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

Antony Jameson

Department of Aeronautics and Astronautics
Stanford University, Stanford, CA

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, 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

$$\frac{du}{dt} = Lu \tag{1}$$

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,

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

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

$$\frac{dv}{dt} = Av \tag{3}$$

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

$$\frac{1}{2}\frac{d}{dt}(v^T v) = v^T Av \tag{4}$$

and stability is established if

$$v^T Av \leq 0 \tag{5}$$

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 $v^T A v$, annihilating all interior contributions, and leaving only boundary terms. Then one seeks boundary operators such that (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 $v^T D v$ vanishes leaving only the boundary terms.

Burgers Equation

The Burgers equation is the simplest example of a nonlinear equation which supports wave motion in opposite directions and the formation of shock awaves, and consequently it provides a very useful example for the analysis of the energy method. Expressed in conservation form, the inviscid Burgers equation is

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0, \qquad a \leq x \leq b, \tag{6}$$

where

$$f(u) = \frac{u^2}{2} \tag{7}$$

and the wave speed is

$$a(u) = \frac{\partial f}{\partial u} = u \tag{8}$$

Boundary conditions specifying the value of u at the left or right boundaries should be imposed if the direction of u is towards the interior at the boundary.

Provided that the solution remains smooth, (6) can be multiplied by u^{k-1} and rearranged to give an infinite set of invariants of the form

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

Here we focus on the first of these

$$\frac{\partial}{\partial t}\left(\frac{u^2}{2}\right)+\frac{\partial}{\partial x}\left(\frac{u^3}{3}\right)=0 \tag{9}$$

This may be integrated over x from a to b to determine the rate of change of the energy

$$E=\int_a^b \frac{u^2}{2}\,dx \tag{10}$$

in terms of the boundary fluxes as

$$\frac{dE}{dt}=\frac{u_a^3}{3}-\frac{u_b^3}{3} \tag{11}$$

This equation fails in the presence of shock waves, as can easily be seen by considering the initial data $u = -x$ in the interval $[-1, 1]$. Then a wave moves inwards from each boundary at unit speed toward the center until a stationary shock wave is formed at $t = 1$, after which the energy remains constant. Thus

$$E(t) = \begin{cases} \frac{1}{3} + \frac{2t}{3}, & 0 \le t \le 1 \\ 1, & t > 1 \end{cases}$$

In order to correct (11) in the presence of a shock wave with left and right states u_L and u_R, equation (9) should be integrated separately on each side of the shock. If the shock is moving at a speed s there is an additional contribution to $\frac{dE}{dt}$ in the amount

$$s\left(\frac{u_L^2}{2}-\frac{u_R^2}{2}\right)=\frac{1}{4}(u_L+u_R)\left(\frac{u_L^2}{2}-\frac{u_R^2}{2}\right)$$

Accordingly

$$\frac{dE}{dt}=\frac{u_a^3}{3}-\frac{u_L^3}{3}+\frac{u_R^3}{3}-\frac{u_b^3}{3}-\frac{1}{4}(u_L+u_R)\left(\frac{u_L^2}{2}-\frac{u_R^2}{2}\right)$$

which can be simplified to

$$\frac{dE}{dt}=\frac{u_a^3}{3}-\frac{u_b^3}{3}-\frac{1}{12}(u_L-u_R)^3 \qquad (12)$$

In the presence of multiple shocks, each will remove energy at the rate $\frac{1}{12}(u_L-u_R)^3$.

As was already observed by Morton and Richtmyer, a skew-symmetric difference operator consistent with (6) for smooth data can be constructed by splitting it between conservation and quasilinear form as

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

Suppose this is discretized on a uniform mesh $x_j = j\Delta x,\ j = 0, 1, \ldots n$. Central differencing of both spatial derivatives at interior points yields the semi-discrete scheme

$$\begin{aligned}\frac{du_j}{dt} &= \frac{1}{6\Delta x}\left(u_{j+1}^2-u_{j-1}^2\right)\\ &\quad+\frac{1}{6\Delta x}u_j\left(u_{j+1}-u_{j-1}\right)=0, \qquad j=1,n-1\end{aligned} \tag{13}$$

Rewriting the quasilinear term as $\frac{1}{6\Delta x}(u_{j+1}u_j - u_j u_{j-1})$ equation (13) and can be expressed in the conservation form

$$\frac{du_j}{dt} + \frac{1}{\Delta x}\left(f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}\right) = 0, \qquad j = 1, n-1 \tag{14}$$

where

$$f_{j+\frac{1}{2}} = \frac{1}{6}\left(u_{j+1}^2 + u_{j+1}u_j + u_j^2\right) \tag{15}$$

and

$$\begin{aligned} \frac{du_0}{dt} + \frac{2}{\Delta x}\left(f_{\frac{1}{2}} - f_0\right) &= 0 \\ \frac{du_n}{dt} + \frac{2}{\Delta x}\left(f_n - f_{n-\frac{1}{2}}\right) &= 0 \end{aligned} \tag{16}$$

where

$$f_0 = \frac{u_0^2}{2}, \qquad f_n = \frac{u_n^2}{2} \tag{17}$$

Now let the discrete energy be represented by trapezoidal integration as

$$E = \frac{\Delta x}{2}\left(\frac{u_0^2}{2} + \frac{u_n^2}{2}\right) + \Delta x \sum_{j=1}^{n-1} \frac{u_j^2}{2} \tag{18}$$

Multiplying equation (14) by u_j and summing by parts

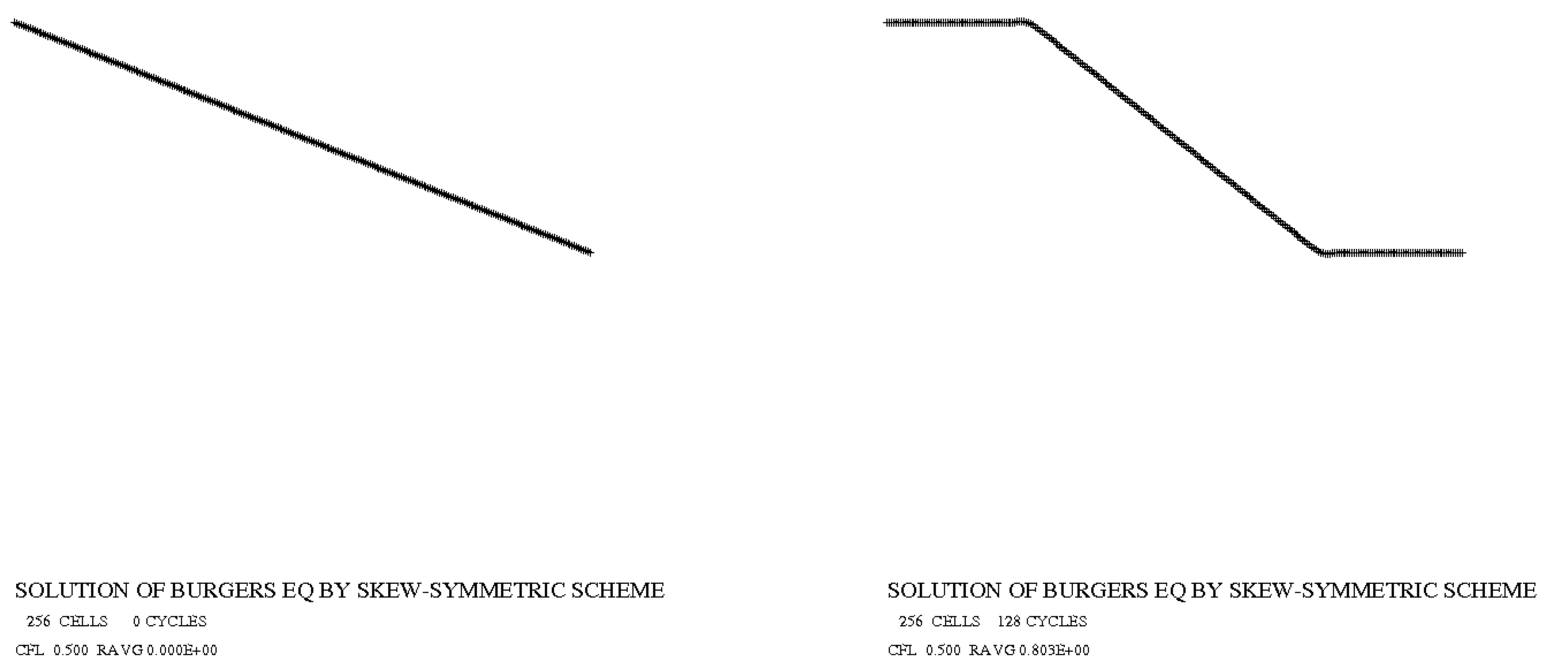
$$\Delta x \sum_{j=1}^{n-1} u_j \frac{du_j}{dt} = -\sum_{j=1}^{n-1} u_j (f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}) = f_{\frac{1}{2}} u_0 - f_{n+\frac{1}{2}} u_n$$

Hence, including the boundary points, we find that

$$\frac{dE}{dt} = \frac{u_0^3}{3} - \frac{u_n^3}{3} \tag{19}$$

which is the exact discrete analog of the continuous energy evolution equation (11).

Evolution of the Solution of the Burgers Equation

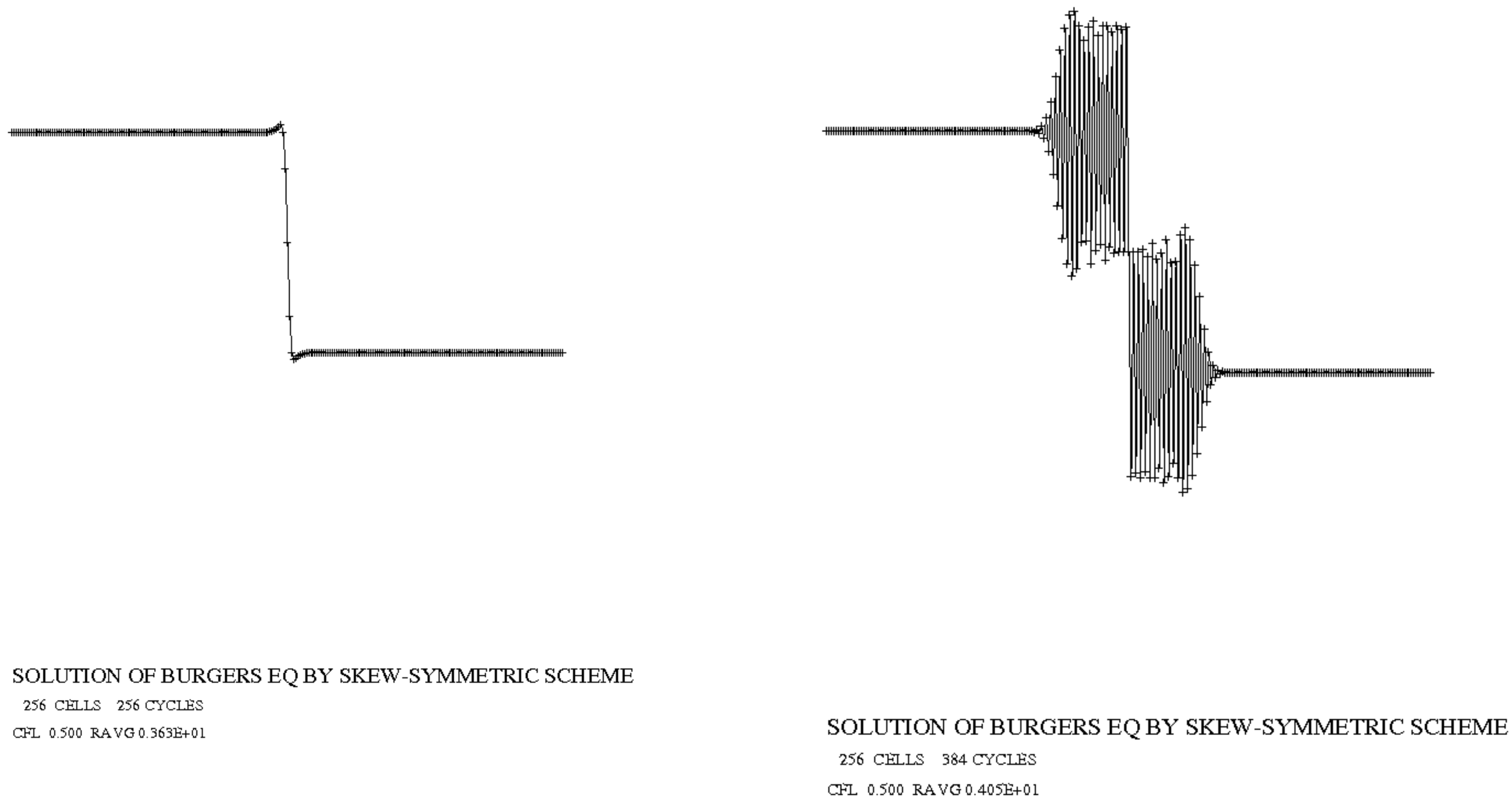


(a) At $t = 0.0$

(b) At $t = 0.5$

Figure 1: Evolution of the solution of the Burgers equation

Evolution of the Solution of the Burgers Equation (Continued)



(a) At $t = 1.0$ (b) At $t = 1.5$

Figure 2: Evolution of the solution of the Burgers equation

Discrete Energy Growth

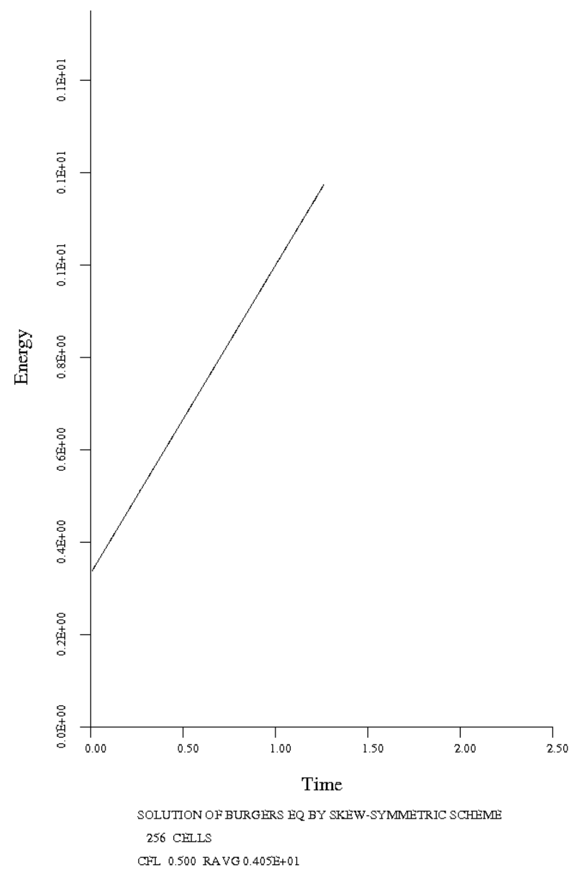


Figure 3: Discrete energy growth

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, that oscillations in the neighborhood of shock waves are eleminated by schemes which are local extremum diminishing (LED) or total variation diminishing (TVD). A semi-discrete scheme is LED if it can be expressed in the form

$$\frac{du_i}{dt} = \sum_j a_{ij}(u_j - u_i) \tag{20}$$

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 (15) is replaced by

$$f_{j+\frac{1}{2}} = \begin{cases} u_j^2 & \text{if} \quad a_{j+\frac{1}{2}} > 0 \\ u_{j+1}^2 & \text{if} \quad a_{j+\frac{1}{2}} < 0 \\ \frac{1}{2}(u_{j+1}^2 + u_j^2) & \text{if} \quad a_{j+\frac{1}{2}} = 0 \end{cases} \tag{21}$$

where the numerical wave speed is evaluated as

$$a_{j+\frac{1}{2}} = \frac{1}{2}(u_{j+1} + u_j) \tag{22}$$

Moreover, the upwind scheme (21) admits a stationary numerical shock structure with a single interior point.

Stanford University, Stanford, CA

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 (15) can be converted to the upwind flux (21) 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

$$\alpha_{j+\frac{1}{2}} = \frac{1}{4} \left| u_{j+1} + u_j \right| - \frac{1}{12} \left(u_{j+1} - u_j \right) \tag{23}$$

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

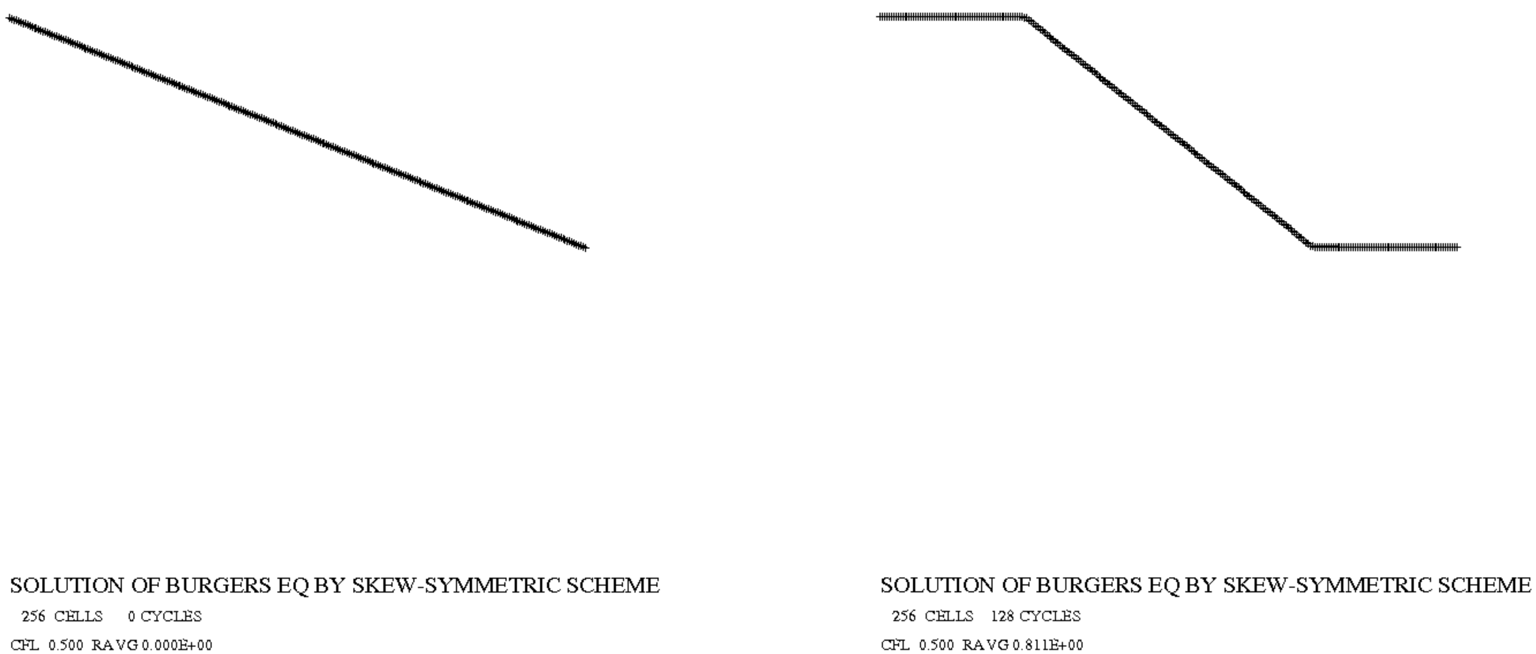
$$s_{j+\frac{1}{2}} = R\left(\Delta u_{j+\frac{3}{2}}, \Delta u_{j-\frac{1}{2}}\right) \tag{24}$$

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

$$R(u,v) = \left| \frac{u-v}{\max\left\{(|u|+|v|), \epsilon\right\}} \right| \tag{25}$$

where ϵ is a tolerance.

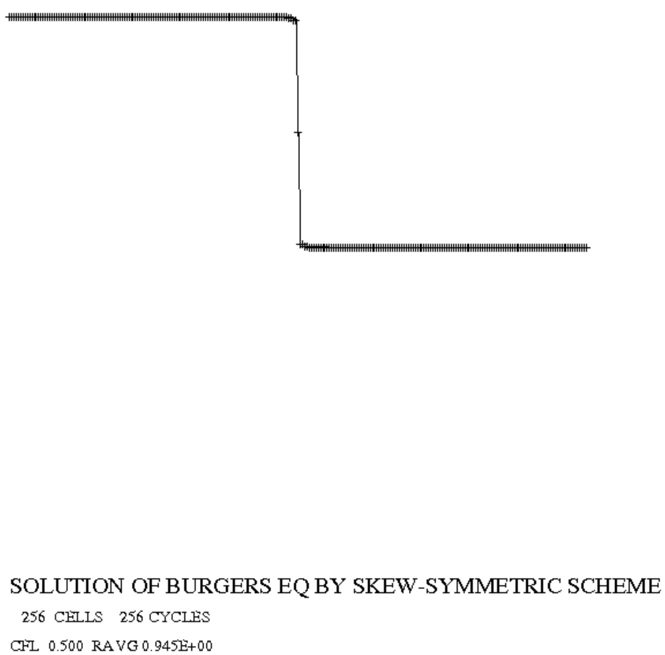
Evolution of the Solution of the Burgers Equation with a Switch



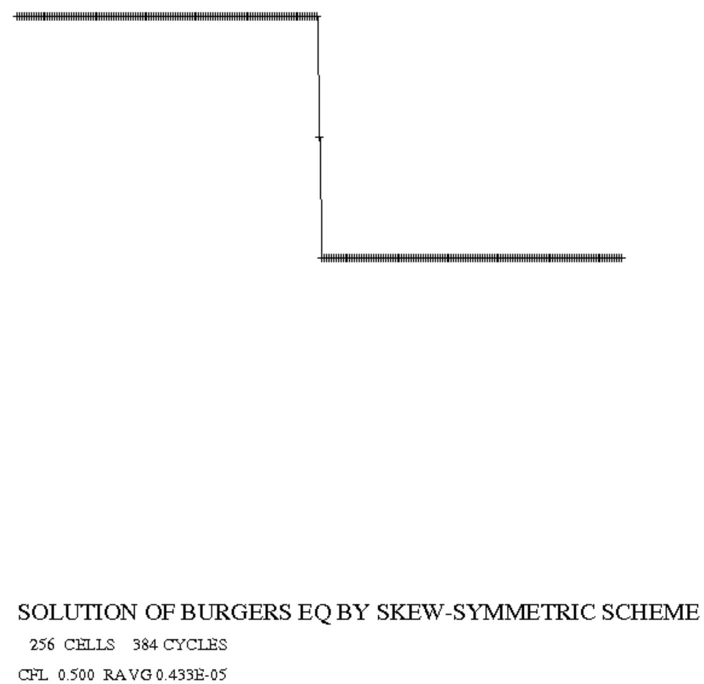
(a) At $t = 0.0$ (b) At $t = 0.5$

Figure 4: Evolution of the Solution of the Burgers Equation with a Switch

Evolution of the Solution of the Burgers Equation with a Switch



(a) At $t = 1.0$



(b) At $t = 1.5$

Figure 5: Evolution of the Solution of the Burgers Equation with a Switch

Discrete Energy Growth with a Limiter

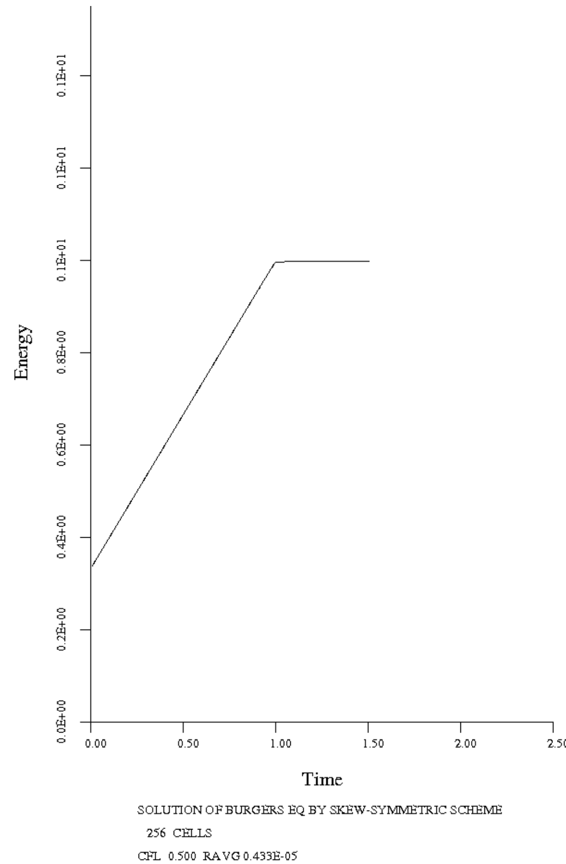


Figure 6: Discrete energy growth with a limiter

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

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = \nu \frac{\partial^2 u}{\partial x} \tag{26}$$

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

$$\frac{dE}{dt} = \frac{u_a^3}{3} - \frac{u_b^3}{3} - \nu \int_a^b \left(\frac{\partial u}{\partial x}\right)^2 dx \tag{27}$$

instead of (11).

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 $\frac{\partial u}{\partial x} = 0$,

$$\begin{aligned} &\frac{1}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}), \qquad j = 2, n-1 \\ &\frac{1}{\Delta x^2}(u_1 - u_0) \qquad \text{at the left boundary,} \\ &\frac{1}{\Delta x^2}(u_n - u_{n-1}) \qquad \text{at the right boundary} \end{aligned} \tag{28}$$

as proposed by Mattsson. Then summing by parts with the convective flux evaluated by (15) as before, the discrete energy balance is found to be

$$\frac{dE}{dt} = \frac{u_0^3}{3} - \frac{u_n^3}{3} - \nu \sum_{j=0}^{n-1} (u_{j+1} - u_j)^2 \tag{29}$$

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 (26) can written as

$$\frac{du_j}{dt} = a_{j+\frac{1}{2}}(u_{j+1} - u_j) + a_{j-\frac{1}{2}}(u_{j-1} - u_j) \tag{30}$$

where

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

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 (20) for a local extremum diminishing scheme if $a_{j+\frac{1}{2}} \geq 0$ and $a_{j-\frac{1}{2}} \geq 0$.

This establishes the Theorem:

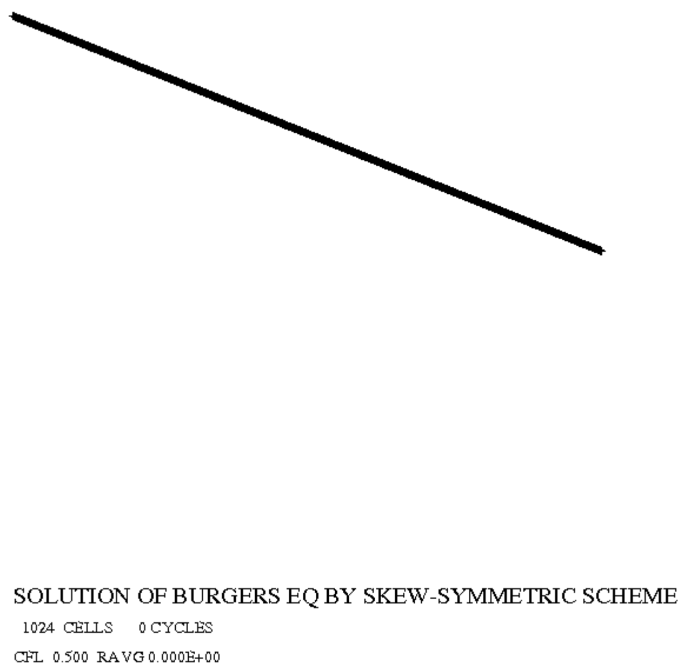
The semi-discrete approximation (14) using the numerical flux (15) and the central difference operator (28) for $\frac{\partial^2 u}{\partial x^2}$ is local extremum diminishing if the cell Reynolds number satisfies the condition

$$\frac{\bar{u}\Delta x}{\nu} \leq 2 \tag{31}$$

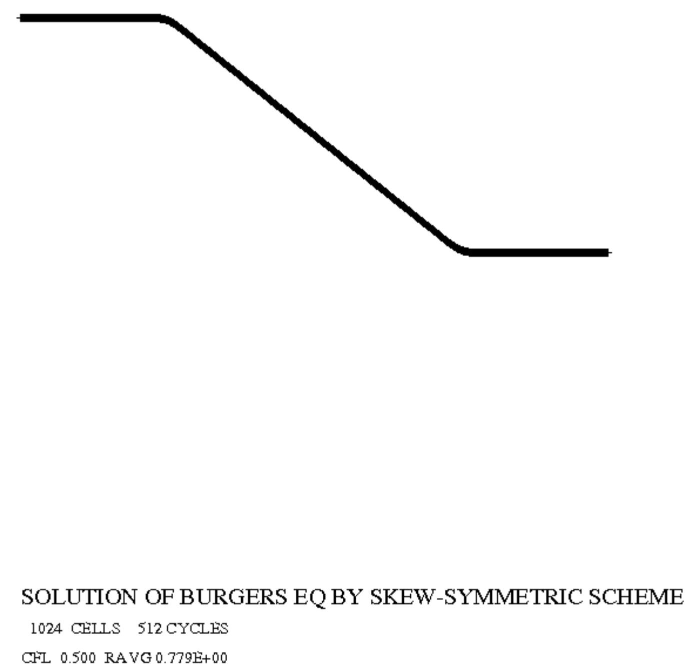
where the local speed is evaluated as

$$\bar{u} = \frac{1}{3}\left|u_{j+1} + u_j + u_{j-1}\right| \tag{32}$$

Evolution of the Solution of the Viscous Burgers Equation



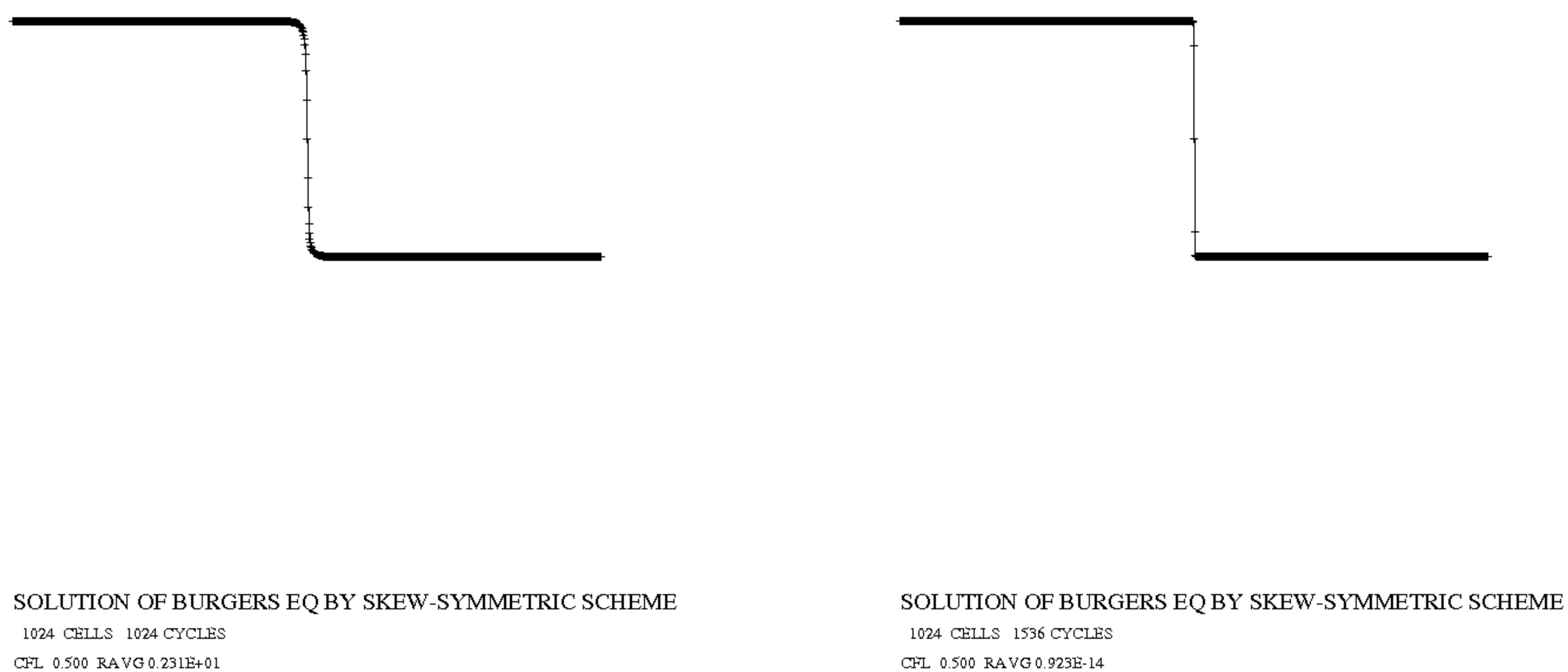
(a) At $t = 0.0$



(b) At $t = 0.5$

Figure 7: Evolution of the Solution of the Viscous Burgers Equation

Evolution of the Solution of the Viscous Burgers Equation



(a) At $t = 1.0$

(b) At $t = 1.5$

Figure 8: Evolution of the Solution of the Viscous Burgers Equation

Discrete Energy Growth for the Viscous Burgers Equation

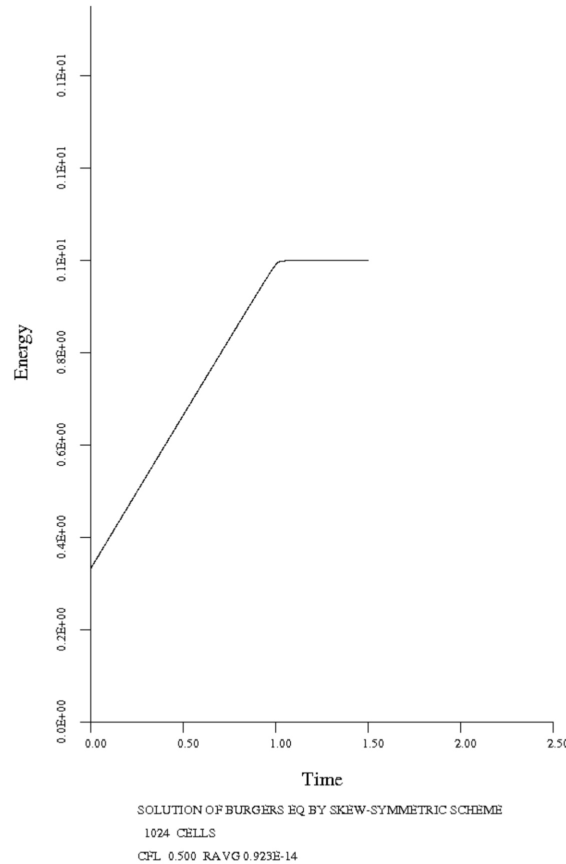


Figure 9: Discrete energy growth for the viscous Burgers equation

The One Dimensional Scalar Conservation Law

Consider the scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \tag{33}$$

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

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

Correspondingly, smooth solutions of (33) also satisfsy

$$\frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x} F(u) = 0 \tag{34}$$

where

$$F_u = u f_u$$

Defining the energy as

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

it follows from (34) that smooth solutions of (33) satisfy the energy equation

$$\frac{dE}{dt} = F(u_a) - F(u_b) \tag{35}$$

Introducing the function $G(u)$ such that

$$G_u = f$$

and multiplying (33) 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

$$F = uf - G, \qquad G = uf - F \tag{36}$$

If shock waves appear in the solution the estimate (35) 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 (34) 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 (36) 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 between the states u_L and u_R such that

$$\bar{f}\left(u_R, u_L\right)\left(u_R - u_L\right) = G\left(u_R\right) - G\left(u_L\right) \tag{37}$$

Then

$$\left.\frac{dE}{dt}\right|_s = -\left\{\frac{1}{2}\left(f_R + f_L\right) - \bar{f}\left(u_R, u_L\right)\right\}\left(u_L - u_R\right) \tag{38}$$

The Roe average can be evaluated as

$$\bar{f}\left(u_R, u_L\right) = \int_0^1 f\left(\hat{u}(\theta)\right) d\theta \tag{39}$$

where

$$\hat{u}(\theta) = u_L + \theta\left(u_R - u_L\right) \tag{40}$$

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,

$$\bar{f}\left(u_R, u_L\right) < \frac{1}{2}\left(f_R + f_L\right) \tag{41}$$

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 (38) that a shock wave always removes energy.

Discretization of a Scalar Conservation Law

Suppose now that (33) is discretized on a grid with cell intervals Δx_j, $j = 1, n$. Consider a semi-discrete conservative scheme of the form

$$\Delta x_j \frac{du_j}{dt} + (f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}) = 0 \tag{42}$$

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 (42) 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

$$f_{j+\frac{1}{2}} = G_{u_{j+\frac{1}{2}}} \tag{43}$$

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

$$G_{u_{j+\frac{1}{2}}}(u_{j+1} - u_j) = G(u_{j+1}) - G(u_j) \tag{44}$$

This is realized by formula (39) 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

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

and define the discrete approximation to the energy as

$$E = \sum_{j=1}^{n} \Delta x_j \frac{u_j^2}{2} \tag{45}$$

Then finally

$$\frac{dE}{dt} = u_1 f_1 - u_n f_n - G_1 + G_n = F_1 - F_n \tag{46}$$

Thus the energy balance (35) is exactly recovered by the discrete scheme. Equations (43) and (44) are satisfied by evaluating the numerical flux by the Roe average (39) between the states u_j and u_{j+1}.

This establishes the theorem:

If the scalar conservation law (33) is approximated by the semi-discrete conservative scheme (42), it also satisfies the semi-discrete energy conservation law (46) if the numerical flux $f_{j+\frac{1}{2}}$ is evaluated by equations (39) and (40).

Entropy and Kinetic Energy Preserving Schemes for the One-Dimensional Gas Dynamics Equations

Consider the gas dynamics equations in the conservation form

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \tag{47}$$

Here the state and flux vectors are

$$u = \begin{bmatrix} \rho \\ \rho v \\ \rho E \end{bmatrix}, \qquad f = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ \rho v H \end{bmatrix} \tag{48}$$

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

$$p = (\gamma - 1)\rho \left(E - \frac{v^2}{2} \right), \qquad H = E + \frac{p}{\rho} \tag{49}$$

where γ is the ratio of specific heats.

In the absence of shock waves the entropy

$$s = \log\left(\frac{p}{\rho^\gamma}\right) \tag{50}$$

is constant, satisfying the advection equation

$$\frac{\partial s}{\partial t} + v\frac{\partial s}{\partial x} = 0 \tag{51}$$

Consider the generalized entropy function

$$h(s) = \rho g(s) \tag{52}$$

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

$$\frac{d^2 g}{ds^2} \bigg/ \frac{dg}{ds} < \frac{1}{\gamma} \tag{53}$$

Then h satisfies the entropy conservation law

$$\frac{\partial}{\partial t}h(u) + \frac{\partial}{\partial x}F(u) = 0 \tag{54}$$

where the entropy flux is

$$F = \rho v g(s) \tag{55}$$

Moreover, introducing the entropy variables

$$w^T = \frac{\partial h}{\partial u} \tag{56}$$

it can be verified that

$$h_u f_u = F_u$$

and hence on multiplying (47) by w^T we recover the entropy conservation law (54) 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,

$$f = \frac{\partial G}{\partial w} \tag{57}$$

and the entropy flux can be expressed as

$$F = f^T w - G \tag{58}$$

Suppose now that (47) is approximated in semi-discrete form on a grid with cell intervals Δx_j, $j = 1, n$ as

$$\Delta x_j \frac{du_j}{dt} + f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} = 0 \tag{59}$$

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 (59) by w^T and sum by parts to obtain

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

Stanford University, Stanford, CA

At interior points evaluate $f^T_{j+\frac{1}{2}}$ as the mean value of $G_{w_{j+\frac{1}{2}}}$ in the sense of Roe such that

$$G_{w_{j+\frac{1}{2}}}\left(w_{j+1}-w_j\right)=G\left(w_{j+1}\right)-G\left(w_j\right) \tag{60}$$

Also evaluate the boundary fluxes as

$$f_{\frac{1}{2}}=f\left(w_1\right), \quad f_{n+\frac{1}{2}}=f\left(w_n\right) \tag{61}$$

Then the interior fluxes cancel, and using (56) amd (58), we obtain the entropy conservation law in the discrete form

$$\sum_{j=1}^{n}\Delta x_j\frac{dh_j}{dt}=F\left(w_1\right)-F\left(w_n\right) \tag{62}$$

G+ $G_{w_{j+\frac{1}{2}}}$ can be constructed to satisfy (60) exactly by evaluating it as the integral

$$G_{w_{j+\frac{1}{2}}} = \int_0^1 G_w\left(\hat{w}(\theta)\right) d\theta \tag{63}$$

where

$$\hat{w}(\theta) = w_j + \theta\left(w_{j+1} - w_j\right) \tag{64}$$

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 the Theorem:

The semi-discrete conservation law (59) satisfies the semi-discrete entropy conservation law (62) is 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 (64), and the boundary fluxes are defined by (61)

Kinetic Energy Preserving Scheme

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

$$\begin{aligned} \frac{\partial k}{\partial t} &= v\frac{\partial}{\partial t}(\rho v) - \frac{v^2}{2}\frac{\partial \rho}{\partial t} \\ &= -\frac{\partial}{\partial x}\left\{v\left(p + \rho\frac{v^2}{2}\right)\right\} + p\frac{\partial v}{\partial x} \end{aligned} \tag{65}$$

Suppose that the semi-discrete conservation scheme (59) is written separately for the continuity and momentum equations as

$$\Delta x_j \frac{d\rho_j}{dt} + (\rho v)_{j+\frac{1}{2}} - (\rho v)_{j-\frac{1}{2}} = 0 \tag{66}$$

$$\Delta x_j \frac{d}{dt}(\rho v)_j + (\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} + p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} = 0 \tag{67}$$

Now multiplying (66) by $\frac{v_j^2}{2}$ and (67) by v_j, adding them and summing by parts,

$$
\begin{aligned}
\sum_{j=1}^{n} \Delta x_j \left(v_j \frac{d}{dt}(\rho v)_j - \frac{v_j^2}{2}\frac{d\rho_j}{dt} \right) &= \sum_{j=1}^{n} \Delta x_j \frac{d}{dt}\left(\rho_j \frac{v_j^2}{2}\right) \\
&= \sum_{j=1}^{n} \frac{v_j^2}{2}\left((\rho v_j)_{j+\frac{1}{2}} - (\rho v_j)_{j-\frac{1}{2}} \right) - \sum_{j=1}^{n} v_j \left((\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} \right) \\
&\quad - \sum_{j=1}^{n} v_j \left(p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} \right) \\
&= -\frac{v_1^2}{2}(\rho v)_{\frac{1}{2}} + v_1(\rho v^2)_{\frac{1}{2}} + v_1 p_{\frac{1}{2}} + \frac{v_n^2}{2}(\rho v)_{n+\frac{1}{2}} - v_n(\rho v^2)_{n+\frac{1}{2}} \\
&\quad - v_n p_{n+\frac{1}{2}} + \sum_{j=1}^{n-1} p_{j+\frac{1}{2}}\left(v_{j+1} - v_j\right) \\
&\quad + \sum_{j=1}^{n-1} \left\{ \frac{1}{2}(\rho v)_{j+\frac{1}{2}}\left(v_{j+1}^2 - v_j^2\right) \frac{1}{2}(\rho v^2)_{j+\frac{1}{2}}\left(v_{j+1} - v_j\right) \right\}
\end{aligned}
\tag{68}
$$

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

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

and will vanish if

$$\left(\rho v^2\right)_{j+\frac{1}{2}}=(\rho v)_{j+\frac{1}{2}}\frac{v_{j+1}+v_j}{2} \tag{69}$$

Now evaluating the boundary fluxes as

$$\begin{aligned}(\rho v)_{\frac{1}{2}} &= \rho_1 v_1 \;,\; \left(\rho v^2\right)_{\frac{1}{2}} = \rho_1 v_1^2 \;,\; p_{\frac{1}{2}} = p_1 \\ (\rho v)_{n+\frac{1}{2}} &= \rho_n v_n \;,\; \left(\rho v^2\right)_{n+\frac{1}{2}} = \rho_n v_n^2 \;,\; p_{n+\frac{1}{2}} = p_n\end{aligned} \tag{70}$$

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

$$\begin{aligned}\sum_{j=1}^{n}\Delta x_j\left(\rho_j\frac{v_j^2}{2}\right) &= v_1\left(p_1+\rho_1\frac{v_1^2}{2}\right)-v_n\left(p_n+\rho_n\frac{v_n^2}{2}\right) \\ &\quad +\sum_{j=1}^{n}p_{j+\frac{1}{2}}(v_{j+1}+v_j)\end{aligned} \tag{71}$$

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

$$p_{j+\frac{1}{2}} = \bar{p} \tag{72}$$

Also if one sets

$$\left(\rho v\right)_{j+\frac{1}{2}} = \bar{\rho}\bar{v} \tag{73}$$

$$\left(\rho v^2\right)_{j+\frac{1}{2}} = \bar{\rho}\bar{v}^2 \tag{74}$$

condition (69) is satisfied. Consistently one may set

$$\left(\rho v H\right)_{j+\frac{1}{2}} = \bar{\rho}\bar{v}\bar{H} \tag{75}$$

The foregoing argument establishes the Theorem:

The semi-discrete conservation law (59) satisfies the semi-discrete kinetic energy global conservation law (71) if the fluxes for the continuity and momentum equations satisfy condition (69) and the boundary fluxes are calculated by equations (70).

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. It has been shown that shock waves in solutions of the Burgers equation will be fully resolved if 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.

Numerical experiments have been 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:

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

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

$$p^* = \frac{\gamma - 1}{\gamma + 1} e^{\frac{s}{\gamma+1}} = \frac{\gamma - 1}{\gamma + 1} \left(\frac{p}{p^\gamma} \right)^{\frac{1}{\gamma+1}}$$

Time Stepping Scheme

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.

Stanford University, Stanford, CA

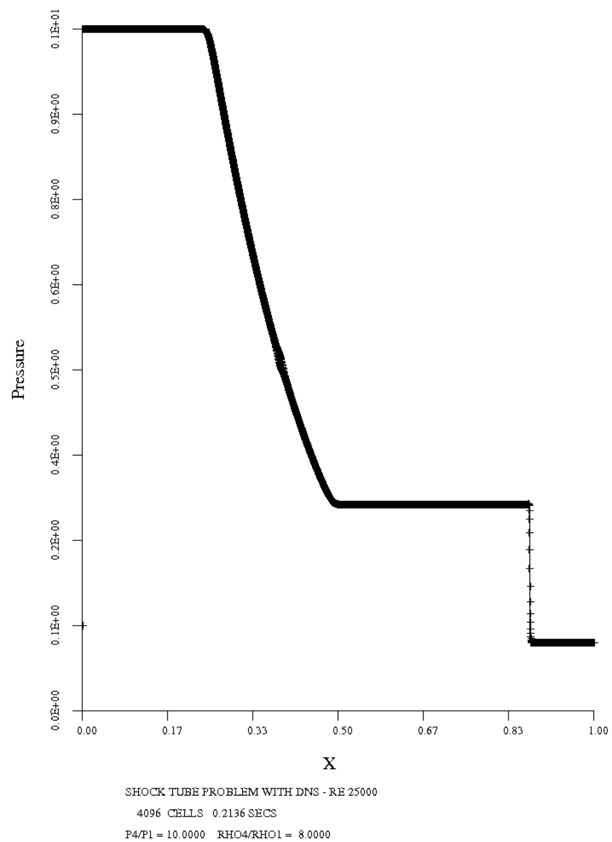
In order to avoid this cost, Shu's total variation diminishing (TVD) scheme was used for the time integration in all the numerical experiments. Writing the semi-discrete scheme in the form

$$\frac{du}{dt} + R(u) = 0 \tag{76}$$

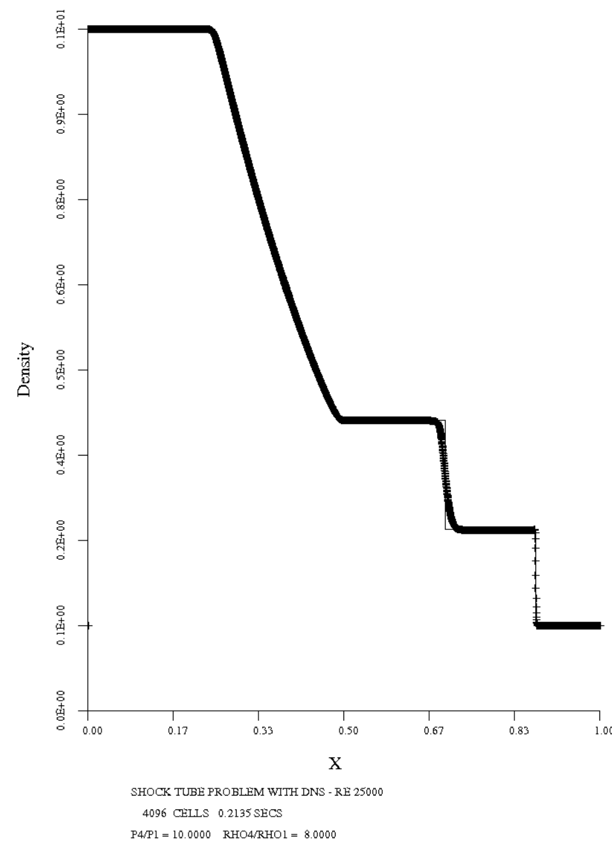
where $R(u)$ represents the discretized spatial derivative, this advances the solution during one time step by the three stage scheme

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

Numerical Results

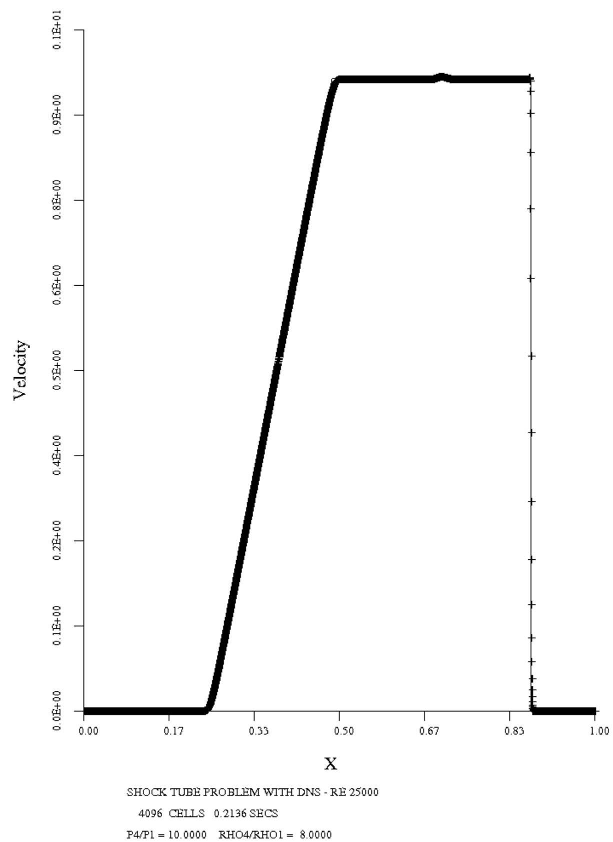


(a) Pressure

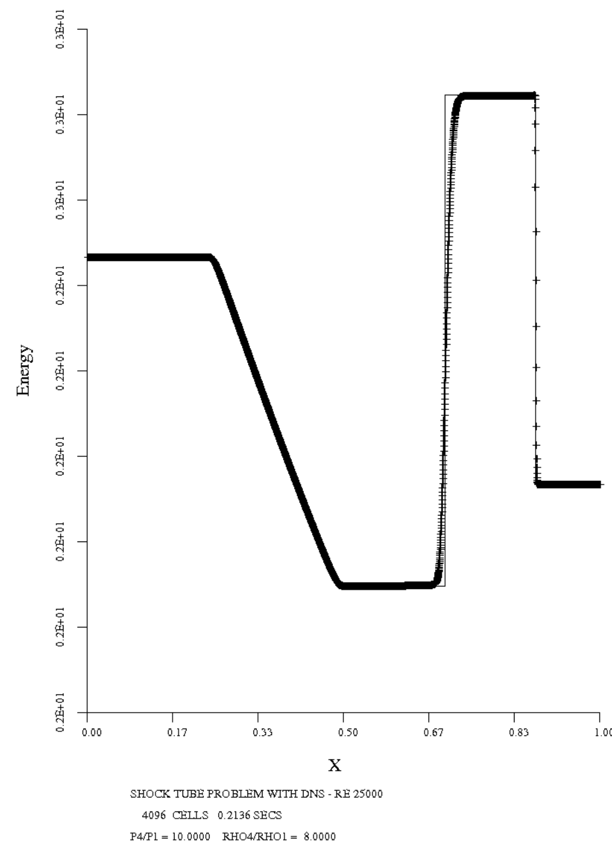


(b) Density

Figure 10: Simple averaging of the flux: 4096 mesh cells, Reynolds number 25000, Computed solution values $+$, Exact inviscid solution $-$

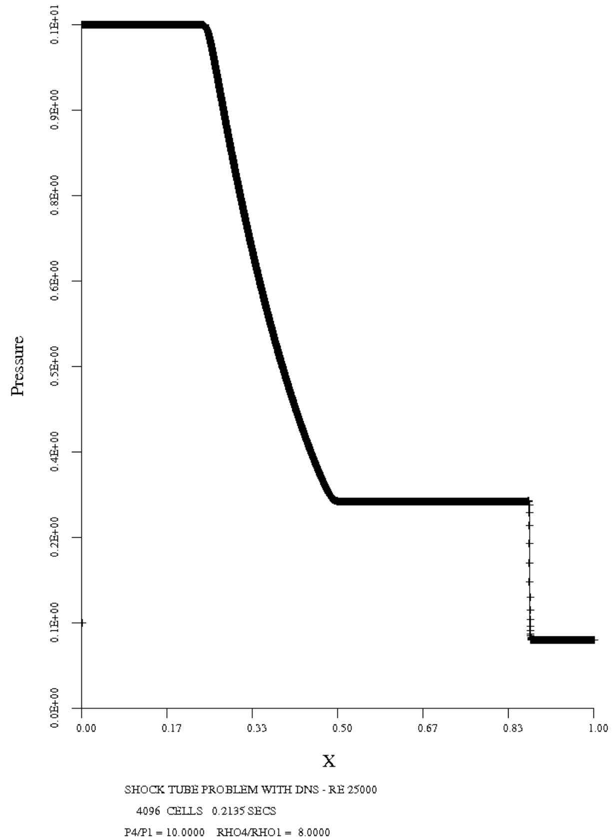


(a) Velocity

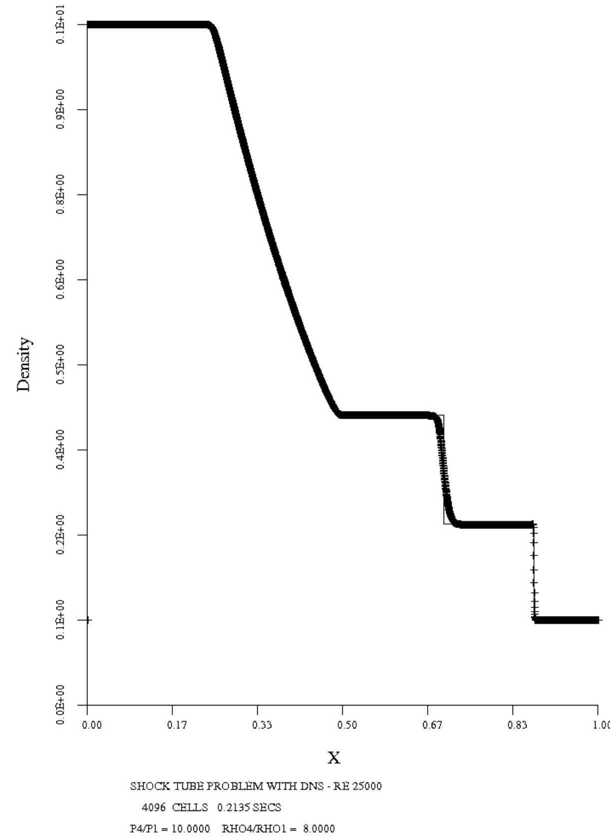


(b) Energy

Figure 11: Simple averaging of the flux: 4096 mesh cells, Reynolds number 25000, Computed solution values $+$, Exact inviscid solution $-$

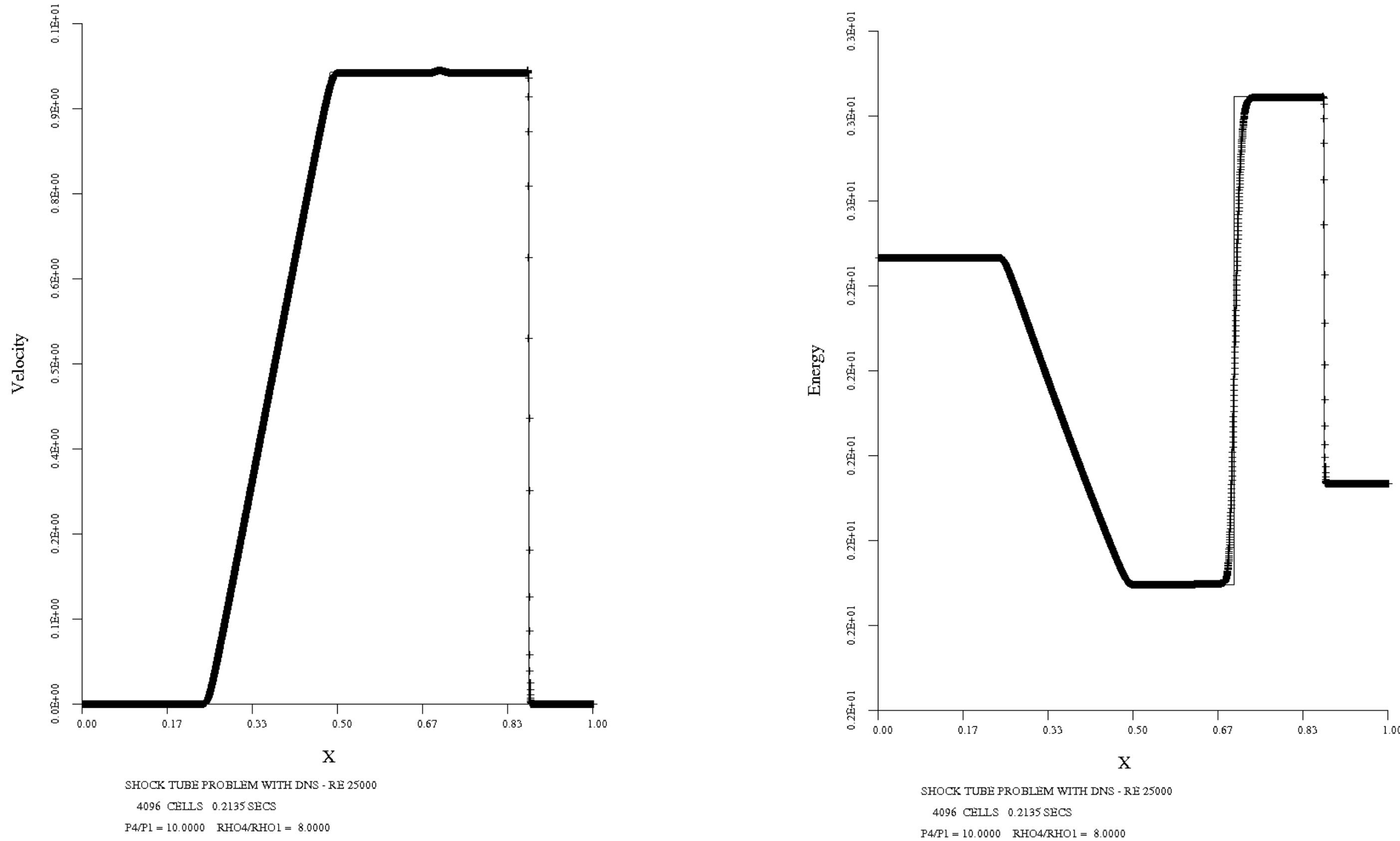


(a) Pressure



(b) Density

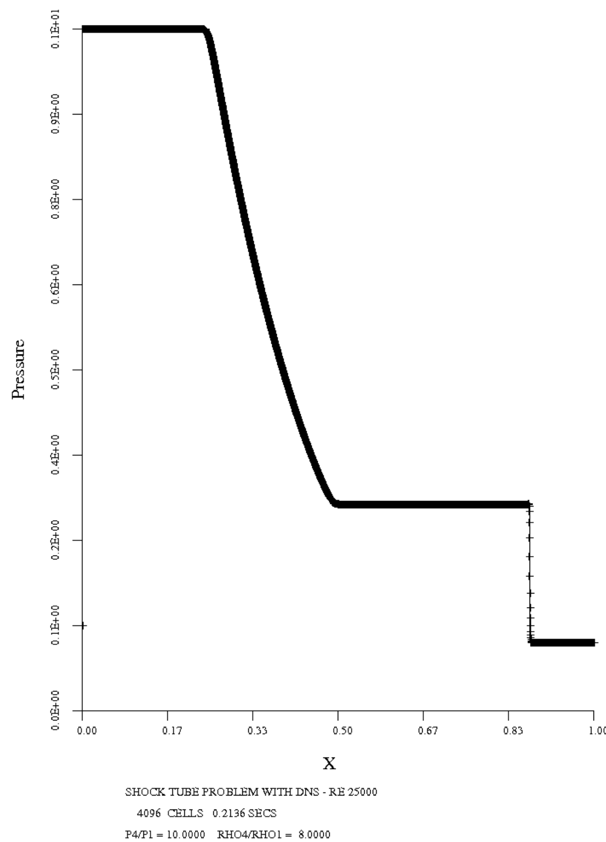
Figure 12: Entropy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −



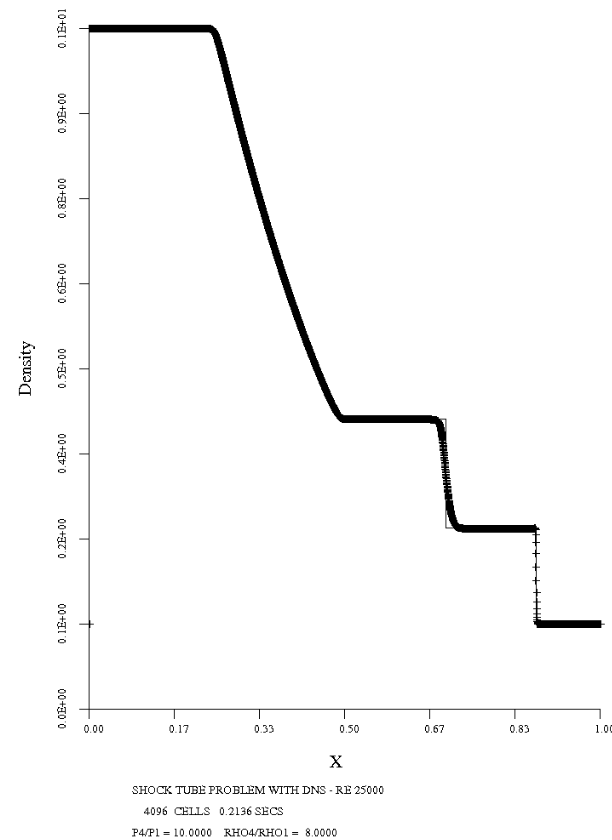
(a) Velocity

(b) Energy

Figure 13: Entropy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −

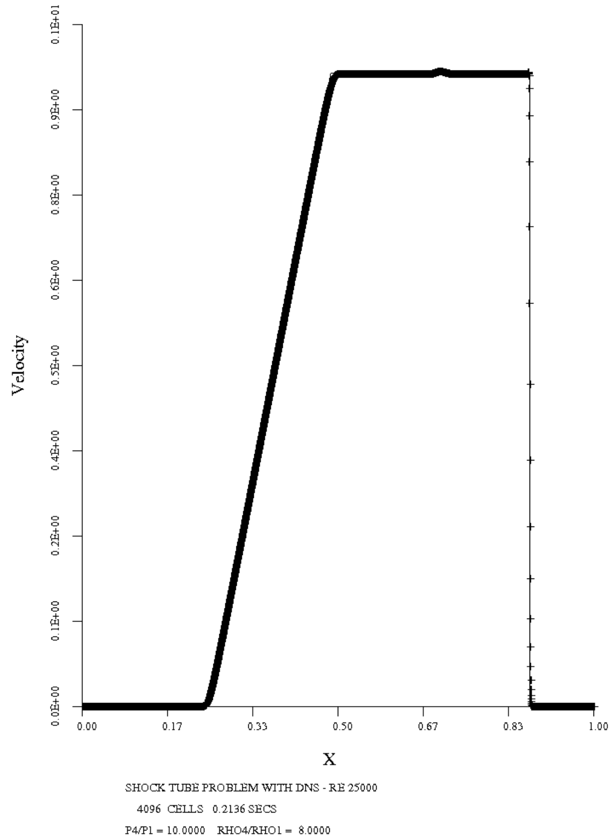


(a) Pressure

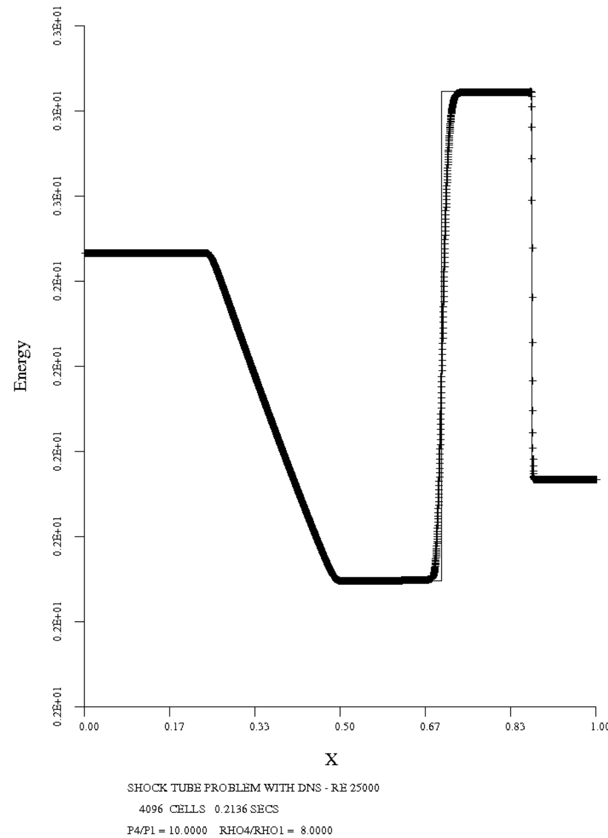


(b) Density

Figure 14: Kinetic energy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values $+$, Exact inviscid solution $-$



(a) Velocity



(b) Energy

Figure 15: Kinetic energy preserving scheme: 4096 mesh cells, Reynolds number 25000, Computed solution values +, Exact inviscid solution −

Conclusions

Conclusion (1)

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 preserve the conservation of 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.

Conclusion (2)

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.

Stanford University, Stanford, CA