Chebyshev Spectral Methods for Limited-Area Models. Part I: Model Problem Analysis

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ABSTRACT

This study considers how spectral methods can be applied to limited-area models using Chebyshev polynomials as basis functions. We review the convergence of Sturm–Liouville series to motivate the use of the Chebyshev polynomials, and describe the tau and collocation projections which allow the use of general (nonperiodic) boundary conditions. These methods are illustrated for a simple model problem, the linear advection equation in one dimension, and numerical results confirm their high accuracy.

Time differencing and efficiency are considered in detail using both asymptotic analysis and numerical results from the model problem. The stability condition for Chebyshev methods with explicit time differencing, often thought to be severe, is shown to be less severe than that for finite difference methods when high accuracy is desired. Fourth-order Runge-Kutta time differencing is the most efficient of the many schemes considered. When the accuracy desired is high enough, Chebyshev spectral methods are more efficient than finite difference methods; numerical results suggest that this may be true in practice even for very modest accuracies.

1. Introduction

Numerical models of the atmosphere begin with a set of governing equations in continuous form which must be discretized in order to solve them on a digital computer. One way to do this is finite difference methods, which represent the dependent variables by their values at discrete gridpoints and approximate the derivatives by finite differences. Alternatively, one can approximate the dependent variables by truncated series expansions in terms of known basis functions. If the basis functions are local, i.e., individually nonzero over only a small part of the computational domain, the method is called a finite element method; if the basis functions are global, i.e., individually nonzero over essentially the whole computational domain, it is called a spectral method.

The primary appeal of spectral methods is their high accuracy. Finite difference and finite element discretizations give algebraic convergence, i.e., the discretization error is \(O(N^{-p})\) where \(N\) is the number of degrees of freedom (gridpoints or basis functions) and \(p\) is a small positive integer giving the order of the method (usually 2 or 4). In contrast, a properly formulated spectral method gives exponential convergence, i.e., the discretization error is \(O(e^{-\alpha N})\) for some positive number \(\alpha\). Thus spectral methods can give very accurate solutions with relatively few degrees of freedom, so they require relatively little storage and are potentially very efficient.

Spectral methods have been used quite successfully in global atmospheric models (e.g., Bourke et al., 1977; Machenhauer, 1979) for studying or predicting the global-scale circulation. With present computer capabilities, however, global models cannot achieve sufficient resolution for the detailed study or prediction of smaller-scale phenomena such as fronts and tropical cyclones. One way to achieve the needed resolution is to restrict the computational domain to less than the entire globe, resulting in a limited-area model. In such a model one must apply lateral boundary conditions at computational boundaries, i.e., boundaries of the computational domain which have no physical counterparts. Formulating these boundary conditions so that they do not distort the solution in the interior of the domain is a difficult task. Unless the behavior of the solution is artificially restricted by applying periodicity or wall conditions, the choice of appropriate basis functions for a spectral method is not readily apparent.

Perhaps for this reason, spectral methods have seldom been used for limited-area atmospheric modeling. DeMaria and Schubert (1984) used a Fourier spectral technique in a primitive equation hurricane model with the simplifying but unrealistic assumption of periodicity in both horizontal directions. Spectral methods based on normal mode expansions also have been used in hurricane modeling (Schubert and DeMaria, 1985); this technique is promising, but requires boundary conditions which reflect propagating gravity waves. However, more general spectral techniques based on Chebyshev polynomial expansions have been developed (e.g., Orszag, 1971a, b; Orszag and Israeli, 1974; Gottlieb and Orszag, 1977). These techniques are ca-
pable of handling quite general boundary conditions, and have been used in a limited-area ocean model based on the barotropic vorticity equation by Haidvogel et al. (1980). The purpose of the present study is to investigate the usefulness of Chebyshev spectral techniques for limited-area atmospheric modeling.

Part I consists of an overview of the basic concepts of spectral models as appropriate for limited-area problems. Section 2 reviews appropriate choices of basis functions and projections, and section 3 demonstrates the Chebyshev spectral methods by applying them to a simple model problem. Questions of time differencing and the resulting overall efficiency are discussed in section 4, and our conclusions are summarized in section 5. In Part II (Fulton and Schubert, 1987) we show how Chebyshev spectral methods can be applied to more complicated problems, using the nonlinear shallow water equations with open boundary conditions as a simple prototype of a general limited-area model based on primitive equations.

2. Spectral discretizations for limited domains

The problems considered in this study consist of partial differential equations of the general form

$$\frac{\partial u(x, t)}{\partial t} + Lu(x, t) = f(u, x, t),$$

(2.1)

where $x$ and $t$ represent space and time coordinates, $u$ is the unknown, $L$ is a linear operator involving space derivatives, and $f$ represents nonlinear terms and/or specified forcing. We want to solve (2.1) on a limited domain in $x$ subject to appropriate boundary and initial conditions. Only one-dimensional problems will be considered in Part I; however, problems in more than one spatial dimension and systems of equations also fit the same conceptual form with $x$ and $u$, respectively, interpreted as vectors. Spectral discretizations for (2.1) are based on approximating the unknown $u$ by a truncated series expansion of the form

$$u_N(x, t) = \sum_{n=0}^{N} \hat{u}_n(t) \phi_n(x),$$

(2.2)

where $\phi_0(x), \ldots, \phi_N(x)$ are fixed basis functions which are global, i.e., individually nonzero over essentially the whole model domain. The spectral coefficients $\hat{u}_0(t), \ldots, \hat{u}_N(t)$ in the expansion (2.2) are determined by requiring that the governing equation (2.1) be approximately satisfied with $u$ replaced by $u_N$; in mathematical terms this amounts to a projection of the true solution $u$ into the space spanned by the basis. We will consistently use the hat notation to denote spectral coefficients as in (2.2). In the following sections we examine the choices of basis functions and projections for problems of the form (2.1).

a. Basis functions

The notion of orthogonality is central to most practical spectral methods. Consequently, basis functions are often chosen as solutions of an appropriate Sturm–Liouville problem. Here we review the convergence of expansions based on such functions in order to choose basis functions suitable for use in general limited-area models.

The general Sturm–Liouville equation is

$$L_{SL} \phi(x) = -(p(x)\phi'(x))' + q(x)\phi(x) = \lambda w(x)\phi(x),$$

(2.3)

where primes denote differentiation with respect to $x$. We seek solutions of this equation on a finite interval $[a, b]$ which corresponds to the limited domain on which a problem of the form (2.1) is to be solved. With suitable boundary conditions and restrictions on the functions $p$, $q$, and $w$, (2.3) has a countably infinite set of solutions $\{\phi_n(x)\}_{n=0}^{\infty}$ corresponding to discrete eigenvalues $\{\lambda_n\}_{n=0}^{\infty}$, with $\lambda_n < \lambda_{n+1}$ and $\lambda_n \to \infty$ as $n \to \infty$. The eigenfunctions are orthogonal in the inner product

$$\langle f, g \rangle_w = \int_a^b f(x)g(x)w(x)dx,$$

(2.4)

and for purposes of analysis it is convenient to assume they are normalized so that $\langle \delta_{mn}, \phi_n \rangle_w = \delta_{mn} (\delta_{mn} = 1$ if $m = n$ and 0 otherwise). Furthermore, they form a complete set in the sense that any suitably smooth function $u(x)$ may be expanded as

$$u(x) = \sum_{n=0}^{\infty} \hat{u}_n \phi_n(x),$$

(2.5)

where

$$\hat{u}_n = \langle u, \phi_n \rangle_w.$$  

(2.6)

This completeness property says that the true solution $u$ of (2.1) may be expressed exactly as an infinite series of such eigenfunctions. However, their usefulness as basis functions for a spectral method depends on how fast the series converges, i.e., how many terms must be retained in a truncated series in order to adequately approximate $u$.

To address this question let $u_N(x)$ denote the series (2.5) truncated after $n = N$. Following Gottlieb and Orszag (1977), we use the Parseval relation to write the error $u - u_N$ in the norm $\| f \|_w = \langle f, f \rangle_w^{1/2}$ generated by the inner product (2.4) as

$$\| u - u_N \|_w^2 = \sum_{n=N+1}^{\infty} \| \hat{u}_n \phi_n \|_w^2 = \sum_{n=N+1}^{\infty} \hat{u}_n^2.$$  

(2.7)

Thus the rate at which the error $\| u - u_N \|_w$ decreases with increasing $N$ is governed by the rate at which the coefficients $\hat{u}_n$ decrease with increasing $n$. In particular, if $\hat{u}_n = O(n^{-r})$ as $n \to \infty$ for some $r > \frac{1}{2}$ then it is easily shown from (2.7) that $\| u - u_N \|_w = O(N^{1/2-r})$ as $N \to \infty$. To estimate $\hat{u}_n$ we substitute for $\phi_n$ in (2.6) from
(2.3) and integrate by parts twice (assuming \(u\) is sufficiently smooth so that this is valid) to obtain

\[
\hat{u}_n = \lambda_n^{-1} (u, w^{-1} L_{SL} \phi_n)_w = \lambda_n^{-1} [(v, \phi_n)_w + B(u, \phi_n)].
\]  
(2.8)

Here \(v = w^{-1} L_{SL} u\) and

\[B(u, \phi_n) = \{p(x)[u'(x)\phi_n(x) - u(x)\phi'_n(x)]\}_{x=0}^{1}.
\]  
(2.9)

The term \((v, \phi_n)_w\) in (2.8) is bounded independent of \(n\), since by the Cauchy–Schwarz inequality \(|(v, \phi_n)_w| \leq \|v\|_w \|\phi_n\|_w\) and \(\|\phi_n\|_w = 1\). The size of the boundary term \(B(u, \phi_n)\) depends in general on the behavior of both the function \(u\) and the eigenfunctions \(\phi_n\) at the boundaries.

If \(p(a) \neq 0\) and \(p(b) \neq 0\) in (2.3) and appropriate linear homogeneous boundary conditions are applied, the Sturm–Liouville problem is regular at both endpoints. Examples of appropriate boundary conditions include periodicity and the conditions

\[
\begin{align*}
\phi(a) \cos \alpha - \phi'(a) \sin \alpha &= 0, \\
\phi(b) \cos \beta + \phi'(b) \sin \beta &= 0
\end{align*}
\]  
(2.10)

where \(\alpha\) and \(\beta\) are specified constants. In this case the eigenvalues and eigenvectors have the asymptotic behavior \(\lambda_n = O(n^2), \phi_n(x) = O(1), \phi'_n(x) = O(n)\) as \(n \to \infty\) (Courant and Hilbert, 1953, pp. 336–339). If \(u\) does not satisfy the boundary conditions applied to the Sturm–Liouville problem, then \(B(u, \phi_n) = O(n)\) and hence \(\hat{u}_n = O(n^{-1})\) if \(u(a) = u(b) = 0\) then \(B(u, \phi_n) = O(1)\) so \(\hat{u}_n = O(n^{-2})\). This slow (algebraic) convergence is a reflection of the Gibbs phenomenon associated with \(u\) not satisfying the boundary conditions satisfied by the expansion functions \(\phi_n\); this phenomenon is discussed in detail in Gottlieb and Orszag (1977). If \(u\) does satisfy the boundary conditions, \(B(u, \phi_n)\) vanishes and the integration by parts argument may be repeated (again assuming \(u\) is sufficiently smooth) to obtain

\[
\hat{u}_n = \lambda_n^{-2} [(z, \phi_n)_w + B(v, \phi_n)],
\]  
(2.11)

where \(z = w^{-1} L_{SL} v\). Again \((z, \phi_n)_w = O(1)\) and \(B(v, \phi_n) = O(n)\), so \(\hat{u}_n = O(n^{-3})\) and the convergence is faster. However, in general the argument may not be repeated again since \(B(v, \phi_n) \neq 0\). Therefore, the rate of convergence of expansions based on eigenfunctions of a regular Sturm–Liouville problem depends both on the smoothness of the function being expanded and on its behavior at the boundaries. This is a generalization of the statement that ordinary Fourier series converge rapidly only if the function being expanded is both smooth and periodic.

If \(p(a) = p(b) = 0\) in (2.3) the Sturm–Liouville problem is singular at both endpoints. In this case \(B(u, \phi_n) = 0\) for any bounded function \(u\), so the integration by parts may be repeated as long as the function being integrated is smooth enough; if \(u\) is infinitely differentiable then \(\hat{u}_n = O(n^{-r})\) for all \(r > 0\) so the convergence is exponential. (Exponential convergence may also be obtained in the regular case with periodic boundary conditions, but only if \(u\) is also periodic.) Therefore, the rate of convergence of expansions based on eigenfunctions of a singular Sturm–Liouville problem depends only on the smoothness of the function being expanded and not on its behavior at the boundaries. Such expansions are therefore appropriate for limited-area spectral models in which the behavior of the solution at the boundary is not artificially restricted by applying periodicity or wall conditions.

The actual choice of basis functions is guided by some practical considerations in addition to those described above. Polynomials are particularly convenient as basis functions, especially since their derivatives are again polynomials and thus are exactly expressible in terms of the basis. Two sets of common orthogonal polynomials satisfy Sturm–Liouville problems which are singular at finite endpoints as discussed above: the Legendre polynomials \(P_n(x)\), for which \([a, b] = [-1, 1]\), \(p(x) = 1 - x^2\), \(q(x) = 0\) and \(w(x) = 1\), and the Chebyshev polynomials \(T_n(x)\), for which \([a, b] = [-1, 1]\), \(p(x) = (1 - x^2)^{1/2}\), \(q(x) = 0\) and \(w(x) = (1 - x^2)^{-1/2}\). Although Legendre series may give better approximations than Chebyshev series at the endpoints (Lanczos, 1973), the latter are usually preferred in limited-area models for the following three reasons. First, Chebyshev series give somewhat better (global) approximations than do Legendre series for the same number of terms. In fact, the Chebyshev approximation of degree \(N\) of a function is very nearly equal to the best approximation which can be obtained by any polynomial of degree \(N\), in the sense of minimizing the maximum pointwise error (Rivlin, 1969). Second, Chebyshev series converge faster than Legendre series when the function being expanded is not smooth (Gottlieb and Orszag, 1977, §3). Third, and perhaps most important, Chebyshev series can be evaluated very efficiently using the Fast Fourier Transform (FFT) algorithm. We will discuss the properties of Chebyshev polynomials in section 3a below.

b. Projections

Having discussed the basis functions in terms of which the dependent variables in a spectral model are to be expanded, we turn now to the approximation methods which relate those expansions to the problem to be solved. Such methods are known as projections, since they project the true solution into the space spanned by the basis functions. Replacing the true solution \(u(x, t)\) in (2.1) with the spectral approximation \(u_N(x, t)\) as given by (2.2) results in the residual

\[
r_N(x, t) = f(x, t) - \frac{\partial u_N(x, t)}{\partial t} - L u_N(x, t),
\]  
(2.12)

which in general is nonzero. The three projections discussed below seek to make the residual approximately zero; they differ in the sense of approximation used.
The Galerkin projection is the classical approximation used in spectral models in spherical geometry (Machenhauer, 1979). It defines \( u_N \) by requiring the residual to be orthogonal to each of the basis functions \( \phi_0, \ldots, \phi_N \) in some inner product \( (, ) \), so the residual is approximately zero in the sense that it has no projection onto the basis functions used in the model. Thus the Galerkin equations are

\[
\left( \frac{\partial u_N}{\partial t} + Lu_N, \phi_n \right) = (f, \phi_n) \quad (n = 0, \ldots, N).
\]

(2.13)

The dependent variables are the spectral coefficients \( \hat{u}_n \); they are initialized by projecting the initial condition \( u(x, 0) = U(x) \) via \( (u_N, \phi_n) = (U, \phi_n) \). If the basis functions are orthonormal in the chosen inner product then (2.13) simplifies to

\[
\frac{d\hat{u}_n}{dt} + \sum_{m=0}^{N} (L\phi_m, \phi_n)\hat{u}_m = (f, \phi_n) \quad (n = 0, \ldots, N).
\]

(2.14)

Solution of these equations is facilitated by choosing the basis functions \( \phi_n \) and inner product \( (, ) \) so that the summation in (2.14) involves relatively few terms. In particular, if the \( \phi_n \) are the normal modes of the system (i.e., the eigenfunctions of \( L \)) then (2.14) reduces to

\[
\frac{d\hat{u}_n}{dt} + \lambda_n \hat{u}_n = (f, \phi_n) \quad (n = 0, \ldots, N)
\]

(2.15)

where \( L\phi_n = \lambda_n \phi_n \). In this manner the equations are decoupled, except for possible coupling through nonlinear terms represented by \( f \).

In the Galerkin projection the boundary conditions of the problem are treated implicitly by building them into the basis functions. That is, the basis functions must be chosen so that they individually satisfy the boundary conditions; these conditions must be linear and homogeneous so they will be satisfied by the linear combination \( u_N \). Since suitable basis functions which individually satisfy open boundary conditions usually cannot be found, the Galerkin approximation is not well suited to many limited-area problems. However, a simple modification removes this difficulty, leading to the tau projection of Lanczos (1938, 1956). In the tau approximation the basis functions need not individually satisfy the boundary conditions of the problem; rather, these conditions are applied explicitly to the truncated series \( u_N \) as a whole. With \( M \) as the number of independent boundary conditions to be applied, these equations simply replace the last \( M \) of equations (2.13). Other than this treatment of the boundary conditions, the Galerkin and tau projections are identical.

In contrast, the collocation projection defines \( u_N \) by requiring the residual to vanish at selected points known as collocation points. Usually it is most convenient to choose basis functions which do not satisfy the boundary conditions of the problem, and then apply these conditions explicitly as in the tau method. Denoting a collocation point by \( \bar{x}_j \), the collocation equations consist of \( N + 1 - M \) equations

\[
\frac{\partial u_N}{\partial t} + Lu_N = f \quad \text{at} \quad x = \bar{x}_j,
\]

(2.16)

together with the \( M \) boundary conditions applied to \( u_N \). In this method the dependent variables are the values \( \hat{u}_j(t) = u_N(\bar{x}_j, t) \) at the collocation points and the boundary values of \( u_N \), rather than the spectral coefficients \( \hat{u}_n \); they are initialized directly from the initial condition on \( u \). We will consistently denote values at collocation points using overbars. Note that the collocation projection uses the series expansion (2.2) only in evaluating \( u_N \). Spectral methods using the collocation projection are often called pseudospectral (Menlées and Orszag, 1979); this terminology emphasizes the connections with classical spectral (Galerkin and tau) methods—global basis functions and exponential convergence—and deemphasizes the connections with finite element collocation methods. The collocation projection is usually very easy to implement, even when the problem to be solved is highly nonlinear.

3. Model problem: the linear advection equation

To illustrate the concepts and methods discussed above we apply them to the one-dimensional linear advection equation

\[
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = f(x, t) \quad (-1 < x < 1)
\]

(3.1a)

with the boundary and initial conditions

\[
u(-1, t) = g(t),
\]

(3.1b)

\[
u(x, 0) = U(x).
\]

(3.1c)

Here \( f \) represents specified forcing and \( g \) and \( U \) are specified boundary and initial values. This problem is the simplest prototype of a limited-area model involving wave or advective processes. When \( f = 0 \) it has the analytical solution

\[
u(x, t) = \begin{cases} U(x - t), & x - t \geq 1, \\ g(t - x - 1), & x - t < -1 \end{cases}
\]

(3.2)

representing propagation or advection in the \(+x\) direction with unit speed.

a. Chebyshev polynomials

From the discussion in section 2a, the Chebyshev polynomials \( T_n(x) \) are appropriate basis functions for this problem. They are defined with the substitution \( x = \cos \theta \) by

\[
T_n(\cos \theta) = \cos(n \theta) \quad (n = 0, 1, \ldots).
\]

(3.3)
As shown in Fig. 1, each $T_n$ has zeros at
$$
\chi_j^{(n)} = \cos \left( \frac{(j + 1/2)\pi}{n} \right) \quad (j = 0, \cdots, n - 1) \quad (3.4)
$$
and extrema at
$$
\tilde{x}_j^{(n)} = \cos \left( \frac{j\pi}{n} \right) \quad (j = 0, \cdots, n) \quad (3.5)
$$
with $T_n(\tilde{x}_j^{(n)}) = (-1)^j$. The Chebyshev polynomials have the orthogonality property
$$
\langle T_m, T_n \rangle = \frac{\pi}{2} c_m \delta_{mn}, \quad c_n = \begin{cases} 2, & n = 0 \\ 1, & n > 0, \end{cases} \quad (3.6)
$$
where $\langle , \rangle$ denotes the Chebyshev inner product
$$
\langle f, g \rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\sqrt{1 - x^2}} dx. \quad (3.7)
$$
In view of (3.6), if a function $\psi(x)$ can be expanded in a Chebyshev series
$$
\psi(x) = \sum_{n=0}^{\infty} \hat{\psi}_n T_n(x) \quad (3.8)
$$
then its spectral coefficients $\hat{\psi}_n$ satisfy
$$
\hat{\psi}_n = \frac{2}{\pi c_n} \langle \psi, T_n \rangle \quad (n = 0, 1, \cdots). \quad (3.9)
$$
Equations (3.8) and (3.9) constitute the continuous Chebyshev transform pair [cf. (2.5) and (2.6)]. For the problem (3.1) we seek an approximate solution in the form of the truncated Chebyshev series
$$
u_n(x, t) = \sum_{n=0}^{N} \hat{u}_{n}(t) T_n(x). \quad (3.10)
$$

### b. The Chebyshev–tau method

The tau approximation to (3.1) in the inner product (3.7) is defined by
$$
\left\{ \frac{\partial u_n}{\partial t} + \frac{\partial u_n}{\partial x}, T_n \right\} = \langle f, T_n \rangle \cdot (n = 0, \cdots, N - 1; t > 0) \quad (n = 0, \cdots, N; t = 0),
$$
$$
\langle u_n, T_n \rangle = \langle U, T_n \rangle \quad (n = 0, \cdots, N; t = 0). \quad (3.11)
$$

The effects of this approximation are easily seen by expanding the residual $r_n$ in a Chebyshev series and using (3.11) to obtain
$$
r_n = f - \frac{\partial u_n}{\partial t} - \frac{\partial u_n}{\partial x} = \tau(t)T_n(x) + \sum_{n=N+1}^{\infty} \hat{f}_n(t) T_n(x),
$$
(3.12)
where the coefficient $\tau(t)$ is uniquely determined by the boundary condition. If $\hat{f}_n$ is small for $n > N$ (i.e., $N$ is large enough to resolve $f$) then the residual $r_n$ is dominated by the term $\tau(t)T_n(x)$; since $T_n(x)$ oscillates with equal amplitude on the interval $[-1, 1]$, the residual is distributed with equal magnitude across the domain. The use of the coefficient $\tau$ by Lanczos is the source of the name "tau method."

Substituting from (3.10) for $u_n$ and using (3.6) and the property $T_n(-1) = (-1)^n$, the tau equations (3.11) reduce to
$$
\frac{d\hat{u}_n}{dt} + \hat{u}_{n}^{(1)} = f_n \quad (n = 0, \cdots, N - 1; t > 0), \quad (3.13a)
$$
$$
\sum_{n=0}^{N} (-1)^n \hat{u}_n = g \quad (t > 0), \quad (3.13b)
$$
$$
\hat{u}_n = \hat{U}_n \quad (n = 0, \cdots, N; t = 0), \quad (3.13c)
$$

where
$$
\hat{u}_n^{(1)} = \frac{2}{\pi c_n} \left\{ \frac{\partial u_n}{\partial x}, T_n \right\} = \frac{2}{c_n} \sum_{m=n+1}^{\infty} m\hat{u}_m \quad (3.14)
$$
denotes the spectral coefficients of the $x$-derivative of $u_n$. To solve this system for the spectral coefficients $\hat{u}_0, \cdots, \hat{u}_N$ using explicit time differencing, one uses (3.13a) to predict new values of $\hat{u}_0, \cdots, \hat{u}_{N-1}$ from those at the previous time level, and then uses (3.13b) to diagnose $\hat{u}_N$. Since the derivative relation (3.14) can be evaluated recursively from
$$
c_{n-1}\hat{u}_{n-1}^{(1)} - \hat{u}_{n+1}^{(1)} = 2m\hat{u}_n \quad (n > 0) \quad (3.15)
$$
starting with $\hat{u}_{N+1}^{(1)} = \hat{u}_{N}^{(1)} = 0$, this (linear) tau model requires only $O(N)$ operations per time step, in spite of the global nature of the spectral approximation.
c. The Chebyshev–collocation method

For the collocation approximation to (3.1) we choose as collocation points the points \( \tilde{x}_j = \tilde{x}_j^{(N)} = \cos(j\pi/N) \)
for \( j = 0, \ldots, N \) at which \( T_N(x) \) has extrema [cf. (3.5)]; this choice allows the necessary transforms to be computed easily, as subsequently discussed. Since \( \tilde{x}_N = -1 \) is the boundary point, the collocation equations are

\[
\frac{d\tilde{u}_j}{dt} + \tilde{u}_j^{(1)}(t) = \tilde{f}_j \quad (j = 0, \ldots, N-1; t > 0),
\]

\[
\tilde{u}_N = g \quad (t > 0),
\]

\[
\tilde{u}_j = \tilde{U}_j \quad (j = 0, \ldots, N; t = 0),
\]

where \( \tilde{u}_j^{(1)}(t) \) denotes the value of the \( x \)-derivative of \( u_N \) at the collocation point \( \tilde{x}_j \). To solve this system for the values \( \tilde{u}_0, \ldots, \tilde{u}_N \) using explicit time differencing, one uses (3.16a) to predict new values \( \tilde{u}_0, \ldots, \tilde{u}_{N-1} \) from those at the previous time level and then uses (3.16b) to diagnose \( \tilde{u}_N \).

In computing the derivative values \( \tilde{u}_j^{(1)} \) one makes use of the spectral representation (3.10) as follows. First, the spectral coefficients \( \tilde{u}_0, \ldots, \tilde{u}_N \) are computed from the values \( \tilde{u}_0, \ldots, \tilde{u}_N \) via the discrete Chebyshev transform

\[
\tilde{u}_n = \frac{2}{N\hat{c}_j} \sum_{j=0}^{N-1} \tilde{u}_j T_n(\tilde{x}_j),
\]

where \( \hat{c}_j = 2 \) for \( j = 0 \) and \( j = N \) and 1 otherwise (note that these coefficients will be different than those in the tau approximation). Next, the recurrence relation (3.15) is used to compute the spectral coefficients \( \tilde{u}_0^{(1)}, \ldots, \tilde{u}_N^{(1)} \) of the derivative. Finally, these coefficients are used to compute the derivative values \( \tilde{u}_0^{(1)}, \ldots, \tilde{u}_N^{(1)} \) via the inverse discrete Chebyshev transform

\[
\tilde{u}_j^{(1)} = \sum_{n=0}^{N} \tilde{u}_n^{(1)} T_n(\tilde{x}_j).
\]

The transforms (3.17) and (3.18) are discrete analogues of the continuous transforms (3.9) and (3.8), respectively. Referring to the values \( \tilde{u}_j \) and coefficients \( \tilde{u}_n \) as “physical space” and “spectral space” representations of \( u_N \), respectively, this calculation can be described as transforming \( u_N \) from physical to spectral space, computing the derivative there, and transforming the result back to physical space. Using the relation (3.3) the discrete Chebyshev transforms can be written as discrete cosine transforms, which in turn can be evaluated using the FFT algorithm, so this whole procedure requires only \( O(N \log N) \) operations.

In results presented below we will identify the Chebyshev–tau and Chebyshev–collocations methods described above by the identifiers TAU and COL, respectively. For this simple linear problem these methods differ only in the treatment of the boundary condition (Gottlieb and Orszag, 1977, §2), as can be seen by transforming (3.16a) using (3.17) and comparing with (3.13a). The more significant differences between these methods for nonlinear problems will be discussed in part II.

d. Numerical results

To illustrate the accuracy of the methods described above we compare them with simple finite difference methods. Specifically, we consider the first-order upstream difference (FD1) scheme

\[
\frac{d\tilde{u}_j}{dt} + \tilde{u}_j - \tilde{u}_{j-1} = \tilde{f}_j,
\]

the second-order centered difference (FD2) scheme

\[
\frac{d\tilde{u}_j}{dt} + \frac{\tilde{u}_{j+1} - \tilde{u}_{j-1}}{2\Delta x} = \tilde{f}_j,
\]

and the fourth-order centered difference (FD4) scheme

\[
\frac{d\tilde{u}_j}{dt} + \frac{-\tilde{u}_{j+2} + 8\tilde{u}_{j+1} - 8\tilde{u}_{j-1} + \tilde{u}_{j-2}}{12\Delta x} = \tilde{f}_j.
\]

Here \( \tilde{f}_j \) denotes values at the gridpoints \( \tilde{x}_j = -1 + j\Delta x \), \( j = 0, \ldots, N \), with \( \Delta x = 2/N \). Note that the centered schemes require computational boundary conditions, which we obtain here by replacing the centered differences in (3.20) and (3.21) by uncentered differences of the same order. In this section we are concerned with space discretization errors only, and hence solve the discretized equations with time steps small enough so that the time discretization errors are negligible in comparison.

The first test case considered here has the analytical solution

\[
u(x, t) = A \exp \left[ -\left( \frac{x - x_0 - \alpha t}{h} \right)^2 \right],
\]

where \( A = h^{-1/2}(\pi/2)^{-1/4} \) so that the continuous \( L_2 \) norm is 1. For all results we use the values \( x_0 = -0.5 \) and \( h = 0.2 \), and set \( f = 0 \) and evaluate the initial and boundary values \( U \) and \( g \) directly from (3.22). Figure 2 shows the approximate solutions at \( t = 1.0 \) obtained by the Chebyshev–collocation method (COL) and the three finite difference methods using \( N = 16 \) and \( N = 24 \), along with the corresponding analytical solution. Chebyshev–tau results are not shown, since they are practically identical to the collocation results for this problem. The spectral method clearly gives a much better approximation than do the difference methods. In particular, the spectral solution does not exhibit the computational dispersion which broadens all of the difference solutions and introduces spurious oscillations in the centered difference methods. Figure 3 shows the corresponding error \( \|u - u_N\|_2 \) as a function of \( N \), using the discrete norm

\[
\|u - u_N\|_2 = \left( \sum_{j=0}^{N} \frac{1}{\hat{c}_j} \left| u(\tilde{x}_j, t) - u_N(\tilde{x}_j, t) \right|^2 \right)^{1/2}.
\]
This is a trapezoidal approximation to the continuous $L_2$ norm using values at the finite difference gridpoints, and hence will be referred to here as the $L_2$ error. As $N$ approaches 32 the error in the spectral solution is decreasing like $10^{-N/4}$, while the finite difference errors are only beginning to approach their asymptotic rates of decrease.

In view of the distribution of zeros and extrema of $T_N(x)$ [cf. (3.4), (3.5)] one could say that the Chebyshev series (3.10) has effective resolution $O(N^{-1})$ near the center of the domain and $O(N^{-2})$ near the boundaries. To see how this nonuniform resolution affects the ability to resolve various solution components we consider a second test case with analytical solution $u(x, t) = \cos[M\pi(x - t)]$.  

Again we set $f = 0$ and evaluate the initial and boundary values $U$ and $g$ directly from (3.24). Figure 4 shows the $L_2$ error at $t = 3.0$ as a function of $N$ and $M$ for the Chebyshev and centered difference methods. Resolving $M$ waves in the domain to an error of no more than 10% requires roughly $N \approx 3M$ for the Chebyshev methods, in agreement with the estimate “$\pi$ polynomials per wavelength” derived by Gottlieb and Orszag (1977, p. 35). In contrast, the fourth- and second-order difference methods require about 10–12 and 30–50 gridpoints per wavelength, respectively, to achieve the same 10% error; this is due primarily to the large phase error (computational dispersion) associated with the centered differences.

The above results show that when modest accuracy is desired Chebyshev spectral methods require far fewer degrees of freedom than do finite difference methods, and that this advantage increases dramatically as the desired accuracy increases. This fact has immediate implications for the amount of computer storage required to obtain accurate solutions. However, the question of the relative efficiency of the methods is more complicated, as it depends on the method chosen for solving the spectral equations. We will examine the questions of time differencing and efficiency in detail in the following section.

4. Time differencing and efficiency

Discretizing the governing equations of a model in space using a spectral method results in a set of ordinary differential equations in time $t$ which may be written in the form

$$\frac{du}{dt} = F(u, t).$$ 

(4.1)
Here the vector $u(t)$ consists of the spectral coefficients (Galerkin and tau projections) or the values at collocation points (collocation projection) of the model variables. Often there are diagnostic relations (i.e., equations not involving time derivatives) in addition to (4.1), such as boundary conditions, which must be satisfied by $u$ for all $t$. If the basis functions of the spectral method are the normal modes of the linear part of the model, then (4.1) reduces to a set of forced oscillation equations [cf. (2.15)] which are coupled only through the nonlinear terms; the linear part of the model can then be solved exactly (e.g., DeMaria and Schubert, 1984; Schubert and DeMaria, 1985). However, such normal mode spectral models usually are feasible only with reflecting or periodic boundary conditions.

With a Chebyshev spectral discretization in space as described in section 3, the model variables are coupled and (4.1) can be solved only approximately (this is also true for the nonlinear terms in normal mode models). Typically one uses a finite difference discretization in time, in which $u(t)$ is represented by values $u^{(k)}$ at discrete time levels $t_k = k\Delta t$, $k = 0, 1, 2, \cdots$, and the time derivative is approximated using finite differences. The resulting scheme is called explicit if it gives $u^{(k+1)}$ explicitly in terms of values at previous time levels $t_k$, $t_{k-1}$, etc.; otherwise, it is called implicit (here, semi-implicit schemes will also be included in the latter cat-
category). Explicit schemes are easy to implement but are only conditionally stable, whereas implicit schemes have better stability properties but are difficult to implement efficiently. We will discuss both types of schemes.

a. Explicit schemes

In choosing an explicit scheme the primary considerations of stability, accuracy, and efficiency are interrelated. Here, we first use an asymptotic analysis to demonstrate the important properties of explicit time differencing for Chebyshev spectral methods as compared with finite difference methods, and then confirm and quantify this analysis with numerical results.

1) ASYMPTOTIC ANALYSIS

Consider the problem of integrating a numerical model of a hyperbolic (wave-like) system in such a way that the error in the numerical solution at a specified time $t$ is at most $10^{-r}$, where $r$ is a specified positive number. Table 1 shows how the required space and time resolution and the resulting total work depend asymptotically on $r$ for both finite difference and Chebyshev–spectral space discretizations. The first row gives the required space resolution $N$. For finite differences of order $p$ in space, the discretization error is $O(N^{-p})$, where $N$ is the number of gridpoints in one dimension, so that $N = O(10^{mp})$. In contrast, for Chebyshev methods the error is $O(10^{-aN})$ for some $a$ so that $N = O(r)$.

Two considerations are involved in choosing the time step $\Delta t$; stability and accuracy. A time differencing scheme (or, more properly, the overall numerical model) is absolutely stable for a fixed time step $\Delta t$ if the numerical solution does not grow in time without bound. This type of stability is appropriate for hyperbolic problems, in which the true (continuous) solution is bounded in time. In general, explicit schemes are only conditionally stable, i.e., absolutely stable only for sufficiently small $\Delta t$. With finite differences in space the stability condition has the form

$$\Delta t = O\left(\frac{\Delta x}{c}\right)$$

where $\Delta x$ is the (spatial) mesh size and $c$ is the maximum speed at which information can propagate in the model. For sufficiently simple problems such conditions can be obtained easily by the von Neumann method (Haltiner and Williams, 1980, §5.5), which considers only a single (spatial) Fourier mode of the solution and ignores boundary conditions. In contrast, deriving stability conditions with Chebyshev discretizations in space requires a more complicated matrix stability analysis (Gottlieb and Orszag, 1977, §9). The resulting conditions have the form

$$\Delta t = O\left(\frac{1}{CN^2}\right)$$

where the length $l$ measures the domain size. This form might be expected, in light of (4.2), since a truncated Chebyshev series of degree $N$ has resolution $O(N^{-2})$ near the boundaries [cf. (3.4) and (3.5)].

It has been argued (e.g., Gottlieb and Orszag, 1977, sec. 9) that the stability condition (4.3) is “severe” compared to (4.2). Indeed, if one simply wants to barely resolve the solution to a particular scale specified by the wavenumber $M$ then both Chebyshev and finite difference models require $N = O(M)$ (although the constants of proportionality are quite different as shown in Fig. 4), and asymptotically the time step required for stability in the Chebyshev model [$\Delta t = O(M^{-2})$] is smaller than in the finite difference model [$\Delta t = O(M^{-1})$]. However, this comparison ignores the difference between exponential and algebraic convergence, which makes it possible to choose $N$ much smaller for the spectral method than for the finite difference method when higher accuracy is desired. Using (4.2) and (4.3) and the estimates of $N$ required for the accuracy $10^{-r}$ given in the first row of Table 1, we can estimate the time step required for stability as shown in the second row. When high enough accuracy is desired (large enough $r$), the time step required for stability in finite difference methods is in fact smaller than that in Chebyshev spectral methods. Thus (4.3) is less “severe” than (4.2) when interpreted in terms of the resolution $N$ needed for accuracy.

Furthermore, one must also take into account the accuracy of the time differencing scheme. With time differences of order $q$ the time discretization error is $O(\Delta t^q)$, so to achieve the accuracy $10^{-r}$ one must choose $\Delta t = O(10^{-aq})$, independent of the space discretization (except when a smaller time step is required for stability). Comparing the time steps required for stability and accuracy in Chebyshev spectral methods as shown in Table 1, we conclude that when high enough accuracy is desired the time step is limited by accuracy rather than stability. Thus, not only is the stability condition (4.3) for Chebyshev spectral methods not “severe”: asymptotically, it is not even the factor which limits the time step.

To compare the efficiency of finite difference and Chebyshev spectral methods, we note that finite dif-

| \(N\) for accuracy \(10^{-r}\) | \(10^{mp}\) | \(r\) | \(r\)
|----------------|-------|-----|-----|
| \(\Delta t\) for stability | \(10^{-mp}\) | \(r^{-2}\) | \(r^{-2}\)
| \(\Delta t\) for accuracy (order \(q\)) | \(10^{mp}\) | \(10^{-q}\) | \(10^{-q}\)
| Stability limit when \(q > p\) | \(r\) small | \(r\) small |
| Work per time step | \(10^{mp}\) | \(r^2\) | \(r\log r\)
| Total work (stability limit) | \(10^{mp}\) | \(r^2\) | \(r^2\log r\)
| Total work (accuracy limit) | \(10^{mp}10^{1q}\) | \(r^210^{1q}\) | \((r \log r)10^{1q}\)
ference methods require $O(N)$ operations per time step, while spectral methods require $O(N^2)$ operations with "slow" transforms (i.e., computing the transforms by simple matrix multiplication) or $O(N \log N)$ operations with fast transforms (i.e., using the FFT algorithm). Using the previous estimates of $N$ and $\Delta t$ we can then estimate the number of operations per time step and the total operations required to compute the solution at a fixed time with error at most $10^{-6}$, as shown in the last three rows of Table 1. From these results we conclude that Chebyshev spectral methods—even with explicit time differencing and "slow" transforms—are inevitably more efficient than finite difference methods, when the accuracy desired is high enough. This asymptotic result is quite general, and basically reflects the exponential convergence of the spectral discretization.

2) NUMERICAL RESULTS

To illustrate the conclusions obtained from the asymptotic analysis we now present numerical results obtained from the model problem of section 3. Table 2 lists the six explicit time differencing schemes considered here, along with their stability conditions for the Chebyshev—collocation and Chebyshev—tau versions of the model problem. The number of "stages" $s$ is the number of times the right-hand side $F$ of (4.1) must be evaluated per time step; since most of the computational work is expended in evaluating $F$, the work per time step is essentially proportional to $s$, and hence the quantity $N^2 \Delta t/s$ gives a measure of the relative efficiency of the time differencing schemes (note that $F$ is different for the collocation and tau methods so their relative efficiencies cannot be compared directly from these numbers). Thus, for the collocation and tau versions the AB2 and FOR schemes, respectively, are the most efficient of the schemes considered when the time step is limited by stability.

However, the time step required for stability may not tell the whole story; the asymptotic analysis of the previous section indicates that when high enough accuracy is desired the time step is limited by accuracy rather than stability. The level of accuracy which requires a smaller time step than that required by stability alone depends in general on the problem being solved, the character of the solution (e.g., its smoothness), and the space and time discretizations chosen. Figure 5 shows the error in the Chebyshev—collocation and Chebyshev—tau solutions of the model problem for the Gaussian test case (3.22) as a function of the time step (scaled by $N$ and $s$ so that the abscissa reflects relative efficiency) for the six time differencing schemes of Table 2. For the collocation method (solid lines), all schemes tested except the AB4 scheme are limited by accuracy for both $N = 16$ and $N = 24$. In contrast, the tau method (dashed lines) requires smaller time steps for stability, so with $N = 16$ only the first-order schemes (FOR and MAT) are limited by accuracy, while with $N = 24$ the second-order schemes (RK2 and AB2) also are somewhat limited by accuracy.

These and similar results for other test cases and other values of $N$ suggest the following choices for ex-

### Table 2. Time differencing schemes tested and stability conditions.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Name</th>
<th>Definition</th>
<th>Order $q$</th>
<th>Stages $s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOR</td>
<td>Forward</td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}_k + \Delta t \mathbf{F}(\mathbf{u}_k)$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>MAT</td>
<td>Matsuno</td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}_k + \Delta t \mathbf{F}(\mathbf{u}_k)$</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>AB2</td>
<td>Second-order</td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}_k + \frac{1}{2} \Delta t (3\mathbf{F}(\mathbf{u}<em>k) - \mathbf{F}(\mathbf{u}</em>{k-1}))$</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Adams–Bashforth</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RK2</td>
<td>Second-order</td>
<td>$\mathbf{u}_{k+1/2} = \mathbf{u}_k + \frac{1}{2} \Delta t \mathbf{F}(\mathbf{u}_k)$</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Runge-Kutta</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AB4</td>
<td>Fourth-order</td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}<em>k + \Delta t \left( \frac{55}{24} \mathbf{F}(\mathbf{u}<em>k) - 9 \mathbf{F}(\mathbf{u}</em>{k-1}) + \frac{37}{3} \mathbf{F}(\mathbf{u}</em>{k-2}) \right)$</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Adams–Bashforth</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RK4</td>
<td>Fourth-order</td>
<td>$\mathbf{u}_{k+1/2} = \mathbf{u}_k + \frac{1}{2} \Delta t \mathbf{F}(\mathbf{u}_k)$</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>Runge-Kutta</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}<em>k + \Delta t \left( \frac{55}{24} \mathbf{F}(\mathbf{u}<em>k) - 9 \mathbf{F}(\mathbf{u}</em>{k-1}) + \frac{37}{3} \mathbf{F}(\mathbf{u}</em>{k-2}) \right)$</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\mathbf{u}_{k+1/2} = \mathbf{u}<em>k + \frac{1}{2} \Delta t \mathbf{F}(\mathbf{u}</em>{k+1/2})$,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\mathbf{u}_{k+2/3} = \mathbf{u}<em>k + \frac{1}{2} \Delta t \mathbf{F}(\mathbf{u}</em>{k+2/3})$,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\mathbf{u}_{k+1} = \mathbf{u}<em>k + \Delta t \left( \frac{55}{24} \mathbf{F}(\mathbf{u}<em>k) - 9 \mathbf{F}(\mathbf{u}</em>{k-1}) + \frac{37}{3} \mathbf{F}(\mathbf{u}</em>{k-2}) \right)$</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>
Fig. 5. $L_2$ errors in the numerical solutions of the model problem (3.1) for the test case (3.22) as functions of $\Delta t$ for the COL (solid lines) and TAU (dashed lines) discretizations with (a) $N = 16$ and (b) $N = 24$, using the explicit time differencing schemes of Table 2 as labeled. The abscissa is scaled by the number of stages to reflect relative efficiency.

Plicit time differencing schemes. For the Chebyshev-collocation method, the time step for most schemes is limited by accuracy as long as $N$ is large enough to minimally resolve the solution (e.g., to better than 10% accuracy); of the schemes tested, the RK4 scheme is the most efficient, often requiring far less work than second-order schemes. For the Chebyshev-\tau method, the time step for most schemes (except first-order schemes) is limited by stability unless relatively high accuracy is desired (e.g., better than 0.1%); the schemes tested, the RK2 and AB2 schemes are the most efficient. However, the RK4 scheme is only slightly less efficient when limited by stability, and can be considerably more efficient when high accuracy is desired.

Finally, the asymptotic analysis of the previous section indicated that when high enough accuracy is desired, Chebyshev methods are more efficient than finite difference methods. The level of accuracy at which this is true in practice depends strongly on the problem, solution, and discretizations as above, and also on the computer system, library (FFT) routines, and the skill of the programmer. To simply demonstrate that Chebyshev methods may be able to compete in efficiency with finite difference methods when modest accuracy is desired, we again consider the model problem of section 3 with the test case (3.22). Figure 6 shows the errors in the Chebyshev-collocation and finite difference solutions as functions of execution time on a CRAY-1 computer; each curve represents errors obtained in separate runs with the same value of $N$ as labeled but different values of $\Delta t$. In each case, RK4 time differencing was used since it required the least work to compute the solution to the level of accuracy of the space discretization error (for the FD2 scheme, some second-order time differencing schemes can result in an overall error less than the space discretization error for a small range of $\Delta t$ just below the stability limit). Tau results are not shown here, since this linear problem involves no transforms and hence the execution time would be misleading. The Chebyshev-collocation method is more efficient than the FD2 method for this problem for accuracies of better than about 5%, and is roughly as efficient as the FD4 method for accuracies of better than 1%.

One additional note about efficiency concerns the method of calculating derivatives in the Chebyshev collocation method. This calculation as normally performed requires two Chebyshev transforms plus the derivative operation in spectral space; furthermore, in order to compute the transforms using the FFT algorithm and take full advantage of symmetry one usually does additional pre- and post-processing (Cooley et al., 1970). Thus it has been suggested (Hussaini et al., 1983) that it may be more efficient to simply generate the matrix which represents the entire collocation derivative operation and multiply by that matrix as needed. Our experience indicates that in one-dimensional problems the matrix procedure (which can be vectorized) is indeed faster than the transform procedure for $N \leq 64$ using an FFT routine coded in FORTRAN, and for $N \leq 32$ using an FFT routine coded in assembly language. Therefore, the matrix procedure was used in generating the results in Fig. 6. However, for multidimensional problems on a CRAY-1 computer, transforms can be computed using the routine FFT99, which is an extremely fast assembly language implementation of the parallel FFT algorithm of Temperton (1983a,b,c). This transform procedure is considerably
faster than the matrix procedure for all $N \geq 8$. Thus the relative efficiencies of the Chebyshev and finite difference methods for the one-dimensional model problem may be somewhat misleading; we expect that for more complicated problems in more dimensions the Chebyshev methods may be more efficient at even more modest levels of accuracy.

b. Modified explicit schemes

The leapfrog scheme was not included above since in its unmodified form it is unconditionally unstable with Chebyshev spectral discretizations in space (Gottlieb and Orszag, 1977, §9). The Asselin–Robert filter (Haltiner and Williams, 1980, p. 147) stabilizes this scheme; in general, the time step allowed by stability increases as the filter parameter $\gamma$ increases. However, the largest stable time step is still less than that of the AB2 scheme, and the heavy filtering ($\gamma > 0.2$) needed to obtain this stability renders the scheme only first-order accurate in time. Thus the leapfrog scheme is not recommended for use in Chebyshev–spectral models.

Two other modified explicit schemes deserve mention since they were introduced specifically for use with spectral methods but are not useful in practice. One is the “partially corrected Adams–Bashforth” scheme proposed by Gazdag (1976), in which a corrector step using only previously computed values is applied to the AB2 scheme. This corrector step indeed stabilizes the physical mode of the solution as claimed, but it also introduces a second computational mode which is unstable except for small time steps. The second scheme, proposed by Gottlieb and Turkel (1980), essentially filters the solution by modifying the Chebyshev derivative relation (3.15); it is claimed to allow
time steps to be “chosen by accuracy requirements alone”. However, a detailed analysis (Fulton and Taylor, 1984) shows that small amounts of filtering do not change the stability properties significantly, while large amounts of filtering render the scheme unconditionally unstable.

c. Implicit schemes

In terms of the accuracy obtained for a given time step, implicit and explicit schemes (of the same order) are roughly comparable. Since implicit schemes are more difficult to program and usually require more work per time step, there is no reason to use them when the time step of explicit schemes is limited by accuracy. However, implicit schemes allow much larger time steps without instability, and hence may be more efficient when the time step of explicit schemes is strongly limited by stability. This is the case for the simple model problem considered here when using the Chebyshev–tau method with only modest accuracy required. For more complicated problems the time step may be limited by stability when the stability condition is related to a physical process which is represented in the model but which is relatively unimportant for the particular problem being studied. For example, if the model admits fast-propagating wave solutions and the physical situation being modeled has very little energy in these modes, the time step may be limited by stability. Similarly, including a “friction” term proportional to the Laplacian of a model variable in a Chebyshev spectral model leads to a stability condition of the form $\Delta t = O(N^{-4})$, which is unduly restrictive if the specific form of friction assumed is merely a somewhat arbitrary representation of general dissipative processes.

Implementing an implicit scheme efficiently in a Chebyshev spectral model can be complicated, since the resulting matrix equations are essentially full due to the global nature of the spectral approximation. Here we give only a brief outline of general approaches which may be useful. These same techniques can be used to solve implicit Chebyshev–spectral equations which arise from diagnostic conditions in balanced models.

Implicit equations in Chebyshev–tau models can sometimes be solved directly. For example, using trapezoidal implicit time differencing for the Chebyshev–tau model (3.13) results in a linear system of equations to be solved at every time step. When the coefficients of the derivative are eliminated using the recurrence relation (3.15), the matrix is tridiagonal except for the first row (which comes from the boundary condition), and ordinary Gaussian elimination can be implemented in $O(N)$ operations (after factorization). This results in a scheme which is absolutely stable for any time step; the time step required for accuracy is similar to that for the collocation method with RK2 time differencing. For nonlinear advection terms one may split the advecting velocity into a specified linear part, which can be treated implicitly, and treat the residual nonlinear term explicitly (Haidvogel, 1979). Implicit equations arising from second derivatives in space also can be converted to essentially tridiagonal form as outlined by Gottlieb and Orszag (1977, §10). Similar procedures may be useful in other one-dimensional problems; however, in more than one dimension iterative methods may be needed (Haidvogel and Zang, 1979).

Implicit equations in Chebyshev–collocation models invariably involve full matrices due to the transforms involved. Direct solution by Gaussian elimination requires $O(N^3)$ operations (after factorization) and hence usually is not practical. Iterative techniques must be carefully designed so that they can use the FFT algorithm in computing the transforms and thus solve the problem in $O(N \log N)$ operations. One such indirect method is the “spectral iteration” method of Orszag (1980) and McCrory and Orszag (1980), which is a defect correction iteration using a finite difference approximation to the spectral operator. Another approach is the spectral multigrid method introduced by Zang et al. (1982, 1984), which combines the powerful multigrid concepts developed by Brandt (1977) and others with spectral discretizations. The relationship between these two methods is discussed briefly in Brandt et al. (1984).

The complexity of the above methods for implementing implicit time differencing in Chebyshev spectral models should be contrasted with the simplicity of such models with explicit time differencing. Unless the size of the time step is excessively limited by stability (e.g., if the velocity scale which determines the stability condition is very much larger than the velocity scale of the part of the solution of physical interest), implicit time differencing may not be worth either the computational cost or the programming effort.

5. Concluding remarks

We have demonstrated the formulation and properties of Chebyshev spectral methods for limited-area models using a simple model problem. The methods are easy to formulate and give very high accuracy using relatively few degrees of freedom. They differ fundamentally from finite difference and finite element methods in that the approximation is global rather than local, which leads to conclusions which differ markedly from what one might expect based on experience with finite differences. For example, the “nonuniform resolution” of the Chebyshev polynomials does not detract from the resolution obtained; indeed, a Chebyshev model with $N$ modes resolves higher wavenumbers than second- or fourth-order centered finite differences over $N$ equally spaced gridpoints, with a sharper distinction between those waves which are resolved accurately and those which are not resolved at all.

Furthermore, the “extra” resolution of the Chebyshev series near the boundaries does not necessarily force one to use implicit time differencing for efficiency.
due to "severe" stability conditions; in fact, the time step required for the Chebyshev–collocation method with explicit time differencing tends to be limited by accuracy rather than stability. Therefore, implicit time differencing is needed for efficiency only in cases where the physics of the problem demands it, i.e., when the model admits modes (such as fast-propagating waves) which limit the stability but which contain very little energy in the physical situation being modeled. These are precisely the same cases which require implicit time differencing for efficiency in finite difference models. However, implementing implicit time differencing in such cases may be more difficult in Chebyshev models due to the global nature of the spectral approximation.

The analysis and numerical results presented here suggest that Chebyshev spectral methods may offer a practical alternative to conventional finite difference methods for limited-area modeling. We have argued that when high enough accuracy is desired the Chebyshev spectral methods are more efficient than finite difference methods, and have presented numerical results which suggest that this may be true in practice for relatively modest accuracy, perhaps for relative errors on the order of five percent. However, the model problem examined here is admittedly extremely simple.

In part II of this study (Fulton and Schubert, 1987) we consider the extension of these methods to more realistic problems, using the nonlinear shallow water equations in two dimensions as a prototype of a primitive-equation limited-area model.

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