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AN UNCONDITIONALLY STABLE IMPLICIT DIFFERENCE SCHEME FOR THE HYDRODYNAMICAL EQUATIONS

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AN UNCONDITIONALLY STABLE IMPLICIT DIFFERENCE SCHEME FOR THE HYDRODYNAMICAL EQUATIONS

by

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Abstract

We solve two hydrodynamical problems. The first involves a shock wave, a contact discontinuity, and a rarefaction wave using an unconditionally stable finite difference scheme. The Courant condition is satisfied everywhere except in one zone behind the shock, where it is violated by factors of 10 and 100. The nonlinear difference equations are solved by Newton's method. The total number of Newton iterations to get to a certain time is apparently independent of the degree to which the normal stability condition is violated in the one zone.

The second problem involves two rarefaction waves moving in opposite directions. One wave moves in a region where the Courant condition is violated by a factor of approximately two. The other wave moves in a region where the Courant condition is satisfied. Numerical results are compared with the analytical solution.

An examination of several runs indicates one explicit time step is about five times as fast as one implicit time step. Therefore, use of the implicit method is indicated when the Courant condition is violated by a factor of 5 or more.

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Table of Contents

Tables

Figures

Chapter I

Introduction

Consider a hydrodynamical problem in which a shock wave or disturbance of some kind is advancing into a material. Suppose that in the neighborhood of the disturbance the sound speed is C_0 and suppose also that there is a relatively quiescent region behind the disturbance in which the sound speed is C_1. Any explicit finite difference method will require

$$\max C \frac{\Delta t}{\Delta x} < 1$$

so that if $C_1 \gg C_0$ one will be forced to follow the uninteresting details of the motion in the quiescent region. An unconditionally stable finite difference method would be useful in such a problem. We present such a method for the equations of nonviscous compressible flow in one-dimensional Lagrangian coordinates.

The Differential Equations

The Lagrangian hydrodynamic equations with time t and mass m as independent variables are:

$$\frac{\partial(1/\rho)}{\partial t} - \frac{\partial u}{\partial m} = 0 \qquad \text{(mass equation)}$$

$$\frac{\partial u}{\partial t} + \frac{\partial p}{\partial m} = 0 \qquad \text{(momentum equation)}$$

$$\frac{\partial I}{\partial t} + p\,\frac{\partial u}{\partial m} = 0 \qquad \text{(energy equation)}$$

The dependent variables are:

ρ = density

u = velocity

p = pressure

I = internal energy

The velocity is defined by

$$u = \frac{\partial x}{\partial t}$$

where x is the coordinate of an element of fluid in the laboratory frame. Differentiating this velocity equation with respect to mass we see from the mass equation that

$$\frac{1}{\rho} = \frac{\partial x}{\partial m}$$

The Difference Equations

To form difference equations from the differential equations we imagine the fluid partitioned into cells of mass m_j where $j = 1,2,\ldots,J$, J being the total number of cells. Subscripts on field variables denote

the value of that particular variable at that space point. For example, $u_{j+1/2}$ denotes the right-hand cell boundary velocity of the j^{th} cell.

Superscripts denote time steps. For example, I_j^{n+1} denotes the internal energy of the j^{th} cell at time $t = (n+1)\Delta t$.

We make the following difference approximations:

$$\frac{\partial u}{\partial t} = -\frac{\partial p}{\partial m}$$

(1)
$$\frac{u_{j+1/2}^{n+1} - u_{j+1/2}^{n}}{\Delta t} = \frac{2\theta\left(p_j^{n+1} - p_{j+1}^{n+1}\right)}{m_j + m_{j+1}} + \frac{2(1-\theta)\left(p_j^{n} - p_{j+1}^{n}\right)}{m_j + m_{j+1}}$$

$$\frac{\partial x}{\partial t} = u$$

(2)
$$\frac{x_{j+1/2}^{n+1} - x_{j+1/2}^{n}}{\Delta t} = \theta u_{j+1/2}^{n+1} + (1-\theta)u_{j+1/2}^{n}$$

$$\frac{1}{\rho} = \frac{\partial x}{\partial m}$$

(3)
$$\rho_j^{n+1} = \frac{m_j}{x_{j+1/2}^{n+1} - x_{j-1/2}^{n+1}}$$

$$\frac{\partial I}{\partial t} = -p\frac{\partial u}{\partial m}$$

(4)
$$\frac{I_j^{n+1} - I_j^{n}}{\Delta t} = \frac{\theta p_j^{n+1}}{m_j}\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right) + \frac{(1-\theta)p_j^{n}}{m_j}\left(u_{j-1/2}^{n} - u_{j+1/2}^{n}\right)$$

This form of the difference equations was chosen because it gives a fairly simple form to the Jacobian matrix. We expect that the Newton iterative method would work just as well for other forms of the equations.

The polytropic gas equation of state is used. Also a pseudo-viscosity term is added to the pressure to spread the shock front. The pressure term then takes the form [1]:

$$(5)\quad p_j^{n+1} = (\gamma-1)\rho_j^{n+1}I_j^{n+1} + \lambda\sqrt{\gamma p_j^n \rho_j^{n+1}}\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right)$$

if

$$\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right) > 0$$

$$p_j^{n+1} = (\gamma-1)\rho_j^{n+1}I_j^{n+1}$$

if

$$\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right) \leq 0$$

Here γ is a constant characteristic of the gas and λ is a constant whose choice will be discussed later.

Rewriting Equations (1) and (4) we have:

$$(6)\quad u_{j+1/2}^{n+1} - u_{j+1/2}^{n} - \frac{2\theta\left(p_j^{n+1} - p_{j+1}^{n+1}\right)\Delta t}{m_j + m_{j+1}} - \frac{2(1-\theta)\left(p_j^{n} - p_{j+1}^{n}\right)\Delta t}{m_j + m_{j+1}} = 0$$

$$(7)\quad I_j^{n+1} - I_j^n - \frac{\theta p_j^{n+1}\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right)\Delta t}{m_j} - \frac{(1-\theta)p_j^n\left(u_{j-1/2}^n - u_{j+1/2}^n\right)\Delta t}{m_j} = 0$$

for $j = 1, 2, \ldots, J$.

Assuming that we know the values of the dependent variables at time n, this gives us a system of 2J simultaneous nonlinear equations in 2J unknowns for the values at time n+1.

Newton's method can be used to solve this system of equations. For a general system of the form

$$f(y) = 0$$

where f and y are vectors Newton's method is an iterative procedure in which the p+1-st iterative $y^{(p+1)}$ is defined by

$$y^{(p+1)} = y^{(p)} + \Delta y$$

where Δy is the solution of the linear system

$$(8)\quad J\Delta y = -f\left[y^{(p)}\right]$$

where

$$J = \left(\frac{\partial f_i}{\partial y_j}\right)$$

evaluated at $y^{(p)}$.

Taking (5) into account we see that (6) and (7) may be written in the form

$$(9)\quad g_j\left(u_{j-1/2}^{n+1},\ u_{j+1/2}^{n+1},\ u_{j+3/2}^{n+1},\ I_j^{n+1},\ I_{j+1}^{n+1}\right) = 0$$

$$(10)\quad \bar{g}_j\left(u_{j-1/2}^{n+1},\ u_{j+1/2}^{n+1},\ I_j^{n+1}\right) = 0$$

In our case we see then that the Jacobian matrix has a particularly simple form, namely that it is block tridiagonal.

$$J = \begin{pmatrix} B_1 & C_1 & & & & & \\ A_2 & B_2 & C_2 & & & & \\ & A_3 & B_3 & C_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & C_{J-1} & \\ & & & & A_J & B_J & \end{pmatrix}$$

where the submatrices are 2 x 2.

$$(11)\quad A_j = \begin{pmatrix} \dfrac{\partial g_j}{\partial u_{j-1/2}} & \dfrac{\partial g_j}{\partial I_{j-1}} \\ \dfrac{\partial \bar{g}_j}{\partial u_{j-1/2}} & \dfrac{\partial \bar{g}_j}{\partial I_{j-1}} \end{pmatrix}$$

$$(12)\quad B_j = \begin{pmatrix} \dfrac{\partial g_j}{\partial u_{j+1/2}} & \dfrac{\partial g_j}{\partial I_j} \\ \dfrac{\partial \bar{g}_j}{\partial u_{j+1/2}} & \dfrac{\partial \bar{g}_j}{\partial I_j} \end{pmatrix}$$

$$(13)\quad C_j = \begin{pmatrix} \dfrac{\partial g_j}{\partial u_{j+3/2}} & \dfrac{\partial g_j}{\partial I_{j+1}} \\ \dfrac{\partial \bar{g}_j}{\partial u_{j+3/2}} & \dfrac{\partial \bar{g}_j}{\partial I_{j+1}} \end{pmatrix}$$

where all differentiations are with respect to the variables u or I at time n+1.

We use the usual scheme to invert a block tridiagonal matrix [2]. Define 2 x 2 matrices as follows:

$$W_1 = B_1^{-1}C_1; \quad W_j = \left(B_j - A_jW_{j-1}\right)^{-1}C_j, \qquad 2 \le j \le J-1$$

$$G_1 = B_1^{-1}f_1; \quad G_j = \left(B_j - A_jW_{j-1}\right)^{-1}\left(f_j - A_jG_{j-1}\right), \qquad 2 \le j \le J$$

If we redefine Δy and f so that

$$f_j = \left(g_j, \bar{g}_0\right), \qquad \Delta y_j = \left(\Delta u_{j+1/2}, \Delta I_j\right)$$

then

$$\Delta y_J = G_J$$

$$\Delta y_j = G_j - W_j \Delta y_{j+1}, \qquad 1 \leq j \leq J-1$$

The p+1-st iterate is obtained by setting

$$u_{j+1/2}^{(p+1)} = u_{j+1/2}^{(p)} + \Delta u_{j+1/2}$$

$$I_j^{(p+1)} = I_j^{(p)} + \Delta I_j$$

Chapter II

Derivation of Matrix Elements and Stability Analysis

We now derive the entries of the 2 x 2 submatrices of the Jacobian matrix. Referring to (6), (7), (11), (12), and (13) we have:

$$A_j = \begin{pmatrix} \dfrac{-2\theta\Delta t}{m_j + m_{j+1}} \left(\dfrac{\partial p_j^{n+1}}{\partial u_{j-1/2}} - \dfrac{\partial p_{j+1}^{n+1}}{\partial u_{j-1/2}} \right) & 0 \\ \dfrac{-\theta\Delta t}{m_j} \dfrac{\partial}{\partial u_{j-1/2}} \left[p_j^{n+1} \left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1} \right) \right] & 0 \end{pmatrix}$$

$$B_j = \begin{pmatrix} 1 - \dfrac{2\theta\Delta t}{m_j + m_{j+1}} \left(\dfrac{\partial p_j^{n+1}}{\partial u_{j+1/2}} - \dfrac{\partial p_{j+1}^{n+1}}{\partial u_{j+1/2}} \right) - \dfrac{2\theta\Delta t}{m_j + m_{j+1}} \left(\dfrac{\partial p_j^{n+1}}{\partial I_j} - \dfrac{\partial p_{j+1}^{n+1}}{\partial I_j} \right) \\ \dfrac{-\theta\Delta t}{m_j} \dfrac{\partial}{\partial u_{j+1/2}} \left[p_j^{n+1} \left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1} \right) \right] \quad 1 - \dfrac{\theta\Delta t}{m_j} \dfrac{\partial}{\partial I_j} \left[p_j^{n+1} \left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1} \right) \right] \end{pmatrix}$$

$$C_j = \begin{pmatrix} \dfrac{-2\theta\Delta t}{m_j + m_{j+1}} \left(\dfrac{\partial p_j^{n+1}}{\partial u_{j+3/2}} - \dfrac{\partial p_{j+1}^{n+1}}{\partial u_{j+3/2}} \right) & \dfrac{-2\theta\Delta t}{m_j + m_{j+1}} \left(\dfrac{\partial p_j^{n+1}}{\partial I_{j+1}} - \dfrac{\partial p_{j+1}^{n+1}}{\partial I_{j+1}} \right) \\ 0 & 0 \end{pmatrix}$$

Here again all differentiations with respect to u and I are to be taken at time n+1.

To complete the derivation we need the various partial derivatives of the pressure terms.

From (2) it follows that

$$(14)\quad x_{j+1/2}^{n+1} - x_{j-1/2}^{n+1} = x_{j+1/2}^{n} - x_{j-1/2}^{n} + \theta\Delta t\left(u_{j+1/2}^{n+1} - u_{j-1/2}^{n+1}\right) + (1-\theta)\Delta t\left(u_{j+1/2}^{n} - u_{j-1/2}^{n}\right)$$

The pressure term may then be written

$$p_j^{n+1} = \frac{(\gamma-1)m_j I_j^{n+1}}{x_{j+1/2}^{n+1} - x_{j-1/2}^{n+1}} + \lambda \sqrt{\frac{\gamma p_j^{n}}{x_{j+1/2}^{n+1} - x_{j-1/2}^{n+1}}} \left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right)$$

if

$$u_{j-1/2} - u_{j+1/2} > 0$$

and

$$p_j^{n+1} = \frac{(\gamma-1)m_j I_j^{n+1}}{x_{j+1/2}^{n+1} - x_{j-1/2}^{n+1}}$$

if

$$u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1} \leq 0$$

A tabulation of the pressure derivatives follows:

$$\frac{\partial p_j^{n+1}}{\partial u_{j+1/2}} = -\frac{(\gamma-1)m_j \theta \Delta t I_j}{\left(x_{j+1/2} - x_{j-1/2}\right)^2} - \lambda\sqrt{\frac{\gamma m_j p_j}{x_{j+1/2} - x_{j-1/2}}}$$

$$-\lambda\theta\Delta t\sqrt{\frac{\gamma m_j p_j}{x_{j+1/2} - x_{j-1/2}}}\ \frac{\left(u_{j-1/2} - u_{j+1/2}\right)}{\left(x_{j+1/2} - x_{j-1/2}\right)}$$

where the last two terms do not appear if $u_{j-1/2} - u_{j+1/2} \leq 0$.

$$\frac{\partial p_{j+1}^{n+1}}{\partial u_{j+1/2}} = -\frac{\partial p_{j+1}^{n+1}}{\partial u_{j+3/2}}$$

$$\frac{\partial p_j^{n+1}}{\partial I_j} = \frac{(\gamma-1)m_j}{\left(x_{j+1/2} - x_{j-1/2}\right)}; \quad \frac{\partial p_{j+1}^{n+1}}{\partial I_j} = 0$$

$$\frac{\partial}{\partial u_{j+1/2}}\left[p_j^{n+1}\left(u_{j-1/2} - u_{j+1/2}\right)\right] = \left(u_{j-1/2} - u_{j+1/2}\right)\frac{\partial p_j^{n+1}}{\partial u_{j+1/2}} - p_j^{n+1}$$

$$\frac{\partial}{\partial I_j}\left[p_j^{n+1}\left(u_{j-1/2}^{n+1} - u_{j+1/2}^{n+1}\right)\right] = \left(u_{j-1/2} - u_{j+1/2}\right)\frac{\partial p_j^{n+1}}{\partial I_j}$$

$$\frac{\partial p_j^{n+1}}{\partial u_{j-1/2}} = -\frac{\partial p_j^{n+1}}{\partial u_{j+1/2}}; \quad \frac{\partial p_{j+1}^{n}}{\partial u_{j-1/2}} = 0$$

$$\frac{\partial}{\partial u_{j-1/2}}\left[p_j^{n+1}\left(u_{j-1/2} - u_{j+1/2}\right)\right] = p_j + \left(u_{j-1/2} - u_{j+1/2}\right)\frac{\partial p_j^{n+1}}{\partial u_{j-1/2}}$$

$$\frac{\partial p_j^{n+1}}{\partial u_{j+3/2}} = 0; \quad \frac{\partial p_{j+1}^{n+1}}{\partial u_{j+3/2}} = -\frac{\partial p_{j+1}^{n+1}}{\partial u_{j+1/2}}$$

$$\frac{\partial p_j^{n+1}}{\partial I_{j+1}} = 0; \quad \frac{\partial p_{j+1}^{n+1}}{\partial I_{j+1}} = \frac{(\gamma-1)m_{j+1}}{x_{j+3/2} - x_{j+1/2}}$$

Thus if we write

$K = \theta\Delta t$

$$\Delta m = \frac{K}{m_j + m_{j+1}}$$

$\Delta u_j = u_{j-1/2} - u_{j+1/2}$

we have:

$$A_j = \begin{pmatrix} 2\Delta m \dfrac{\partial p_j^{n+1}}{\partial u_{j+1/2}} & 0 \\ -\dfrac{K}{m_j}\left(-\Delta u_j \dfrac{\partial p_j^{n+1}}{\partial u_{j+1/2}} + p_j\right) & 0 \end{pmatrix}$$

$$B_j = \begin{pmatrix} 1 - 2\Delta m\left(\dfrac{\partial p_j^{n+1}}{\partial u_{j+1/2}} + \dfrac{\partial p_{j+1}^{n+1}}{\partial u_{j+3/2}}\right) & \dfrac{-2\Delta m(\gamma-1)m_j}{x_{j+1/2} - x_{j-1/2}} \\ -\dfrac{K}{m_j}\left(\Delta u_j \dfrac{\partial p_j^{n+1}}{\partial u_{j+1/2}} - p_j\right) & 1 - \dfrac{K\Delta u_j(\gamma-1)}{x_{j+1/2} - x_{j-1/2}} \end{pmatrix}$$

$$C_j = \begin{pmatrix} 2\Delta m \dfrac{\partial p_{j+1}^{n+1}}{\partial u_{j+3/2}} & \dfrac{2\Delta m(\gamma-1)m_{j+1}}{x_{j+3/2} - x_{j+1/2}} \\ 0 & 0 \end{pmatrix}$$

The method described in Chapter I is used to invert this matrix.

Stability Analysis

As has been pointed out [3] a rigorous stability analysis for the hydrodynamical difference equations has not been carried out. This analysis proceeds in the same manner as that done by Fromm [1].

We assume that the field variables vary slightly from their true values.

Let:

$$u_{j+1/2} = u_0\left(1 + \xi_{j+1/2}\right), \qquad \xi \ll 1$$

$$\rho_j = \rho_0\left(1 + \epsilon_j\right), \qquad \epsilon \ll 1$$

$$I_j = I_0\left(1 + \delta_j\right), \qquad \delta \ll 1$$

For simplicity assume that the cell masses are equal; $m_j = m = \rho_0 \delta x_0$.

We substitute these values in the difference equations and get the equations of first variation, dropping all higher order terms.

$$x^n_{j+1/2} - x^n_{j-1/2} = \frac{m_j}{\rho^n_j} = \frac{\rho_0 \delta x_0}{\rho_0\left(1+\epsilon^n_j\right)} = \delta x_0\left(1-\epsilon^n_j\right)$$

Then (14) becomes

$$(15)\quad \epsilon^{n+1}_j - \epsilon^n_j = \frac{\theta \delta t u_0}{\delta x_0}\left(\xi^{n+1}_{j-1/2} - \xi^{n+1}_{j+1/2}\right) + \frac{(1-\theta)\delta t u_0}{\delta x_0}\left(\xi^n_{j-1/2} - \xi^n_{j+1/2}\right)$$

We define the Courant number $\mu = \dfrac{C_0 \delta t}{\delta x_0}$ where C_0 is the local sound speed.

Then (15) becomes

$$(16)\quad \epsilon^{n+1}_j - \epsilon^n_j = \frac{\theta \mu u_0}{C_0}\left(\xi^{n+1}_{j-1/2} - \xi^{n+1}_{j+1/2}\right) + \frac{(1-\theta)\mu u_0}{C_0}\left(\xi^n_{j-1/2} - \xi^n_{j+1/2}\right)$$

The first variation of the energy equation (7) is

$$(17)\quad I_0\left(\delta_j^{n+1} - \delta_j^n\right) = \frac{\theta\delta t}{m} p_j^{n+1} u_0\left(\xi_{j-1/2}^{n+1} - \xi_{j+1/2}^{n+1}\right) + \frac{(1-\theta)\delta t}{m} p_j^n u_0\left(\xi_{j-1/2}^n - \xi_{j+1/2}^n\right)$$

For p_j^n we substitute

$$(\gamma-1)\rho_0 I_0\left(1 - \delta_j^n + \epsilon_j^n\right) + \lambda\rho_0 u_0 C_0\left(\xi_{j-1/2}^n - \xi_{j+1/2}^n\right)$$

Upon simplification (17) becomes

$$(18)\quad \delta_j^{n+1} - \delta_j^n = \frac{(\gamma-1)\rho_0 u_0 \delta t}{m}\left[\theta\left(\xi_{j-1/2}^{n+1} - \xi_{j+1/2}^{n+1}\right) + (1-\theta)\left(\xi_{j-1/2}^n - \xi_{j+1/2}^n\right)\right]$$

Finally we get the first variation of the momentum equation by substitution into (6) and again dropping higher order terms.

$$\begin{aligned}(19)\quad \xi_{j+1/2}^{n+1} - \xi_{j+1/2}^n = \frac{\theta\delta t}{mu_0}\Bigg\{&(\gamma-1)\rho_0 I_0\left[\left(\epsilon_j^{n+1} - \epsilon_{j+1}^{n+1}\right) + \left(\delta_j^{n+1} - \delta_{j+1}^{n+1}\right)\right] \\ &+ \lambda\rho_0 C_0 u_0\left[\left(\xi_{j-1/2}^{n+1} - \xi_{j+1/2}^{n+1}\right) - \left(\xi_{j+1/2}^{n+1} - \xi_{j+3/2}^{n+1}\right)\right]\Bigg\} \\ &+ \frac{(1-\theta)\delta t}{m}\Bigg\{(\gamma-1)\rho_0 I_0\left[\left(\epsilon_j^n - \epsilon_{j+1}^n\right) + \left(\delta_j^n - \delta_{j+1}^n\right)\right] \\ &+ \lambda\rho_0 C_0 u_0\left[\left(\xi_{j-1/2}^n - \xi_{j+1/2}^n\right) - \left(\xi_{j+1/2}^n - \xi_{j+3/2}^n\right)\right]\Bigg\}\end{aligned}$$

At this point we do the usual thing. We assume that the coefficients are constant and that the solution of these three equations of first variation can be written in a Fourier series. If so, then each term of the series is a solution and we look at a typical term to see what conditions must be satisfied to make it a solution.

We assume that

$$\xi_{j+1/2}^{n} = \xi e^{ik(j+1/2)} r_1^n$$

$$\epsilon_j^n = \epsilon e^{ikj} r_2^n$$

$$\delta_j^n = \delta e^{ikj} r_3^n$$

and consider only the special case $r_1 = r_2 = r_3 = r$.

Substitution of these values into (16), (18), and (19) yields after simplification

$$(1-r)\epsilon - \left[\frac{(r\theta+1-\theta)\ 2i \sin k/2\ \mu u_0}{c_0}\right] \xi = 0$$

$$\left[-\frac{2ic_0\mu \sin k/2\ (r\theta+1-\theta)}{u_0\gamma}\right]\epsilon + \left[1 - 4\lambda\mu \sin^2 k/2\ (r\theta+1-\theta) - r\right]\xi$$

$$+ \left[-\frac{2ic_0\mu \sin k/2\ (r\theta+1-\theta)}{u_0\gamma}\right]\delta = 0$$

$$\left[-\frac{2i(\gamma-1)u_0\mu \sin k/2\ (r\theta+1-\theta)}{c_0}\right]\xi + (1-r)\delta = 0$$

For this system of homogeneous linear equations to have a non-trivial solution it is necessary that its coefficient matrix be singular.

$$\begin{vmatrix} 1-r & -\dfrac{2i\mu u_0 \sin k/2\,(r\theta+1-\theta)}{c_0} & 0 \\ -\dfrac{2ic_0\mu \sin k/2\,(r\theta+1-\theta)}{u_0\gamma} & 1-4\lambda\mu \sin^2 k/2\,(r\theta+1-\theta)-r & -\dfrac{2ic_0\mu \sin k/2\,(r\theta+1-\theta)}{u_0\gamma} \\ 0 & -\dfrac{2i(\gamma-1)u_0\mu \sin k/2\,(r\theta+1-\theta)}{c_0} & 1-r \end{vmatrix} = 0$$

Expanding this determinant we get:

$$(1-r)\left[1-r-4\lambda\mu \sin^2 k/2\,(r\theta+1-\theta)\right] + 4\mu^2 \sin^2 k/2\,(r\theta+1-\theta)^2 = 0$$

For full generality at this point we would have to study the roots of this quadratic equation for arbitrary θ. This is somewhat difficult. The two cases of most importance are $\theta = 1/2$ and $\theta = 1$. Let $\sin^2 k/2 = \tau^2$.

For $\theta = 1/2$ the equation reduces to

$$r^2\left(1 + 2\lambda\mu\tau^2 + \mu^2\tau^2\right) + r\left(2\mu^2\tau^2 - 2\right) + \left(1 - 2\lambda\mu\tau^2 + \mu^2\tau^2\right) = 0$$

$$r = \frac{1 - \mu^2\tau^2 - 2\mu\tau\sqrt{\lambda^2\tau^2 - 1}}{1 + 2\lambda\mu\tau^2 + \mu^2\tau^2}$$

Case (1): If $\lambda^2\tau^2 < 1$, then r is complex

$$|r|^2 = \frac{(1 - \mu^2\tau^2)^2 + 4\mu^2\tau^2(1 - \lambda^2\tau^2)}{(1 + 2\lambda\mu\tau^2 + \mu^2\tau^2)^2}$$

$$= \frac{1 - 2\lambda\mu\tau^2 + \mu^2\tau^2}{1 + 2\lambda\mu\tau^2 + \mu^2\tau^2} < 1$$

Case (2): If $\lambda^2\tau^2 \geq 1$, then r is real.

To have $r < 1$ we need

$$2\lambda\mu\tau^2 + \mu^2\tau^2 > -\mu^2\tau^2 \pm 2\mu\tau\sqrt{\lambda^2\tau^2 - 1} \quad \text{or} \quad \lambda\tau + \mu\tau > \pm\sqrt{\lambda^2\tau^2 - 1}$$

But $\lambda\tau > \sqrt{\lambda^2\tau^2 - 1}$, so indeed $r < 1$. The proof for the case $\theta = 1$ is similar.

Notice here that $r < 1$, independent of μ, the Courant number. This shows that we have verified a necessary condition for this method to be unconditionally stable, namely, for solutions of the equations of first variation having the form we have prescribed.

Chapter III

Discussion of Numerical Results

The first problem used to test the scheme is the one used in [2]. Here we have two constant states separated by a discontinuity. The configuration at 40 cycles is a shock moving with speed 1.24, a contact discontinuity at the point of initial discontinuity, and a rarefaction wave.

The initial conditions for this problem are:

$\gamma = 1.4$

$\Delta t = 0.337$ (the Courant value)

$J = 50$ (25 cells to the left of the interface and 25 cells to the right).

Material on left	Material on right
$m_j = 1$	$m_j = 1$
$\rho_j = 0.5$	$\rho_j = 0.4454$
$p_j = 3.528$	$p_j = 0.5714$
$u_j = 0.698$	$u_j = 0$
$I_j = 19.756$	$I_j = 2.857$

Tables 1, 2, and 3 give the velocities, densities, and internal energies for several different calculations.

The Lax-Wendroff figures refer to the values obtained using the scheme of Reference 4.

Exact refers to the analytical values.

Explicit refers to values obtained using one of the explicit schemes of Reference 1.

Imp_1 refers to calculations done with all 50 cells having mass one.

To test numerically the unconditional stability of the implicit difference scheme a thin cell having the same density, but only a tenth the mass and width of the other cells, was put into cell 20. This means that the Courant condition was violated there by a factor of approximately ten. Imp_2 refers to calculations done with this thin cell.

Imp_3 is similar to Imp_2, the only difference being that this time cell 20 was given mass and width one-hundredth that of the other cells. Thus the Courant condition was violated by a factor of approximately one hundred. As can be seen from the results for Imp_2 and Imp_3, no instability appeared in the calculation. When the explicit method was run with a thin cell, large fluctuations appeared and eventually two cell boundaries crossed near the thin cell.

Since Newton's method involves evaluating the elements of a large matrix and then inverting it, another method for solving the system of simultaneous nonlinear equations was considered, namely, the method of nonlinear overrelaxation as described in [5]. If one has a system of k algebraic equations

$$f_i(x_1, x_2, \ldots, x_k) = 0, \quad i = 1,2,\ldots,k$$

each having one continuous derivative, then the generalization of ordinary overrelaxation suggested by Lieberstein for the nonlinear system is

$$x_1^{(n+1)} = x_1^{(n)} - \omega \frac{f_1\left[x_1^{(n)}, x_2^{(n)}, \ldots, x_k^{(n)}\right]}{f_{11}\left[x_1^{(n)}, x_2^{(n)}, \ldots, x_k^{(n)}\right]}$$

$$x_2^{(n+1)} = x_2^{(n)} - \omega \frac{f_2\left[x_1^{(n+1)}, x_2^{(n)}, \ldots, x_k^{(n)}\right]}{f_{22}\left[x_1^{(n+1)}, x_2^{(n)}, \ldots, x_k^{(n)}\right]}$$

etc., where $f_{ii} = \partial f_i / \partial x_i$. Here superscripts on variables denote the n^{th} iterate and n+1-st iterate and ω is the relaxation parameter.

It was hoped that this method would be faster than Newton's method for solving the system of nonlinear equations. As Lieberstein points out, the rate of convergence of this method depends rather critically on the choice of ω. For our choice of $\omega = 1$ the overrelaxation method was actually slower than Newton's method, but a more careful study of how to choose ω in an optional manner would probably make the overrelaxation method faster than Newton's method.

Figure 1 gives the velocity profile for Imp_1 superimposed on the exact solution. Figure 2 gives the density profile for Imp_1 superimposed on the exact solution.

Figure 3 gives the velocity profile near the shock front for $\theta = 1/2$ and three different values of λ. In general a large value of λ gives a smoother profile near the shock front but spreads the shock over several cells. A smaller λ gives a sharper shock front but has more oscillation. Some intermediate value of λ gives the best compromise between these two effects. We have found that for $\theta = 1/2$ a smaller λ can be used than for the explicit case. This is clear from Figure 3. To test the explicit case we needed to take $\lambda = 0.7$ and even then some oscillations appeared near the shock front, but for the implicit case $\lambda = 0.5$ gave a fairly sharp shock front with practically no oscillation.

Several trials were run with $\theta = 1$. The most notable differences in the results are that (1) they are somewhat less accurate than for $\theta = 1/2$ and (2) it was found that the pseudo-viscosity term was unnecessary and $\lambda = 0$ gave the sharpest shock front with little oscillation.

The reduced accuracy may be understood when one considers that for $\theta = 1/2$ all the differences are centered and the truncation errors are of order $(\Delta t)^3$. For any other choice of θ some second-order truncation error is present. One should then expect more accurate results for $\theta = 1/2$ than for any other choice of θ.

The result that $\lambda = 0$ is the best choice means that the implicit scheme itself contributes an effective viscosity term when $\theta = 1$.

Table 4 gives the velocity profile for $\theta = 1$, $\lambda = 0$ and $\lambda = 0.5$.

The total number of Newton iterations required to get to t = 13.48 is approximately 120 for Imp_1, Imp_2, and Imp_3 and for $\theta = 0.5$ and $\theta = 1$. This number is thus apparently independent of the degree to which the Courant condition is violated in zone 20.

The convergence criterion used required that the maximum percentage change in any value of μ or I be less than 1% on one Newton iteration. This generally required three Newton iterations for each time cycle. When this criterion was relaxed to the point of requiring the maximum percentage change to be less than 10% the final results were changed at most by a unit or two in the fourth significant digit. For this criterion only two Newton iterations were required for each time cycle.

When the stricter convergence criterion is used timing experiments have indicated that the explicit method is approximately five times faster per time step than the implicit scheme. In this case use of the implicit scheme is indicated when the Courant condition is to be violated by a factor of 5 or more.

With the less stringent convergence criterion the explicit method is only about three times as fast as the implicit method. Thus if this convergence criterion gives sufficient accuracy, and in practice it has, use of implicit scheme is indicated when the Courant condition is to be violated by a factor of 3 or more.

In practice the rate of convergence has been approximately quadratic, the maximum percentage change being roughly squared each time. Also in practice the Jacobian matrix has proved to be diagonally dominant.

This partially accounts for the accuracy of the inversion routine and the rapidity of convergence of Newton's method.

The second problem involves one gas, half of which is initially at rest, the other half initially moving with constant velocity. The configuration at 40 cycles is two rarefaction waves moving in opposite directions at a sound speed which is C = 0.316.

The gas initially at rest is divided into 90 cells of mass 0.1. The gas which is initially moving is divided into 10 cells of mass 1.0. Other initial conditions are:

$\gamma = 1.4$ $\quad \theta = 0.5$

$\mu t = 0.5$ $\quad \lambda = 0$

Finely celled gas	Coarsely celled gas
$\rho_j = 1.0$	$\rho_j = 1.0$
$u_j = 0.0$	$u_j = 2.0$
$p_j = 0.0714$	$p_j = 0.0714$
$I_j = 0.1786$	$I_j = 0.1786$

Figure 4 gives the plot of the density at time t = 20 from the numerical results and also the analytical values. It can be seen that no instabilities have appeared in the finely divided material even though the Courant condition is violated by a factor of approximately two.

One difficulty apparent from the graph is that the implicit scheme seems to lag behind the true solution in the finely divided region. Evidently the scheme does not allow signals to be propagated at sound speed in such a finely divided material. This may be the fault of the form of the difference equations, since they are nonconservative.

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4. Lax, P. and Wendroff, B., "Systems of Conservation Laws," Communications on Pure and Applied Mathematics, May 1960, pp. 217-237.
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Table 1 Velocity

Cell	Lax Wendroff	Explicit	Exact	Imp_1	Imp_2	Imp_3
1	0.702	0.698	0.698	0.702	---	---
2	0.709	0.699	0.698	0.707	0.709	0.709
3	0.725	0.703	0.698	0.720	0.719	0.721
4	0.754	0.716	0.698	0.747	0.743	0.746
5	0.800	0.752	0.698	0.794	0.788	0.793
6	0.866	0.826	0.822	0.865	0.857	0.864
7	0.948	0.938	0.984	0.961	0.950	0.960
8	1.045	1.075	1.130	1.075	1.063	1.074
9	1.150	1.223	1.342	1.203	1.190	1.202
10	1.259	1.372	1.453	1.335	1.322	1.334
11	1.366	1.512	1.528	1.463	1.452	1.463
12	1.463	1.616	1.528	1.568	1.611	1.568
13	1.541	1.613	1.528	1.611	1.588	1.612
14	1.589	1.588	1.528	1.586	1.563	1.587
15	1.596	1.563	1.528	1.561	1.546	1.562
16	1.566	1.548	1.528	1.545	1.537	1.546
17	1.525	1.538	1.528	1.537	1.533	1.538
18	1.508	1.533	1.528	1.533	1.531	1.534
19	1.518	1.530	1.528	1.531	1.531	1.532
20	1.534	1.528	1.528	1.529	1.530 1.529	1.530 1.530

21	1.529	1.526	1.528	1.528	1.528	1.529
22	1.526	1.525	1.528	1.527	1.527	1.527
23	1.528	1.527	1.528	1.526	1.526	1.527
24	1.528	1.532	1.528	1.526	1.526	1.526
25	1.528	1.520	1.528	1.526	1.526	1.526
26	1.528	1.526	1.528	1.525	1.526	1.526
27	1.528	1.527	1.528	1.525	1.525	1.525
28	1.528	1.528	1.528	1.525	1.525	1.526
29	1.528	1.527	1.528	1.525	1.526	1.527
30	1.528	1.525	1.528	1.526	1.526	1.527
31	1.528	1.529	1.528	1.526	1.526	1.526
32	1.527	1.532	1.528	1.526	1.526	1.526
33	1.528	1.522	1.528	1.525	1.525	1.526
34	1.527	1.530	1.528	1.526	1.525	1.526
35	1.527	1.512	1.528	1.525	1.525	1.526
36	1.528	1.531	1.528	1.528	1.527	1.529
37	1.533	1.524	1.528	1.524	1.524	1.525
38	1.526	1.529	1.528	1.528	1.529	1.528
39	1.519	1.472	1.528	1.508	1.508	1.509
40	1.576	1.518	1.528	1.522	1.523	1.527
41	1.546	1.298	1.528	1.432	1.432	1.423
42	0.850	0.725	0	0.558	0.558	0.547
43	0.108	0.136	0	0.114	0.114	0.111
44	0.006	0.018	0	0.019	0.019	0.019
45	0.000	0.002	0	0.003	0.003	0.003

Table 2 Density

Cell	Lax Wendroff	Explicit	Exact	Imp_1	Imp_2	Imp_3
1	0.445	0.445	0.445	0.445	---	---
2	0.444	0.445	0.445	0.445	0.445	0.445
3	0.442	0.445	0.445	0.444	0.444	0.444
4	0.438	0.444	0.445	0.441	0.441	0.441
5	0.432	0.440	0.445	0.436	0.437	0.436
6	0.423	0.431	0.426	0.428	0.429	0.429
7	0.413	0.418	0.407	0.418	0.419	0.418
8	0.401	0.402	0.388	0.404	0.406	0.405
9	0.388	0.384	0.370	0.389	0.391	0.390
10	0.376	0.367	0.350	0.374	0.375	0.374
11	0.363	0.351	0.345	0.358	0.360	0.359
12	0.352	0.338	0.345	0.345	0.347	0.346
13	0.343	0.334	0.345	0.337	0.337	0.337
14	0.338	0.338	0.345	0.336	0.336	0.336
15	0.337	0.339	0.345	0.339	0.339	0.339
16	0.341	0.341	0.345	0.342	0.341	0.342
17	0.345	0.343	0.345	0.343	0.343	0.343
18	0.347	0.344	0.345	0.344	0.344	0.344
19	0.346	0.345	0.345	0.344	0.344	0.344
20	0.344	0.345	0.345	0.344	0.345 0.345	0.344 0.345
21	0.344	0.345	0.345	0.344	0.345	0.345

22	0.345	0.345	0.345	0.345	0.345	0.345
23	0.344	0.345	0.345	0.345	0.345	0.345
24	0.344	0.345	0.345	0.345	0.345	0.345
25	0.346	0.345	0.345	0.345	0.345	0.345
26	1.212	1.170	1.304	1.213	1.218	1.170
27	1.287	1.225	1.304	1.242	1.247	1.225
28	1.295	1.259	1.304	1.264	1.269	1.259
29	1.292	1.284	1.304	1.280	1.283	1.284
30	1.294	1.289	1.304	1.290	1.292	1.289
31	1.295	1.289	1.304	1.296	1.296	1.299
32	1.297	1.286	1.304	1.301	1.301	1.304
33	1.300	1.296	1.304	1.304	1.303	1.306
34	1.302	1.294	1.304	1.305	1.305	1.306
35	1.304	1.304	1.304	1.306	1.306	1.308
36	1.306	1.294	1.304	1.303	1.303	1.304
37	1.307	1.292	1.304	1.305	1.305	1.306
38	1.306	1.286	1.304	1.294	1.294	1.296
39	1.299	1.307	1.304	1.306	1.306	1.309
40	1.335	1.248	1.304	1.261	1.261	1.266
41	1.326	1.194	1.304	1.313	1.313	1.312
42	0.831	0.964	0.500	0.841	0.841	0.834
43	0.540	0.628	0.500	0.568	0.568	0.566
44	0.503	0.518	0.500	0.511	0.512	0.511
45	0.500	0.502	0.500	0.502	0.502	0.502

Table 3 Internal Energy

Cell	Lax Wendroff	Explicit	Imp_1	Imp_2	Imp_3
1	19.78	19.76	19.76	---	---
2	19.77	19.76	19.75	19.76	19.76
3	19.74	19.75	19.72	19.73	19.73
4	19.67	19.73	19.68	19.69	19.68
5	19.55	19.68	19.59	19.60	19.59
6	19.40	19.54	19.45	19.47	19.45
7	19.21	19.32	19.26	19.28	19.26
8	18.98	19.02	19.01	19.03	19.01
9	18.74	18.69	18.72	18.75	18.73
10	18.49	18.34	18.42	18.45	18.43
11	18.25	18.01	18.12	18.15	18.12
12	18.02	17.73	17.85	17.87	17.85
13	17.92	17.60	17.67	17.68	17.67
14	17.73	17.65	17.66	17.65	17.65
15	17.73	17.70	17.72	17.71	17.72
16	17.79	17.75	17.77	17.77	17.77
17	17.89	17.79	17.80	17.80	17.80
18	17.92	17.81	17.82	17.82	17.81
19	17.90	17.82	17.82	17.82	17.82
20	17.86	17.82	17.83	17.83 17.83	17.83 17.83
21	17.86	17.82	17.83	17.83	17.83
22	17.88	17.83	17.84	17.83	17.83

23	17.90	17.83	17.84	17.84	17.84
24	17.90	17.81	17.84	17.84	17.84
25	17.78	17.80	17.86	17.86	17.85
26	5.086	5.266	5.074	5.074	5.052
27	4.789	5.026	4.954	4.955	4.938
28	4.763	4.880	4.871	4.871	4.852
29	4.770	4.803	4.813	4.813	4.797
30	4.765	4.772	4.772	4.772	4.761
31	4.757	4.747	4.747	4.747	4.738
32	4.748	4.730	4.730	4.729	4.723
33	4.739	4.732	4.722	4.721	4.716
34	4.734	4.731	4.719	4.718	4.711
35	4.729	4.733	4.720	4.720	4.713
36	4.727	4.732	4.716	4.716	4.707
37	4.729	4.717	4.722	4.722	4.715
38	4.725	4.710	4.710	4.710	4.701
39	4.717	4.715	4.727	4.728	4.723
40	4.769	4.667	4.663	4.664	4.661
41	4.698	4.472	4.738	4.738	4.728
42	3.948	3.908	3.788	3.788	3.770
43	2.973	3.087	3.030	3.030	3.025
44	2.863	2.887	2.884	2.884	2.883
45	2.857	2.861	2.861	2.861	2.861

Table 4 Velocity

Cell	$\theta=1$ $\lambda=0$	$\theta=1$ $\lambda=0.5$
1	0.780	0.775
2	0.793	0.788
3	0.819	0.813
4	0.858	0.851
5	0.909	0.900
6	0.972	0.961
7	1.044	1.032
8	1.125	1.106
9	1.210	1.195
10	1.298	1.282
11	1.382	1.365
12	1.456	1.440
13	1.511	1.498
14	1.542	1.534
15	1.551	1.547
16	1.546	1.546
17	1.541	1.543
18	1.540	1.540
19	1.539	1.538
20	1.539	1.536
21	1.538	1.535
22	1.538	1.534
23	1.538	1.533
24	1.538	1.533
25	1.538	1.532
26	1.538	1.532
27	1.538	1.532
28	1.538	1.532

Table 4 (Cont.)

29	1.538	1.532
30	1.538	1.532
31	1.538	1.532
32	1.538	1.532
33	1.538	1.532
34	1.538	1.532
35	1.538	1.532
36	1.538	1.531
37	1.538	1.529
38	1.538	1.521
39	1.537	1.489
40	1.552	1.382
41	1.177	1.079
42	0.262	0.581
43	0.029	0.213
44	0.003	0.064
45	0.000	0.018
46	0.000	0.005
47	0.000	0.001
48	0.000	0.000
49	0.000	0.000
50	0.000	0.000

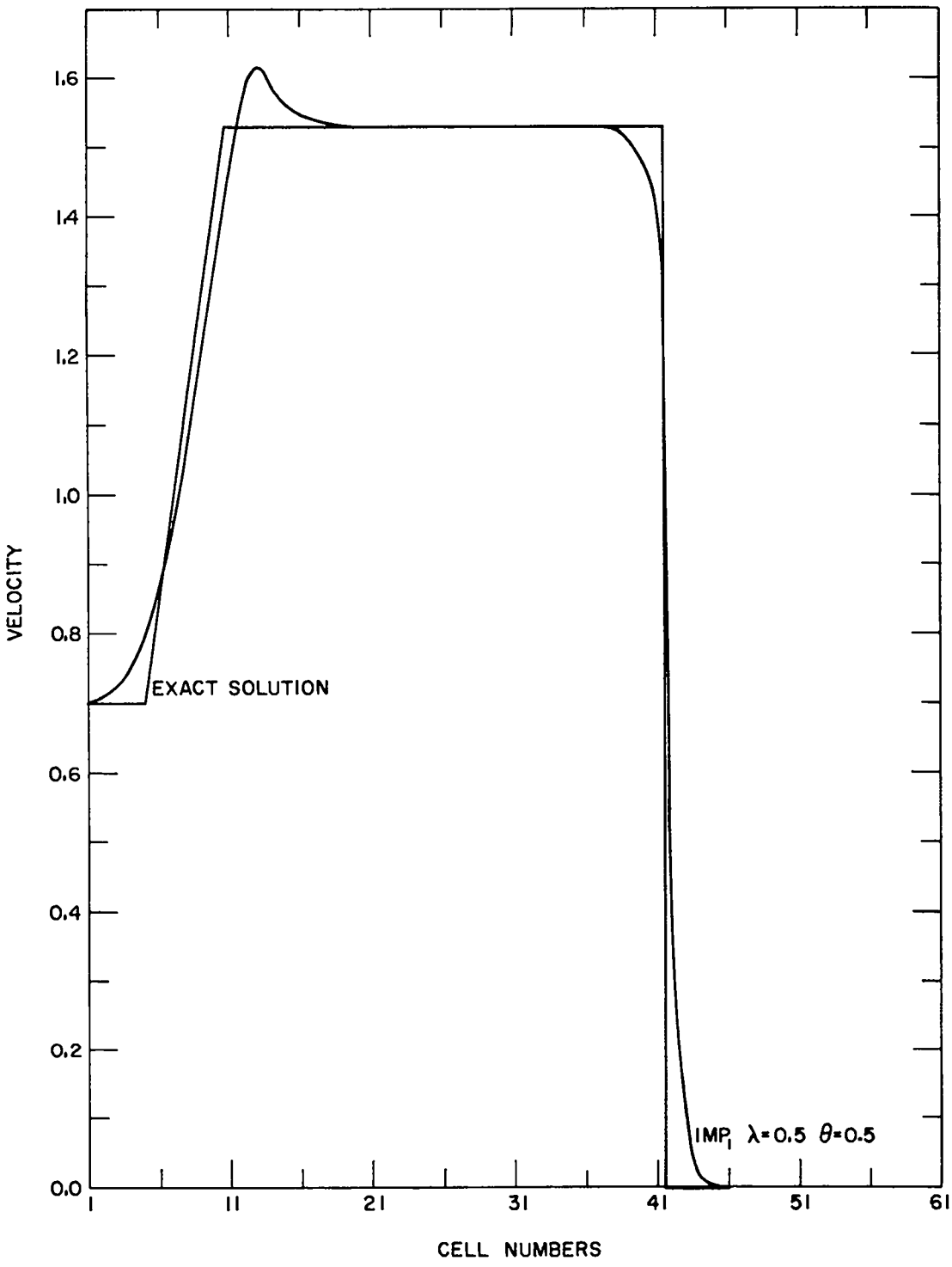

Fig. 1. Velocity profile at time t = 13.48 for problem 1.

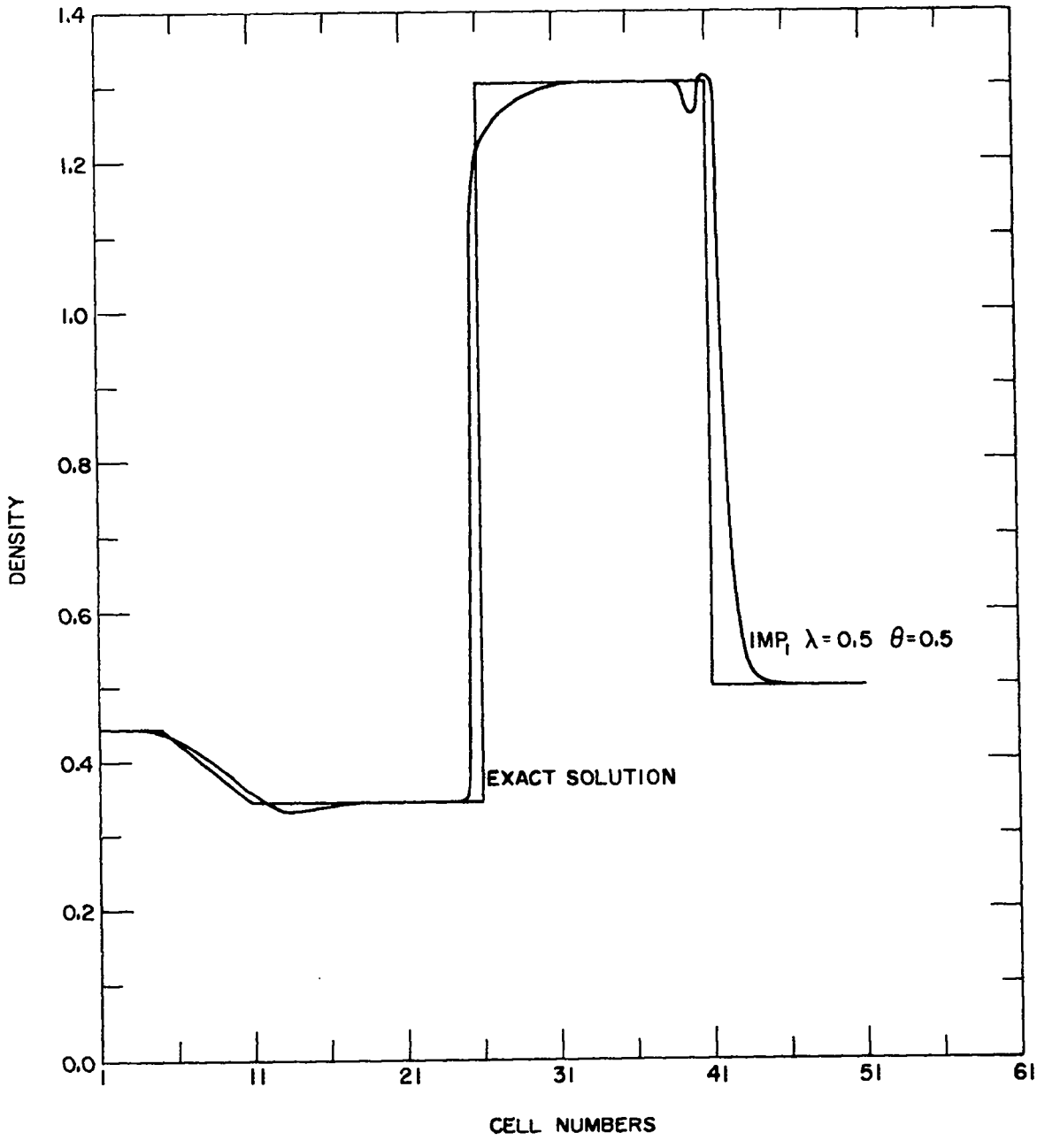

Fig. 2. Density profile at time t = 13.48 for problem 1.

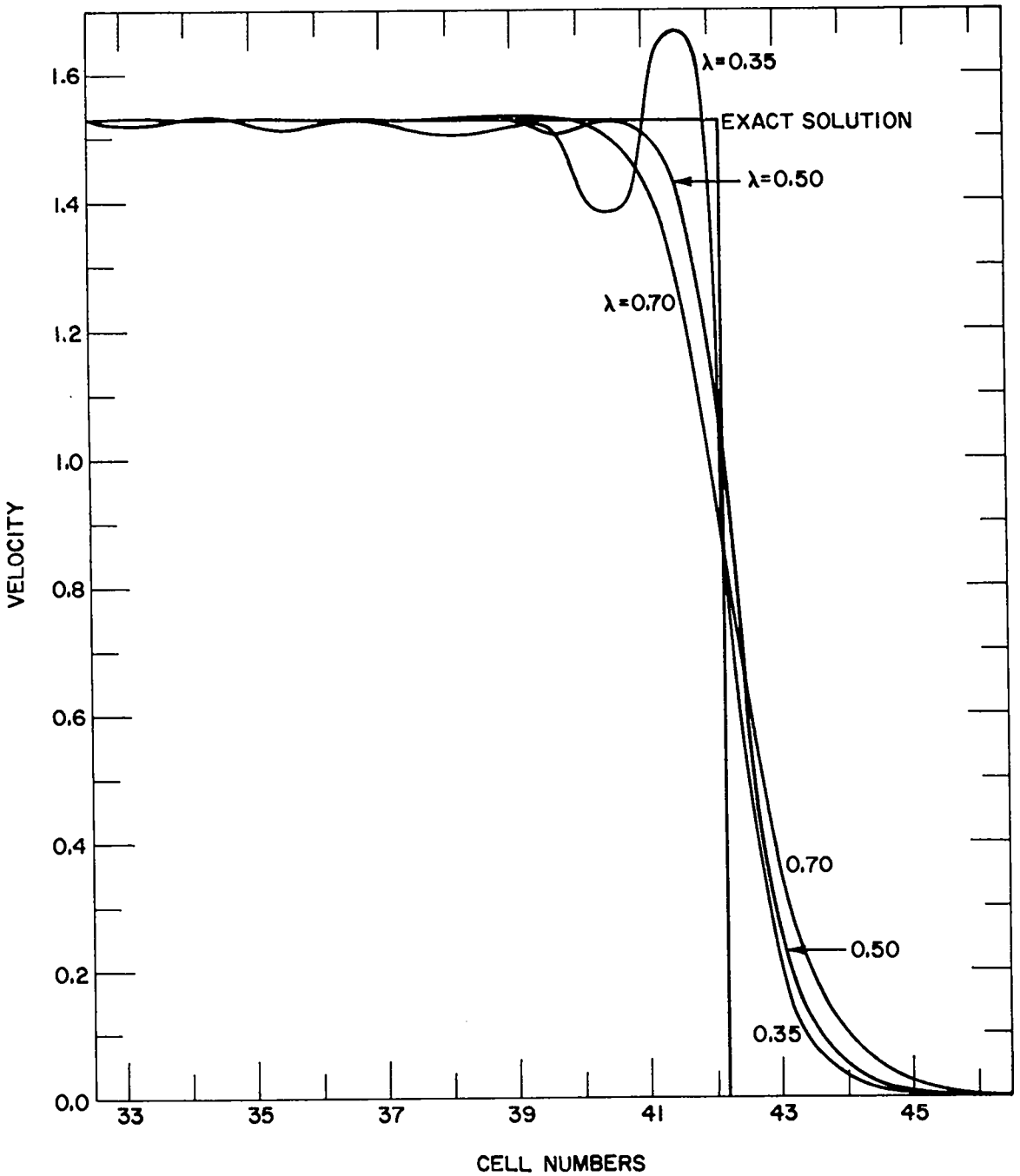

Fig. 3. Velocity profile of the shock front at t = 13.48 for various choices of λ.

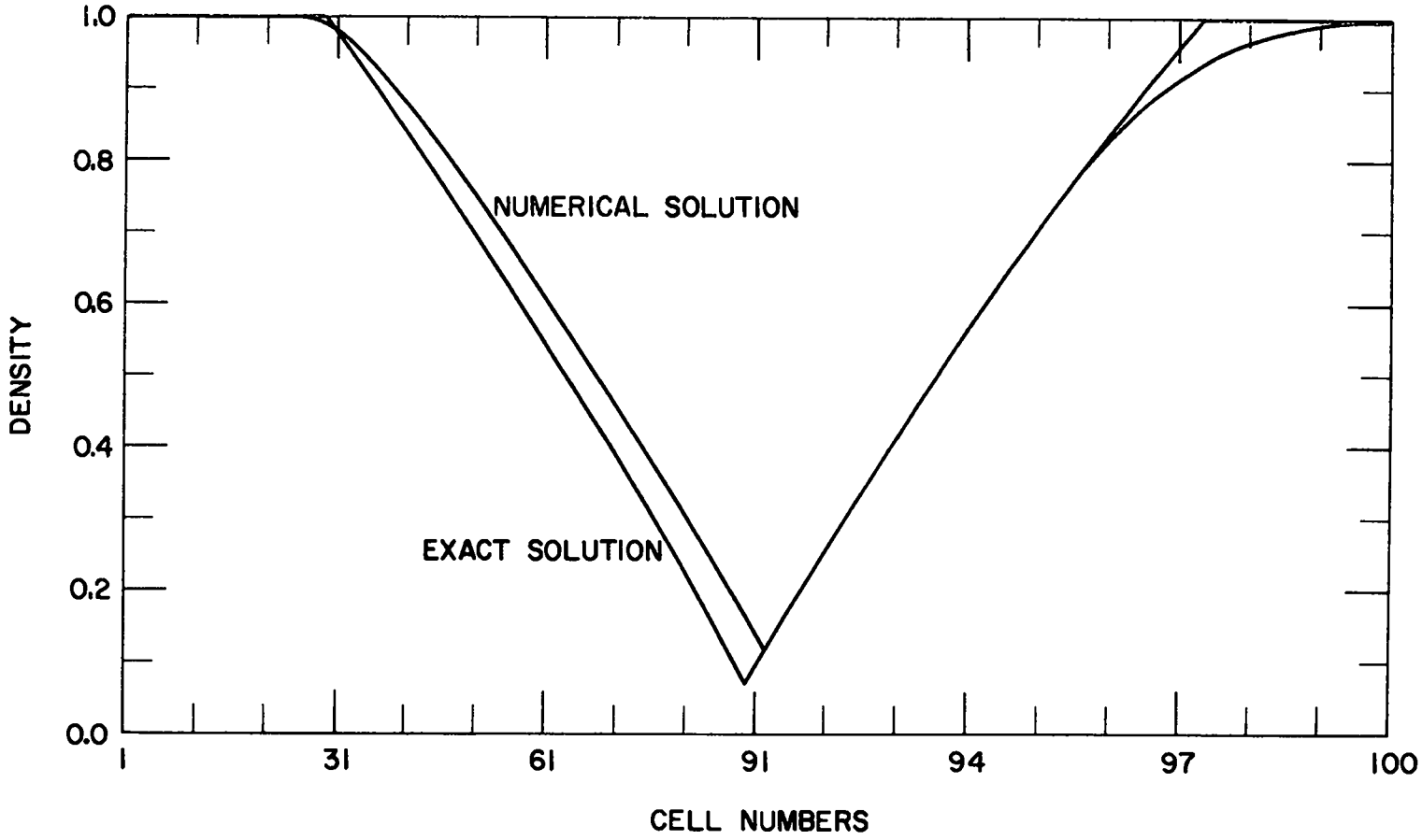

Fig. 4. Density profile for problem 2 at time t = 20.