = \alpha(k,t), \quad (2-17) \]

where \( \alpha(k,0) = \alpha(k) + \beta(k,0) \). If the basis functions are \( g(k) e^{i k x} \) then the conversion back to real space will become:

\[ \varphi(x,t) = \int_{-\infty}^{\infty} \alpha(k) g(k) e^{i(kx - \sigma(k)t)} \, dk 
+ \int_{-\infty}^{\infty} \beta(k,t) g(k) e^{i k x} \, dk. \]

The first term can be treated by the generalized Filon scheme since the slowly varying part, \( \alpha(k) g(k) \), does not become highly oscillatory in \( k \) with time. The second term is more difficult. If, for example one were to evaluate it using Filon quadrature to treat the space dependence analytically, aliasing would eventually result. This is due to the fact that the "slowly-varying" function, \( \beta(k,t) \), would become increasingly oscillatory (in \( k \)) with time. This can be explained as follows. The development of high-frequency oscillations in the transform is a manifestation of the fact that the real space solution has had time to propagate away from the region of interest. For example consider an isolated extremum of the real space solution \( \varphi(x,t) \). If at \( t = 0 \) this feature is located at \( x = 0 \), and if the equations allow propagation, then at \( t = t_0 \) it will be centred at a different value of \( x \), say \( x_0 \). Then at \( t = 0 \):
\[ \varphi(x) \propto \int_{-\infty}^{\infty} A(k) e^{ikx} \, dk \]

and at \( t = t_0 \):

\[ \varphi(x-x_0) \propto \int_{-\infty}^{\infty} A(k) e^{ik(x-x_0)} \, dk \]

Therefore the transform which was \( A(k) \) at \( t = 0 \) must become \( A(k) e^{-ikx_0} \) at \( t = t_0 \). If an average propagation speed, \( c_0 \), is defined then \( x_0 = ct_0 \) and the transform is seen to become increasingly oscillatory as the extremum propagates away or, equivalently, as time increases. Although this cannot be avoided it can be delayed by choosing \( \theta(k,0) \) such that the function \( \theta(k,t) \) varies slowly with time. The initial tendency of \( \theta(k,t) \) can be set to zero by a proper choice of the function \( \alpha(k) \) using (2-16) and (2-17). In fact, this procedure can be carried out for higher orders as well. Setting \( \frac{\partial^2 \theta}{\partial t^2}(k,0) = 0 \) one obtains:

\[ \alpha(k) = \alpha(k,0) - \frac{d(k,0)}{i \sigma(k)} + \frac{1}{(i \sigma(k))^2} \frac{\partial d(k,0)}{\partial t} \]

\[ + \cdots + \frac{(-1)^h}{(i \sigma(k))^h} \frac{\partial^{h+1} d(k,0)}{\partial t^{h+1}} \]
This technique is analogous to normal mode initialization where $a(k,0)$ is adjusted such that $\alpha(k) = 0$. In this way, $\beta(k,t)$ will develop small-scale $k$-structure as slowly as possible. According to the above discussion this is equivalent to ensuring that the average propagation speed is small for this contribution. Clearly this has only been done at $t = 0$. If the forcing excites high-speed wave modes at a later time, aliasing will rapidly become a problem. If, for example, at some subsequent time, $\gamma$, the function $\beta(k,\gamma)$ begins to oscillate rapidly with respect to the $k$-space resolution, $\Delta k$, then it can once more be partitioned as in (2-16). In this case:

$$a(k,t) = \alpha(k) e^{-i \gamma(k)t} + \gamma(k) e^{-i \gamma(k)(t-\gamma)} + \delta(k,t)$$

where $\lim_{\delta t} \delta(k,t)$ is set to zero thereby determining $\gamma(k)$. The new term involving $\gamma(k)$ can be treated using the quadrature scheme discussed in appendix A. The other term, $\delta(k,t)$ is for $t \approx \gamma$ slowly varying in time and therefore contains only the low-frequency modes. Rapid $k$-oscillations begin to occur when the real space solution has a significant amount of energy at large coordinate values. The high-frequency waves have large group velocities. It is therefore essential that the transform be periodically partitioned in the above fashion to remove these modes from the term whose specific time dependence is
not known. If this is done it remains slowly varying in time.

Eventually the partitioning procedure will be of no use. This is due to the fact that even the slowest modes will have propagated to large coordinate values. Requiring the function \( \xi(k,t) \) to have a zero tendency at time intervals \( t = nT \) will guarantee that it be slowly varying in time. However, it will be rapidly oscillatory in \( k \). At this point aliasing will be unavoidable and the numerical procedure breaks down.

The final result is that this method maintains accuracy for a much longer time period than simple domain truncation. The latter breaks down as soon as the fast modes have propagated to large distances.
CHAPTER 3: SIMPLE INFINITE-DOMAIN ATMOSPHERIC MODELS

3.1. Infinite Vertical Domain

The most potentially useful application of the above numerical techniques would be to describe variations in the vertical on a semi-infinite domain. In this case the unphysical high-frequency gravity waves generated by inaccurate initial data, forcing and nonlinear interactions would quickly propagate out of the computational domain leaving only the modes of meteorological interest.

Although infinite vertical domain models are potentially more useful, further numerical investigation was confined to a more simple infinite horizontal domain for illustrative purposes.

3.2. Barotropic Shallow-Water Model with an Infinite Horizontal Domain

3.2.1. Mathematical Formulation
The shallow water equations are:

$$ \frac{\partial u_D}{\partial t} - f v_D = -\frac{\partial h_D}{\partial x} - \nabla_D \cdot \nabla_D u_D \quad (3-1) $$

$$ \frac{\partial v_D}{\partial t} + f u_D = -\frac{\partial h_D}{\partial y} - \nabla_D \cdot \nabla_D v_D \quad (3-2) $$

$$ \frac{\partial h_D}{\partial t} + \rho_0 \nabla_D \cdot \nabla_D = -\nabla_D \cdot \nabla_D h_D - \rho_D \nabla_D \cdot \nabla_D \quad (3-3) $$

assuming that there is no spatial variation in which is twice the rotation frequency. Also, \( \nabla_D = u_j + v_j \), the fluid height \( H = h_0 + h \), \( \rho = gh \), \( \rho_0 = gh_0 \) and

$$ \int_D H \, dx \, dy = h_0 \int_D dx \, dy $$

A non-dimensional form of the system can be obtained by introducing the scaling: \( u_\ast = \varepsilon \sqrt{\rho_0} \), \( v_\ast = \varepsilon \sqrt{\rho_0} \); \( T_\ast = L \sqrt{\rho_0} \) and \( f = \frac{2 \Omega L}{\sqrt{\rho_0}} \), where \( L \) is the length scale in \( x \) and \( y \). Then:

$$ \frac{\partial X}{\partial t} + i \mathcal{L} X = -\varepsilon N(X) \quad (3-4) $$
where \[ X = \begin{pmatrix} \varphi \\ u \\ v \end{pmatrix} \] (3-5)

\[ L = \begin{pmatrix} 0 & -i & 0 \\ -i & -c \frac{\partial}{\partial x} & -i \\ 0 & \frac{\partial}{\partial y} & -i \end{pmatrix} \] (3-6)

and \[ N(X) = (\nabla \cdot \nabla) X + \nabla \cdot \nabla \begin{pmatrix} \varphi \\ 0 \\ 0 \end{pmatrix} \] (3-7)

The domain, D, was \(-\infty < x < \infty; 0 \leq y \leq 1\). The eigenvalues and associated eigenvectors are derived in appendix B. They are given by

\[ Y_n^l(k) = \sqrt{2} \frac{e^{ikx}}{\omega} \begin{pmatrix} f \sin \pi nx \\ \pi \cosh \pi n y \\ -ik \sinh n y \end{pmatrix} \]
\[ \gamma_n^2(k) = \frac{e^{ikx}}{\omega (\omega^2 + f^2 k^2)^{1/2} (k^2 + n^2 \pi^2)^{1/2}} \left( \frac{(\omega^2 - f^2) \omega \cos \pi y - f \sin \pi y}{\omega (\omega^2 + f^2 k^2)^{1/2} (k^2 + n^2 \pi^2)^{1/2}} \right) \]

\[ \gamma_n^3(k) = \frac{e^{ikx}}{\omega (\omega^2 + f^2 k^2)^{1/2} (k^2 + n^2 \pi^2)^{1/2}} \left( \frac{(\omega^2 - f^2) \omega \cos \pi y - f \sin \pi y}{\omega (\omega^2 + f^2 k^2)^{1/2} (k^2 + n^2 \pi^2)^{1/2}} \right) \]

\[ \gamma_n^4(k) = \left( \frac{f}{e^{2f} - 1} \right)^{1/2} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} e^{fy} e^{ikx} \]

\[ \gamma_n^5(k) = \left( \frac{f}{1 - e^{-2f}} \right)^{1/2} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} e^{-fy} e^{ikx} \]

The eigenvalues are \( \lambda_1 = 0; \lambda_2 = u; \lambda_3 = -u \) where \( u = (k^2 + n^2 \pi^2 + f^2)^{1/2} \); \( \lambda_4 = -k \) and \( \lambda_5 = k \).

Defining the scalar product as:
\[(X, Y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle X, Y \rangle \, dy \, dx,\]

where \(\langle x, y \rangle = x_1 \cdot y_1 + x_2 \cdot y_2 + x_3 \cdot y_3\), one can convert from real space to spectral space and vice-versa via:

\[a_n^c(k, t) = \langle Y^n_c(k), X \rangle\]

and

\[X = \sum_{n=1}^{3} \sum_{\zeta=0}^{\infty} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk + \sum_{n=1}^{3} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk\]

(3-9)

In practice (3-9) can be simplified using the reality conditions. One can easily show that:

\[\sum_{n=1}^{3} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk = 2 \sum_{n=1}^{3} \text{Re} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk\]

and

\[\sum_{n=1}^{3} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk = 2 \sum_{n=1}^{3} \text{Re} \int_{-\infty}^{\infty} a_n^c(k, t) \, Y^n_c(k, \bar{\zeta}) \, dk.\]

This allows \(k\) to be restricted to positive values.
3.2.2. The Linear Model

Numerical experiments were performed using the linear equation:

\[
\frac{\partial X}{\partial t} + i \mathcal{L} X = 0
\]  

(3-10)

Interesting results can be obtained using only the linear terms since linear propagation of high-frequency gravity waves on an infinite domain is not easily simulated numerically.

Some aspects of a fully nonlinear model are discussed in section 3.2.3.

3.2.2.1. Initialization and Steady-State Configuration

Taking the scalar product of equation (3-10) and the basis vectors and using the self-adjoint property of \( \mathcal{L} \) gives the linear spectral equations:

\[
\frac{\partial \alpha(k,t)}{\partial t} + i \sigma(k) \alpha(k,t) = 0
\]

(3-11)

The solutions are \( \alpha(k,t) = \alpha(k,0)e^{-\sigma(k)t} \). For a more complicated case (3-11) would involve some sort of numerical time-stepping. If the assumption is made that
the spectral equations can always be accurately solved, then attention can be directed to the question of the spectral to real space conversion. The first step is to assume the initial conditions on the real space vector \( X(x,y,t) \). Since the transform coefficients \( a_n^k \) are given by the scalar product of \( X(x,y,t) \) with the basis functions \( Y_n^k \), a good deal of simplification results if \( X(x,y,t) \) is assumed initially to have only one non-zero component. The conditions \( u(x,y,0) = v(x,y,0) = 0 \) and \( \varphi(x,y,0) = \varphi_0(x,y) \), where \( \varphi_0(x,y) \) is some height field localized near \( x = 0 \), were used. This describes a height field which is not in geostrophic balance with the velocity field. As a result geostrophic, gravity and Kelvin modes are excited.

As time increases, the gravity and Kelvin waves quickly propagate away from the origin, whereas the geostrophic modes, having \( \sigma = 0 \), remain. At large times the motion at small \( x \) is completely geostrophic. The final geostrophic state can be determined from the initial conditions via the conservation of potential vorticity. Taking \( \frac{\partial}{\partial x} \) of the first of equations (3-4) and adding it to \( -\frac{\partial}{\partial y} \) of the second with \( \epsilon = 0 \) gives \( \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + f \varphi \varphi' = 0 \), where \( \varphi = \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \) is the vorticity. Use of the 3rd component of (3-4) with \( \epsilon = 0 \) to eliminate the divergence term yields:
\[ \frac{\partial}{\partial t} (\xi - \Phi \Psi) = 0 \quad (3-12) \]

At \( t = 0 \), \( \xi - \Phi \Psi = -f \phi_0(x, y) \) and as \( t \to \infty \) the motion will be geostrophic and therefore non-divergent. In this case a stream function \((x, y)\) can be introduced:

\[
\xi = -\frac{\partial \Phi(x, y)}{\partial y}, \quad \psi = \frac{\partial \Phi(x, y)}{\partial x}
\]

and

\[
\xi - \Phi \Psi = (\nabla^2 - f^2) \Phi(x, y)
\]

Since (3-12) states that the quantity \( \xi - \Phi \Psi \) is constant, its initial value is equal to its value at large times for all points. For the points near the origin this can be stated as follows:

\[
(\nabla^2 - f^2) \Phi(x, y) = -f \phi_0(x, y)
\]

(3-13)

Clearly the stream function must satisfy the boundary conditions \( v(x, 0) = v(x, 1) = 0 \). The appropriate basis functions for \( v(x, y) \) in \( y \) are therefore \( \sin \pi y \), ie

\[
v(x, y) = \sum_{n=1}^{\infty} \tilde{v}_n(x) \sin \pi y = \frac{\partial \Phi(x, y)}{\partial x}
\]
Therefore:

\[
\tilde{f}(x, y) = \sum_{k=1}^{\infty} \left( \int \tilde{\psi}_k(x) \, dx \right) \sin \pi y
\]

\[
= \sum_{k=1}^{\infty} \tilde{\psi}_k(x) \sin \pi y
\]

Thus, \( \sin \pi y \) are the appropriate basis functions for \( \tilde{f}(x, y) \) as well.

Considerable simplification results if the function \( \psi_0(x, y) \) can be represented by a single wavenumber in \( y \). The form \( \psi_0(x, y) = \tilde{\psi}(x) \cdot \sin \pi y \) was chosen arbitrarily. Equation (3-13) now reads:

\[
\sum_{k=1}^{\infty} \left[ \tilde{\psi}_k''(x) - \left( \frac{\xi^2 + \eta^2 \pi^2}{\alpha_k^2} \right) \tilde{\psi}_k(x) \right] \sin \pi y
\]

\[
= - \int \tilde{\psi}(x) \sin \pi y
\]

(3-14)

For convenience define

\[
\alpha_k^2 = \left( \frac{\xi^2 + \eta^2 \pi^2}{\alpha_k^2} \right)
\]

Multiplying equation (3-14) by \( \sin \pi y \) and integrating from \( y = 0 \) to \( y = 1 \), one obtains:

\[
\tilde{\psi}_m''(x) - \alpha_m^2 \tilde{\psi}_m(x) = \begin{cases} 
- \int \tilde{\psi}(x) & \text{if } m = 1 \\
0 & \text{if } m = 1
\end{cases}
\]
The homogeneous solution is: \( \tilde{\psi}_m(x) = A_m e^{ax} + B_m e^{-ax} \).

However, since the boundary conditions in \( x \) are that \( \varphi, u \) and \( v \) vanish as \( x \) approaches \( \pm \infty \), both \( A_m \) and \( B_m \) must be zero. Therefore, \( \tilde{\psi}_m(x) = 0 \) if \( m \neq 1 \) and only the particular solution to

\[
\tilde{\psi}_1(x) - a^2 \tilde{\psi}_1(x) = -\int \tilde{\varphi}(x) \quad (3-15)
\]

need be sought.

The equation (3-15) gives the final geostrophic state in terms of the initial condition chosen. It was used to determine \( \tilde{\varphi}(x) \) based on a simple profile for \( \tilde{\psi}(x) \). The essential property required is that \( \tilde{\psi}(x) \) be a localized function representing the region of interest in the computational domain. For this reason the Gaussian function, \( \tilde{\psi}_1(x) = A e^{-\frac{1}{2}x^2} \), was chosen. This gives \( \varphi(x,y,0) = \varphi_0(x,y) = \tilde{\varphi}(x) \Delta_k \pi y = \frac{A}{\pi} \left( 2b^2 + a^2 - 4a^2 \right) e^{-\frac{1}{2}x^2} \sin \pi y \), where \( a^2 = f^2 + \pi^2 \) and \( b \) is the width parameter of the Gaussian function chosen as the final steady-state.

Now that the vector \( X(x,y,0) \) has been specified, the initial values in the spectral representation follow:

\[
\alpha_1(k) = \frac{-1}{2\sqrt{2\pi}} \frac{A}{b} \omega_1 e^{-\frac{k^2}{4b^2}}
\]
\[ a_1^2(k) = \frac{\alpha}{4\sqrt{\pi}} \frac{A}{b} \frac{k(k^2 + \pi^2)^{1/2}}{(\omega^2 + \pi^2 + f^2 k^2)^{1/2}} e^{-k^2/4b^2} \]

\[ a_2^2(k) = -\frac{\alpha}{2\sqrt{\pi}} \frac{A}{b} \frac{\omega^2}{f(f^2 + \pi^2)} \frac{M}{1-n^2} [1 + (-1)^n] e^{-k^2/4b^2} \]

\[ a_3^2(k) = a_1^2(k) \]

\[ a_4^2(k) = -a_2^2(k) \]

\[ a_5^2(k) = a_4^2(k) \]

\[ a_6^2(k) = a_1^2(k) \]

where \( n = 2, 4, 6, \ldots \) and \( \omega_i = (k^2 + \pi^2 + f^2)^{1/2} \) and \( \omega = (k^2 + n^2 \pi^2 + f^2)^{1/2} \).

3.2.2.2. Numerical Results

The real space vector can be determined via:
\[
X(x,y,t) = 2 \text{Re} \int_0^\infty \left( a_1(k,t) \gamma_1(k \tilde{r}) + a_2(k,t) \gamma_2(k \tilde{r}) + a_3(k,t) \gamma_3(k \tilde{r}) \right) \, dk
+ \sum_{\ell=2,4,6} \left( a_0(k,t) \gamma_0(k \tilde{r}) + a_0(k,t) \gamma_0(k \tilde{r}) \right) \, dk
\]

The first term in the integrand represents the geostrophic contribution. It does not vary in time in the linear model and was calculated using Filon quadrature with \( e^{ikx} \) as the rapidly varying part. The next two integrals and the infinite sum represent the rightward and leftward propagating gravity waves. They are of the form considered in section 2.2.1 and were treated using the generalized Filon quadrature for dispersive waves outlined in appendix A. Finally, the last two terms describe the two Kelvin waves. Since, for these modes, \( \xi = \pm \text{Re} \), the rapid oscillation takes the form \( e^{ik(x+ct)} \). They are therefore not dispersive and were treated using Filon quadrature in its original form.

The values used were: the rotation parameter, \( f = 1 \); the \( k \)-space resolution, \( \Delta k = 3.0 \); the number of points, \( N = 11 \); \( k \) minimum = 0; \( k \) maximum = 30; the Gaussian width parameter, \( b = 6 \); its amplitude, \( A = 1 \) and the computations were performed on a grid extending from \( x = -0.8 \) to \( x = +0.8 \) with \( \Delta x = 0.125 \) and \( y = 0 \) to \( y = 1 \) with \( \Delta y = 0.125 \). The infinite sum of gravity waves was truncated after 4 terms.
Figure 6 shows the initial height field chosen in section 3.2.2.1 along with its truncated version. At \( t = 0 \), the oscillation \( e^{ikx(t)} \) is simply a constant and the integrals are rather easy to perform. At subsequent small values of \( t \) the generalized-Filon evaluation can be compared to the use of Filon quadrature itself where the factor \( e^{ikx(t)} \) is included in the slowly varying part of the integral. Since \( G(k) = \pm (k^2 + n^2 + f^2)^{1/2} \), the \( k \)-space oscillation frequency is \( \frac{kt}{(k^2 + n^2 + f^2)^{1/2}} \).

Considering the values used, this quantity reaches a maximum value of approximately \( \pm t \). If 5 points are required to accurately represent one wavelength, then the Filon approximation will begin to break down at around \( t = .5 \). This can be observed in Figure 7 and 8 which show good agreement between the generalized-Filon and Filon schemes at \( t = .04 \) and \( .32 \) respectively. In Figures 9 and 10, at \( t = 1.3 \) and \( 2.6 \) respectively, treating \( e^{G(k)t} \) as slowly varying in \( k \) becomes invalid. The Filon evaluation shows unphysically large height values which are entirely due to aliasing. The generalized-Filon scheme, on the other hand shows a progressive trend towards smaller displacement values as the high amplitude wave packets move away from the origin. The subsequent generalized-Filon height fields in figure 11 show a continuation of this trend. Figure 12 shows that by \( t = 100 \), the height field-
Figure 6: Comparison between the numerical evaluation of the initial height field a) with the field itself b)
Figure 7: a) Generalized-Pilon and
b) Pilon schemes at $t = .04$
Figure 8: a) Generalized-Filon and
b) Filon schemes at $t = 0.32$
Figure 9: a) Generalized-Filon and b) Filon schemes at t = 1.3
Figure 10: a) Generalized-Filon and
b) Filon schemes at $t = 2.6$
Figure 11: Generalized-Filon scheme at t = 5, 10, 20
Figure 12: A comparison between
a) the generalized-Filon evaluation at $t = 100$, and
b) the steady-state solution
is essentially identical to the steady-state Gaussian chosen in section 3.2.2.1.

3.2.3. The Nonlinear Model

Since the atmosphere and atmospheric models in general are nonlinear, the treatment of these terms in a spectral model on an infinite domain is discussed. In this case the full model equations are given by (3-4):

\[ \frac{\partial X}{\partial t} + \mathbf{L} X = - \epsilon \mathbf{N}(X) \]

The spectral equations will now be of the form:

\[ \frac{\partial a_p(k, t)}{\partial t} + \mathbf{L}_p(k) a_p(k, t) = \]

\[ - \epsilon \sum_{r_1} \sum_{r_2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c(k, k', k'') a_{r_1}^{\lambda}(k, t) a_{r_2}^{\lambda}(k', t) \, dk \, dk'' \]

(3-16)

where the \( c_{r_1}^{\lambda}(k, k', k'') \) are non-zero only if:

\[ (k_1 + q_{r_1} \pi_j) + (k_2' + q_{r_1} \pi_j') + (k_3' + q_{r_1} \pi_j) = 0 \]

In this case the right hand side of (3-16) can be simplified. Equation (3-16) is of the form of the linear forced problem, discussed in section 2.3 with:
\( d(k,t) = -\varepsilon(Y_r(k),N(X)) \). In this case however, a priori knowledge of the forcing function is impossible since it evolves with the spectral amplitudes. Accurate treatment of the nonlinear problem is impossible since in order to separate the integrand into a slowly varying function modulating a rapid oscillation one must know the form of the rapid oscillation, specifically, how it changes with time. The transform can be partitioned as in section 2.3 to give

\[ \alpha_{\rho}^f(k,t) = \alpha(k) e^{-\varepsilon \tilde{\sigma}_{\rho}(k)t} + \beta_{\rho}^f(k,t), \quad (3-17) \]

where

\[ \frac{d}{dt} \beta_{\rho}^f(k,t) + i \tilde{\sigma}_{\rho}(k) \beta_{\rho}^f(k,t) = d(k,t), \]

and

\[ \frac{\partial}{\partial t} \beta_{\rho}^f(k,c) = 0. \]

This ensures that \( \beta_{\rho}^f(k,t) \) develops rapid \( k \)-oscillations as slowly as possible.

In the case of models which accurately represent the atmosphere, the amplitudes of the geostrophic modes should be much larger than those of the gravity modes. Therefore, the nonlinear terms should be dominated by interactions between geostrophic modes and so, to leading order, \( d(k,t) \) should vary only slowly with time. By setting the initial tendency of \( \beta_{\rho}^f(k,t) \) equal to zero one determines the
function $\omega(k)$ in equation (3-17). The term involving $\omega(k)$ is easily treated using the special quadrature schemes described above. In present-day initialization schemes (see for example Machenhauer 1977) an iterative procedure is used to adjust the set of functions $a_{\tau, k, 0}$ such that $\omega(k) = 0$. This totally removes the linear part of the motion and is essential for models with unphysical upper boundary conditions.

The proposed method of dealing with the fully nonlinear problem would be to partition the transform via equation (3-17). The linear part of the motion is easily dealt with and the forced part will develop small-scale k-structure as slowly as possible. Periodically, when this becomes a problem, the forced part of the transform is once again partitioned into a rapid oscillation of frequency $\omega(k)$ and an unspecified time-dependent part. In this way the fast modes excited since the last partitioning procedure propagate away without reflection. After each such procedure a new term to be treated via the quadrature scheme in appendix A is created. Also, the contribution from the earlier terms becomes negligible as the energy contained in them has propagated to great distances. They can thus be discarded at the same rate they are created after a certain time.

Since the fast modes have been removed, the rest of
the transform reaches large heights only after a relatively long period of time. At this point aliasing is unavoidable and spurious modes will occur.
CHAPTER 4: CONCLUSIONS

In light of the conclusions reached above with respect to linear and nonlinear wave propagation on infinite domains it seems reasonable to suggest that the initial data be decomposed into fast and slow mode contributions. The high-frequency, nearly linear fast modes should then be treated according to the technique outlined above. In the case of the low-frequency, highly nonlinear slow modes, the spectral formulation will inevitably lead to spurious reflected modes which develop slowly.

In the particular case of atmospheric models with an infinite vertical domain, if the domain extends high enough, it has been found that the longest Rossby waves can be accurately treated for all times (Kirkwood and Derome 1977). This is due to the trapping of these waves by physical processes at work in the model. For this reason domain truncation in real space or a finite resolution in k-space should be acceptably accurate at least for these modes. If attention is directed to transient Rossby waves however, the methods of section 3.2.3 provide an alternative to the use of a radiation boundary condition.

When atmospheric models are initialized with real data, instrumental inaccuracy and the interpolation scheme
used to determine grid point values from surrounding synoptic station observations introduce error. This error manifests itself in the form of spurious high-frequency gravity waves. In order to obtain accurate vertical motion fields at small times, these modes must be removed by any one of a number of techniques (Haltiner and Martin 1980). If, after this, the initial gravity wave transforms are partitioned according to (3.17) then any remaining energy in the fast modes would quickly propagate away. Meanwhile, if the average propagation speed of the slow modes remains small then the numerical k-space quadrature should remain accurate until \( t = t_e \). If, on the other hand, the nonlinear terms excite high-frequency modes at an intermediate time, \( t_o (0 < t_o < t_e) \), then due to the large group velocities of these modes, the k-space transform would begin to oscillate rapidly. This could be controlled by the partitioning process outlined in section 2.3.

Errico (1984) has shown that in inviscid finite domain models, equipartition of energy between gravity and Rossby modes results. This is suppressed by dissipation in modern NWP models. Otherwise it would result in a continuous rise in energy of the fast modes. If energy were allowed to leak out of the computational domain less dissipation would be required. Such a model may perhaps give more realistic results.
Another potential application of spectral techniques on infinite domains would be localized models, for example mesoscale models, in which one or both of the horizontal coordinates would be taken as infinite. For some applications the various wave phenomena propagating away from the domain of interest near the centre of the grid must be prevented from reflecting back in. This is often done using radiation boundary conditions. These spectral techniques may provide the only possible alternative. Their application would be restricted to cases where the motion at the centre of the grid is not influenced by the surroundings. Also, the success of the method depends on the ability to extract the nearly linear fast mode behaviour from the total transform. This requires a relatively large frequency spread between the slow and fast modes.

Based on the potential benefits of the techniques applied to localized models or the problem of the upper boundary condition in NWP and GCM models, it seems reasonable to say that further investigation is warranted. The next step would be a numerical investigation of a nonlinear model initialized with typical Rossby and gravity wave spectra.
APPENDIX A

FILON QUADRATURE GENERALIZED FOR DISPERSION

Since the integrals of interest are of the form:

\[ \mathcal{I} = \int_{-\infty}^{\infty} A_k e^{i(kx - \tau(k)t)} dk \]

the quadrature formula will be developed using this notation. The first step, as in Filon quadrature, is to separate the range of integration into double subintervals of width \(2\Delta k\) where \(\Delta k\) is the distance between sampled values of \(A(k)\).

\[ \mathcal{I} = \sum_{k_{n}-\Delta k}^{k_{n}+\Delta k} \int A(k) e^{i(kx - \tau(k)t)} dk = \sum_{k_{n}-\Delta k}^{k_{n}+\Delta k} \mathcal{I}_n \]

where \(k_n = n\Delta k + k_{\min}\) and \(k_{\max} = N\Delta k + k_{\min}\). Over each double subinterval \((k)\) is expanded about \(k_n\). The resolution, \(\Delta k\), must be chosen such that both \(\tau(k)\) and \(A(k)\) are accurately represented by 3 terms of their respective Taylor expansions. Thus:

\[ \mathcal{I}_n = \int_{k_n-\Delta k}^{k_n+\Delta k} A(k) e^{i(kx - \tau(k)t)} dk = e^{i\phi_n(k)} \int_{k_n-\Delta k}^{k_n+\Delta k} A(k) e^{i\phi_n(k)} dk, \]

where the phase function, \(\phi_n(k)\), can be approximated via:
where
\[ a_k = \frac{1}{2} \] 
\[ b_k = \frac{1}{2} \] 
\[ c_k = \frac{1}{2} \]

The contribution can once more be rewritten:

\[ \Omega = \mathcal{A} \left[ b_{k-1} k \Delta k + c_k^2 (k-1)^2 \right] \int_{k-\Delta k}^{k} \] 

For each double subinterval three values of \( A(k) \) are available: \( A(k_0 - \Delta k) \), \( A(k_0) \) and \( A(k_0 + \Delta k) \). Parabolic arcs are fitted to these values according to:

\[ A_k(k) = \alpha_k + \beta_k (k - k_0) + \gamma_k (k - k_0)^2 \]

where
\[ \alpha_k = A(k) \]
\[ \beta_k = \frac{A(k_0 + \Delta k) - A(k_0 - \Delta k)}{2 \Delta k} \]
\[ \gamma_k = \frac{A(k_0 + \Delta k) - 2A(k_0) + A(k_0 - \Delta k)}{2 \Delta k^2} \]

After replacing \( k - k_0 \) by a new variable \( s \) and completing the square, one obtains:

\[ \Omega = \mathcal{A} \int_{-\Delta k}^{\Delta k} \left[ c_{\Delta k} + \frac{b_{\Delta k}}{2} \right] ds. \]
At this point a new variable of integration, \( u \), is introduced:

\[
\mu = \frac{C_n \cdot \mu - \frac{b_n}{2C_n}}{\sqrt{2}}
\]

The limits of integration become:

\[
\mu_0 = \frac{t - 1}{\sqrt{2}C_n} \left( -C_n^2 + \frac{b_n}{2C_n} \right) ; \quad \mu_1 = \frac{t - 1}{\sqrt{2}} \left( C_n^2k + \frac{b_n}{2C_n} \right)
\]

In this case

\[
\begin{align*}
\int_x^\infty & = \frac{\sqrt{2}}{(t^{-1}C_n)} e^{\left( \frac{t^{-2}}{2C_n^2} \right) \mu_0^2} \int_{\mu_0}^{\mu_1} \left[ x \cdot \left( \frac{\ell \cdot \mu}{t^{-1}C_n} - \frac{b_n}{2C_n} \right)^2 \right] e^{-u^2} \, du \\
& = \frac{\sqrt{2}}{(t^{-1}C_n)} e^{\left( \frac{t^{-2}}{2C_n^2} \right) \mu_0^2} \int_{\mu_0}^{\mu_1} \left( \mu + \Phi \mu + \overline{\Phi} \mu^2 \right) e^{-u^2} \, du \quad (A-2)
\end{align*}
\]

where

\[
\begin{align*}
\xi & \equiv \frac{\mu^2}{t^{-2}} - \frac{\beta_n b_n}{2C_n^2} + \frac{\delta_n b_n^2}{4C_n^2} \\
\Phi & \equiv \frac{\sqrt{2}}{t^{-1}} \left( \frac{\beta_n \cdot \mu}{C_n} - \frac{\delta_n b_n}{C_n^2} \right) \\
\overline{\Phi} & \equiv \frac{\delta_n b_n}{C_n^2}
\end{align*}
\]

Since all of the integrals can be expressed in terms of \( \int e^{-u^2} \, du \) and an integrated term, one can write:
The integral from \( K_{\text{min}} \) to \( K_{\text{max}} \) can then be calculated by performing the sum:

\[
I = \sum_{k=1}^{N-1} I_k
\]

Assuming that the resolution, \( \Delta k \), is adequate to describe \( A(k) \) and \( \mathcal{F}(k) \), then the integration is easily performed once the relevant values of

\[
F_A(\xi) = \int_{0}^{\xi} e^{-u^2} du
\]

have been supplied. One has only to calculate and tabulate the functions in order to evaluate the real space parameters. Note that the values of \( x \) and \( t \) are contained in the limit, \( \xi \). In this way one calculates the appropriate \( \xi \) given \( x \) and \( t \) and then performs some sort of interpolation between tabulated values to find \( F(\xi) \). If the functions are calculated accurately, then accuracy is maintained for all values of \( x \) and \( t \).
The value of $\jmath$ is given by:

$$\jmath \equiv \frac{c-i}{\sqrt{2}} \left( \pm c \Delta k + \frac{b}{2c} \right)$$

where $c = \left( \sqrt{-\frac{1}{2}} \right)$ is either purely real or imaginary. Therefore $\jmath$ can be written as $\jmath = \mu (1+i)$, where $\mu$ is real.

As a result:

$$F(\mu(1+i)) = \int_0^\infty e^{-\mu^2} \, d\mu$$

$$= \frac{\sqrt{\pi}}{2} \left[ \left( C\left(\frac{2\mu}{\sqrt{\pi}}\right) + S\left(\frac{2\mu}{\sqrt{\pi}}\right) \right) \\
+ i \left( C\left(\frac{2\mu}{\sqrt{\pi}}\right) - S\left(\frac{2\mu}{\sqrt{\pi}}\right) \right) \right]$$

where

$$C(x) = \int_0^x \cos \frac{\pi t^2}{2} \, dt$$

and

$$S(x) = \int_0^x \sin \frac{\pi t^2}{2} \, dt$$

are Fresnel integrals (Abramowitz & Stegun 1964) and

$$F(\mu(1-i)) = F^*(\mu(1+i))$$

Also, some simplification is afforded by the fact that $F(-\jmath) = -F(\jmath)$. If $\mu$ is less than one, $F(\mu(1+i))$ can be quite accurately represented by 6 terms of its Taylor
series expansion. If \( \mu \) is larger than two, five terms of its asymptotic series suffice. For \( \mu \) between one and two, the integrals were calculated using Simpson's rule with \( \Delta \mu = 0.0004 \). The values were stored at intervals of 0.04 which implies that 26 tabulated values were all that was required. The programme simply performed a linear interpolation between neighbouring tabulated values.

Due to the change of variable in the integration, the quadrature scheme is not valid if \( C = 0 \). If \( C^2 \Delta k^2 < 0.17 \) the programme substitutes a 3-term series expansion for the factor \( e^{-C^2(k-k_\mu)^2} \) in equation (A-1). Also, the error in evaluating the difference between the two error functions is magnified if \( C^2 \Delta k^2 \) is small compared to \( b_n \Delta k \). In the case where \( \frac{C^2 \Delta k}{b_n} < 0.002 \), the above Taylor series approximation for \( e^{-C^2(k-k_\mu)^2} \) was also made. The local frequency of oscillation near \( k_\mu \) is \( b_n + 2C^2(k-\mu^2) \). Given that \( C^2 \Delta k < b_n \), the frequency near \( k_\mu \) is approximately \( b_n \). If \( b_n \) is small, the contribution to the total integral is large, but since \( C^2 \Delta k < b_n \), \( C^2 \Delta k \) is very small and the Taylor series approximation is valid. On the other hand, if \( b_n \) is large then \( C^2(k-\mu)^2 \) may be too large to approximate \( e^{-C^2(k-k_\mu)^2} \) accurately by a few terms of its Taylor expansion. However, this inaccuracy only results if the contribution of this subinterval is negligible. The switching value of 0.002 was found by trial and error using the atmospheric
model dispersion relation for gravity waves described in chapter 3. The condition $\frac{C_s^2 \Delta k}{\kappa} < .002$ can be rewritten as:

$$\frac{-\frac{1}{2} \frac{\partial^2 \sigma}{\partial k^2} \frac{\Delta k}{\kappa} + \frac{\sigma}{\kappa} \frac{t}{\kappa}}{X} < .002$$

Thus the Taylor expansion is used at small times and for regions of $k$-space where the waves are not very dispersive.
APPENDIX B

SHALLOW-WATER MODEL BASIS FUNCTIONS AND EIGENVALUES

To construct the basis functions consideration is made of the linear equation. For ε = 0, (3-4) has two types of solution:

a) \( X \sim X e^{(kx + \frac{f}{2} - \sigma t)} \)

and b) \( X \sim X e^{-aF} e^{(kx - \sigma t)} \) \hspace{1cm} (B-1)

Substituting the form a) into (3-6) yields

\[
\mathcal{L} = \begin{pmatrix} 0 & k & \ell \\ k & 0 & i\ell \\ \ell & -i\ell & 0 \end{pmatrix}
\]

The eigenvalues and associated eigenvectors are:

\[
\sigma_1 = 0 \hspace{1cm} \mathbf{x}' = \omega^{-1} \begin{pmatrix} 1 \\ -\ell \\ i\ell \end{pmatrix}
\]

\[
\sigma_{2,3} = \pm \omega \hspace{1cm} \mathbf{x}^{2,3} = \omega^{-1} \begin{pmatrix} \omega^2 f^2 \\ \sqrt{2} (k^2 + 1) \ell \\ \ell \end{pmatrix} \left( \begin{array}{c} \mathcal{G}_{1,3,k} + i\ell \mathcal{G} \\ \mathcal{G}_{2,1} + i\ell \mathcal{G} \end{array} \right) \hspace{1cm} (B-2)
\]

where \( \omega = (k^2 + 1^2 + f^2)^{1/2} \). Since \( \mathcal{L} \) is self-adjoint, the eigenvectors are orthogonal:

\[
< \mathbf{x}', \mathbf{x}'' > = \mathbf{x}_1^* \mathbf{x}_1' + \mathbf{x}_2^* \mathbf{x}_2' + \mathbf{x}_3^* \mathbf{x}_3' = \delta_{ij}
\]
They also have the properties:

\[ \chi^1(\vec{k}) = \chi^1(-\vec{k}) \]
\[ \chi^2(\vec{k}) = \chi^3(-\vec{k}) \]
\[ \chi^3(\vec{k}) = \chi^2(-\vec{k}) \]

where \( \vec{K} = k_1\hat{i} - j\hat{j} \). The geometry used described an infinitely long channel of unit width. The appropriate boundary conditions which the eigenvectors must satisfy is that the transverse velocity be zero at the walls:

\[ v(x,0,t) = v(x,1,\epsilon) = 0 \]

This can be achieved if the third component is proportional to \( \sin n\pi y \) where \( n = 0,1,2, \ldots \). This involves taking a linear combination of two eigenvectors with the same eigenvalue:

\[ Y_i^{(k)}(k,\vec{r}) = \alpha_j^{(k)}(k) \chi^j e^{(kx,j \pi y - \omega t)} + \beta_j^{(k)}(k) \chi^j e^{-(kx,j \pi y - \omega t)} \]

where the index \( i \) refers to the eigenvalue determined in (B-2): \( i = 1 \) is the zero frequency geostrophic mode, and \( i = 2,3 \) are the rightward and leftward propagating gravity modes respectively. If the above combination of eigenvectors is labeled \( Y_i^{(k)}(k) \) where \( i \) represents the type of mode, \( j \) is the \( y \)-wavenumber divided by \( \pi \), and if the scalar product is defined as in section 3.2.1, then the desired orthogonality property is:

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The coefficients $d_j^i(k)$, $\beta^i_j(k)$ are then given by

$$d_j^i(k) = \frac{c}{\sqrt{2}}, \quad \beta_j^i(k) = -\frac{c}{\sqrt{2}}.$$  

$$d_j^2,3(k) = \frac{c}{\sqrt{2}} \frac{\omega_i k + i k}{(\omega_i^2 k^2 + \lambda_i k^2)^{1/2}} \quad \beta_j^2,3(k) = \frac{c}{\sqrt{2}} \frac{\omega_i k - i k}{(\omega_i^2 k^2 + \lambda_i k^2)^{1/2}}$$

The three modes described above do not form a complete set of basis vectors. There is another set of modes for which the solution takes on the form $b_1$ in equation (B-1). Substitution of this form into the linear equations yields.

$$\sigma_{y,5} = \pm \sqrt{f^2 + k^2 - \alpha^2}$$

The boundary conditions $v(x,0,t) = v(x,1,t) = 0$ can be satisfied only if $\alpha = \pm f$. In this case

$$\sigma_{y,5} = \pm k.$$  

Substitution of these values into the linear problem yields eigenvectors in which $v(x,y,t)$ vanishes everywhere. The solutions are Kelvin waves and are described by:

$$\sigma_{y,5} = \pm k \quad \chi_{y,5}^* = \sigma_{y,5} \left( \begin{array}{c} 1 \\ \mp 1 \\ 0 \end{array} \right)$$

where $\chi_{y,5}$ is chosen such that the basis functions are
orthonormal.

\[ \chi^4 = \left( \frac{f}{e^{2f} - 1} \right)^{1/2} \quad \chi^5 = \left( \frac{f}{1 - e^{-2f}} \right)^{1/2} \]

With the addition of the 2 Kelvin waves, the set of basis functions is now complete. The full orthonormal set is given by equation (3-8) in Section 3.2.1.
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