Boundary Effects in Regional Spectral Models

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ABSTRACT

The choice of an appropriate spectral spatial discretization is governed by considerations of accuracy and efficiency. The purpose of this article is to discuss the boundary effects on regional spectral methods. In particular, we consider the Chebyshev τ and sinusoidal- or polynomial-subtracted sine–cosine expansion methods. The Fourier and Chebyshev series are used because of the orthogonality and completeness properties and the existence of fast transforms. The rate of convergence of expansions based on Chebyshev series depends only on the smoothness of the function being expanded, and not on its behavior at the boundaries. The sinusoidal- or polynomial-subtracted sine–cosine expansion Tatsumi-type methods do not, in general, possess the exponential-convergence property. This is due to the fact that the higher derivatives of the polynomial- or sinusoidal-subtracted function are not periodic in a model with time-dependent boundary conditions. The discontinuity in derivatives causes the slow convergence of the expanded series (Gibbs phenomenon). When a large disturbance is near the boundary so that derivative discontinuities in the expanded function are large, the Tatsumi-type method causes not only erroneous numerical values in the outgoing boundary, but also spurious oscillations in the incoming boundary region. When the wave is away from the boundary, low resolution in the Tatsumi-type method converges exponentially, just as with the Chebyshev τ method. High-resolution solutions of the Tatsumi-type method do not, however, yield high accuracy due to the discontinuity in higher derivatives of the expanded function.

1. Introduction

With the advent of the fast Fourier transform (FFT) and the spectral transform method (Orszag 1970), the spectral method has emerged as a viable alternative to finite-difference and finite-element methods for numerical solution of atmospheric problems. This is especially true for global atmospheric modeling. There are three areas in which spectral discretization is superior to other types of discretization (with the exception of semi-Lagrangian gridpoint techniques) in global models: 1) the spectral method eliminates pole problems; 2) the computational cost of enlarging the model time step by the semi-implicit, implicit zonal advection and high-wavenumber damping techniques is trivial and with present computer capability, only the global model with spectral discretization allows the physical parameterization package (with the exception of radiation) to be called every time step; 3) spectral models have high accuracy and efficiency that comes from the "exponential-convergence" property. The shortcoming of global spectral models is the lack of a fast Legendre transform. The $O(M^3)$ operational counts for the Legendre transform makes the spectral model inefficient as the model resolution M (number of waves around the earth) increases to the order of 200 for inviscid models. At present, almost all of the operational global models and GCMs are based on the spectral method with spherical harmonics basis functions.

Despite the popularity of the spectral method for global models, most of the research and operational limited-area models are based on finite-difference or finite-element methods. The main obstacles are the time-dependent boundary conditions and the implementation of semi-implicit methods. Tatsumi (1986) develops a sinusoidal-subtracted Fourier sine–cosine series-expansion method for limited-area modeling. To reduce the Gibbs phenomenon, a boundary relaxation (smoothing) scheme is employed. Tatsumi argues that the boundary smoothing is not an important part of the method and his method can be contrasted with the polynomial-subtracted Fourier sine–cosine series expansion that is discussed by Gottlieb and Orszag (1977). Fulton and Schubert (1987a,b) present a summary of Chebyshev spectral methods, including discussions and demonstrations of technique implementation, accuracy, and stability. They also develop a Chebyshev spectral shallow-water model in a limited

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domain, and it yields good results without any boundary smoothing. The purpose of this paper is to study the boundary effects on limited-area spectral methods. In particular, we will discuss the exponential-convergence property in the polynomial- or sinusoidal-subtracted sine–cosine expanded methods. We will use a simple calculation to explore situations in which derivatives of an expanded function are discontinuous at a time-dependent lateral boundary. Section 2 gives the analysis, and in section 3 numerical results without boundary smoothing or filtering are presented. The summary is given in section 4.

2. Analysis of boundary effects

The formulation of a spectral method involves the choice of the basis function and projection operator. In other words, which series will we use to approximate the unknown functions? The fundamental requirement is the "completeness" of the series. Namely, any suitable smooth function can be expressed exactly as an infinite sum of the series. The projection operators are used to find the coefficients of the series expansion. Three commonly used projections are Galerkin, pseudospectral (collocation), and tau.

In addition to the completeness of the basis functions, the orthogonality property is central to most practical spectral methods. Consequently, basis functions are often chosen as solutions of an appropriate Sturm–Liouville problem. To efficiently implement the spectral method in an atmospheric model, we need fast transforms and rapid convergence for the chosen basis function. The fast transform cuts down the computational cost of projection (finding the spectral coefficients), while rapid convergence guarantees the efficiency and accuracy of the spectral method. Due to the existence of fast transforms, Fourier and Chebyshev series are well suited for atmospheric spectral modeling. In the following, we will present arguments that show how the boundary conditions affect the speed of convergence of various basis functions. More detailed analyses can be found in Lanczos (1956), Gottlieb and Orszag (1977), and Fulton and Schubert (1987a).

We consider the general Sturm–Liouville equation in limited domain $[a, b]$

$$L\phi(x) = -[p(x)\phi'(x)]' + q(x)\phi(x) = \lambda w(x)\phi(x), \quad (2.1)$$

where primes denote differentiation with respect to x. With suitable boundary conditions and restrictions on functions $p(x)$, $q(x)$ and $w(x)$, (2.1) has a countable infinite set of solutions $\phi(x)_{n=0}^{\infty}$ corresponding to discrete eigenvalues $\lambda_{n_n=0}^{\infty}$. The eigenfunctions ϕ_n from (2.1) form a complete set and are orthonormal in the inner product

$$(\phi_i, \phi_j)_w = \int_a^b \phi_i(x)\phi_j(x)w(x)dx = \delta_{ij}, \quad (2.2)$$

where $\delta_{ij} = 1$ if $i = j$, and 0 otherwise. Thus, any suitable function can be expanded as

$$u(x) = \sum_{n=0}^{\infty} \hat{u}_n\phi_n(x), \quad (2.3)$$

where

$$\hat{u}_n = (u, \phi_n)_w. \quad (2.4)$$

The speed of convergence can be estimated by the rate at which the spectral coefficient $\hat{u}_n$ decreases with increasing n. To estimate the magnitude of $\hat{u}_n$, we substitute for ϕ_n in (2.4) from (2.1) and integrate by parts twice (assuming u is sufficiently smooth) to obtain

$$\hat{u}_n = \lambda_n^{-1}(u, w^{-1}L\phi_n)_w = \lambda_n^{-1}[(v, \phi_n)_w + B(u, \phi_n)]. \quad (2.5)$$

Here $v = w^{-1}Lu$ and

$$B(u, \phi_n) = p(x)[u'(x)\phi_n(x) - u(x)\phi_n'(x)]_{x=a}^{x=b}. \quad (2.6)$$

In the case of the Chebyshev series $p(x) = (1 - x^2)^{1/2}$ in the domain $[-1, 1]$ and $p(-1) = p(1) = 0$, the boundary term $B(u, \phi_n)$ in (2.6) always vanishes for any bounded function u. Thus, integration by parts for the $\lambda_n^{-1}[(v, \phi_n)_w]$ term may be repeated as long as the function being integrated is smooth enough. Since the term $(v, \phi_n)_w$ in (2.5) is bounded independent of n and 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), we have $\hat{u}_n < O(n^{-m})$ if u is m times differentiable. This is the desired property of exponential convergence. Namely, the convergence rate of Chebyshev series depends only on the smoothness of the function being expanded.

In the case of the Fourier series $p(x) = 1 \neq 0$, the exponential convergence may also be obtained in the case with periodic conditions, but only if a smooth function u is also periodic. When u does not satisfy the periodic condition that is common in atmospheric limited-area models, then $B(u, \phi_n) = O(n)$ and $\hat{u}_n = O(n^{-1})$, which yields a very slow convergence rate. If $u(a) = 0$ and $u(b) = 0$, then $B(u, \phi_n) = O(1)$ and $\hat{u}_n = O(n^{-2})$. This slow (algebraic) convergence is a reflection of the Gibbs phenomenon associated with u not satisfying the boundary conditions satisfied by the expansion function ϕ_n.

In the Tatsumi-type method, a sinusoidal function or polynomial is introduced to satisfy the time-dependent lateral boundary conditions. After subtracting the additional basis, the function that satisfies the homogeneous condition (i.e., $u = 0$ or $u' = 0$ at the boundary) is used for the sine–cosine expansion and for performing the calculation as with the spectral method. This additional basis introduced will certainly help reduce the Gibbs phenomenon at the boundary. This procedure, however, in general cannot realize the exponential-convergence property, because the higher derivatives of the function being expanded by sine–cosine series may not be continuous at the boundary. Thus, we expect the Gibbs phenomenon near the boundary in the Tatsumi-type method. In the next section we use the simple advection equation to illustrate the point.

3. Model problem

We consider the one-dimensional linear advection equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad (3.1a)$$

in the domain $[-1, 1]$ with the initial condition

$$u(x, t = 0) = \exp\left[-\left(\frac{x + 0.5}{0.2}\right)^2\right], \quad (3.1b)$$

and the boundary condition

$$u(-1, t) = g(t) = \exp\left[-\left(\frac{-0.5 - t}{0.2}\right)^2\right]. \quad (3.1c)$$

The analytical solution of this problem is

$$u_{\text{ana}}(x, t) = \exp\left[-\left(\frac{x + 0.5 - t}{0.2}\right)^2\right]. \quad (3.2)$$

This is the simplest model involving wave or advective processes. The incoming boundary condition (3.1c) is specified according to the analytical solution $u_{\text{ana}}(-1, t)$. The analytic solution is used only at the inflow boundary. No boundary condition is needed at $x = 1$. This is an open boundary situation in the sense that any wave should propagate out of the domain without any difficulty. We will solve the above problem with polynomial-subtracted (PST), sinusoidal-subtracted (SST) sine-series expansion of the Tatsumi-type method and Chebyshev τ method. We will also include the fourth-order finite-difference method (FD4) in our calculations for comparison.

a. Numerical methods

If $N + 1$ is the number of grid points used in the calculation, the FD4 scheme is

$$\frac{d\bar{u}_j}{dt} + \frac{-\bar{u}_{j+2} + 8\bar{u}_{j+1} - 8\bar{u}_{j-1} + \bar{u}_{j-2}}{12\Delta x} = 0 \quad (3.3)$$

for $j = 2, \cdots, N - 2$. The fourth-order one-sided difference is used for $j = 0, 1, N - 1$, and N points. Here, $\bar{u}_j$ denotes values at the grid points $x_j = -1 + j\Delta x$, $(j = 0, \cdots, N)$, with $\Delta x = 2/N$.

For the τ method, the dependent variable $u(x, t)$ is approximated by the series expansion

$$u_N(x, t) = \sum_{n=0}^{N} \hat{u}_n(t) T_n(x), \quad (3.4)$$

where the $T_n(x)$ are the Chebyshev polynomials defined on the interval $-1 \leqslant x \leqslant 1$ by $T_n(x) = \cos(n\phi)$ with $x = \cos\phi$. Let us define the Chebyshev inner product of two functions $p(x)$ and $q(x)$ as

$$\langle p, q \rangle = \int_{-1}^{1} \frac{p(x)q(x)}{(1 - x^2)^{1/2}} dx. \quad (3.5)$$

The spectral coefficient $\hat{u}_n(t)$ is given by

$$\hat{u}_n(t) = \frac{2}{\pi c_n} \langle u(x, t), T_n(x) \rangle, \quad (3.6)$$

with
$$c_n = \begin{cases} 2, & n = 0 \\ 1, & n > 0 \end{cases}.$$

With the above definition, the τ equations for our model problem are

$$\frac{d\hat{u}_n}{dt} + \hat{u}_n^{(1)} = 0$$
$$(n = 0, 1, \cdots, N - 1; t > 0), \quad (3.7a)$$

$$(-1)^N \hat{u}_N = g(t) - \sum_{n=0}^{N-1} (-1)^n \hat{u}_n \quad (t > 0), \quad (3.7b)$$

$$\hat{u}_n(0) = \frac{2}{\pi c_n} \langle u(x, t = 0), T_n(x) \rangle$$
$$(n = 0, 1, \cdots, N; t = 0), \quad (3.7c)$$

where

$$\hat{u}_n^{(1)} = \frac{2}{c_n} \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{N} m\hat{u}_m \quad (3.8)$$

denotes the spectral coefficients of the x derivative of u_N. Equations (3.7a) and (3.7b) indicate that the last mode $\hat{u}_N$ is determined by the requirement that the whole series satisfies the boundary condition. To solve this system for the spectral coefficients $\hat{u}_0, \ldots, \hat{u}_N$ using explicit time differencing, one uses (3.7a) to predict new values of $\hat{u}_0, \ldots, \hat{u}_{N-1}$ from those at the previous time level, then uses (3.7b) to diagnose $\hat{u}_N$. The derivative relation (3.8) yields the (backward) recurrence formula

$$c_{n-1}\hat{u}_{n-1}^{(1)} - \hat{u}_{n+1}^{(1)} = 2n\hat{u}_n$$
$$(n = 1, 2, \cdots, N - 1), \quad (3.9)$$

with the starting values $\hat{u}_{N+1}^{(1)} = \hat{u}_N^{(1)} = 0$. Despite the global nature of the spectral approximation, the evaluation of (3.8) by (3.9) allows N values of $\hat{u}_n^{(1)}$ to be computed in $O(N)$ operations. To evaluate the spectral coefficients of an arbitrary function, discretization of (3.6) is needed. The physical points used for a fast discrete Chebyshev transform are $\bar{x}_j = \cos(j\pi/N)$ for $j = 0, \cdots, N$. These grids have irregular spacing that are of $O(1/N^2)$ near the boundary.

The PST and SST methods employed here are the same as those illustrated in Gottleib and Orszag (1977) and Tatsumi (1986). The two methods differ only in the choice of basis functions that satisfy the time-dependent boundary conditions. For the PST scheme, we seek the solutions of (3.1a)–(3.1c) as the sum of a linear polynomial and a sine series

$$u(x, t) = \frac{\bar{u}(1, t) - g(t)}{2} x + \frac{\bar{u}(1, t) + g(t)}{2} + \sum_{n=1}^{N} \tilde{v}_n(t) \sin\left[n\left(\frac{\pi}{2} x + \frac{\pi}{2}\right)\right], \quad (3.10)$$

where $\bar{u}(1, t)$ is the computed value at $x = 1$ by the PST method. For the SST method, we follow Tatsumi (1986) and seek solutions of (3.1a)–(3.1c) as the sum of a time-dependent sinusoidal function and a sine series. The time-dependent sinusoidal basis is

$$h_{\sin}(x, t) = \frac{\bar{u}(1, t) - g(t)}{2} \sin\left(\frac{\pi}{2} x\right) + \frac{\bar{u}(1, t) + g(t)}{2}. \quad (3.11)$$

These additional time-dependent bases are introduced to satisfy the time-dependent lateral boundary conditions and thus to allow the subtracted functions to be expanded in sine series. Note that the subtracted function may be continuous in its function values at the boundary, but there is no guarantee that they will be continuous in the functions' higher derivatives.

b. *Numerical results*

The fourth-order Runge–Kutta time-integration scheme is used here, with the time step chosen to be very small so that the errors in the computation are dominated by spatial-discretization errors.

Figure 1 gives the numerical solutions of the model

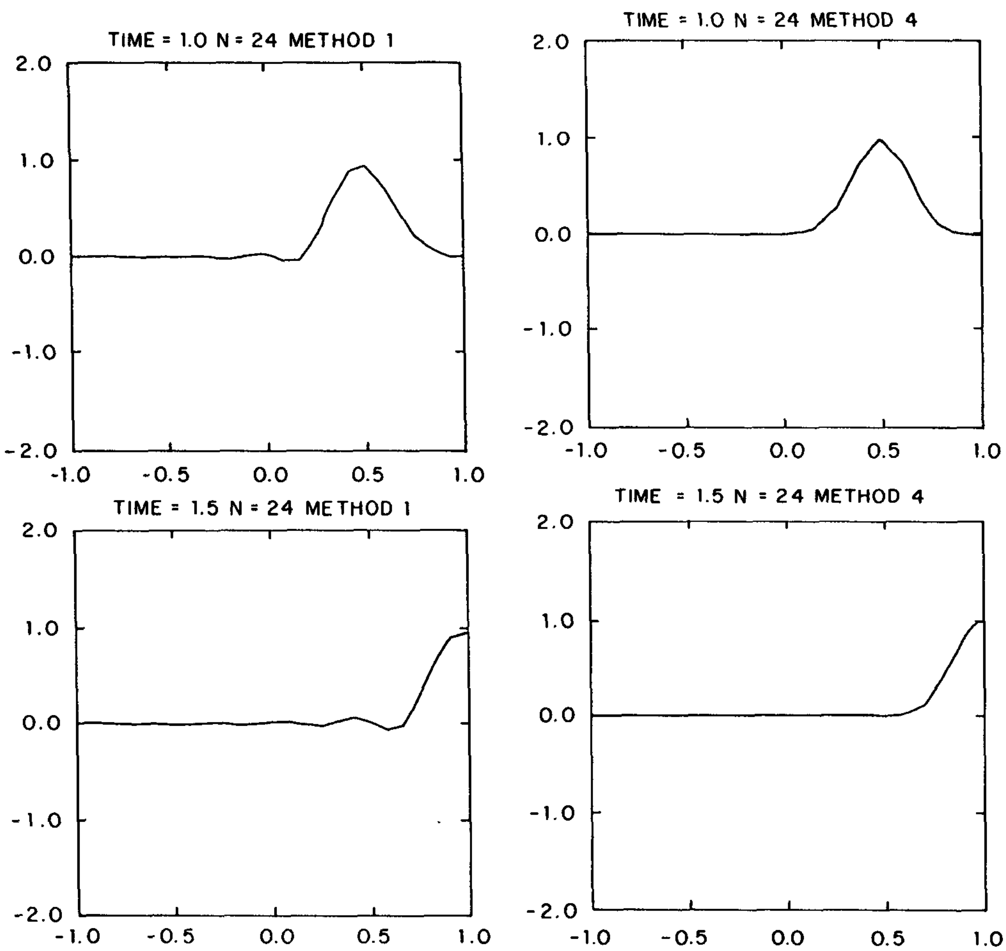

FIG. 1. Numerical solutions of the model problem (3.1a)–(3.1c) with $N = 24$ at $t = 1.0$ and $t = 1.5$ for (a) FD4 method and (b) Chebyshev τ method.

problem (3.1a)–(3.1c) with $N = 24$ at $t = 1.0$ and $t = 1.5$ for the FD4 method and the Chebyshev τ method. The analytic solution (not shown) moves with a constant speed and structure. The τ method clearly gives a much better approximation than does the difference method. In particular, the τ solution does not exhibit the computational dispersion that broadens and introduces spurious oscillations in the FD4 solution. Both the FD4 and τ method let the wave go out of the domain smoothly.

Figure 2 presents the numerical solutions of the SST method at $t = 1.0$, $t = 1.2$, $t = 1.4$, and $t = 1.5$ with $N = 24$. At $t = 1.0$, the numerical solution of SST resembles the τ solution, which is very accurate. This is in agreement with Tatsumi's calculation of the one-dimensional advection equation with a solitary wave. Tatsumi (1986), however, uses zero boundary conditions throughout the time during which the pulse hits the boundary. This suggests that his result is a product of his methods and the application of boundary smoothing. To isolate the boundary effects in the Tatsumi method, we do not use any boundary relaxation in our calculations even though boundary smoothing may be a nonnegligible part of the Tatsumi method. When the wave approaches the right boundary at $t = 1.2$, $t = 1.4$, and $t = 1.5$, Gibbs phenomenon occurs due to the large discontinuity in the function derivatives. This Gibbs phenomenon not only gives erroneous values in the outgoing boundary region, but it also gives false oscillations in the incoming boundary region. The PST method yields similar results, so they are not shown here.

The corresponding root-mean-square error is shown in Fig. 3 as a function of the number of grid points N for $t = 1.0$ and $t = 1.5$. The algebraic convergence of the FD4 and the exponential convergence of the τ method are obvious. As N approaches 32, the error in the τ method is decreasing like $10^{-N/4}$, while the finite-difference errors are only beginning to approach their asymptotic rate of decrease. The SST or PST methods converge even more slowly than the FD4 method at $t = 1.5$. This is due to the fact that the derivatives of the polynomial- or sinusoidal-subtracted functions are not continuous at the boundary. This discontinuity is es-

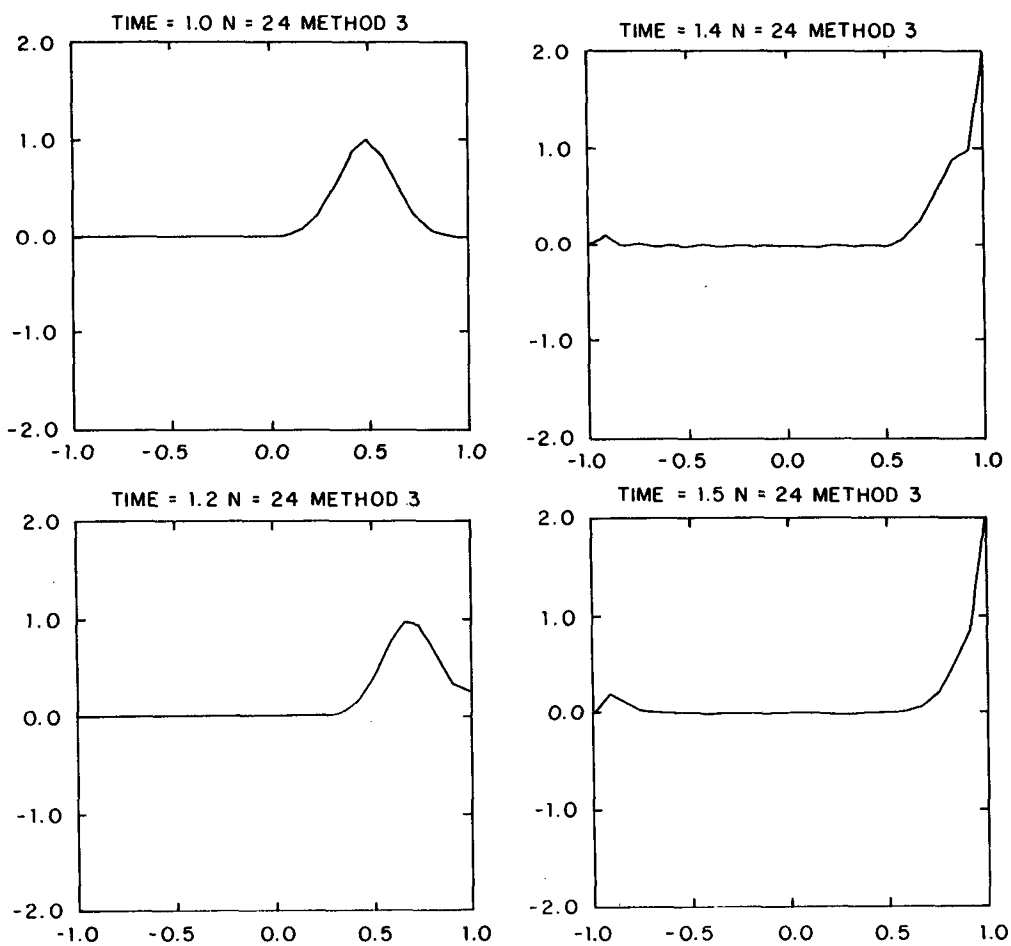

FIG. 2. Numerical solutions of the model problem (3.1a)–(3.1c) with $N = 24$ at $t = 1.0$, $t = 1.2$, $t = 1.4$, and $t = 1.5$ for SST method.

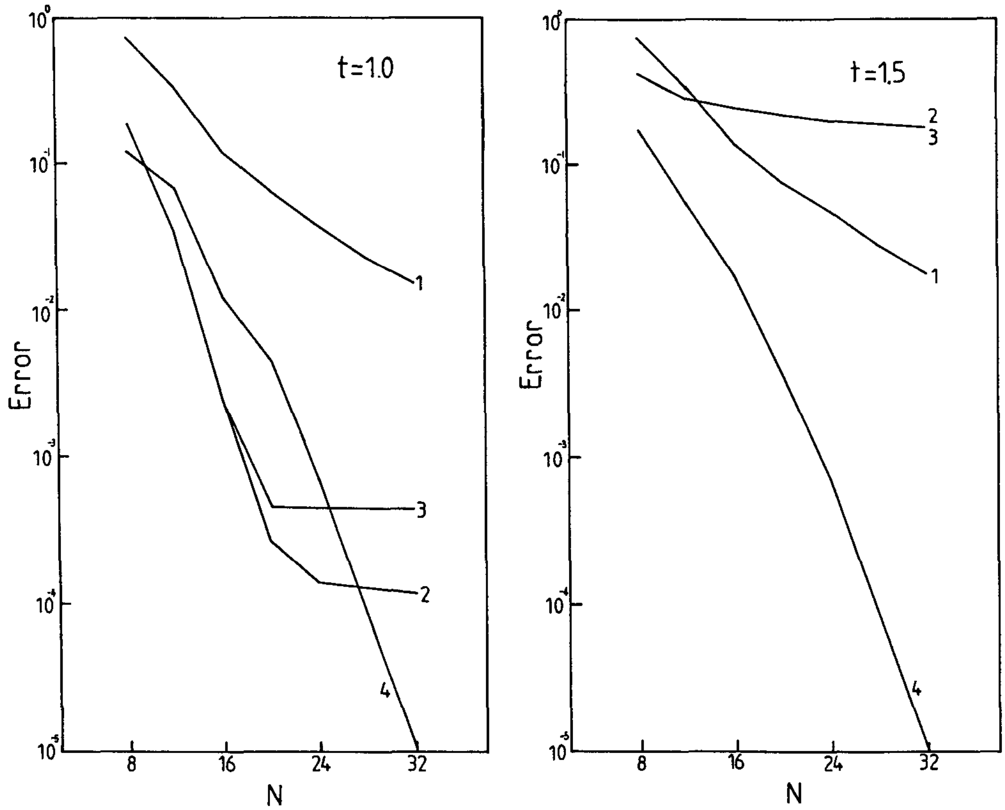

FIG. 3. Root-mean-square errors in the numerical solutions of the model problem (3.1) as functions of N at (a) $t = 1.0$ and (b) $t = 1.5$. Curve 1 is the FD4 method, curve 2 the PST method, curve 3 the SST method, and curve 4 the τ method.

pecially large when the wave approaches the right boundary. Thus, the slow convergence rate (Gibbs phenomenon) distorts the solution considerably. When the wave is away from the right boundary as at $t = 1.0$, the discontinuity of the expanded function's derivatives at the boundary is small. The SST and PST do possess rapid convergence for $N < 20$. Because the equal grid spacing used in the sine transform is smaller than the irregular grid spacing used in the Chebyshev transform at the center of the domain, the SST and PST methods yield results that are better than the τ method for $N < 20$. Both the SST and the PST methods, however, have very slow convergence rates for $N > 20$ again due to the Gibbs phenomenon. In a situation when high accuracy is desired [e.g., $O(10^{-4})$ in our model problem] the efficiency of the Tatsumi-type method is questionable.

Finally, we test the time-step stability of the above methods. Figure 4 gives the root-mean-square error as a function of time step for $N = 16$ at $t = 1.0$. When the time step is small, the flat lines reflect the spatial-discretization error of the methods for $N = 16$ at $t = 1.0$. Figure 4 illustrates that the τ method has a more restricted stability constraint. This is expected from the fact that the grid spacing is of $O(1/N^2)$.

4. Concluding remarks

Spectral models seek the solution to a differential equation in terms of a series of known, smooth functions. The basis function is often chosen from the eigenfunctions of the Sturm–Liouville problem for reasons of orthogonality and completeness. The primary appeal of the spectral method is the accuracy and efficiency associated with the fast transform and the rapid convergence rate for the chosen basis functions. The Fourier and Chebyshev series that allow fast transform calculations are often used for spectral methods. When the expanded function is sufficiently smooth, the Chebyshev series possesses the exponential-convergence property regardless of the boundary conditions imposed. The exponential-convergence property holds for Fourier series only when the expanded function is smooth and periodic.

In terms of regional spectral modeling, the Tatsumi-type methods based on sinusoidal- or polynomial-subtracted sine–cosine expansions do not, in general, possess the exponential-convergence property. The slow convergence of the expanded series comes from the fact that the higher derivatives of the function are not continuous at the boundary (periodic) in a regional

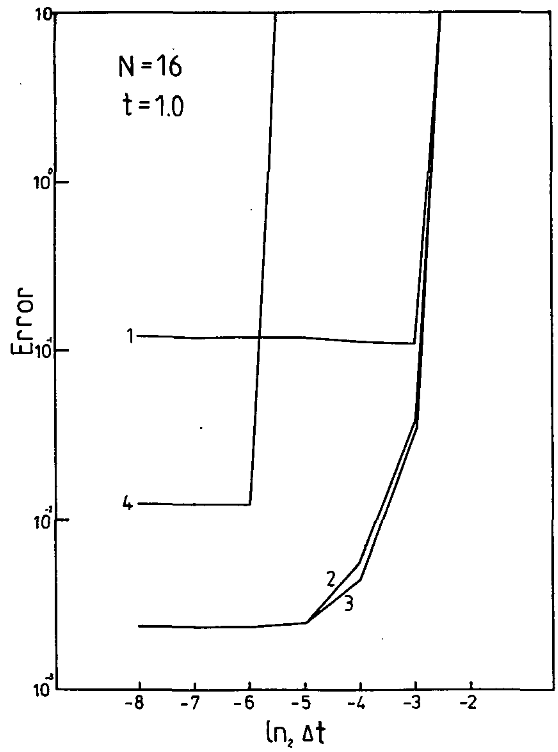

FIG. 4. Root-mean-square errors in the numerical solutions of the model problem (3.1a)–(3.1c) as functions of time step Δt. Curve 1 is the FD4 method, curve 2 the PST method, curve 3 the SST method, and curve 4 the τ method.

model with time-dependent lateral boundary conditions. When the discontinuity is large, the Tatsumi-type method causes the wrong computed solution in outgoing boundary regions and false oscillations on the incoming boundary regions due to Gibbs phenomenon. When the disturbance is away from the boundary and the discontinuity is small, the method with low resolution converges exponentially just as does the τ method. The high-resolution solutions of the Tatsumi-type method have a very slow convergence rate and do not yield high accuracy accordingly. The Tatsumi-type method is not suited for the purpose of high-accuracy modeling.

The main focus of this article is to use the simplest model to illustrate the boundary effects in the Tatsumi-type spectral method. We have not explored the effect of aliasing in the transform method, or the effect of boundary smoothing in the Tatsumi-type method. Since we have not discussed the implementation of efficient semi-implicit time-integration schemes in regional spectral models and since the explicit time step in the Tatsumi-type method is larger than in the τ method, it is beyond the scope of the present work to determine which spectral method is more suitable for regional modeling. We will study these effects in the future. In general, the selection of numerical methods can be made only with knowledge of the particular application, including accuracy requirements and solution characteristics.

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