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An Application of the Arnoldi's Method to a Geophysical Fluid Dynamics Problem

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A new method to find solutions of large linear systems, based on a projection on the Krylov subspace, is shown to be successful when applied to the linearized barotropic and baroclinc primitive equations. These sets of equations are widely used in the simulation of the dynamics of the atmosphere. The scheme consists of projecting the original linear system on the Krylov subspace, thereby reducing the dimensionality of the matrix to be inverted in order to obtain the solution. The iterative Arnoldi's method reaches a solution even using a Krylov subspace ten times smaller than the original space of the problem. This generality allows us to treat the important problem of propagation of linear waves in the atmosphere from a more general point of view. A larger class (nonzonally symmetric) of basic states can now be treated for the baroclinic primitive equations. These kinds of problems leading to large unsymmetrical linear system of order 10000 or more can now be successfully tackled by the Krylov approach. Numerical results of a General Circulation Model, linearized around a nonsymmetrical basic state, are here shown for various numbers of degrees of freedom.

1. INTRODUCTION

The effects of external forcings on large scale atmospheric circulation has been an interesting and important subject in dynamic meteorology. In the late 1970s there has been a resurgence of interest for the linearized approach to the problems; a number of investigators have found that stationary weve propagation derived from linear models yields a considerable insight into the dynamics of circulation.

For meteorological application two-dimensional and three-dimensional systems are used. In the former case only the Navier–Stokes equations on a spherical surface are considered. The fluid is supposed horizontally nondivergent, and thermodynamical effects are ignored. This is called a barotropic system. In the latter case the Navier–Stokes equations for a fluid of finite thickness on the sphere are used. To close the system the thermodynamics and continuity equations are added and the hydrostatic approximation is made. This system is called the primitive equations system or, briefly, the baroclinic system. A quite comprehensive list of references of linear studies in this framework may be found in Held [19].

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These kinds of models are usually linearized around a basic state that varies only in the latitudinal direction for the barotropic case and in both the vertical and latitudinal directions for the baroclinic case. The equations become separable in one variable, the longitude, and so the solution can be expressed as a Fourier series in terms of longitudinal waves. The equations are then solved for each longitudinal wavenumber. The numerical methods developed for these cases involve the reduction of the equations to a matrix form. An analytical calculation of matrix elements is presented by Lindzen and Kuo [11], that was also used by Simmons [17] and Nigam [13], while Hoskins and Karoly [9] used a spectral General Circulation Model (GCM) to compute the elements of the matrix without computing the interactions analytically. The size of the matrix to be inverted for each wavenumber was on the order of a few hundreds. All of these examples included the solution of a large, sparse, matrix (block diagonal in the wavenumber representation) and in all cases only direct methods, based on Gaussian elimination, were used.

The time-mean state of the real atmosphere is, however, far from being independent of longitude, so it is natural to try to remove this limitation from the assumptions for the basic flow. However, by doing so we lost the advantage of the block-diagonal symmetry. The matrix is not sparse any more and we cannot treat each wavenumber separately. Yet the barotropic case is still treatable without a special consideration, as Branstator [3] and Navarra and Miyakoda [12] did. Even some baroclinic case is treatable if an approximate version of system (2.3)–(2.6), such as the quasigeostrophic system, is used (as in Federiksen [6]). However, this is not the case for the primitive equations. The order of the matrix, for a linear model of resolution comparable with that of a low resolution spectral GCM, may exceed 10000. Direct methods are impractical and even storage of the matrix is difficult. If a finite-difference numerical scheme is used the matrix may have a sparse structure, but if a spectral representation is used the sparseness is generally lost. In general, the matrix is expected to be unsymmetrical and, possibly, indefinite. Direct methods are ruled out because of the difficulty of computing and storing the elements of the matrix. By the same token, iterative methods that involve simultaneous operations on the elements of the matrix have to be excluded. The situation also precludes pre-conditioning methods since it is difficult to construct a pre-conditioning operator in compact form.

What we present here is an application of a method belonging to the class of algorithms based on oblique projections on a Krylov subspace, the Arnoldi's method. The algorithm is originally due to Saad [16] and what is described here is its application to the barotropic and baroclinc case. One feature that makes this algorithm very suitable for a geophysical application is that the matrix A need not be computed explicitly. In this algorithm only the vectors Ax are needed in the construction of the Krylov subspace. As we will see in the following this operation may be performed numerically by using a linearized version of a Global Circulation Model. Section 2 will describe the physical models and the details of the numerical representation. Section 3 will describe Arnoldi's method, and Section 4 will present the results of the numerical experiments.

2. The Physical Equations

We will take two kinds of problems. The first one is described by the non-divergent barotropic equation for the two-dimensional flow on a rotating sphere, viz.

$$\frac{\partial}{\partial t}(\zeta) + \nabla \cdot (\mathbf{v}\zeta + f\mathbf{v}) = F(\phi, \lambda) - K\nabla^2\zeta - \varepsilon\zeta, \tag{2.1}$$

where ζ is the vertical component of the relative vorticity; ∇ is the horizontal gradient operator in spherical coordinates; F is an external prescribed forcing; $\mathbf{v} = (u, v)$, is the horizontal velocity vector, and f is the Coriolis parameter defined as $2\Omega \sin \phi$, Ω is the earth angular velocity and ϕ is the latitude. For the linearized case to be discussed in the following, the dissipation terms already written for completeness in (2.1), become important. The basic flow used in the linear equations includes zero wind lines that need to be treated with the inclusion of small scale dissipation, $-K\nabla^2\zeta$; also, the generation of wave trains so long that could return back to the forcing region, causing a resonance, is to be avoided by damping the waves with a $-\varepsilon\zeta$ term, as in [8]. Since the flow is assumed horizontally non divergent ($\nabla \cdot \mathbf{v} = 0$), it is possible to define a streamfunction ψ, such that

$$\nabla^2\psi = \zeta,$$

$$u = -\frac{1}{a}\frac{\partial \psi}{\partial \phi}, \qquad v = \frac{1}{a\cos\lambda}\frac{\partial \psi}{\partial \lambda}$$

so that Eq. (2.1) may be written

$$\frac{\partial}{\partial t}(\nabla^2\psi) + J(\psi, \nabla^2\psi + f) = F - K\nabla^4\psi - \varepsilon\nabla^2\psi, \tag{2.2}$$

where $J(\psi, \nabla^2\psi)$ is the Jacobian operator in spherical coordinates

$$J(\psi, \nabla^2\psi) = \frac{1}{a^2\cos\phi}\left[\frac{\partial \psi}{\partial \lambda}\frac{\partial}{\partial \phi}(\nabla^2\psi) - \frac{\partial}{\partial \lambda}(\nabla^2\psi)\frac{\partial \psi}{\partial \phi}\right].$$

Problems involving finite-difference representations of Jacobians arising in ODE codes have also been considered by Gear and Saad [20].

In the second problem, we consider a system of equations which is normally used in numerical weather prediction. This set of equations represents a three-dimensional compressible fluid on a rotating sphere, driven by heating. The model is based on the "transform" spectral technique. Bourke [1, 2] developed this model for the barotropic and for the baroclinc case. However, the particular model used in this paper is the GCM built by Gordon and Stern [7] and, therefore, we will follow their description of the essential parts of the procedure.

First, the set of equations is written in terms of vorticity ζ, divergence D, temperature T and logarithm of surface pressure $q = \log(p_s)$, using as vertical coordinate the normalized pressure $\sigma = p/p_s$,

$$\frac{\partial \zeta}{\partial t} = -\nabla \cdot (\hat{k} \times \mathbf{S}) - K_\zeta \nabla^4 \zeta, \tag{2.3}$$

$$\frac{\partial D}{\partial t} = \nabla \cdot (\mathbf{S}) - \nabla^2 (E + \phi) - K_D \nabla^4 D, \tag{2.4}$$

$$\frac{\partial T}{\partial t} = -\mathbf{v} \cdot \nabla T - \dot{\sigma} \frac{\partial T}{\partial \sigma} + \frac{RT}{c_p} \frac{\omega}{p} + \frac{Q}{c_p} - K_T \nabla^4 T, \tag{2.5}$$

$$\frac{\partial q}{\partial t} = -\tilde{\mathbf{v}} \cdot \nabla q - \nabla \cdot \tilde{\mathbf{v}}, \tag{2.6}$$

$$\frac{\omega}{p} = \frac{\dot{\sigma}}{\sigma} + (\mathbf{v} - \tilde{\mathbf{v}}) \cdot \nabla q - \nabla \cdot \tilde{\mathbf{v}}, \tag{2.7}$$

$$\dot{\sigma} = -\int_0^\sigma (D - \tilde{D})\, d\sigma - \int_0^\sigma (\mathbf{v} - \tilde{\mathbf{v}}) \cdot \nabla q \, d\sigma, \tag{2.8}$$

$$\frac{\partial \phi}{\partial \sigma} = -\frac{RT}{\sigma}, \tag{2.9}$$

$$E = \frac{(u^2 + v^2)}{2}, \tag{2.10}$$

$$\mathbf{S} = -(\zeta + f)\hat{k} \times \mathbf{v} - \dot{\sigma} \frac{\partial \mathbf{v}}{\partial \sigma} - RT \nabla q. \tag{2.11}$$

Here ω is the vertical pressure velocity, ϕ the geopotential, R the gas constant, c_p the specific heat capacity at costant pressure, $\hat{k}$ the vertical unit vector,

$$(\tilde{\ }) = \int_0^1 \cdots d\sigma$$

the vertical average operator, Q the heating. The heating Q is the only forcing of the system; in the following, we will be interested only in the case when Q is a prescribed function independent of time, but otherwise unrestricted.

Vertical derivatives are treated by finite-differencing so that the variables (ζ, D, T, q) are specified at discrete levels. Boundary conditions are applied at the bottom and the top of the atmosphere as $\dot{\sigma} = 0$. The variables are then expressed in terms of spherical harmonics at each level. Vorticity, for instance, is written

$$\zeta = \sum_{m=0}^{J} \sum_{n=|m|}^{|m|+J} ((\zeta_n^m)^R \cos(m\lambda) + (\zeta_n^m)^I \sin(m\lambda))\, P_n^m(\cos\phi). \tag{2.12}$$

The parameter J describes the order of the truncation and is therefore a measure of the total number of degrees of freedom in the system. Substituting the spherical harmonics expansion in (2.1) or (2.3)–(2.11) and projecting variables on the spherical harmonics, we obtain a system of ordinary differential equations for the spherical harmonic coefficients, that can be written symbolically as

$$\dot{x} = N(x) + f. \tag{2.13}$$

The vectors x, f represent the spherical harmonic coefficients for all variables and the heating function at all levels. N is a symbolic writing for the nonlinear operator on the r.h.s. of (2.3)–(2.6). The equations are then simplified by linearizing (2.13) around a certain time-independent basic state. It is necessary to postulate a forcing $\bar{f}$ that makes the basic state $\bar{x}$ a solution of the full stationary equation $N(\bar{x}) = \bar{f}$. Dissipation, in the form of Rayleigh friction $-\varepsilon(\sigma)(\zeta, D)$ and Newtonian cooling $-\gamma(\sigma)T$ is usually added to account for ground dissipation and for radiation cooling. Small scale dissipation is also included as a ∇^4 term for vorticity, divergence and temperature.

The equations for the perturbation x' can then be written

$$\dot{x} = L_{\bar{x}}(x') - f', \tag{2.14}$$

where L is the spectral representation of a linear differential operator with variable coefficients that depend on the basic state. The expression of L in continuous form is given in the Appendix.

The stationary equation is now obtained by setting the time derivative term in (2.14) to zero. Dropping primes one obtains

$$L_{\bar{x}}(x) = f$$

whose numerical representation is given by a real matrix equation

$$Ax = f. \tag{2.15}$$

Equation (2.15) is the basic equation to which the Krylov subspace method will be applied.

The problem is now reduced to solving a linear system whose order is given by the total number of variables, namely the total number of independent spherical harmonic coefficients. According to relation (2.12) there are $2(J+1)$ real coefficients for each $m \neq 0$ and since there are three variables (ζ, D, T) with vertical dependence expressed at K vertical levels, and one two-dimensional variable q, the total length of the block for a certain wavenumber m is given by $2(J+1)(3K+1)$, where K is the total number of vertical levels in the model, i.e., $K=9$. The zonal block $(m=0)$ is special because these coefficients are only $(J+1)$ and $(\zeta_0^0)_k$, $(D_0^0)_k$, q_0^0 are not considered. The length of the $m=0$ block is therefore $(J+1)(3K+1)-2K-1$. If the vector x is ordered by wavenumber

m, $x = (\alpha^{(1)}, \alpha^{(2)}, \ldots, \alpha^{(m)}, \ldots, \alpha^{(J)})$ where $\alpha^{(m)}$ are the coefficients for all variables and levels corresponding to wavenumber m, then the structure of A will be

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1J} \\ A_{21} & A_{22} & & A_{2J} \\ \vdots & & \ddots & \vdots \\ A_{J1} & A_{J2} & \cdots & A_{JJ} \end{pmatrix},$$

where the diagonal block A_{JJ} describes the effect of the wavenumber $m = 0$ of the basic state onto the wavenumber J of the perturbation. In the sonally symmetric case considered by other authors $A_{mm'} = 0$ for $m \neq m'$, so the matrix is block-diagonal. In the case considered here $A_{mm'} \neq 0$ for all m, m', even if some of the elements are small. The matrix is not sparse and it is not banded. It is not known to be diagonally dominant, but the dissipation chosen will project on the diagonal elments of each block increasing the chances for diagonal dominancy.

The total length of the vector x is then obtained by summing over all m

$$L = (J+1)(3K+1) - 2K - 1 + \sum_{m=1}^{J} 2m(J+1)(3K+1),$$

i.e., $L = (2J+1)(J+1)(3K+1) - 2K - 1$. Table I represents the length of vectors for various truncations of the baroclinic spectral model.

The problem is so large that direct methods are unpractical. Very few iterative methods for large nonsymmetrical systems have been developed. Elman [21] gives a review of some of the methods available. Chebyshev iterations [10] require estimates of the bounds on the spectrum of A, and this itself is a rather difficult problem in the case treated here. In general these methods converge if the matrix is nonsymmetric positive definite, i.e., the real parts of all the eigenvalues are of the same sign. A priori, it is not rigorously known if the matrix treated here has this property or not. Since the Krylov subspace methods can be applied to the more general case, one of them, the Arnoldi's method, has been selected for this application. However, in the indefinite case convergence is not proved and the algorithm may break down [22]. In general, A will be only known implicitly through the finite difference or the spectral representation of the operator L_x. As it will be discussed in detail in the following, the Krylov subspace method does not require explicitly the elements of A. In fact, no operation on them is needed by the algorithm, only the result of the transformation $x \to z = Ax$ is used in the procedure. So, for a given x, Ax is easily accessible, but A itself is not. In this case, the calculation of Ax has been accomplished by using a linearized version of the spectral model by Gordon and Stern [7].

TABLE I

Truncation order J	1	3	7	15
Dimension of A	149	765	3341	13869

3. The Arnoldi's Method

Originally, the concept of the Krylov suspace was developed by Krylov ([10], for an English treatment see Faddeva, [51]) and Arnoldi [18] as a way to find the eigenvalues and the eigenvectors of a matrix. Only recently it has been pointed out that algorithms based on the Krylov subspace idea are very powerful tools to find approximations of eigenelements of large nonsymmetrical matrices (Saad [15]; Ruhe [14]) and that such algorithms may be applied to the solution of large, non-symmetrical, linear systems as well (Saad [22, 16]). The latest approach is the one that we have used in the application of this paper.

Let us consider a linear equation

$$Ax = f, \tag{3.1}$$

where A is a matrix of order n, and x, f are vectors of length n. The solution x to the equation has to be found among all the n-dimensional vectors belonging to the vector space R^n. The matrix A itself is to be considered as a linear transformation on the elements of the vector space.

To illustrate the Arnoldi method, let us assume the orthonormal basis in R^n, $U = (u_1, u_2, \ldots, u_n)$ and perform a change of coordinate so that in the new coordinate system equation (3.1) will be

$$U^{\mathrm{T}} A U b = U^T f, \tag{3.2}$$

where the matrix U^{T} denotes the transpose of the orthogonal matrix U. Therefore

$$b = (U^{\mathrm{T}} A U)^{-1} U^{\mathrm{T}} f \tag{3.3}$$

the solution is then given by

$$x = Ub = b_1 u_1 + b_2 u_2 + \cdots + b_n u_n. \tag{3.4}$$

In general, a change in coordinates does not give much advantage since Eq. (3.2) still require finding n coefficients. The question is whether it is possible to find a special coordinate system in which many of the b's are identically zero, and so only a smaller number, say m, of coefficients are sufficient to reconstruct the solution of the original system. In practice, many of the b's are small and we can neglect them without appreciably affecting the precision of the solution. The Arnoldi method provides an algorithm that yields such a basis, reducing the problem to finding only m coefficients instead of n.

Following Saad [16] we will try to sketch the essential points of the algorithm. Defining the Krylov subspace by $V = (v_0, Av_0, \ldots, A^{m-1} v_0)$ and an initial guess by $x^{(0)}$, we want to find an approximate solution of $Ax = f$ of the form $x^{(1)} = x^{(0)} + y^{(1)}$ where $y^{(1)} \in \mathrm{Span}(V)$, or $y^{(1)} = Vc^{(1)}$. The coefficients c are obtained by solving the Galerkin condition

$$V^{\mathrm{T}} A V c^{(1)} = V^{\mathrm{T}} r^{(0)}, \tag{3.5}$$

where $r^{(0)} = Ax^{(0)} - f$. We can see from (3.5) that though v_0 is in principle arbitrary, the choice $v_0 = r^{(0)}$ is convenient.

If the solution is not accurate enough, then a larger value of m must be used. It may happen that even with the largest m allowed by the computing system the precision of the solution is still not satisfactory. In this case the method can be made iterative. We set

$$\begin{aligned} x^{(2)} &= x^{(1)} + y^{(2)}, \\ r^{(1)} &= Ax^{(1)} - f, \end{aligned} \tag{3.6}$$

and form another Krylov subspace with $v_0 = r^{(1)}$ to obtain another Galerkin condition for $y^{(2)}$

$$\begin{aligned} V^{\mathrm{T}} A V c^{(2)} &= V^{\mathrm{T}} r^{(1)}, \\ y^{(2)} &= V c^{(2)}, \end{aligned}$$

and so on. In practice, it is not necessary to perform the matrix multiplications to get $V^{\mathrm{T}}AV$. The Arnoldi's algorithm provides the elements of an approximate representation of $V^{\mathrm{T}}AV$ that has the structure of a Hessenberg matrix. In fact, using the Arnoldi's algorithm one can build an orthonormal basis $V = (v_1, v_2, \ldots, v_m)$ of the Krylov subspace, K, in the following way. For the first element v_1,

$$v_1 = \frac{v_0}{\|v_0\|}$$

for the second element v_2

$$\begin{aligned} w &= (Av_1 - (Av_1, v_1)v_1), \\ v_2 &= \frac{w}{\|w\|}, \end{aligned}$$

for the third element v_3

$$\begin{aligned} w &= (Av_2 - (Av_2, v_1)v_1 - (Av_2, v_2)v_2), \\ v_3 &= \frac{w}{\|w\|}, \end{aligned}$$

and so on. In general we write

$$\begin{aligned} w &= Av_j - \sum_{i=1}^{j} h_{ij} v_i, \\ v_{j+1} &= \frac{w}{h_{j+1,j}}, \end{aligned} \tag{3.7}$$

where

$$\begin{aligned} h_{ij} &= (Av_j, v_i) \qquad \text{for} \quad i \leqslant j, \\ h_{j+1,j} &= \|w\| \qquad \text{for} \quad j = 1,\ldots, m. \end{aligned} \tag{3.8}$$

We have indicated with $(\cdot, \cdot)$ the scalar product in R^n and with $\|\cdot\|$ the norm associated with it.

The operator $V^{\mathrm{T}}AV$ is the restriction of the matrix A to the m-dimensional Krylov space K. Since V forms an orthonormal set it is not difficult to show the following relation

$$AV = VH + h_{m+1,m} v_{m+1} e_m^{\mathrm{T}}, \tag{3.9}$$

where we have denoted by e_m^{T} the mth row of the identity matrix I in m dimensions and H is the Hessenberg matrix whose coefficient are the h_{ij} defined by (3.8). It is an approximation to $V^{\mathrm{T}}AV$ and so we can solve, instead of (3.5)

$$Hc^{(1)} = V^{\mathrm{T}} r^{(0)} \tag{3.10}$$

that together with $y^{(1)} = Vc^{(1)}$, yields an approximate solution to (3.1). Equation (3.10) is an equation for $c^{(1)}$, i.e., an m-dimensional vector, and so we have reduced the size of the linear system from n to m. Since H is a Hessenberg matrix only $n(n+1)/2 + (n-1)$ elements are needed to store it in memory. Furthermore a very efficient row-wise Gaussian elimination, particularly suitable for vector processors, may be implemented to solve system (3.10).

Note that (3.7) and (3.8) imply that $h_{m+1,m}$, will be zero if the vector Av_m is linearly dependent on the preceeding $v_1,\ldots, v_m$, vectors in the sequence (3.7). When this happens then $AV = VH$, and (3.10) gives the exact solution of (3.1). In practice the loss of linear independence will take place gradually, and the solution of Eq. (3.10) gives approximate solutions to (3.1).

The term $h_{m+1,m}$ will be zero in exact arithmetic if m is equal to n. The important factor is the speed of the convergence. General conclusions on the speed are difficult to obtain. Saad [15, 16] gives estimate for special distributions of the eigenvalues of the matrix A. The effectiveness of this approach is somewhat limited by the fact that, for large problems, the size of the Krylov subspace (i.e., m) is limited by a particular computer capacity and even for the largest possible m, the attained precision may not be satisfactory. The remedy is to make the calculation scheme iterative, as it has been described earlier. The iteration as it has been set up in (3.6) is not a stationary iterative scheme, since the matrix $V^{\mathrm{T}}AV$ changes at each iteration. The starting vector for the construction of the Krylov space determines the matrix for that iteration. No general results for the convergence of this scheme are available. In the nonsymmetric positive definite case convergence has been observed experimentally.

It can be shown that the Krylov subspace method reduces to an algorithm that is very close to Richardson's scheme if the Krylov subspace is very small. In general

the larger the Krylov subspace, the better, since the convergence is faster at large m. For marginal problems ($m \approx n$) the projection part is more important and so a good precision may be achieved even with only one iteration. For very large matrix problems, the ratio m/n becomes small (less than 0.1) and then the iteration becomes important. It is interesting to note that the iteration (3.8) is not optimal. In fact, at each iteration we construct a Krylov space that is different from the previous ones, but it is not orthogonal to them. Therefore the corrections we are getting at each step are not optimum.

4. Numerical Experiments

As a first example, the Krylov method is applied to the barotropic equation (2.1) linearized around an asymmetric basic state, obtained by a previous long-term integration of the full nonlinear equation (2.1). The model is an hemispheric, spectral model, with resolution $J = 15$. The dimension of the equivalent matrix, i.e., the number of unknowns, is 248.

The convergence will be monitored by testing the residual norm of the approximate solution given at each iteration by

$$R^{IT} = \frac{\|Ax^{IT} - f\|}{\|Ax^{IT}\|}$$

Small values of R^{IT} mean that the solution is not changing much from one iteration to another. This residual can slightly underestimate the correctness of the solution because it gives the same weight to large and small component of x. In other words, it is a criterion that test the solution uniformly, regardless of the magnitude of the various components. Nonetheless, R is the convergence indicator that will be used throughout this section.

The calculations have been performed on the CDC 205 system at the Geophysical Fluid Dinamics Laboratory, Princeton, NJ, in single precision, with a 48 bits mantissa. The orthogonal vector system V is stored on disk, but everything else is core-contained.

In Fig. 1, R^{IT} is plotted as the algorithm develops for the barotropic case. The coefficient of dissipation used here is $K = 4 \times 10^6$ m^2 sec^{-1}, and $\varepsilon = 15$ day^{-1}. In the abscissa is the total number of steps, defined to be the product of the dimension of the Krylov subspace m, by the number of the iteration N. All experiments, except the case labeled A, have zero as an initial guess. The convergence is quite good. It is clear, however, that the best convergence rates are attained for large m/n ratios, where n is the dimension of the total problem, i.e., 248. Below a certain threshold the rate is not sensitive much to m; in the $m = 32$ and $m = 15$ cases speeds are very similar. The experiment A is for random initial guess. It converges slower than the companion experiment with the same m, but with zero initial guess.

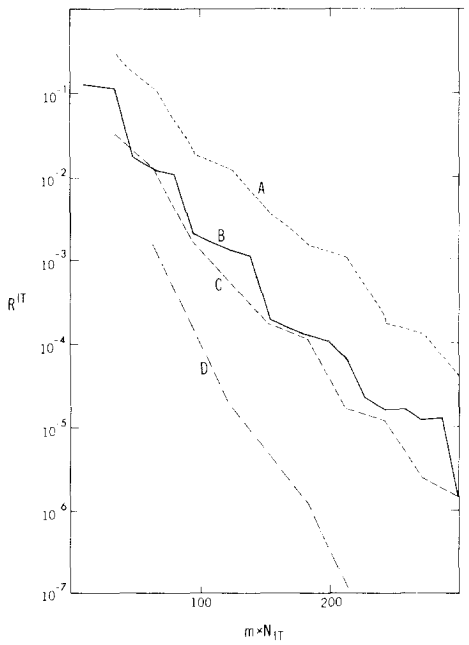

FIG. 1. Barotropic, nonseparable case. Convergence of the Krylov method for the barotropic equation. R^{IT} is plotted in logarithmic scale as a function of the total number of steps, defined as the product of the dimension of the Krylov space m and the iteration number N_{IT}. This format will be the same for all the remaining convergence figures. In this case $n = 248$. Various sizes of the Krylov subspace are used. Experiment A has $m = 32$ and randomly chosen initial guess. Experiments B, C, D are for $m = 15$, $m = 31$, and $m = 62$, respectively, and zero initial guess.

In the next examples we are going to discuss the baroclinic primitive equation system (2.21). We can expect from the physical characteristics of this system that it is more difficult than the barotropic case. It is known that in the case of a no motion, isothermal basic state, the baroclinic equations have eigenvalues that range in absolute value over several order of magnitude, from 10^{-3} (gravity waves) to 10^{-7} (Rossby waves). The more complicated basic state used here should not change this situation too much. The barotropic system should have a smaller range of eigenvalues and so it should be better conditioned than the baroclinic case.

The value of the coefficient of the Rayleigh friction $\varepsilon(\sigma)$ is a linear function of the level number, and it goes from 5 day^{-1} at the botton level to 50 day^{-1} at the top level. The Newtonian cooling $\gamma(\sigma)$ is also linear in the level number and it ranges from 5 day^{-1} at the bottom level to 10 day^{-1} at the top level. Small scale dissipation is modeled by the ∇^4 term and it has the same coefficient of 2.338×10^{16} m^4 sec^{-1} for vorticity, divergence and temperature. This is the standard setting of the friction parameters that is used in most of the following experiments.

New values will be explicitly stated where necessary. The forcing on the r.h.s. is given by a distribution of heating localized in latitude and longitude

$$Q(\lambda, \theta, \sigma) = A \sin(\pi\sigma)\left[\sin\frac{\pi(\lambda-\lambda_1)}{\lambda_2-\lambda_1}\sin\frac{\pi(\theta-\theta_1)}{\theta_2-\theta_1}\right]^2, \qquad \theta_1<\theta<\theta_2, \quad \lambda_1<\lambda<\lambda_2, \tag{4.1}$$

where σ is the vertical coordinate and λ, θ are the longitude and the latitude.

The basic state used in the first three examples is a solid rotation corresponding to a vorticity of $0.4\times10^{-5}\,\text{sec}^{-1}$ and a uniform temperature of 173°K which leads to separable equations. Next, another separable case is considered, but with a more complicated structure. Finally, asymmetric basic states, resulting in non-separable equations and therefore in a dense, non-symmetrical A will be treated.

Figure 2 shows the behavior of the iterations for the baroclinic primitive equation model for truncation $J=1$ ($n=149$). The size of the Krylov space is important in controlling the convergence. It is interesting to note that for very small subspace the Krylov method tends to the Richardson's iteration method. It appears that the Krylov method is successful where the Richardson's algorithm would have failed. As speculated, the baroclinic case is more difficult than the barotropic one and so

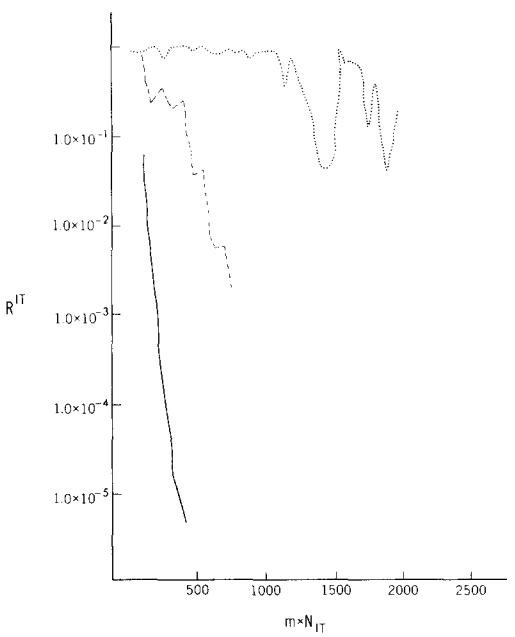

FIG. 2. Baroclinic, separable case. Convergence of the residual norms for the linearized primitive equations (2.15). The truncation is $J=1$, $n=149$. Different Krylov subspaces are used. Dotted, dashed and solid line are for experiments with $m=50$, $m=75$ and $m=100$.

the convergence is slower and the residual norms do not reach the extremely small values recorded previously.

The R1 system, though representing the simplest nontrivial case, is not going to be of great scientific relevance and it is therefore necessary to proceed to higher resolution models that represent the basic mathematical tool for a great variety of geophysical problems.

Figure 3 shows the convergence for the R7, 9 vertical levels, primitive equation model. The solid line is for a zero initial guess, while the dotted line has for initial guess a R3 solution obtained previously by a direct method. The choice of a better initial guess is beneficial to accelerate the convergence of the solution. In this case $n = 3341$ and $m = 1000$, so that the ratio is 0.3. Finally, in Fig. 4 the result for the case of a R15 and 9 level is shown with a ratio $m/n \approx 0.1$, since $n = 13869$.

As a further test the algorithm was used to reproduce the result by Nigam [13], using the same heating and mean flow. The spectral model with $J = 15$ and 9 vertical levels, for a total number of degrees of freedom $n = 13869$ was used. Eq. (2.3)–(2.6) are essentially the set used by Nigam, even if an exact comparison is not possible due to the different numerical formulation of the two models. Figure 5

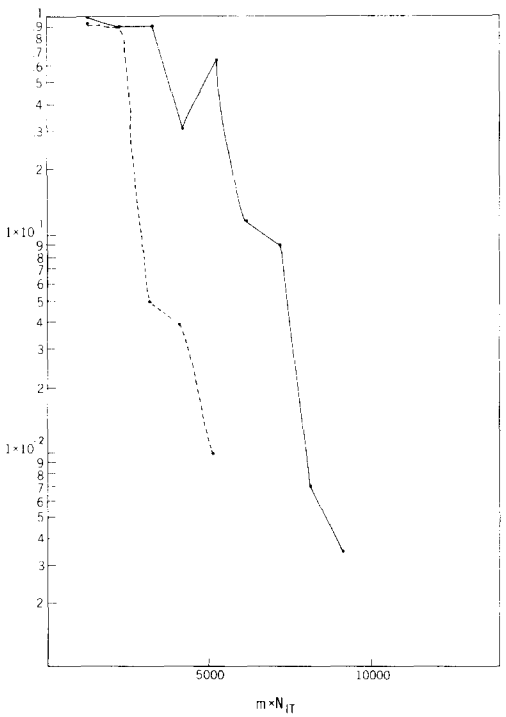

FIG. 3. Baroclinic, separable case. As in Fig. 2, but for $J = 7$, $n = 3341$, $m = 1000$. Solid line is for zero initial guess while the dotted line is an experiment with a low truncation solution, $J = 3$, as initial guess.

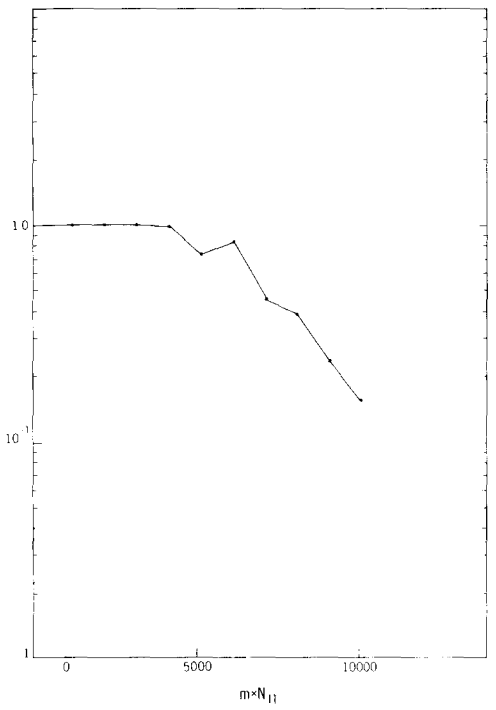

FIG. 4. Baroclinic, separable case. As in Fig. 2, but for $J = 15$, $n = 13869$, $m = 1000$. A zero initial guess is assumed.

shows the convergence in this case, where m/n is again ≈ 0.1. The initial guess is a $J = 7$ solution obtained previously by direct methods. After 6 iterations the solution is very close to Nigam's at inspection, and the R^{IT} has dropped an order of magnitude. The breaking down of the R^{IT} by wavenumber (not shown) provided evidence that the error is larger on the higher longitudinal wavenumbers and smaller on the low wavenumber components. In the problem of the general circulation of the atmosphere, the relevant physical information is carried by the large scale pattern corresponding to low wavenumbers. The spectral distribution of R^{IT} indicates that the Arnoldi's method converges faster on the physically relevant low wavenumber portion of the solution.

As a last test with the separable basic states the solution of a $J = 7$, 9 level model obtained with the Krylov method was compared with a solution calculated with a LU-decomposition. The former and the latter agreed to 3–4 decimal places.

The preceding examples were concerned with separable equations. It is now possible to drop the restriction of symmetry in the basic state and attack the non-separable set of equations. The basic state used here is obtained by time-averaging a set of nonlinear integrations of Eqs. (2.3)–(2.11) with truncation $J = 15$ performed with the GFDL spectral model, described by Gordon and Stern [7]. The basic state has strong variation both in the vertical and in the horizontal.

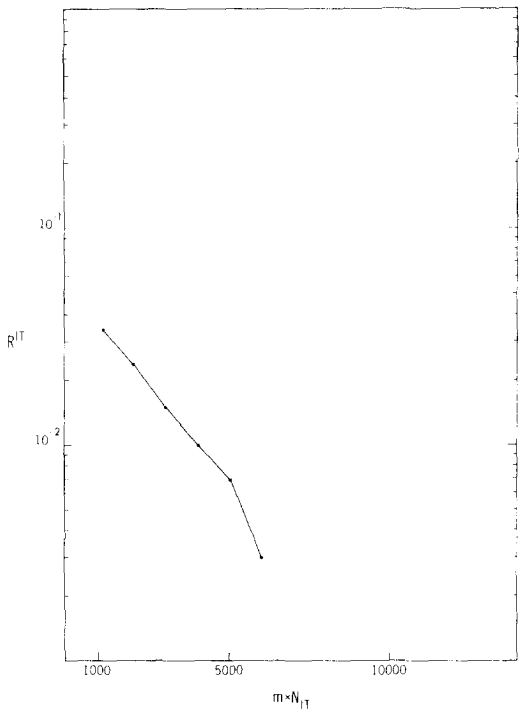

FIG. 5. Baroclinic, separable case. Convergence for the experiment reproducing Nigam (1983) result. The model is a $J = 15$ with $n = 13869$. The Krylov space dimension is $m = 1000$. Initial guess is a low truncation solution ($J = 7$) obtained previously.

It is necessary to use higher values of dissipation to achieve convergence with the size of the Krylov space that we have chosen, $m = 1000$. Rayleigh friction $\varepsilon(\sigma)$ and Newtonian cooling $\gamma(\sigma)$ are left with the same functional dependence, but they are multiplied uniformly by a factor 3.0 and 2.0, respectively. The ∇^4 coefficient is multiplied by a factor 10.0. The physical problem is not altered by this increase. Dissipation is a model-dependent parameter and values of this size have been used before in meteorological studies. The coefficient of the ∇^4 operator has a value close to the one used by Grose *et al.* [24] and the values of the Newtonian cooling and Rayleigh dumping are similar to the values used by Gill [23] in his study of the equatorial circulation. They are therefore appropriate in the equatorial areas, but a little too strong in the upper troposphere in the midlatitudes. The wavetrains emanating from the tropics are then attenuated in their propagation, but they are still very well developed. In Fig. 8 it is possible to see how the wave is clearly propagating far away from the source and all over the northern hemisphere.

These values do not represent the threshold for convergence, but rather a practical minimum. Below these values the convergence may be very slow. Other experiments, not shown, indicate that increasing the dissipation results in faster

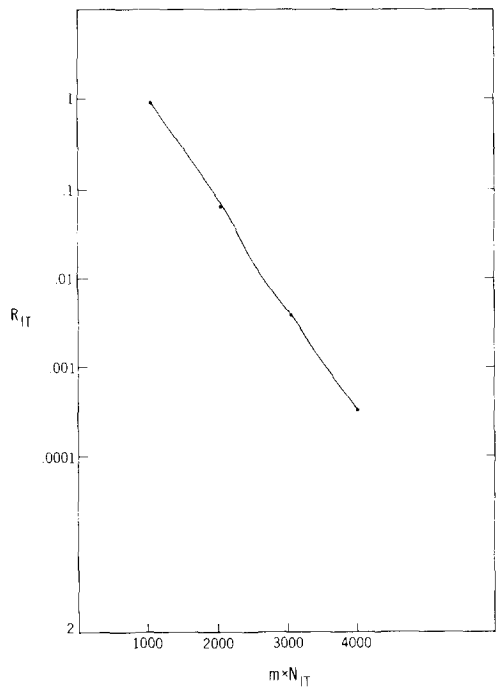

FIG. 6. Baroclinic, nonseparable case. Convergence of the residual norms of the iterates for the Krylov method, for the asymmetric, non separable, basic state. In this case $J = 7$, $n = 3341$ and $m = 1000$. The initial guess is irrelevant.

convergence rate. More study is however needed to clarify completely the role played by dissipation in the algorithm.

Figure 6 shows the convergence for the $J = 7$ model, 9 level, with a ratio $m/n \approx 0.3$, since $n = 3341$. The curve is typical of a set of several such solutions obtained with the same basic state, but for different forcings on the right-hand side. The forcings were varied by modifying the geographical location of the center of the distribution (4.1). The initial guess here is a solution obtained for another forcing.

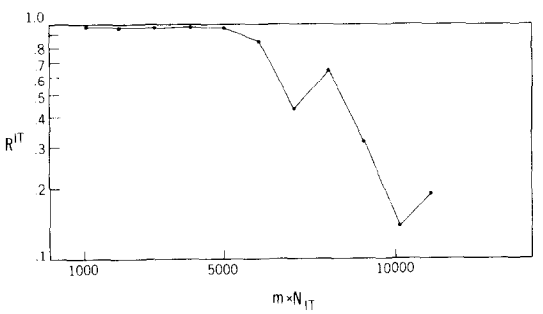

FIG. 7. Baroclinic, nonseparable case. As in Fig. 6, but for $J = 15$, $n = 13869$, $m = 1000$.

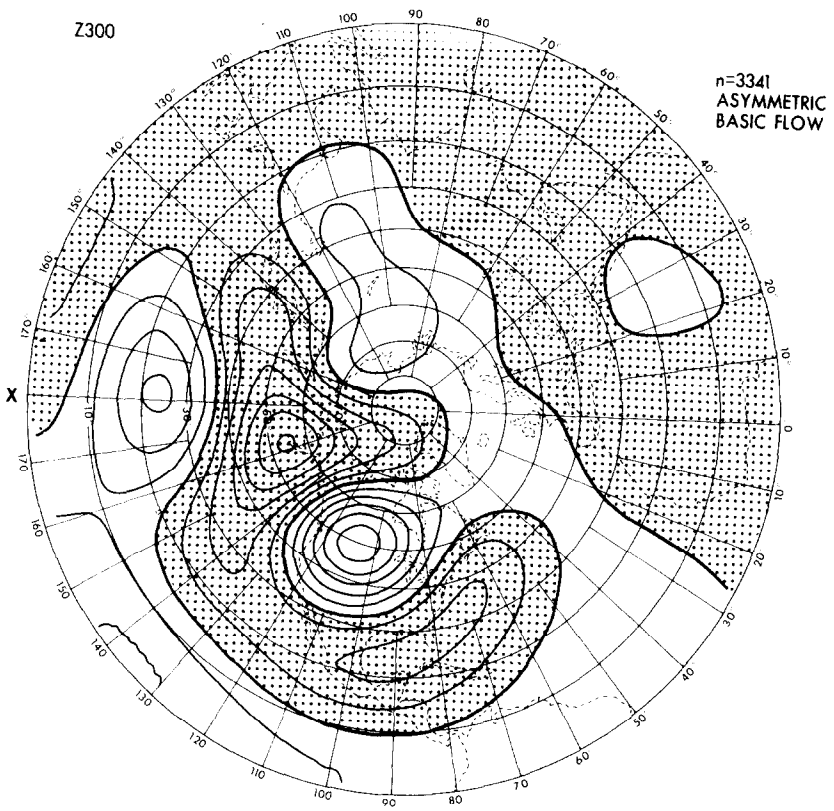

FIG. 8. Typical geopotential heigh pattern obtained from the Krylov method (J = 7, nonseparable case). Contour is 5 meters. The forcing is a dipole centered at the cross. Negative areas are shaded.

The convergence rates do not depend on the initial guess and four iterations are enough to achieve a good precision.

The convergence of the solution in a higher truncation case ($J = 15$, 9 levels) is illustrated in Fig. 7; m/n is ≈ 0.1 and again it is the high wavenumber part of the solution that slows down the convergence. It is necessary to perform 11 iterations before reaching small values of the residual norms.

A typical height field at 300 mb pressure level is plotted on a polar stereograpic projection in Fig. 8. Wavetrains are properly developed and they propagate quite far from the source. The source is a dipole, centered at the equator. The positive center is to the east, while the negative center is to the west of the cross. The two centers have a spatial distribution given by Eq. (4.1) and the same amplitude. The solution is not entirely different from Hoskins and Karoly [9] results, but the differences due to the asymmetric basic state are not negligible.

It is important to note that these asymmetric solution could not have been obtained by other methods. Since A, especially in the $J = 7$ case, is probably not nonsymmetric positive definite, its spectrum is not contained into one complex half-

plane, so simple iteration methods fail. It is interesting to point out that the matrix $V^{\mathrm{T}}AV$ provides an approximation to the eigenvalues of A [15]. This information is available at the extra cost of computing the eigenvalues of the Hessemberg matrix H. Some care should be taken because in the general case it is not possible to conclude that the spectrum of A lies in a half plane if the spectrum of $V^{\mathrm{T}}AV$ does. This happens only if A is a normal matrix.

The Arnoldi's algorithm fills in a gap between direct methods and iteration methods. These two extreme cases are two particular limits of the iterative Arnoldi's method. The former is realized when $m \approx n$, and the latter when $m \ll n$, in this last case a scheme very similar to Richardson's method is obtained. When $m \ll n$ it is not possible to reach a solution for the asymmetric basic state used and with the level of dissipation chosen. A fortiori, the Richardson's method would have met the same lack of success. If the ratio m/n is not too small, the Krylov method is capable of treating indefinite cases, by realizing a sort of trade off between direct and iterative methods.

5. Conclusions

The Krylov subspace method is useful for solving large linear systems resulting from the discretization of linear barotropic and baroclinic models. It has the capability of expanding the class of treatable basic states by including asymmetric flows. Even very large problems, with a total number of degrees of freedom of the order of 10000, can be treated satisfactorily. It is particularly effective for problems in which the storage is just beyond the capacity of the fast memory of the computer.

It does not require any explicitly storage of the matrix A, but only calculation of the application of the matrix to a vector, Ax, and usually this task may be resolved by an external routine. In fact, a time-dependent numerical model provides this information by computing the right-hand side of Eq. (2.14) (with $f' = 0$), usually in the form of a time tendency. It is possible, then, to implement the method by modifying a preexisting numerical model without extensive recoding. This is particularly desirable in geophysical problems where codes for complicated multilevel models have been developed so extensively. The application is not limited to a spectral model, but it may be applied also to a grid-point model.

The convergence of the method is controlled by the dissipation terms and by the dimension of the Krylov subspace compared to the total space. The dissipation factor is more important if the projection is made on a Krylov subspace that is much smaller than the total space. In this case the iteration part is more important than the projection part and convergence may be limited to nonsymmetric positive definite cases.

APPENDIX

We now describe how to obtain Eq. (2.14). We divide the flow fields into the time-independent basic state, denoted by the subscript b, and a deviation, denoted, for convenience, with the same symbols (ζ, D, T, q). These splitted variables are then inserted in Eqs. (2.3)–(2.11) and, retaining only first order ters in the equations for the deviation, we arrive at the explicit form of $L=(L_\zeta, L_D, L_T, L_q)$,

$$L_\zeta = -\hat{k}\cdot\nabla\times\left[-\zeta\hat{k}\times\mathbf{v}_b-(f+\zeta_b)\hat{k}\times\mathbf{v}-\dot{\sigma}\frac{\partial\mathbf{v}_b}{\partial\sigma}-\dot{\sigma}_b\frac{\partial\mathbf{v}}{\partial\sigma}\right.$$

$$\left.-RT_b\nabla q-RT\nabla q_b\right]-\varepsilon(\sigma)\zeta-K_\zeta\nabla^4\zeta, \tag{A.1}$$

$$L_D=\nabla\cdot\left[-\zeta\hat{k}\times\mathbf{v}_b-(f+\zeta_b)\hat{k}\times\mathbf{v}-\dot{\sigma}\frac{\partial\mathbf{v}_b}{\partial\sigma}-\dot{\sigma}_b\frac{\partial\mathbf{v}}{\partial\sigma}\right.$$

$$\left.-RT_b\nabla q-RT\nabla q_b\right]-\varepsilon(\sigma)D-K_D\nabla^4D-\nabla^2\phi-\nabla^2(\mathbf{v}\cdot\mathbf{v}_b), \tag{A.2}$$

$$L_T=-\mathbf{v}_b\cdot\nabla T-\mathbf{v}\cdot\nabla T_b-\dot{\sigma}_b\frac{\partial T}{\partial\sigma}-\dot{\sigma}\frac{\partial T_b}{\partial\sigma}$$

$$+\frac{R}{c_p}\left[T_b\left(\frac{\omega}{p}\right)+T\left(\frac{\omega}{p}\right)_b\right]-\gamma(\sigma)T-K_T\nabla^4T, \tag{A.3}$$

$$L_q=-\tilde{\mathbf{v}}\cdot\nabla q_b-\tilde{\mathbf{v}}_b\cdot\nabla q-\nabla\cdot\tilde{\mathbf{v}} \tag{A.4}$$

and also

$$\frac{\omega}{p}=\frac{\dot{\sigma}}{\sigma}+(\mathbf{v}-\tilde{\mathbf{v}})_b\cdot\nabla q+(\mathbf{v}-\tilde{\mathbf{v}})\cdot\nabla q_b-\nabla\cdot\mathbf{v}$$

$$\dot{\sigma}=-\int_0^\sigma(D-\tilde{D})\,d\sigma-\int_0^\sigma(\mathbf{v}-\tilde{\mathbf{v}})_b\cdot\nabla q\,d\sigma-\int_0^\sigma(\mathbf{v}-\tilde{\mathbf{v}})\cdot\nabla q_b\,d\sigma,$$

$$\frac{\partial\phi}{\partial\sigma}=-\frac{RT}{\sigma}.$$

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