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On the Boundary Treatment in Spectral Methods for Hyperbolic Systems*

CLAUDIO CANUTO AND ALFIO QUARTERONI

Istituto di Analisi Numerica del C.N.R., Pavia, Italy

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Spectral methods have been successfully applied to the simulation of slow transients in gas transportation networks. Implicit time advancing techniques are naturally suggested by the nature of the problem. The aim of this paper is to clarify the correct treatment of the boundary conditions in order to avoid any stability restriction originated by the boundaries. The Beam and Warming and the Lerat schemes are unconditionally linearly stable when used with a Chebyshev pseudospectral method. Engineering accuracy for a gas transportation problem is achieved at Courant numbers up to 100.

1. INTRODUCTION

Spectral methods have been recently applied to the numerical simulation of the unsteady flow of a gas in long distance transportation networks (see [1]). The regularity properties of the solution [12] make spectral methods particularly effective for this class of problems. Engineering accuracy is achieved at a lower computational cost than by using more conventional finite-order methods.

Transients occurring in the normal operation of pipeline networks are usually slow. This happens because variations imposed on the physical variables at the boundaries are very slow. Moreover, their propagation toward the interior is damped by the presence of a strong friction effect.

These reasons, as well as the need to avoid the severe stability conditions which arise from the use of explicit methods for spectral methods, make it highly desirable to use implicit methods in time. If a method is considered which is unconditionally stable for the pure initial value problem, the boundary conditions have to be incorporated into the numerical scheme in such a way that no spurious stability restriction is introduced.

Theoretical and experimental results on the numerical treatment of boundary conditions for finite difference approximations of hyperbolic systems are widely available in the literature. In [8], Gottlieb, *et al.* address the issue of correctly

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imposing the boundary conditions in terms of the physical variables, rather than in terms of the "characteristic" ones. They show that the boundary conditions can be properly imposed within a finite difference or finite element method which is explicit in time, by a procedure of *boundary corrections* at the end of each time step. There is computational evidence that their procedure works for spectral methods as well (see, e.g., [1]).

It is the present authors' impression that implicit time advancing methods have not received sufficient attention in [8], hence the reading of that paper may lead to some misunderstanding about the practical implementation of the boundary conditions in implicit methods. As a matter of fact, the *boundary corrections* proposed there destroy unconditional stability, as it will be documented below.

The purpose of this paper is to discuss in more detail the correct implementation of the boundary conditions within an implicit time advancing scheme when a Chebyshev collocation method is used in space. We stress that the only unconditionally stable treatment of the boundary conditions consists of imposing at each endpoint the prescribed physical conditions together with certain linear combinations of the physical differential equations. The coefficients of these combinations are those which express the incoming characteristic variables in terms of the physical ones. Thus the equations at the boundaries have to be incorporated into the matrix to be inverted at each time step.

The Beam and Warming scheme and a class of Lerat-type schemes have been chosen in the following discussion as time-marching methods for the time discretization of a linear 2×2 hyperbolic system. An application to a gas transient simulation of industrial interest is also presented.

2. The Boundary Treatment on a Linear Problem

The following simple hyperbolic system has been widely considered in the literature as a model for more complex situations:

$$w_t + Aw_x = 0, \qquad -1 < x < 1,\ t > 0, \tag{2.1}$$

where

$$w = (w_1, w_2)^T, \qquad A = \begin{pmatrix} \frac{1}{2} & 1 \\ 1 & \frac{1}{2} \end{pmatrix}. \tag{2.2}$$

The system is supplemented by an initial condition

$$w(x, 0) = w^0(x), \qquad -1 < x < 1, \tag{2.3}$$

and the boundary conditions

$$w_1(-1, t) = w_1(1, t) = 0, \qquad t > 0. \tag{2.4}$$

The initial-boundary value problem (2.1)–(2.4) is well posed (see, e.g., [5]); more precisely, for each $t>0$ one has

$$\int_{-1}^{1} |w(x,t)|^2\,dx \leqslant \int_{-1}^{1} |w^0(x)|^2\,dx. \tag{2.5}$$

The matrix A has two eigenvalues of opposite sign

$$\lambda_1 = \tfrac{3}{2}, \qquad \lambda_2 = -\tfrac{1}{2}. \tag{2.6}$$

It can be diagonalized as

$$A = T\Lambda T^{-1} \tag{2.7}$$

with

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2), \qquad T = T^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{2.8}$$

The system (2.1) can be written in diagonal form as

$$z_t + \Lambda z_x = 0, \tag{2.9}$$

where

$$z = (u, v)^T = T^{-1} w \tag{2.10}$$

are the characteristic variables. The boundary conditions (2.4) become

$$(u+v)(-1,t) = (u+v)(+1,t) = 0, \qquad t>0. \tag{2.11}$$

We consider a spatial approximation of (2.1) based on the Chebyshev collocation method at the points

$$x_j = \cos\frac{j\pi}{N}, \qquad j = 0,\ldots, N. \tag{2.12}$$

For each $t>0$, the approximate solution, which we still denote by $w(x,t)$, will be a couple of polynomials of degree N in the x variable. The degree N will be kept fixed throughout the paper. We denote by

$$D = \{d_{ij}\}_{0 \leqslant i,j \leqslant N} \tag{2.13}$$

the matrix of the Chebyshev pseudospectral derivative at the points (2.12) (see, e.g., [9]). We recall that if an N-degree polynomial w is identified with the vector $\mathbf{w}$ of its values at the points (2.12), then $D\mathbf{w}$ is the vector of the values of w_x at the same points.

We will now introduce time discretization methods for the previous system.

Hereafter, we will say that a method is stable for a given Δt if the computed solutions w^n at the times $t_n = n\,\Delta t$ satisfy an estimate of the form

$$\|w^n\|_{L^2(-1,1)} \leqslant C, \qquad n = 1, 2, 3....$$

with C independent of n. Unconditional stability will mean stability for all $\Delta t > 0$.

We first give numerical evidence to the fact that if the boundary correction procedure described in [8] is applied within an implicit time advancing method, a severe stability restriction occurs.

The differential system (2.1) is collocated at all the points (2.12) (including the boundary points) and advanced in time by one step of the Beam and Warming method [2], which here reduces to the classical Cranck–Nicolson scheme

$$\tilde{w}_j^{n+1} + \frac{\Delta t}{2} A(\tilde{w}_x^{n+1})_j = w_j^n - \frac{\Delta t}{2} A(w_x^n)_j, \qquad j = 0,..., N. \tag{2.14}$$

(Let us recall for further reference that the Beam and Warming scheme applied to the conservation law $w_t + f(w)_x = 0$ is, before space discretization,

$$\Delta w^n + \frac{\Delta t}{2} (A(w^n)\,\Delta w^n)_x = -\Delta t f(w^n)_x, \tag{2.15}$$

where $\Delta w^n = w^{n+1} - w^n$ and $A(w) = f'(w)$.)

The interior values are retained, i.e., $w_j^{n+1} = \tilde{w}_j^{n+1}$ for $j = 1,..., N-1$, whereas the boundary values $\tilde{w}_0^{n+1}$ and $\tilde{w}_N^{n+1}$ are corrected by solving the linear systems

$$\begin{aligned} (w_1)_0^{n+1} &= 0 \\ (w_1)_0^{n+1} + (w_2)_0^{n+1} &= (\tilde{w}_1)_0^{n+1} + (\tilde{w}_2)_0^{n+1} \end{aligned} \tag{2.16}$$

and

$$\begin{aligned} (w_1)_N^{n+1} &= 0 \\ (w_1)_N^{n+1} - (w_2)_N^{n+1} &= (\tilde{w})_N^{n+1} - (\tilde{w}_2)_N^{n+1}. \end{aligned} \tag{2.17}$$

Numerical experiments show that this method is stable only if

$$\Delta t \leqslant 0.74\,\Delta t_*,$$

where $\Delta t_* = 16/3N^2$ is the stability limit for the modified Euler method. Although the Cranck–Nicolson method is A-stable for a scalar equation, the stability condition introduced by the boundary treatment is more severe than that of an explicit method.

We observe here a phenomenon which is well known for finite difference schemes as well. Namely, the coupling of an explicit treatment of the boundary conditions with an implicit interior scheme may result in a reduction of the stability limit for the pure interior scheme.

The proper way to treat the boundary conditions is naturally derived using the characteristic form (2.9) of the hyperbolic system. In this case it is possible to represent the spatially discretized system as an ODE system in the form

$$\frac{d\mathbf{z}}{dt} + M\mathbf{z} = 0, \tag{2.18}$$

where the matrix M already takes into account the boundary conditions. It is clear that if M is diagonalizable and has the spectrum in the right complex half plane, then any A-stable time discretization method yields an unconditionally stable scheme for (2.18). In turn, this gives rise to an unconditionally stable scheme for the physical system (2.1)–(2.4), via the transformation (2.10).

It is well known that the Chebyshev collocation method at the points (2.12) for the scalar initial boundary value problem

$$\begin{aligned} u_t + u_x &= 0, \qquad -1 < x < 1,\ t > 0 \\ u(-1, t) &= 0 \\ u(x, 0) &= u^0(x) \end{aligned} \tag{2.19}$$

gives stable numerical results. (Unfortunately, so far no proof of an estimate of the type (2.5) is known for this method. A stability result involving a modified Chebyshev norm can be found in [10].) The method can be written as an ODE system in the form

$$\frac{d\mathbf{u}}{dt} + \tilde{D}\mathbf{u} = 0, \tag{2.20}$$

where $\mathbf{u} = (u_0, ..., u_{N-1})^{\mathrm{T}}$ and $\tilde{D}$ is the submatrix of D obtained by deleting the last row and column. Thus the differential equation is collocated at the interior points and at the outflow boundary point $x = 1$. The matrix $\tilde{D}$ has distinct eigenvalues with strictly positive real parts, hence, any A-stable time discretization method will produce stable solutions with no stability restriction.

In analogy with the scalar case, the spatial discretization of the system (2.9) is

$$\begin{aligned} (u_t + \tfrac{3}{2}u_x)(x_j, t) &= 0, \qquad j = 0, ..., N-1 \\ (v_t - \tfrac{1}{2}v_x)(x_j, t) &= 0, \qquad j = 1, ..., N \\ v(x_0, t) &= -u(x_0, t) \\ u(x_N, t) &= -v(x_N, t). \end{aligned} \tag{2.21}$$

In order to cast this system into the form (2.18) we eliminate the unknowns u_N and v_0 through the boundary conditions. Hence, we set

$$\mathbf{z} = (u_0, ..., u_{N-1}, v_1, ..., v_N)^{\mathrm{T}} \tag{2.22}$$

and

$$M=\left[\begin{array}{c|c|c}
\tfrac{3}{2}d_{ij} & 0 & -\tfrac{3}{2}d_{iN} \\
\hline
\tfrac{1}{2}d_{l0} \quad 0 & & -\tfrac{1}{2}d_{lm}
\end{array}\right], \qquad \begin{array}{l} j=0,\ldots,N-1,\ i=0,\ldots,N-1, \\ l=1,\ldots,N,\ m=1,\ldots,N \end{array}$$

The eigenvalues of M have been computed for increasing values of N. They were found to be distinct and with non-negative real parts.

It follows that the Beam and Warming scheme will produce unconditionally stable approximate solutions of (2.21). They are defined by the system

$$u_j^{n+1}+\frac{3}{2}\frac{\Delta t}{2}(u_x^{n+1})_j=u_j^n-\frac{3}{2}\frac{\Delta t}{2}(u_x^n)_j, \qquad j=0,\ldots,N-1 \tag{2.24.1}$$

$$v_j^{n+1}-\frac{1}{2}\frac{\Delta t}{2}(v_x^{n+1})_j=v_j^n+\frac{1}{2}\frac{\Delta t}{2}(v_x^n)_j, \qquad j=1,\ldots,N \tag{2.24.2}$$

$$u_N^{n+1}=-v_N^{n+1} \tag{2.24.3}$$

$$v_0^{n+1}=-u_0^{n+1}. \tag{2.24.4}$$

We now go back to the physical equations using the transformation (2.10). At each interior point both the characteristic equations are collocated, hence we get

$$w_j^{n+1}+\frac{\Delta t}{2}A(w_x^{n+1})_j=w_j^n-\frac{\Delta t}{2}A(w_x^n)_j, \qquad j=1,\ldots,N-1. \tag{2.25}$$

At the boundary point x_0, Eq. (2.24.1) with $j=0$ becomes

$$\tau_{11}\left[w^{n+1}+\frac{\Delta t}{2}Aw_x^{n+1}\right]_1+\tau_{12}\left[w^{n+1}+\frac{\Delta t}{2}Aw_x^{n+1}\right]_2$$
$$=\tau_{11}\left[w^n-\frac{\Delta t}{2}Aw^n\right]_1+\tau_{12}\left[w^n-\frac{\Delta t}{2}Aw_x^n\right]_2, \tag{2.26}$$

where we have set $T^{-1}=\{\tau_{hk}\}_{1\leqslant h,k\leqslant 2}$. Similarly at x_N Eq. (2.24.2) with $j=N$ gives

$$\tau_{21}\left[w^{n+1}+\frac{\Delta t}{2}Aw_x^{n+1}\right]_1+\tau_{22}\left[w^{n+1}+\frac{\Delta t}{2}Aw_x^{n+1}\right]_2$$
$$=\tau_{21}\left[w^n-\frac{\Delta t}{2}Aw_x^n\right]_1+\tau_{22}\left[w^n-\frac{\Delta t}{2}Aw_x^n\right]_2. \tag{2.27}$$

Finally we have the physical boundary conditions

$$(w_1)_0^{n+1} = (w_1)_0^{n+1} = 0. \tag{2.28}$$

We conclude that at each boundary point the equation to be added to the prescribed boundary condition is obtained by collocating a linear combination of the physical equations after their discretization by the Beam and Warming scheme. The coefficients of this linear combination are entries of the matrix T^{-1} defined by (2.10).

This is the correct extension to an implicit time advancing scheme of the boundary treatment proposed in [8] for explicit schemes.

A class of time discretization schemes of implicit type has been recently proposed by Lerat for finite difference approximations of hyperbolic systems (see [11, 4]). The interest of such methods lies in the fact that unconditional stability (in time) is achieved by including a second derivative term (in space) into the scheme. Unlike the Beam and Warming method, Lerat's schemes are dissipative in the sense of Kreiss, hence spurious oscillations are automatically damped.

We will introduce hereafter the analogs of a subclass of Lerat schemes in the case of spatial discretizations by the Chebyshev collocation method. The previous considerations on the treatment of the boundary conditions will guide us in defining a scheme which is unconditionally stable in time.

Let us recall that for the conservation law

$$w_t + f(w)_x = 0 \tag{2.29}$$

a class of methods of Lerat's type reads as (see [11])

$$\Delta w^n + \beta \frac{\Delta t^2}{2} (A^2(w^n) \cdot \Delta w_x^n)_x = -\Delta t f(w^n)_x + \frac{\Delta t^2}{2} (A^2(w^n)\, w_x^n)_x, \tag{2.30}$$

where $\Delta w^n = w^{n+1} - w^n$, $A(w) = f'(w)$ and β is a negative parameter. The method is obtained from the two-term Taylor formula for w at $t = t_n$. Time derivatives are replaced by space derivatives using (2.29) and w^n is replaced by $w^n + \beta\, \Delta w^n$ in the second-order term.

The same idea can be used in deriving a "Lerat method" for solving a general ODE system like (2.18). Precisely one gets

$$z^{n+1} + \beta \frac{\Delta t^2}{2} M^2 z^{n+1} = z^n - \Delta t M z^n + (1+\beta) \frac{\Delta t^2}{2} M^2 z^n. \tag{2.31}$$

The stability properties of this method are easily investigated by a normal mode analysis. The characteristic root of the method is

$$\rho = \frac{1 - \lambda + (1+\beta)\, \lambda^2/2}{1 + \beta\, \lambda^2/2}, \tag{2.32}$$

where $\lambda = \Delta t \mu$ and μ stands for an eigenvalue of M. If $\beta = -\frac{1}{2}$, a cancellation occurs and the characteristic root is

$$\rho = \left(1 + \frac{\lambda}{2}\right) \Big/ \left(1 - \frac{\lambda}{2}\right) \tag{2.33}$$

hence $|\rho| \leqslant 1$ iff $\mathbb{R}\mathrm{e}\, \lambda \geqslant 0$. It follows that for $\beta = -\frac{1}{2}$ the Lerat discretization (2.31) of (2.18) is unconditionally stable when M is the matrix associated to the Chebyshev collocation spatial discretization. The expression (2.33) of the characteristic root shows that the Lerat scheme coincides with the Beam and Warming scheme on the model equation (2.1), i.e., whenever the coefficient matrix A is constant, so that it commutes with differentiation. The two methods differ for the conservation law (2.29), as it can be seen by comparing (2.15) and (2.30).

If $\beta \neq -\frac{1}{2}$, ρ has a singularity at $\lambda = \pm\sqrt{2/|\beta|}$ hence the scheme is only conditionally stable. Since the eigenvalues of the pseudospectral Chebyshev derivative are uniformly bounded away from the origin [6, Sect. 2], stability is guaranteed if Δt is chosen sufficiently large.

Finally, let us observe that $|\rho| \leqslant 1$ for all $\beta \leqslant -\frac{1}{2}$ if λ is imaginary. Hence, all the Lerat schemes are unconditionally stable when used with a Fourier method in space.

Remark. The previous analysis shows that unconditional stability is achieved (at least for $\beta = -\frac{1}{2}$) if the stabilizer term in (2.31) is built up by the *square* of the *matrix of the pseudospectral derivative including the boundary conditions*. Instead, one could think of a stabilizer term which simply involves the second derivative operator (in analogy to the finite difference case, see [4]) with no boundary condition or, say, Dirichlet boundary conditions. The resulting linear system would be of classical elliptic type, for which efficient solution techniques are available. Unfortunately, such a method turns out to be unstable.

Finally, we recall that the scheme (2.31) can be transformed into an equivalent scheme in terms of the physical unknowns using again the transformation (2.10).

The use of a method like (2.31) in several space dimensions leads to a stabilizing matrix M^2 whose condition number is $O(N^4)$. Hence a preconditioned iterative technique is in order. The effective preconditioning of hyperbolic problems is yet a research area (see [7, 13]).

3. Extension to Nonlinear Systems

Assume now that the system to be solved is

$$w_t + A(w)\, w_x + g(w) = 0, \tag{3.1}$$

where $g(w)$ is a vector and $A(w)$ is a 2×2 matrix which can be diagonalized as

$$A(w) = T(w)\, \Lambda(w)\, T^{-1}(w) \tag{3.2}$$

with $A(w) = \text{diag}\{\lambda, \mu\}$, $\lambda, \mu \in \mathbb{R}$, $\lambda\mu < 0$. The treatment of the boundary conditions described in the previous section can be applied here, provided the linear combinations of the physical equations at the boundary points involve as coefficients the entries of the matrix $T^{-1}(w^n)$.

The Beam and Warming method was used to simulate a 1 hr transient of isentropic methane gas in a pipe of lentgh 250 km and diameter 0.5 m. Denoting by ρ the density of the gas and by u its velocity, the equation of motion are (see, e.g., [1])

$$\begin{aligned} \rho_t + (\rho u)_x &= 0 \\ (\rho u)_t + (p + \rho u^2)_x + f\rho u|u| &= 0, \end{aligned} \tag{3.3}$$

where the Moody friction factor f is equal to 0.01.

System (3.3) is supplemented by an equation of state, which gives the pressure as a function of the temperature (supposed to be known) and the density. The flow is initially steady and corresponds to an inflow pressure $p = 70$ bar and to a flow-rate per unit cross area $q = 244.462$ Kg/m^{2}s. The boundary conditions simulate the packing of the pipe: the downstream flow-rate is unchanged, while the upstream flow-rate is increased linearly by 30% in 360 s, then kept constant at $q = 317.8$ Kg/m^{2}s.

Normalizing the spatial domain to the interval $(-1, 1)$ we write (3.3) as

$$w_t + \frac{2}{L}\{F(w)\}_x + G(w) = 0, \qquad -1 < x < 1,\ t > 0, \tag{3.4}$$

where

$$w = \begin{pmatrix} \rho \\ q \end{pmatrix},\ F(w) = \begin{pmatrix} q \\ p + qu \end{pmatrix},\ G(w) = \begin{pmatrix} 0 \\ (f/2d) \cdot (q|q|/\rho) \end{pmatrix}$$

and $q = \rho u$. Fixing a time step $\Delta t > 0$, we set $t^n = n\,\Delta t$ and we define w^n to be a couple of polynomials of degree N in space which approximate $w(t^n)$. We define $\Delta w^n = w^{n+1} - w^n$, $A = \partial F/\partial w$ (the Jabobian of F), and $B = \partial G/\partial w$.

The implicit Beam and Warming scheme gives at the interior collocation points (2.12),

$$\begin{aligned} &\Delta w^n + \frac{\Delta t}{2}\{\partial_N[A(w^n)\,\Delta w^n] + B(w^n)\,\Delta w^n\} \\ &\quad = -\Delta t\{\partial_N[F(w^n)] + G(w^n)\} \qquad \text{for} \quad x = x_j,\ 1 \leqslant j \leqslant N-1. \end{aligned} \tag{3.5}$$

Here ∂_N denotes the pseudospectral Chebyshev differentiation, i.e., $\partial_N \phi$ is the derivative of the polynomial ϕ_N which interpolates the function ϕ at the nodes (2.12). The boundary conditions are treated with the method previously described, namely the linear characteristic combination of the physical equations is prescribed

TABLE I

Comparison between Beam and Warming and Modified Euler Time Discretizations, with the Chebyshev Collocation Method in Space. Exact $p_{\text{inflow}} = 74.8080...$

		Implicit		Explicit	
N	α	p_{inflow}	CPU time	p_{inflow}	CPU time
8	1.	74.8084	$0.83\ E-2$	74.8076	$0.58\ E-2$
	10.	74.806	$0.88\ E-3$		
	25.	74.797	$0.37\ E-3$		
	50.	74.778	$0.19\ E-3$		
	100.	74.509	$0.11\ E-3$		
	200.	74.103	$0.87\ E-4$		
	300.	73.071	$0.57\ E-4$		
16	1.	74.8080	$0.38\ E-1$	74.8080	$0.12\ E-1$
	10.	74.806	$0.39\ E-2$		
	25.	74.798	$0.16\ E-2$		
	50.	74.752	$0.86\ E-3$		
	100.	74.651	$0.51\ E-3$		
	200.	74.274	$0.28\ E-3$		
	300.	73.458	$0.21\ E-3$		
32	1.	74.8080	$0.79\ E\ \varnothing$	74.8080	$0.98\ E-1$
	10.	74.8080	$0.83\ E-1$		
	25.	74.807	$0.33\ E-1$		
	50.	74.805	$0.17\ E-1$		
	100.	74.798	$0.89\ E-2$		
	200.	74.752	$0.45\ E-2$		
	500.	74.460	$0.19\ E-2$		
	750.	74.360	$0.13\ E-2$		

at the boundary together with the boundary values of the flow-rate q, which are given from data.

Table I contains the values of the computed inflow pressure for different values of N and Δt. The exact value is 74.8080.... The time step Δt has the form $\Delta t = \alpha\, \Delta t_*$, where Δt_* is the stability limit of the modified Euler method for the same problem. The CPU times (in hr) on the Honeywell 6040 at the University of Pavia are also reported. The columns on the right contain the computed values and corresponding CPU times produced by the modified Euler method, using $\Delta t = 0.9 \Delta t_*$.

These results show that the Beam and Warming method considered in this paper is unconditionally stable and more convenient than an explicit method of the same order for attaining accuracies of industrial interest. Further results will appear elsewhere.

Note. The scheme of Lerat's type corresponding to the choice $\beta = -\frac{1}{2}$ in (2.31) has been independently proposed in the context of spectral methods in [3]. We thank one of the referees for bringing this reference to our attention.

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