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PREFACE

This volume is a collection of papers presented at the Symposium on Numerical Boundary Condition Procedures held at Ames Research Center, NASA, October 19-20, 1981. The purpose of this symposium was to provide a forum for the presentation and interchange of recent technical findings in the field of numerical boundary approximations. The symposium was held in conjunction with the Symposium on Multigrid Methods, and both were sponsored by the Applied Computational Aerodynamics and Computational Fluid Dynamics Branches at Ames.

Probably, the single most important aspect in the successful application of any numerical technique in solving gas dynamic problems is the proper treatment of the impermeable and permeable boundaries that encompass the computational line, plane, or volume. Papers were solicited in this research area which utilized new or existing numerical boundary condition procedures for various types of boundaries and governing equations.

It is apparent from the contributed papers that computational fluid dynamicists as well as numerical analysts are quite active in this discipline. The papers cover a wide spectrum of research on topics that include numerical procedures for treating inflow and outflow boundaries, steady and unsteady discontinuous surfaces such as shock waves and slip surfaces, far field boundary conditions, and multiblock grids. In addition, papers were presented which consider the effects of numerical boundary approximations on stability, accuracy, and convergence rate of the numerical solution.

The symposium presented three invited and over nineteen contributed papers. The invited speakers were Dr. A. Bayliss, Prof. G. Moretti, and Prof. B. Gustafsson. Nearly all of the papers presented at the symposium appear in this proceedings. Those which do not, will appear as a supplement.

Paul Kutler

TABLE OF CONTENTS

N81-33874 D/8

UNCONDITIONAL INSTABILITY OF INFLOW-DEPENDENT BOUNDARY CONDITIONS IN DIFFERENCE APPROXIMATIONS TO HYPERBOLIC SYSTEMS*

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ABSTRACT

In this paper we study the stability of finite difference approximations to initial-boundary hyperbolic systems. As is well-known, a proper specification of boundary conditions for such systems is essential for their solutions to be well-defined. We prove a discrete analogue of the above - if the numerical boundary conditions are consistent with an inflow part of the problem, they render the overall computation unstable. An example of the inviscid gasdynamics equations is considered.

1. INTRODUCTION - WELL DEFINED HYPERBOLIC SYSTEM

We consider the first order hyperbolic system

(1.1a) $$\frac{\partial u}{\partial t} + A(x)\frac{\partial u}{\partial x} = F(x,t), \quad t > 0 ,$$

with initial data

(1.1b) $$u(x,0) = f(x), \quad t = 0 ,$$

in the first quarter of the plane $0 \leq x < \infty$. Here $u \equiv u(x,t)$ is the N-dimensional vector of unknowns and by hyperbolicity we mean that the (nonsingular) coefficient matrix $A \equiv A(x)$ is similar to a real diagonal Λ

(1.2) $$TAT^{-1} = \Lambda \equiv \mathrm{diag}(\lambda_1,\ldots,\lambda_N),$$
$$\lambda_1 > \cdots > \lambda_\ell > 0 > \lambda_{\ell+1} > \cdots > \lambda_N, \quad \lambda_j \equiv \lambda_j(x) .$$

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The system (1.1a) - rewritten in its characteristic form

$$\frac{\partial \tilde{u}}{\partial t} + \Lambda \frac{\partial \tilde{u}}{\partial x} = \tilde{F} \tag{1.3}$$

($\tilde{}$ denotes multiplication by T on the left), asserts that the characteristic variables $\tilde{u}_j$ are uniquely determined by the forcing terms $\tilde{F}_j$ along the characteristic curves $\dot{x}_j(t) + \lambda_j(x_j) = 0$. The last $N - \ell$ of these curves are outgoing curves impinging on the boundary $x = 0$ from the right, each of which carries one piece of initial data; thus, exactly $N - \ell$ pieces of information flow toward the left boundary $x = 0$; these are the last $N - \ell$ <u>outflow</u> components of $\tilde{u}$ associated with $\dot{x}_j = -\lambda_j > 0_{|\ell<j\leq N}$. It therefore follows that for the system (1.1) to be uniquely solvable, exactly ℓ <u>additional</u> pieces of information must be provided at the boundary $x = 0$,

$$Bu_{|x=0} = G, \quad \text{rank } [B] = \ell . \tag{1.4a}$$

The requirement of these boundary conditions to be on top of the predetermined outflow components can be expressed as follows (Hersh [1]):

For all nontrivial ϕ in the eigenspace Φ^+ spanned by the eigenvectors $\{\phi_j\}_{j=1}^{\ell}$ associated with the positive eigenvalues $\{\lambda_j\}_{j=1}^{\ell}$, we have

$$B\phi \neq 0 . \tag{1.4b}$$

Had the system (1.1a) been given to us in its characteristic form (1.3), the boundary conditions (1.4) then can be reformulated as the standard reflection

$$\tilde{u}^+ = \tilde{B}\tilde{u}^- + \tilde{G} \tag{1.5}$$

where $\tilde{u} = (\tilde{u}^+, \tilde{u}^-)$ partitioned corresponding to its inflow and outflow parts. The first ℓ <u>inflow</u> characteristic variables $\tilde{u}^+$ are then everywhere determined via (1.5) and (1.1b) along the ingoing characteristics $\dot{x}_j = -\lambda_j < 0_{|1\leq j\leq\ell}$; combined with the $N - \ell$ outflow pieces of data, the solution u is then well defined throughout the region of integration.

<u>Example</u>. The linearized inviscid 1 - D gasdynamics equations take the primitive form[1]

$$\frac{\partial u}{\partial t} + A \frac{\partial u}{\partial x} = F, \quad 0 < x < \infty, \quad t > 0 \tag{E.1a}$$

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(1) Neglecting low order terms due to the linearization.

where $u \equiv (\rho,U,p)^t$ are the density velocity and pressure respectively, F stands for the external forces and

$$(E.1b) \qquad A = \begin{bmatrix} \eta & \xi & 0 \\ 0 & \eta & 1/\xi \\ 0 & \gamma\zeta & \eta \end{bmatrix} \qquad \gamma = \text{ratio of specific heats}$$

with $(\xi,\eta,\zeta)^t$ denoting the corresponding variables we linearize about. The system is hyperbolic since A is diagonalizable by

$$T = \begin{bmatrix} c^2 & 0 & -1 \\ 0 & \xi c & 1 \\ 0 & -\xi c & 1 \end{bmatrix}, \qquad c = \sqrt{\gamma\zeta/\xi}$$

$$TAT^{-1} \equiv \text{diag}(\eta,\eta + c,\eta - c) \ .$$

We consider the subsonic inflow case $0 < \eta < c$; two boundary conditions are required at $x = 0$ to complement the only predetermined outflow variable $\tilde{u}_3 \equiv p - \xi cU$ associated with $\lambda_3 \equiv \eta - c < 0$. While prescribing the two conditions one should neither set boundary values for the predetermined $p - \xi cU_{|x=0}$, nor should he prescribe only $U_{|x=0}$ and $p_{|x=0}$ (or otherwise the two independent relations will again set values for $p - \xi cU_{|x=0}$). Failure to satisfy either one of the above constraints will either imply inconsistency, or at best, the consistent condition will give no new information and we will still be missing one piece of data at the boundary. Both cases are saved by requiring (1.4b) to hold:

For all $u \equiv (\rho,U,p)^t \neq 0$ in $\text{span}\{\phi_1,\phi_2\}$ where $\phi_1 = (2\xi c,0,0)^t$, $\phi_2 = (\xi c,c^2,\xi c^3)^t$ corresponding to $\lambda_1 = \eta > 0$, $\lambda_2 = \eta + c > 0$ we should have $Bu \neq 0$. Indeed, requiring $B\phi_1 \neq 0$ amounts to the requirement of not imposing $U_{|x=0}$ and $p_{|x=0}$ alone (i.e, without involving $\rho_{|x=0}$), while $B\phi_2 \neq 0$ (or -- which is the same thing -- $B(2\phi_2 - \phi_1) \neq 0$) prevent us from prescribing $p - \xi cU_{|x=0}$. We are then assured that we have two genuinely additional boundary conditions complementing the third predetermined outflow one (for more details we refer to [2]).

In this paper we study difference approximations to the hyperbolic system (1.1). We show that when our numerical boundary conditions are zeroth-order accurate with an inflow part of the problem, they render the overall computation unstable -- a discrete analogue of the necessary condition (1.4b). In the next section we set the exact mathematical framework for our discussion, and proof of the main theorem is given in Section 3.

This paper was written while visiting the Mathematics Research Center, University of Wisconsin-Madison, Madison Wisconsin, and I thank the Center and its Director, J. Nohel for their hospitality.

2. WELL DEFINED DIFFERENCE APPROXIMATIONS-STATEMENT OF MAIN THEOREM

We would like to solve (1.1), (1.4) by difference approximations. In order to do so, we introduce a mesh size $\Delta x > 0$ and a time step $\Delta t > 0$ such that $\lambda \equiv \Delta t/\Delta x = \text{const}$. Using the notation $v_\nu(t) \equiv v(\nu\Delta x, t)$ we approximate (1.1) by a consistent two-step solvable basic scheme of the form

$$\sum_{j=-r}^{p} A_j(x_\nu)v_{\nu+j}(t + \Delta t) = \sum_{j=-r}^{p} A_j(x_\nu)v_{\nu+j}(t) + \Delta t H_\nu(t), \tag{2.1a}$$

$$\nu = r, r + 1, \ldots .$$

Starting with the initial data

$$v_\nu(t = 0) = f_\nu, \qquad \nu = 0,1,\ldots , \tag{2.1b}$$

the scheme (2.1a) is then used to advance in time. To enable our calculation, the r boundary values $\{v_\nu(t + \Delta t)\}_{\nu=0}^{r-1}$ are required at each time step, and these are obtained from solvable boundary conditions of the form

$$\sum_{j=0}^{q} B_{j\nu}(x_\nu)v_j(t + \Delta t) = \sum_{j=0}^{q} B_{j\nu}(x_\nu)v_j(t) + \Delta t H_\nu(t), \tag{2.1c}$$

$$\nu = 0,1,\ldots,r - 1 .$$

Usually for obtaining $v_0(t + \Delta t)$ one complements the $N - \ell$ inflow values taken from (1.4) by additional ℓ consistent outflow relations and in case of higher order basic scheme, $r > 1$, extra boundary conditions as in (2.1c) must be provided for both the outflow and inflow components of $\{v_\nu(t + \Delta t)\}_{\nu=1}^{r-1}$.

We now have an overall difference approximation consisting of interior scheme (2.1a) together with boundary conditions (2.1c) and the main property we would like our approximation to have is stability; that is, we want small initial perturbations not to excite our homogeneous computation but rather to have only a small comparable affect. For, it is the stability which guarantees the convergence of our results to the exact solution of (1.1), (1.4), as we refine the mesh $\Delta x, \Delta t \to 0$. In fact, lack of stability is most likely to cause our computation to diverge. We therefore make the natural

Assumption. The basic scheme (2.1a) is stable for the pure Cauchy problem $-\infty < \nu < \infty$[(1)].

We are now left with the task of determining whether our boundary conditions (2.1c) maintain the assumed interior stability overall, or either our careless boundary treatment renders the overall computation unstable. During the last decade since the appearance of the works of Kreiss and his coworkers, [3]-[5], which introduce a stability theory for approximations to such mixed problems, many safe procedures to handle the outflow components were analyzed (e.g. [5]-[8]). Here however, we are interested in the inflow components whose boundary calculation is required when either the exact inflow conditions (1.4) are not known or when extra inflow values must be provided at $\{x_\nu\}_{\nu=1}^{r-1}$. Our main result is basically a negative one telling what one should not do.

Theorem. If the boundary conditions (2.1c) are zeroth-order accurate with an inflow component of system (1.1), i.e., there exists $\phi_*^+ \in \Phi^+$ such that

$$\sum_{j=0}^{q} [\mathcal{B}_{j\nu} - B_{j\nu}]\phi_*^+\Big|_{x=0} = 0, \qquad \nu = 0,1,\dots,r-1, \tag{2.2}$$

then the overall approximation (2.1) is unstable.

The above theorem is clearly the discrete analogue of the necessary requirement (1.4b) for well-posedness; both reflect the independence of the inflow boundary values on the differential equation. In the special case of explicit one-leveled boundary extrapolation it was first proved by Kreiss [9] for the scalar case, and extended substantially by Burns [10] for the vector case. Here we give a simplified version of her proof for the general two-leveled implicit approximation. The assumption made in [10, Assumption 3.2], that $\mathcal{A}_j$, A_j are polynomials in A, is removed here so our result is also valid for multileveled multidimensional approximations, as can be shown using the standard devices which for simplicity are omitted. Finally we give a direct estimate of the unstable polynomial growth of the computed solution. Even though such growth by itself may be accepted as weak instability, it is rejected here due to the possible reflections at the other (right) boundary which will then result into the untolerable exponential instability [5].

As an example, consider any standard 5-point interior scheme approximating the system (E.1a) above. Two dimensional inflow eigenspace is to be determined at (x_1,t) and - in case the exact inflow conditions are not known - at (x_0,t) as well. According to the above theorem, any attempt to calculate the missing values in an inflow-dependent manner, that

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(1) Local stability around $x = 0$ is in fact enough - see Section 3.

is using zeroth-order accurate conditions for either $\rho c^2 - p$, $\xi c U + p$ or any combination of them will result into instability.

We close this section by finally noting that in general the boundary conditions (2.1c) are obtained using consistent discretizations of the two sources available to us - the differential system (1.1a) augmented by the inflow boundary conditions (1.4). By the above theorem, the approximated inflow boundary values cannot be calculated in an inflow-dependent manner by a consistent discretization of solely the inflow part of system (1.1a); one must take into account also the outflow data via conditions (1.4). A detailed procedure along these lines to achieve these values with any degree of accuracy is described in [8].

3. UNCONDITIONAL INSTABILITY-PROOF OF MAIN THEOREM

From the nature of our negative result it is sufficient to restrict attention to the case localized about $x = 0$, since it is the constant coefficient case $\mathcal{A}_j \equiv \mathcal{A}_j(0)$, $A_j \equiv A_j(0)$, $\mathcal{B}_{j\nu} \equiv \mathcal{B}_{j\nu}(0)$, $B_{j\nu} \equiv B_{j\nu}(0)$, which infers the instability of the general case.

The solution of the homogeneous approximation (2.1) with vanishing interior initial data $f_\nu \big|_{|\nu>r} = 0$ ($\underline{f} \equiv (f_0,\ldots,f_{r-1})^t$ yet to be determined) is given by the Cauchy formula

$$(3.1) \qquad v_\nu(t) = \frac{1}{2\pi i}\int_\Gamma z^n \varphi_\nu(z)\,dz, \qquad t = n\cdot\Delta t\ .$$

Here Γ is any contour enclosing the spectrum of the underlying difference operator and $\{\varphi_\nu(z)\}_{\nu=0}^\infty$, $\sum_{\nu=0}^\infty |\varphi_\nu|^2 < \infty$ obeys the resolvent equation

$$(3.2a) \qquad \sum_{j=-r}^{p} (z\mathcal{A}_j - A_j)\varphi_{\nu+j}(z) = 0, \qquad \nu = r, r+1, \ldots ,$$

together with the side conditions

$$(3.2b) \qquad \sum_{j=0}^{q} (z\mathcal{B}_{j\nu} - B_{j\nu})\varphi_j(z) = f_\nu, \qquad \nu = 0,1,\ldots,r-1\ .$$

Equation (3.2a) is an ordinary difference equation with constant coefficient matrices; its most general $\underline{\ell_2\text{-bounded}}$ solution is given by [11]

$$(3.3) \qquad \varphi_k(z) = X(z)L^k(z)\underline{\sigma}, \qquad k = 0,1,\ldots ,$$

where we employed the assumption of the Cauchy stability. Here $X(z)$

consists of Nr columns vectors - they are the N-dimensional Jordan chains $\{\phi_m(z)\}_{m=1}^{Nr}$ associated with the characteristic eigenvalue problem[1]

(3.4) $$\sum_{j=-r}^{p} (zA_j - A_j)\kappa_m^j(z)\phi_m(z) = 0 \;;$$

$L(z)$ is an Nr-dimentional matrix consisting of the Jordan blocks associated with the eigenvalues $\kappa_m(z)$; and $\underset{\sim}{\sigma}$ is an Nr-dimensional free vector yet to be determined by Nr boundary conditions (3.2b):

(3.5a) $$D(z)\underset{\sim}{\sigma} = \underset{\sim}{f}, \qquad D(z) = [D_0(z),\dots,D_{r-1}(z)]^t$$

where

(3.5b) $$D_\nu(z) = \sum_{j=0}^{q} (zB_{j\nu} - B_{j\nu})X(z)L^j(z), \qquad \nu = 0,1,\dots,r-1 \;.$$

The key of the instability proof lies in the study of the singular point $z = 1$; indeed in what follows we will show that $z = 1$ is an eigenvalue of the problem whose eigenprojection has a polynomial growth; this in turn implies the unstable polynomial growth of the whole difference operator. In order to do so, we are now going to use the consistency condition to gain more precise information about the behaviour near $z = 1$.

In [5] it was proved by the assumption of Cauchy stability, that the matrix $L(z)$ in the neighbourhood of $z = 1$ takes the form [5, Theorem 9.1]

(3.6a) $$L(z) = \begin{bmatrix} L_+(z) & 0 \\ 0 & L_0(z) \end{bmatrix} ,$$

where using the consistency of the interior scheme it follows that the ℓ-dimensional $L_+(z)$ is of the form [5, Theorem 9.3]

(3.6b) $$L_+(z) = I - (\lambda\Lambda^+)^{-1}(z - 1) + \mathcal{O}(z - 1)^2 ,$$

while the $(Nr - \ell) \times (Nr - \ell)$ $L_0(z)$ satisfies

(3.6c) $$L_0^*(z)L_0(z) < (1 - \delta)I, \qquad \delta > 0 \;.$$

Consider the first ℓ column vectors $\phi_m(z)_{|1 \le m \le \ell}$ in $X(z)$ which we

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[1] By consistency it is enough to consider only simple Jordan chains around $z = 1$ - see below.

denote by $X_+(z)$. Inserting the corresponding eigenvalues of $L_+(z)$ from (3.6b), $\kappa_m(z) = 1 - (\lambda\lambda_m)^{-1}(z-1) + O(z-1)^2$, into (3.4), and using the consistency of the basic scheme which amounts to the standard

$$\sum_{j=-r}^{p} [A_j - A_j] = \sum_{j=-r}^{p} [j(A_j - A_j) - \lambda A_j A] = 0 ,$$

we arrive to

$$(z-1) \cdot \sum_{j=-r}^{p} A_j [I - zA\lambda_m^{-1}]\phi_m(z) = O(z-1)^2 .$$

By the solvability $\sum_{j=-r}^{p} A_j e^{ij\theta}\big|_{\theta=0} = \Sigma A_j$ is nonsingular; dividing by $(z-1)\Sigma A_j$ we obtain that

(3.7) $$X_+(z) = X_+(1) + O(z-1), \quad X_+(1) \in \Phi^+ ,$$

where $X_+(1)$ consists of the ℓ column vectors $\phi_m(1) \equiv \phi_m$ - the eigenvectors of A corresponding to its positive eigenvalues $\lambda_m > 0$.

We now claim that $[D(z)]^{-1}$ is singular at $z = 1$. To see that we take τ to be an Nr-dimensional vector whose first ℓ scalar components, τ_+, are uniquely determined as the solution of (see (2.2))

$$X_+(1)\tau_+ = \phi_*^+ ,$$

and the remaining $Nr - \ell$ components are taken to zero. Taking into account (3.6b) and (3.7) we then find by (2.2)

(3.8a) $$D(z)\tau_+ = \sum_{j=0}^{q} (B_{j\nu} - B_{j\nu})X_+(1)\tau_+ + O(z-1) = O(z-1)$$

and hence for $d(z) \equiv \det[D(z)]$ we conclude that

(3.8b) $$d(z) = O(z-1)^s \qquad s \geq 1 .$$

The proof of the theorem is almost at our hands now; we consider that part of the solution corresponding to the eigenprojection associated with $z = 1$:

(3.9a) $$w_\nu(t) = \frac{1}{2\pi i} \int_{|z-1|=\varepsilon} z^n \varphi_\nu(z)\,dz, \quad \nu = 0,1,\ldots, \quad t = n\cdot\Delta t ,$$

where by (3.3), (3.5), $\varphi_\nu(z)$ has the <u>analytic</u> representation $([D(z)]^{-1} \equiv \mathcal{D}(z)/d(z))$

$$(3.9b) \qquad \varphi_\nu(z) = [X_+(z), X_0(z)] \begin{bmatrix} L_+(z) & 0 \\ 0 & L_0(z) \end{bmatrix}^\nu \mathcal{D}(z)\underset{\sim}{f}/d(z) .$$

Taking (3.8b) into account, the residue theorem implies

$$(3.10) \qquad w_\nu(t) = \sum_{k=0}^{s-1} \binom{n}{k} \cdot \mathrm{Res}\left[(z-1)^k \varphi_\nu(z)\right]_{|z=1}$$

and since by (3.6b) $L_+(z = 1) = I$ we finally conclude

$$(3.11) \qquad \|w(t)\| \geq \left[\sum_{\nu=0}^{(n+1)\cdot r} |w_\nu(t)|^2\right]^{1/2} \geq \mathrm{const.}[t/\Delta t]^s \|\underset{\sim}{f}\| .$$

REMARKS

(i) As in [10] one can show that also in our case, the resolvent condition $\|\varphi(z)\| \leq \mathrm{const.}(|z| - 1)^{-1}$ is violated. Indeed using the representation (3.9b) and employing the equivalent H-norm,

$$\|\psi(z)\|_H = \left[\sum_{\nu=0}^{\infty} \psi_\nu^*(z) H(z) \psi_\nu(z)\right]^{1/2}, \quad \text{with} \quad H(z) \equiv [X_+(z)X_+^*(z)]^{-1}, \quad \text{one}$$

gets $\|\varphi(z)\| \geq \mathrm{const.}|z - 1|^{-3/2}$.

(ii) Unlike the case of one-leveled boundary extrapolation [10, Section 5], it does not follow that the more accurate the boundary conditions with an inflow part of our problem, the worse is the singular behaviour at $z = 1$ - the R.H.S. of (3.8a) remains unaffected in the genuinely two-leveled case.

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