Energy Estimates for Nonlinear Conservation Laws with Applications to Solutions of the Burgers Equation and One-Dimensional Viscous Flow in a Shock Tube by Central Difference Schemes

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Abstract

This work revisits an idea that dates back to the early days of scientific computing, the energy method for stability analysis. It is shown that if the scalar non-linear conservation law

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

is approximated by the semi-discrete conservative scheme

$$\frac{du_j}{dt} + \frac{1}{\Delta x}\left(f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}\right) = 0$$

then the energy of the discrete solution evolves at exactly the same rate as the energy of the true solution, provided that the numerical flux is evaluated by the formula

$$f_{j+\frac{1}{2}} = \int_0^1 f(\hat{u}) d\theta$$

where

$$\hat{u}(\theta) = u_j + \theta(u_{j+1} - u_j).$$

With careful treatment of the boundary conditions, this provides a path to the construction of non-dissipative stable discretizations of the governing equations. If shock waves appear in the solution, the discretization must be augmented by appropriate shock operators to account for the dissipation of energy by the shock waves. In the case of the viscous Burgers equation, it is also shown that shock waves can be fully resolved by non-dissipative discretizations of this type with a fine enough mesh, such that the cell Reynolds number ≤ 2. The results are extended to the equations of gas dynamics. Two schemes are proposed, entropy preserving (EP) and kinetic energy preserving (KEP). Both are applied to the direct numerical simulation of one-dimensional viscous flow in a shock-tube.

1 Introduction

A prime focus in the development of computational fluid dynamics (CFD) for aeronautics has been the simulation of transonic and supersonic flows which generally contain shock waves, contact discontinuities and slip-lines. The need to capture discontinuities without introducing oscillations has driven the development of a comprehensive theory for the formulation of shock capturing schemes, stemming from the pioneering work of Godunov [1], and including contributions by Boris, Van Leer, Roe, Harten, Liou and Jameson, among others [2, 3, 4, 5, 6, 7, 8]. These schemes generally add artificial diffusion either explicitly, or implicitly via upwind operators, in order to satisfy total variation diminishing (TVD) or local extremum diminishing (LED) properties [7, 8]. However, they suffer the drawback that the artificial diffusion may degrade the accuracy of viscous flow simulations. On the other hand it seems that if the conservation law has an accompanying energy estimate, it should be possible to construct discrete schemes which satisfy the same estimate, and must therefore be stable without the need to introduce artificial diffusion, at least as long as the solution remains smooth.

The use of energy estimates to establish the stability of discrete approximations to initial value problems has a long history. The energy method is discussed in the classical book by Morton and Richtmyer [10], and it has been emphasized by the Uppsala school under the leadership of Kreiss and Gustafsson. Consider a well posed intitial value problem of the form

$$\frac{du}{dt} = Lu \tag{1.1}$$

where u is a state vector, and L is a linear differential operator in space with approximate boundary conditions. Then forming the inner product with u,

$$\left(u, \frac{du}{dt}\right) = \frac{1}{2}\frac{d}{dt}(u,u) = (u, Lu) \tag{1.2}$$

If L is skew self-adjoint, $L^* = -L$, and the right hand side is

$$\frac{1}{2}(u, Lu) + \frac{1}{2}(u, L^*u) = 0$$

Then the energy $\frac{1}{2}(u,u)$ cannot increase.

If (1.1) is approximated in semi-discrete form on a mesh as

$$\frac{dv}{dt} = Av \tag{1.3}$$

where v is the vector of the solution values of the mesh points, the corresponding energy balance is

$$\frac{1}{2}\frac{d}{dt}(v^T v) = v^T A v \tag{1.4}$$

and stability is established if

$$v^T A v \leq 0 \tag{1.5}$$

A powerful approach to the formulation of discretizations with this property is to construct A in a manner that allows summation by parts (SBP) of $v^T Av$, annihilating all interior contributions, and leaving only boundary terms. Then one seeks boundary operators such that (1.5) holds. In particular suppose that A is split as

$$A = D + B$$

where D is an interior operator and B is a boundary operator. Then if D is skew-symmetric, $D^T = -D$, the contribution $v^T Dv$ vanishes leaving only the boundary terms.

Skew-symmetric and SBP operators of both second and higher order have been devised for a variety of problems. The benefits of kinetic energy preserving schemes for the treatment of incompressible viscous flow has also been emphasized by Moin and Stanford's Center for Turbulence Research. Honein and Moin have also examined skew-symmetric schemes for compressible flow [11]. SBP operators are typically constructed by splitting the equations into a part in conservation form and a part in quasilinear form. For example, the inviscid Burgers equation is written as

$$\frac{\partial u}{\partial t} + \frac{2}{3}\frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) + \frac{1}{3}u\frac{\partial u}{\partial x} = 0$$

Then the use of second order central difference operators for both parts at every interior point, and one sided operators at each boundary yields an SBP operator.

In nonlinear problems for which the solution may develop shock waves it is generally beneficial to preserve conservation form in the discretization. According to the theorem of Lax and Wendroff [12], this will assure that the discrete solution satisfies the correct shock jump conditions, provided that it converges in the limit as the mesh interval is reduced to zero. In any case it is highly desirable to maintain global conservation properties of the

true solution in the discrete solution. Small errors in the global conservation of mass, for example, can lead to large errors in the solution of flows in ducts.

The author has developed general procedures for constructing semi-discrete schemes for conservation laws in conservation form such that the discrete solution also exactly satisfies a discrete global conservation law for a generalized energy or entropy function. In order to take advantage of this approach, it is first necessary to identify an appropriate energy principle for the governing equations. If shock waves appear in the solution the energy principle will need to be modified to allow for their effect on the energy or entropy balance. Moreover, in the light of Godunov's theorem that monotonically varying discrete shocks can only be obtained by locally first-order accurate schemes, the basic discretization scheme will need to be augmented by appropriate shock operators.

Section 2 presents the formulation for a general nonlinear conservation law for a scalar state variable,

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

assuming that the flux $f(u)$ is a convex function of u. An energy estimate is derived for solutions containing shock waves. Then it is shown that a semi-discrete equation in the conservation form

$$\Delta x_j \frac{du_j}{dt} + f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} = 0$$

satisfies a corresponding discrete energy estimate if the numerical flux is calculated as

$$f_{j+\frac{1}{2}} = \int_0^1 f\left(\hat{u}(\theta)\right) d\theta$$

where

$$\hat{u}(\theta) = u_j + \theta \left(u_{j+1} - u_j\right)$$

The theory is verified by numerical tests for the Burgers equation. In the inviscid case the scheme needs to be augmented by a shock operator to prevent the growth of oscillations near the shock. In the viscous case it is shown that the shock will be fully resorved by the central difference scheme if a sufficiently fine mesh is used.

In inviscid compressible fluid flow the total energy, consisting of the sum of the internal and kinetic energy, is conserved, not just the kinetic energy. Correspondingly, it follows from the governing equations that entropy is conserved if no shock waves are formed. In a recent paper [13] the author showed that a semi-discrete scheme in conservation form can be constructed so that it globally conserves a generalized entropy function in a smooth

flow. Such an entropy preserving (EP) scheme is obtained by an appropriate formulation of the numerical fluxes across the interfaces between the grid cells. It requires the use of entropy variables in the evaluation of the flux, although the standard conservative variables are updated at each time step. There is some latitude in the definition of the generalized entropy function $h(u)$ of the state vector u. Harten [14] has given conditions guaranteeing that $h(u)$ is a convex function, so that the solution cannot become unbounded if $h(u)$ remains bounded. Multiplying the governing equations for $\frac{\partial u}{\partial t}$ by $w^T = \frac{\partial h}{\partial u}$ then produces the evolution equation for $\frac{\partial h}{\partial t}$, while w^T represents the entropy variables. Entropy variables have been used by Hughes, Mallet and Franca [15], and also by Gerritsen and Olsson [16], who proposed a non conservative entropy preserving scheme.

Although a bound on the kinetic energy does not assure a bound on the solution in a compressible flow, correct simulation of the evolution of kinetic energy is a crucial requirement for accurate simulations of turbulence, where there is an energy cascade between the different eddy scales. In another paper [17] the author has shown that the interface fluxes of a semi-discrete conservative scheme can be constructed in an alternative way which assures that the global discrete kinetic energy evolves in a manner that exactly corresponds to the true equation for kinetic energy. There is some latitude in the definition of the fluxes for such a kinetic energy preserving (KEP) scheme, provided that the fluxes for the continuity and momentum equations satisfy a compatibility condition. Section 3 presents the formulation of these schemes for the one-dimensional gas dynamics equations.

In Section 4 both the EP and the KEP schemes are applied to the direct numerical simulation (DNS) of one-dimensional viscous flow in a shock tube. It is demonstrated in numerical experiments that both schemes can successfully resolve the shock wave, contact discontinuity and expansion fan without adding any artificial diffusion, provided that a fine enough mesh is used with a number of cells of the order of the Reynolds number. Numerical results for simulations at Reynolds number of 25000 based on the speed of sound on a mesh with 4096 cells indicate that the KEP scheme performs better than the EP scheme for this flow. Both schemes can be extended to multi-dimensional finite volume discretizations on general grids. The proofs are given in [13] and [17].

2 Energy estimates and conservative central difference schemes for one-dimensional scalar conservation laws

Consider the scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \tag{2.1}$$

$$u(x,0) = u_0(x),$$

$$u \qquad \text{specified at inflow boundaries.}$$

Writing (2.1) in the quasilinear form

$$\frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0$$

where $a(u) = \frac{\partial f}{\partial u}$, it can be seen that it describes the propagation of u along characteristics

$$x - a(u)t = \xi$$

at the wave speed $a(u)$. We shall restrict attention to the case where $f(u)$ is a convex function of u such that $\frac{\partial f^2}{\partial u^2} > 0$, and $a(u_L) > a(u_R)$ if $u_L > u_R$. Then shock waves may appear in the solution if waves overrun each other and the characteristics converge. A shock with left and right states u_L and u_R satisfies the jump condition

$$f_R - f_L = s\,(u_R - u_L) \tag{2.2}$$

where s is the shock speed, and the entropy condition that $u_L > u_R$.

Correspondingly, smooth solutions of (2.1) also satisfsy

$$\frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x} F(u) = 0 \tag{2.3}$$

where

$$F_u = u f_u$$

since multiplying (2.1) by u yields

$$u\frac{\partial u}{\partial t} + u f_u \frac{\partial u}{\partial x} = 0$$

Defining the energy as

$$E = \int_a^b \frac{u^2}{2} dx$$

it follows from (2.3) that smooth solutions of (2.1) satisfy the energy equation

$$\frac{dE}{dt} = F(u_a) - F(u_b) \tag{2.4}$$

Introducing the function $G(u)$ such that

$$G_u = f$$

and multiplying (2.1) by u we obtain

$$\begin{aligned} u\frac{\partial u}{\partial t} + u\frac{\partial f}{\partial x} &= \frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x}(uf) - f\frac{\partial u}{\partial x} \\ &= \frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x}(uf) - G_u\frac{\partial u}{\partial x} \\ &= \frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x}(uf - G) \\ &= 0 \end{aligned}$$

Thus F and G can be identified as

$$F = uf - G, \qquad G = uf - F \tag{2.5}$$

For the inviscid Burgers equation

$$F = \frac{u^3}{3}, \qquad G = \frac{u^3}{6}$$

If shock waves appear in the solution the estimate (2.4) no longer holds. Consider a solution containing a shock wave with left and right states u_L and u_R, with corresponding flux vectors

$$f_L = f(u_L), \qquad f_R = f(u_R)$$

Equation (2.1) should then be integrated separately on each side of the shock wave. Moreover there is an additional contribution to $\frac{dE}{dt}$ due to the shock motion at the speed

$$s = \frac{f_R - f_L}{u_R - u_L}$$

This is

$$s\left(\frac{u_L^2}{2}-\frac{u_R^2}{2}\right)=-\frac{1}{2}\left(f_R-f_L\right)\left(u_R+u_L\right)$$

Thus

$$\frac{dE}{dt}=F\left(u_a\right)-F\left(u_L\right)+F\left(u_R\right)-F\left(u_b\right)-\frac{1}{2}\left(f_R-f_L\right)\left(u_R+u_L\right)$$

Substituting formula (2.5) for F, we find that the contribution due to the shock wave is

$$\left.\frac{dE}{dt}\right|_s=G\left(u_R\right)-G\left(u_L\right)-\frac{1}{2}\left(f_R+f_L\right)\left(u_R-u_L\right)$$

Suppose now that $f=\frac{\partial G}{\partial u}$ is evaluated as an average in the sense of Roe [4] between the states u_L and u_R such that

$$\bar{f}\left(u_R,u_L\right)\left(u_R-u_L\right)=G\left(u_R\right)-G\left(u_L\right) \tag{2.6}$$

Then

$$\left.\frac{dE}{dt}\right|_s=-\left\{\frac{1}{2}\left(f_R+f_L\right)-\bar{f}\left(u_R,u_L\right)\right\}\left(u_L-u_R\right) \tag{2.7}$$

The Roe average can be evaluated as

$$\bar{f}\left(u_R,u_L\right)=\int_0^1 f\left(\hat{u}(\theta)\right)d\theta \tag{2.8}$$

where

$$\hat{u}(\theta)=u_L+\theta\left(u_R-u_L\right) \tag{2.9}$$

since then

$$\begin{aligned} G\left(u_R\right)-G\left(u_L\right) &= \int_0^1 G_u\left(\hat{u}(\theta)\right)\hat{u}_\theta d\theta \\ &= \int_0^1 G_u\left(\hat{u}(\theta)\right)d\theta\left(u_R-u_L\right) \end{aligned}$$

Under the assumption that $f(u)$ is a convex function of u,

$$\bar{f}\left(u_R,u_L\right)<\frac{1}{2}\left(f_R+f_L\right) \tag{2.10}$$

because

$$\frac{1}{2}\left(f_R+f_L\right)=\int_0^1\left(f_L+\theta\left(f_R,f_L\right)\right)d\theta$$

and for $0 < \theta < 1$

$$f\left(\hat{u}(\theta)\right) < f_L + \theta\left(f_R - f_L\right)$$

It then follows from equation (2.7) that a shock wave always removes energy.

For the inviscid Burgers equation

$$\left.\frac{dE}{dt}\right|_s = -\frac{1}{12}\left(u_L - u_R\right)^3$$

Suppose now that (2.1) is discretized on a grid with cell intervals Δx_j, $j = 1, n$. Consider a semi-discrete conservative scheme of the form

$$\Delta x_j \frac{du_j}{dt} + \left(f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}\right) = 0 \tag{2.11}$$

where the numerical flux $f_{j+\frac{1}{2}}$ is a function of u_i over a range bracketing u_j such that $f_{j+\frac{1}{2}} = f(u)$ whenever u is substituted for the u_i, thus satisfying Lax's consistency condition. Multiplying (2.11) by u_j and summing by parts over the interior points we obtain

$$\begin{aligned}\sum_{j=1}^{n} \Delta x_j u_j \frac{du_j}{dt} &= -\sum_{j=1}^{n} u_j (f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}) \\ &= u_1 f_{\frac{1}{2}} - u_n f_{n+\frac{1}{2}} + \sum_{j=1}^{n-1} f_{j+\frac{1}{2}}(u_{j+1} - u_j)\end{aligned}$$

Now define the numerical flux as

$$f_{j+\frac{1}{2}} = G_{u_{j+\frac{1}{2}}} \tag{2.12}$$

where $G_{u_{j+\frac{1}{2}}}$ is the mean value of G_u in the range from u_j to u_{j+1} such that

$$G_{u_{j+\frac{1}{2}}}(u_{j+1} - u_j) = G(u_{j+1}) - G(u_j) \tag{2.13}$$

This is realized by formula (2.8) with $u_L = u_j$, $u_R = u_{j+1}$. Then, denoting $G(u_j)$ by G_j,

$$\begin{aligned}\sum_{j=1}^{n} \Delta x_j u_j \frac{du_j}{dt} &= u_1 f_{\frac{1}{2}} - u_n f_{n+\frac{1}{2}} + \sum_{j=1}^{n-1} (G_{j+1} - G_j) \\ &= u_1 f_{\frac{1}{2}} - u_n f_{n+\frac{1}{2}} - G_1 + G_n\end{aligned}$$

Now let the boundary fluxes be evaluated as

$$f_{\frac{1}{2}} = f(u_1), \qquad f_{n+\frac{1}{2}} = f(u_n)$$

and define the discrete approximation to the energy as

$$E = \sum_{j=1}^{n} \Delta x_j \frac{u_j^2}{2} \tag{2.14}$$

Then finally

$$\frac{dE}{dt} = u_1 f_1 - u_n f_n - G_1 + G_n = F_1 - F_n \tag{2.15}$$

Thus the energy balance (2.4) is exactly recovered by the discrete scheme. Equations (2.12) and (2.13) are satisfied by evaluating the numerical flux by the Roe average (2.8) between the states u_j and u_{j+1}. Thus we have established Theorem 2.1:

Theorem 2.1 *If the scalar conservation law* (2.1) *is approximated by the semi-discrete conservative scheme* (2.11)*, it also satisfies the semi-discrete energy conservation law* (2.15) *if the numerical flux* $f_{j+\frac{1}{2}}$ *is evaluated by equations* (2.8) *and* (2.9)*.*

It follows from (2.10) that $f_{j+\frac{1}{2}}$ is strictly less than the arithmetic average $\frac{1}{2}(f(u_{j+1}) + f(u_j))$ if $u_{j+1} \neq u_j$.

In the case of Burgers equation formulas (2.8) and (2.9) yield the numerical flux

$$f_{j+\frac{1}{2}} = \frac{u_{j+1}^2 + u_{j+1}u_j + u_j^2}{6} \tag{2.16}$$

and

$$\frac{1}{2}(f(u_{j+1}) + f(u_j)) - f_{j+\frac{1}{2}} = \frac{1}{12}(u_{j+1} - u_j)^2$$

The formulation so far does not include the boundary conditions. Suppose that boundary data $u = g_0$ should be imposed at x_0 if the left boundary x_0 is an inflow boundary, and correspondingly $u = g_n$ should be imposed at x_n if the right boundary x_n is an inflow boundary. It is convenient to introduce the positive and negative wave speeds

$$a^+(u) = \max(a(u), 0), \qquad a^-(u) = \min(a(u), 0)$$

Then we modify the equations at the boundary points by adding simultaneous approximation

terms (SAT), so that we solve for u_1 and u_n by the equations

$$\begin{aligned} \Delta x_1 \frac{du_1}{dt} + (f_{\frac{3}{2}} - f_{\frac{1}{2}}) + \tau a_0^+ (u_0 - g_0) = 0 \\ \Delta x_n \frac{du_n}{dt} + (f_{n+\frac{1}{2}} - f_{n-\frac{1}{2}}) - \tau a_0^- (u_n - g_n) = 0 \end{aligned} \tag{2.17}$$

where the parameter τ determines the amount of the penalty if the boundary condition is not satisfied exactly. It is shown in [13] that the choice $\tau = 2$ ensures that the rate of change of the discrete energy does not exceed the rate of change of the true energy.

Numerical experiments have been conducted to verify the stability of the semi-discrete scheme (2.11) and (2.16) with the boundary conditions (2.17) for the solution of the inviscid Burgers equation. Shu's total variation diminishing (TVD) scheme [18], was used for time integration. Writing the semi-discrete scheme in the form

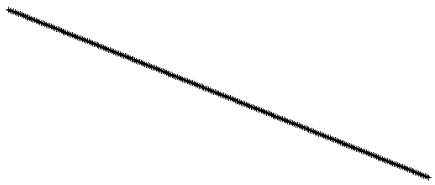
$$\frac{du}{dt} + R(u) = 0 \tag{2.18}$$

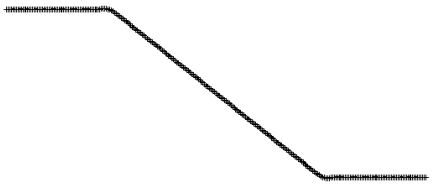
where $R(u)$ represents the discretized spatial derivative, this advances the solution during one time step by the three stage scheme

$$\begin{aligned} u^{(1)} &= u^{(0)} - \Delta t\, R(u^{(0)}) \\ u^{(2)} &= \frac{3}{4}u^{(0)} + \frac{1}{4}u^{(1)} - \frac{1}{4}\Delta t\, R(u^{(1)}) \\ u^{(3)} &= \frac{1}{3}u^{(0)} + \frac{2}{3}u^{(2)} - \frac{2}{3}\Delta t\, R(u^{(2)}) \end{aligned}$$

where $u^{(0)}$ and $u^{(3)}$ denote the solution of the beginning and the end of the time step. If (2.18) satisfies the TVD property with forward Euler time stepping, Shu's scheme is also TVD for time steps satisfying the CFL condition $|a|\frac{\Delta t}{\Delta x} \leq 1$.

Figure 2.1 displays snap shots of the solution with initial data $u = -x$ in $[-1, 1]$ at times $t = 0, .5, 1, 1.5$ using a grid with 256 intervals. The true solution is a straight line connecting wave fronts moving inwards from both boundaries at unit speed until a shock is formed at $t = 1$. It can be seen that the discrete solution closely tracks the true solution prior to the formation of the shock. After the shock is formed the discrete solution develops strong oscillations in a zone expanding outward from the shock towards both boundaries. This is consistent with the fact that according to equation (2.15), the discrete energy continues to grow at the rate $\frac{2}{3}t$ when $t > 1$ as illustrated in Figure 2.2, and the energy must be absorbed in the solution.



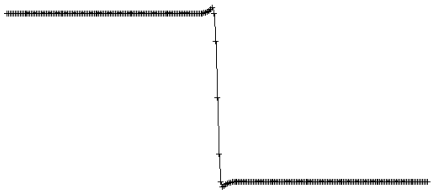


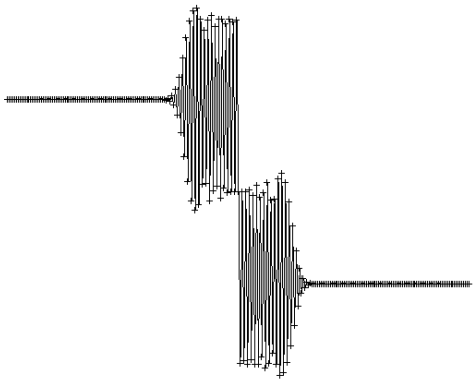
SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
256 CELLS 0 CYCLES
CFL 0.500 RAVG 0.000E+00

SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
256 CELLS 128 CYCLES
CFL 0.500 RAVG 0.803E+00

(a) At $t = 0.0$

(b) At $t = 0.5$





SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
256 CELLS 256 CYCLES
CFL 0.500 RAVG 0.363E+01

SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
256 CELLS 384 CYCLES
CFL 0.500 RAVG 0.405E+01

(c) At $t = 1.0$

(d) At $t = 1.5$

Figure 2.1: Evolution of the solution of the Burgers equation

It is evident that the scheme must be modified to preserve stability in the presence of shock waves. It is well known from shock capturing theory [7, 8], that oscillations in the neighborhood of shock waves are eleminated by schemes which are local extremum dimin-

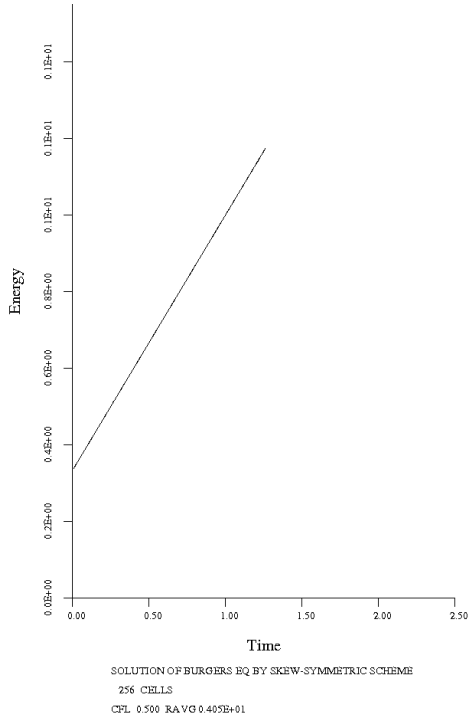


Figure 2.2: Discrete energy growth

ishing (LED) or total variation diminishing (TVD). A semi-discrete scheme is LED if it can be expressed in the form

$$\frac{du_i}{dt} = \sum_j a_{ij}(u_j - u_i) \tag{2.19}$$

where the coefficients $a_{ij} \geq 0$, and the stencil is compact, $a_{ij} \neq 0$ when i and j are not nearest neighbors. This property is satisfied by the upwind scheme in which the numerical flux (2.16) is replaced by

$$f_{j+\frac{1}{2}} = \begin{cases} u_j^2 & \text{if} \quad a_{j+\frac{1}{2}} > 0 \\ u_{j+1}^2 & \text{if} \quad a_{j+\frac{1}{2}} < 0 \\ \frac{1}{2}(u_{j+1}^2 + u_j^2) & \text{if} \quad a_{j+\frac{1}{2}} = 0 \end{cases} \tag{2.20}$$

where the numerical wave speed is evaluated as

$$a_{j+\frac{1}{2}} = \frac{1}{2}(u_{j+1} + u_j) \tag{2.21}$$

Moreover, the upwind scheme (2.20) admits a stationary numerical shock structure with a

single interior point.

The LED condition only needs to be satisfied in the neighborhoods of local extrema, which may be detected by a change of sign in the first differences $\Delta u_{j+\frac{1}{2}} = u_{j+1} - u_j$. A shock operator which meets these requirements can be constructed as follows. The numerical flux (2.16) can be converted to the upwind flux (2.20) by the addition of a diffusive term of the form

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} \Delta u_{j+\frac{1}{2}}.$$

The required coefficient is

$$\alpha_{j+\frac{1}{2}} = \frac{1}{4} |u_{j+1} + u_j| - \frac{1}{12} (u_{j+1} - u_j) \tag{2.22}$$

In order to detect an extremum introduce the function

$$R(u, v) = \left| \frac{u - v}{|u| + |v|} \right|^q$$

where q is an integer power. $R(u, v) = 1$ whenever u and v have opposite signs. When $u = v = 0$, $R(u, v)$ should be assigned the value zero. Now set

$$s_{j+\frac{1}{2}} = R\left(\Delta u_{j+\frac{3}{2}}, \Delta u_{j-\frac{1}{2}}\right) \tag{2.23}$$

so that $s_{j+\frac{1}{2}} = 1$ when $\Delta u_{j+\frac{3}{2}}$ and $\Delta u_{j-\frac{1}{2}}$ have opposite signs which will generally be the case if either u_{j+1} or u_j is an extremum. In a smooth region where $\Delta u_{j+\frac{3}{2}}$ and $\Delta u_{j-\frac{1}{2}}$ are not both zero, $s_{j+\frac{1}{2}}$ is of the order Δx^q, since $\Delta u_{j+\frac{3}{2}} - \Delta u_{j-\frac{1}{2}}$ is an undivided difference. In order to avoid activating the switch at smooth extrema, and also to protect against division by zero, $R(u, v)$ may be redefined as

$$R(u, v) = \left| \frac{u - v}{\max\{(|u| + |v|), \epsilon\}} \right| \tag{2.24}$$

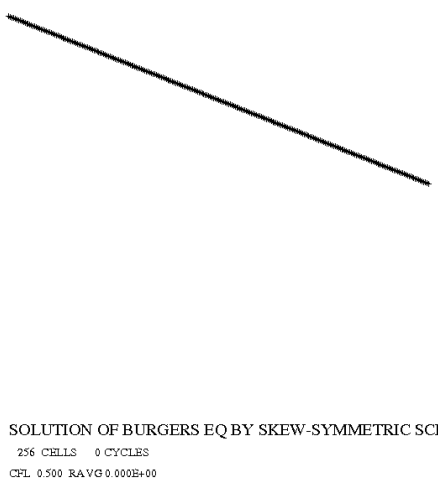
where ϵ is a tolerance [7].

Finally the diffusion term is modified to

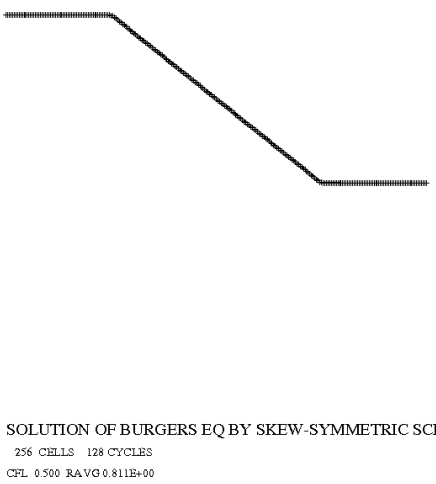
$$d_{j+\frac{1}{2}} = \max(s_{j+\frac{3}{2}}, s_{j+\frac{1}{2}}, s_{j-\frac{1}{2}}) \alpha_{j+\frac{1}{2}} \Delta u_{j+\frac{1}{2}}$$

Thus the coeffcient is reduced to a magnitude of order Δx^q in smooth regions, while it has the value $\alpha_{j+\frac{1}{2}}$ in the neighborhood of a shock. The value $q = 8$ has proved satisfactory in

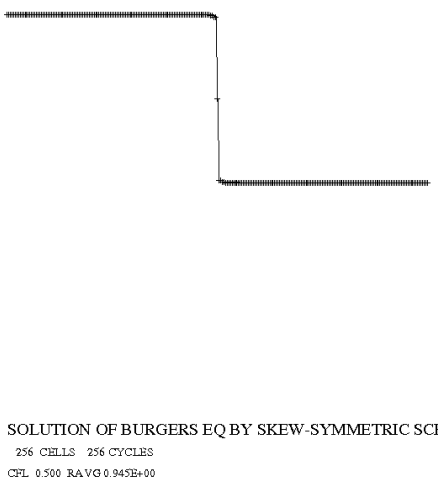
numerical experiments.



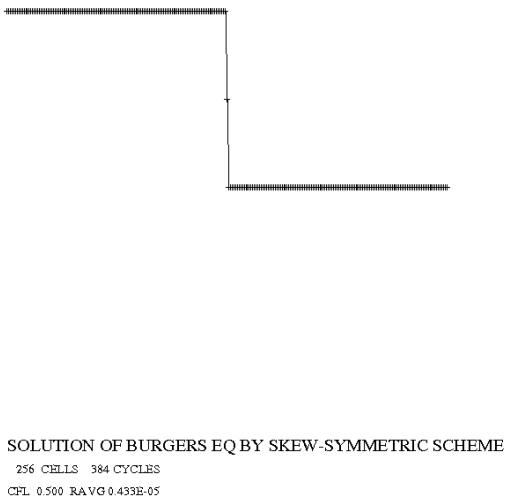
(a) At $t = 0.0$



(b) At $t = 0.5$



(c) At $t = 1.0$



(d) At $t = 1.5$

Figure 2.3: Evolution of the solution of the Burgers equation with a switch

Figure 2.3 shows the evolution of the discrete solution for the same case as Figure 2.1, with initial data $u = -x$ in $[-1, 1]$, using the shock operator defined by equations (2.22-2.24).

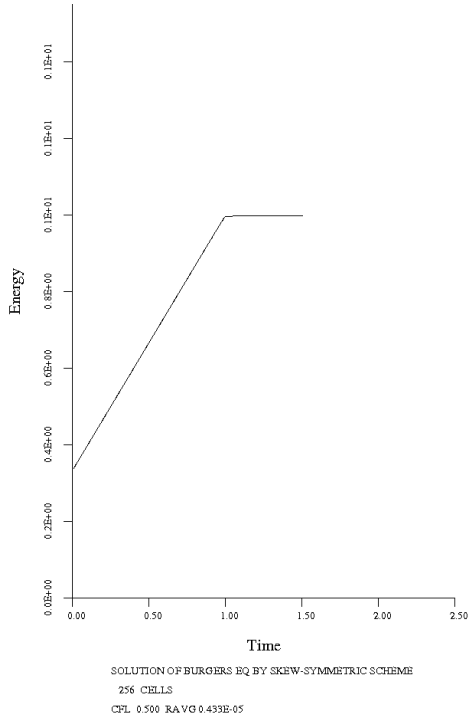


Figure 2.4: Discrete energy growth with a limiter

A stationary shock with a single interior point is formed when $t = 1$ as expected. Figure 2.4 confirms that the discrete energy grows at the rate $\frac{2t}{3}$ until the shock forms and then remains constant. The difference between the discrete energy and the true energy of the stationary solution is $-\frac{1}{2}\Delta x$ because of the zero value in the middle of the discrete shock. Once the numerical shock structure is established the additional diffusive terms only contribute to $\frac{du_j}{dt}$ at the three points $s-1$, s and $s+1$ comprising the shock, for which

$$u_{s-1} = 1, \qquad u_s = 0, \qquad u_{s+1} = -1$$

The only non-zero values of $\Delta u_{j+\frac{1}{2}}$ are

$$\Delta u_{s-\frac{1}{2}} = -1, \qquad \Delta u_{s+\frac{1}{2}} = -1$$

Also

$$\begin{aligned} a_{s-\frac{1}{2}} &= -\frac{1}{2}, & \alpha_{s-\frac{1}{2}} &= \frac{1}{3} \\ a_{s+\frac{1}{2}} &= -\frac{1}{2}, & \alpha_{s+\frac{1}{2}} &= \frac{1}{3} \end{aligned}$$

Thus the additional contribution to $\frac{dE}{dt}$ due to the shock is

$$\begin{aligned}\sum_{s=-1}^{1} u_s \left(\alpha_{s+\frac{1}{2}} \Delta u_{s+\frac{1}{2}} - \alpha_{s-\frac{1}{2}} \Delta u_{s-\frac{1}{2}}\right) &= \alpha_{s-\frac{1}{2}} u_{s-1} \Delta u_{s-\frac{1}{2}} - \alpha_{s+\frac{1}{2}} u_{s+1} \Delta u_{s+\frac{1}{2}} \\ &= -\frac{2}{3}\end{aligned}$$

This exactly cancels the contribution of $\frac{2}{3}$ from the boundaries, so that the total rate of change of the discrete energy is zero.

In the case of the viscous Burgers equation with the viscosity coefficient ν

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = \nu \frac{\partial^2 u}{\partial x} \tag{2.25}$$

the energy balance is modified by the viscous dissipation. Multiplying by u, and integrating the right hand side by parts with $\frac{\partial u}{\partial x} = 0$ at each boundary, the energy balance equation assumes the form

$$\frac{dE}{dt} = \frac{u_a^3}{3} - \frac{u_b^3}{3} - \nu \int_a^b \left(\frac{\partial u}{\partial x}\right)^2 dx \tag{2.26}$$

instead of (2.4). Suppose that $\frac{\partial^2 u}{\partial x^2}$ is discretized by a central difference operator at interior points with one sided formulas at the boundaries corresponding to $\frac{\partial u}{\partial x} = 0$, as proposed by Mattsson [19]. Then summing by parts with the convective flux evaluated by (2.16) as before, the discrete energy balance is found to be

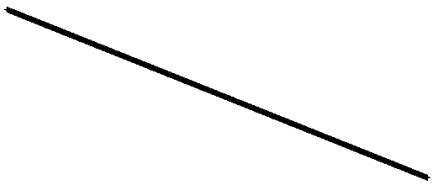
$$\frac{dE}{dt} = \frac{u_1^3}{3} - \frac{u_n^3}{3} - \nu \sum_{j=1}^{n-1} (u_{j+1} - u_j)^2 \tag{2.27}$$

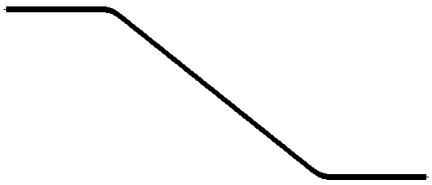
This enables the possibility of fully resolving shock waves without the need to add any additional numerical diffusion via shock operators. The convective flux difference $f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}$ can be factored as

$$\frac{1}{3\Delta x}(u_{j+1} + u_j + u_{j-1})(u_{j+1} - u_{j-1})$$

Accordingly the semi-discrete approximation to equation (2.25) can written as

$$\frac{du_j}{dt} = a_{j+\frac{1}{2}}(u_{j+1} - u_j) + a_{j-\frac{1}{2}}(u_{j-1} - u_j) \tag{2.28}$$



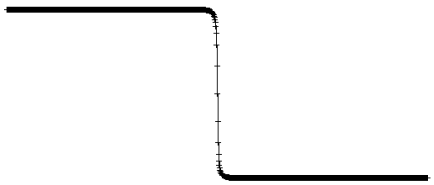


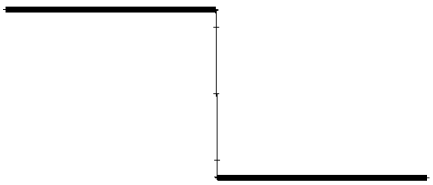
SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
1024 CELLS 0 CYCLES
CFL 0.500 RAVG 0.000E+00

SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
1024 CELLS 512 CYCLES
CFL 0.500 RAVG 0.779E+00

(a) At $t = 0.0$

(b) At $t = 0.5$





SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
1024 CELLS 1024 CYCLES
CFL 0.500 RAVG 0.231E+01

SOLUTION OF BURGERS EQ BY SKEW-SYMMETRIC SCHEME
1024 CELLS 1536 CYCLES
CFL 0.500 RAVG 0.923E-14

(c) At $t = 1.0$

(d) At $t = 1.5$

Figure 2.5: Evolution of the solution of the viscous Burgers equation

where

$$a_{j+\frac{1}{2}} = \frac{\nu}{\Delta x^2} - \frac{u_{j+1} + u_j + u_{j-1}}{3\Delta x}$$

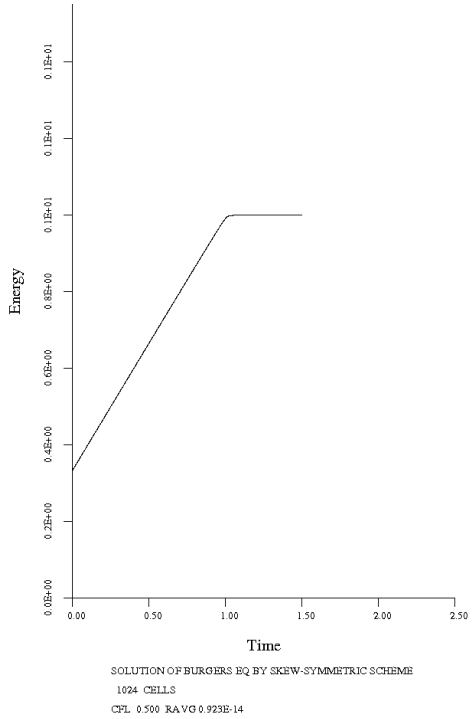


Figure 2.6: Discrete energy growth for the viscous Burgers equation

and

$$a_{j-\frac{1}{2}} = \frac{\nu}{\Delta x^2} + \frac{u_{j+1} + u_j + u_{j-1}}{3\Delta x}$$

The semi-discrete approximation satisfies condition (2.19) for a local extremum diminishing scheme if $a_{j+\frac{1}{2}} \geq 0$ and $a_{j-\frac{1}{2}} \geq 0$. This establishes theorem 2.2:

Theorem 2.2 *The semi-discrete approximation* (2.11) *using the numerical flux* (2.16) *and the central difference operator for* $\frac{\partial^2 u}{\partial x^2}$ *is local extremum diminishing if the cell Reynolds number satisfies the condition*

$$\frac{\bar{u}\Delta x}{\nu} \leq 2 \tag{2.29}$$

where the local speed is evaluated as

$$\bar{u} = \frac{1}{3}\left|u_{j+1} + u_j + u_{j-1}\right| \tag{2.30}$$

It has been confirmed by numerical experiments that shock waves are indeed fully resolved with no oscillation if the cell Reynolds number satisfies condition (2.29). Figure 2.5 shows the evolution of the discrete viscous Burgers equation using this scheme for the same

initial data as before, $u = -x$ in $[-1, 1]$. The Reynolds number $\frac{uL}{\nu}$ based on the boundary velocity $u = \pm 1$ and the length of the interval was 2048, and the solution was calculated on a uniform mesh with 1024 intervals, so that the cell Reynolds number condition (2.29) was satisfied in the entire domain. It can be seen that a stationary shock wave is formed at the time $t = 1$, and it is finally resolved with three interior points. Correspondingly the energy becomes constant after the shock wave is formed, as can be seen in Figure 2.6.

3 Entropy and kinetic energy preserving schemes for the one-dimensional gas dynamics equations

This section presents the formulation of fully conservative schemes for one-dimensional gas dynamics which are either entropy preserving (EP) or kinetic energy preserving (KEP). In both cases the global conservation property is obtained by proper construction of the interface flux between each pair of neighboring cells. The detailed proofs for these schemes have been given in [13] and [17], but in order to facilitate the comparison of the EP and KEP schemes they are outlined here for the one-dimensional gas dynamics equations.

Consider the gas dynamics equations in the conservation form

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \tag{3.1}$$

Here the state and flux vectors are

$$u = \begin{bmatrix} \rho \\ \rho v \\ \rho E \end{bmatrix}, \qquad f = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ \rho v H \end{bmatrix} \tag{3.2}$$

where ρ is the density, v is the velocity and p, E and H are the pressure, energy and enthalpy. Also

$$p = (\gamma - 1)\rho \left(E - \frac{v^2}{2} \right), \qquad H = E + \frac{p}{\rho} \tag{3.3}$$

where γ is the ratio of specific heats.

In the absence of shock waves the entropy

$$s = \log \left(\frac{p}{\rho^\gamma} \right) \tag{3.4}$$

is constant, satisfying the advection equation

$$\frac{\partial s}{\partial t} + v \frac{\partial s}{\partial x} = 0 \tag{3.5}$$

Consider the generalized entropy function

$$h(s) = \rho g(s) \tag{3.6}$$

where it has been shown by Harten [14] that h is a convex function of u provided that

$$\frac{d^2g}{ds^2}\Big/\frac{dg}{ds} < \frac{1}{\gamma} \tag{3.7}$$

Then h satisfies the entropy conservation law

$$\frac{\partial}{\partial t}h(u) + \frac{\partial}{\partial x}F(u) = 0 \tag{3.8}$$

where the entropy flux is

$$F = \rho v g(s) \tag{3.9}$$

Moreover, introducing the entropy variables

$$w^T = \frac{\partial h}{\partial u} \tag{3.10}$$

it can be verified that

$$h_u f_u = F_u$$

and hence on multiplying (3.1) by w^T we recover the entropy conservation law (3.8) where now the Jacobian matrix

$$\frac{\partial f}{\partial w} = f_u u_w$$

is symmetric. Accordingly f can be expressed as the gradient of a scalar function G,

$$f = \frac{\partial G}{\partial w} \tag{3.11}$$

and the entropy flux can be expressed as

$$F = f^T w - G \tag{3.12}$$

Different choices of the entropy function $g(s)$ have been discussed by Harten [14], Hughes, Franca and Mallet [15], and Gerritsen and Olsson [16].

Suppose now that (3.1) is approximated in semi-discrete form on a grid with cell intervals Δx_j, $j = 1, n$ as

$$\Delta x_j \frac{du_j}{dt} + f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} = 0 \tag{3.13}$$

where the numerical flux $f_{j+\frac{1}{2}}$ is a function of u_i over a range of i bracketing j. In order to construct an entropy preserving (EP) scheme multiply (3.13) by w^T and sum by parts to

obtain

$$\begin{aligned}\sum_{j=1}^{n} \Delta x_j w_j^T \frac{du_j}{dt} &= -\sum_{j=1}^{n} \Delta x_j w_j^T \left(f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} \right) \\ &= w_1^T f_{\frac{1}{2}} - w_n^T f_{n+\frac{1}{2}} + \sum_{j=1}^{n-1} f_{j+\frac{1}{2}}^T \left(w_{j+1} - w_j \right)\end{aligned}$$

At interior points evaluate $f_{j+\frac{1}{2}}^T$ as the mean value of $G_{w_{j+\frac{1}{2}}}$ in the sense of Roe [4] such that

$$G_{w_{j+\frac{1}{2}}} \left(w_{j+1} - w_j \right) = G\left(w_{j+1} \right) - G\left(w_j \right) \tag{3.14}$$

Also evaluate the boundary fluxes as

$$f_{\frac{1}{2}} = f\left(w_1 \right), \quad f_{n+\frac{1}{2}} = f\left(w_n \right) \tag{3.15}$$

Then the interior fluxes cancel, and using (3.10) and (3.12), we obtain the entropy conservation law in the discrete form

$$\sum_{j=1}^{n} \Delta x_j \frac{dh_j}{dt} = F\left(w_1 \right) - F\left(w_n \right) \tag{3.16}$$

$G_{w_{j+\frac{1}{2}}}$ can be constructed to satisfy (3.14) exactly by evaluating it as the integral

$$G_{w_{j+\frac{1}{2}}} = \int_0^1 G_w \left(\hat{w}(\theta) \right) d\theta \tag{3.17}$$

where

$$\hat{w}(\theta) = w_j + \theta \left(w_{j+1} - w_j \right) \tag{3.18}$$

since then

$$\begin{aligned}G\left(w_{j+1} \right) - G\left(w_j \right) &= \int_0^1 G_w \left(\hat{w}(\theta) \right) w_\theta d\theta \\ &= \int_0^1 G_w \left(\hat{w}(\theta) \right) d\theta \left(w_{j+1} - w_j \right)\end{aligned}$$

Thus we obtain:

Theorem 3.1 *The semi-discrete conservation law* (3.13) *satisfies the semi-discrete entropy*

conservation law (3.16) *if the numerical flux is calculated as*

$$f_{j+\frac{1}{2}} = \int_0^1 f\hat{w}(\theta)d\theta, \quad j = 1, n-1$$

where $\hat{w}(\theta)$ *is defined by* (3.18)*, and the boundary fluxes are defined by* (3.15)

The construction of a kinetic energy preserving (KEP) scheme requires a different approach in which the fluxes of the continuity and momentum equations are separately constructed in a compatible manner. Denoting the specific kinetic energy by k,

$$k = \rho\frac{v^2}{2}, \quad \frac{\partial k}{\partial u} = \left[-\frac{v^2}{2}, v, 0\right]$$

Thus

$$\begin{aligned} \frac{\partial k}{\partial t} &= v\frac{\partial}{\partial t}(\rho v) - \frac{v^2}{2}\frac{\partial \rho}{\partial t} \\ &= -\frac{\partial}{\partial x}\left\{v\left(p + \rho\frac{v^2}{2}\right)\right\} + p\frac{\partial v}{\partial x} \end{aligned} \tag{3.19}$$

Suppose that the semi-discrete conservation scheme (3.13) is written separately for the continuity and momentum equations as

$$\Delta x_j \frac{d\rho_j}{dt} + (\rho v)_{j+\frac{1}{2}} - (\rho v)_{j-\frac{1}{2}} = 0 \tag{3.20}$$

$$\Delta x_j \frac{d}{dt}(\rho v)_j + (\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} + p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} = 0 \tag{3.21}$$

Now multiplying (3.20) by $\frac{v_j^2}{2}$ and (3.21) by v_j, adding them and summing by parts,

$$\begin{aligned}
\sum_{j=1}^{n} \Delta x_j \left(v_j \frac{d}{dt}(\rho v)_j - \frac{v_j^2}{2} \frac{d\rho_j}{dt} \right) &= \sum_{j=1}^{n} \Delta x_j \frac{d}{dt} \left(\rho_j \frac{v_j^2}{2} \right) \\
&= \sum_{j=1}^{n} \frac{v_j^2}{2} \left((\rho v_j)_{j+\frac{1}{2}} - (\rho v_j)_{j-\frac{1}{2}} \right) - \sum_{j=1}^{n} v_j \left((\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} \right) \\
&\quad - \sum_{j=1}^{n} v_j \left(p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} \right) \\
&= - \frac{v_1^2}{2} (\rho v)_{\frac{1}{2}} + v_1 (\rho v^2)_{\frac{1}{2}} + v_1 p_{\frac{1}{2}} + \frac{v_n^2}{2} (\rho v)_{n+\frac{1}{2}} - v_n (\rho v^2)_{n+\frac{1}{2}} - v_n p_{n+\frac{1}{2}} \\
&\quad + \sum_{j=1}^{n-1} \left\{ \frac{1}{2} (\rho v)_{j+\frac{1}{2}} \left(v_{j+1}^2 - v_j^2 \right) - \frac{1}{2} (\rho v^2)_{j+\frac{1}{2}} \left(v_{j+1} - v_j \right) \right\} \\
&\quad + \sum_{j=1}^{n-1} p_{j+\frac{1}{2}} \left(v_{j+1} - v_j \right) \qquad (3.22)
\end{aligned}$$

Each term in the first sum containing the convective terms can be expanded as

$$\left\{ (\rho v)_{j+\frac{1}{2}} \frac{v_{j+1} + v_j}{2} - (\rho v^2)_{j+\frac{1}{2}} \right\} \left(v_{j+1} - v_j \right)$$

and will vanish if

$$(\rho v^2)_{j+\frac{1}{2}} = (\rho v)_{j+\frac{1}{2}} \frac{v_{j+1} + v_j}{2} \qquad (3.23)$$

Now evaluating the boundary fluxes as

$$\begin{array}{lllllllll}
(\rho v)_{\frac{1}{2}} & = & \rho_1 v_1 & , & (\rho v^2)_{\frac{1}{2}} & = & \rho_1 v_1^2 & , & p_{\frac{1}{2}} & = & p_1 \\
(\rho v)_{n+\frac{1}{2}} & = & \rho_n v_n & , & (\rho v^2)_{n+\frac{1}{2}} & = & \rho_n v_n^2 & , & p_{n+\frac{1}{2}} & = & p_n
\end{array} \qquad (3.24)$$

(3.22) reduces to the semi-discrete kinetic energy conservation law

$$\begin{aligned}
\sum_{j=1}^{n} \Delta x_j \left(\rho_j \frac{v_j^2}{2} \right) &= v_1 \left(p_1 + \rho_1 \frac{v_1^2}{2} \right) - v_n \left(p_n + \rho_n \frac{v_n^2}{2} \right) \\
&\quad + \sum_{j=1}^{n} p_{j+\frac{1}{2}} \left(v_{j+1} + v_j \right) \qquad (3.25)
\end{aligned}$$

Denoting the arithmetic average of any quantity q between $j+1$ and j as

$$\bar{q} = \frac{1}{2}\left(q_{j+1} + q_j\right)$$

the interface pressure may be evaluated as

$$p_{j+\frac{1}{2}} = \bar{p} \tag{3.26}$$

Also if one sets

$$\begin{aligned} (\rho v)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v} && (3.27)\\ \left(\rho v^2\right)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v}^2 && (3.28) \end{aligned}$$

condition (3.23) is satisfied. Consistently one may set

$$(\rho v H)_{j+\frac{1}{2}} = \bar{\rho}\bar{v}\bar{H} \tag{3.29}$$

The foregoing argument establishes

Theorem 3.2 *The semi-discrete conservation law* (3.13) *satisfies the semi-discrete kinetic energy global conservation law* (3.25) *if the fluxes for the continuity and momentum equations satisfy condition* (3.23) *and the boundary fluxes are calculated by equations* (3.24).

Condition (3.23) allows some latitude in the construction of the fluxes. For example it is also satisfied if one sets

$$\begin{aligned} (\rho v)_{j+\frac{1}{2}} &= \overline{\rho v}\\ \left(\rho v^2\right)_{j+\frac{1}{2}} &= \overline{\rho v}\bar{v}\\ (\rho v H)_{j+\frac{1}{2}} &= \overline{\rho v}\bar{H} \end{aligned}$$

instead of equations (3.27−3.29).

4 Direct numerical solution of one-dimensional viscous flow in a shock tube

This section presents the results of numerical experiments in which both the entropy preserving (EP) and the kinetic energy preserving (KEP) schemes have been applied to the direct numerical simulation (DNS) of one-dimensional viscous flow in a shock tube. In Section 2 was shown that shock waves in solutions of the Burgers equation will be cleanly represented if the local cell Reynolds number $Re_c \leq 2$. The compressible Navier-Stokes equations are not amenable to such a simple analysis, but it can still be expected that the number of mesh cells needed to fully resolve shock waves and contact discontinuities will be proportional to the Reynolds number, given that the shock thickness is proportional to the coefficient of viscosity, as has been shown by G.I. Taylor and W.D. Hayes [20, 21].

In the numerical experiments the viscous stress was calculated at each cell interface by discretizing the velocity and temperature gradient on a compact stencil as

$$\left(\frac{\partial v}{\partial x}\right)_{j+\frac{1}{2}} = \frac{1}{\Delta x}\left(v_{j+1} - v_j\right)$$
$$\left(\frac{\partial T}{\partial x}\right)_{j+\frac{1}{2}} = \frac{1}{\Delta x}\left(T_{j+1} - T_j\right)$$

The coefficient of viscosity was calculated as a function of the temperature by Sutherland's law

$$\mu = 1.461 \times 10^{-6} \frac{T^{3/2}}{(T + 110.3)}$$

taking $\lambda = -\frac{2}{3}\mu$, the viscous stress and heat flux assume the form

$$\sigma_{j+\frac{1}{2}} = \frac{4}{3}\mu \left(\frac{\partial u}{\partial x}\right)_{j+\frac{1}{2}}$$
$$q_{j+\frac{1}{2}} = -\kappa \left(\frac{\partial T}{\partial x}\right)_{j+\frac{1}{2}}$$

where the coefficient of heat conduction κ was obtained from the Prandtl number Pr as

$$\kappa = \frac{\mu c_p}{Pr}$$

The Prandtl number was taken to be .75.

Numerical experiments were performed using three different flux formulas

1. Simple averaging:
$$f_{j+\frac{1}{2}} = \frac{1}{2}\left(f\left(u_{j+1}\right) + f\left(u_j\right)\right)$$

2. The entropy preserving (EP) scheme:
$$f_{j+\frac{1}{2}} = \int_0^1 f\left(\hat{w}(\theta)\right) d\theta$$
where w denote the entropy variables and
$$\hat{w}(\theta) = w_j + \theta\left(w_{j+1} - w_j\right)$$

3. The kinetic energy preserving (KEP) scheme:
$$\begin{aligned}\left(\rho v\right)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v} \\ \left(\rho v^2\right)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v}^2 \\ \left(\rho v H\right)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v}\bar{H}\end{aligned}$$

In the EP scheme the entropy variables were taken to be
$$w^T = \frac{\partial h}{\partial u}$$
where
$$h = \rho e^{\frac{s}{\gamma+1}} = \rho\left(\frac{p}{\rho^\gamma}\right)^{\frac{1}{\gamma+1}}$$
Accordingly the entropy variables assume the comparatively simple form
$$w = \frac{p^*}{p}\begin{bmatrix} u_3 \\ -u_2 \\ u_1 \end{bmatrix}, \quad u = \frac{p}{p^*}\begin{bmatrix} w_3 \\ -w_2 \\ w_1 \end{bmatrix}$$
where
$$p^* = \frac{\gamma-1}{\gamma+1}e^{\frac{s}{\gamma+1}} = \frac{\gamma-1}{\gamma+1}\left(\frac{p}{p^\gamma}\right)^{\frac{1}{\gamma+1}}$$

It was remarked in [13] that the energy or entropy preserving property could be impaired by the time discretization scheme. One solution to this difficulty is to use an implicit time-

stepping scheme of Crank-Nicolson type in which the spatial derivatives are evaluated using the average value of the state vectors between the beginning and the end of each time step,

$$\bar{u}_j = \frac{1}{2}\left(u_j^{n+1} + u_j^n\right)$$

This requires the use of inner iterations in each time step. In order to avoid this cost, Shu's total variation diminishing (TVD) scheme [18] was used for the time integration in all the numerical experiments. Writing the semi-discrete scheme in the form

$$\frac{du}{dt} + R(u) = 0 \tag{4.1}$$

where $R(u)$ represents the discretized spatial derivatives, this advances the solution during one time step by the three stage scheme

$$\begin{aligned} u^{(1)} &= u^{(0)} - \Delta t\, R(u^{(0)}) \\ u^{(2)} &= \frac{3}{4}u^{(0)} + \frac{1}{4}u^{(1)} - \frac{1}{4}\Delta t\, R(u^{(1)}) \\ u^{(3)} &= \frac{1}{3}u^{(0)} + \frac{2}{3}u^{(2)} - \frac{2}{3}\Delta t\, R(u^{(2)}) \end{aligned}$$

The test case for the numerical experiments was the well known example originally proposed by Sod [22]. The shock tube extends over the range $0 \le x \le 1$, with a discontinuity in the initial data at $x = .5$. The left and right states are

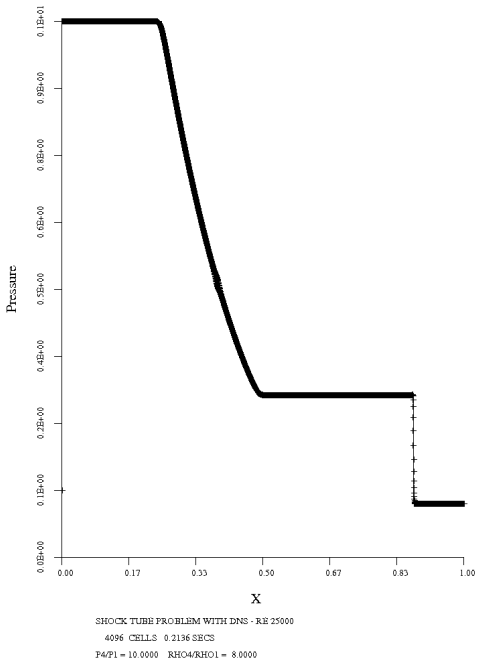
$$\begin{aligned} p_L &= 1.0, & p_R &= .1 \\ \rho_L &= 1.0, & \rho_R &= .125 \\ v_L &= 0, & v_R &= 0 \end{aligned}$$

The Reynolds number is based on the speed of sound of the left state

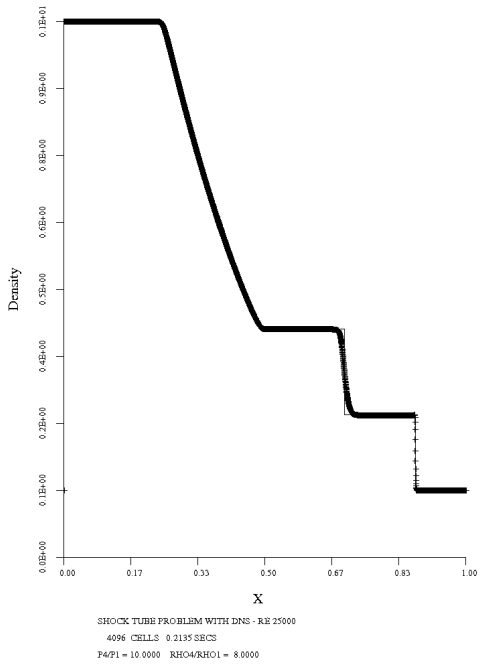
$$Re = \frac{\rho_L c_L}{\mu}, \qquad c_L = \sqrt{\frac{\gamma p_L}{\rho_L}}$$

The numerical experiments confirm that the EP and KEP schemes both enable direct numerical simulation (DNS) of the viscous flow in the shock tube, provided that a fine enough mesh is used, while significant oscillations can be observed in the solution when simple flux averaging is used (scheme 1). It is interesting that the oscillations are primary observed in the expansion region. As a representative example, Figures 4.1−4.3 show the solutions

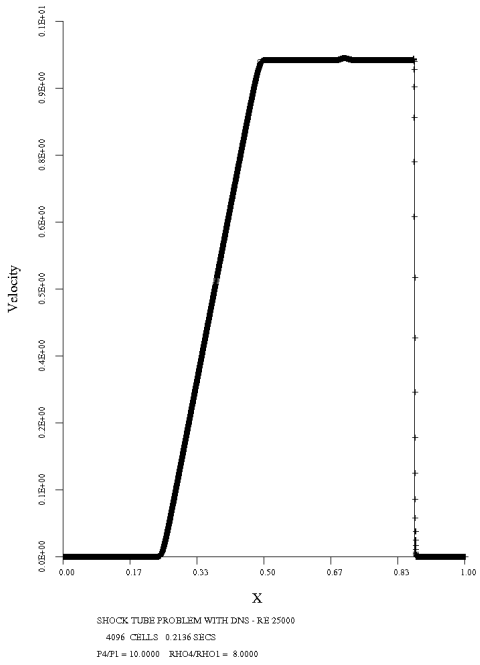
for a Reynolds number $Re = 25000$ which were obtained with the three schemes on a grid with 4096 cells, at the time $t = .2136$. The figures also display the exact inviscid solution with a solid line.With simple flux averaging there are oscillations in the entropy (measured by $\frac{p}{\rho^\gamma} - \frac{p_0}{\rho_0^\gamma}$ of the order of .01. With the EP scheme these oscillations are reduced to the order of .001, while with the KEP scheme they are further reduced to the order of .0001. When the Reynolds number is increased to 1 million, and the calculations are performed on a mesh with 204800 cells, it remains true that the only observable oscillations appear in the expansion region, but with reduced amplitude, while the three schemes exhibit the same order of merit. On the other hand it has been found that the oscillations in the expansion region are amplified as the Reynolds number and number of mesh cells are reduced.



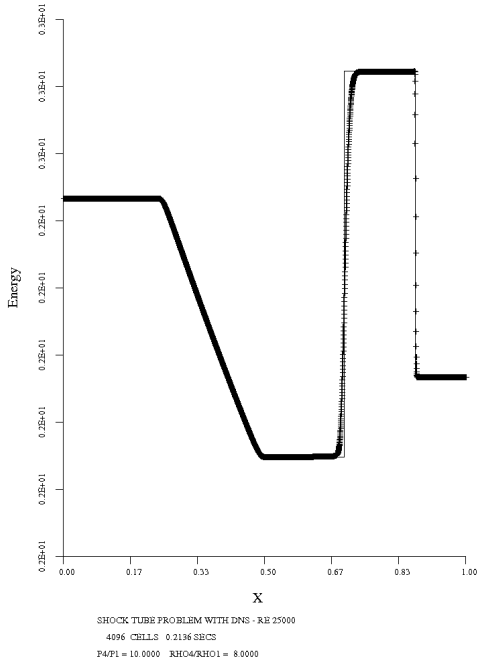
(a) Pressure



(b) Density

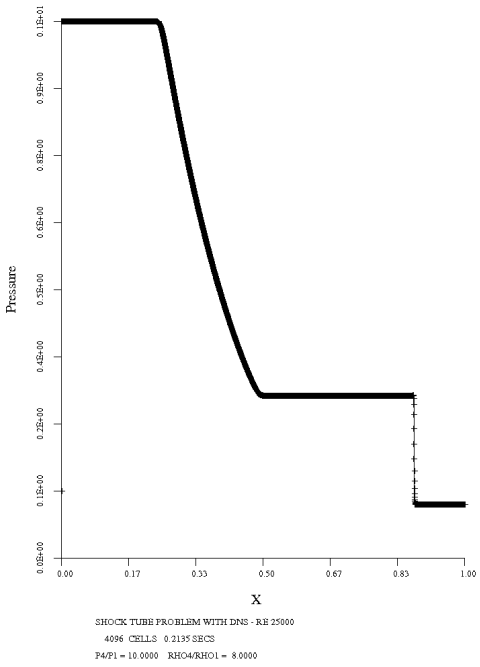


(c) Velocity

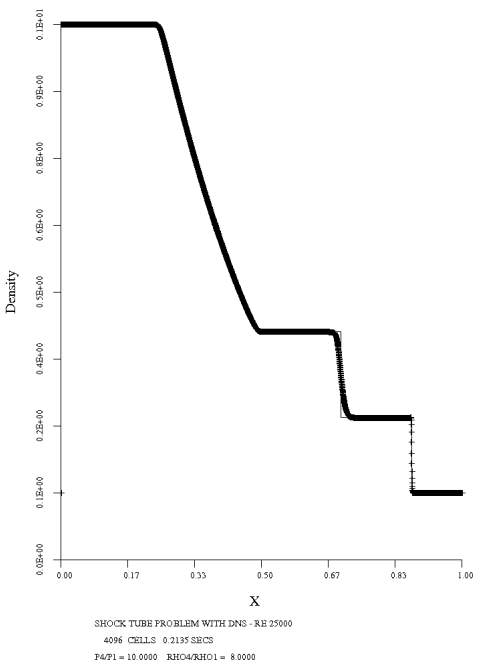


(d) Energy

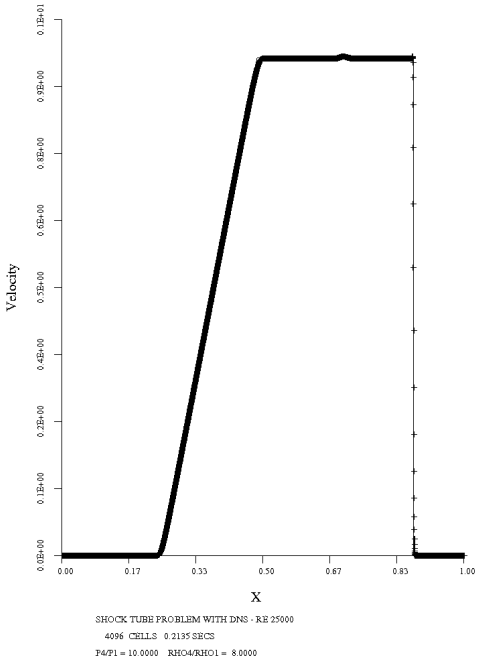
Figure 4.1: Simple averaging of the flux: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −



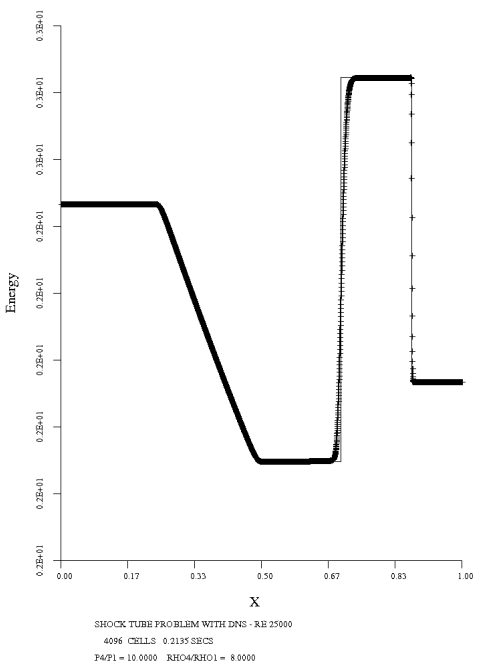
(a) Pressure



(b) Density

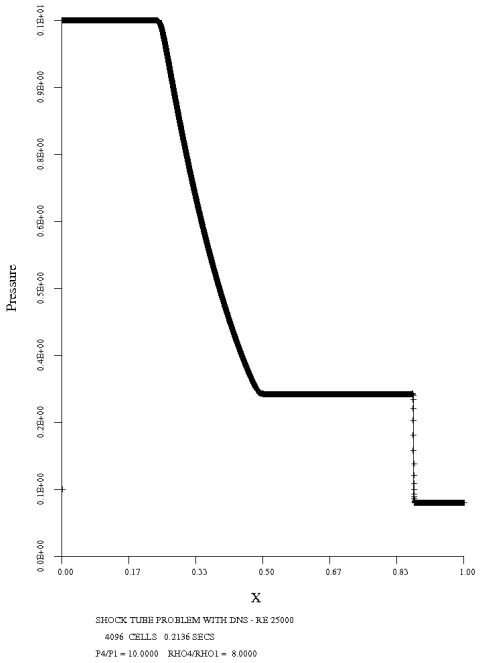


(c) Velocity

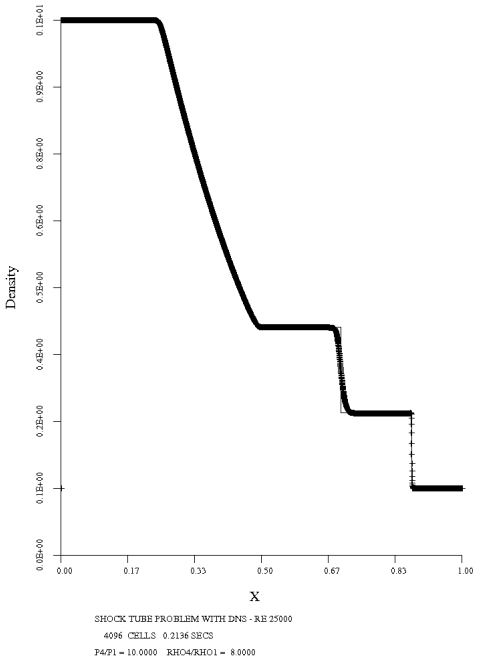


(d) Energy

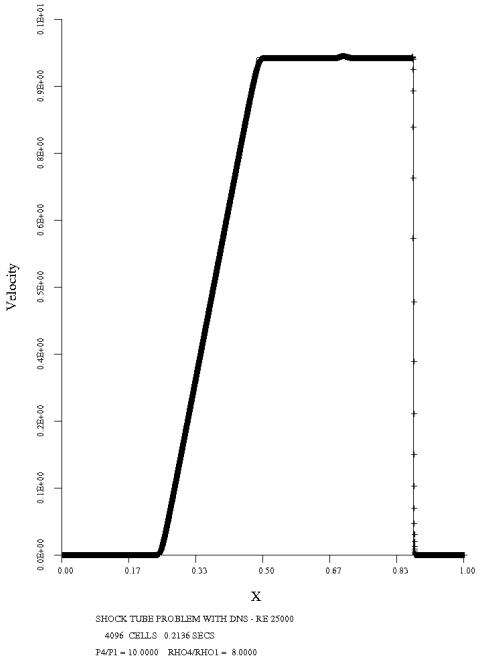
Figure 4.2: Entropy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −



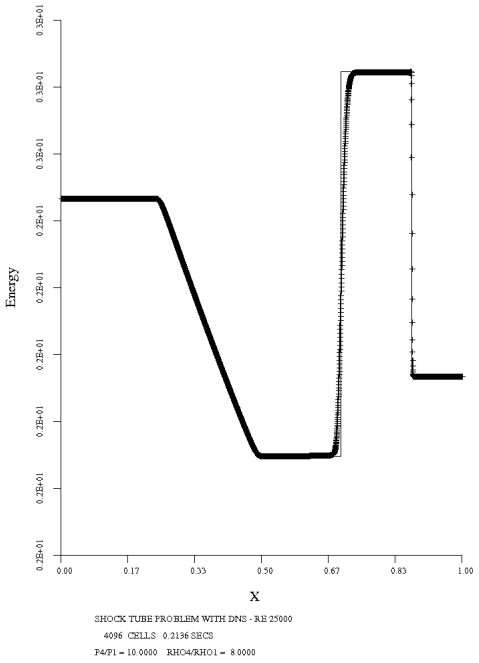
(a) Pressure



(b) Density



(c) Velocity



(d) Energy

Figure 4.3: Kinetic energy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −

5 Conclusion

The derivations in this paper establish that it is possible to construct semi-discrete approximations to the compressible Navier-Stokes equations in conservation form which also discretely conserve either entropy (the EP scheme) or kinetic energy (the KEP scheme). Both these schemes enable the direct numerical simulation of one-dimensional viscous flow in a shock tube, provided that the number of cells in the computational mesh is of the order of the Reynolds number.

The performance of both the EP and the KEP schemes improves as the Reynolds number and the number of mesh cells are simultaneously increased. For the model problem examined in this paper, one-dimensional viscous flow in a shock tube, the KEP scheme performs better than the EP scheme.

The Kolmogoroff scale for the small eddies that can persist in a viscous turbulent flow is of the order of $\frac{1}{Re^{\frac{3}{4}}}$. Accordingly it appears that by using a mesh with the order of Re^3 cells, direct numerical simulation (DNS) of viscous turbulent flow with shock waves will be feasible in the future for high Reynolds number flows. Current high-end computers attain computing speeds of the order of 100 teraflops (10^{14} floating point operations/second). This is about 1 million times faster than high-end computers 25 years ago. A further increase by a factor of million to 10^{20} flops could enable DNS of viscous compressible flow at a Reynolds number of 1 million. This is still short of the flight Reynolds numbers of long range transport aircraft in the range of $50 - 100$ million, but the eventual use of DNS for compressible turbulent flows can clearly be anticipated.

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