I.O.S.

QUASI-GEOSTROPHIC OCEAN MODELS EMPLOYING SPECTRAL METHODS
PART I — THEORETICAL BACKGROUND

BY

C.F. ROGERS

REPORT NO. 191

1984

NATURAL ENVIRONMENT RESEARCH COUNCIL

INSTITUTE OF OCEANOGRAPHIC SCIENCES

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When citing this document in a bibliography the reference should be given as follows:-

ROGERS, C.F. 1984 Quasi-geostrophic ocean models employing spectral methods. *Institute of Oceanographic Sciences, Report*, No. 191, 57pp.

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WORMLEY

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This work was supported jointly by the SERC and NERC while the author was on secondment at IOS (Wormley).

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Introduction

This report describes a set of three quasi-geostrophic models designed for oceanographic use. In the vertical variables are expanded in terms of the normal modes of a linearized flat bottom and unforced ocean. In the horizontal spectral techniques are employed using Fourier or Chebyshev functions. The three model oceans which are considered are:

(a) A doubly periodic ocean in the E-W and N-S directions.

(b) A channel ocean periodic in the E-W direction.

(c) A basin ocean.

Each model is designed to run with an arbitrary number of vertical modes and a number of degrees of freedom in the horizontal equal to 2^n (n integer). The number of degrees of freedom in the N-S and E-W directions may be chosen independently. All three models have been coded in as similar a way as possible consistent with their inherent differences and are implemented to run on the CRAY-1 Computer System.

The representation of the quasi-geostrophic dynamics in terms of vertical normal modes and spectral expansions has a number of advantages over alternative and more conventional approaches. First the choice of a vertical normal mode representation has the advantage that a basic state with continuous density stratification can be efficiently treated. Moreover, the modal representation offers the advantage of being optimally calibrated in situations in which two or more physical processes are operating (e.g. bottom topography and nonlinearity) (Flierl, 1978).

The use of spectral expansions for representing the horizontal variation of variables relies mainly on the substantial improved accuracy that such techniques offer over finite difference or finite element methods of comparable number of degrees of freedom. The remarkable accuracy of spectral methods is a result of the rapid convergence one obtains with expansions of smooth functions in series of smooth orthogonal functions. The remainder of such series after N terms in general goes to zero more rapidly than any power of $^1/_N$ as $N \to \infty$ (Gottlieb & Orszag, 1977). In contrast the error associated with a finite difference representation with the same number of degrees of freedom goes like $^1/_{N^2}$ for central difference schemes.

A further aspect makes the use of Chebyshev polynomials attractive for non-periodic ocean domains. The representation of the planetary vorticity effect (β-term) by Chebyshev polynomials is a more accurate procedure owing to the absence of the Gibbs phenomena at the boundaries (Haidvogel 1978). The use of Chebyshev polynomials has the further advantage of providing enhanced resolution at the boundaries where the resolution of narrow boundary currents is often required in oceanographic applications.

The above techniques must however, in order to be useful, be as efficient as finite difference methods of similar degrees of freedom. This aspect is ensured for our applications by the use of Fast Fourier transform algorithms which may also be used to construct Fast Chebyshev transforms (Fast cosine transforms). The solution of the associated Helmholtz equations in the basin and channel models may also be performed competitively in comparison with alternative techniques of equivalent accuracy (Haidvogel & Zang, 1979).

Dynamical Equations

The quasi-geostrophic ocean models considered in this report are based on the quasi-geostrophic equations which are an approximate set of equations derived from the primitive equations of geophysical fluid dynamics. They share with the primitive equations the assumption of hydrostatic balance but in addition further restrict the allowed characteristic velocity scale U and the length scale L. Indeed the quasi-geostrophic equations may be derived from the primitive equations as a first-order approximation in a formal expansion in small Rossby number, $R_0 = U/f_0L \ll 1$. Consistently the time-scales of motion are assumed to be slow relative to the inertial period f_0^{-1} and the aspect ratio of the motion $\delta = H/_L \ll 1$ is regarded as a small quantity (Pedlosky, 1979). Furthermore, the latitudinal extent of the ocean models considered here are restricted to be less than fully global $L/_a \ll 1$. Hence, the so-called β-plane approximation may be made in which only the first order change in the Coriolis term with latitude is retained. A number of derivations of the quasi-geostrophic equations are available in the literature and those to be found in the Evolution of Physical Oceanography (Edited by Warren and Wunsch 1981) are recommended. We present below the quasi-geostrophic equations in order to establish our notation.

The quasi-geostrophic equations are a set of coupled equations for the dynamic geostrophic pressure p, density fluctuations ρ' and the vertical velocity w. In standard depth coordinates and β-plane geometry the horizontal velocities are simply

$$u = -p_y/_{f_0} \qquad v = p_x/_{f_0} \tag{1}$$

and the density fluctuation are described by the hydrostatic equation

$$\rho' = -\rho_o P_z/g \tag{2}$$

where ρ_o is the mean density of the ocean. The vorticity and conservation of density equations are

$$\partial_t \nabla^2 p + \frac{1}{f_o} J(p, \nabla^2 p) + \beta p_x - f_o^2 w_z = 0 \tag{3}$$

and

$$\partial_t p_z + \frac{1}{f_o} J(p, p_z) + w N^2(z) = 0 \tag{4}$$

where $N^2(z) = -\frac{g}{\bar{\rho}} \cdot \frac{d\bar{\rho}}{dz}$ is the mean Brunt-Väisälä frequency; J is the Jacobian operator describing horizontal advection; and ∇^2 is the horizontal Laplacian relating the dynamic pressure to the vorticity $\nabla^2 p$. $\bar{\rho} = \bar{\rho}(z)$ is the density stratification of the motionless mean state about which the fluctuations take place. Elimination of the vertical velocity between the equations (3) and (4) produces the standard quasi-geostrophic potential vorticity equation

$$\frac{\partial}{\partial t}\left(\nabla^2 + \frac{\partial}{\partial z} \cdot \frac{f_o^2}{N^2} \frac{\partial}{\partial z}\right) p + \frac{1}{f_o} J\left(p, \left[\nabla^2 + \frac{\partial}{\partial z} \cdot \frac{f_o^2}{N^2} \frac{\partial}{\partial z}\right] p\right) + \beta p_x = 0 \tag{5}$$

In the absence of forcing and dissipation this equation simply expresses the conservation of potential vorticity following the two-dimensional geostrophic motion i.e.

$$\frac{D_g}{Dt} Q = 0 \tag{6}$$

where
$$\frac{D_g}{Dt} = \frac{\partial}{\partial t} + \frac{1}{f_0} J(p, \ )$$

and
$$Q = \nabla^2 p + f_0 + \beta y + \frac{\partial}{\partial z}\left(\frac{f_0^2}{N^2} \cdot \frac{\partial p}{\partial z}\right)$$

Normal Mode Representation

In the standard form of the quasi-geostrophic equation, eq.(5), N, the Brunt-Väisälä frequency, is a function of depth only. Normal modes describing the vertical structure arise from linearising the equations, since the equation then admits a solution of separable form, $p = \alpha(x,y,t)\, F(z)$, where the boundary condition p_{zt} =0 at z =0, $-H$ translates into F_z =0 at $z = 0, -H$. The equation for the vertical structure functions $F(z)$ is a Sturm-Liouville type equation,

$$\frac{\partial}{\partial z}\left(\frac{f_0^2}{N^2} \cdot \frac{\partial F_i}{\partial z}\right) + \lambda_i F_i = 0 \tag{7}$$

with $\partial_z F_i = 0 \quad , z = 0, -H$

Here λ_i and F_i are the ith eigenvalue (separation constant) and eigenfunction of the system. These functions form a complete orthonormal set of functions for all reasonable density structures. In terms of these functions the general solution to the nonlinear problem (as well as the forced problem if the right-hand side is also expanded in the same set of functions) may be represented by

$$p = \sum_{i=0}^{M-1} \alpha_i(x,y,t)\; F_i(z) \tag{8}$$

The precise form of the modes and values of the separation constants depends on the assumed form of the density structure. As an example, the modes for a simple analytic form of the density structure are given in Appendix F. This appendix also contains a numerical scheme for calculating the modes of a more general density profile. In all cases the set of modes consist of one barotropic mode (F_0 =1, λ_0 =0) and an infinite set of baroclinic modes (F_i , λ_i ; $\lambda_i >$ 0 all $i>0$) with increasing values of λ_i and increasing numbers of crossing points between z =0 and $-H$. Substitution of (8) directly into (5) results in the equation below;

$$\partial_t(\nabla^2-\lambda_k)\alpha_k + \frac{1}{f_0}\sum_{i,j} J(\alpha_i, [\nabla^2-\lambda_j]\,\alpha_j)\xi_{ijk} + \beta\partial_x\alpha_k = 0 \tag{9}$$

for the horizontal part of each vertical mode. Note that ($\nabla^2 - \lambda_k$) α_k gives the vorticity field of the kth mode. The constants ξ_{ijk} are the vertical structure constants defined as

$$\xi_{ijk} \equiv \langle F_i F_j F_k \rangle = \frac{1}{H}\int_{-H}^{0} F_i(z)\, F_j(z)\, F_k(z)\, dz \tag{10}$$

The inclusion of boundary conditions specifying w at $z = 0$ or $z = -H$ requires special care (Flierl 1978). These will, however, be dealt with in greater detail at a later stage. Equation (9) forms the basis of each of the three models; doubly periodic, channel and basin. The solution procedure differs between the three models only because of the different lateral boundary conditions. Before discussing the vertical and horizontal structure problems in greater detail, the constants of motion of the model system of equations will be presented.

Constants of motion

For the adiabatic and unforced system (9) the equations conserve total energy if appropriate boundary conditions are imposed. Multiplying equation (9) by α_k and integrating over the model domain one can show that for the kth mode,

$$\partial_t \frac{1}{2} \iint dx\,dy \, [\nabla\alpha_k . \nabla\alpha_k + \lambda_k \alpha_k^2] - \iint dx\,dy \sum_{ij}^{1} \xi_{ijk} J(\alpha_k, \alpha_i) \eta_j = 0 \quad (11)$$

provided α_k is periodic or spatially constant along the boundary (at most a function of time). The terms involving divergencies then vanish. The Jacobian terms represent the energy exchanges between modes. The total energy, obtained after summing over all modes k , is conserved because ξ_{ijk} and $J(\alpha_k, \alpha_i)$ have opposite symmetry. Thus,

$$\partial_t \frac{1}{2} \iint dx\,dy \sum_{k}^{1} [\nabla\alpha_k . \nabla\alpha_k + \lambda_k \alpha_k^2] = 0 \quad (12)$$

In a similar manner the modal enstrophy equation is found by multiplying equation (9) by $\eta_k = (\nabla^2 - \lambda_k)\alpha_k$ and integrating over the domain.

$$\partial_t \frac{1}{2} \iint dx\,dy \, \eta_k^2 - \iint dx\,dy \sum_{ij}^{1} \xi_{ijk} J(\eta_k, \eta_i) \alpha_j + \iint dx\,dy \, \nabla . \underset{\sim}{Q} = 0 \quad (13)$$

where $\quad \underset{\sim}{Q} = \hat{\imath} \; \frac{\beta}{2} \left(\frac{\partial \alpha_K}{\partial x} \right)^2$

if the boundary conditions on α_K are as already employed. If α_K is periodic in the east-west direction this divergence term vanishes and after summing over all modes the enstrophy of the system is conserved i.e.

$$\partial_t \frac{1}{2} \sum_K \iint dx\,dy \; \eta_K^2 = 0 \qquad (14)$$

However, for a bounded domain in the east-west direction enstrophy is not conserved. This arises because a Rossby wave packet reflected from a meridional boundary preserves its energy but increases its total wave number, thereby increasing its enstrophy.

Spectral Methods

As already mentioned in the introduction, equation (9) is solved using spectral methods. In these methods the dependent variable, in our case $\alpha_K(x, y, t)$, is represented as a truncated series of known functions of the independent variables x and y. In general one may choose either a set of functions which satisfy the boundary conditions individually (Galerkin method) or apply the boundary conditions as constraints on the expansion coefficients (Tau method). For the doubly periodic ocean the periodic boundary conditions are most conveniently imposed by the choice of a Fourier series representation. This provides an example of the former method. However, our use of Chebyshev polynomials in the channel and basin oceans provides an example of the latter method. Here the individual Chebyshev polynomials do not satisfy the boundary conditions imposed on the problem (typically $\alpha_k = 0$ on the boundary). Instead the boundary conditions are represented by constraints on the expansion coefficients of the representation. These differences will be seen more clearly in the next sections which describe the methods in greater detail.

Doubly Periodic Ocean

For the doubly periodic ocean the streamfunction of the ith mode (eq. 9) is represented as a truncated Fourier series. Dropping the i suffix the expression for $\alpha_i(x, y)$ is

$$\alpha(x,y,t) = \sum_{\|k\| \leq K} \sum_{\|\ell\| \leq K} \hat{\alpha}_{k\ell}(t)\, e^{ikx}\, e^{i\ell y} \qquad (15)$$

on the domain $0 \leq x \leq 2\pi$

$0 \leq y \leq 2\pi$

where k and ℓ are integers and $\|k\| \leq K$ implies $-K \leq k < K$. $\hat{\alpha}_{k\ell}$ represent the Fourier coefficients in the transform space. If x and y are determined on the uniform grid $x_n = \frac{2\pi n}{2K}$, $y_m = \frac{2\pi m}{2K}$ then to conform with FFT transform algorithms a computational set of Fourier coefficients $a_{k\ell}$ is introduced. The relationship between $\hat{\alpha}_{k\ell}$ and $a_{k\ell}$ is described in more detail in appendix G.

$$\alpha_{nm} = \alpha(x_n, y_m) = (-1)^{n+m} \sum_{k=0}^{N-1} \sum_{\ell=0}^{N-1} a_{k\ell}\, e^{\frac{2\pi i k n}{N}} \cdot e^{\frac{2\pi i \ell m}{N}} \qquad (16)$$

where $N = 2K$ and $a_{k+K,l+K} = \hat{\alpha}_{kl}$. Since α_{nm} is real the expansion coefficients a_{kl} satisfy the conjugate relation.

$$a_{kl} = a^{*}_{N-k,N-l} \tag{17}$$

This property reassures us that only N^2 variables need be stored.

In the doubly periodic ocean model the spectral functions diagonalise the Laplacion operator. Hence employing a leapfrog time scheme the transform space form of eq. (9) becomes

$$-(k^2+l^2)\left(\frac{\hat{\alpha}^{n+1}_{kl} - \hat{\alpha}^{n-1}_{kl}}{2\Delta t}\right) + i\beta k \hat{\alpha}^{n}_{kl} + \hat{J}^{n}_{kl} = 0 \tag{18}$$

Here $\hat{\alpha}^{n}_{kl}$ represents the value of the streamfunction at the nth time-step and $\hat{J}^{n}_{kl}$ represents the total nonlinear transform space contribution. We may consequently step-forward in time given $\hat{\alpha}_{kl}$ at two previous time levels provided $\hat{J}^{n}_{kl}$ is known from $\hat{\alpha}^{n}_{kl}$. We discuss the determination of $\hat{J}^{n}_{kl}$, together with the time-stepping procedure in greater detail at a later stage.

Chebyshev Channel Model

For a channel ocean model in which the flow is bounded in the N-S direction by impenetrable walls we need to impose the boundary condition $\alpha = 0$ along the zonal boundaries. The flow is assumed to be periodic in the E-W direction. A possible choice of spectral functions in this case is a truncated mixed Fourier-Chebyshev expansion of the form

$$\alpha(x,y) = \sum_{\|k\| \leq K} \sum_{m=0}^{N} \hat{\alpha}_{km}\, e^{ikx}\, T_m(y) \tag{19}$$

on the domain: $-1 \leq y \leq 1$

$0 \leq x \leq 2\pi$

If a mixed spatial grid is introduced

$$x_n = \frac{2\pi n}{2K} \qquad n = 0, 1 \ldots 2K-1$$

$$y_j = \cos\left(\frac{\pi j}{N}\right) \qquad j = 0, 1 \ldots N \tag{20}$$

we may make use of the important relation between Chebyshev polynomials and cosine functions.

$$\alpha_{nj} \equiv \alpha(x_n, y_j) = (-1)^n \sum_{k=0}^{N-1} \sum_{m=0}^{N} a_{km}\, e^{\frac{2\pi i k n}{N}} \cos\left(\frac{\pi j m}{N}\right) \tag{21}$$

Since α_{nj} is real the expansion coefficients a_{km} satisfy

$$a_{km} = a^{*}_{N-k,m} \tag{22}$$

Although this representation possesses advantages for representing baroclinic modes the spectral functions no longer diagonalise the Laplacian operator. To solve this problem we represent the potential vorticity in the ith mode by $\eta = (\nabla^2 - \lambda)\alpha$, and substitute into eq. (9). Approximating the time derivative by a leap-frog scheme

$$\frac{\hat{\eta}^{n+1}_{km} - \hat{\eta}^{n-1}_{km}}{2\Delta t} + ik\beta\,\hat{\alpha}^{n}_{km} + \hat{J}^{n}_{km} = 0 \qquad (23)$$

where $\hat{\eta}$ is the spectral expansion coefficient of η. Hence knowing $\hat{\eta}^n$, $\hat{\eta}^{n-1}$ and $\hat{\alpha}^n$; and assuming we may determine $\hat{J}^n$ from $\hat{\alpha}^n$ and $\hat{\eta}^n$ we may step-forward in time if $\hat{\alpha}^{n+1}$ can be found from $\hat{\eta}^{n+1}$. Substitution of eq (19) and its equivalent for η into the above Helmholtz equation relating α and η gives,

$$(-k^2-\lambda)\,\hat{\alpha}_{km} + \frac{1}{c_m}\sum_{\substack{p=m+2\\ p+m\ \text{even}}}^{N} p(p^2-m^2)\,\hat{\alpha}_{kp} = \hat{\eta}_{km} \qquad (24)$$

$$0 \leq m \leq N-2 \; ; \; \|k\| \leq K$$

where $c_0=2$, $c_n=1$ for $n \geq 1$. We have made use of the properties of Chebyshev polynomials collected in appendix A to represent the 2nd derivative in the y-direction. Note that although there are $2K\times(N+1)$ coefficients in (19) we only have $2K\times(N-1)$ equations in (24). The other $4K$ equations are provided by the boundary condition $\alpha = 0$ on $y = \pm 1$. The property $T_n(\pm 1) = (\pm 1)^n$ implies,

$$\sum_{\substack{p=0\\ p\ \text{even}}}^{N} \hat{\alpha}_{kp} = \sum_{\substack{p=1\\ p\ \text{odd}}}^{N} \hat{\alpha}_{kp} = 0 \quad , \; \|k\| \leq K \qquad (25)$$

When the boundary conditions are combined with equation (24) the $2K_*(N+1)$ coefficients $\hat{\alpha}_{kp}$ are completely determined. This method of dropping the equations for the highest modes and determining them directly from the boundary conditions is equivalent to the tau method.

The solution of the set of equations (24) is straightforward although it is best to first transform the system to a quasitridiagonal form (see Appendix D). The system can be decomposed into N independent systems of equations, one for each value of k. Furthermore, for fixed k each system can be written as (Gottlieb & Orszag (1977), Haidvogel (1978)),

$$q\, \ell_n \hat{\alpha}_{k,n-2} + (1 - q\, d_n)\hat{\alpha}_{k,n} + q\, u_n \hat{\alpha}_{k,n+2} = \hat{f}_{kn} \qquad (26)$$

$$2 \leq n \leq N$$

where

$$\ell_n = \frac{c_{n-2}}{4n(n-1)}$$

$$d_n = \frac{e_{n+2}}{2(n^2-1)}$$

$$u_n = \frac{e_{n+4}}{4n(n+1)}$$

$$\hat{f}_{kn} = \ell_n \hat{\eta}_{k,n-2} - d_n \hat{\eta}_{k,n} + u_n \hat{\eta}_{k,n+2}$$

and

$$q = -(k^2 + \lambda)$$

The even and odd terms in this system of equations decouple and thus may be treated separately. Each of these subsystems consists of a tridiagonal set of equations accompanied by a row of 1's arising from the boundary conditions. These quasitridiagonal systems can be solved by a Gaussian elimination and further details are contained in Appendix C.

Barotropic Sine Channel Model

For some purposes in which only a barotropic model is required a sine expansion in the N-S direction provides an economical alternative to the Chebyshev model already described. It also provides better resolution in the middle of the channel which may be an advantage for some applications. For baroclinic applications, however, the streamfunction is not necessarily zero on the boundaries. The stream function represented as a sine expansion will always be zero on the channel walls and although this may be overcome using a mixed sine/cosine representation the uniformity of approach is lost (White, 1978). For the barotropic case, the sine representation does possess, however, the advantage of requiring no solution of a Poisson equation. The barotropic streamfunction is then represented as a mixed Fourier-Sine expansion of the form

$$\alpha(x,y) = \sum_{\|k\| \leq K} \sum_{m=0}^{N} \hat{\alpha}_{km} \, e^{ikx} \sin(my) \tag{27}$$

on the domain $0 \leq y \leq \pi$

$0 \leq x \leq 2\pi$

The spatial grid is now uniform in both directions

$$x_n = \frac{2\pi n}{2K} \qquad n = 0, 1 \ldots 2K-1$$
$$y_j = \frac{\pi j}{N} \qquad j = 0, 1 \ldots N \tag{28}$$

The values of the stream function on this grid are:

$$\alpha_{nj} \equiv \alpha(x_n, y_j) = (-1)^n \sum_{k=0}^{N-1} \sum_{m=0}^{N} \hat{\alpha}_{km} \, e^{\frac{2\pi i k n}{N}} \sin\left(\frac{m j \pi}{N}\right) \tag{29}$$

and the coefficients are also conjugate symmetric as in previous cases. As in the doubly periodic model the Laplacian is diagonal in this representation and we may employ a leapfrog time scheme directly on the streamfunction. Derivative operations on the streamfunction may also be found easily in the E-W direction but those in the N-S direction require extra care. These are required for the evaluation of the non-linear Jacobian terms and as the derivative in the N-S direction converts the representation into a cosine series a cosine transform algorithm is required to determine physical space values of the arrays. These are already available for the Chebyshev models and may be employed in the determination of the Jacobian advective terms.

Basin Model

For a basin ocean model we bound the flow with impenetrable meridional as well as zonal walls. In order to impose these constraints we have employed an extension of the Chebyshev channel model. We chose in this case to represent the streamfunction as a double Chebyshev expansion of the form

$$\alpha(x,y) = \sum_{n=0}^{N} \sum_{m=0}^{N} \hat{\alpha}_{nm} T_n(x) T_m(y) \tag{30}$$

on the domain $-1 \leq y \leq 1$

$-1 \leq x \leq 1$

For the non-uniform spacial grid

$$x_i = \cos\left(\frac{\pi i}{N}\right) \quad i = 0,1 \ldots N$$

$$y_j = \cos\left(\frac{\pi j}{N}\right) \quad j = 0,1 \ldots N \tag{31}$$

This representation is equivalent to a double cosine-transform

$$\alpha_{ij} \equiv \alpha(x_i y_j) = \sum_{n=0}^{N} \sum_{m=0}^{N} \hat{\alpha}_{nm} \cos\left(\frac{\pi i n}{N}\right) \cos\left(\frac{\pi m j}{N}\right) \tag{32}$$

Consequently we may use FFT transforms to determine $\hat{\alpha}_{nm}$.

In this representation the β-term and non-linear advection terms may be calculated by making use of the derivative algorithms for Chebyshev series (see Appendix A). Like the Chebyshev channel model the Laplacian operator associated with the solution of the Helmholtz equation

$$(\nabla^2 - \lambda)\alpha = \eta \quad , \quad \alpha = 0 \quad \text{on the boundaries} \tag{33}$$

is not diagonalised by this choice of spectral functions. Furthermore, the spectral functions in the x-direction are no longer eigenfunctions of ∂_x^2-operator. To overcome this latter difficulty we follow Haidvogel (1978) and first introduce discrete eigenfunctions of the ∂_x^2 -operator which satisfy homogeneous boundary conditions. It should be noted that the discrete eigenfunctions may be introduced in either the E-W or N-S directions. The analysis described below assumes discrete eigenfunctions in the E-W direction. To obtain N-S discrete eigenfunctions it is sufficient to transpose the matrices F and A in equations (36) and (38). It has generally been found preferable to use N-S discrete eigenfunctions as errors associated with the discrete representation propagate less readily as linear Rossby waves. Although this procedure incurs extra processing it need only be performed once and so is well suited to the situation of repeated solution of equation (33). The eigenvalue problem of the ∂_x^2 -operator is

$$\partial_x^2 u_\nu = \lambda_\nu u_\nu \quad ; \quad u_\nu(\pm 1) = 0 \tag{34}$$

If $$u_\nu(x) = \sum_{n=0}^{N} e_{n\nu} T_n(x)$$

there are (N-1) non-zero eigenvalues and eignvectors $\underset{\sim}{e}_\nu^T$ = ($e_{0\nu}$, $e_{1\nu}$,.... $e_{N\nu}$).The determination of the $e_{n\nu}$ and λ_ν is described in greater detail in Appendix (E). The eigenfunctions $u_\nu(x)$ are now used to partially diagonalise the Laplacian operator. To do this the streamfunction α and the vorticity η are expanded in the modified double spectral functions

$$\begin{aligned} \alpha(x,y) &= \sum_{n=0}^{N-2} \sum_{m=0}^{N} b_{nm}\ u_n(x)\ T_m(y) \\ \eta(x,y) &= \sum_{n=0}^{N-2} \sum_{m=0}^{N} g_{nm}\ u_n(x)\ T_m(y) \end{aligned} \tag{35}$$

The coefficients g_{nm} and $\hat{\eta}_{nm}$ ($0 \leqslant n \leqslant N-2,\ 0 \leqslant m \leqslant N$) are related by

$$G = E^{-1} F \tag{36}$$

where G and F are the matrices of g_{nm} and $\hat{\eta}_{nm}$ and E^{-1} is the (N-1)x(N-1) inverse of E (the coefficients e_{nm} minus its last two rows). With this representation equations analogous to the Chebyshev channel model are obtained

$$(\lambda_n - \lambda)\, b_{nm} + \frac{1}{c_m} \sum_{\substack{q=m+2 \\ q+m \text{ even}}}^{N} q(q^2 - m^2)\, b_{nq} = g_{nm} \tag{37}$$

$$0 \leqslant n \leqslant N-2$$

and

$$0 \leqslant m \leqslant N-2$$

$$\sum_{\substack{q=0 \\ q \text{ even}}}^{N} b_{nq} = \sum_{\substack{q=1 \\ q \text{ odd}}}^{N} b_{nq} = 0 \qquad 0 \leqslant n \leqslant N-2$$

These equations can be handled as described in that section. We can, therefore, obtain b_{nm}(0<n<N-2, 0< m<N) by the same quasitridiagonal solution algorithm. The Chebyshev coefficients $\hat{\alpha}_{nm}$ can be recovered by performing the matrix multiplication

$$A = E\, B \tag{38}$$

where A is the matrix $\hat{\alpha}_{nm}$(0<n<N-2, 0< m<N). To obtain the remaining terms

$\hat{\alpha}_{N,m}$ and $\hat{\alpha}_{N-1,m}$ for $0 \leq m \leq N$ the boundary condition relationships are used.

Boundary conditions

Associated with the spectral methods discussed in the previous sections further consideration must be given to the appropriate lateral boundary conditions. In addition, the boundary conditions on w at $z = 0$ or $z = -H$ in forced applications must also be examined.

Including the possibility of Ekman pumping forced by wind stress the top boundary condition is,

$$w = w_E(x,y,t) = \frac{1}{\rho_0 f_0} \cdot \mathrm{curl}_z \underset{\sim}{\tau} \qquad \text{at} \quad z = 0 \tag{39}$$

At the bottom of the ocean topography and Ekman layer friction are included with the specification

$$w = \frac{1}{f_0}\left[J(p,b) + \sqrt{\frac{\nu}{2f_0}}\; \nabla^2 p \right] \quad \text{at} \quad z = -H \tag{40}$$

Here $b(x,y)$ is the deviation of the bottom from level (i.e. the true bottom is at $z = -H + b$) and ν is the eddy viscosity appropriate to the bottom Ekman layer. As shown by Flierl (1978) the inclusion of these forcing effects modifies equation (9) in the following manner:

$$\begin{aligned} &\left\{ \partial_t [\nabla^2 - \lambda_k] + \beta \partial_x \right\} \alpha_k + \frac{1}{f_0} \sum_{ij} J(\alpha_i, [\nabla^2 - \lambda_j]\alpha_j)\, \xi_{ijk} \\ &= \frac{f_0^2}{H} F_k(0)\, w_E \;-\; \frac{f_0}{H} F_k(-H) \sum_i \left[J(\alpha_i, b) + \sqrt{\frac{\nu}{2f_0}}\; \nabla^2 \alpha_i \right] F_i(-H) \end{aligned} \tag{41}$$

We shall now consider the appropriate lateral boundary conditions for the streamfunction. It is only lateral friction parameterizations such as

Laplacian friction or biharmonic friction which require additional boundary conditions. For the case of a doubly periodic ocean periodicity in the E-W and N-S directions for each mode is sufficient. For models with impenetrable boundaries the streamfunction must be spatially constant in order that the normal geostrophic velocity vanishes on the boundary. Hence to 1st order in the Rossby number

$$\alpha_k \Big|_{\text{boundary}} = c_k(t) \qquad k = 0, 1, \ldots M-1 \tag{42}$$

For the barotropic mode this constant may be set to zero without loss of generality (Pedlosky, 1979). For the remaining baroclinic modes c_k, $k = 1, \ldots$ McWilliams (1977) has shown that the time-varying functions must be chosen to satisfy that there be no vertical mass flux through the ocean. The mass continuity equation to 1st order in the Rossby number implies

$$\iint dx\,dy\; w = 0 \qquad \text{for all } z$$

If w is expressed in normal modes we obtain

$$\iint dx\,dy\; w_k = 0 \qquad \text{for all baroclinic modes}$$

Equation (4) further implies that

$$\partial_t \iint dx\,dy\; \alpha_k = 0 \qquad \text{for all } t$$

or

$$\iint dx\,dy\; \alpha_k = \text{constant} = \iint dx\,dy\; \alpha_k \Big|_{t=0} \tag{43}$$

This constant is zero if α_k is zero at $t=0$. That is the initial state of the ocean is at rest.

The full solution for the baroclinic modes may be written as a sum of a particular solution α_k^p (with $\alpha_k^p = 0$ on the boundary) and a homogeneous solution (with α_k^h =1 on the boundary). The actual baroclinic solution is then

$$\alpha_k = \alpha_k^p + c_k \alpha_k^h \tag{44}$$

where

$$c_k = - \frac{\iint dx\,dy\, \alpha_k^p}{\iint dx\,dy\, \alpha_k^h} \qquad \text{assuming } \alpha_k = 0 \text{ at } t=0 \tag{45}$$

The homogeneous solutions satisfy

$$(\nabla^2 - \lambda_k)\,\alpha_k^h = 0 \qquad \text{with } \alpha_k^h = 1 \text{ on the boundary} \tag{46}$$

These solutions, α_k^h, need be determined only once as a preprocessing step at the beginning of a simulation. They may be determined by first subtracting one from the solution i.e. $\alpha_k^h = \phi_k + 1$ and solving

$$(\nabla^2 - \lambda_k)\,\phi_k = \lambda_k \qquad \text{with } \phi_k = 0 \text{ on the boundary} \tag{47}$$

The solution algorithms for the Helmholtz equation are used to solve this problem.

Lateral Dissipation

Lateral dissipation mechanisms are often required in highly turbulent flows or flows with significant non-linear transfers in order to dissipate the enstrophy that inevitably builds up at small scales or large horizontal mode numbers. We may adopt two approaches to this problem. Scale-selective parameterizations may be introduced into the dynamical equations themselves or a filter procedure may be applied to the vorticity field, thereby removing the smaller scales of motion. For the doubly periodic ocean the introduction of Laplacian friction ($\nabla^4 \alpha_k$) or biharmonic friction ($\nabla^6 \alpha_k$) incurs very little increased computational cost since the Fourier representation diagonalises these operators. However, for the Basin or channel ocean models each new power of ∇^2 implies an extra Helmholtz solution at each time-step. Furthermore, the inclusion of explicit dissipation increases the order of the dynamical equations. Consequently additional ill-defined boundary conditions must be imposed (Marshall 1982). Consequently for the ocean models described in this report a compromise has been made. For the basin ocean model Laplacian friction is explicitly included and further implicit dissipation is provided by applying a filter to the vorticity field. Basin ocean models are available with a choice of zero vorticity or zero gradient vorticity boundary conditions i.e.

$$\begin{aligned} \eta_k \big|_{\text{boundary}} &= 0 && \text{zero vorticity} \qquad (48) \\ \frac{\partial \eta_k}{\partial n}\Big|_{\text{boundary}} &= 0 && \text{zero gradient vorticity} \end{aligned}$$

Modifications to the Helmholtz solution algorithm have been made to accommodate the zero gradient boundary condition.

We have adopted the filtering procedure successfully applied by Haidvogel, Robinson and Schulman (1980) to the vorticity field.

$$\hat{\eta}_{nm}(\text{filtered}) = f_n f_m \hat{\eta}_{nm}$$

where the spectral filter

$$f_n = 1 - \exp(-\kappa[N^2 - n^2]) \tag{49}$$

and $\kappa = \dfrac{2.3}{[N^2 - n_{90}^2]}$ gives 10% reduction of the n_{90} mode.

Non-linear advection

The non-linear advection of each mode receives contributions from all other modes coupled through the vertical density structure. In equation (9) this means that each modal equation contains the contribution

$$\sum_{ij} J(\alpha_i, \eta_j)\, \xi_{ijk} \tag{50}$$

where $\eta_j = (\nabla^2 - \lambda_j)\alpha_j$ and $J(\alpha_i, \eta_j) = \partial_x \alpha_i\, \partial_y \eta_j - \partial_y \alpha_i\, \partial_x \eta_j$

The Jacobian $J(\alpha_i, \eta_j)$ is calculated at each time-step for each mode in spectral space. In order to determine the contribution for each mode the Jacobian terms are evaluated from the spectral space components of η_j and α_i. The arrays are transformed to real space where the nonlinear products are evaluated locally. Finally a transformation back to spectral space is performed. An algorithm such as this to evaluate non-linear contributions is known as a pseudo-spectral approximation. The evaluation of the nonlinear products in real space introduces aliassing errors into the Jacobians which may lead to aliassing instability. We may adopt two approaches to overcome this problem; either we remove the aliassing errors completely or constrain them so that an instability does not develop. The former, however, may only be done at the cost of using twice as many transform operations. Furthermore, the method of de-aliassing assumes a uniform grid in real space. We have consequently implemented a fully alias-free Jacobian only for the doubly periodic ocean.

The second approach makes use of the analogy with the well-known Arakawa finite-difference forms of the Jacobian (Arakawa, 1966). We may construct a set of pseudo-spectral nonlinear approximations to the Jacobian which conserve either energy, enstrophy or both for orthonormal spectral functions with respect to unit weight. For example, the form:

$$J(\alpha,\eta) = \partial_y(\alpha_x \eta) - \partial_x(\alpha_y \eta) \tag{51}$$

may be used to construct an aliassed approximation to the Jacobian which conserves energy. The aliassing errors have been shown to be small for the case of 2-D turbulence (Fox and Orszag, 1973). Strict energy conservation is guaranteed only for orthonormal functions with unit weight. The weight function for Chebyshev polynomials is quite different - $w(x) = (1-x^2)^{-1/2}$ and energy will no longer be conserved. However, non-conservation associated with Chebyshev spectral techniques rarely exceeds one part in 10^5 (Haidvogel, 1977).

The nondimensional equations

The complete quasi-geostrophic potential vorticity equation, eq (41), is scaled with length scales L_x and L_y, and the time scale, $T = (\beta L_x)^{-1}$. Laplacian lateral friction is included for completeness. Asterisks denote dimensional variables.

$$x^* = L_x x \equiv L x$$

$$y^* = L_y y \equiv \left(\frac{L_y}{L_x}\right) \cdot L y$$

$$t^* = T t$$

The non-dimensional potential vorticity equation may be written:

$$\{\partial_t [\nabla^2 - \lambda_k] + \partial_x\} \phi_k + R \sum_{ij} J(\phi_i, [\nabla^2 - \lambda_j] \phi_j) \xi_{ijk}$$

$$= F_k(0) \operatorname{curl}_z \underset{\sim}{\tau} + LF . \nabla^4 \phi_k$$

$$- F_k(-H) \sum_i [G \, J(\phi_i, \frac{b}{H}) + BF \, \nabla^2 \phi_i] F_i(-H) \quad (52)$$

where $\operatorname{curl}_z \underset{\sim}{\tau} = \partial_x \tau^y - \left(\frac{L_x}{L_y}\right) \partial_y \tau^x$

and $\nabla^2 \equiv \partial_x^2 + \left(\frac{L_x}{L_y}\right)^2 \partial_y^2$

The non-dimensional constants and scaling factors are given below:

$$\alpha_K^* = \left(\frac{f_o \tau_o}{\rho_o H \beta} \right) \phi_K$$

$$\underset{\sim}{T}^* = \tau_o \underset{\sim}{T}(x,y)$$

$$\lambda_K^* = L^{-2} . \lambda_K$$

$$R = \frac{\tau_o}{\rho_o L^3 \beta^2 H} . \left(\frac{L_x}{L_y} \right)$$

$$G = \frac{f_o}{\beta L} . \left(\frac{L_x}{L_y} \right)$$

$$BF = \frac{1}{\beta L} . \varepsilon = \left(\frac{1}{\beta L} \right) \left(\frac{f_o}{H} \sqrt{\frac{\nu}{2 f_o}} \right)$$

$$LF = \frac{A_4}{\beta L^3}$$

The computational domain for the basin model is $(-1,+1)^2$; for the doubly periodic model $(0,2\pi)^2$ and for the Chebyshev channel model $(-1,+1)x(0,2\pi)$. Table I gives typical values of the non-dimensional constants for a square basin of depth H = 5 km and wind stress $\tau_0 = 10^{-1} Nm^{-2}$. The horizontal velocities are scaled with the Sverdrup velocities

$$U = \left(\frac{\tau_o}{\beta H \rho_o L} \right) \quad \text{and} \quad V = \left(\frac{\tau_o}{\beta H \rho_o L} \right) \left(\frac{L_x}{L_y} \right)$$

TABLE I

Non-dimensional constants for a square basin

Constants	L=500 km	L=1000 km
R	0.4×10^{-3}	0.5×10^{-4}
BF($\varepsilon=10^{-7}s^{-1}$)	10^{-2}	0.5×10^{-2}
LF($A_4=100\ m^2s^{-2}$)	4×10^{-5}	0.5×10^{-5}
G	10.0	5.0

Time differencing techniques

The ocean models described in this report generally use a 'leap-frog' approximation to represent the rate of change of relative vorticity in eq (52):

$$\left(\frac{\partial \eta}{\partial t}\right)^n \approx \frac{\eta^{n+1} - \eta^{n-1}}{2\Delta t} \tag{53}$$

which is accurate to second order. An explicit forward step is performed at the beginning of an integration or on commencement of a further integration. Additional forward steps may be taken, when necessary, in order to suppress the computational mode associated with the 'leap-frog' approximation.

The bottom frictional term is treated semi-implicitly for barotropic ocean models, although for baroclinic models a lagged procedure is considered easier to implement. Unlike finite difference methods lateral frictional terms in spectral models must be treated semi-implicitly in order to correctly implement the higher order boundary conditions. All other contributions to the potential vorticity equation are treated explicitly. Examples of the time-differencing procedures for basin or channel oceans are given below. For the doubly periodic ocean the time-stepping may be expressed directly in terms of the streamfunction. The examples below are expressed in real space and are derived from eq (52), whereas computationally the time-step procedure is applied in transform space.

(a) A barotropic ocean with bottom friction

$$\begin{aligned}\zeta_o^{n+1} &= \left(\frac{1-\Delta t.\, BF}{1+\Delta t.\, BF}\right)\zeta_o^{n-1} + \frac{2\Delta t}{(1+\Delta t \cdot BF)}\Big(\partial_x \phi_o^n + R\, J(\phi_o^n, \zeta_o^n) \\ &\qquad + \operatorname{curl}_z \underset{\sim}{\tau} - G\, J(\phi_o^n, \tfrac{b}{H})\Big) \\ \zeta_o^{n+1} &= \nabla^2 \phi_o^{n+1}\end{aligned} \tag{54}$$

(b) A barotropic ocean with bottom and lateral friction.

$$\chi_{+}^{n+1} = -\chi_{-}^{n-1} + \frac{2}{LF} \cdot \left(\partial_x \phi_o^n + R\, J(\phi_o^n, \zeta_o^n) + \operatorname{curl}_z \underset{\sim}{\tau} - G\, J(\phi_o^n, \tfrac{b}{H}) \right)$$

$$\chi_{\pm}^{n+1} = \nabla^2 \zeta_o^{n+1} \mp \frac{(1 \pm \Delta t . BF)}{LF . \Delta t} \zeta_o^{n+1} \tag{55}$$

$$\zeta_o^{n+1} = \nabla^2 \phi_o^{n+1}$$

A Helmholtz equation is first solved to determine ζ from the time-step variable χ and finally Poisson's equation is solved to determine the stream function.

(c) General case

Since the bottom frictional contribution to the K th vertical mode equation, eq (45), involves a sum over all vertical modes the semi-implicit treatment of this term is less straightforward for the general baroclinic case. Treating this contribution lagged by one time-step avoids this difficulty and maintains computational stability. The higher order lateral friction, however, must still be treated semi-implicitly.

$$\begin{aligned} \chi_{+}^{n+1} = -\chi_{-}^{n-1} &+ \frac{2}{LF}\Big(\partial_x \phi_K^n + R \sum_{ij}{}' \xi_{ijK} J(\phi_i^n, \eta_j^n) - F_K(0) \operatorname{curl}_z \underset{\sim}{\tau} \\ &+ F_K(-H) \sum_i{}' \left[G\, J(\phi_i^n, \tfrac{b}{H}) + BF\, \nabla^2 \phi_i^{n-1} \right] F_i(-H) \Big) \end{aligned} \tag{56}$$

where

$$\chi_{\pm} = \nabla^4 \phi_K \pm \frac{1}{\Delta t . LF} \nabla^2 \phi_K \mp \frac{\lambda_K}{\Delta t . LF} . \phi_K$$

To regain the streamfunction at the new time level the solution of two Helmholtz equations involving the auxiliary field Θ is required. Thus,

$$\chi_{+}^{n+1} = \nabla^2 \theta^{n+1} - B\,\theta^{n+1}$$

$$\theta^{n+1} = \nabla^2 \phi_{K}^{n+1} - A\,\phi_{K}^{n+1}$$

where

$$A = \frac{1 - \sqrt{1 - 4\Delta t.LF.\lambda_K}}{2\Delta t.LF} \sim \lambda_K + O(\Delta t.LF)$$

$$B = \frac{1}{\Delta t.LF} - \lambda$$

determines the streamfunction ϕ_{K}^{n+1}. The vorticity η^{n+1}, required for the non-linear advection, is approximately given by θ^{n+1}. It may, however, be determined exactly once ϕ^{n+1} has been found.

(d) Time-step constraints

The time differencing techniques described above are subject to certain stability restrictions. The most important, the so called CFL-constraint (Courtant, Friedrich, Levy) restricts the ratio of Δx / Δt to be greater than the fastest velocity in the ocean. This might be, for example, the advective velocity or a phase velocity. For ocean models with variable effective grid spacing increased resolution may increase the severity of this constraint. The fastest velocity in the basin ocean model may be the phase velocity of the basin modes or for significantly non-linear flows the advective velocity. We present below estimates of the CFL-constraint for various basin model parameters.

(i) Rossby basin modes

The Rossby basin modes are solutions to the linear problem

$$\partial_t(\nabla^2-\lambda)\phi + \partial_x\phi = 0 \tag{57}$$

with $\phi = 0$ on the boundaries $-1 \leq {x \atop y} \leq 1$. Non-dimensional coordinates are assumed in this section. The solution is easily constructed

$$\phi_{nm} = \sin\frac{n\pi}{2}(x+1)\sin\frac{m\pi}{2}(y+1)\cos\left(\frac{x}{2\omega_{nm}} + \omega_{nm}t\right) \tag{58}$$

where

$$\omega_{nm} = \frac{1}{2\left[\lambda + \frac{\pi^2}{4}(n^2+m^2)\right]^{1/2}}$$

and the phase velocity is

$$c_{nm} = -\frac{1}{2\left[\lambda + \frac{\pi^2}{4}(n^2+m^2)\right]}$$

The fastest mode corresponds to the barotropic (1,1)-mode with phase velocity

$$c_{11} = -\frac{1}{\pi^2}$$

implying the CFL-constraint: $\Delta t < \Delta x\, \pi^2$

In terms of dimensional variables

$$\Delta t^* < \frac{\Delta x^*}{L} \cdot \frac{\pi^2}{L\beta}$$

For the Chebyshev basin ocean with $(N+1)$ Chebyshev polynomials in each direction the smallest Δx is

$$\Delta x \sim \frac{1}{2}\left(\frac{\pi}{N}\right)^2$$

The corresponding largest time-step Δt^* for a 1000 km basin and 33 Chebyshev polynomials is 1.32 hrs. Table II gives a comparison of largest allowed time-step for various sized oceans and number of degrees of freedom. It should be emphasised that this is only a constraint if the basin modes are excited.

(ii) Advective velocity

In performing integrations in which significant non-linear flows develop advective velocities may become sufficiently large as to exceed the CFL-constraint. For the non-dimensional scaling described in the previous section the velocities are scaled with the Sverdrup velocity.

$$U = \left(\frac{\tau_0}{\beta H \rho_0 L} \right)$$

Furthermore, the CFL-constraint implies

$$U \partial_x \phi < \frac{\Delta x^*}{\Delta t^*}$$

or in non-dimensional form

$$R \partial_x \phi < \frac{\Delta x}{\Delta t}$$

The strength of the advective velocities that actually develop in an integration will, of course, depend on the strength of the wind forcing or other forcing mechanism together with the strength of the dissipative mechanisms. It may be possible to make estimates of these velocities from linear solutions to the problem in hand. Table III indicates, however, that excessive resolution in the boundary layer severely restricts the permissible time-step for advective velocities of 1-2 m s^{-1}. Consequently care must be exercised in the choice of number of Chebyshev polynomials for a given basin size in order that the boundary layers are not over resolved.

TABLE II

Basin mode-CFL constraint

Basin size (km)	17 $\Delta x=1.9x10^{-2}$	33 $\Delta x=4.8x10^{-3}$	65 $\Delta x=1.2x10^{-3}$	129 $\Delta x=3.0x10^{-4}$
1000	5.28	1.32	0.33	0.08
2000	2.64	0.66	0.17	0.04
4000	1.32	0.33	0.08	0.02

TABLE III

Largest Δt^* (hrs) for a given advective velocity

Advective velocity (ms^{-1})	2.5 km	5.0 km	10.0 km	20.0 km
10^{-1}	6.95	13.90	27.8	55.6
1.0	0.70	1.39	2.78	5.56
2.0	0.35	0.70	1.39	2.78

Conclusion

This report describes the theoretical background to a set of three quasi-geostrophic ocean models which use spectral methods to represent the horizontal variation of the dynamic pressure. In addition the depth variation is represented in terms of the normal modes of a linearized flat bottom and unforced ocean. The modal vorticity equations, eq (11) or eq (52) form the basic dynamical equations describing the evolution of the ocean systems. The full three dimensional structure is regained by summing over all the contributing normal modes.

A further report will describe applications of the models and their implementation on the CRAY-1 computer system.

APPENDIX A

Properties of Chebyshev Polynomial Expansions

The Chebyshev polynomial of degree n , $T_n(x)$, is defined by

(A1) $$T_n(\cos\theta) = \cos n\theta$$

Thus, $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2-1$, $T_3(x) = 4x^3-3x$, $T_4(x) = 8x^4-8x^2+1$ and so on. The Chebyshev polynomials are the solutions of the differential equation

(A2) $$(1-x^2)^{1/2} \frac{d}{dx} (1-x^2)^{1/2} \frac{dT_n}{dx} + n^2 T_n = 0$$

that are bounded at $x = \pm 1$. They satisfy the orthogonality relation

(A3) $$\int_{-1}^{1} T_n(x)\, T_m(x)\, (1-x^2)^{-1/2}\, dx = \frac{\pi}{2} c_n \delta_{nm}$$

where $c_0=2$, $c_n = 1$ for $n>0$. Some properties of Chebyshev polynomials are

(A4) $$T_{n+1}(x) = 2x\, T_n(x) - T_{n-1}(x)$$

(A5) $$|T_n(x)| \leq 1 \quad ; \quad |T_n'(x)| \leq n^2$$

(A6) $$\frac{d^p}{dx^p} T_n(\pm 1) = (\pm)^{n+1} \prod_{k=0}^{p-1} (n^2-k^2)/(2k+1)$$

(A7) $$\left| \frac{d^p}{dx^p} T_n(x) \right| = O(n^{2p}), \quad n \to \infty \quad p \text{ fixed } |x| \leq 1$$

(A8)
$$T_n(\pm 1) = (\pm 1)^n \quad , \quad T_{2n}(0) = (-1)^n \quad , \quad T_{2n+1}(0) = 0$$
$$T_{2n}'(0) = 0 \quad , \quad T_{2n+1}'(0) = (-1)^n n$$

The following formulae relate the expansion coefficients a_n in the series

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x) \qquad |x| \leq 1$$

to the expansion coefficients b_n of

$$Lf(x) = \sum_{n=0}^{\infty} b_n T_n(x) \qquad |x| \leq 1$$

for various linear operators L. We use the constants c_n and d_n defined by

$$c_0 = 2 \quad , \quad c_n = 1 \quad (n>0) \quad , \quad c_n = 0 \quad (n<0)$$
$$d_n = 1 \quad (n \geq 0) \quad , \quad d_n = 0 \quad (n<0)$$

Some formulae are:

(A9) $$Lf = f'(x) \quad : \quad c_n b_n = 2 \sum_{\substack{p=n+1 \\ p+n \text{ odd}}}^{\infty} p\, a_p$$

(A10) $$Lf = f''(x) \quad : \quad c_n b_n = \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} p(p^2-n^2)\, a_p$$

(A11) $$Lf = x f(x) \quad : \quad b_n = \frac{1}{2}\left(c_{n-1} a_{n-1} + a_{n+1} \right)$$

(A12) $$Lf = x^2 f(x) \quad : \quad b_n = \frac{1}{4}\left(c_{n-2} a_{n-2} + (c_n + c_{n-1}) a_n + a_{n+2} \right)$$

(A13) $$Lf = x^4 f(x) \; : \quad b_n = \frac{1}{16}\Big\{ c_{n-4} a_{n-4} + (c_{n-3} + c_{n-2}^2 + 2c_{n-2}) a_{n-2}$$
$$+ (c_{n-2} + 2c_{n-1} + c_{n-1}^2 + c_n^2 + c_n) a_n + (c_{n-1} + c_n + c_{n+1} + c_{n+2}) a_{n+2} + a_{n+}$$

(A14)
$$Lf = \frac{f(x) - f(0)}{x} \; : \quad c_n b_n = 2 \sum_{\substack{p=n+1 \\ p+n \text{ odd}}}^{\infty} (-1)^{(p-n-1)/2} \cdot a_p$$

(A15)
$$Lf = \frac{f(x) - f(0) - f'(0)x}{x^2} \; : \quad c_n b_n = 2 \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} (p-n)(-1)^{(p-n-2)/2} \cdot a_p$$

(A16)
$$Lf = \frac{f'(x) - f'(0)}{x} \; : \quad c_n b_n = 4 \sum_{\substack{p=n+2 \\ p-n \equiv 2 \bmod 4}}^{\infty} p\, a_p$$

(A17)
$$Lf = \frac{f'(x) - f'(0) - f''(0)x}{x^2} \; :$$
$$c_n b_n = 2 \sum_{\substack{p=n+3 \\ p-n \equiv 3 \bmod 4}}^{\infty} (p-n+1)\, p\, a_p - \sum_{\substack{p=n+5 \\ p-n \equiv 1 \bmod 4}}^{\infty} (p-n-1)\, p\, a_p$$

(A18)
$$Lf = x f'(x) \; : \quad c_n b_n = n a_n + 2 \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} p\, a_p$$

(A19) $$Lf = x^2 f'(x) \; : \; b_n = \frac{1}{2}\Big\{ (n-1) a_{n-1} + (n+1)(1 + d_{n-1} + c_{n-1}) a_{n+1}$$
$$+ 4 \sum_{\substack{p=n+3 \\ p+n \text{ odd}}}^{\infty} p\, a_p \Big\}$$

(A20) $$Lf = x f''(x) \quad : \quad c_n b_n = 2n(n+1) a_{n+1} + \sum_{\substack{p=n+3 \\ p+n \text{ odd}}}^{\infty} p(p^2-n^2-1) a_p$$

(A21)

$$Lf = x^2 f''(x) \quad : \quad c_n b_n = n(n-1) a_n + \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} p(p^2-n^2-2) a_p$$

(A22)

$$Lf = \frac{f(x)}{1-x^2}, \quad \text{with } f(\pm 1) = 0 \quad : \quad c_n b_n = -2 \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} (p-n) a_p$$

Also, if we expand $f^{(q)}(x)$ as in

$$\frac{d^q}{dx^q} f(x) = \sum_{n=0}^{\infty} a_n^{(q)} T_n(x)$$

then

(A23) $$c_{n-1} a_{n-1}^{(q)} - a_{n+1}^{(q)} = 2n\, a_n^{(q-1)} \quad , n \geq 1$$

APPENDIX B

Transform Techniques

The transform techniques employed by the spectral methods are based on the existence of algorithms for Fast Fourier Transforms and assume that such subroutines are readily available. Such subprogrammes are available on the CRAY-1 Computer System and are written in the Cray Assembly Language (CAL) for operation under the Cray Operating System (COS). The subroutines are addressed by a conventional FORTRAN call statement. Three subroutines are available, namely

CFFT2 Complex to Complex ($x_j \rightarrow y_k$)

$$y_k = \sum_{j=0}^{N-1} x_j \cdot \exp\left(\pm i \frac{2\pi}{N} jk\right) \quad k = 0, \ldots N-1$$

CRFFT2 Complex to Real ($x_j \rightarrow y_k$)

$$y_k = \sum_{j=0}^{N-1} x_j \cdot \exp\left(\pm i \frac{2\pi}{N} jk\right) \quad k = 0, \ldots N-1$$

$$y_k \text{ real} \;;\quad x_j = x^*_{N-j}$$

RCFFT2 Real to Complex ($x_j \rightarrow y_k$)

$$y_k = 2 \sum_{j=0}^{N-1} x_j \cdot \exp\left(\pm i \frac{2\pi}{N} jk\right) \quad k = 0, \ldots N/2$$

$$x_j \text{ real} \;;\quad y_k = y^*_{N-k}$$

Further details may be found in the CRAY-1 Library reference manual. For the doubly periodic model these subroutines may be used immediately to define 2-dimensional transforms. For spectral expansions employing sine, Chebyshev or cosine functions pre-and post-processing is required. A summary of the steps required is given below and further details are provided by Cooley, Lewis and Welch (1970).

For the oceanographic applications described in this report the transforms required are two-dimensional. Two-dimensional transforms based on the repreated application of the above subroutines are available although it has been found possible to obtain improved efficiency using the Fast Fourier Transform routine developed by Clive Temperton (1983). This routine called FFT77 provides useful time savings of between 2 and 3. Double cosine, cosine-Fourier and double Fourier transforms have been developed and are incorporated into each of the ocean models.

Finite Chebyshev Transform and Inverse

The finite Chebyshev series is $Y(x) = \sum_{n=0}^{N} \hat{Y}_n T_n(x) \quad -1 \leq x \leq 1$

If collocation points $x_j = \cos\left(\frac{\pi j}{N}\right) \quad j = 0,1 \ldots N$ are introduced

$$Y(j) \equiv Y(x_j) = \sum_{n=0}^{N} \hat{Y}_n \cos\left(\frac{\pi n}{N} j\right) \quad j = 0,1 \ldots N$$

Formally $Y(j)$ is made into a real even sequence over twice the range $Y(j), j=0,\ldots$ 2N-1 using $Y(j) = Y(2N-j)$.

To compute the cosine transform

(a) Form the complex conjugate even sequence $X(j)$ where

$$X(j) = Y(2j) + [Y(2j+1) - Y(2j-1)]i$$

for j = 0,1...N-1 (only j = 0,1,... $N/2$ terms need be formed). Only $Y(0)$ ... $Y(N)$ need be given.

(b) Input $\frac{X^*(j)}{N}$ to the CRFFT2 routine

Output is the real sequence A(n), n=0,...N.

(c) Form $\hat{Y}(n) = \frac{1}{2}\left\{[A(n) + A(-n)] - [A(n) - A(-n)]/\left(2\sin\left(\frac{\pi n}{N}\right)\right)\right\}$

$$n = 1, \ldots N-1 \quad ; \quad A(-n) = A(N-n)$$

(d) Determine

$$\hat{Y}(0) = \frac{1}{2}(A_1 + A_2)$$
$$\hat{Y}(N) = \frac{1}{2}(A_1 - A_2)$$

from

$$A_1 = A(0)$$
$$A_2 = \frac{1}{N}\sum_{j=0}^{N-1} Y(2j+1) = \frac{2}{N}\sum_{j=0}^{N/2-1} Y(2j+1)$$

Inverse

given $\hat{Y}(n) \quad n = 0,1 \ldots N$

(a) Determine

$$A_1 = \hat{Y}(0) + \hat{Y}(N) = A(0)$$

$$A_2 = \hat{Y}(0) - \hat{Y}(N)$$

(b) Form

$$A(n) = [\hat{Y}(n) + \hat{Y}(N-n)] - [\hat{Y}(n) - \hat{Y}(N-n)](2\sin(\frac{\pi n}{N}))$$

(c) Input $A(n)$, $n = 0,1, \ldots N-1$ to the RCFFT2 routine. Output is the complex even sequence $\frac{X^*(j)}{N}$.

(d) Form $Y(j), j = 0, \ldots N$ from $X(j)$, $j = 0, \ldots N/2$

$Y(2j) = \text{Real } X(j) \qquad j = 0, \ldots N/2$

and

$$Y(2j+1) = Y(2j-1) + \text{Im } X(j), \quad j = 1, \ldots N/2 - 1$$

assuming $Y(1)$ is given

$Y(1)$ is determined from, $\quad Y(1) = A_2 - \frac{2}{N} \sum_{i=1}^{N/2-1} \text{Im } X(i) \left(\frac{N}{2} - i\right)$

Finite Sine Transform and Inverse

(a) sine transform

(i) Form the complex conjugate odd sequence $X(j)$ where

$$X(j) = -[Y(2j+1) - Y(2j-1)] + Y(2j); \qquad j = 1, \ldots N/2 - 1.$$

and

$$X(0) = -2Y(1)$$

$$X(N/2) = 2Y(N-1)$$

(ii) Input X^* to the CRFFT2 routine. Output is the real sequence

$$A(n) \quad n = 0, 1, \ldots N$$

(iii) Form $\hat{Y}(n) = \frac{1}{2}\left\{ [A(n) - A(-n)] - [A(n) + A(-n)]/(2\sin(\frac{\pi n}{N}))\right\}$

$\hat{Y}(0) = \hat{Y}(N) = 0$ $\qquad n = 1, \ldots N-1$

(b) Inverse

given $\hat{Y}(n)$, $n = 0, 1, \ldots N$

(i) $A(0) = 0$

(ii) Form $A(n) = [\hat{Y}(n) - \hat{Y}(N-n)] - [\hat{Y}(n) + \hat{Y}(N-n)]\,(2\sin(\frac{\pi n}{N}))$

$n = 1, \ldots N-1$

(iii) Input $A(n)$, $n = 0, 1 \ldots N-1$ to the RCFFT2 routine. Output is the complex odd sequence $\frac{X^*(j)}{N}$

(iv) Form $Y(j)$, $j = 0, 1 \ldots N$ from $X(j)$, $j = 0, 1 \ldots N/2$

$Y(2j) = \operatorname{Im} X(j)$ $\qquad j = 0, \ldots N/2$

$Y(2j+1) = Y(2j-1) - \text{Real } X(j)$ $\qquad j = 1, \ldots N/2$

given $Y(1) = -\frac{1}{2} X(0)$

APPENDIX C

Quasi-Tridiagonal Solver

The solution of a quasitridiagonal system of linear equations is required for models involving Chebyshev spectral functions. The quasi-tridiagonal set of N linear equations take the form

$$\begin{pmatrix} D_1 & E_1 & 1 & 1 & \cdots & \cdots & 1 & 1 \\ C_2 & D_2 & E_2 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & C_3 & D_3 & E_3 & \cdots & \cdots & 0 & 0 \\ & & & \ddots & & & \vdots & \vdots \\ & & & & \ddots & & D_{N-1} & E_{N-1} \\ & & & & & & C_N & D_N \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ \\ \\ X_N \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ \\ \\ B_N \end{pmatrix}$$

where $D_1 = E_1 = 1$ and $B_1 = 0$

Assuming all C_I are non-zero, we first perform an elimination step for K=1,N-1

$$KP1 = K+1$$

$$T = -D_K / C_{KP1}$$

$$D_{KP1} = T \times D_{KP1} + E_K$$

$$E_{KP1} = T \times E_{KP1} + 1$$

$$B_{KP1} = T \times B_{KP1} + B_K$$

where '=' is interpreted as replace. After elimination we obtain the triangular matrix

$$\begin{pmatrix} D_1' & E_1' & 1 & 1 & 1 & \cdots & 1 & 1 & 1 \\ 0 & D_2' & E_2' & 1 & 1 & \cdots & 1 & 1 & 1 \\ 0 & 0 & D_3' & E_3' & 1 & \cdots & 1 & 1 & 1 \\ & & & \ddots & & \ddots & & \vdots & \\ & & & & & & & D_{N-1}' & E_{N-1}' \\ & & & & & & & & D_N' \end{pmatrix}$$

Back-substitution may then be performed for KK = 1,N-1

$$B_N = B_N / D_N$$

$$SUM = 0$$

$$K = N - KK$$

$$B_K = (B_K - E_K \times B_{K+1} - SUM)/D_K$$

$$SUM = SUM + B_{K+1}$$

The output vector is B_K . If any $C_I = 0$ all are zero and the input vector $B_I, I = 2, \ldots N$ is the solution vector and $B_1 = -\sum_{I=2}^{N} B_I$

APPENDIX D

Quasi-Tridiagonal Transformation

It is a simple algebraic exercise to show that the system of equations represented by (24) or (37) may be put into quasi-tridiagonal form. It is sufficient for our purposes to consider only one index i.e.

$$\frac{1}{c_n} \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{N} p\,(p^2-n^2)\,a_p \;+\; \alpha\, a_n \;=\; f_n \qquad 0 \leqslant n \leqslant N-2$$

For simplicity consider only the even terms and define

$$S_q = \sum_{\substack{p=q \\ p \text{ even}}}^{N} p\,(p^2-n^2)\; a_p$$

then $\quad$ for $\quad 2 \leqslant n \leqslant N-4$

(i)

$$\frac{1}{c_{n+2}}\, S_{n+4} \;-\; \frac{4(n+1)}{c_{n+2}} \sum_{\substack{p=n+4 \\ p \text{ even}}}^{\prime} p\,a_p \;+\; \alpha\, a_{n+2} \;=\; f_{n+2}$$

(ii)

$$\frac{1}{c_{n-2}}\, S_n \;+\; \frac{4(n-1)}{c_{n-2}} \sum_{\substack{p=n \\ p \text{ even}}}^{\prime} p\,a_p \;+\; \alpha\, a_{n-2} \;=\; f_{n-2}$$

We have also

$$\sum_{\substack{p=n \\ p \text{ even}}}^{\prime} p\,a_p \;=\; n\,a_n + (n+2)\,a_{n+2} + \sum_{\substack{p=n+4 \\ p \text{ even}}}^{\prime} p\,a_p$$

$$S_n = S_{n+2} = 4(n+2)(n+1)\,a_{n+2} + S_{n+4}$$

and $\quad S_{n+2} = c_n f_n - \alpha\, a_n\, c_n$

Adding (i) and (ii) in suitable combinations to remove the middle sum leads quite simply to

$$\alpha \frac{c_{n+2}\, a_{n+2}}{4n(n+1)} + \left(1 - \frac{\alpha c_n}{2(n^2-1)}\right) a_n + \alpha \frac{c_{n-2}\, a_{n-2}}{4n(n-1)}$$

$$= \frac{c_{n+2}\, f_{n+2}}{4n(n+1)} - \frac{c_n f_n}{2(n^2-1)} + \frac{c_{n-2}\, f_{n-2}}{4n(n-1)}$$

This system of equations is valid for $2<n<N-4$ and to obtain the appropriate equations for $n=N-2$ and N the original equation is used. We obtain finally,

$$\alpha\, e_{n+4}\, a_{n+2} + \left(1 - \frac{\alpha\, e_{n+2}}{2(n^2-1)}\right) a_n + \alpha \frac{a_{n-2}\, c_{n-2}}{4n(n-1)}$$

$$= \frac{e_{n+4}\, f_{n+2}}{4n(n+1)} - \frac{e_{n+2}\, f_n}{2(n^2-1)} + \frac{c_{n-2}\, f_{n-2}}{4n(n-1)}$$

Here $e_n = 1$ for $n<N$, $e_n = 0$ for $n > N$. In combination with the boundary condition constraints we arrive at the quasi-tridiagonal system described in the main text.

APPENDIX E

Discrete ∂_x^2 - eigenvalue problem

The basin Chebyshev spectral model utilises the discrete eigenvalues and eigenfunctions of the continuous problem

$$\partial_x^2 u_\nu = \lambda_\nu u_\nu \quad , \quad u_\nu(\pm 1) = 0$$

obtained by setting $u_\nu(x) = \sum_{n=0}^{N} e_{n\nu} T_n(x)$. This assumption implies

$$\frac{1}{c_n} \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{N} p(p^2-n^2)\, e_{p\nu} = \lambda_\nu e_{n\nu} \qquad 0 \leqslant n \leqslant N-2$$

and the boundary conditions are

$$\sum_{p \text{ even}} e_{p\nu} = \sum_{p \text{ odd}} e_{p\nu} = 0$$

The same quasitridiagonal transformation may be applied to the above problem as has already been described for the Helmholtz equation system. We obtain the system of equations:

$$e_n = \lambda \left[\ell_n e_{n-2} - d_n e_n + u_n e_{n+2} \right]$$
$$2 \leqslant n \leqslant N$$

together with the accompanying boundary conditions. e_N and e_{N-1} may be eliminated from the above equations by use of the boundary conditions and the equations represent a standard eigenvalue problem of order N-1 with eigenvalues λ_ν. Consequently we have a set of N-1 eigenvalues and eigenfunctions

$$u_\nu(x) = \sum_{n=0}^{N} e_{n\nu} T_n(x) \qquad \nu = 0, 1 \ldots N-2$$

The matrix $E = \{ e_{n\nu} \}$ $n, \nu = 0, 1 \ldots N-2$ and its inverse may then be used to perform the transformation described in the main body of the text. It should be noted that the transformation is not orthogonal since the Chebyshev functions are not orthonormal with unit weight. Since the discrete eigenfunctions possess definite parity under co-ordinate transformation

$x \rightarrow -x$ the matrices E and E^{-1} contain elements which are alternatingly zero and nonzero. This property can be used to speed up the matrix multiplications by a factor of 2.

APPENDIX F

Vertical Structure Functions

The vertical structure functions and constants for a simple analytic Brunt-Väisälä frequency N^2 is given below. Finally the numerical procedure for more realistic vertical variations of N^2 is given.

(a) Constant Brunt-Vaisala frequency N^2

$$F_{n}(z) = A_n \cos\left(\frac{n\pi}{N}\right)z$$

$$n = 0, 1, \dots M-1$$

where

$$\lambda_n = \frac{f_0}{N} \cdot \frac{n\pi}{H} \qquad \text{and} \qquad A_0 = 1, \quad A_n = \sqrt{2},\ n = 1, \dots M-1$$

The vertical structure constants between baroclinic modes are

$$\xi_{ijk} = \frac{1}{\sqrt{2}}\left[\delta_{k,i+j} + \delta_{k,|i-j|}\right], \quad ijk = 1, \dots M-1$$

(b) Numerical vertical Structure Determination

The second-order differential equation describing the vertical structure is expressed in finite-difference form on the grid

$$z_i = -i\left(\frac{H}{N}\right) \qquad i = 0, 1, \dots N$$

and N_i is the Brunt-Vaisala frequency on the finite difference grid. With

$$S_i = \frac{N_i^2}{f_0^2}, \quad A_i = S_i^{-1}, \quad B_i = -\frac{1}{S_i^2} \cdot \frac{dS_i}{dz}$$

the difference equation is

$$\left[\frac{A_i}{(\Delta z)^2} + \frac{B_i}{2\Delta z} \right] F_{i+1} - \frac{2A_i}{(\Delta z)^2} F_i + \left[\frac{A_i}{(\Delta z)^2} - \frac{B_i}{2\Delta z} \right] F_{i-1} + \lambda F_i = 0$$

$$i = 0, 1, \ldots N$$

The above difference equation is expressed as a tri-diagonal (NxN) matrix with the derivative boundary conditions

$$F_{-1} = F_1 \quad , \quad F_{N+1} = F_{N-1}$$

determining the end-point values. A standard NAG eigenvalue subroutine is used to determine the first eigenvalues between $0 \leq \lambda \leq \lambda_{max}$ and their associated eigenvectors. The vertical structure constants are determined by simple numerical quadrature.

(c) Vertical Structure Constants

The total number of non-trivial vertical structure constants for M-modes is 4(M-1)+(M-1)(M-2) + $^1/6$(M-1)(M-2)(M-3); this number is 4, 10, 19, 32, .. for M = 2, 3, 4, 5, ... However, a number of these constants are unity so that the number of constants to be determined is reduced considerably for small values of M. For the M-mode problem we have M matrices each (MxM) of the form:

$$K = 0 \qquad \langle F_i F_j F_0 \rangle = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{pmatrix}$$

$$K = 1 \qquad \langle F_i F_j F_1 \rangle = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 1 & \xi_{111} & \xi_{121} & \cdots \\ 0 & \xi_{121} & \xi_{221} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

$$K = 2 \qquad \langle F_i F_j F_2 \rangle = \begin{pmatrix} 0 & 0 & 1 & \cdots \\ 0 & \xi_{112} & \xi_{122} & \cdots \\ 1 & \xi_{122} & \xi_{222} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

$$\vdots$$

where the symmetry of ξ_{ijk} has been employed. The elements which are neit zero or one consist of the (M-1) vectors of diagonal elements ξ_{iik} and (M-1) upper halves of the symmetric matrices ξ_{ijk} $(j>i)$. The latter eleme can be arranged into (M-1) vectors for convenience. Although this grouping the vertical structure constants does not exploit their full symme completely it does separate the coupling into diagonal and non-diago contributions.

APPENDIX G

Physical and computational modes

In the report we often need to evaluate discrete Fourier transforms such as

$$u_j = \sum_{\|k\| \leqslant K} u(k)\, e^{ikx_j} \qquad j = 0,1 \ldots 2K-1$$

where $\|k\| \leqslant K$ is defined as $-K \leqslant k < K$ and $x_j = 2\pi j/(2K)$.

On the other hand, fast Fourier transform codes are usually written to evaluate

$$A_j = \sum_{n=0}^{N-1} a_n\, e^{\frac{2\pi i n j}{N}} \qquad j = 0, \ldots N-1$$

The correspondence is stated explicitly below and it is these coefficients which are employed in the computations. Set N=2K and define the computational wavenumber k' by k'=k+K. Setting $a_{k'} = u(k)$, $\|k\| \leqslant K$ i.e.

$$\begin{aligned} a_{2K-1} &= u(K-1) \\ &\vdots \\ a_0 &= u(-K) \end{aligned}$$

it follows that

$$u_j = (-1)^j \sum_{k'=0}^{N-1} a_{k'}\, e^{\frac{2\pi i k' j}{N}}$$

Conversely

$$u(k) = \frac{1}{N} \sum_{j=0}^{N-1} u_j\, e^{\frac{-2\pi i j k''}{N}}$$

where $k'' = k$ if $0 \leq k < K$

$k'' = k+N$ if $-K \leq k < 0$

Note also $a_{k'} = a^*_{N-k'}$ $(0 < k' < N)$, $a_0 = a_0^*$

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