Formulation of Kinetic Energy Preserving Conservative Schemes for Gas Dynamics and Direct Numerical Simulation of One-dimensional Viscous Compressible Flow in a Shock Tube Using Entropy and Kinetic Energy Preserving Schemes

Antony Jameson

Stanford University
Aerospace Computing Laboratory
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Abstract

This paper follows up on the author's recent paper "The Construction of Discretely Conservative Finite Volume Schemes that also Globally Conserve Energy or Enthalpy". In the case of the gas dynamics equations the previous formulation leads to an entropy preserving (EP) scheme. It is shown in the present paper that it is also possible to construct the flux of a conservative finite volume scheme to produce a kinetic energy preserving (KEP) scheme which exactly satisfies the global conservation law for kinetic energy. A proof is presented for three dimensional discretization on arbitrary grids. Both the EP and KEP schemes have been applied to the direct numerical simulation of one-dimensional viscous flow in a shock tube. The computations verify that both schemes can be used to simulate flows with shock waves and contact discontinuities without the introduction of any artificial diffusion. The KEP scheme performed better in the tests.

1 Introduction

Stemming from the pioneering work of Godunov [1], procedures for the construction of non-oscillatory shock capturing schemes are by now well established [2, 3, 4, 5, 6]. In general they add artificial diffusion either explicitly ot implicitly via upwind operators in order to satisfy total variation diminishing (TVD) or local extremum diminishing (LED) properties [7, 8]. However there is a risk that the artificial diffusion may compromise the accuracy of viscous flow simulations. If the discrete scheme can be constructed to satisfy a global energy estimate of some kind, then it should by stable, at least for smooth solutions, without the need for artificial viscosity. The use of energy estimates to establish stability has a long history, and it is discussed in the classical book of Morton and Richtmyer [9].

One route to achieving discrete energy estimates is to use difference operators which have a skew-symmetric form. Typically these operators are derived by splitting the governing equations in a mixture of conservation and quasilinear form [10]. However, in the treatment of compressible flows with shock waves it is beneficial to write the discrete equations in conservation form. According to the theorem of Lax and Wendroff [11], this is sufficient to guarantee that the discrete solution satisfies the correct shock jump conditions as long as it converges in the limit as the mesh interval is reduced.

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 [12] 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 [13] has given conditions such $h(u)$ 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 [14], and also by Gerritsen and Olsson [15], 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 the present work it is 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 2 presents the derivation of the entropy preserving (EP) and kinetic energy preserving (KEP) schemes for the one dimensional gas dynamics equations. In Section 3 the formulation of the KEP scheme is extended to multi-dimensional viscous compressible flow simulations on arbitrary grids. The KEP property is again assured by a compatibility condition between the fluxes for the continuity and momentum equations. The proof is completed by showing that the finite volume scheme satisfies a discrete Gauss theorem for the pressure and stress terms, provided that these are both evaluated at the cell interfaces by arithmetic averages of their values in the neighboring cells.

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. Representative numerical calculations include simulations at a Reynolds number in the range 2500–100000 based on the speed of sound on meshes with 512–16384 cells.

2 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 proof for the EP scheme has been given in [12], but in order to facilitate the comparison of the EP and KEP schemes it is outlined here

Consider the gas dynamics equations in the conservation form

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

Here the state and flux vectors are

$$u = \begin{bmatrix} \rho \\ \rho v \\ \rho E \end{bmatrix}, \qquad f = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ \rho v H \end{bmatrix} \tag{2.2}$$

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

$$p = (\gamma - 1)\rho \left(E - \frac{v^2}{2} \right), \qquad H = E + \frac{p}{\rho} \tag{2.3}$$

where γ is the ratio of specific heats.

In the absence of shock waves the entropy

$$s = \log \left(\frac{p}{\rho^\gamma} \right) \tag{2.4}$$

is constant, satisfying the advection equation

$$\frac{\partial s}{\partial t} + v \frac{\partial s}{\partial x} = 0 \tag{2.5}$$

Consider the generalized entropy function

$$h(s) = \rho g(s) \tag{2.6}$$

where it has been shown by Harten [13] that h is a convex function of u provided that

$$\frac{d^2g}{ds^2}\Big/\frac{dg}{ds} < \frac{1}{\gamma} \tag{2.7}$$

Then h satisfies the entropy conservation law

$$\frac{\partial}{\partial t}h(u) + \frac{\partial}{\partial x}F(u) = 0 \tag{2.8}$$

where the entropy flux is

$$F = \rho v g(s) \tag{2.9}$$

Moreover, introducing the entropy variables

$$w^T = \frac{\partial h}{\partial u} \tag{2.10}$$

it can be verified that

$$h_u f_u = F_u$$

and hence on multiplying (2.1) by w^T we recover the entropy conservation law (2.8) 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,

$$f = \frac{\partial G}{\partial w} \tag{2.11}$$

and the entropy flux can be expressed as

$$F = f^T w - G \tag{2.12}$$

Different choices of the entropy function $g(s)$ have been discussed by Harten [13], Hughes, Franca and Mallet [14], and Gerritsen and Olsson [15].

Suppose now that (2.1) is approximated in semi-discrete form on a grid with cell intervals Δx_j, $j = 1, n$ as

$$\Delta x_j \frac{du_j}{dt} + f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} = 0 \tag{2.13}$$

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

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

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

$$G_{w_{j+\frac{1}{2}}}\left(w_{j+1}-w_j\right)=G\left(w_{j+1}\right)-G\left(w_j\right) \tag{2.14}$$

Also evaluate the boundary fluxes as

$$f_{\frac{1}{2}}=f\left(w_1\right),\quad f_{n+\frac{1}{2}}=f\left(w_n\right) \tag{2.15}$$

Then the interior fluxes cancel, and using (2.10) amd (2.12), we obtain the entropy conservation law in the discrete form

$$\sum_{j=1}^{n}\Delta x_j\frac{dh_j}{dt}=F\left(w_1\right)-F\left(w_n\right) \tag{2.16}$$

$G_{w_{j+\frac{1}{2}}}$ can be constructed to satisfy (2.14) exactly by evaluating it as the integral

$$G_{w_{j+\frac{1}{2}}}=\int_0^1 G_w\left(\hat{w}(\theta)\right)d\theta \tag{2.17}$$

where

$$\hat{w}(\theta)=w_j+\theta\left(w_{j+1}-w_j\right) \tag{2.18}$$

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 2.1 *The semi-discrete conservation law* (2.13) *satisfies the semi-discrete entropy conservation law* (2.16) *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* (2.18)*, and the boundary fluxes are defined by* (2.15)

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

$$\begin{aligned}\frac{\partial k}{\partial t} &= v\frac{\partial}{\partial t}(\rho v) - \frac{v^2}{2}\frac{\partial \rho}{\partial t} \\ &= -\frac{\partial}{\partial x}\left\{v\left(p + \rho\frac{v^2}{2}\right)\right\} + p\frac{\partial v}{\partial x} \end{aligned} \tag{2.19}$$

Suppose that the semi-discrete conservation scheme (2.13) is written separately for the continuity and momentum equations as

$$\Delta x_j \frac{d\rho_j}{dt} + (\rho v)_{j+\frac{1}{2}} - (\rho v)_{j-\frac{1}{2}} = 0 \tag{2.20}$$

$$\Delta x_j \frac{d}{dt}(\rho v)_j + (\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} + p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} = 0 \tag{2.21}$$

Now multiplying (2.20) by $\frac{v_j^2}{2}$ and (2.21) by v_j, adding them and summing by parts,

$$\begin{aligned}
\sum_{j=1}^{n} \Delta x_j \left(v_j \frac{d}{dt}(\rho v)_j - \frac{v_j^2}{2}\frac{d\rho_j}{dt} \right) &= \sum_{j=1}^{n} \Delta x_j \frac{d}{dt}\left(\rho_j \frac{v_j^2}{2} \right) \\
&= \sum_{j=1}^{n} \frac{v_j^2}{2}\left((\rho v_j)_{j+\frac{1}{2}} - (\rho v_j)_{j-\frac{1}{2}} \right) - \sum_{j=1}^{n} v_j \left((\rho v^2)_{j+\frac{1}{2}} - (\rho v^2)_{j-\frac{1}{2}} \right) \\
&\quad - \sum_{j=1}^{n} v_j \left(p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} \right) \\
&= -\frac{v_1^2}{2}(\rho v)_{\frac{1}{2}} + v_1 (\rho v^2)_{\frac{1}{2}} + v_1 p_{\frac{1}{2}} + \frac{v_n^2}{2}(\rho v)_{n+\frac{1}{2}} - v_n (\rho v^2)_{n+\frac{1}{2}} - v_n p_{n+\frac{1}{2}} \\
&\quad + \sum_{j=1}^{n-1} \left\{ \frac{1}{2}(\rho v)_{j+\frac{1}{2}} \left(v_{j+1}^2 - v_j^2 \right) - (\rho v^2)_{j+\frac{1}{2}} \left(v_{j+1} - v_j \right) \right\} \\
&\quad + \sum_{j=1}^{n-1} p_{j+\frac{1}{2}} \left(v_{j+1} - v_j \right)
\end{aligned} \tag{2.22}$$

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

$$(\rho v^2)_{j+\frac{1}{2}} = (\rho v)_{j+\frac{1}{2}} \frac{v_{j+1} + v_j}{2} \tag{2.23}$$

Now evaluating the boundary fluxes as

$$\begin{array}{lllllllll}
(\rho v)_{\frac{1}{2}} & = & \rho_1 v_1 & , & (\rho v^2)_{\frac{1}{2}} & = & \rho_1 v_1^2 & , & p_{\frac{1}{2}} & = & p_1 \\
(\rho v)_{n+\frac{1}{2}} & = & \rho_n v_n & , & (\rho v^2)_{n+\frac{1}{2}} & = & \rho_n v_n^2 & , & p_{n+\frac{1}{2}} & = & p_n
\end{array} \tag{2.24}$$

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

$$\begin{aligned}
\sum_{j=1}^{n} \Delta x_j \left(\rho_j \frac{v_j^2}{2} \right) &= v_1 \left(p_1 + \rho_1 \frac{v_1^2}{2} \right) - v_n \left(p_n + \rho_n \frac{v_n^2}{2} \right) \\
&\quad + \sum_{j=1}^{n} p_{j+\frac{1}{2}} \left(v_{j+1} + v_j \right)
\end{aligned} \tag{2.25}$$

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

$$p_{j+\frac{1}{2}} = \bar{p} \tag{2.26}$$

Also if one sets

$$\begin{aligned} (\rho v)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v} && (2.27)\\ \left(\rho v^2\right)_{j+\frac{1}{2}} &= \bar{\rho}\bar{v}^2 && (2.28) \end{aligned}$$

condition (2.23) is satisfied. Consistently one may set

$$(\rho v H)_{j+\frac{1}{2}} = \bar{\rho}\bar{v}\bar{H} \tag{2.29}$$

The foregoing argument establishes

Theorem 2.2 *The semi-discrete conservation law* (2.13) *satisfies the semi-discrete kinetic energy global conservation law* (2.25) *if the fluxes for the continuity and momentum equations satisfy condition* (2.23) *and the boundary fluxes are calculated by equations* (2.24)*.*

Condition (2.23) 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 (2.27)–(2.29).

3 Kinetic energy preserving (KEP) scheme for multi-dimensional viscous flow

The extension of the entropy preserving (EP) scheme to multi-dimensional gas dynamics on general grids has been given in [12]. In this section it is shown how to extend the kinetic energy preserving (KEP) scheme to multi-dimensional viscous compressible flow. Denote the density, velocity components, pressure, energy and enthalpy by p, v^i, p, E and H, where the superscript i is used to denote the i^{th} coordinate direction. This is convenient because subscripts will be needed to denote the grid location. Repeated superscripts will be used to indicate summation over the coordinate directions. Also

$$p = (\gamma - 1)\left(\rho E - \frac{{v^i}^2}{2}\right), \quad H = E + \frac{p}{\rho} \tag{3.1}$$

The viscous stress tensor is

$$\sigma^{ij} = \mu\left(\frac{\partial v^i}{\partial x^j} + \frac{\partial v^j}{\partial x^i}\right) + \lambda\delta^{ij}\frac{\partial v^k}{\partial x^k} \tag{3.2}$$

where δ^{ij} is the Kronecker delta, and μ and λ are the viscosity coefficients. Usually $\lambda = -\frac{2}{3}\mu$. The heat flux is

$$q^j = -\kappa\frac{\partial T}{\partial x^j} \tag{3.3}$$

where T is the temperature and κ is the coefficient of heat conduction. The governing equations can now be written in conservation form as

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x^i} f^i(u) = 0 \tag{3.4}$$

where the state and flux vectors are

$$u = \begin{bmatrix} \rho \\ \rho v^1 \\ \rho v^2 \\ \rho v^3 \\ \rho E \end{bmatrix}, \qquad f^i = \begin{bmatrix} \rho v^i \\ \rho v^i v^1 - \sigma^{i1} + p\delta^{i1} \\ \rho v^i v^2 - \sigma^{i2} + p\delta^{i2} \\ \rho v^i v^3 - \sigma^{i3} + p\delta^{i3} \\ \rho v^i H - v^j\sigma^{ij} - q^j \end{bmatrix} \tag{3.5}$$

The kinetic energy is again denoted by k where

$$k = \rho \frac{v^{i^2}}{2}, \qquad \frac{\partial k}{\partial u} = \left[-\frac{v^{i^2}}{2}, v^1, v^2, v^3, 0 \right] \tag{3.6}$$

and the kinetic energy conservation law is

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x^j} \left\{ v^j \left(p + \rho \frac{v^{i^2}}{2} \right) + v^i \sigma^{ij} \right\} = p \frac{\partial v^j}{\partial x^j} - \sigma^{ij} \frac{\partial v^i}{\partial x^j} \tag{3.7}$$

Suppose now that the domain is covered by a grid, and the equations are discretized in finite volume form. The discrete variables may be associated either with nodes, each of which is surrounded by a control volume, or with the control volumes themselves. In the first case the control volumes may be taken as dual cells where the nodes are the vertices of the primary cells. In the second case the control volumes are simply the primary cells, and the discrete variables may be regarded as cell averages. Each interior control volume, say o, is bounded by faces (not necessarily planar) with a directed face area S_{op} for the face separating the control volumes o and p. Each boundary control volume is closed by an outer face with directed area S_o which is the negative of the sum $\sum_p S_{op}$ of the face areas between o and its neighbors. The control volumes may be tetrahedral, hexahedral or of mixed polyhedral form.

The semi-discrete finite volume scheme to be considered has the form

$$vol_o \frac{du_o}{dt} + \sum_p S^i_{op} f^i_{op} = 0 \tag{3.8}$$

for every interior control volume, where S^i_{op} are the projected areas of the face S_{op} in the coordinate directions. At a boundary control volume b there is an additional contribution $S^i_b f^i_b$, where the boundary flux vector will be evaluated as

$$f^i_b = f^i \left(u_b \right) \tag{3.9}$$

Multiplying (3.8) by

$$w^T_o = \left(\frac{\partial k}{\partial u} \right)_o \tag{3.10}$$

and summing over the nodes

$$\sum_o vol_o \frac{dk_o}{dt} = -\sum_o w_o^T \sum_p S_{op}^i \, f_{op}^i - \sum_b w_b^T \, S_b^i \, f_b^i \tag{3.11}$$

where the last sum represents the contribution of the boundaries.

Every interior face appears twice in the sums on the right hand side of (3.11) with opposite signs for its discrete face area. Thus its contribution is

$$\left(w_p^T - w_o^T\right) S_{op}^i \, f_{op}^i \tag{3.12}$$

Consider now contributions of the convective terms to (3.12). these are

$$\left(v_p^j - v_o^j\right) S_{op}^i \left(\rho v^i v^j\right)_{op} - \frac{1}{2}\left(v_p^{j^2} - v_o^{j^2}\right) S_{op}^i \left(\rho v^i\right)_{op}$$
$$= \left(v_p^j - v_o^j\right) S_{op}^i \left\{\left(\rho v^i v^j\right)_{op} - \frac{1}{2}\left(\rho v^i\right)_{op}\left(v_p^{j^2} - v_o^{j^2}\right)\right\}$$

Thus the convective contributions of the interior faces will vanish if

$$\left(\rho v^i v^j\right)_{op} = \frac{1}{2}\left(\rho v^i\right)_{op}\left(v_p^j + v_o^j\right) \tag{3.13}$$

Defining the average of any quantity q between its values at o and p as

$$\bar{q} = \frac{1}{2}\left(q_p + q_o\right) \tag{3.14}$$

condition (3.13) will be satisfied if one set

$$\left(\rho v^i\right)_{op} = \bar{\rho}\bar{v}^i \tag{3.15}$$
$$\left(\rho v^i v^j\right)_{op} = \bar{\rho}\bar{v}^i\bar{v}^j \tag{3.16}$$

To complete the derivation it is now necessary to examine the contributions of the pressure and stress tensor to (3.11). These can be expressed as

$$\sum_o v_o^T \sum_p S_{op}^i P_{op}^i - \sum_b v_b^T S_b^i P_b^i \tag{3.17}$$

where

$$v = \begin{bmatrix} v^1 \\ v^2 \\ v^3 \end{bmatrix}, \qquad P^i = \begin{bmatrix} p\delta^{i1} - \sigma^{i1} \\ p\delta^{i2} - \sigma^{i2} \\ p\delta^{i3} - \sigma^{i3} \end{bmatrix} \tag{3.18}$$

Let P^i_{op} be evaluated as

$$P^i_{op} = \frac{1}{2}\left(P^i_p + P^i_o\right) = \bar{P}^i \tag{3.19}$$

The first term in (3.17) is now

$$-\frac{1}{2}\sum_o v^T_o P^i_o \sum_p S^i_{op} - \frac{1}{2}\sum_o v^T_o \sum_p P^i_p S^i_{op}$$

At every interior control volume o the fluxes $v^T_p S^i_{op} P^i_o$ generated by its neighbors can be associated with o, so the contributions at o can be written as

$$-\frac{1}{2} v^T_o P^i_o \sum_p S^i_{op} + \frac{1}{2} v^T_p \sum S^i_{op} P^i_o$$

Here $\sum_p S^u_{op} = 0$ because it is the sum of the face areas of a closed volume. Thus one can add $v^T_o P^i_o \sum_p S^i_{op}$ to obtain

$$\frac{1}{2} P^{i^T}_o \sum_p \left(v_p + v_o\right) S^i_{op} = \sigma^{ij}_o \sum_p \bar{v}^j S^i_{op} + p_o \sum_p \bar{v}^i S^i_{op}$$

This represents the finite volume discretization of

$$p\frac{\partial v^i}{\partial x^i} - \sigma^{ij}\frac{\partial v^j}{\partial x^i}$$

for the control volume o. A boundary control volume b receives the contributions

$$\frac{1}{2} P^{i^T}_b \sum_p v_p S^i_{bp}$$

from the neighbors while it returns the contributions

$$-\frac{1}{2} P^{i^T}_b v_b \sum_p S^i_{bp} - P^{i^T}_b v_b S^i_b$$

giving the total

$$\begin{aligned}
&\frac{1}{2}P_b^{i^T}\sum_p (v_p+v_b)\,S_{op}^i - P_b^{i^T}v_b\sum_p S_{bp}^i - P_b^{i^T}v_bS_b^i \\
&\qquad = \frac{1}{2}P_b^{i^T}\sum_p (v_p+v_b)\,S_{bp}^i + P_b^{i^T}v_bS_b^i - P_b^{i^T}v_bS_b^i \\
&\qquad = \sigma_b^{ij}\left(\sum_p \bar{v}^j S_{bp}^i + v_b^j S_b^i\right) + P_b\left(\sum_p \bar{v}^i S_{bp}^i + v_b^i S_b^i\right) - \sigma_b^{ij}v_b^j S_b^i - P_p v_b^i S_b^i
\end{aligned}$$

Combining this result with the result for the interior control columes, and including the convective terms for the boundaries, we finally obtain the semi-discrete global kinetic energy conservation law

$$\begin{aligned}
\sum_o vol_o\frac{dk_o}{dt} =& \sum_b S_o^i\left\{v_o^i\left(p_o+\rho_o\frac{v_o^{i^2}}{2}\right) - v_o^i\sigma_o^{ij}\right\} \\
&+\sum_o\left(p_o\sum_p \bar{v}^i S_{op}^i - \sigma_o^{ij}\sum_p \bar{v}^j S_{op}^i\right)
\end{aligned} \tag{3.20}$$

where the first sum on the right hand side over the boundary control volumes represent the flux through the boundaries and the second sum is the finite volume discretization of

$$\int_D\left(p\frac{\partial v^i}{\partial x^i} - \sigma^{ij}\frac{\partial v^j}{\partial x^i}\right)dV$$

This establishes theorem 3.1

Theorem 3.1 *The semi-discrete conservation law* (3.8) *satisfies the semi-discrete global kinetic energy conservation law* (3.20) *if the interface fluxes satisfy condition* (3.13) *and the boundary fluxes are evaluated by equation* (3.9)*.*

Note that the discrete viscous terms

$$-\sum_o \sigma^{ij}\sum_p \bar{v}^j S_{op}^i$$

guarantee dissipation of the discrete energy because $\sum_p \bar{v}^j S_{op}^i$ is the consistent discretization of $\frac{\partial v^j}{\partial x^i}$ in the control volume. Then splitting $\frac{\partial v^j}{\partial x^i}$ into its symmetric and anti-symmetric parts

as

$$\frac{\partial v^j}{\partial x^i} = \frac{1}{2}\left(\frac{\partial v^j}{\partial x^i} + \frac{\partial v^i}{\partial x^j}\right) + \frac{1}{2}\left(\frac{\partial v^j}{\partial x^i} - \frac{\partial v^i}{\partial x^j}\right)$$

the contribution of the viscous terms amounts to

$$-\sum_o \left\{ \frac{1}{2}\mu \left(\frac{\partial v^j}{\partial x^i} + \frac{\partial v^i}{\partial x^j}\right)\left(\frac{\partial v^j}{\partial x^i} + \frac{\partial v^i}{\partial x^j}\right) + \lambda \left(\frac{\partial v^k}{\partial x^k}\right)^2 \right\}$$

Setting $\lambda = -\frac{2}{3}\mu$ this is

$$\sum_o \frac{1}{2}\mu \left(\frac{\partial v^j}{\partial x^i} + \frac{\partial v^i}{\partial x^j} - \frac{2}{3}\delta^{ij}\frac{\partial v^k}{\partial x^k}\right)^2$$

The discretization of the viscous terms covered by the proof does not have the most compact possible stencil. Consequently it might allow an updamped odd-even mode.

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 an analysis of discrete solution methods for the viscous Burgers equation [12] it was established that the EP scheme will satisfy the conditions for a local extremum diminishing (LED) scheme if the local cell Reynolds number $Re_c \leq 2$. Here Re_c is defined as

$$\frac{v\Delta x}{\nu}$$

where v is the velocity and ν is the kinematic viscosity. This indicates the need to use a mesh with a number of cells proportional to the global Reynolds number $\frac{vL}{\nu}$, where L is the global length scale.

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 [16, 17].

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

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

$$w = \frac{p^*}{p} \begin{bmatrix} u_3 \\ -u_2 \\ u_1 \end{bmatrix}, \qquad u = \frac{p}{p^*} \begin{bmatrix} w_3 \\ -w_2 \\ w_1 \end{bmatrix}$$

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 [12] 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 derivative, this advances the solution during one time step by the three stage scheme

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

The test case for the numerical experiments was the well known example originally proposed by Sod [19]. The shock tube extends over the range $0 \leq x \leq 1$, with a discontinuity

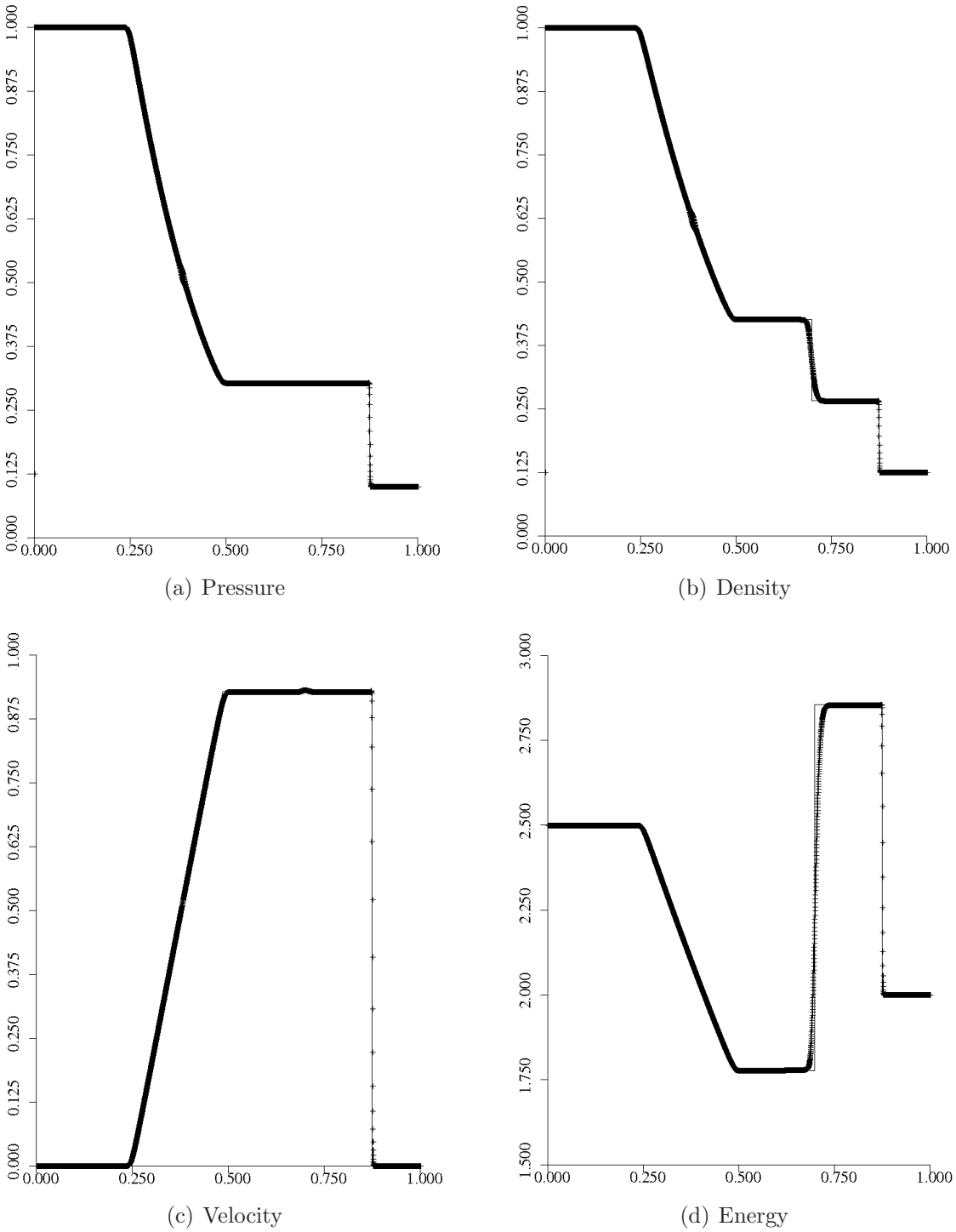
in the initial data at $x = .5$. The left and right states are

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

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 the oscillations in the expansion region are amplified as the Reynolds number and number of mesh cells are reduced, as is illustrated in Figures 4.4–4.6. In all cases (surprisingly to the author) the KEP scheme performs better than the EP scheme for this model problem, while simple flux averaging is inadequate.



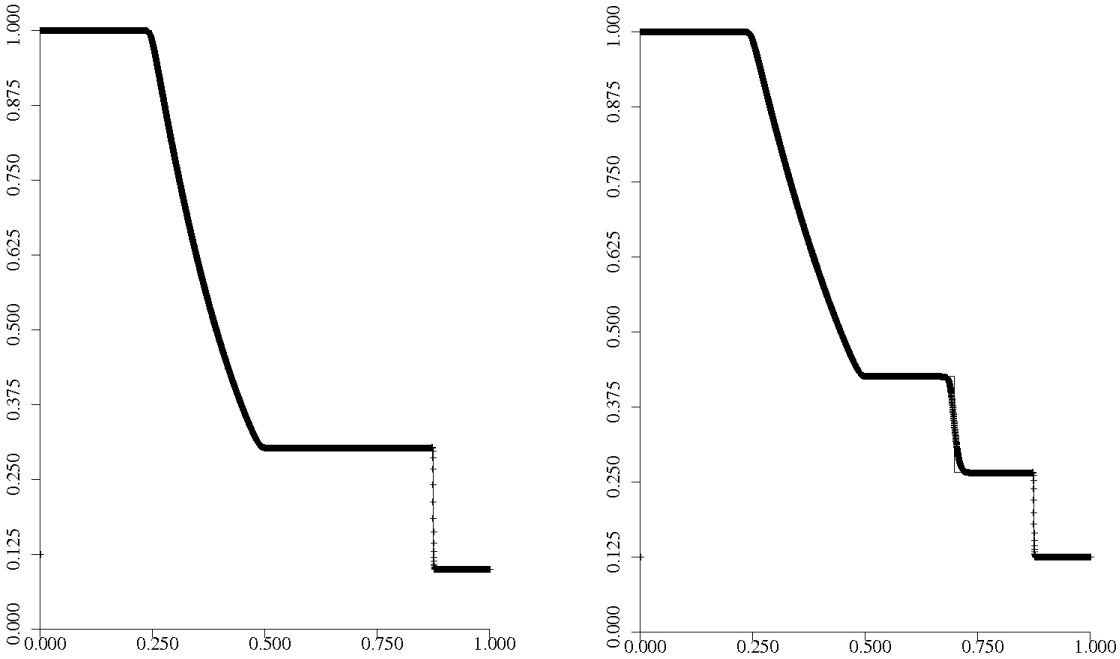
(a) Pressure

(b) Density

(c) Velocity

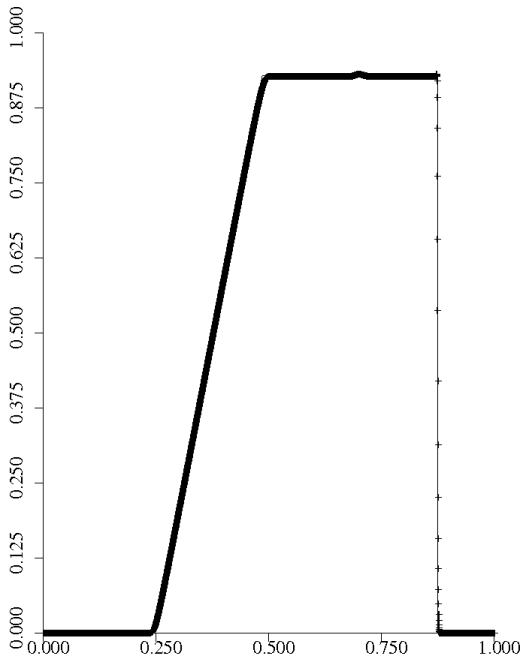
(d) Energy

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

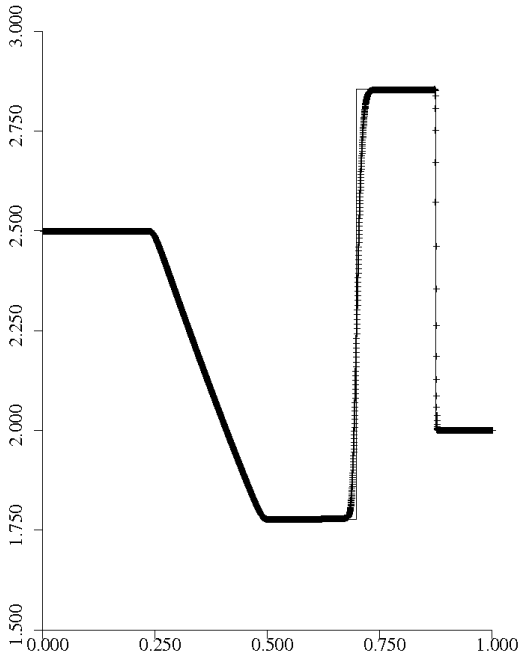


(a) Pressure

(b) Density

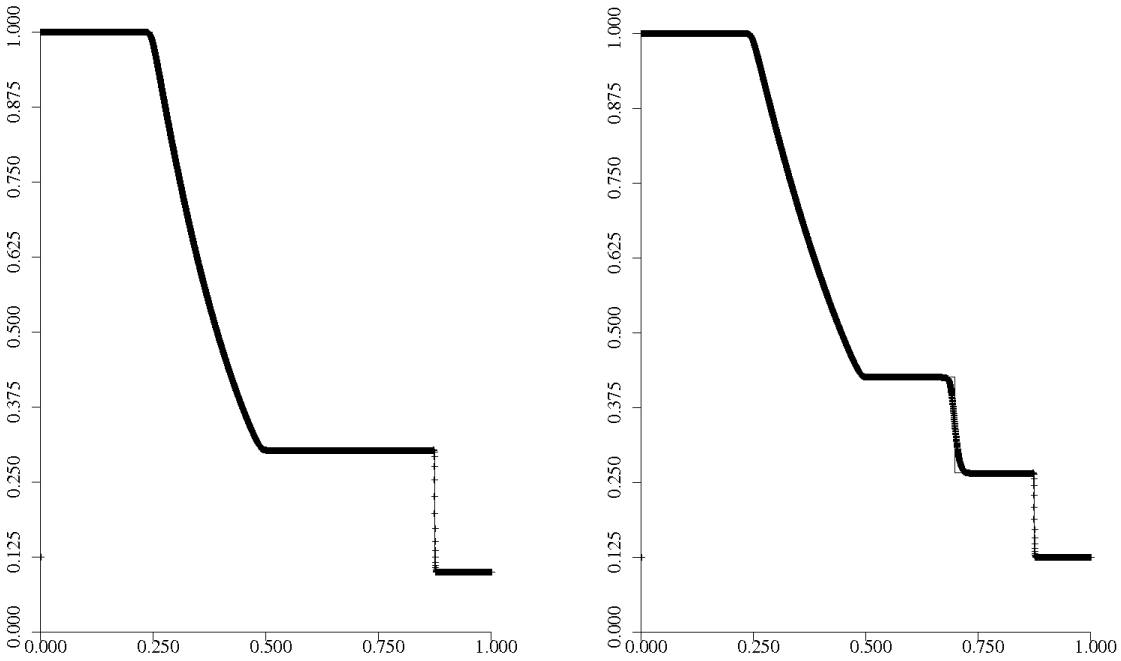


(c) Velocity



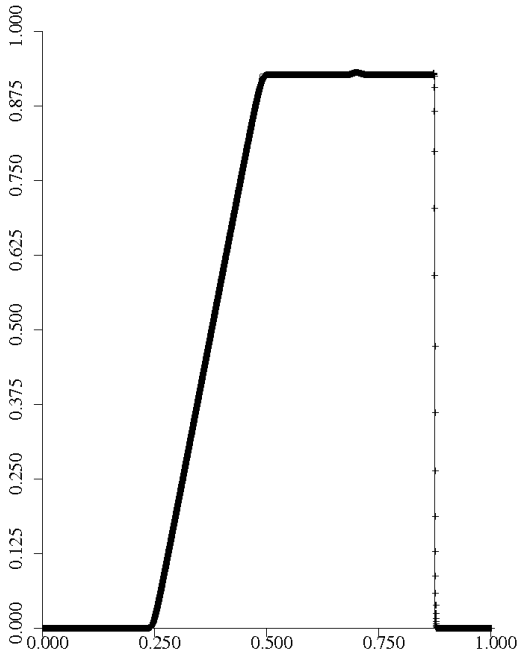
(d) Energy

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

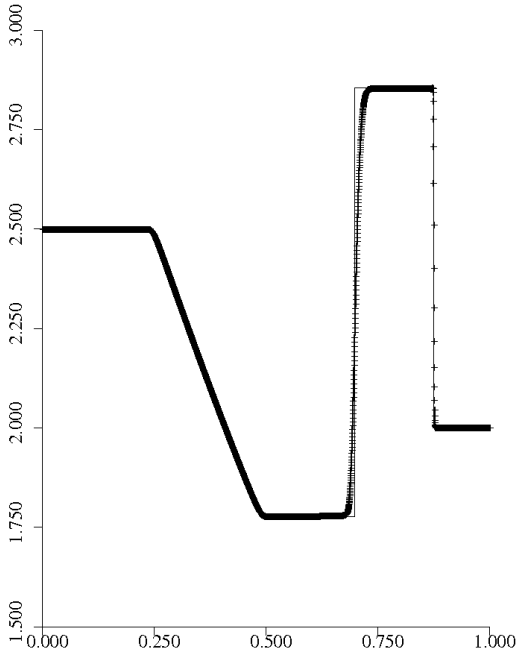


(a) Pressure

(b) Density

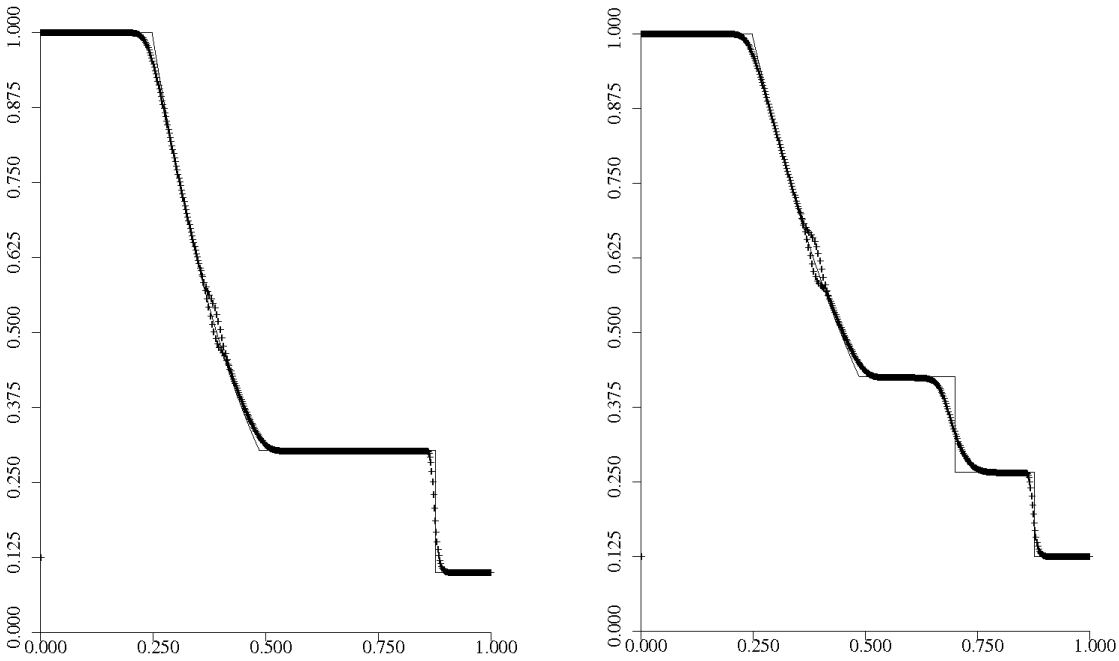


(c) Velocity



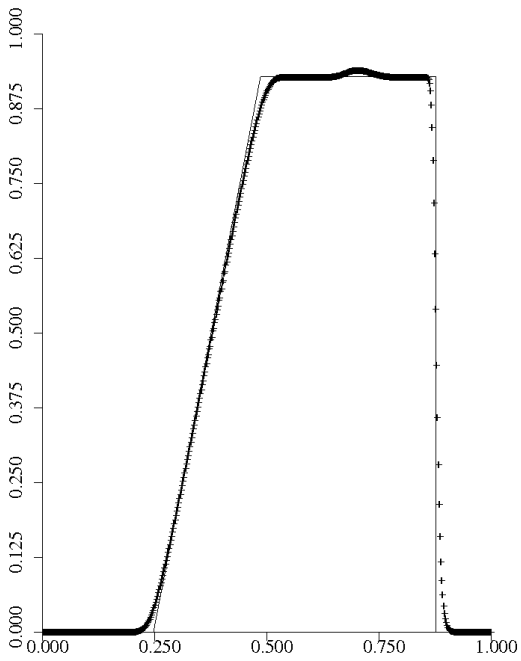
(d) Energy

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

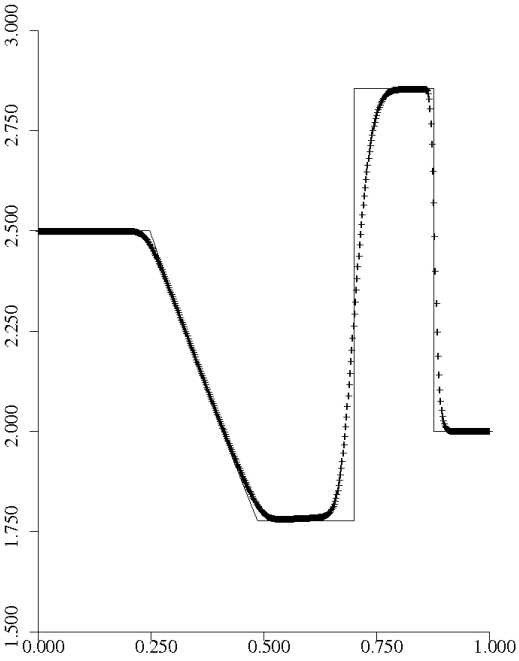


(a) Pressure

(b) Density

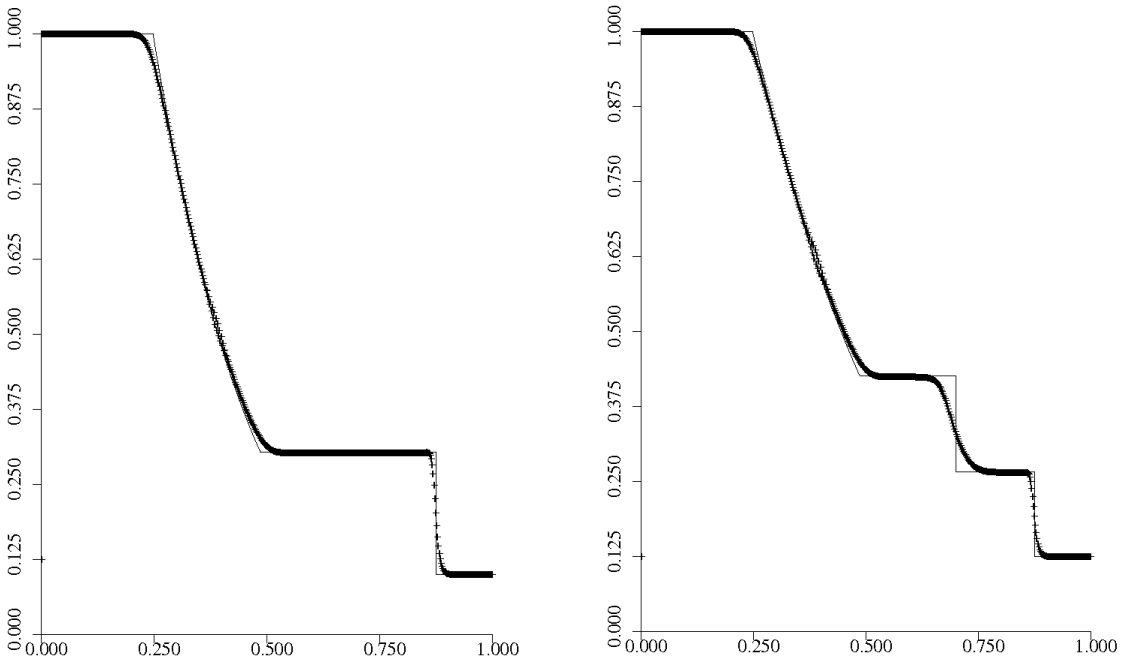


(c) Velocity



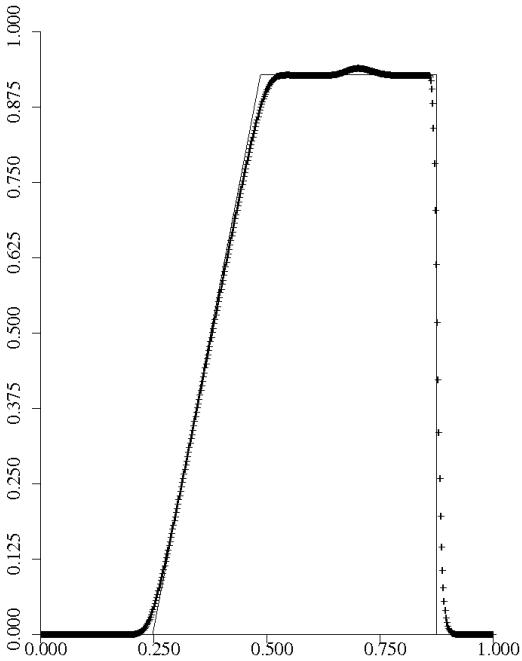
(d) Energy

Figure 4.4: Simple averaging of the flux (coarse mesh): 512 mesh cells, Reynolds number 2500, Computed solution values +, Exact inviscid solution —

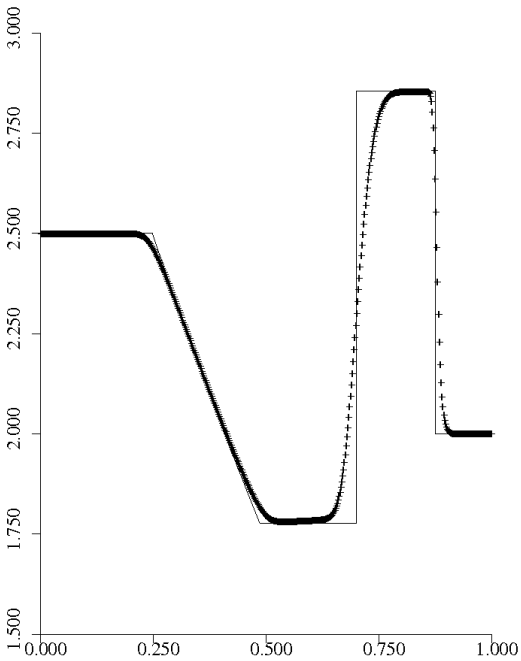


(a) Pressure

(b) Density

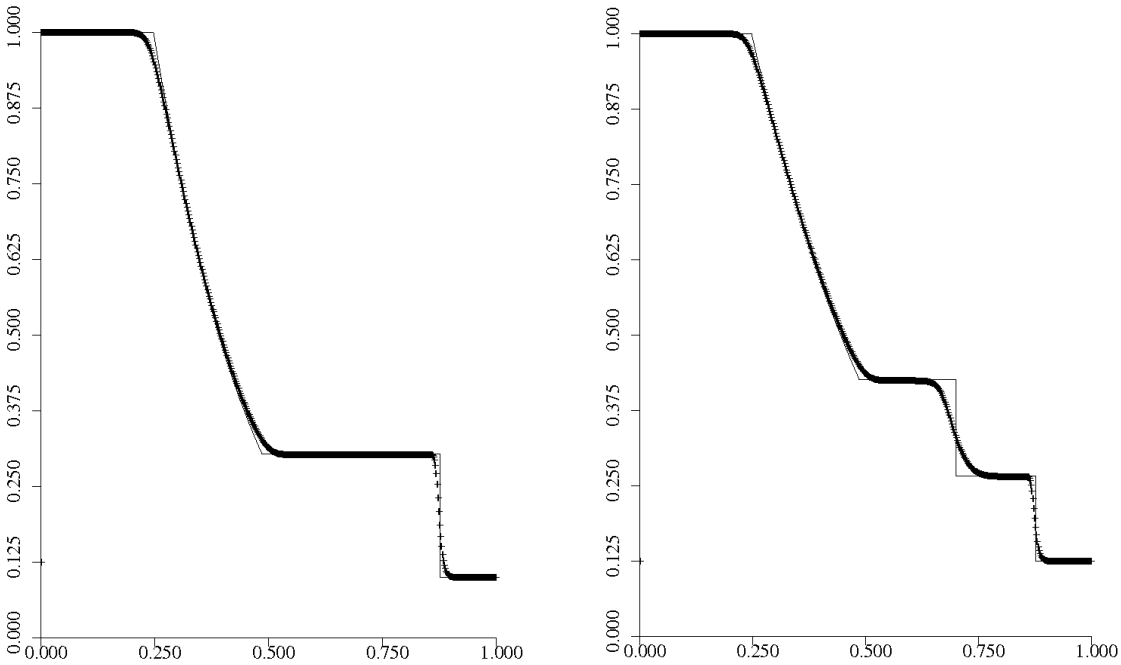


(c) Velocity



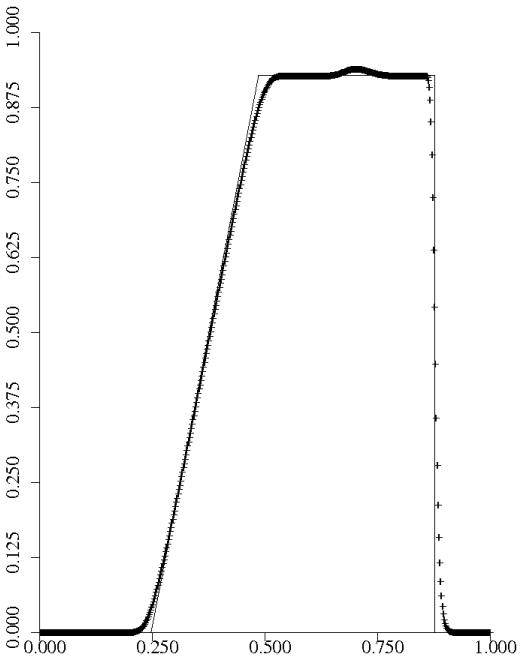
(d) Energy

Figure 4.5: Entropy preserving scheme (coarse mesh): 512 mesh cells, Reynolds number 2500, Computed solution values +, Exact inviscid solution —

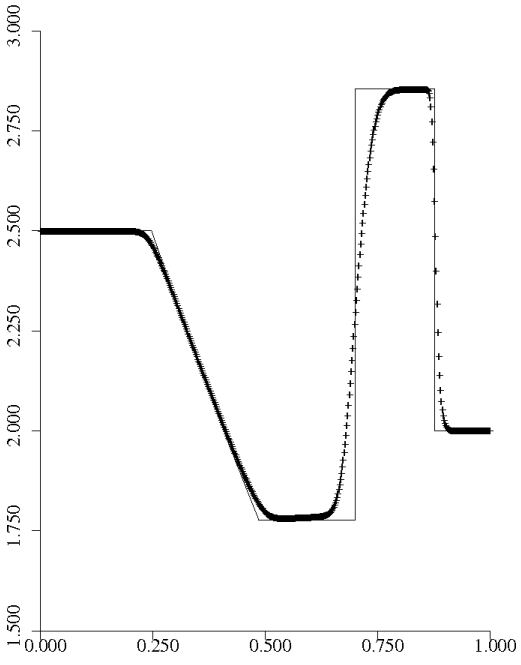


(a) Pressure

(b) Density



(c) Velocity



(d) Energy

Figure 4.6: Kinetic energy preserving scheme (coarse mesh): 512 mesh cells, Reynolds number 2500, Computed solution values +, Exact inviscid solution —

5 Conclusion

As a sequel to [12], 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.

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

Acknowledgement

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