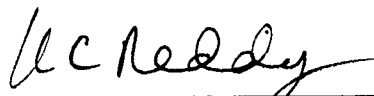


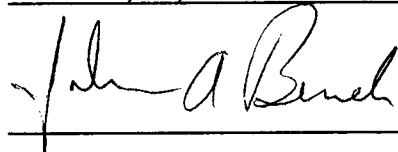
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**A LOCAL LAGRANGIAN FINITE VOLUME METHOD FOR THE
NUMERICAL SOLUTION OF CONSERVATION LAWS**

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Blair Henry Rollin

December 1992

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ABSTRACT

An analytical cell averaging approach is applied to a local Lagrangian finite volume formulation of conservation laws describing the flow of a compressible fluid. After discretization, the approach eliminates the need for pointwise evaluation of fluxes and coupled with nonoscillatory interpolating functions, yields an accurate, conservative, stable scheme. This is done without the addition of any terms not derived from a direct discretization of terms in the original conservation law and without decoupling the system into characteristic fields. The development of the scheme is motivated and documented and its viability demonstrated by application to two one-dimensional fluid flow problems.

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CHAPTER I

INTRODUCTION AND PURPOSE

The purpose of this treatise is threefold; to motivate and document the development of a new numerical method developed to solve the equations describing the flow of compressible fluids, formalize the present state of this algorithm, and demonstrate its viability by applying the algorithm to simple compressible fluid flow applications.

It should be stressed that the material presented here represents only an initial investigation of ideas that may prove useful in the future. Years of work by many skilled mathematicians, scientists and engineers is required to refine a computational algorithm to the point at which it can be applied to the complex real world flow problems being tackled routinely in laboratories across the world today.

Since late 1990, K. C. Reddy of The University of Tennessee Space Institute and the author have been developing a novel approach to solving the compressible flow equations based on a Lagrangian finite volume in space-time on fixed grids[1][2][3]. The algorithm is particularly elegant in that, unlike most popular schemes used today, it relies on no additional terms not present in the original equations to provide stability. Nor is it necessary to decouple the equations into characteristic fields. By adopting a cell averaged approach to a unique formu-

lation of the equations, great strides in accuracy and stability have been made. Indeed, the analytical formulation of the governing physical conservation laws itself stabilizes the numerical algorithm.

CHAPTER II

LAGRANGIAN FORMULATIONS

In this chapter we wish to justify the use of Lagrangian formulations of fluid flow conservation laws as the basis for numerical discretization.

The Euler equations, a coupled system of three PDE's,

$$(1) \quad \nabla \circ \langle \mathbf{E}, \mathbf{Q} \rangle = \mathbf{0}, \nabla \equiv \left\langle \frac{\partial}{\partial x}, \frac{\partial}{\partial t} \right\rangle$$

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}, \mathbf{E} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (e + p)u \end{pmatrix}, p = (\gamma - 1)(e - \rho u^2/2),$$

describe the flow of a one-dimensional inviscid perfect gas. If we assume that entropy is constant in our region of interest then it can be shown[4][5] that they, can be written as a homogeneous coupled system of two nonlinear ordinary differential equations from which it follows that

$$u + \frac{2}{\gamma - 1}c = b_1 = \text{constant} \quad \text{along} \quad \frac{dx}{dt} = u + c$$

$$u - \frac{2}{\gamma - 1}c = b_2 = \text{constant} \quad \text{along} \quad \frac{dx}{dt} = u - c$$

$$c = \left(\frac{\gamma p}{\rho} \right)^{1/2}.$$

Constant entropy implies, by definition,

$$\frac{p}{\rho^\gamma} = b_3 = \text{constant} \quad \text{along} \quad \frac{dx}{dt} = u.$$

Writing this system in terms of the primitive variables (ρ, u, p) , we see that the determinant of the Jacobian of the transformation is given by

$$\det \frac{\partial(b_1, b_2, b_3)}{\partial(\rho, u, p)} = \det \begin{pmatrix} -\frac{\gamma p}{\rho^{\gamma+1}} & 0 & \frac{1}{\rho^\gamma} \\ -\frac{(\gamma-1)}{2\rho} \left(\frac{\gamma p}{\rho}\right)^{1/2} & 1 & \frac{(\gamma-1)}{2} \left(\frac{\gamma}{\rho p}\right)^{1/2} \\ \frac{(\gamma-1)}{2\rho} \left(\frac{\gamma p}{\rho}\right)^{1/2} & 1 & -\frac{(\gamma-1)}{2} \left(\frac{\gamma}{\rho p}\right)^{1/2} \end{pmatrix}$$

$$= \frac{\gamma-1}{\rho^{\gamma+1}} \left\{ (\gamma-1) \left(\frac{\gamma p}{\rho}\right)^{1/2} \right\}.$$

We may assume that the primitive variables ρ and p never vanish. Since the Jacobian given above never vanishes, and assuming the conservation variables to be sufficiently smooth in our region of interest, we may apply the inverse function theorem which tells us the transformation is invertible. Then, with the additional hypothesis that $u \neq 0$, the determinant of the Jacobian of the transformation

$$\mathbf{F}(\rho, \rho u, e) = \begin{pmatrix} \rho \\ u \\ p \end{pmatrix}$$

given by $\frac{1}{2}\rho u^2$ never vanishes. Therefore the solution is completely specified and locally the domain of dependance of the PDE, Equation (1), is bounded by a cone with edges $\frac{dx}{dt} = u + c$ and $\frac{dx}{dt} = u - c$. So in a differential sense the domain of dependance is symmetrically located about the pathlines of the flow $\frac{dx}{dt} = u$.

Along similar lines, we may extend the domain of dependance analysis for linear systems presented by LeVeque[6]. If we linearize Equation (1) about some state indicated by the subscript o , the equation becomes

$$\mathbf{Q}_t + \frac{\partial E}{\partial \mathbf{Q}_o} \mathbf{Q}_x = \mathbf{O}.$$

The coefficient matrix of this system is diagonalizable with real distinct eigenvalues u_o , $u_o + c_o$ and $u_o - c_o$. So, if

$$\frac{\partial E}{\partial Q_o} = R_o \Lambda_o R_o^{-1}$$

then

$$Q_t + R_o \Lambda_o R_o^{-1} Q_x = O,$$

$$\Rightarrow R_o^{-1} Q_t + \Lambda_o R_o^{-1} Q_x = O,$$

$$\Rightarrow \partial_t(R_o^{-1} Q) + \Lambda_o \partial_x(R_o^{-1} Q) = O,$$

$$\Rightarrow \partial_t(V) + \Lambda_o \partial_x(V) = O,$$

$$V = R_o^{-1} Q.$$

This is a system of three decoupled linear constant coefficient advection equations, each of whose solutions is just

$$V_p(x, t) = V_p(x - \lambda_{o_p} t, 0)$$

where λ_{o_p} is the p^{th} diagonal element of Λ_o . Then the p^{th} component of the solution is just

$$\begin{aligned} Q_p(x, t) &= \sum_{i=1}^3 R_{o_p, i} V_i(x, t) = \sum_{i=1}^3 R_{o_p, i} V_i(x - \lambda_{o_i} t, 0) \\ &= \sum_{i=1}^3 R_{o_p, i} \sum_{k=1}^3 R_{o_i, k}^{-1} Q_k(x - \lambda_{o_i} t, 0). \end{aligned}$$

So $Q(x, t)$ depends only on the values of Q at the points $(x'_i, 0)$, $x'_i = x - \lambda_{o_i} t \quad \forall i$. Now assume that the initial data is smooth. If we were forced to estimate $Q(x, t)$ by choosing one value from the initial data to represent it, that value certainly must come from those whose domain is the domain of dependance of $Q(x, t)$. The only reasonable choice for smooth initial data from values at the points $(x - (u_o + c_o)t, 0)$, $(x - u_o t, 0)$, $(x - (u_o - c_o)t, 0)$, would be that value of Q at $(x - u_o t, 0)$, in center of the domain of dependance. This is Q evaluated along $\frac{dx}{dt} = u_o$. These observations make a Lagrangian formulation of the equations a natural choice for the basis of numerical discretization.

Alternatively, we may take another point of view with regards to Equation (1) which shows that a unique Lagrangian formulation transforms the system of three PDE's into a quite simplified system of three ODE's.

Let us integrate these equations over a quasi-arbitrary space-time volume V shown in Figure (1). The quasi-arbitrary nature is apparent in the following description. Let V be bounded spatially by arbitrary curves parameterized by r , say

$$\tau_L = x_L(r)\hat{i} + t_L(r)\hat{j}, \quad \tau_R = x_R(r)\hat{i} + t_R(r)\hat{j}$$

where the subscripts R and L refer to right and left respectively, with the stipulations that $t_{L,R}$ increase with the parameter and $\tau_{L,R}$ do not intersect, and bounded temporally by straight lines connecting τ_L and τ_R at r and $r + \Delta r$.

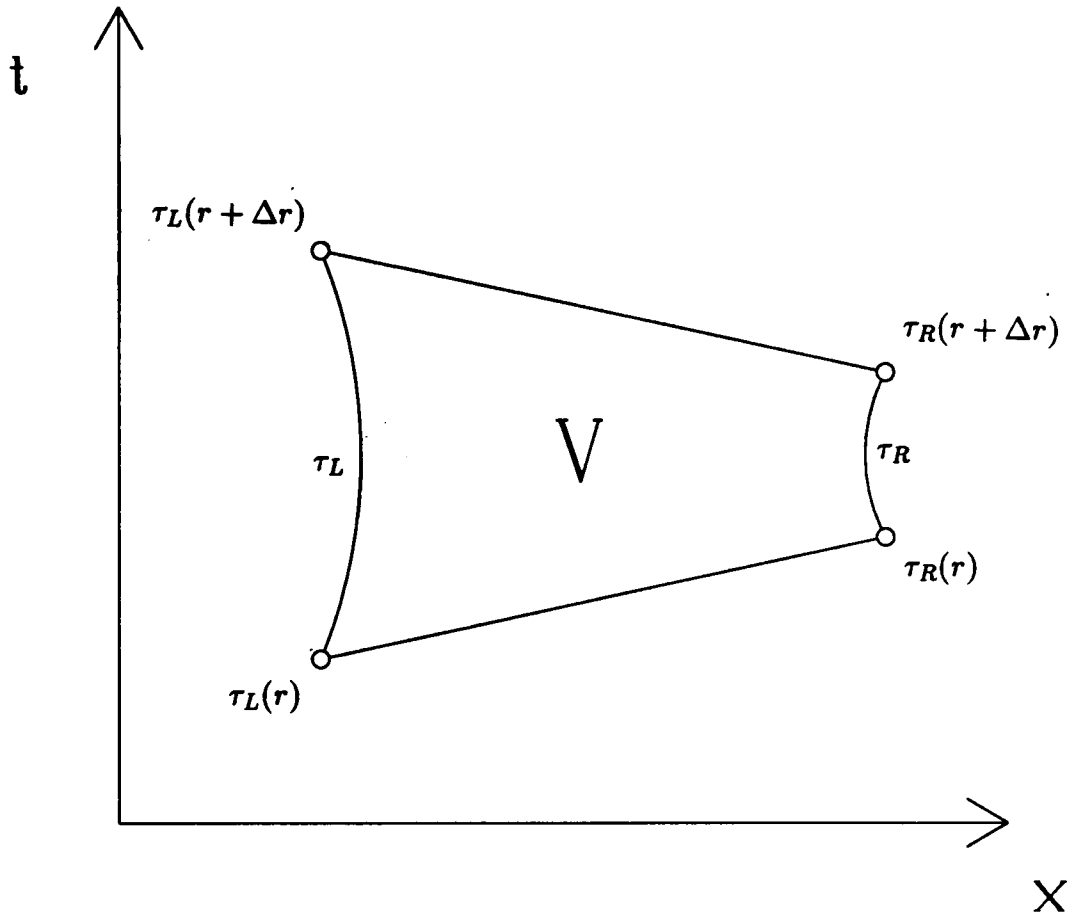


Figure 1. A quasi-arbitrary volume in space-time.

Define

$$\Delta x(\alpha) = x_R(\alpha) - x_L(\alpha)$$

$$\Delta t(\alpha) = t_R(\alpha) - t_L(\alpha)$$

$$m(\alpha) = \frac{\Delta t(\alpha)}{\Delta x(\alpha)}.$$

Integrating

$$\nabla \circ \langle \mathbf{E}, \mathbf{Q} \rangle = \mathbf{O}, \quad \nabla \equiv \left\langle \frac{\partial}{\partial x}, \frac{\partial}{\partial t} \right\rangle$$

over V yields

$$\oint_{\partial V} \langle \mathbf{E}, \mathbf{Q} \rangle \circ \mathbf{n} ds = \mathbf{O}.$$

Defining $'$ to indicate differentiation with respect to the parameter, $\mathbf{n}$ is such that $\mathbf{n} \circ \tau'_{R,L} = \mathbf{O}$, $\|\mathbf{n}\| = 1$, and has outward orientation along $\tau_{L,R}$, and is constant with outward orientation along the top and bottom edges of V . Along

$\tau_{L,R}$,

$$\mathbf{n} = \begin{cases} \frac{\langle -t'_L, x'_L \rangle}{\|\langle -t'_L, x'_L \rangle\|} & \text{along } \tau_L \\ \frac{\langle t'_R, -x'_R \rangle}{\|\langle t'_R, -x'_R \rangle\|} & \text{along } \tau_R \end{cases}$$

and

$$ds^2 = dx^2 + dt^2 = \frac{dx^2}{dr^2} dr^2 + \frac{dt^2}{dr^2} dr^2$$

$$\Rightarrow ds = (x'^2_{L,R} + t'^2_{L,R})^{1/2} dr.$$

So

$$\mathbf{n} ds = \begin{cases} \langle -t'_L, x'_L \rangle dr & \text{along } \tau_L \\ \langle t'_R, -x'_R \rangle dr & \text{along } \tau_R. \end{cases}$$

At the top and bottom of V ,

$$\mathbf{n} = \begin{cases} \frac{\langle -\Delta t(r+\Delta r), \Delta x(r+\Delta r) \rangle}{\|\langle -\Delta t(r+\Delta r), \Delta x(r+\Delta r) \rangle\|} & \text{top} \\ \frac{\langle \Delta t(r), -\Delta x(r) \rangle}{\|\langle \Delta t(r), -\Delta x(r) \rangle\|} & \text{bottom} \end{cases}$$

and

$$ds^2 = dx^2 + dt^2 = dx^2 + \left(\frac{dt}{dx}\right)^2 dx^2 = \left(1 + \left(\frac{\Delta t}{\Delta x}\right)^2\right) dx^2$$

$$\Rightarrow ds = (\Delta x^2 + \Delta t^2)^{1/2} \frac{dx}{\Delta x}$$

where the arguments of Δx and Δt have been omitted for convenience. So

$$\begin{aligned} nds &= \begin{cases} \langle -\frac{\Delta t(r + \Delta r)}{\Delta x(r + \Delta r)}, 1 \rangle dx & \text{top} \\ \langle \frac{\Delta t(r)}{\Delta x(r)}, -1 \rangle dx & \text{bottom} \end{cases} \\ &= \begin{cases} \langle -m(r + \Delta r), 1 \rangle dx & \text{top} \\ \langle m(r), -1 \rangle dx & \text{bottom.} \end{cases} \end{aligned}$$

Now our surface integral expansion is given by

$$\begin{aligned} \oint_{\partial V} \langle \mathbf{E}, \mathbf{Q} \rangle \circ nds &= O = \\ \int_{x_L(r+\Delta r)}^{x_R(r+\Delta r)} \langle \mathbf{E}, \mathbf{Q} \rangle \circ \langle -m(r + \Delta r), 1 \rangle dx &- \int_{x_L(r)}^{x_R(r)} \langle \mathbf{E}, \mathbf{Q} \rangle \circ \langle -m(r), 1 \rangle dx + \\ \int_r^{r+\Delta r} \langle \mathbf{E}, \mathbf{Q} \rangle_R \circ \langle t'_R, -x'_R \rangle(\bar{r}) d\bar{r} &+ \int_r^{r+\Delta r} \langle \mathbf{E}, \mathbf{Q} \rangle_L \circ \langle -t'_L, x'_L \rangle(\bar{r}) d\bar{r} = \\ \int_{x_L(r+\Delta r)}^{x_R(r+\Delta r)} (\mathbf{Q} - m(r + \Delta r)\mathbf{E}) dx &- \int_{x_L(r)}^{x_R(r)} (\mathbf{Q} - m(r)\mathbf{E}) dx + \\ (-\mathbf{Q}x' + \mathbf{E}t')_R(r_R)\Delta r &- (-\mathbf{Q}x' + \mathbf{E}t')_L(r_L)\Delta r = O \end{aligned}$$

where $r_{R,L}$ are in $(r, r + \Delta r)$ and given by the mean value theorem. Dividing

the above equation by Δr we have

$$\begin{aligned} &\frac{\int_{x_L(r+\Delta r)}^{x_R(r+\Delta r)} (\mathbf{Q} - m(r + \Delta r)\mathbf{E}) dx - \int_{x_L(r)}^{x_R(r)} (\mathbf{Q} - m(r)\mathbf{E}) dx}{\Delta r} + \\ &(-\mathbf{Q}x' + \mathbf{E}t')_R(r_R) - (-\mathbf{Q}x' + \mathbf{E}t')_L(r_L) = O. \end{aligned}$$

As $\Delta r \rightarrow 0$, $r_{R,L} \rightarrow r$, so

$$\lim_{\Delta r \rightarrow 0} \frac{\int_{x_L(r+\Delta r)}^{x_R(r+\Delta r)} (\mathbf{Q} - m(r + \Delta r)\mathbf{E}) dx - \int_{x_L(r)}^{x_R(r)} (\mathbf{Q} - m(r)\mathbf{E}) dx}{\Delta r} +$$

$$\lim_{\Delta r \rightarrow 0} (-\mathbf{Q}x' + \mathbf{E}t')_R(r_R) - (-\mathbf{Q}x' + \mathbf{E}t')_L(r_L) =$$

$$(2) \quad \frac{d}{dr} \int_{x_L(r)}^{x_R(r)} (\mathbf{Q} - m(r)\mathbf{E})dx + \\ (-\mathbf{Q}x' + \mathbf{E}t')_R(r) - (-\mathbf{Q}x' + \mathbf{E}t')_L(r) = \mathbf{O}.$$

We have transformed the original system of PDE's to one of ODE's.

Now let us examine this equation.

$$\frac{d}{dr} \int_{x_L(r)}^{x_R(r)} (\mathbf{Q} - m(r)\mathbf{E})dx + \\ \begin{pmatrix} \rho(ut' - x') \\ \rho u(ut' - x') + pt' \\ e(ut' - x') + put' \end{pmatrix}_R (r) - \begin{pmatrix} \rho(ut' - x') \\ \rho u(ut' - x') + pt' \\ e(ut' - x') + put' \end{pmatrix}_L (r) = \mathbf{O}.$$

We wish to solve the resulting form of this equation numerically. Thus the equation should be readily discretizable and have as simple a form as possible. To simplify the equation we might hope that $m(r) = 0$ and $x' = ut'$. If the system is to be discretized in time we certainly must have $t_R(r) = t_L(r), \forall r$. The choice $r = t$ and $t_R = t_L = t$ satisfies this requirement for discretization and $\Delta t(r) = 0 \Rightarrow m(r) = 0$. Moreover, if $\frac{dx}{dt} = u$ at both R and L then $x' = ut'$ simplifying the equations just as we had hoped.

Therefore, by performing a volume integration in a Lagrangian context we have simplified Equation (1) considerably. We have

$$(3) \quad \frac{d}{dt} \int_{x_L(t)}^{x_R(t)} \mathbf{Q}(x, t)dx + \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix}_R (t) - \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix}_L (t) = \mathbf{O}$$

where x_R and x_L satisfy $\frac{dx_{R,L}}{dt} = u(x_{R,L}(t), t)$, as a reformulation of Equation (1).

Integrating this equation in time from time t to $t + \Delta t$ we see that the path-lines described by $\frac{dx_{R,L}}{dt} = u(x_{R,L}(t), t)$ define our volume V which will hereafter be referred to as a local Lagrangian finite volume (LLFV), or Lagrangian finite volume. The corresponding integral form of Equation (3) is

$$(4) \quad \int_{x_L(t+\Delta t)}^{x_R(t+\Delta t)} Q(x, t + \Delta t) dx - \int_{x_L(t)}^{x_R(t)} Q(x, t) dx + \int_t^{t+\Delta t} F_R(s) ds - \int_t^{t+\Delta t} F_L(s) ds = O,$$

with

$$(5) \quad \mathbf{F} = -Q\mathbf{u} + \mathbf{E} = \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix}.$$

We may include a source term to the equation in the following manner. For

$$(6) \quad Q_t + E_x = S,$$

we have

$$\frac{\partial}{\partial t} Q + \frac{\partial}{\partial x} (E - \int_{x_0}^x S(\eta, t) d\eta) = O,$$

where x_0 is some fixed point in our domain. Now integrate this equation over a Lagrangian finite volume from times t to $t + \Delta t$. The new term

$$- \int_t^{t+\Delta t} \int_{x_0}^{x_R(s)} S(x, s) dx ds + \int_t^{t+\Delta t} \int_{x_0}^{x_L(s)} S(x, s) dx ds$$

will be included in our surface integral expansion, Equation (4). Then move this term to the right hand side of Equation (4).

Alternatively, leave the source term on the right hand side of Equation (6). Integrate both sides over our Lagrangian finite volume. In either case, the right side of our new equation is given by

$$\int_t^{t+\Delta t} \int_{x_L(s)}^{x_R(s)} S(x, s) dx ds.$$

Thus the equation including the source term corresponding to Equation (4) is

$$(7) \quad \int_{x_L(t+\Delta t)}^{x_R(t+\Delta t)} Q(x, t + \Delta t) dx - \int_{x_L(t)}^{x_R(t)} Q(x, t) dx + \\ \int_t^{t+\Delta t} F_R(s) ds - \int_t^{t+\Delta t} F_L(s) ds = \int_t^{t+\Delta t} \int_{x_L(s)}^{x_R(s)} S(x, s) dx ds.$$

Dividing the new term by Δt ,

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_t^{t+\Delta t} \int_{x_L(s)}^{x_R(s)} S(x, s) dx ds = \\ \lim_{\Delta t \rightarrow 0} \frac{\frac{\partial}{\partial \Delta t} \int_t^{t+\Delta t} \int_{x_L(s)}^{x_R(s)} S(x, s) dx ds}{\frac{\partial}{\partial \Delta t} \Delta t} = \\ \int_{x_L(t)}^{x_R(t)} S(x, t) dx.$$

In this way we see that the equation corresponding to Equation (3) including the source term is

$$(8) \quad \frac{d}{dt} \int_{x_L(t)}^{x_R(t)} Q(x, t) dx + \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix}_R (t) - \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix}_L (t) = \int_{x_L(t)}^{x_R(t)} S(x, t) dx.$$

CHAPTER III

A LAGRANGIAN FINITE VOLUME FORMULATION FOR THE EULER EQUATIONS

3.1 A Basis for Discretization

Referring again to the one-dimensional Euler equations, Equation (1), we wish to integrate these equations on a fixed, uniform, space-time grid over cells that are bounded by particle paths and by time levels n and $n+1$ as shown in Figure (2).

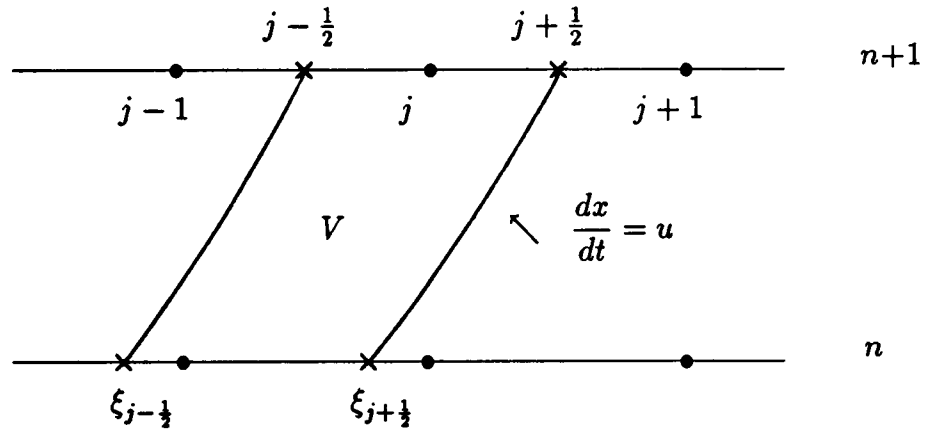


Figure 2. A Lagrangian finite volume in space-time centered at node x_j .

Define

$$h = x_{j+1/2} - x_{j-1/2}, \quad \Delta t = t^{n+1} - t^n$$

and $x_{R,L}$ the solutions to the differential equation

$$\frac{dx}{dt} = u, \quad \text{with} \quad x_{R,L}(t^{n+1}) = x_{j\pm 1/2}.$$

Integrating backward in time we define

$$(9) \quad \xi_{j\pm 1/2} = x_{R,L}(t^n).$$

Now we write Equation (4) making explicit the dependance on x_j as

$$(10) \quad \int_{x_{j-1/2}}^{x_{j+1/2}} Q(x, t^{n+1}) dx - \int_{\xi_{j-1/2}(x_j)}^{\xi_{j+1/2}(x_j)} Q(x, t^n) dx + \\ \int_{t^n}^{t^{n+1}} F(x_R(t), t) dt - \int_{t^n}^{t^{n+1}} F(x_L(t), t) dt = O,$$

where F is defined by Equation (5).

3.2 Discretization in Time

From the definition of $x_{R,L}$

$$\int_{t^n}^{t^{n+1}} x'_{R,L} dt = \int_{t^n}^{t^{n+1}} u(x_{R,L}(t), t) dt \\ \Rightarrow \quad \xi_{j\pm 1/2} = x_{j\pm 1/2} - \int_{t^n}^{t^{n+1}} u(x_{R,L}(t), t) dt.$$

Approximating the integral on the right by the trapezoidal rule yields

$$(11) \quad \xi_{j\pm 1/2} = x_{j\pm 1/2} - \bar{u}_{j\pm 1/2} \Delta t,$$

$$\bar{u}_{j\pm 1/2} = (u_{j\pm 1/2}^{n+1} + u(\xi_{j\pm 1/2}, t^n))/2.$$

With this approximation we are assuming the characteristics $x_{R,L}$ to be straight lines of slope $\frac{dx}{dt} = \bar{u}_{j\pm 1/2}$. Integrating the second two terms in Equation (10) similarly, we have,

$$(12) \quad \int_{x_{j-1/2}}^{x_{j+1/2}} Q(x, t^{n+1}) dx - \int_{\xi_{j-1/2}(x_j)}^{\xi_{j+1/2}(x_j)} Q(x, t^n) dx + \bar{F}_{j+1/2} \Delta t - \bar{F}_{j-1/2} \Delta t = O,$$

where

$$\bar{F}_{j\pm 1/2} = (F_{j\pm 1/2}^{n+1} + F(\xi_{j\pm 1/2}, t^n))/2,$$

and again the so called flux vector F is defined by Equation (5).

3.3 Conservative Differencing

To preserve global conservation properties in space, regardless of how we evaluate $Q(x_{j\pm\frac{1}{2}}, t^{n+1})$ and $Q(\xi_{j\pm\frac{1}{2}}, t^n)$, we perform the evaluation consistently on each cell at any given time step. In terms of conservation, this leaves a great deal of flexibility in the method of evaluation. For example, we could use linear interpolation between the nodes to evaluate $Q(x_{j\pm\frac{1}{2}}, t^{n+1})$ and cubic interpolation to evaluate $Q(\xi_{j\pm\frac{1}{2}}, t^n)$. Conservation dictates that we evaluate $Q(x_{j\pm\frac{1}{2}}, t^{n+1})$ and $Q(\xi_{j\pm\frac{1}{2}}, t^n)$ the same way on the j^{th} and $j \pm 1^{st}$ cells.

To preserve conservation in time, at any time level t^n we fix an approximating function for Q and use it for all integrations. The solution at time t^n is integrated twice, once at the top of the cells at time step n , and once at the bottom of the cells at time step $n + 1$. If we assume that $Q(x, t^n)$ is a piecewise constant function with value $Q(x_j, t^n)$ in $(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$ at time step n (when $Q(x, t^n)$ is at the top of the cells), we may integrate it exactly. If we then assume that $Q(x, t^n)$ is a piecewise linear continuous function between the nodes at time step $n + 1$ (when $Q(x, t^n)$ is at the bottom of the cells), and integrate this by the trapezoidal rule we are left with a scheme that is not conservative in time and consequently, does not capture shock speeds correctly. This is due to the nonlinearity of the equations. This method will be conservative in time if the trapezoidal integration is performed at uniformly spaced locations separated by h . This is simply because both methods of integration produce the same result

in this case as is seen by the following demonstration. In particular this occurs when $\frac{dx}{dt} = \text{constant}$.

Consider a discrete function $\{q_j\}$ with domain all of $\mathcal{R}$, that vanishes outside a bounded interval. Interpreting the function to be piecewise constant within each cell $(x_{j-1/2}, x_{j+1/2})$,

$$\int_{\mathcal{R}} q dx = \sum_{j=-\infty}^{\infty} q_j h.$$

Next assume the function to be piecewise linear with values $\{q_j\}$ given at the nodes and use the trapezoidal rule to integrate the function over the points $\{\xi_{j+1/2}\}$, where we will use the convention that $\xi_{j+1/2}$ is in the interval $[x_j, x_{j+1})$. The interpolated values are given by

$$y_i = \frac{q_{i+1} - q_i}{h} (\xi_{i+1/2} - x_{i+1}) + q_{i+1}.$$

So the trapezoidal rule gives

$$\begin{aligned} \int_{\mathcal{R}} q dx &= \sum_{j=-\infty}^{\infty} (y_{j-1} + y_j) \frac{h}{2} = \frac{1}{2} \sum_{j=-\infty}^{\infty} [(q_j - q_{j-1})(\xi_{j-1/2} - x_j) + q_j h + \\ &\quad (q_{j+1} - q_j)(\xi_{j+1/2} - x_{j+1}) + q_{j+1} h] \\ &= \frac{1}{2} \sum_{j=-\infty}^{\infty} [(q_{j+1} - q_{j-1})(\xi_{j+1/2} - x_{j+1}) + (q_j + q_{j+1})h] \\ &= \frac{1}{2} \sum_{j=-\infty}^{\infty} q_j h + \frac{1}{2} \sum_{j=-\infty}^{\infty} q_{j+1} h = \sum_{j=-\infty}^{\infty} q_j h. \end{aligned}$$

The important observation necessary to obtain this result is that the locations at which the interpolation is performed are evenly spaced so that $\xi_{j+1/2} - \xi_{j-1/2} = h = x_j - x_{j-1} \quad \forall j$, which implies equality of the coefficients in our sum.

As stated previously, for nonlinear problems however, this will not be the case. The distance between adjacent ξ locations will vary with u and in general, will not be constant.

We do, however, have the freedom to use different approximating functions at different time levels provided that the approximating function is fixed with respect to the x -grid and the type of approximating function used remains fixed for all evaluations.

With these rules in mind, when the cells abut in time and space, no numerical sources will appear and the scheme will be globally conservative. We also observe that we may use different approximating functions for integration than those used to interpolate the fluxes and the scheme will remain conservative.

3.4 The Scalar Wave Equation

Let us consider a simple case temporarily and observe some results from this scheme applied to the scalar one-way wave equation.

We wish to solve the linear wave equation

$$(13) \quad \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad a = \text{constant}.$$

The exact solution being $u_0(x - at)$ where $u_0(x)$ is the initial condition, we observe that the initial profile just moves along with velocity a . The characteristics $\frac{dx}{dt} = a$ form the boundary of our volume of integration between times t^{n+1} and t^n . Heuristically, we may think of a fluid of density u moving with constant speed a and form our volume of integration in the $x - t$ plane as shown in Figure (3).

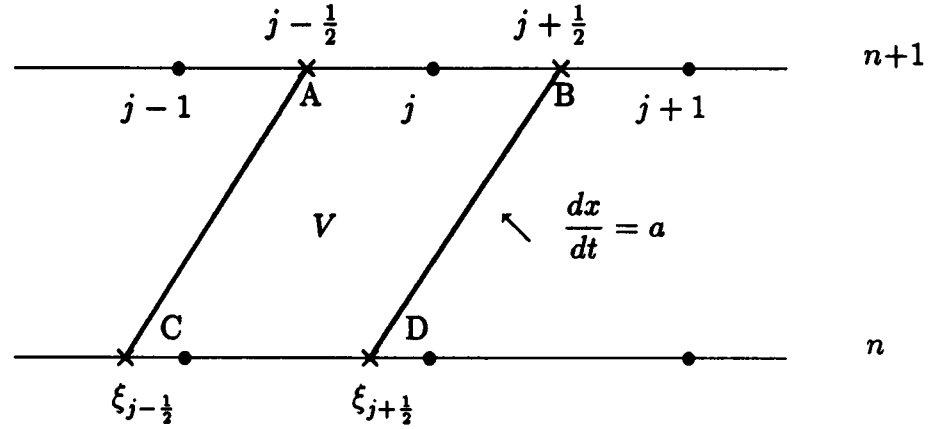


Figure 3. A Lagrangian finite volume for the scalar wave equation.

Rewriting equation (13) as

$$\nabla \circ \langle au, u \rangle = 0, \nabla \equiv \left\langle \frac{\partial}{\partial x}, \frac{\partial}{\partial t} \right\rangle$$

we have $\int_V \nabla \circ \langle au, u \rangle dV = 0$, or

$$(14) \quad \oint_{\partial V} \langle u, au \rangle \circ \mathbf{n} ds = 0.$$

The surface integral is to be performed about V . Thus $\mathbf{n} ds$ about ∂V is given by

$$\mathbf{n} ds = \begin{cases} \langle 0, 1 \rangle dx & \text{along A B} \\ \langle 1, -a \rangle dt & \text{along D B} \\ \langle 0, -1 \rangle dx & \text{along C D} \\ \langle -1, a \rangle dt & \text{along C A.} \end{cases}$$

Thus Equation (14) yields

$$\int_{x_{j-1/2}}^{x_{j+1/2}} u^{n+1} dx + \int_{\xi_{j+1/2}}^{x_{j+1/2}} (au - au) dt + \int_{\xi_{j-1/2}}^{x_{j-1/2}} (-au + au) dt - \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx = 0,$$

or

$$(15) \quad \int_{x_{j-1/2}}^{x_{j+1/2}} u^{n+1} dx = \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx,$$

with $\xi_{j\pm 1/2}$ given by

$$\xi_{j\pm 1/2} = x_{j\pm 1/2} - a\Delta t.$$

Alternatively, we can arrive at this result in a simpler manner. Observe that for Equation (13), Equation (1) is a scalar equation with $Q = u$ and $E = au$. Again choosing $t = r$ yields $t'_{R,L} = 1$. Then, if $x' = at'$, our result is the first component of Equation (3). An integration in time gives Equation (15).

Let us define some terms that will facilitate our analysis of the scheme.

Let $\{U_j\}$ and $\{V_j\}$ be two discrete grid functions generated by a method of the form

$$(16) \quad U_j^{n+1} = L(U_j^n)$$

where L is a linear operator.

If

$$V_j^n \geq U_j^n \quad \forall j \quad \Rightarrow \quad V_j^{n+1} \geq U_j^{n+1} \quad \forall j$$

then the method is said to be monotone.

Define the l_1 -norm of a discrete function as

$$\|U\|_1 = h \sum_{j=-\infty}^{\infty} |U_j|$$

where we assume that $\{U_j\}$ vanishes outside of some bounded set. If $\{U_j\}$ and $\{V_j\}$ are any such functions then so is $\{(U - V)_j\}$. The method is said to be l_1 -contracting if

$$\|U^{n+1} - V^{n+1}\|_1 \leq \|U^n - V^n\|_1$$

for any such functions.

The total variation of a discrete function $\{U_j^n\}$ is defined to be

$$TV(U^n) = \sum_{j=-\infty}^{\infty} |U_{j+1}^n - U_j^n|.$$

The method given by Equation (16) is said to be total variation diminishing or *TVD* if

$$TV(U^{n+1}) \leq TV(U^n).$$

For the time being let us assume that the approximating functions on which we are to perform the integration are piecewise constant within each fixed grid cell. Then we have the following result.

The method given by Equation (15) is TVD on the scalar equation , Equation (19).

To establish the result suppose U_j^n and V_j^n are grid functions with the following property,

$$U_j^n \leq V_j^n \quad \forall j.$$

Then

$$U_j^{n+1} = \frac{1}{h} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} U^n dx \leq \frac{1}{h} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} V^n dx = V_j^{n+1} \quad \forall j.$$

Therefore, the method given by Equation (15) with piecewise constant approximations in each fixed grid cell is a monotone method. Combining this with the results[6] that

$$\text{monotone} \quad \Rightarrow \quad l_1\text{-contracting} \quad \Rightarrow \quad TVD$$

substantiates the claim.

Another consequence[6] of monotonicity is that

A monotone method is at most first order accurate.

Therefore, the method described above is at most first order accurate for arbitrary CN , where CN is the Courant-Friedrichs-Lewy number or Courant number, $CN = \frac{a\Delta t}{\Delta x}$.

We now establish another result. We introduce the notational index m such that $x_m \leq \xi_{j+1/2} \leq x_{m+1}$. For the first case assume that $\xi_{j+1/2} \leq x_{m+1/2}$. Then the method is given by

$$\begin{aligned} u_j^{n+1} &= \frac{1}{h} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx = \\ \frac{1}{h} [h - (a\Delta t - (j - m)h)] u_m^n + [a\Delta t - (j - m)h] u_{m-1}^n &= \\ [1 - (CN - (j - m))] u_m^n + [CN - (j - m)] u_{m-1}^n, \end{aligned}$$

Since $\xi_{j+1/2} \leq x_{m+1/2}$ it follows that

$$\begin{aligned} 1 > \frac{1}{2} &\geq [(a\Delta t - (j - m)h) \frac{1}{h}] \geq 0 \\ \Rightarrow \quad 1 > CN - (j - m) &\geq 0 \end{aligned}$$

and

$$CN - (j - m) = 0 \quad \text{iff} \quad CN \in \mathcal{Z}.$$

For a sinusoidal wave mode the method (15) has form

$$\begin{aligned} V_\alpha^{n+1} e^{ij\xi} &= V_\alpha^n e^{i(m-1)\xi} [a\Delta t - (j - m)h] \frac{1}{h} + \\ V_\alpha^n e^{im\xi} [h - (a\Delta t - (j - m)h)] \frac{1}{h}. \end{aligned}$$

$$\Rightarrow \quad \frac{V_{\alpha}^{n+1}}{V_{\alpha}^n} = e^{i(m-j)\xi} [e^{-i\xi}(CN - (j - m)) + (1 - (CN - (j - m)))].$$

Let C be the parameter defined by $C = CN - (j - m)$. Then C obeys the inequality $1 > C \geq 0$ and vanishes only for $CN \in \mathcal{Z}$.

$$\begin{aligned} \left| \frac{V_{\alpha}^{n+1}}{V_{\alpha}^n} \right|^2 &= |e^{i(m-j)\xi}|^2 |e^{-i\xi}C + (1 - C)|^2 \\ &= 1 - 4C(1 - C)\sin^2 \xi/2. \end{aligned}$$

Since $1 > C \geq 0$,

$$\Rightarrow \quad 4C(1 - C) \geq 0 \quad \text{and} \quad \left| \frac{V_{\alpha}^{n+1}}{V_{\alpha}^n} \right|^2 \leq 1,$$

the equality holds *iff* $CN \in \mathcal{Z}$.

The case $x_{m+1/2} \leq \xi_{j+1/2}$ goes entirely similarly and produces the same amplification factor with the same conditions on C . We have demonstrated the following.

The method given by Equation (15) with piecewise constant approximating functions on the fixed grid is unconditionally stable on Equation (13). Moreover, it is dissipative of order two for noninteger CN and nondissipative for $CN \in \mathcal{Z}$.

The next result is a product of the following truncation error analysis. It extends the previous results.

The method given by Equation (15) with piecewise constant solution on the fixed grid is consistent with Equation (13) and truncation error is of order h for $CN < 1$. The leading error term is of a diffusive nature. For $CN = 1$, however, truncation error is of order h^2 and it is not diffusive.

We will assume that $a > 0$, $CN \leq 1$ and expand the function u in a Taylor series about u^* , the function evaluated in the center of the cell at the point $(x_j - \frac{a\Delta t}{2}, t^{n+1/2})$.

Define

$$\begin{aligned} L_h[u_h] &= \frac{1}{h\Delta t} \{u_j^{n+1}h - \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx\} \\ &= \frac{1}{h\Delta t} \{u_j^{n+1}h - a\Delta t u_{j-1}^n - (h - a\Delta t)u_j^n\}, \end{aligned}$$

and

$$L[u] = u_t + au_x = 0.$$

Then

$$\begin{aligned} u_j^{n+1} &= u^* + \frac{\Delta t}{2} u_t^* + \frac{a\Delta t}{2} u_x^* + \\ &\quad \frac{\Delta t^2}{8} u_{tt}^* + \frac{a\Delta t^2}{4} u_{tx}^* + \frac{a^2\Delta t^2}{8} u_{xx}^* + \mathcal{O}(h^3), \\ u_j^n &= u^* - \frac{\Delta t}{2} u_t^* + \frac{a\Delta t}{2} u_x^* + \\ &\quad \frac{\Delta t^2}{8} u_{tt}^* - \frac{a\Delta t^2}{4} u_{tx}^* + \frac{a^2\Delta t^2}{8} u_{xx}^* + \mathcal{O}(h^3), \\ u_{j-1}^n &= u^* - \frac{\Delta t}{2} u_t^* - (h - \frac{a\Delta t}{2}) u_x^* + \\ &\quad \frac{\Delta t^2}{8} u_{tt}^* + \frac{\Delta t}{2} (h - \frac{a\Delta t}{2}) u_{tx}^* + \frac{1}{2} (h - \frac{a\Delta t}{2})^2 u_{xx}^* + \mathcal{O}(h^3). \end{aligned}$$

So

$$\begin{aligned} L_h[u_h] &= (u_t^* + au_x^*) + \frac{1}{2}(a^2\Delta t - ah)u_{xx}^* + \mathcal{O}(h^2) \\ &= (u_t^* + au_x^*) + \frac{a}{2}(a\Delta t - h)u_{xx}^* + \mathcal{O}(h^2). \end{aligned}$$

Thus

$$L_h[u_h] = L[u^*] + \frac{a}{2}(a\Delta t - h)u_{xx}^* + \mathcal{O}(h^2),$$

and for $CN = 1$, $a\Delta t = h$. This establishes the claim.

If $CN \leq 1$ it is easily seen that the method given by Equation (15) is just the familiar first order upwind method. With this observation none of these results are surprising.

We may increase accuracy to $\mathcal{O}(h^2)$, if a piecewise linear continuous approximations are chosen for integration purposes. This is seen by the following demonstration.

We add to our list of Taylor series representations the equations given below.

$$\begin{aligned}
 u_{j+1}^{n+1} &= u^* + \frac{\Delta t}{2} u_t^* + \left(h + \frac{a\Delta t}{2}\right) u_x^* + \\
 &\quad \frac{\Delta t^2}{8} u_{tt}^* + \frac{\Delta t}{2} \left(h + \frac{a\Delta t}{2}\right) u_{tx}^* + \frac{1}{2} \left(h + \frac{a\Delta t}{2}\right)^2 u_{xx}^* + \mathcal{O}(h^3), \\
 u_{j-1}^{n+1} &= u^* + \frac{\Delta t}{2} u_t^* - \left(h - \frac{a\Delta t}{2}\right) u_x^* + \\
 &\quad \frac{\Delta t^2}{8} u_{tt}^* - \frac{\Delta t}{2} \left(h - \frac{a\Delta t}{2}\right) u_{tx}^* + \frac{1}{2} \left(h - \frac{a\Delta t}{2}\right)^2 u_{xx}^* + \mathcal{O}(h^3), \\
 u_{j+1}^n &= u^* - \frac{\Delta t}{2} u_t^* - \left(h + \frac{a\Delta t}{2}\right) u_x^* + \\
 &\quad \frac{\Delta t^2}{8} u_{tt}^* - \frac{\Delta t}{2} \left(h + \frac{a\Delta t}{2}\right) u_{tx}^* + \frac{1}{2} \left(h + \frac{a\Delta t}{2}\right)^2 u_{xx}^* + \mathcal{O}(h^3).
 \end{aligned}$$

Since

$$\int_{x_{j-1/2}}^{x_{j+1/2}} u^{n+1} = \frac{3h}{4} u_j^{n+1} + \frac{h}{8} u_{j-1}^{n+1} + \frac{h}{8} u_{j+1}^{n+1}$$

for a piecewise linear approximation, define our operator

$$L_h[u_h] = \frac{1}{h\Delta t} \left\{ \frac{3h}{4} u_j^{n+1} + \frac{h}{8} u_{j-1}^{n+1} + \frac{h}{8} u_{j+1}^{n+1} - \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx \right\}.$$

For simplicity assume that $CN \leq \frac{1}{2}$. Then $\xi_{j+1/2} \in [x_j, x_{j+1}]$ and $\xi_{j-1/2} \in [x_{j-1}, x_j]$. So the interpolated values based on piecewise linear approximations at the ξ locations are given by

$$u(\xi_{j+1/2}, t^n) = (u_{j+1}^n - u_j^n) \left(\frac{1}{2} - CN \right) + u_j^n,$$

$$u(\xi_{j-1/2}, t^n) = (u_{j-1}^n - u_j^n)\left(\frac{1}{2} + CN\right) + u_j^n,$$

and the integral above is given by

$$\int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u^n dx = \frac{1}{2}(u_j^n + u(\xi_{j-1/2}, t^n))\left(\frac{h}{2} + a\Delta t\right) + \frac{1}{2}(u_j^n + u(\xi_{j+1/2}, t^n))\left(\frac{h}{2} - a\Delta t\right).$$

Therefore, after some manipulation,

$$L_h[u_h] = k_1 u_j^{n+1} + k_2 u_{j+1}^{n+1} + k_2 u_{j-1}^{n+1} + k_3 u_j^n + k_4 u_{j-1}^n + k_5 u_{j+1}^n,$$

where the constants are given by

$$\begin{aligned} k_1 &= \frac{3}{4\Delta t}, \\ k_2 &= \frac{1}{8\Delta t}, \\ k_3 &= -\frac{1}{2\Delta t}\left[\left(\frac{1}{2} + CN\right)\left(1 + \left(\frac{1}{2} - CN\right)\right) + \left(\frac{1}{2} - CN\right)\left(1 + \left(\frac{1}{2} + CN\right)\right)\right], \\ k_4 &= -\frac{1}{2\Delta t}\left(\frac{1}{2} + CN\right)^2, \\ k_5 &= -\frac{1}{2\Delta t}\left(\frac{1}{2} - CN\right)^2. \end{aligned}$$

Now, carrying out the arithmetic it is easy to show that

$$L_h[u_h] = L[u^*] + \mathcal{O}(h^2).$$

3.5 Results

These analytical results are demonstrated numerically for a test problem. First we solve the scalar wave equation by the numerical scheme of Equation (15) with initial conditions $u(x, 0) = \sin(4x)$ and a simulation of infinite domain.

Figures (4) and (5) show the results of the method given by Equation (15) with piecewise constant approximating functions applied to Equation (13). Figure (4) shows the results with 100 spatial grid points over 5 unit lengths at Courant number 5.5 after 20 time steps.

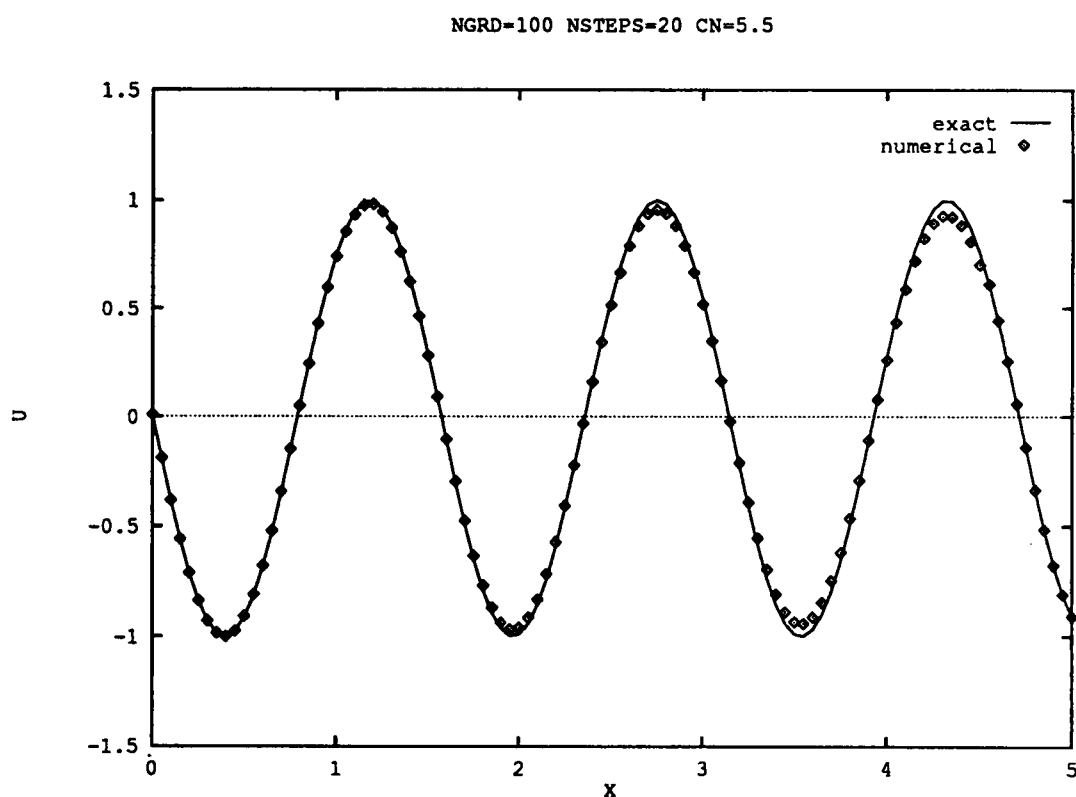


Figure 4. Results using piecewise constant approximating functions with $CN=5.5$ after 20 time steps and sinusoidal initial conditions.

Figure (5) shows the results on the same grid after the same number of time steps, this time using a Courant number of 5 . The solution is virtually exact for the case with integer CN and dissipative for the earlier case with noninteger CN.

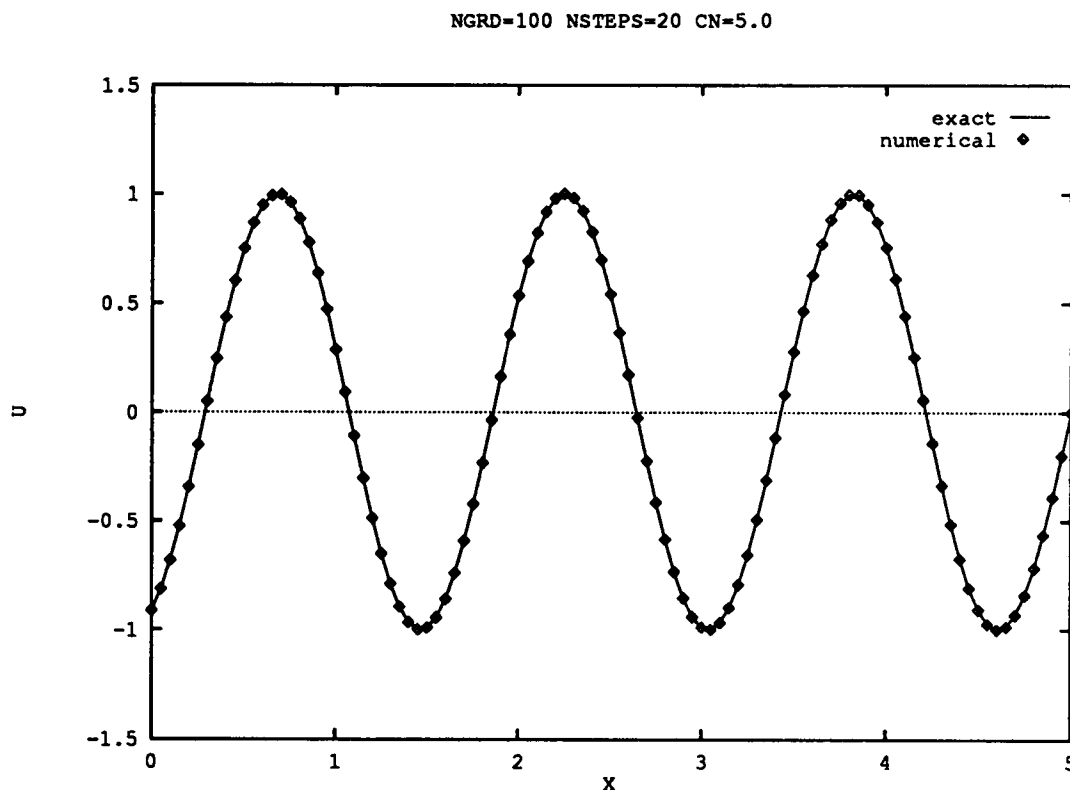


Figure 5. Results using piecewise constant approximating functions with $CN=5$ after 20 time steps and sinusoidal initial conditions.

Results for the same problem using the method given by Equation (15) but assuming piecewise linear continuous approximations are shown in Figure (6). Note that the solution is virtually exact. Unlike the piecewise constant solution, this is true regardless of the Courant number.

NGRD=100 NSTEPS=20 CN=5.5

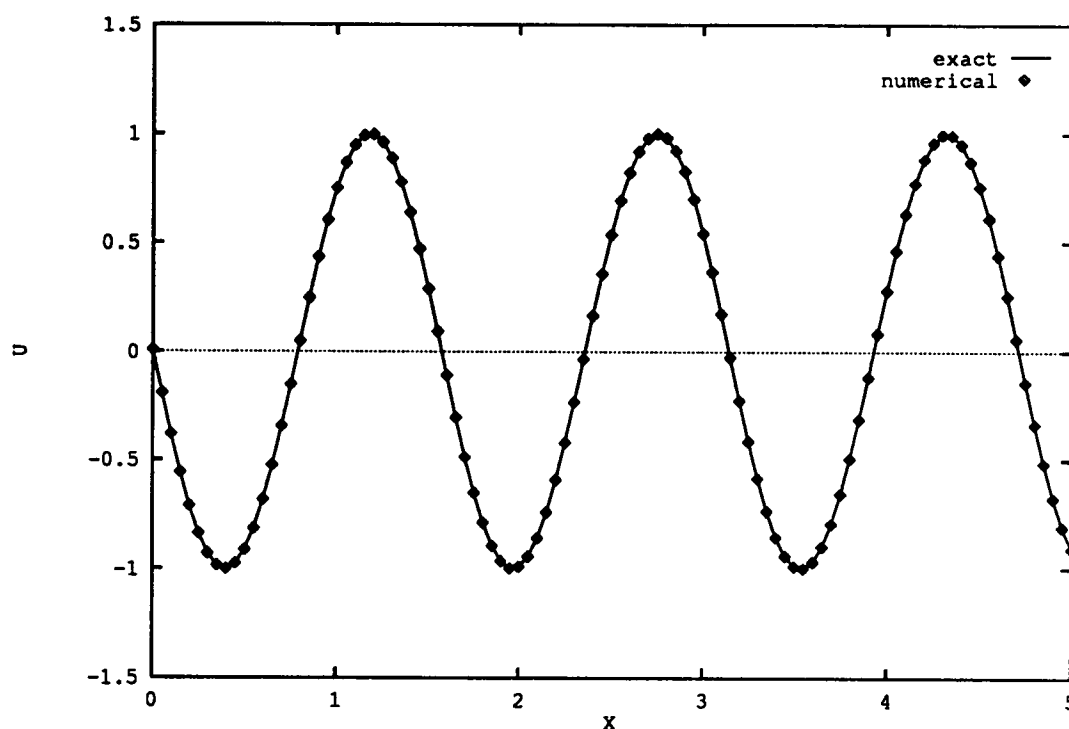


Figure 6. Results using piecewise linear approximating functions with $CN=5.5$ after 20 time steps and sinusoidal initial conditions.

These results seem to indicate the method of choice to be that of Equation (15) using piecewise linear approximations for all Courant numbers. However, the next set of results point out some difficulties.

We apply the same methods, on the same grid, to square wave initial condition,

$$u(x,0) = \begin{cases} 1 & 1 < x \leq 1.5 \\ 0 & \text{elsewhere.} \end{cases}$$

Figure (7) shows the results using piecewise constant approximation with non-integer Courant number, $CN = 1.5$ after 30 time steps. Again the solution is

quite diffusive but entirely stable and nonoscillatory.

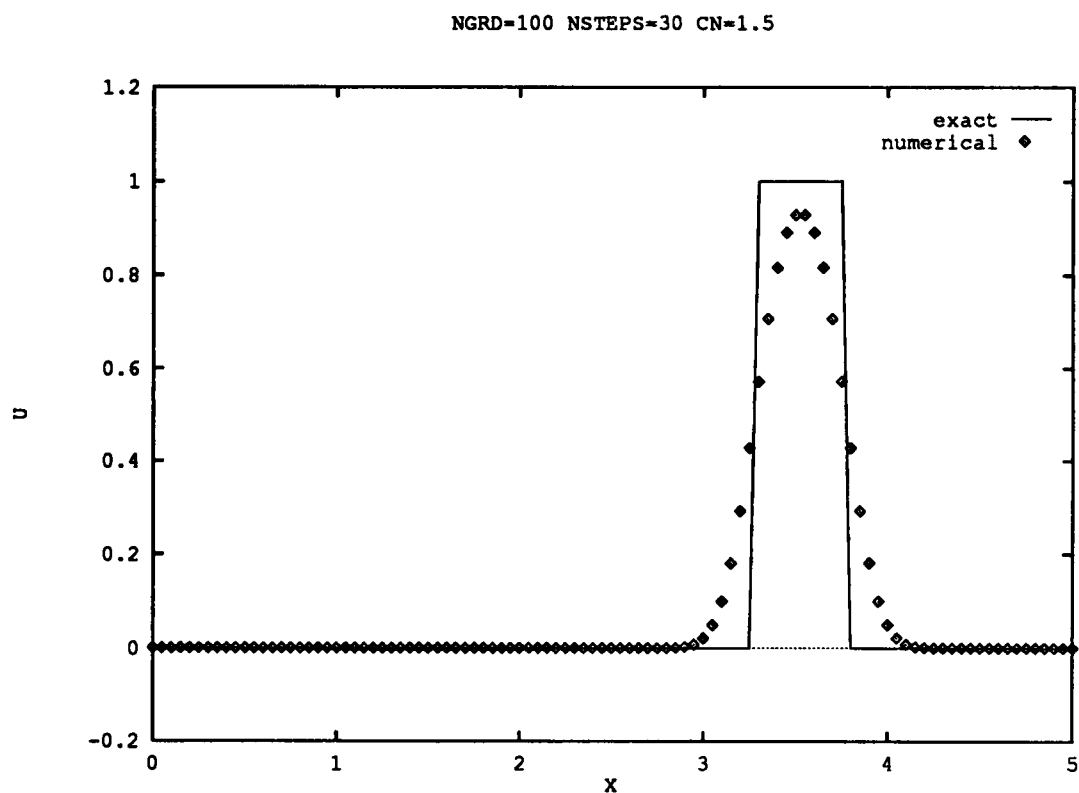


Figure 7. Results using piecewise constant approximating functions with $CN=1.5$ after 30 time steps and square wave initial conditions.

Figure (8) shows the same case using integer Courant number, $CN = 1$. The solution is virtually exact, stable and nonoscillatory. These results are consistent with our analysis.

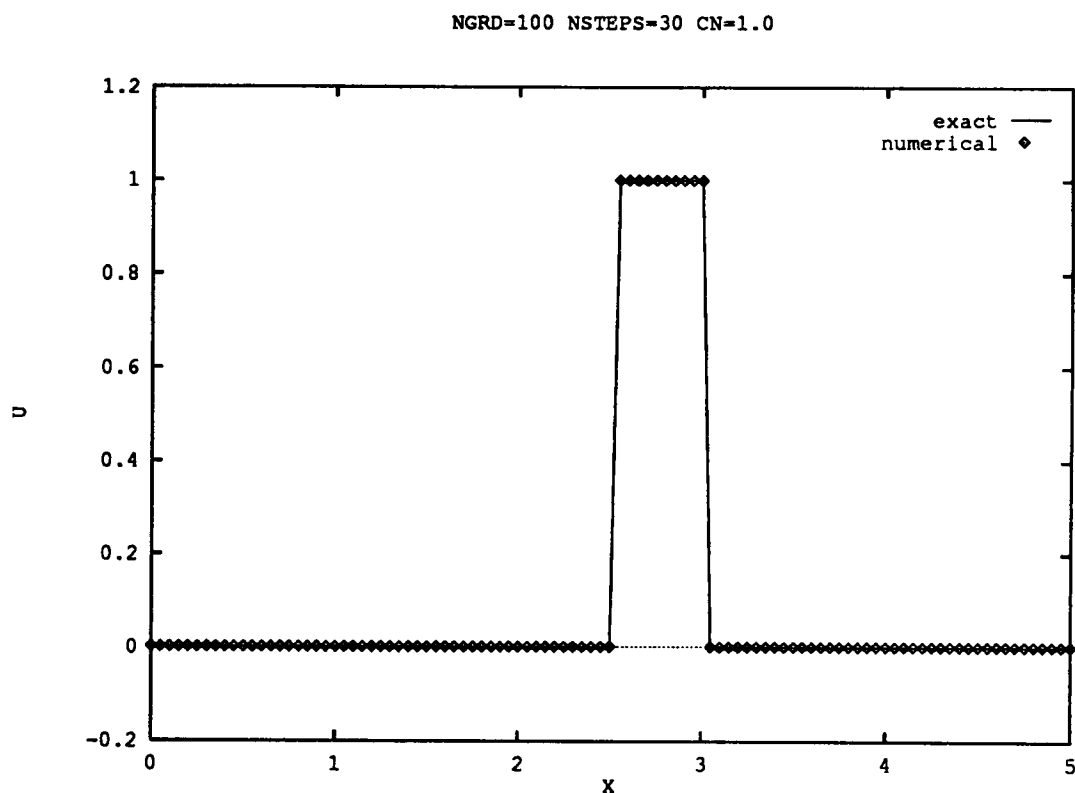


Figure 8. Results using piecewise constant approximating functions with $CN=1.0$ after 30 time steps and square wave initial conditions.

However, when a piecewise linear approximation is used, we see from Figure (9) that though the solution is nondiffusive and fairly accurate, overshoots and undershoots appear around discontinuities.

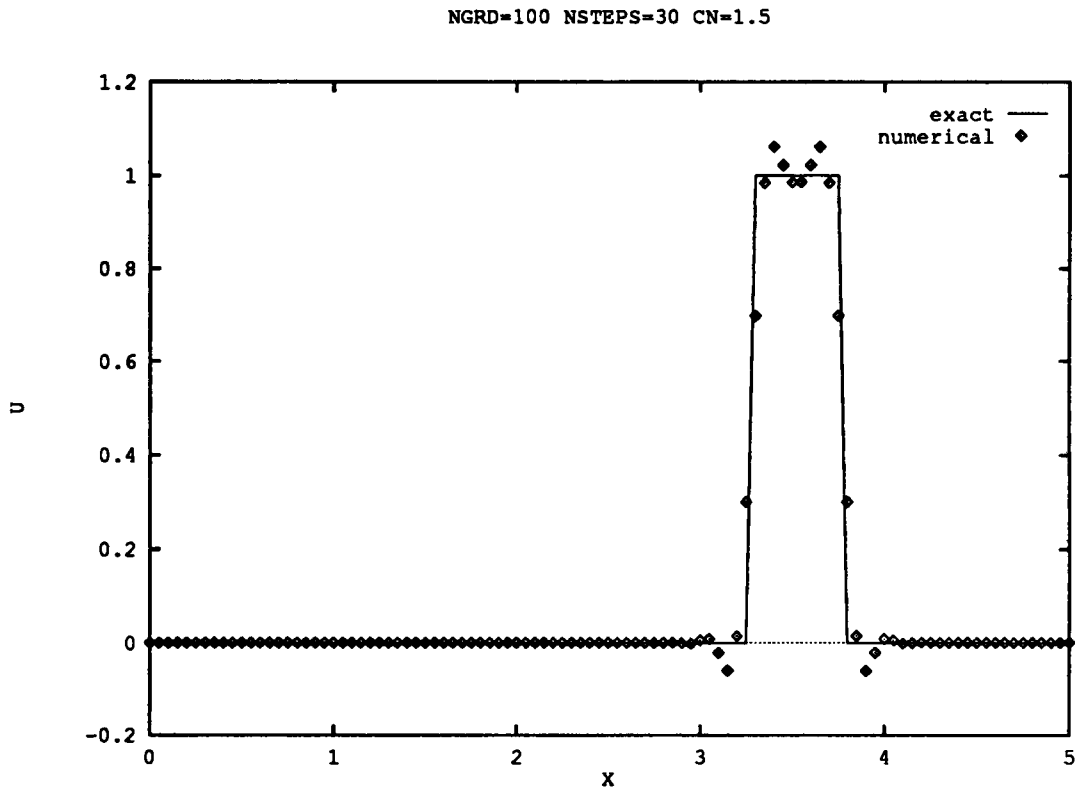


Figure 9. Results using piecewise linear approximating functions with $CN=1.5$ after 30 time steps and square wave initial conditions.

In summary, the two previous test cases demonstrate the increase in accuracy achieved by using the piecewise linear continuous approximations and the accuracy and stability of using an integer Courant number with piecewise constant approximations. It is also apparent that with piecewise linear approximating functions we begin to develop oscillatory behavior for discontinuous solutions. The result shown in Figure (9) leads one to believe that this method using piecewise linear continuous approximations would not perform well on fluid flow problems involving shocks. To test this, the method given by Equation (12)

is applied to the familiar shock-tube problem of Sod[7].

The shock-tube problem describes the one dimensional adiabatic flow of an inviscid perfect gas with initial conditions of two constant states separated by a discontinuity. The problem may be solved analytically and so represents a good test for a numerical algorithm.

Figure (10) shows the density of a gas determined by applying the method given by Equation (12) to this problem with $u_l = u_r = 0$, $\rho_l = 1$ $\rho_r = 0.125$, $p_l = 100000$ $p_r = 10000$. Here we have assumed piecewise constant approximations for integration purposes and used linear interpolation to determine the flux values at the ξ locations. For the nonlinear Euler equations, we see that the method is conservative and stable. It captures shocks and contact discontinuities though both are smeared similar to all well known first order methods. Note that unlike the linear test cases even though an integer Courant number was used, the solution is dissipative. The solution does not substantially change for other CN , though for CN much greater than 1.5 the method becomes unstable.

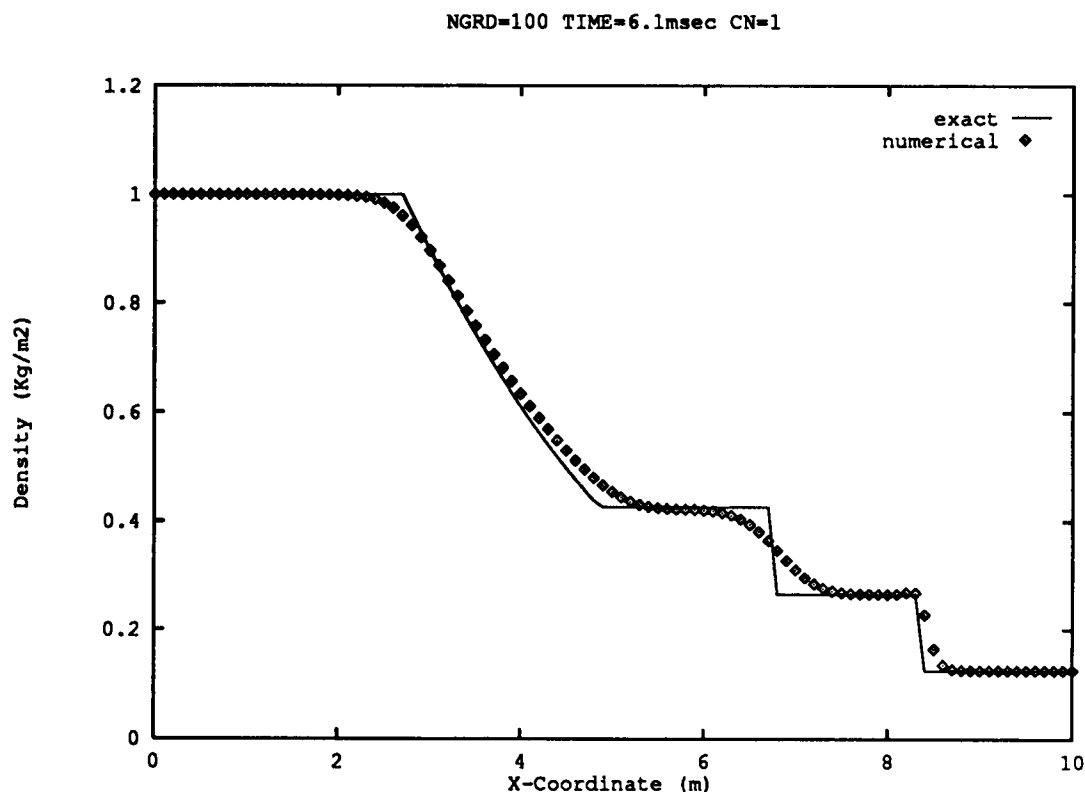


Figure 10. Density in the shock-tube with piecewise constant integration and linear interpolation of fluxes.

We suspect that using piecewise linear approximations would be unstable. Indeed, the method using piecewise linear continuous approximations for both integration and interpolation purposes is unstable on these non-linear vector equations.

So in terms of formal accuracy on the scalar equation, using piecewise constant approximating functions for integration provides $\mathcal{O}(h)$ accuracy and that using piecewise linear continuous approximating functions provides $\mathcal{O}(h^2)$ accuracy. But the latter is unstable for some important nonlinear test cases. Following ideas of the so-called MUSCL and flux-limited schemes[8], the pre-

vious two results suggest that a piecewise linear slope-limited approximation might provide the desired accuracy we seek and also retain the stability shown with piecewise constant integration. However, this method has also proved to be unstable for certain initial conditions though it is highly accurate for others. It is suspected that this may have something to do with using different approximating functions to perform the integrations than those used to evaluate the fluxes.

To this end, an attempt to solve the shock-tube problem is made using piecewise linear slope-limited approximations for integration and interpolation purposes. If a ξ location happened to coincide with a half node, the average value of the left and right interpolant is used. However, this method proved to be unstable for any initial conditions. In fact, even using piecewise constant approximations with this type of interpolation proves unstable.

Though it is still not clear why it is unstable, a conjecture is that it may be due in part to the pointwise evaluation of fluxes from discontinuous functions as will be discussed in the next chapter.

The basic local Lagrangian scheme is further refined by considering a cell averaged approach to develop more accurate and robust solution strategies.

CHAPTER IV

A CELL AVERAGED APPROACH

4.1 Motivation

It is observed that when the piecewise constant approximations are used for both integration and interpolation the method is also unstable (recall that this choice is stable if linear interpolation is used). When a discontinuous function is used for interpolation an ambiguity arises in determining a function value at a discontinuity. Moreover, precise location of the argument is critical in the sense that a very small change in the argument could produce a very large change in the corresponding ordinate. This is clearly undesirable in an iterative process.

With these thoughts in mind we now develop the present form of the algorithm.

4.2 The Cell Averaged Conservation Law

We start with Equation (8) and integrate it from t^n to t^{n+1} . Let x be any point in our domain and define x_R the solution to

$$\frac{dx_R}{dt} = u \quad x_R(t^{n+1}) = x + h/2,$$

and define

$$\xi_R(x) = x_R(t^n).$$

Similar equations hold for x_L, ξ_L . We have

$$(17) \quad \int_{x-\frac{h}{2}}^{x+\frac{h}{2}} Q(z, t^{n+1}) dz - \int_{\xi_L(x)}^{\xi_R(x)} Q(z, t^n) dz + \\ \int_{t^n}^{t^{n+1}} F(x_R(t), t) dt - \int_{t^n}^{t^{n+1}} F(x_L(t), t) dt = \\ \int_{t^n}^{t^{n+1}} \int_{x_L(t)}^{x_R(t)} S(\eta, t) d\eta dt$$

where F is again defined by Equation (5). Now we average Equation (17) over cell j from $x_{j-1/2}$ to $x_{j+1/2}$.

$$(18) \quad \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{x-h/2}^{x+h/2} Q(z, t^{n+1}) dz dx - \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{\xi_L(x)}^{\xi_R(x)} Q(z, t^n) dz dx + \\ \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} F(x_R(t), t) dt dx - \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} F(x_L(t), t) dt dx = \\ \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} \int_{x_L(t)}^{x_R(t)} S(\eta, t) d\eta dt dx.$$

Note that $x_{R,L}(t)$ are implicitly defined to be functions of x through the initial conditions of their defining differential equations. No approximations have been made so far. This is an exact reformulation of the original conservation law given by Equation (1).

Consider the term

$$\frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} F(x_R(t), t) dt dx$$

and its counterpart with x_L . When

$$x = x_{j-1/2}, \begin{cases} x_R(t^{n+1}) = x_{j-1/2} + h/2 = x_j \\ x_L(t^{n+1}) = x_{j-1/2} - h/2 = x_{j-1}. \end{cases}$$

When

$$x = x_{j+1/2}, \begin{cases} x_R(t^{n+1}) = x_{j+1/2} + h/2 = x_{j+1} \\ x_L(t^{n+1}) = x_{j+1/2} - h/2 = x_j. \end{cases}$$

So, for example, the first term signifies the double integral of F over the region in the $x-t$ plane bounded in time by the lines $t = t^n$ and $t = t^{n+1}$ and bounded spatially by pathlines intersecting $t = t^{n+1}$ at x_j and x_{j+1} . Notice that this formulation eliminates the need for pointwise evaluation of fluxes. Instead it requires flux integral averages along pathlines in a banded zone. As we shall see, these approximations lead to discrete equations which will be solved iteratively.

4.3 Approximation and Discretization

Using the midpoint rule we have the following results for the first two terms and the last term in Equation (18).

$$(19) \quad \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{x-h/2}^{x+h/2} Q(z, t^{n+1}) dz dx = \int_{x_{j-1/2}}^{x_{j+1/2}} Q(x, t^{n+1}) dx + \mathcal{O}(h^2)$$

$$(20) \quad \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{\xi_L(x)}^{\xi_R(x)} Q(z, t^n) dz dx = \int_{\xi_L(x_j)=\xi_{j-1/2}}^{\xi_R(x_j)=\xi_{j+1/2}} Q(x, t^n) dx + \mathcal{O}(h^2)$$

$$(21) \quad \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} \int_{x_L(t)}^{x_R(t)} S(\eta, t) d\eta dt dx = \int_{t^n}^{t^{n+1}} \int_{x_L(t)}^{x_R(t)} S(\eta, t) d\eta dt|_{x=x_j} + \mathcal{O}(h^2)$$

provided Q and S are sufficiently smooth. Again, the notation indicating that the third term is to be evaluated at $x = x_j$ means that $x_{R,L}(t)$ are implicitly defined so that $x_{R,L}(t^{n+1}) = x_{j\pm 1/2}$.

Recall the approximation $\xi_{j\pm 1/2} = x_{j\pm 1/2} - \bar{u}_{j\pm 1/2}\Delta t$, in Equation (11) associated with Equation (12). $\bar{u}$ may be interpreted as an average value of u in the region of flux integration this region being the characteristics $x_{R,L}$ intersecting $x_{j\pm 1/2}$. The regions of flux integration for Equation (18) are those described at the end of the previous section. With this motivation we redefine

$$\xi_{j\pm 1/2} = x_{j\pm 1/2} - \bar{u}_{j\pm 1/2}\Delta t,$$

where $\bar{u}_{j\pm 1/2}$ are now defined to be the average value of u in the regions of flux integration described in the previous section. Similarly

$$\xi_j = \xi_R(x_{j-1/2}) = \xi_L(x_{j+1/2}) = x_j - \bar{u}_j\Delta t$$

where $\bar{u}$ is defined to be the average value of u in the region bounded by pathlines intersecting $x_{j\pm 1/2}$ at t^{n+1} . This is the region where the source term is to be integrated. These regions are depicted in Figures (11) and (12).

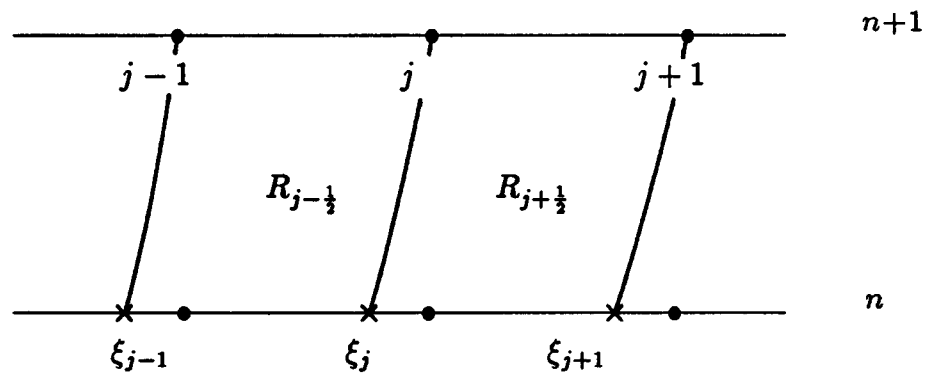


Figure 11. Regions of flux integration.

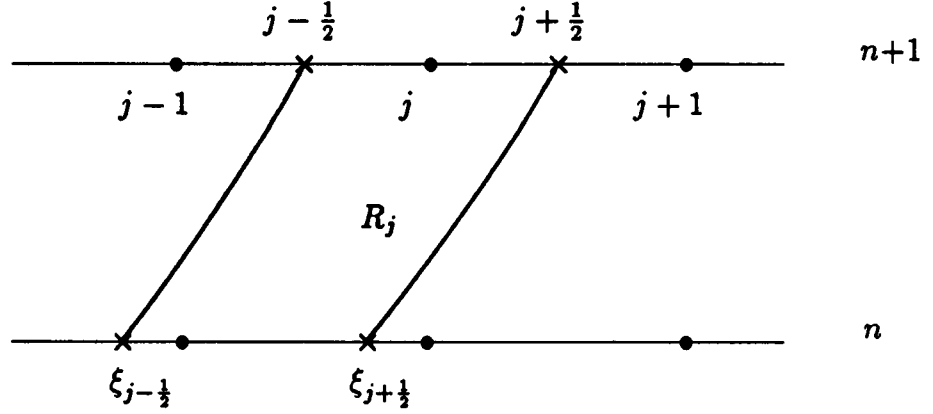


Figure 12. Region of source integration.

We may now formally define

$$R_{j+1/2} = \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{x_R(t^n)}^{x_R(t^{n+1})} dx_R dx,$$

$$R_{j-1/2} = \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{x_L(t^n)}^{x_L(t^{n+1})} dx_L dx,$$

and

$$R_j = \int_{x_j}^{x_{j+1}} \int_{x_L(t^n)}^{x_L(t^{n+1})} dx_L dx = \int_{x_{j-1}}^{x_j} \int_{x_R(t^n)}^{x_R(t^{n+1})} dx_R dx.$$

These are simply the definitions of the area of the regions shown in Figures (11) and (12). For example, let us examine the definition of $R_{j+1/2}$. For any

$$x \in (x_{j-1/2}, x_{j+1/2}),$$

$$\int_{x_R(t^n)}^{x_R(t^{n+1})} dx_R$$

is just the length of the pathline of the flow intersecting $t = t^{n+1}$ at $x + h/2$ between time levels n and $n + 1$. Integrating these over the cell gives the area

enclosed by $t = t^n$ and $t = t^{n+1}$ and the pathlines of the flow intersecting x_j and x_{j+1} at time level $n + 1$.

It is now clear that we will need to integrate various dependent variables over the regions shown in Figures (11) and (12). For simplicity we consider the integration of the generic dependent variable f over the region R_j in Figure (12). At any stage of the iteration we have an estimate of the solution at time t^{n+1} and we know the solution at t^n . Because of the Lagrangian formulation it is evident that assuming the solution to be constant along any given pathline in $((n - 1/2)\Delta t, (n + 1/2)\Delta t)$ would be a better assumption than assuming it constant along $x = \text{constant}$ in the same time interval. Therefore, we divide the region R_j into two parts, $\bar{R}_j$, that region of R_j in $((n + 1/2)\Delta t, (n + 1)\Delta t)$ and $\underline{R}_j$, that region of R_j in $(n\Delta t, (n + 1/2)\Delta t)$. We now make the approximations

$$\int \int_{\bar{R}_j} f d\bar{R}_j \approx \frac{\bar{R}_j}{\Delta x(t^{n+1})} \int_{x_L(t^{n+1})}^{x_R(t^{n+1})} f dx = \frac{\bar{R}_j}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} f(x, t^{n+1}) dx$$

$$\int \int_{\underline{R}_j} f d\underline{R}_j \approx \frac{\underline{R}_j}{\Delta x(t^n)} \int_{x_L(t^n)}^{x_R(t^n)} f dx = \frac{\underline{R}_j}{\delta \xi_j} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} f(x, t^n) dx$$

where

$$\Delta x(t) = x_R(t) - x_L(t)$$

$$\delta \xi_j = \xi_{j+1/2} - \xi_{j-1/2}$$

i.e.; f is assumed constant in the regions $\bar{R}_j$ and $\underline{R}_j$ with value equal to the average value of f at t^{n+1} in $(x_{j-1/2}, x_{j+1/2})$, and the average value of f in

$(\xi_{j-1/2}, \xi_{j+1/2})$ at t^n , respectively. The integral of f over the regions $\bar{R}_{j\pm 1/2}$, $\underline{R}_{j\pm 1/2}$ is defined entirely similarly.

Therefore we may approximate the last two terms in the left hand side of Equation (18) and the term in the right hand side of Equation (21) by

$$\begin{aligned} & \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} \mathbf{F}(x_R(t), t) dt dx \approx \\ & \frac{1}{h} \left\{ \frac{\underline{R}_{j+1/2}}{\delta \xi_{j+1/2}} \int_{\xi_j}^{\xi_{j+1}} \mathbf{F}(x, t^n) dx + \frac{\bar{R}_{j+1/2}}{h} \int_{x_j}^{x_{j+1}} \mathbf{F}(x, t^{n+1}) dx \right\}, \\ & \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} \mathbf{F}(x_L(t), t) dt dx \approx \\ & \frac{1}{h} \left\{ \frac{\underline{R}_{j-1/2}}{\delta \xi_{j-1/2}} \int_{\xi_{j-1}}^{\xi_j} \mathbf{F}(x, t^n) dx + \frac{\bar{R}_{j-1/2}}{h} \int_{x_{j-1}}^{x_j} \mathbf{F}(x, t^{n+1}) dx \right\}, \end{aligned}$$

and

$$\begin{aligned} & \int_{t^n}^{t^{n+1}} \int_{x_L(t)}^{x_R(t)} \mathbf{S}(\eta, t) d\eta dt|_{x=x_j} \approx \\ & \left\{ \frac{\underline{R}_j}{\delta \xi_j} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} \mathbf{S}(x, t^n) dx + \frac{\bar{R}_j}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{S}(x, t^{n+1}) dx \right\}. \end{aligned}$$

4.4 The Local Lagrangian Finite Volume Method

The preceding discussion has now led us to the following approximation to Equation (18).

$$\begin{aligned} (22) \quad & \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{Q}(x, t^{n+1}) dx - \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} \mathbf{Q}(x, t^n) dx + \\ & \frac{1}{h} \left\{ \frac{\underline{R}_{j+1/2}}{\delta \xi_{j+1/2}} \int_{\xi_j}^{\xi_{j+1}} \mathbf{F}(x, t^n) dx + \frac{\bar{R}_{j+1/2}}{h} \int_{x_j}^{x_{j+1}} \mathbf{F}(x, t^{n+1}) dx \right\} - \end{aligned}$$

$$\frac{1}{h} \left\{ \frac{\underline{R}_{j-1/2}}{\delta \xi_{j-1/2}} \int_{\xi_{j-1}}^{\xi_j} F(x, t^n) dx + \frac{\overline{R}_{j-1/2}}{h} \int_{x_{j-1}}^{x_j} F(x, t^{n+1}) dx \right\} -$$

$$\left\{ \frac{\underline{R}_j}{\delta \xi_j} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} S(x, t^n) dx + \frac{\overline{R}_j}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} S(x, t^{n+1}) dx \right\} = O$$

where $\delta \xi_{j+1/2} = \xi_{j+1} - \xi_j$ and $\delta \xi_j = \xi_{j+1/2} - \xi_{j-1/2}$. Note that the R 's can be written in terms of the ξ 's as follows.

$$(23) \quad \overline{R}_{j+1/2} = \frac{3h\Delta t}{8} + \frac{\Delta t}{8}(\xi_{j+1} - \xi_j) \quad \overline{R}_j = \frac{3h\Delta t}{8} + \frac{\Delta t}{8}(\xi_{j+1/2} - \xi_{j-1/2}).$$

$$(24) \quad \underline{R}_{j+1/2} = \frac{h\Delta t}{8} + \frac{3\Delta t}{8}(\xi_{j+1} - \xi_j) \quad \underline{R}_j = \frac{h\Delta t}{8} + \frac{3\Delta t}{8}(\xi_{j+1/2} - \xi_{j-1/2}).$$

Equation (22) is the Local Lagrangian Finite Volume (LLFV) method. We now have nearly everything sufficiently defined so that the iterative process may begin to solve the implicit equations. We need only to choose a solution set on which to perform the integrations required in Equation (22) and a method of integration.

4.5 The Approximating Functions

For the approximation process we choose approximating functions devised by Harten and Osher[9]. These are piecewise linear slope-limited in each cell, constructed from the cell averages of each of the components of $\mathbf{Q}$, and provide $\mathcal{O}(h^2)$ approximation to the components of $\mathbf{Q}$. Moreover, they have the property that the cell averages of the functions are an $\mathcal{O}(h^3)$ approximation to the cell averages of the components of $\mathbf{Q}$. These approximating functions can be shown

to be essentially nonoscillatory in the sense that the number of local extrema in the solution to the nonlinear scalar equation will not increase when used in conjunction with the authors method.

It is also demonstrated by the authors that the method given by Equation (15) to solve the scalar equation, Equation (13), using these approximating functions is a monotonicity preserving method. Though not as strong a result as TVD, this property assures us that spurious oscillations will not occur when the method is applied to a step function.

Because of their form, the terms in the right side of Equations (19) and (20) can be evaluated exactly in terms of the cell averages of Q . Thus we seek to find the solution in terms of the cell averages of Q . From this point onward we will interpret Q_j to mean the cell average of the Q function in the j^{th} cell.

It should be noted that if the components of Q are considered to be piecewise linear in each grid cell, then the components of the flux vectors are simply rational functions in each grid cell and hence could be integrated analytically. However, for simplicity the remaining terms are integrated by two point Gaussian quadrature in each subinterval in which Q is continuous. This should not affect the accuracy of the scheme.

It is a well known result[10] that for an n -point Gauss-Legendre quadrature

rule, the error in the formula is given by

$$\int_a^b f(x)dx - \sum_{i=1}^n w_i f(x(u_i)) = \frac{(b-a)}{2} \left(\frac{b-a}{2}\right)^{2n} \frac{f^{(2n)}(\xi)}{(2n+2)!} \int_{-1}^1 (u-u_1)^2 \dots (u-u_n)^2 du$$

where $\xi \in (a, b)$ and we are assuming a sufficiently smooth function $f(x)$. The $\{w_i\}$ are the weights of the quadrature formula and the $\{u_i\}$ are the roots of the n^{th} degree Legendre polynomial.

Now, suppose we want to use the n -point quadrature as a composite rule over a domain $[A, B]$ where we assume that $|f^{(2n)}(x)|$ is bounded on $[A, B]$ by C .

Dividing the domain into k subintervals of length h and applying the n -point quadrature rule to each subinterval we have a total error bounded by

$$k \frac{h}{2} \left(\frac{h}{2}\right)^{2n} \bar{C} \quad \text{where}$$

$$\bar{C} = C \int_{-1}^1 (u-u_1)^2 \dots (u-u_n)^2 du$$

and $\bar{C}$ is independent of the length h .

Therefore, we may conclude that with respect to the grid size h , the error introduced due to the 2-point quadrature can be considered of $\mathcal{O}(h^4)$ for sufficiently smooth flux and source functions.

4.6 Method of Solution

As stated previously, because of the coupling of the solution at time level $n + 1$ and the location of the ξ 's at time level n , it is necessary to solve the resulting implicit equations iteratively. The Locally Implicit Method (LIM) developed by Reddy[11] and Reddy and Benek[12] was chosen as the method of solution.

A heuristic derivation of the coefficients used in the LIM will now be presented. Familiarity with the Locally Implicit Method itself is assumed. We fix the ξ locations at the current iteration level for the linearization and assume that $\mathbf{S} = \mathbf{O}$ in Equation (22).

$$(25) \quad \int_{x_{j-1/2}}^{x_{j+1/2}} Q^{n+1} dx = h Q_j^{n+1} = (Q_j^{(m)} + \Delta Q_j) h$$

where the ΔQ_j symbol in this equation and the following represents an iterative change in Q_j .

Since $\mathbf{F} = -\mathbf{Q}u + \mathbf{E}$,

$$\begin{aligned} (26) \quad \mathbf{F}^{n+1} &= \mathbf{F}^{(m)} + \Delta \mathbf{F} = \mathbf{F}^{(m)} - (\Delta(\mathbf{Q}u) - \Delta \mathbf{E}) \\ &= \mathbf{F}^{(m)} - \left(\mathbf{Q} \frac{\partial u}{\partial \mathbf{Q}} + u\mathbf{I} - \mathbf{A} \right) |^{(m)} \Delta \mathbf{Q} \\ &= \mathbf{F}^{(m)} + \mathbf{B}^{(m)} \Delta \mathbf{Q} \\ \mathbf{B}^{(m)} &= - \left(\mathbf{Q} \frac{\partial u}{\partial \mathbf{Q}} + u\mathbf{I} - \mathbf{A} \right) |^{(m)} \end{aligned}$$

and $\mathbf{A}$ is the Jacobian matrix $\frac{\partial \mathbf{E}}{\partial \mathbf{Q}}$.

So Equation (22) can be written

$$\begin{aligned}
 (27) \quad h\Delta \mathbf{Q}_j &+ \frac{\overline{R}_{j+1/2}^{(m)}}{h^2} \int_{x_j}^{x_{j+1}} \mathbf{B}^{(m)} \Delta \mathbf{Q} dx - \frac{\overline{R}_{j-1/2}^{(m)}}{h^2} \int_{x_{j-1}}^{x_j} \mathbf{B}^{(m)} \Delta \mathbf{Q} dx \\
 &= -[\mathbf{Q}_j^{(m)} h - \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} \mathbf{Q}^n dx \\
 &\quad + \frac{\overline{R}_{j+1/2}^{(m)}}{h\delta\xi_{j+1/2}} \int_{\xi_j}^{\xi_{j+1}} \mathbf{F}^n dx + \frac{\overline{R}_{j+1/2}^{(m)}}{h^2} \int_{x_j}^{x_{j+1}} \mathbf{F}^{(m)} dx \\
 &\quad - \frac{\overline{R}_{j-1/2}^{(m)}}{h\delta\xi_{j-1/2}} \int_{\xi_{j-1}}^{\xi_j} \mathbf{F}^n dx - \frac{\overline{R}_{j-1/2}^{(m)}}{h^2} \int_{x_{j-1}}^{x_j} \mathbf{F}^{(m)} dx] \\
 &= RHS^{(m)}.
 \end{aligned}$$

Applying the trapezoidal rule to the integrals on the left we have

$$\begin{aligned}
 h\Delta \mathbf{Q}_j &+ \frac{\overline{R}_{j+1/2}^{(m)}}{2h} \{\mathbf{B}_j^{(m)} \Delta \mathbf{Q}_j + \mathbf{B}_{j+1}^{(m)} \Delta \mathbf{Q}_{j+1}\} - \frac{\overline{R}_{j-1/2}^{(m)}}{2h} \{\mathbf{B}_j^{(m)} \Delta \mathbf{Q}_j + \mathbf{B}_{j-1}^{(m)} \Delta \mathbf{Q}_{j-1}\} \\
 &= \{h\mathbf{I} + (\frac{\overline{R}_{j+1/2}^{(m)} - \overline{R}_{j-1/2}^{(m)}}{2h} \mathbf{B}_j^{(m)})\} \Delta \mathbf{Q}_j + \frac{\overline{R}_{j+1/2}^{(m)}}{2h} \mathbf{B}_{j+1}^{(m)} \Delta \mathbf{Q}_{j+1} - \frac{\overline{R}_{j-1/2}^{(m)}}{2h} \mathbf{B}_{j-1}^{(m)} \Delta \mathbf{Q}_{j-1} \\
 &= RHS^{(m)}.
 \end{aligned}$$

For left to right sweeps $\Delta \mathbf{Q}_{j-1}$ has already been determined. So $\Delta \mathbf{Q}_{j-1}$ and its coefficient are moved to the right side of Equation (24). When the approximations involved in simplifying the coefficient of $\Delta \mathbf{Q}_{j-1}$ are reversed the terms associated with any function, say f , $f_{j-1}^{(m)}$ and Δf_{j-1} sum to give the value of f

at the current iteration level, that is $f_{j-1}^{(m+1)}$. The argument is entirely similar for right to left sweeps. Thus for left to right sweeps

$$\begin{aligned} & \{hI + (\frac{\overline{R}_{j+1/2}^{(m)} - \overline{R}_{j-1/2}^{(m)}}{2h} B_j^{(m)})\} \Delta Q_j + \frac{\overline{R}_{j+1/2}^{(m)}}{2h} B_{j+1}^{(m)} \Delta Q_{j+1} \\ & = RHS^{m*} \end{aligned}$$

and for left to right sweeps

$$\begin{aligned} & \{hI + (\frac{\overline{R}_{j+1/2}^{(m)} - \overline{R}_{j-1/2}^{(m)}}{2h} B_j^{(m)})\} \Delta Q_j - \frac{\overline{R}_{j-1/2}^{(m)}}{2h} B_{j-1}^{(m)} \Delta Q_{j-1} \\ & = RHS^{m*} \end{aligned}$$

where the m^* superscript to RHS indicates that the current iterate in the term RHS given by Equation (27) is to be evaluated at the latest available estimate, be it given by the (m) or $(m + 1)$ iteration level.

Making the approximations

$$B_{j+1}^{(m)} \Delta Q_{j+1} \approx B_j^{(m)} \Delta Q_j$$

for right to left sweeps and

$$B_{j-1}^{(m)} \Delta Q_{j-1} \approx B_j^{(m)} \Delta Q_j$$

for left to right sweeps, we have

$$\{hI + \frac{(2\overline{R}_{j+1/2}^{(m)} - \overline{R}_{j-1/2}^{(m)})}{2h} (A - uI - Q \frac{\partial u}{\partial Q})|_j^{(m)}\} \Delta Q_j$$

$$= C_{lr} \Delta Q_j = RHS^{m*}$$

and for right to left sweeps

$$\left\{ hI + \frac{(\bar{R}_{j+1/2}^{(m)} - 2\bar{R}_{j-1/2}^{(m)})}{2h} (A - uI - Q \frac{\partial u}{\partial Q}) \right\}_j^{(m)} \Delta Q_j$$

$$= C_{rl} \Delta Q_j = RHS^{m*}.$$

The notation C_{lr} and C_{rl} has been introduced to represent the coefficients of ΔQ_j in the above equations.

There is a fair amount of flexibility in the LIM. In general we want to use a norm of the above coefficient matrices as a coefficient for the local iteration in order to avoid matrix inversions. Though it can be classified as a quasi-Newton iteration and some interesting analytical results can be derived regarding the LIM[13], there is no way at present to derive a unique coefficient that will guarantee convergence of the process. Also, the inequalities in the following discussion help guide us to a coefficient which will prevent the process from diverging, but they certainly may produce less than optimal convergence rates. We do our best to make the derivation concrete but ultimately the proof is in the pudding. If we drive RHS^{m*} to zero we have solved the equations and achieved our immediate goal. Any approximations made in the derivation of the coefficients will not effect the solution assuming the iteration converges.

We may simplify the coefficient matrices in the above equations with the help of the following observation.

Suppose a scalar function $f(w_1, \dots, w_k) \neq 0$ is homogeneous of degree n . Let $W = \begin{pmatrix} w_1 \\ \vdots \\ w_k \end{pmatrix}$. If $(\frac{\partial f}{\partial W})^T \neq 0$ then $W \frac{\partial f}{\partial W}$ has eigenvalue nf with corresponding eigenvector W .

Proof:

$$W \frac{\partial f}{\partial W} W = W((\frac{\partial f}{\partial W})^T)^T W = W(W^T (\frac{\partial f}{\partial W})^T)^T. \text{ By Eulers Theorem}$$

$$W^T (\frac{\partial f}{\partial W})^T = nf. \quad \blacksquare$$

Since $u = \frac{\rho u}{\rho}$ is homogeneous of degree 0, using this result we may replace $B_j^{(m)}$ in the previous equations by $(A - uI) |_j^{(m)}$, so that

$$C_{rl} = \{hI + \frac{(\bar{R}_{j+1/2}^{(m)} - 2\bar{R}_{j-1/2}^{(m)})}{2h} (A - uI) |_j^{(m)}\}$$

and

$$C_{lr} = \{hI + \frac{(2\bar{R}_{j+1/2}^{(m)} - \bar{R}_{j-1/2}^{(m)})}{2h} (A - uI) |_j^{(m)}\}.$$

Let C represent the coefficient matrix above, either C_{rl} or C_{lr} , and k represent the corresponding term $2\bar{R}_{j+1/2}^{(m)} - \bar{R}_{j-1/2}^{(m)}$ or $\bar{R}_{j+1/2}^{(m)} - 2\bar{R}_{j-1/2}^{(m)}$.

The eigenvalues of $A - uI$ are 0 and $\pm c$ where $c = (\frac{\gamma p}{\rho})^{1/2}$ is the speed of sound. So, dropping subscripts,

$$C = hI + |\frac{k}{2h}|(A - uI)$$

and the spectral radius of C is $h + |\frac{k}{2h}|c$. Then in any norm,

$$h + |\frac{k}{2h}|c \leq \|C\| \leq h + |\frac{k}{2h}|\|A - uI\|.$$

So for $\forall \varepsilon > 0$, there exists a norm which we will denote as the ω norm, such that

$$(28) \quad h + \left| \frac{k}{2h} \right| c_j^{(m)} \leq \|C\|_\omega \leq h + \left| \frac{k}{2h} \right| (c_j^{(m)} + \varepsilon).$$

Alternatively, we may derive a similar result which may help assist us in understanding future observations. The spectral radius of

$$hI + \left| \frac{k}{2h} \right| B$$

is $h + \left| \frac{k}{2h} \right| \left(\frac{\gamma-1}{\gamma} \right)^{1/2} c$, so in any norm,

$$\begin{aligned} h + \left| \frac{k}{2h} \right| \left(\frac{\gamma-1}{\gamma} \right)^{1/2} c &\leq \|C\| \leq h + \left| \frac{k}{2h} \right| \|B\| \\ &\leq h + \left| \frac{k}{2h} \right| (\|A - uI\| + \|Q \frac{\partial u}{\partial Q}\|). \end{aligned}$$

For any $\varepsilon_1 > 0$ there exists an α norm such that

$$\|C\|_\alpha \leq h + \left| \frac{k}{2h} \right| (\|A - uI\|_\alpha + \varepsilon_1),$$

since $Q \frac{\partial u}{\partial Q}$ has zero as a triple eigenvalue. The α norm has been chosen for this ε_1 and is some unknown consistent matrix norm whose existence is guaranteed[14].

Similarly, for any $\varepsilon_2 > 0$ there exists a β norm such that

$$\|A - uI\|_\beta \leq c + \varepsilon_2.$$

So $\exists \mu \geq 1$ such that

$$\frac{1}{\mu} \|A - uI\|_\beta \leq \|A - uI\|_\alpha \leq \mu \|A - uI\|_\beta \leq \mu(c + \varepsilon_2).$$

Then

$$(29) \quad h + \left| \frac{k}{2h} \right| \left(\frac{\gamma - 1}{\gamma} \right)^{1/2} c \leq \|C\|_{\beta} \leq \mu \left[h + \left| \frac{k}{2h} \right| (\varepsilon_1 + \mu(c + \varepsilon_2)) \right].$$

Consider these results given by Equations (28) and (29). Since the ε 's were arbitrary we approximate write Equation (28) as

$$(30) \quad \|C\|_{\omega} \approx h + \left| \frac{k}{2h} \right| c_j^{(m)}$$

and the largest estimate of $\|C\|_{\beta}$ as

$$(31) \quad \|C\|_{\beta} \approx \mu h + \left| \frac{k}{2h} \right| \mu^2 c_j^{(m)}.$$

Considering Equation (31), since $\mu \geq 1$, the direction of the inequalities suggest that we try $\mu = 1$. This yields Equation (30). However, Equation (31) also suggests that we may find it useful to under-relax the iteration.

From the previous heuristic analysis we use the following iterative equations for the LIM,

$$(32) \quad \left(h + \left| \frac{2\bar{R}_{j+1/2}^{(m)} - \bar{R}_{j-1/2}^{(m)}}{2h} \right| c_j^{(m)} \right) \Delta Q_j = R H S^{m*} \quad \text{for left to right sweeps}$$

and

$$(33) \quad \left(h + \left| \frac{\bar{R}_{j+1/2}^{(m)} - 2\bar{R}_{j-1/2}^{(m)}}{2h} \right| c_j^{(m)} \right) \Delta Q_j = R H S^{m*} \quad \text{for right to left sweeps.}$$

Again, as long as the iteration converges any approximations made will not effect the solution. Note that for free stream flow, the above coefficients degenerate to $h + \frac{\Delta t}{2} c_j^{(m)}$.

In the results to be presented several different coefficients, sweep-dependant and non-sweep-dependant, were tried. The coefficients presented here induced convergence that was at least as fast as any others tried. Moreover, these coefficients provided convergence of the LIM under a wider range of initial conditions than any others tried. As will be mentioned in the appendix, it is of particular interest that for some difficult cases, it was necessary to under-relax the residual to attain convergence.

CHAPTER V

RESULTS

Before examining the results on two nonlinear fluid flow problems, let us examine the results of the cell averaged LLFV method applied to the scalar wave equation, Equation (13). Note that there are no fluxes to be averaged and the algorithm just degenerates to that given by Equation (15) using the approximating functions of Harten and Osher[9] for integration. As noted previously, this scheme is monotonicity preserving. Figure (13) shows the solution for a square wave initial condition using the same parameters as the corresponding examples shown in Chapter III. Observe that the solution is entirely nonoscillatory like the piecewise constant case yet much more accurate. Its accuracy is comparable to that of the piecewise linear continuous case but no oscillations appear at the discontinuities.

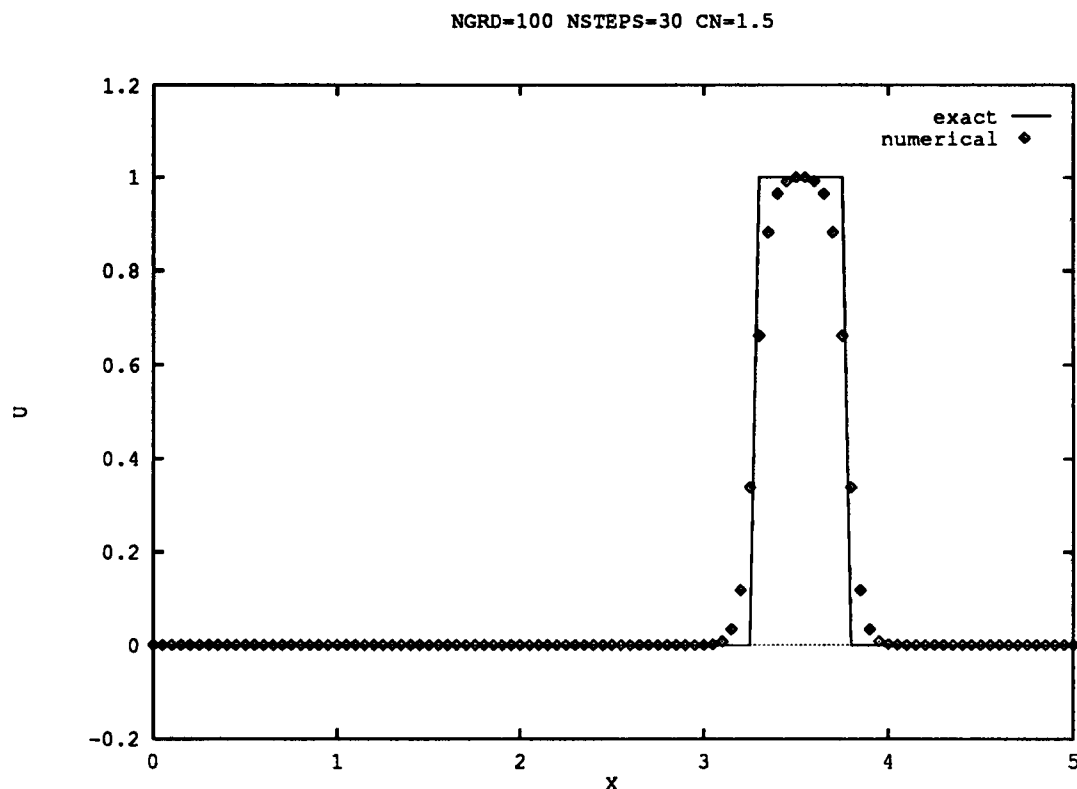


Figure 13. Effects on a square wave using nonoscillatory approximating functions.

The algorithm was applied to two nonlinear test cases, the familiar shock-tube problem[7] and the quasi-one-dimensional nozzle flow problem[15], both of which have analytical solutions.

5.1 The Shock-Tube Problem

We wish to solve the Euler equations, Equation (1), on an infinite domain with initial conditions of two constant states separated by a discontinuity in the

components of $\mathbf{Q}$. In Equation (22) $\mathbf{F}$ is given by Equation (5) and $\mathbf{S} = \mathbf{O}$. The density solution for initial conditions $p_L = 10^5; \rho_L = 1; p_R = 10^3; \rho_R = 0.01; u_L = u_R = 0$, is shown in Figure (14). Note that the solution is highly accurate but virtually nonoscillatory. The contact discontinuity is reasonably well resolved.

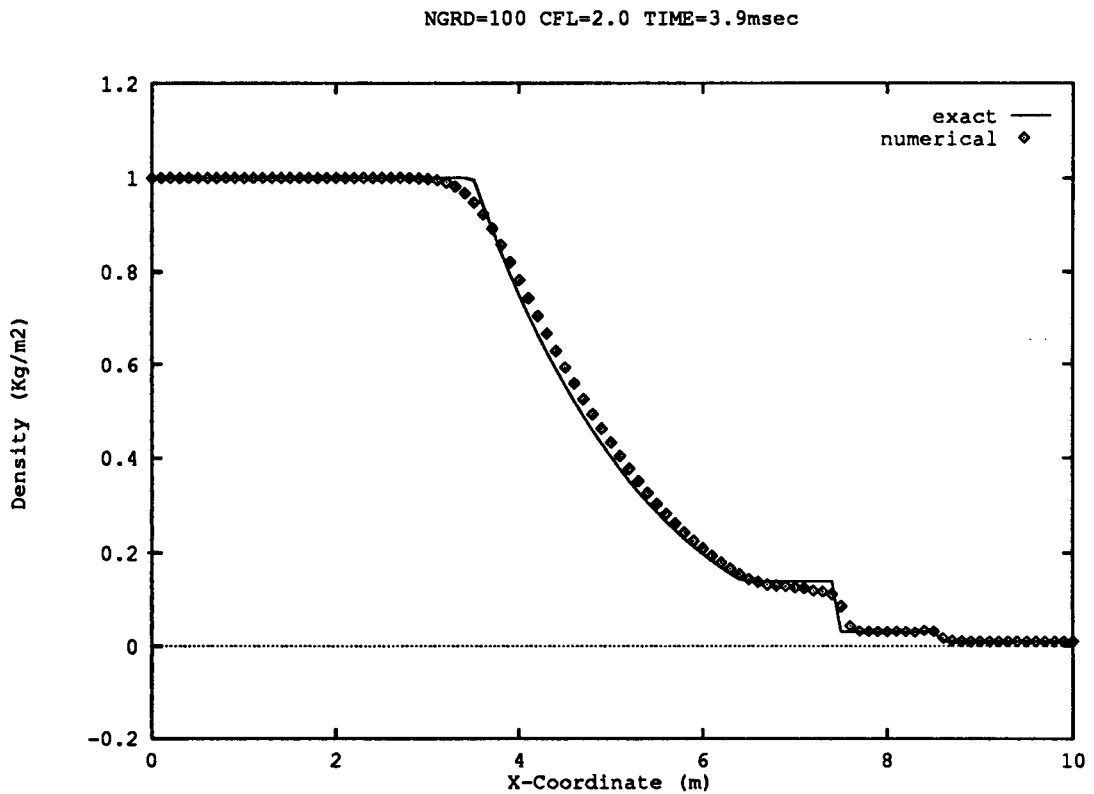


Figure 14. Density in the shock-tube with a strong shock.

The density solution for initial conditions $p_L = 10^5; \rho_L = 1; p_R = 10^4; \rho_R =$

0.125; $u_L = u_R = 0$, is shown in Figure (15). Again the solution is quite good.

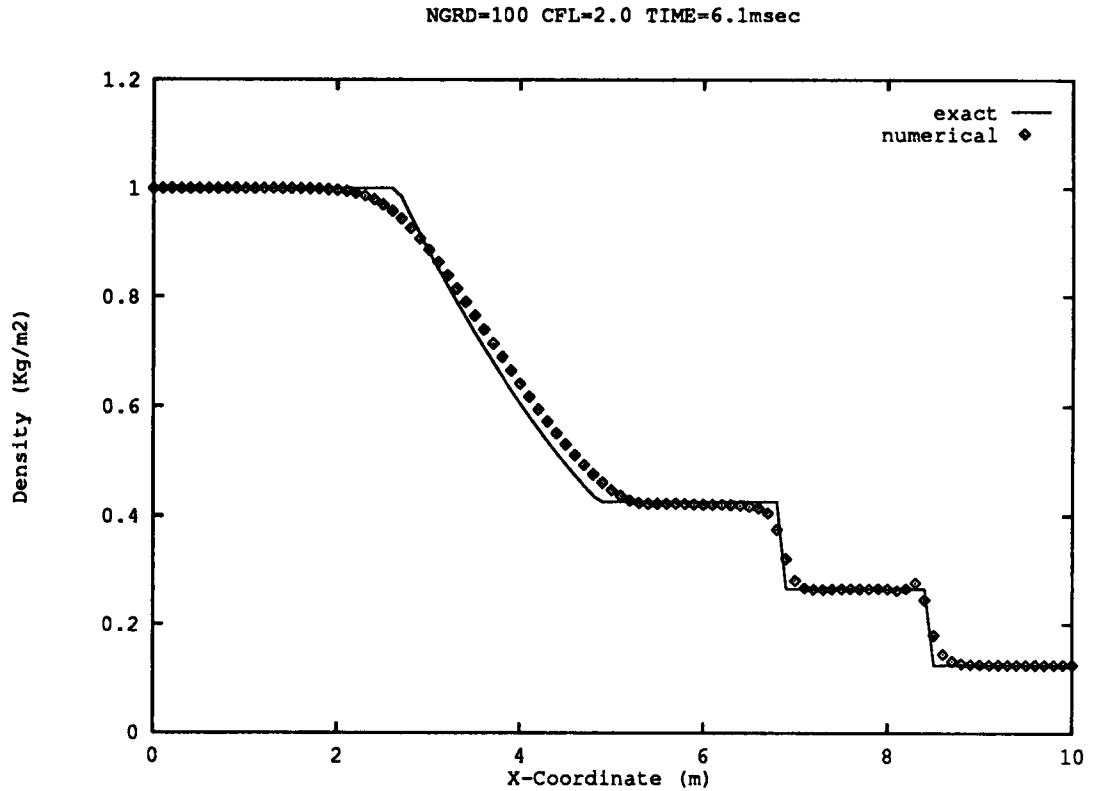


Figure 15. Density in the shock-tube with a weak shock.

As an informal comparison, the same test case as shown in Figure (15) is solved using a second order accurate TVD scheme based on Roe averaging designed by Yee, Warming and Harten[16]. This code was written by the Com-

putational Fluid Dynamics group at CALSPAN Corp./AEDC Operations.

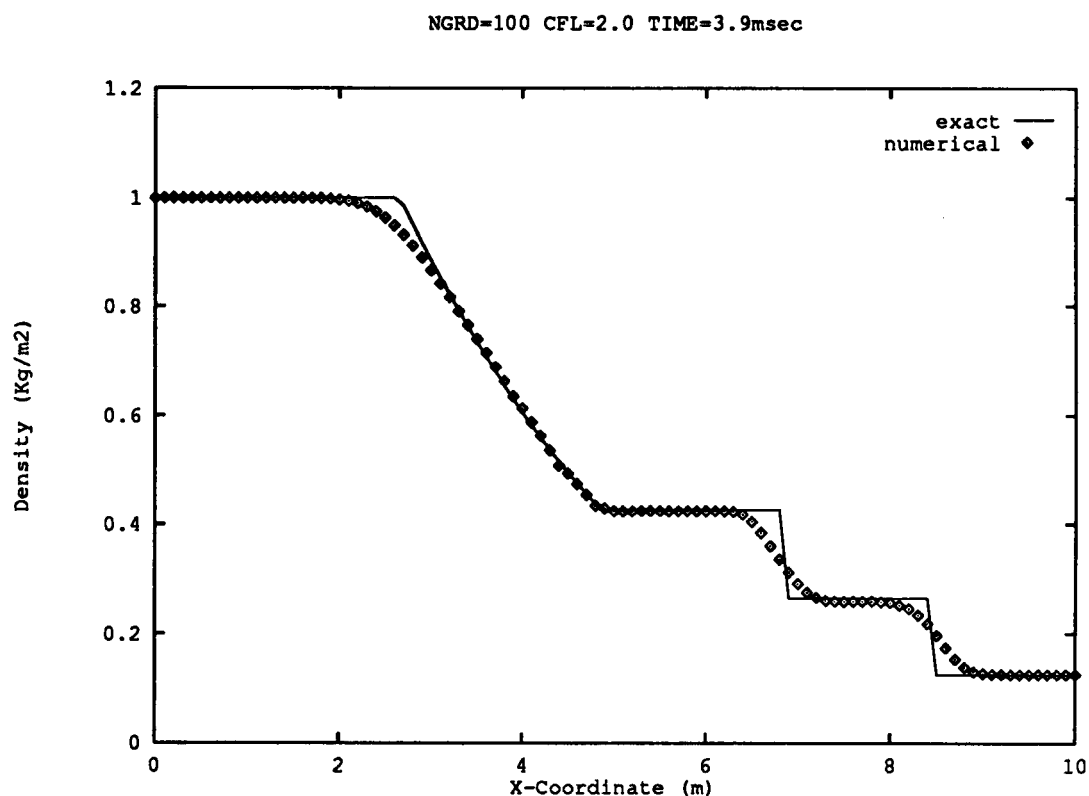


Figure 16. Density in the shock-tube with a weak shock
solved by a second order accurate TVD scheme.

Though neither solution is clearly superior to the other, the solution produced by the LLFV method does compare favorably in terms of resolution of the shock and contact discontinuity.

5.2 The Quasi-One-Dimensional Nozzle Flow Problem

The quasi-one-dimensional nozzle flow equations can be written as $Q_t +$

$E_x = S$ where

$$Q = \alpha \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}, E = \alpha \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (e + p)u \end{pmatrix}, S = \begin{pmatrix} 0 \\ p\alpha' \\ 0 \end{pmatrix},$$

and $\alpha(x)$ is the crosssectional area of the nozzle. The source term appearing in the nozzle flow equations is due to the averaging effects of approximating a two-dimensional varying area nozzle by one-dimensional equations. The equations were solved in a diverging duct with domain $x \in [0, 10]$ and the area of the duct given by $\alpha(x) = 1.398 + 0.347 \arctan[0.8(x - 4)]$. Empirical knowledge has indicated that the same coefficients used for the shock tube problem, those given by Equations (32) and (33), are appropriate and work well for the nozzle flow problem. These were used and indeed did provide convergence. Both test cases to follow use inlet conditions $T_0 = 300K; p_0 = 1bar; A^* = 0.8$. For the first test case outlet boundary conditions are determined to locate a shock at $x = 4$. Though a routine exercise, determination of these conditions will be stated here for completeness. All equations are derived by Zucker[15].

We assume a supersonic expansion to $x = 4$ at which point

$$\frac{\alpha(4)}{A^*} = \frac{1}{M} \left(\frac{2}{\gamma + 1} + \frac{\gamma - 1}{\gamma + 1} M^2 \right)^{\frac{\gamma + 1}{2(\gamma - 1)}}$$

may be solved iteratively for the supersonic Mach number at the shock. The normal shock relation

$$M_2^2 = \frac{M_1^2 + \frac{2}{\gamma - 1}}{\frac{2\gamma}{\gamma - 1} M_1^2 - 1}$$

where M_1 is the supersonic Mach number and M_2 is the subsonic Mach number then determines the Mach number immediately after the shock. Through the isentropic relations

$$p_0 = p(1 + \frac{\gamma - 1}{2} M^2)^{\frac{\gamma}{\gamma - 1}}$$

$$t_0 = t(1 + \frac{\gamma - 1}{2} M^2)$$

and the normal shock relations

$$t_2 = t_1 \frac{(1 + \frac{\gamma - 1}{2} M_1^2)}{(1 + \frac{\gamma - 1}{2} M_2^2)}$$

$$p_2 = p_1 \frac{(1 + \gamma M_1^2)}{(1 + \gamma M_2^2)}$$

we determine the total pressure and total temperature after the shock.

$$\frac{\alpha(4)}{A^{*'}} = \frac{1}{M_2} \left(\frac{2}{\gamma + 1} + \frac{\gamma - 1}{\gamma + 1} M_2^2 \right)^{\frac{\gamma + 1}{2(\gamma - 1)}}$$

then determines our new sonic reference area $A^{*'}$. Then the subsonic solution to

$$\frac{\alpha(10)}{A^{*'}} = \frac{1}{M} \left(\frac{2}{\gamma + 1} + \frac{\gamma - 1}{\gamma + 1} M^2 \right)^{\frac{\gamma + 1}{2(\gamma - 1)}}$$

determines the exit Mach number and the isentropic relations given above completely determine the exit conditions. Figure (17) shows the steady state Mach number distribution as generated by the LLFV method versus the exact solution for this problem.

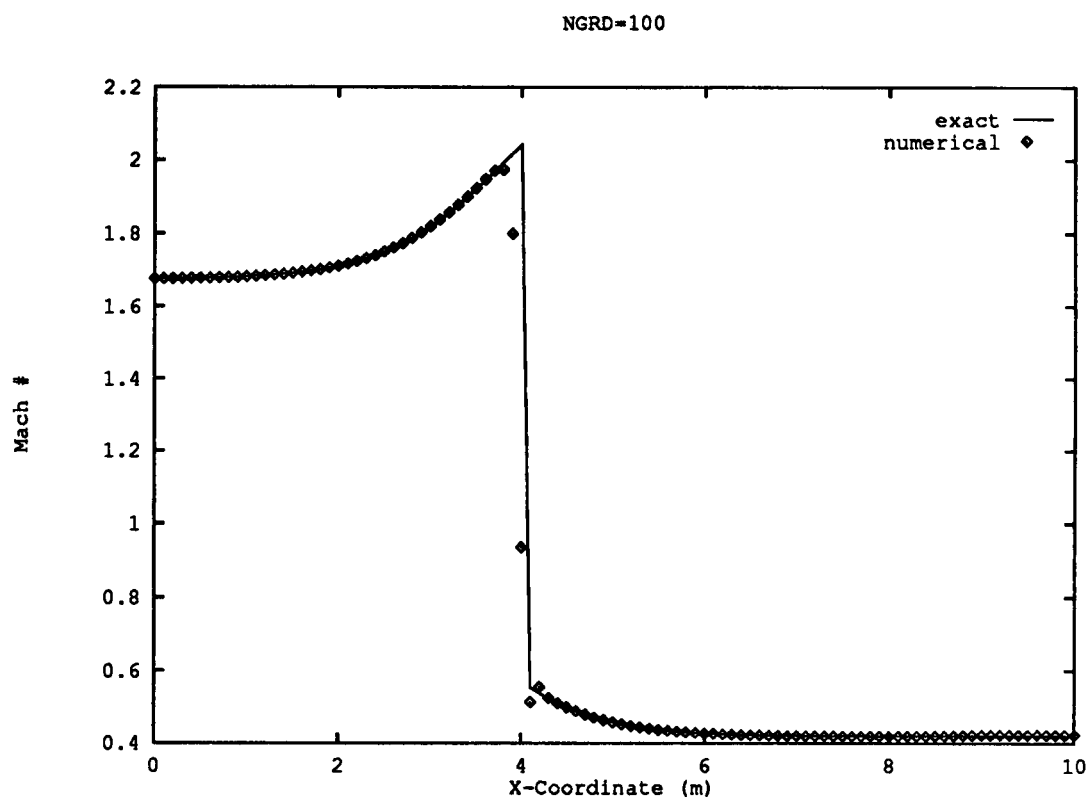


Figure 17. Transonic flow in a diverging duct.

Figure (18) shows the steady state Mach number distribution for the same inlet conditions but with a pure supersonic expansion. In both cases the solution is quite good though a small oscillation appears near the shock in Figure (17).

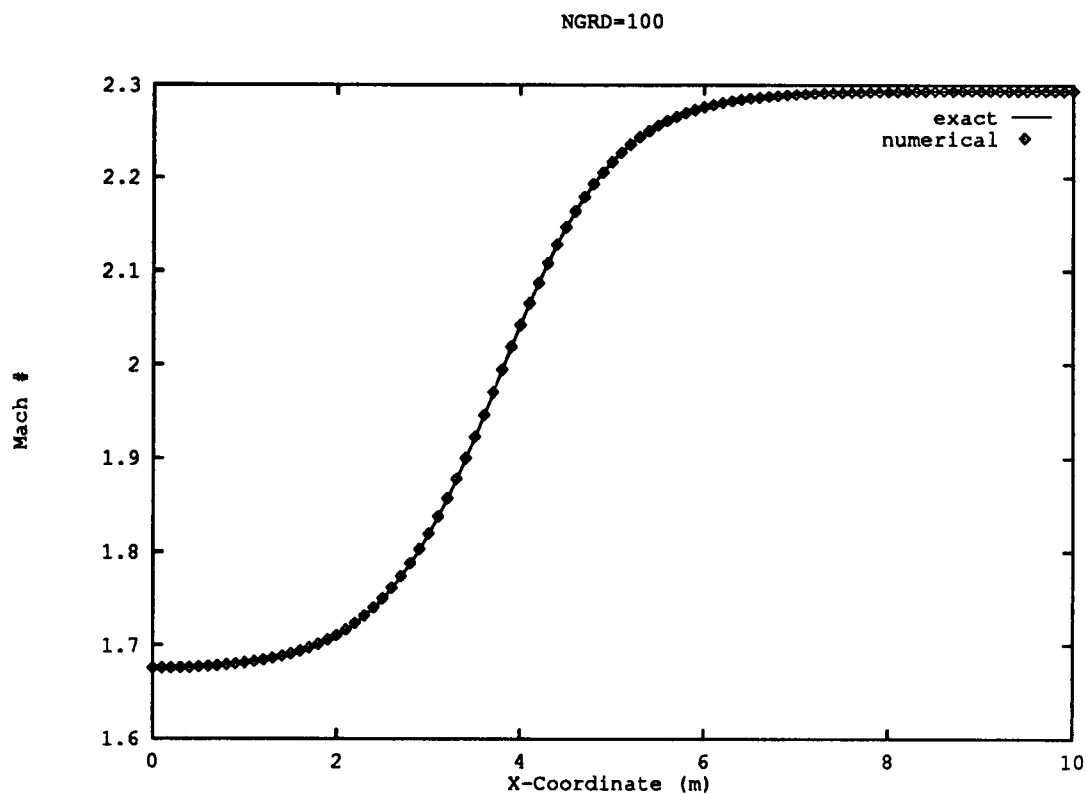


Figure 18. A pure supersonic expansion.

No convergence studies were undertaken. $CN = 1$ was used due to the difficulty in imposing boundary conditions with large time steps. In this thesis effects of various boundary conditions on the LLFV method are not studied.

CHAPTER VI

CONCLUSIONS

The purpose of this thesis was only to formally motivate and document the development of the LLFV algorithm and investigate its viability on some simple fluid flow applications. We have seen that it provides a mathematically elegant, numerically stable method of solution for conservation laws. The results indicate that the accuracy is certainly greater than first order and so it may be categorized as a high order accurate scheme. However, the novelty of the scheme is its most important feature.

The LLFV method captures the entropy satisfying solution to the fluid flow conservation laws without additional terms being included in the discretized form of the original equations and without decoupling the system into characteristic fields. This is a significant achievement.

The main ideas that should be emphasised are the reformulation of the PDE to an ODE which is symmetric about the center of the domain of dependence of the original hyperbolic system, the analytical averaging of the equation to eliminate reliance on pointwise evaluation of quantities, and the use of nonoscillatory approximating functions.

The applications presented here serve only to demonstrate that the basic ideas behind the method are sound. In order to apply the method to realistic

flow problems several significant hurdles must be overcome.

Though extension to two dimensions is foreseeable, extension to three dimensions will undoubtedly prove more cumbersome. Our finite volumes will be in four dimensional space.

The LLFV method has demonstrated its ability to produce stable solutions with large time steps. This is a very desirable feature for steady state applications. Therefore, in any number of dimensions future work must concentrate on implementing boundary conditions in conjunction with small and large time steps.

Even after these problems are solved, there is no guarantee that it will prove superior to existing algorithms.

There is one result that should be mentioned in closing. After absorbing the results presented the reader may be left with a disconcerting feeling about the connection between the approximating functions and the integration of the fluxes. As demonstrated in Chapter III, using piecewise constant approximations for integration purposes and linear interpolation between nodes to determine the fluxes produces a stable algorithm. However, as mentioned, if the piecewise constant approximations are also used for interpolation of the fluxes the algorithm is unstable. This immediately raises the question of whether a simpler slope-limited approximating function, where the slopes are defined by

$$s_j = \minmod(\delta u_{j+1/2}, \delta u_{j-1/2})/h$$

s_j being the slope of the piecewise linear interpolant in the j^{th} cell, δ the central difference operator, would be adequate for the LLFV method in its cell averaged form presented in Chapter IV. The answer is no. The algorithm is not stable when these limiters are used to define the slopes of the approximating function.

Conversely, is the simpler form of the algorithm described in Chapter III stable if we use the approximating functions devised by Harten and Osher[9] and determine the fluxes by interpolation using the same functions? Again the answer is no. Thus, it may be concluded that both integration of the fluxes, and the proper approximating functions are necessary for stability and that neither alone is sufficient.

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REFERENCES

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APPENDIX

APPENDIX

DETAILS ON THE IMPLEMENTATION OF THE ALGORITHM

In this appendix we will discuss the implementation of the algorithm to the shock-tube problem and the quasi-one-dimensional nozzle flow problem discussed in Chapter VI. It is not meant to be a quantitative study of the effects of the numerous twists that can be used in the implementation of the algorithm to these problems. It is meant only to give a qualitative idea of the effects of several different implementations that might occur to someone trying to solve these problems, and most importantly, to document what worked.

To implement the algorithm to the problems mentioned above, four major details must be addressed. They are:

- i) What values are to be used for $Q^{(m)}$, $m = 0$, the initial guess for the LIM iteration?
- ii) How do we initially estimate the ξ locations?
- iii) How do we handle the boundaries of the computational domain?
- iv) What quantities do we update after the residual given by Equation (27) has been computed?

First we will discuss the shock-tube problem. Many of the ideas will carry over

to the nozzle problem.

Let the nodes in the domain of the problem be numbered from 0 to $jmax$. We are only concerned with obtaining a solution at time t such that $Q(ih, t) = Q(ih, 0)$ for $i \in \{0, \dots, left\} \cup \{right, \dots, jmax\}$ where $left$ and $right$ are integers such that $0 < left < right < jmax$. Typically, $left \approx 10\%jmax$ and $right \approx 90\%jmax$. This is simply because we know from the exact solution that the properties remain constant sufficiently far away from the initial discontinuity for a bounded time interval. Physically this is obvious since the information is being propagated by waves of finite speed. Denote the l^{th} component of the numerical solution at time t and spatial locations j by Q_j^l and the exact value as EX_j^l . For comparison purposes, define

$$ER = \left(\sum_{j=0}^{jmax} \sum_{l=1}^3 \frac{(Q_j^l - EX_j^l)^2}{3(jmax + 1)} \right)^{1/2}.$$

To solve the coupled system, Equation (14), by the LIM we must have an initial guess for the solution at t^{n+1} , that is $Q^{(0)}$. Two different methods have been tried. The simplest is just to let $Q_j^{(0)} = Q_j^n \forall j$. The second method is more involved.

To justify it and other results I rely on the assumption developed in Chapter II that locally, $Q(x_j, t^{n+1})$ is approximately equal to the value of Q at t^n along the pathline intersecting (x_j, t^{n+1}) . I also assume that Q does not vary much locally, which is a good assumption in most parts of the domain.

With these assumptions $\underline{R}_j \approx \overline{R}_j \approx \frac{h\Delta t}{2}$ and $\delta\xi_j \approx h$. So

$$\begin{aligned}\bar{u}_j &= \left\{ \frac{\underline{R}_j}{\delta\xi_j} \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u(x, t^n) dx + \frac{\overline{R}_j}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx \right\} / (\underline{R}_j + \overline{R}_j) \\ &\approx \frac{1}{2h} \left\{ \int_{\xi_{j-1/2}}^{\xi_{j+1/2}} u(x, t^n) dx + \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx \right\} \\ &\approx \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx = \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{Q_2(x, t^{n+1})}{Q_1(x, t^{n+1})} dx.\end{aligned}$$

Again, since Q doesn't vary much locally,

$$\begin{aligned}&\frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx \\ &= \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{Q_2(x, t^{n+1})}{Q_1(x, t^{n+1})} dx \approx \frac{Q_2(x_j, t^{n+1})}{Q_1(x_j, t^{n+1})} dx \approx u_j^{n+1}.\end{aligned}$$

Now, suppose $\xi_j \in [x_m, x_{m+1}]$. Consistent with our assumptions, $u(\xi_j, t^n)$ can be reasonably well estimated by linear interpolation between $u(x_m, t^n)$ and $u(x_{m+1}, t^n)$. Denoting $u(x_m, t^n)$ by u_m^n and $u(x_{m+1}, t^n)$ by u_{m+1}^n , we can write

$$u(\xi_j, t^n) \approx (u_{m+1}^n - u_m^n) \frac{(\xi_j - x_m)}{h} + u_m^n,$$

and from our first hypothesis $u(\xi_j, t^n) \approx u_j^{n+1}$. Then

$$\xi_j \approx (u_j^{n+1} - u_m^n) \frac{h}{(u_{m+1}^n - u_m^n)} + x_m$$

and since

$$\xi_j = jh - \bar{u}_j \Delta t \approx jh - u_j^{n+1} \Delta t$$

we have

$$u_j^{n+1} \approx \frac{(j-m)u_{m+1}^n + (m+1-j)u_m^n}{1 + (u_{m+1}^n - u_m^n) \frac{\Delta t}{h}}.$$

Now, choose m near j and evaluate u_j^{n+1} from the above expression. Then $\xi_j \approx jh - u_j^{n+1}\Delta t$ can be evaluated. If $\xi_j \in [x_m, x_{m+1}]$, we have satisfied the relationship. If not, we repeat the process until the correct m is found. When it is, we linearly interpolate the components of Q at the ξ_j locations for our initial guess.

$$Q_j^{(0)} = Q^l(\xi_j, t^n) \quad \text{for } l \in \{1, 2, 3\}, j \in \{left, \dots, right\}.$$

It was found that if the solutions computed using the two different initialization procedures converged, then ER in both solutions differed by less than 1%. However, the algorithm is capable of producing good solutions at relatively high CN numbers. For instance, a fairly smooth solution could be obtained on typical problems[7] with $CN = 6$. In the cases where a large CN is used, the linear initialization procedure described above would lead to a converged solution. In contrast, the first method mentioned, zero order time extrapolation, results in a divergent solution.

It is now an appropriate time to note several other points.

When using a large CN , it is necessary to give the code a 'soft start'. We choose a small CN to start with, CN_i . Typically $CN_i = 0.1$. Then we gradually increase this to CN by taking 5 or 10 time steps with the temporary value of CN , CN_{temp} , given by a cubic polynomial with a local minimum of CN_i and a local maximum of CN .

When using very large time steps it is also necessary to under-relax the residual given by RHS in Equation (27) with a typical under-relaxation parameter of 0.4. This may be explained by the analysis leading to Equation (31). Of course this slows convergence at each time step. Much research has determined that 3 symmetric sweeps of the LIM are sufficient to obtain a converged solution. With under-relaxation, instead of using 3 symmetric sweeps, the domain is swept until the quantity

$$\sum_{j=left}^{right} \sum_{i=1}^3 \frac{(\frac{RHS_{i,j}^*}{coeff})^2}{3(right - left)}$$

where $coeff$ is determined by either Equation (32) or (33), is sufficiently small, typically less than 100.

Now we address the question of how to initially estimate the ξ locations.

After initializing the dependant variable at the beginning of each time step, we make the following approximations.

$$\bar{u}_j \approx \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx$$

and

$$\bar{u}_{j+1/2} \approx \frac{1}{h} \int_{x_j}^{x_{j+1}} u(x, t^{n+1}) dx.$$

Then the ξ locations are determined using these values.

For the shock-tube problem, the boundaries of the domain can be considered the nodes $left - 1$ and $right + 1$. In order to apply the algorithm to the nodes

$\{left, \dots, right\}$ we must have knowledge of ξ_{left-1} and $\xi_{right+1}$. Since we are concerned with solving the problem for times t such that the solution is constant in a neighborhood of the points (x_j, t) , for $j \in \{0, \dots, left\} \cup \{right, \dots, jmax\}$ (in fact $u = 0$), we may assume that $\underline{R}_j \approx \bar{R}_j$ for such j . Again

$$\int_{\xi_{j-1/2}}^{\xi_{j+1/2}} Q(x, t^n) dx \approx \int_{x_{j-1/2}}^{x_{j+1/2}} Q(x, t^{n+1}) dx.$$

So we fix $\xi_j = jh - \bar{u}_j \Delta t$ where

$$\bar{u}_j = \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^{n+1}) dx$$

for $j = left - 1, right + 1$.

Now we turn to the question of what quantities to update after the residual given by Equation (23) has been computed and the current value of $Q_j^{(m)}$ has been updated.

The structure of the limiters used in the approximating functions is such that the scheme has 5 point coupling at the $n+1$ time level for fixed ξ locations. Since the interpolants are linear in each cell the ξ_j locations are independent of the slopes of the interpolants, for fixed $\xi_{j+1/2}$. However, the $\xi_{j+1/2}$ locations are not independent of the slopes of interpolants for fixed ξ_j . Therefore, this suggests that we should update the limiters at x_j and its 4 neighboring nodes. Then ξ_j and $\xi_{i+1/2}$ for $i \in \{j-3, \dots, j+2\}$. Of course it should not hurt to update as many ξ locations as we please, but it is computationally inefficient.

In practice, observations indicate that the scheme converges just as fast when only ξ_j and $\xi_{j\pm 1/2}$ are updated. Here again, convergence was judged by using three symmetric sweeps at each time step and comparing ER for each solution. Varying the number of ξ 's updated typically accounted for a change of less than 1% in ER .

It might occur to the inquisitive reader that the order in which the ξ 's are updated might effect convergence. In all investigations the $\xi_{i+1/2}$ locations were updated in a left to right sequence. No studies were undertaken to observe any effects of varying this sequence. Whether ξ_j or $\xi_{j\pm 1/2}$ were updated first proved to have no effect.

As mentioned previously, most of the techniques used in the shock-tube problem are applicable to the nozzle flow problem which we now address.

There is some conceptual difficulty in dealing with boundaries. For example, at an inflow boundary, using large time steps would lead to pathlines extending out of the computational domain to their intersections with the previous time level. The LLVF method has demonstrated the potential to be particularly useful in maintaining stable solutions with large time steps. More research will be necessary before these problems are overcome.

The quasi-one-dimensional nozzle flow problem is solved in order to test how the algorithm performs on a steady state equation with a source term. Of course convergence speed is intimately linked with the time step size, never the

less, to circumvent the problem of boundary conditions for the time being, the following methods are used.

With the techniques described for the shock-tube problem the exit boundary presents no problem though we must specify how the quantities in cell j_{max} are to be determined. Just substitute $left = j_{max} - 1$ in the previous discussion to locate the ξ 's. This is justified since the area of the nozzle is practically constant in the neighborhood of the exit, hence nearly uniform flow in this region. So, combining this with the observation that we are only interested in a steady state solution justifies the approximation

$$\bar{u}_{j_{max}} \approx \frac{1}{h} \int_{x_{j_{max}-1/2}}^{x_{j_{max}+1/2}} u(x, t^{n+1}) dx,$$

at least for small time steps.

Since we want ξ_{left-1} to remain in our domain, we simply set $left = 2$, use the exact solution at nodes 0 and 1 for supersonic inflow, and restrict CN so that $CN \leq 1$. This is consistent with the theory of Riemann invariants since no information may propagate from the interior upstream in supersonic flow. Then since the area in the neighborhood of the entrance is also nearly constant we assume

$$\bar{u}_1 \approx \frac{1}{h} \int_{x_{1/2}}^{x_{3/2}} u(x, t^{n+1}) dx.$$

In this manner ξ_{left-1} and $\xi_{right+1}$ are approximated initially. However, since the solution is changing this may be too gross an approximation particularly at

the exit boundary. Therefore, to update $\xi_{left-1} = \xi_1$ and $\xi_{right+1} = \xi_{jmax}$ we use

$$\bar{u}_1 \approx \frac{1}{2h} \int_{x_{1/2}}^{x_{3/2}} u(x, t^{n+1}) dx + \frac{1}{2h} \int_{\xi_1 - \frac{h}{2}}^{\xi_1 + \frac{h}{2}} u(x, t^n) dx$$

and

$$\bar{u}_{jmax} \approx \frac{1}{2h} \int_{x_{jmax-1/2}}^{x_{jmax+1/2}} u(x, t^{n+1}) dx + \frac{1}{2h} \int_{\xi_{jmax} - \frac{h}{2}}^{\xi_{jmax} + \frac{h}{2}} u(x, t^n) dx.$$

Regardless of supersonic or subsonic outflow, the exit boundary conditions are set using the theory of Riemann invariants. When quantities are extrapolated from the interior they are always extrapolated to the exit boundary using first order extrapolation in space. In the case of a subsonic exit, if the exit pressure was simply fixed and ρ and ρu were extrapolated from the interior, waves appeared to propagate from the boundary into the interior. However, subsonic exit boundary conditions based on Riemann invariants do work well.

No test cases involving subsonic inflow have been considered. Though these ideas may adapt themselves to this problem, they will have to be carefully considered.

VITA

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