JOURNAL OF COMPUTATIONAL PHYSICS 73, 289–305 (1987)

A Representation and Approximation of the Solutions of Hyperbolic Differential Equations

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Received February 13, 1986; revised October 29, 1986

A representation is obtained for a weak solution of a hyperbolic system of partial differential equations in two variables with the mixed initial and boundary values being specified. The procedure is based on obtaining and inverting the Stieltjes transform of the solution. A numerical scheme to approximate the solution is developed, based on some properties of the representation and the method of characteristics. The method is illustrated by considering the equations that describe fluid flow in an ideal shock tube. © 1987 Academic Press, Inc.

1. INTRODUCTION

Considerable attention has been paid to developing methods to obtain numerical approximations to the solutions of quasi-linear, hyperbolic partial differential equations. In the classical method of characteristics, the quasi-linearity is exploited to reduce the problem to approximating the fixed point of an integral operator [1, p. 464]. The characteristic curves are determined by solving ordinary differential equations. Numerical approximations to the derivatives and the integrals encountered reduce the formalism to a computational procedure [2]. In a finite difference scheme, which covers a large number of procedures, the original partial differential equation is discretized by replacing the derivatives by some finite difference approximations to them. Numerical experimentations with some of the earlier methods demonstrated that they tend to smear the discontinuities of the solutions or introduce spurious oscillations to an unacceptable degree [3,4]. Subsequent improvements over the earlier techniques, which have grown into a large body of literature, overcame these difficulties to a large extent. Also, some convergence results have been obtained for a few of the methods falling in this category [5, 6]. The random choice method of Glimm [7] was developed from the Riemann representation of the solution [1, p. 453]. This scheme enables one to assume a discontinuous profile for an approximate solution. In a numerical experiment with an ideal shock tube, the procedure was found to approximate the solution reasonably well, except for the location of the discontinuities [3]. However, this method takes two to three times more computing time than the finite difference schemes considered in Ref. [3] and it is complicated to use.

0021-9991/87 $3.00
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In the present article, we consider a hyperbolic system of quasi-linear differential equations in two variables, with mixed initial and boundary values being specified. A representation of the solution is obtained by constructing and inverting its Stieltjes transform, which is well defined for a function of bounded variation. Quasi-linearity combined with the representation yields a fixed point equation for the solution. The formalism is then reduced to a computationally feasible form by comparing it with the method of characteristics. In view of some of the properties of the transform and the resulting representation, one may assume a discontinuous or a piecewise continuous profile for the approximation. Two approximations thus obtained, may be combined to yield an improved approximation (cf. Appendix). A scheme is developed to obtain the approximate values numerically and illustrated by considering the conservation laws describing fluid flow in an ideal shock tube.

2. The Stieltjes Transform

Some standard properties of the Stieltjes transform that will be needed are stated here. Let $h(x)$ be a function of bounded variation; then $H(z)$, defined by the Stieltjes integral

$$H(z)=\int_a^b \frac{dh(x)}{z-x}, \tag{1}$$

is called the Stieltjes transform of dh. Here $a=-\infty$ and $b=\infty$ are allowed. The function $H(z)$ is analytic in the complement of $[a, b]$. If $h(x)$ is constant on any subinterval of $[a, b]$, it is included in the region of analyticity of $H(z)$. According to the Stieltjes inversion formula [8],

$$\begin{aligned}\bar{h}(s)-\bar{h}(r)&=-\frac{1}{\pi}\lim_{\varepsilon\to 0}\int_r^s dy\,\mathrm{Im}\cdot H(y+i\varepsilon)\\ &=\lim_{\varepsilon\to 0}\int_{a'}^{b'} dh(x)\left[\tan^{-1}\frac{x-s}{\varepsilon}-\tan^{-1}\frac{x-r}{\varepsilon}\right],\end{aligned} \tag{2a}$$

where $\bar{h}(x)=\frac{1}{2}[h(x+0)+h(x-0)]$ and $[a', b']$ is any interval included in $[a, b]$ that includes $[r, s]$. It is clear that, at all points of its continuity, $h(x)=\bar{h}(x)$ and, if x is a point of discontinuity, then $\bar{h}(x)$ is the mean of the left and right limits. With this understanding, the bar from $\bar{h}(x)$ will be dropped. The inversion formula determines $h(x)$ uniquely at all of its points of continuity except for an additive constant. By observing that $H(z^*)=H^*(z)$, (2a) may be written as

$$h(s)-h(r)=\frac{1}{2\pi i}\int_{\Gamma_{sr}} dz\,H(z) \tag{2b}$$

where Γ_{sr} denotes the contour running from s to r on the upper side of the real axis and from r to s on the lower side.

Let $P_n(x)$, $n=0, 1, 2, \ldots$ be the orthogonal polynomials associated with dh. Then $H_n(z)$, given by

$$H_n(z)=\frac{1}{P_n(z)}\int_a^b dh(x)\,\frac{P_n(x)-P_n(z)}{x-z}, \tag{3}$$

defines the $[n, n]$ Padé approximant to $H(z)$ [9] and $H_n(z)\to_{n\to\infty} H(z)$ for each z in the complement of $[a, b]$. Also [8]

$$h_n(s)-h_n(r)=\frac{1}{2\pi i}\int_{\Gamma_{sr}} dz\, H_n(z)\xrightarrow[n\to\infty]{} h(s)-h(r) \tag{4a}$$

and, with a continuous $g(x)$,

$$\int_a^b dh_n(x)\, g(x)\xrightarrow[n\to\infty]{}\int_a^b dh(x)\, g(x). \tag{4b}$$

The zeros of the polynomials $P_n(x)$ are in $[a, b]$; as a consequence, $h_n(x)$ is a step function with jump discontinuities located at the zeros. Some flexibility can be exercised in locating the discontinuity points [10]; however, since this approximation provides only a motivation for the one used here, we shall not elaborate on it further.

3. Representation of the Solution

Consider a hyperbolic system of quasi-linear partial differential equations in variables t in $[0, T]$ and x in $[0, 1]$:

$$\frac{\partial \Phi}{\partial t}+\bar{A}(x, t; \Phi)\frac{\partial \Phi}{\partial x}=\bar{S}(x, t; \Phi), \tag{5a}$$

where Φ, $\bar{S}$ are m-vectors and $\bar{A}$, an $m\times m$ matrix with real eigenvalues. Let ϕ be defined by

$$\phi=\phi'(x, t)-(1-x)\,\phi'(0, t)-x\phi'(1, t)$$

where $\phi'(x, t)=\Phi(x, t)-\Phi(x, 0)$; then (5a) reduces to an equivalent equation

$$\frac{\partial \phi}{\partial t}+A(x, t; \phi)\frac{\partial \phi}{\partial x}=S(x, t; \phi) \tag{5b}$$

with $\phi(x, 0)=\phi(0, t)=\phi(1, t)=0$, $A(x, t; \phi)=A(x, t; \Phi)$, and

$$S=\bar{S}-\left[\frac{\partial}{\partial t}+A\frac{\partial}{\partial x}\right](\Phi-\phi).$$

For convenience of exposition, we shall restrict ourselves to (5b); corresponding expressions for Φ are obtained by substituting for ϕ. Also $\Phi(x, 0)$ and an appropriate subset of $\{\Phi_\mu(0, t), \Phi_\mu(1, t)\}$, $\mu = 1$ to m, will be assumed to be given so that a weak solution of (5a) and, hence, that of (5b), exists [1, p. 471]. Here Φ_μ denotes the μth component of Φ. By definition of hyperbolicity, there are m linearly independent eigenvectors corresponding to the (real) eigenvalues of A [1, p. 424]. It is then straightforward to construct an invertible matrix B such that $BAB^{-1} = A^d$, where A^d is a diagonal matrix [4]. The eigenvalues of A and A^d will be denoted by λ^μ, $\mu = 1$ to m. Let $W = B(\phi)\,\phi$; then (5b) is equivalent to

$$\frac{\partial W}{\partial t} + A^d(\phi)\frac{\partial W}{\partial x} = B(\phi)\,S(\phi) + \left[\frac{\partial B(\phi)}{\partial t} + A^d(\phi)\frac{\partial B(\phi)}{\partial x}\right]\phi = S'(\phi). \tag{6}$$

For a fixed value of μ, the solution of Eq. (6) may be obtained by solving the scalar equation

$$L(v)\,\sigma(v) = \frac{\partial\sigma(v)}{\partial t} + \lambda(v)\frac{\partial\sigma(v)}{\partial x} = s(v) \tag{7}$$

with $\sigma(x, 0; v) = \sigma(0, t; v) = \sigma(1, t; v) = 0$ and v is an arbitrary function in some neighborhood of ϕ. The solution component W_μ of (6) is obtained for each value of μ, by letting $\lambda(v) = \lambda^\mu(\phi)$, $s(v) = S'_\mu(\phi)$ in (7), to obtain $\sigma(\phi) = W_\mu$, which determines $\phi = B^{-1}(\phi)\,W$. In the following, we obtain $\sigma(v)$ as the image of v under a transformation and thus reduce (5) to a fixed-point equation.

Consider (7) for a fixed function v and, at first, assume λ to be an absolutely continuous function and s, a square-integrable function of x and t. Let $\mathscr{H}$ be the Hilbert space of the square integrable functions of x and t on $[0, 1] \times [0, T]$, let L' be the restriction of L to the absolutely continuous functions with the same boundary conditions as on σ, and let $L^\dagger$ be the adjoint of L' in $\mathscr{H}$. The symbol (,) will denote the scalar product in $\mathscr{H}$. Also, let $\hat{f}$ be a solution of

$$(L^\dagger \hat{f}(z, T))(x, t) = -\frac{\partial \hat{f}}{\partial t} - \frac{\partial}{\partial x}(\lambda \hat{f}) = \frac{1}{(z-x)^2} = (\psi(z))(x, t) \tag{8}$$

with $\hat{f}(z, T; x, T) = 0$ and values at $x = 0, 1$ being arbitrary. It follows from (7) and (8) that

$$\begin{aligned}(s, \hat{f}(z, T)) &= (L\sigma, \hat{f}(z, T)) = (\sigma, L^\dagger \hat{f}(z, T)) = (\sigma, \psi(z))\\ &= -\int_0^T dt \int_0^1 \frac{d\sigma(x, t)}{z - x}.\end{aligned}$$

Thus the Stieltjes transform, defined by (1), of $d\sigma(x, T)$ is given by

$$\int_0^1 \frac{d\sigma(x, T)}{z - x} = -\frac{\partial}{\partial T}(\sigma, \psi(z)) = -\left(s, \frac{\partial \hat{f}(z, T)}{\partial T}\right) = -(s, f(z, T)). \tag{9}$$

From (8), $\hat{f}$ is the solution of

$$\hat{f}(z, T; x, t) = \frac{(T-t)}{(z-x)^2} + \int_t^T dt' \frac{\partial}{\partial x} (\lambda \hat{f}(z, T))(x, t').$$

A differentiation with respect to T together with the identity $\hat{f}(z, T; x, T) = 0$ yields

$$f(z, T; x, t) = \frac{1}{(z-x)^2} + \int_t^T dt' \frac{\partial}{\partial x} (\lambda f(z, T))(x, t'),$$

i.e.,

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} (\lambda f) = 0$$

and

$$f(z, T; x, T) = (\psi(z))(x, T). \tag{10}$$

Using the inversion formula (2b), one has, from (9), for a fixed $\bar{x}$, that

$$\sigma(\bar{x}, T; v) = -\frac{1}{2\pi i} \int_{\Gamma_{\bar{x}}} dz (s(v), f(z, T; v)) \tag{11}$$

where $\Gamma_{\bar{x}} = \Gamma_{\bar{x}.0}$ and $\sigma(0, T) = 0$.

For the general case, $\lambda(v)$ may be approximated by a sequence of absolutely continuous functions, $s(v)$ by the square-integrable ones, and f by the resulting sequence of solutions of (10). The representation given by (11) makes sense as long as the scalar product is well defined.

The function W_μ is obtained from (11) by replacing v by ϕ. Since $\phi = B^{-1}(\phi) W$, a fixed-point equation for ϕ is given by

$$\phi = B^{-1}(\phi) \mathscr{L}\phi$$

where

$$(\mathscr{L}\phi)_\mu = W_\mu = -\frac{1}{2\pi i} \int_{\Gamma_{\bar{x}}} dz (S'_\mu(\phi), f^\mu(z, T; \phi)). \tag{12}$$

Here f^μ is the solution of (10) with $\lambda = \lambda^\mu(\phi)$.

Let $\hat{P}_n(x)$ be the orthogonal polynomials with respect to $d\sigma(x, T; v)$; $\hat{P}_n$ depends on μ and v. If one replaces $\psi(z)$ by $\psi_n(z)$, given by

$$(\psi_n(z))(x, t) = \frac{d}{dx} \frac{1}{\hat{P}_n(z)} \frac{\hat{P}_n(x) - \hat{P}_n(z)}{x - z}$$

in the above treatment, then a moment approximant, σ_n (discontinuous), to σ results in

$$\sigma_n(\bar{x}, T; v) = -\frac{1}{2\pi i}\int_{\Gamma_{\bar{x}}} dz(s(v), f_n(z, T; v)), \tag{13}$$

where f_n is the solution of (10) with $\psi(z)$ replaced by $\psi_n(z)$. From (4a), $\sigma_n \to_{n\to\infty} \sigma$. As above, a fixed-point equation for the corresponding approximation ϕ_n to ϕ is given by

$$\phi_n = B^{-1}(\phi_n)\,\mathscr{L}_n \phi_n,$$

where

$$(\mathscr{L}_n \phi_n)_\mu = (W_n)_\mu = -\frac{1}{2\pi i}\int_{\Gamma_{\bar{x}}} dz(S'_\mu(\phi_n), f_n^\mu(z, T; \phi_n)). \tag{14}$$

Here again, f_n^μ is the solution of (10) with $\lambda = \lambda^\mu(\phi_n)$ and $\psi(z) = \psi_n(z; \phi_n)$.

4. Reduction to the Method of Characteristics

Some reduction of the scalar product is desirable to develop a computationally feasible scheme to obtain an approximation to ϕ based on (12) or (14). A fixed-point equation, $\phi = B^{-1}(\phi)\,\mathscr{L}^c\phi$, for ϕ may also be obtained by the method of characteristics for sufficiently smooth S_0 and A^d. In the following, we show that there is a representation of the scalar product in (12) that reduces $\mathscr{L}$ to $\mathscr{L}^c$. For this, it is sufficient to consider the expression given by (11) for σ and a fixed v.

With $\tilde{s} = s/\lambda$, (11) becomes

$$\sigma(\bar{x}, T) = -\frac{1}{2\pi i}\int_{\Gamma_x} dz \int_0^1 dx \int_0^T dt\, \tilde{s}(x, t)\,\lambda(x,t) f(z, T; x, t). \tag{15}$$

The solution f of (10) may be obtained by the method of characteristics, to yield

$$f(z, T; x, t) = \frac{1}{[z - \hat{x}(x, t; T)]^2}\exp\left[\int_t^T dt'\,\lambda_x(x(\hat{x}, t; t'), t')\right],$$

where $\lambda_x = \partial\lambda(x, t)/\partial x$ and $(\hat{x}, t')$ is the characteristic curve defined by

$$\frac{d\hat{x}}{dt_1} = \lambda(\hat{x}, t_1), \qquad \hat{x}(x, t; t) = x,$$

i.e.,

$$\hat{x}(x, t; t_1) = x + \int_t^{t_1} dt'\,\lambda(\hat{x}(x, t; t'), t'). \tag{16}$$

It follows that

$$\int_0^T dt\, \lambda(x, t) f(z, T; x, t) = -\int_0^T dt \frac{\partial \hat{x}(x, t; T)}{\partial t} \frac{1}{[z - x(\hat{x}, t; T)]^2}$$
$$= \frac{1}{z - \hat{x}(x, 0; T)} - \frac{1}{z - x}. \tag{17}$$

Now assume that for each x there is a $\tau(x)$ such that

$$\int_0^T dt\, \tilde{s}(x, t)\, \lambda(x, t) f(z, T; x, t) = \tilde{s}(x, \tau(x)) \int_0^T dt$$
$$\times \lambda(x, t) f(z, T; x, t).$$

For sufficiently smooth functions, existence of such a $\tau(x)$ follows from the mean value theorem. Then from (15) and (17) one has that

$$\sigma(\bar{x}, T) = \frac{1}{2\pi i} \int_{\Gamma_{\bar{x}}} dz \int_0^1 d\rho(x) \left[\frac{1}{z - x} - \frac{1}{z - \hat{x}(x, 0; T)} \right]$$
$$= \lim_{\varepsilon \to 0} \int_0^1 d\rho(x) \left[\tan^{-1} \frac{x - \bar{x}}{\varepsilon} - \tan^{-1} \frac{\hat{x}(x, 0; T) - \bar{x}}{\varepsilon} \right] \tag{18}$$

where $\rho(x) = \int_0^x dy\, \tilde{s}(y, \tau(y))$.

On the other hand, if the same manipulations are used to reduce (13), one obtains

$$\sigma(\bar{x}, T) = \lim_{n \to \infty} \int_0^1 d\rho(x) \int_{\Gamma_{\bar{x}}} \frac{dz}{\hat{P}_n(z)} \left[\frac{\hat{P}_n(x) - \hat{P}_n(z)}{x - z} - \frac{\hat{P}_n(\hat{x}) - \hat{P}_n(z)}{\hat{x} - z} \right]$$
$$= \lim_{n \to \infty} \int_0^1 d\rho(x)\, \theta_n(x), \tag{19}$$

where $\hat{x} = \hat{x}(x, 0; T)$. Equations (18) and (19) both, in conjunction with (2a) and (4a), respectively, lead to

$$\sigma(\bar{x}, T) = \rho(\bar{x}) - \rho(\tilde{x}(\bar{x})), \tag{20}$$

where $\tilde{x}$ is the inverse of $\hat{x}(x, 0; T)$, i.e., $\tilde{x}(\hat{x}(x, 0; T)) = x$.

By setting $\hat{x}(x, 0; T) = \bar{x}$ in (16), one obtains

$$\tilde{x}(\bar{x}) = \bar{x} - \int_0^T dt'\, \lambda(\hat{x}(\tilde{x}, 0; t'), t'). \tag{21}$$

It is now straightforward to check that, if $(x, \tau(x))$ is the characteristic curve joining $(\tilde{x}, 0)$ and $(\bar{x}, T)$ and (7) is solved by the method of characteristics, then (20) results.

Although the manipulations leading to (18), (19), and (20) are valid for a smooth ρ, the expressions are valid as long as ρ is a function of bounded variation; $\hat{x}$ and $\tilde{x}$ are clearly continuous functions of x, even for a (bounded) λ that has discontinuities. Thus, by the usual limiting process, a ρ with discontinuities is admissible in (18), (19), and (20).

5. Numerical Scheme

Let $\{x_k\}$, $k=0, 1, ..., N$ be a set of grid points. Our aim is to compute $\phi(x_k)=\phi(x_k, t_0+\Delta t)$ with $\phi(x_k, t_0)$ being given. At each time point, by setting $t_0=0$ and $\Delta t=T$, the derivations of Sections 3 and 4 are valid as such. A standard and, in most cases, the simplest procedure to solve a fixed-point equation is by iteration. In the present situation, one may start with some approximate value ϕ_0 to ϕ and obtain one, $W_\mu(\phi_0)$, to $W_\mu(\phi)$ for each fixed value of μ. Thus, a $W(\phi_0)$ is obtained that yields an approximation $B^{-1}(\phi_0)\, W(\phi_0)$ to ϕ. At the next step, the new approximation replaces ϕ_0. This process is continued until a satisfactory level of accuracy is achieved. We shall take $\phi_0(x_k)=\phi(x_k, 0)=0$, i.e., $\Phi_0(x_k)=\Phi(x_k, 0)$, and, for convenience in the computation, separate the first approximation and further iterative corrections to $\sigma(\phi)$. Let

$$\rho_0(x)=\int_0^x dy\, \tilde{s}(y, \tau(y); \phi_0)$$

and

$$\rho_1(x)=\rho(x)-\rho_0(x)-[B(\phi)-B(\phi_0)]\,\phi.$$

Then (20) may be written as

$$\sigma(\bar{x}, T)=\sigma^0(\bar{x}, T)+\sigma^1(\bar{x}, T) \tag{22}$$

where

$$\sigma^{0,1}(x, T)=\rho_{0,1}(x)-\rho_{0,1}(\tilde{x}(x))$$

and

$$\sigma=[B(\phi)\,\phi]_\mu.$$

If ϕ_0 is close to ϕ, the dominant term in σ is σ^0.

Since no confusion will arise, $\Delta_k=x_k-x_{k-1}$ will also denote the interval $[x_{k-1}, x_k]$. Let $p_k=x_k-\tilde{x}(x_k)$ as defined by (21), and $|p_k|\leqslant\Delta_k, \Delta_{k+1}$. This restriction does not allow time steps exceeding the Courant limit. The formalism has room for relaxing this restriction, but we shall not pursue it for the present. At each stage of iteration, (21) is a fixed-point equation in $\tilde{x}$, which may itself be solved by the same procedure with some starting value, e.g., x_k. It is clear that $\tilde{x}(x_k)$ is in Δ_k or Δ_{k+1}. Assuming that $\rho_0(x_k)$ is accurately determined for each k value, the evaluation of σ^0 thus reduces to a problem of interpolation. Evaluation of the iterative correction σ^1 also reduces to the same problem, as shown by the example in Section 6. The general case differs from this one only in algebraic details. However, since σ^1 is small for a sufficiently small value of T, somewhat cruder approximations may be used. In the following, we concentrate on an accurate determination of σ^0.

Standard methods of interpolation assume some profile, e.g., a piecewise linear for ρ_0. This should introduce diffusion at each time step. Here, we develop an interpolation scheme based on a discontinuous profile for ρ_0. The value of σ^0 is given by

$$\sigma^0(x_k, T) = \int_{\tilde{x}(x_k)}^{x_k} d\rho_0(x) = \int_a^b d\rho_0(x)\, \theta(x_k, \tilde{x}; x), \tag{23}$$

where $\theta(a', b'; x)$ is the step function, which is equal to one in the interval $[a', b']$ and zero otherwise; $[a, b]$ may be any interval contained in $[0, 1]$ such that $x_k, \tilde{x}$ are in it.

Similarly the following expression for σ^0 is obtained, starting with (19):

$$\sigma^0(x_k, T) = \lim_{n \to \infty} \int_a^b d\rho_0(x)\, \theta_n(x). \tag{24}$$

The function $\theta_n(x)$ is the sum of a polynomial in x and the one in $\tilde{x}(x, 0; T)$, and $\tilde{x}$ is a continuous function of x, even for a discontinuous λ. Hence, $\theta_n(x)$ is a continuous function of x. Now, let $\rho_l(x)$ be a moment approximant (discontinuous) to ρ_0. Then

$$\sigma^0(x_k, T) = \lim_{n, l \to \infty} \sigma^0_{n,l}(x_k, T) = \lim_{n, l \to \infty} \int_0^1 d\rho_l(x)\, \theta_n(x). \tag{25}$$

It is clear that σ^0_{nl} is obtained by replacing θ with a continuous θ_n and ρ_0 with a discontinuous ρ_l in (23). A direct evaluation of σ^0_{nl} based on (25) is not possible for it requires the knowledge of the moments of σ. Also, it is not computationally attractive, or even feasible, to obtain an accurate moment approximant to ρ_0 because ρ_0 is assumed to be known only at $\{x_k\}$. The main import of the present representation, therefore, remains the realization of a possibility of approximating σ_0 by replacing ρ_0 with a discontinuous ρ_a and θ with a continuous θ_a in (23).

By reducing the interval of integration $[a, b]$ to one cell containing $x_k, \tilde{x}(x_k)$, one has that

$$\sigma_a(x_k, T) = \int_{x'}^{x_k} d\rho_a(x)\, \theta_a(x_k, \tilde{x}(x_k); x), \tag{26}$$

where $x' = x_{k-1}$ for $p_k > 0$ and $x' = x_{k+1}$ for $p_k < 0$; for $p_k = 0$, $\sigma_a(x_k, T) = 0$. Also, let $\Delta = \Delta_k, p_k > 0$; $\Delta = \Delta_{k+1}, p_k < 0$; and $\alpha_k = |p_k|/\Delta$, $\gamma(x) = (x - x')/\Delta$. Set $\rho_a(x_k) = \rho_0(x_k)$ for each value of k, and let $\rho_a(x)$ have one point of discontinuity, as yet unspecified, in each of the intervals Δ_k with a jump $[\rho_0(x_k) - \rho_0(x_{k-1})]$. For a sufficiently large value of N, this should approximate $\rho_0(x)$ well. For $\alpha_k = 1$, it follows from (23) that $\sigma^0(x_k, T) = \rho_0(x_k) - \rho_0(x')$. It would be desirable to preserve this exactness property.

Equation (26) may be written as

$$\sigma_a(x_k, T) = \int_0^1 d\rho_a(\gamma)\, \theta_a(1, 1 - \alpha_k; \gamma).$$

Let $\beta_k = (\xi_k - x_k)/(\Delta_{k+1})$, where ξ_k is the point of discontinuity of $\rho_a(x)$ in Δ_{k+1}, $\beta = \beta_{k-1}$ for $p_k > 0$, and $\beta = 1 - \beta_k$ for $p_k < 0$; we have that

$$\sigma_a(x_k, T) = \theta_a(1, 1 - \alpha_k; \beta)[\rho_0(x_k) - \rho_0(x')]. \tag{27}$$

In view of the aforementioned difficulties, θ_a and β_k are determined by somewhat heuristic arguments. Consider setting

$$\theta_a(1, 1 - \alpha; \gamma) = \begin{cases} \dfrac{\alpha}{1-\alpha}\gamma & \gamma \leqslant 1 - \alpha \\[2ex] 1 - \dfrac{1-\alpha}{\alpha}(1 - \gamma) & \gamma \geqslant 1 - \alpha. \end{cases} \tag{28}$$

The function θ_a thus defined has the following properties: For $\alpha = 1$, $\theta_a = 1$ for each $\gamma \neq 0$, implying that the exactness property is preserved with any choice of $\beta \neq 0$. For each α and $\beta = 1 - \alpha_k$, $\sigma_a(x_k, T)$ reduces to the value given by the linear interpolation of $\rho_0(x)$; thus (27) includes one of the standard approximations. For each α, θ_a has range $[0, 1]$: hence for any semimonotonic $g(\gamma)$ that does not have discontinuities at 0, 1 and $(1 - \alpha)$, there is a β' such that

$$\int_0^1 dg(\gamma)\, \theta(1, 1 - \alpha; \gamma) = \theta_a(1, 1 - \alpha; \beta')\; (g(1) - g(0)).$$

If $g(\gamma)$ is uniquely defined at these points, then they are not excluded. Piecewise semimonotonicity of $\rho_0(x)$ on each of the intervals Δ_k is a milder requirement than piecewise linearity. For each $\alpha = 0, 1$, θ_a is invertible; therefore, β' is uniquely determined by $g(\gamma)$ and α. Invertibility of θ_a will help determine adequate values of β_k in the following section. As a consequence of these properties, (28) offers an attractive choice for θ_a.

The procedure thus reduces to obtaining an approximation $\hat{\sigma}_a$ to σ, given by

$$\hat{\sigma}_a(x_k, T) = \sigma_a(x_k, T; \phi_0) + \sigma_a^1(x_k, T; \phi_0, \phi_a), \tag{29}$$

where σ_a^1 is an approximation to σ^1 and σ_a is given by (27).

Let $\mathcal{O}(t)$ be a one-parameter group of transformations that determines $\{\phi(x_k, t'+t)\}$ from a knowledge of $\{\phi(x_k, t')\}$; i.e., $\phi(x, t'+t) = \mathcal{O}(t)\,\phi(x, t')$, where $\phi(x, t) = \{\phi(x_k, t)\}$. We have obtained an approximation $\mathcal{O}_a$ to $\mathcal{O}$ except for the determination of $\{\beta_k\}$. While a judicious choice of values for β_k may be made, a more adequate criterion for their determination is desirable. At the initial time point, these values may be assumed to be known, for they are determined by the initial data. At other time points, let $-T'$ be the time point preceding zero in the present coordinate system for the time variable. The invertibility of $\mathcal{O}(t)$ implies that $\phi(x, -T') = \mathcal{O}(-T')\ \phi(x, 0)$, since $\phi(x, 0)$ is obtained by the operation $\phi(x, 0) = \mathcal{O}(T')\ \phi(x, -T')$. We require that $\mathcal{O}_a$ be invertible to determine $\{\beta_k\}$.

Let $\phi_a(x, -T')$ be the approximation to $\phi(x, -T')$, which determines $\phi(x, 0)$ in the present scheme. The requirement of invertibility of $\mathcal{O}_a$ is equivalent to

$$\begin{aligned}\sigma'(x_k, -T') &= [B(\phi_0(x_k))\,\phi_a(x_k, -T')]_\mu \\ &= \hat{\sigma}_a(x_k, -T') \\ &= \sigma_a(x_k, -T'; \phi_0) + \sigma_a^1(x_k, -T'; \phi_0, \phi_a(x, -T'))\end{aligned} \tag{30}$$

for each fixed μ. Let $(x'(x_k), 0)$ and $(x_k, -T')$ be on the same characteristic curve; $x'(x_k)$ is the counterpart for $-T'$ of $\tilde{x}(x_k)$ for T. Further, let p'_k and α'_k be defined for $-T'$ as p_k and α_k were for T. Then

$$\hat{\sigma}_a(x_k, -T') = \theta_a(1, 1-\alpha'_k, \beta')[\rho_0(x_k) - \rho_0(x')], \tag{31}$$

where $\beta', x' = 1-\beta_k, x_{k+1}$ for $p'_k < 0$ and $\beta', x' = \beta_k, x_{k-1}$ for $p'_k > 0$. Thus

$$\begin{aligned}\theta'_a &= \theta_a(1, 1-\alpha'_k, \beta') \\ &= [\sigma'(x_k, -T') - \sigma_a^1(x_k, -T'; \phi_0, \phi_a(x, -T'))]\,/(\rho_0(x_k) - \rho_0(x')).\end{aligned} \tag{32}$$

All of the quantities on the right side of (32) are known; hence, no iteration is required, although it is needed for the forward computation. The value of β' is now obtained by inverting θ_a:

$$\beta' = \begin{cases} \dfrac{1-\alpha'_k}{\alpha'_k}\,\theta'_a & \theta'_a \leqslant \alpha'_k \\[2ex] 1 - \dfrac{\alpha'_k}{1-\alpha'_k}(1-\theta'_a) & \theta'_a \geqslant \alpha'_k. \end{cases} \tag{33}$$

If a value for β' in the interior of $[0, 1]$ is not found, then a judicious choice may be made, e.g., $\beta_k = \frac{1}{2}$ or $1-\alpha'_k$.

In the above, we have described a procedure to obtain a value for σ_a assuming a discontinuous profile for ρ_a and a continuous approximation to θ_a. An alternative value for σ_a may be obtained, by the same procedure, by interchanging the roles of ρ and θ. The two approximations may be used to derive an improved value using a variational principle. We explain these modifications in the Appendix.

6. Example

To illustrate the procedure described in Section 5, we will consider the conservation equations describing one-dimensional, inviscid, compressible fluid flow, namely

$$\frac{\partial \Phi}{\partial t}+\frac{\partial F(\Phi)}{\partial x}=0, \tag{34}$$

where Φ is a three-dimensional vector with its components Φ_1, Φ_2, and Φ_3 being the mass, momentum, and energy density, respectively; $F_1=\Phi_2$, $F_2=\frac{1}{2}(3-\gamma)\times\Phi_2^2/\Phi_1+(\gamma-1)\,\Phi_3$, and $F_3=\gamma\Phi_2\Phi_3/\Phi_1-\frac{1}{2}(\gamma-1)\,\Phi_2^3/\Phi_1^2$; γ is the ratio of the specific heats. For an ideal gas, $\gamma=1.4$ and the initial conditions for the shock tube of References [3, 4] are

$$\Phi_1(x,0)=1, \qquad \Phi_2(x,0)=0,\ \Phi_3(x,0)=\frac{1}{\gamma-1} \qquad 0\leqslant x<0.5$$

$$\Phi_1(x,0)=0.125, \quad \Phi_2(x,0)=0,\ \Phi_3(x,0)=0.1/(\gamma-1) \quad 0.5<x\leqslant 1.$$

The standard boundary conditions [11] imply that $\Phi_2(0,t)=\Phi_2(1,t)=0$, and Φ_3 is given as a function of Φ_1 at the end points or vice versa. By setting $A_{\mu\nu}=\partial F_\mu/\partial\Phi_\nu$ and making the substitutions according to Eqs. (5a) and (5b), (34) reduces to (5b). With $u=\Phi_2/\Phi_1$ and c given by

$$c^2=\gamma(\gamma-1)(\Phi_3/\Phi_1-\tfrac{1}{2}u^2)$$

the eigenvalues are given by $\lambda^1=u-c$, $\lambda^2=u$, and $\lambda^3=u+c$, and B is easily constructed from the eigenvectors of A.

With the present initial conditions, an advantage may be taken from the fact that, for a period of time, $\Phi(0,t)=\Phi(0,0)$ and $\Phi(1,t)=\Phi(1,0)$. The case for more general initial conditions and/or for an arbitrary point in time differs from the present one only in some algebraic details. Also, to simplify the exposition further, a distinction between the exact and approximate quantities will not be made in the following.

Consider (21) with $\bar{x}=x_k$ and μ having a fixed value. Then

$$\tilde{x}(x_k)=x_k-\int_0^T dt'\,\lambda^\mu(x,t').$$

Assuming λ^μ along the characteristic to be smooth enough that the integral may be approximated accurately, for small values of T, using the trapezoidal rule, we have that

$$\tilde{x}(x_k)=x_k-\frac{T}{2}\,[\lambda^\mu(\tilde{x}(x_k),0)+\lambda^\mu(x_k,T)]. \tag{35}$$

The value of $x'(x_k)$ is obtained by replacing T with $-T'$ and $\tilde{x}(x_k)$ with $x'(x_k)$ in (35), which may then be solved by iteration. Now, σ_a^1 of (29) is given by

$$\sigma_a^1(x_k, T) = \int_{\tilde{x}(x_k)}^{x_k} [dB(x, \tau(x))(\Phi(x, \tau(x)) - \Phi(x, 0)) - (B(x, \tau(x)) - B(x, 0))\, d\Phi_0(x)]_\mu - [(B(x_k, T) - B(x_k, 0))\, \phi(x_k, T)]_\mu.$$

Using again the trapezoidal rule, one has that

$$\begin{aligned}\sigma_a^1(x_k, T) = \tfrac{1}{2}\{ &[B(x_k, T) - B(\tilde{x}(x_k), 0)](\Phi(x_k, T) - \Phi(x_k, 0)) \\ &- (B(x_k, T) - B(x_k, 0))[\Phi(x_k, 0) - \Phi(\tilde{x}(x_k), 0)]\}_\mu \\ &- [(B(x_k, T) - B(x_k, 0))\, \phi(x_k, T)]_\mu. \end{aligned} \tag{36}$$

Again T, $\tilde{x}(x_k)$ may be replaced by $-T'$, $x'(x_k)$ to yield $\sigma_a^1(x_k, -T')$ in (36). An advantage of (35) and (36) is that the evaluation of $\tilde{x}(x_k)$ and $\sigma^1(x_k, T)$ has been reduced to interpolation of quantities at zero time and iteration at point x_k. Computation of $x'(x_k)$ and $\sigma_a(x_k, -T')$ does not need iteration with respect to time. Interpolation may be carried out by a standard procedure or by the method described in Section 5 with a judicious choice of discontinuities. In view of the smallness of the iterative corrections, this should be satisfactory. Now, the jumps are given by

$$\rho_0(x_k) - \rho_0(x') = -\int_{x'}^{x_k} B(\Phi_0)\, d\Phi_0(x). \tag{37}$$

Since B is a continuous function of Φ_0, the jumps may be accurately determined by standard numerical methods.

Equations (35)–(37), together with (32)–(33), yield the values of $\{\beta_k\}$. After having determined $\{\beta_k\}$, (27), (29), (35)–(37) for T can be used to determine an iterative approximation to $\sigma = (B(\phi_0)\, \phi)_\mu$, which, for each μ value, enables one to compute the same to ϕ and hence Φ.

7. Results and Discussion

Results computed by the present method for the example in Section 6 are shown in Figs. 1 to 3, together with the exact values. One hundred equidistant positions in [0, 1] were taken for $\{x_k\}$, and the time steps were chosen so that the maximum Courant number equaled 0.75. The values of $\{\beta_k\}$ were computed approximately by dropping σ_a^1 in (32). This saved considerable computing time and reduced storage requirements without affecting the results significantly.

Although there is some discrepancy between the exact and computed values, presumably as a consequence of several approximations made, significant

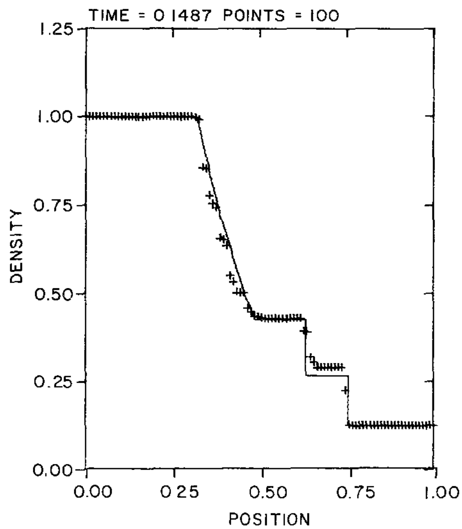

FIG. 1. Mass density profile, computed by the present method (+) and the exact values (solid line).

improvements over some of the other methods are observed: spurious oscillations are absent, the resolution and accuracy of the location of the discontinuities are excellent; the constant state is adequately realized; and the diffusion is minimal. Among all the methods discussed in Ref. [3], only Glimm's method preserves these properties, but the location of the discontinuities is significantly in error. The present method without iterations also preserves these properties to a large extent,

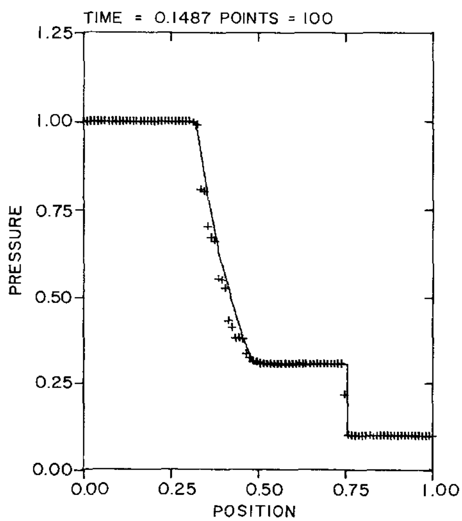

FIG. 2. Pressure profile, computed by the present method (+) and the exact values (solid line).

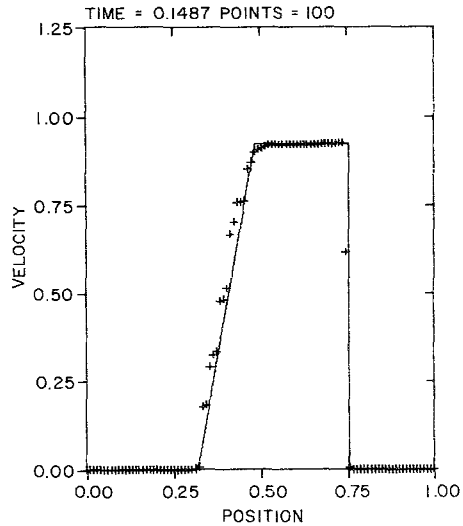

FIG. 3. Velocity profile, computed by the present method (+) and the exact values (solid line).

but the values in the constancy region were less accurate. The computing time for the present scheme without iterations compares favorably with one-step finite-difference methods. With iterations sufficient to achieve the accuracy indicated in Figs. 1 to 3, computing time remains less than that required by the hybrid scheme reported in Ref. [4]. An increase in the Courant number to 0.9 and a reduction in the number of grid points to 50 affected the results only slightly but resulted in a considerable saving in computing time—in the present case, a factor of three reduction. Storage requirements are quite modest, involving only the grid points and the values of Φ at the grid points at times $-T'$, 0, and T, in addition to a few $m(=3)$-vectors.

While our aim was to develop a computationally attractive scheme to approximate numerically the solutions of a system of quasi-linear hyperbolic partial differential equations, the representation obtained in Section 3 may be used for a qualitative study of weak solutions. The numerical procedure depends heavily on the interpolation method obtained in Section 5, which may also be applicable to other problems.

APPENDIX

Consider (23) and let $\eta = \sigma^0(x_k, T)/(\rho_0(x_k) - \rho_0(x'))$ and $\zeta(\gamma) = [\rho_0(x_k) - \rho_0(x(\gamma))]/(\rho_0(x_k) - \rho_0(x'))$; then

$$\eta = -\int_0^1 d\zeta(\gamma)\, \theta(\gamma) \tag{A.1}$$

$$= \int_0^1 \zeta(\gamma)\, d\theta(\gamma), \tag{A.2}$$

where $\theta(\gamma)=\theta(1, 1-\alpha_k; \gamma)$ and x', γ, α_k are as in (26)–(27). By replacing θ with θ_a and $\zeta(\gamma)$ with $[1-\theta(1, \beta; \gamma)]$ in (A.1), we obtain an approximation $\eta_1=\theta(1, 1-\alpha_k, \beta)$ to η given by (27). Alternatively, replacing $\zeta(\gamma)$ with $\zeta_a=[1-\theta_a(1, \beta; \gamma)]$ and leaving $\theta(\gamma)$ unchanged in (A.2) yield another approximation $\eta_2=1-\theta_a(1, \beta; 1-\alpha_k)$ to η. An efficient use of the two may be made by using the variational principle as follows. At first we assume ζ and θ to be the absolutely continuous functions of γ; the final expressions admit functions with discontinuities.

Let $\mathscr{H}_\gamma$ be the Hilbert space of square-integrable functions of γ on [0, 1] equipped with the usual scalar product denoted by $\langle\, , \rangle$. Let C be an operator on $\mathscr{H}_\gamma$ and

$$C\gamma=\xi, \qquad C^\dagger\chi'=\xi',$$

where $C^\dagger$ is the adjoint of C. Then the functionals F_1 and F_2 defined by

$$F_1(\chi_a, \chi'_a)=\langle\chi'_a, \xi\rangle+\langle\xi', \chi_a\rangle-\langle\chi'_a, C\chi_a\rangle \tag{A.3}$$

and

$$F_2(\chi_a, \chi'_a)=\frac{\langle\chi'_a, \xi\rangle\langle\xi', \chi_a\rangle}{\langle\chi'_a, C\chi_a\rangle} \tag{A.4}$$

are stationary with respect to small variations of χ_a and χ'_a about the exact solutions χ and χ' and $F_1(\chi, \chi')=F_2(\chi, \chi')=\langle\chi', \xi\rangle=\langle\xi', \chi\rangle$. Thus, if $\langle\chi'_a, \xi\rangle$ and $\langle\xi', \chi_a\rangle$ are first-order-accurate approximations, F_1 and F_2 are second-order accurate. Note that, for certain forms of χ_a and χ'_a, the stationary values of F_1 and F_2 are the same [12].

Let $C=-d/d\gamma$, defined on absolutely continuous functions that vanish at 1, and thus $C^\dagger=d/d\gamma$, defined on functions that vanish at zero; then $\eta=\langle\theta, C\zeta\rangle=\langle C^\dagger\theta, \zeta\rangle$. Thus, variational expressions for η may be obtained by further substituting $\chi_a=\zeta_a$, $\chi'_a=\theta_a$, $\xi=-\delta(\gamma-\beta)$, $\xi'=\delta(\gamma-(1-\alpha_k))$ in (A.3) and (A.4), where δ denotes the Dirac delta function. This results in $(\chi'_a, \xi)=\eta_1$, $(\xi', \chi_a)=\eta_2$, and

$$\langle\chi'_a, C\chi_a\rangle=\langle\theta_a, C\zeta_a\rangle=\begin{cases}\eta_2+\dfrac{1}{2}\dfrac{1-2\beta}{1-\beta}\cdot\dfrac{\alpha\beta}{1-\alpha} & \beta\leqslant 1-\alpha\\[2ex] \eta_2+\dfrac{1}{2}\dfrac{1-2\beta}{\beta}\cdot\dfrac{1-\alpha}{\alpha}(1-\beta) & \beta\geqslant 1-\alpha.\end{cases} \tag{A.5}$$

One may also consider θ_a and ζ_a to be parameter dependent, and their values may be determined by requiring F_1 or F_2 to be stationary. Similar considerations apply to θ'_a in (32).

ACKNOWLEDGMENTS

The author is thankful to Dr. S. R. Mulpuru for several helpful discussions, to Dr. W. G. Mathers for a critical reading of the manuscript, and to Dr. W. T. Hancox for encouragement.

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