Positivity and Stability Analysis of LSKUM in One and Two Dimensions.

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Abstract

Numerical schemes for fluid flows must preserve the positivity of density and pressure. This is a weak stability condition and is the first step towards establishing an entropy inequality. It also allows us to derive a rigorous CFL condition. Positivity of finite volume methods based on Kinetic Theory has been established in [2] and some general results have been given for finite volume methods in [6]. It must be remarked that very few numerical methods for Euler equations are positivity preserving. In the present work, the positivity and stability of first order LSKUM [3, 4] in one- and two-dimensions is established under a CFL-like condition, though the stability results are not very strong. The analysis leads to the discovery of many length scales which are integral averages of the node spacings, and are used in the definition of the CFL number. In 2-D, the concept of a *genuine connectivity* is defined which can be used to obtain a *good* connectivity for LSKUM.

1 Some Terminalogy in 1-D

Consider a one dimensional grid $\mathcal{G}$, the coordinates of the points being $\{x_i \mid i \in \mathcal{G}\}$. For each $i \in \mathcal{G}$, there exist a set of points $\mathcal{C}_i = \{j \mid j \in \mathcal{G}\}$ which are said to be in the connectivity of point i. Further, each $\mathcal{C}_i$ is divided into $\mathcal{L}_i$ and $\mathcal{R}_i$, so that $\mathcal{C}_i = \mathcal{L}_i \cup \mathcal{R}_i$, and

$$\mathcal{L}_i = \{j \in \mathcal{C}_i \mid \Delta x_{ji} \leq 0\}$$

$$\mathcal{R}_i = \{j \in \mathcal{C}_i \mid \Delta x_{ji} \geq 0\}$$

where

$$\Delta(\cdot)_{ji} = (\cdot)_j - (\cdot)_i$$

We also define the following terms[1].

$$D_{l_i} = \sum_{j \in \mathcal{L}_i} \Delta x_{ji}^2, \quad D_{r_i} = \sum_{j \in \mathcal{R}_i} \Delta x_{ji}^2 \tag{1.1}$$

$$S_{l_i} = -\sum_{j \in \mathcal{L}_i} \Delta x_{ji}, \quad S_{r_i} = \sum_{j \in \mathcal{R}_i} \Delta x_{ji} \tag{1.2}$$

With these terms, we define two lengths which will be useful in the analysis.

$$l_i = \frac{D_{l_i}}{S_{l_i}}, \quad r_i = \frac{D_{r_i}}{S_{r_i}}$$

[1] All summations are over j unless indicated otherwise

Note that l_i and r_i are convex combinations of the Δx_{ji} so that the following inequalities are valid:

$$\min_{j \in \mathcal{L}_i} |\Delta x_{ji}| \leq l_i \leq \max_{j \in \mathcal{L}_i} |\Delta x_{ji}|$$

$$\min_{j \in \mathcal{R}_i} |\Delta x_{ji}| \leq r_i \leq \max_{j \in \mathcal{R}_i} |\Delta x_{ji}|$$

Finally, we define another length as follows.

$$h_i = \frac{l_i r_i}{l_i + r_i}$$

Since h_i is the harmonic mean of l_i, r_i, we have the following inequalities,

$$h_i \leq l_i, \qquad h_i \leq r_i$$

2 First Order LSKUM in One-Dimension

Consider the Boltzmann equation in one-dimension without the collision term,

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = 0$$

The above equation can be rewritten after splitting the velocity v into positive and negative parts,

$$\frac{\partial f}{\partial t} + \frac{v + |v|}{2} \frac{\partial f}{\partial x} + \frac{v - |v|}{2} \frac{\partial f}{\partial x} = 0$$

Using least squares for the x-derivatives we obtain the first order update formula for the velocity distribution function,

$$f_i^{n+1} = f_i^n - \Delta t \left[\frac{v + |v|}{2} \left(\frac{\sum \Delta x_{ji} \Delta f_{ji}^n}{\sum \Delta x_{ji}^2} \right)_{\mathcal{L}_i} + \frac{v - |v|}{2} \left(\frac{\sum \Delta x_{ji} \Delta f_{ji}^n}{\sum \Delta x_{ji}^2} \right)_{\mathcal{R}_i} \right] \tag{2.1}$$

and the appropriate stencil is indicated in figure (1). The conserved variables are obtained

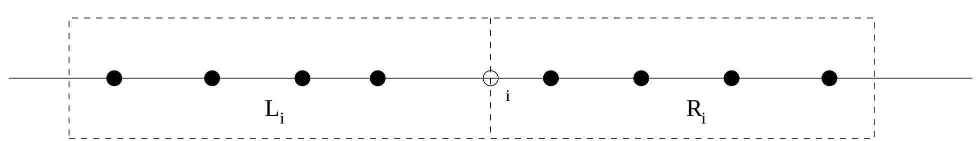

Figure 1: Split stencil for 1-D

by taking ψ-moments of f_i^{n+1},

$$U_i^{n+1} = \int_{\mathbb{R} \times \mathbb{R}^+} \psi f_i^{n+1} \mathrm{d}v \mathrm{d}I = \begin{bmatrix} \rho_i^{n+1} \\ (\rho u)_i^{n+1} \\ e_i^{n+1} \end{bmatrix}$$

where

$$\psi = \begin{bmatrix} 1 \\ v \\ I + v^2/2 \end{bmatrix}$$

The update equation for U is

$$U_i^{n+1} = U_i^n - \Delta t \left[\left(\frac{\sum \Delta x_{ji} \Delta F_{ji}^+}{\sum \Delta x_{ji}^2} \right)_{\mathcal{L}_i}^n + \left(\frac{\sum \Delta x_{ji} \Delta F_{ji}^-}{\sum \Delta x_{ji}^2} \right)_{\mathcal{R}_i}^n \right] \tag{2.2}$$

The split fluxes $F^\pm$ are given by [5]

$$F^\pm = \int_{\mathbb{R}\times\mathbb{R}^+} \psi f v^\pm \mathrm{d}v \mathrm{d}I, \quad \text{where} \quad v^\pm = (v \pm |v|)/2$$

Let us define the following quantities,

$$|F| = F^+ - F^- \tag{2.3}$$

and

$$W = \begin{bmatrix} \rho \\ e \end{bmatrix} \tag{2.4}$$

$$\Phi = \begin{bmatrix} F_\rho \\ F_e \end{bmatrix} \tag{2.5}$$

with obvious definitions for $\Phi^\pm$, and

$$|\Phi| = \max\{\Phi^+, -\Phi^-\} \tag{2.6}$$

where the maximum is to be taken in terms of each component, i,e,

$$|\Phi| = \begin{bmatrix} \max\{F_\rho^+, -F_\rho^-\} \\ \\ \max\{F_e^+, -F_e^-\} \end{bmatrix}$$

3 Solution Space

We assume that the solution space $\mathcal{W} \subset \mathbb{R}^m$ satisfies the following hypothesis.
H1. $\mathcal{W}$ is an open subset of $\mathbb{R}^m$.
H2. $\forall p, q \in \mathcal{W}$, $\forall \alpha, \beta \in \mathbb{R}^{+\star}$, $\alpha p + \beta q \in \mathcal{W}$.
H3. $p \in \mathcal{W} \Longrightarrow -p \notin \mathcal{W}$.

For the case of Euler equations in 1-D, the solution space is

$$\mathcal{W} = \{U \in \mathbb{R}^3 : U_1 \geq 0, U_3 \geq U_2^2/(2U_1)\} \tag{3.1}$$

and it can be verified that it satisfies all the above three hypotheses.

4 A partial-order relation on $\mathbb{R}^m$

Let $p, q \in \mathbb{R}^m$. p is said to be lower than q if and only if $q - p \in \mathcal{W}$ or $p = q$. It is denoted as $p \preceq q$. Conversley, p is said to be greater than q if and only if $p - q \in \mathcal{W}$ or $p = q$. This is denoted as $p \succeq q$.

Using hypothesis H1, H2, H3, we can easily prove that,
P1. $\forall p, q, r, s \in \mathbb{R}^m$, $\forall \alpha, \beta \in \mathbb{R}^{+\star}$, $p \preceq r$ and $q \preceq s \Longrightarrow \alpha p + \beta q \preceq \alpha r + \beta s$.
P2. $\forall p, q \in \mathbb{R}^m$, $p \preceq q \Longleftrightarrow -p \succeq -q$.
P3. $\forall p \in \mathbb{R}^m$, $p \in \mathcal{W} \Longleftrightarrow p \succ 0$.

Lemma 1 *If $\rho \ge 0$ and $T \ge 0$, then*

$$F^+ \succeq 0 \tag{4.1}$$

for $1 < \gamma \le 3$.

Proof: By definition

$$F^+_\rho = \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v(vf) \ge 0$$

Consider

$$\begin{aligned}
\mu &= 2F^+_\rho F^+_e - (F^+_m)^2 \\
&= 2\left(\int vf\mathrm{d}v\mathrm{d}I\right)\left(\int v(I + v^2/2)f\mathrm{d}v\mathrm{d}I\right) - \left(\int v^2 f\mathrm{d}v\mathrm{d}I\right)^2 \\
&\ge \left(\int (vf)\mathrm{d}v\mathrm{d}I\right)\left(\int v^3 f\mathrm{d}v\mathrm{d}I\right) - \left(\int v^2 f\mathrm{d}v\mathrm{d}I\right)^2 \\
&\ge 0, \quad \text{by Cauchy-Schwarz inequality}
\end{aligned}$$

This proves that $F^+ \succeq 0$.

Lemma 2 *Under the conditions of lemma (4) and $|F|$ as defined by equation (2.3), we have, for $\alpha, \beta \in [0,1]$*

$$\alpha F^+ - \beta F^- \preceq |F| \tag{4.2}$$

Proof: We note that

$$\alpha F^+ \preceq F^+$$
$$-\beta F^- \preceq -F^-$$

so that

$$\alpha F^+ - \beta F^- \preceq F^+ - F^- = |F|$$

and hence the lemma is proved.

Lemma 3 [Estivalezes and Villedieu] *Let d represent the number of space dimensions and F represent one component of the flux. Then, for $1 < \gamma \le 3$*

$$|F| \preceq \lambda(U)U \tag{4.3}$$

where

$$\lambda(U) = 2\left(|\vec{u}| + \frac{2d+1}{2}\sqrt{\frac{RT}{2\pi}}\right) \tag{4.4}$$

Proof: Let F denote the x-component of the flux, and $(\bar{\rho}, \bar{m}, \bar{e})$ represent the components of $|F|$. Then for $\tau \in \mathbb{R}^+$,

$$
\begin{aligned}
\rho - \tau\bar{\rho} &= \rho - \tau \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I \\
&\geq \rho \left(1 - \tau \left(|\vec{u}| + \sqrt{\frac{2RT}{\pi}}\right)\right) \\
&> 0 \text{ if } \tau < \left(|\vec{u}| + \sqrt{\frac{2RT}{\pi}}\right)^{-1}
\end{aligned}
$$

Next, let

$$(e - \tau\bar{e})(\rho - \tau\bar{\rho}) - \frac{1}{2}(m - \tau\bar{m})^2 = A + B - \tau C + \tau^2 D$$

$$
\begin{aligned}
A &= (\rho - \tau\bar{\rho}) \left(\int_{\mathbb{R}^d \times \mathbb{R}^+} I f \mathrm{d}\vec{v}\mathrm{d}I - \tau \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| I F \mathrm{d}\vec{v}\mathrm{d}I\right) \\
&\geq (\rho - \tau\bar{\rho}) \left(1 - \tau \left(|\vec{u}| + \sqrt{\frac{2RT}{\pi}}\right)\right) \rho I_o \\
&> 0 \text{ if } \tau < \left(|\vec{u}| + \sqrt{\frac{2RT}{\pi}}\right)^{-1} \\
D &= \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| \frac{v^2}{2} f \mathrm{d}\vec{v}\mathrm{d}I - \frac{1}{2}\sum_{i=1}^{d} \left(\int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| v_i f \mathrm{d}\vec{v}\mathrm{d}I\right)^2 \\
&\geq 0 \\
B &= \int_{\mathbb{R}^d \times \mathbb{R}^+} f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{v^2}{2} f \mathrm{d}\vec{v}\mathrm{d}I - \frac{1}{2}\sum_{i=1}^{d} \left(\int_{\mathbb{R}^d \times \mathbb{R}^+} v_i f \mathrm{d}\vec{v}\mathrm{d}I\right)^2 \\
&= \frac{d}{2}\rho^2 RT \\
C &= \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{v^2}{2} f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I + \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{v^2}{2} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} f \mathrm{d}\vec{v}\mathrm{d}I \\
&\quad - \sum_{i=1}^{d} \left(\int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| v_i f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} v_i f \mathrm{d}\vec{v}\mathrm{d}I\right) \\
&= \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{(v-u)^2}{2} f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I + \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{(v-u)^2}{2} |v_1| f \mathrm{d}\vec{v}\mathrm{d}I \int_{\mathbb{R}^d \times \mathbb{R}^+} f \mathrm{d}\vec{v}\mathrm{d}I \\
&\leq \frac{d}{2}\rho^2 RT \left(2|\vec{u}| + \frac{2d+1}{d}\sqrt{\frac{2RT}{\pi}}\right)
\end{aligned}
$$

Putting all these together, we obtain,

$$A + B - \tau C + \tau^2 D \geq \frac{d}{2}\rho^2 RT \left(1 - \tau \left(2|\vec{u}| + \frac{2d+1}{d}\sqrt{\frac{2RT}{\pi}}\right)\right)$$

and hence

$$\lambda(U) = 2\left(|\vec{u}| + \frac{2d+1}{d}\sqrt{\frac{RT}{2\pi}}\right)$$

Definition [CFL Number]
The CFL number σ is defined as

$$\sigma = \min_{i \in \mathcal{G}} \frac{\Delta t \lambda(U_i)}{h_i} \tag{4.5}$$

Theorem 1 *If $\rho_i^n \geq 0$, $T_i^n \geq 0$, $i \in \mathcal{G}$, then under the CFL condition*

$$\sigma^n \leq 1 \tag{4.6}$$

the first order LSKUM is positivity preserving for $1 < \gamma \leq 3$, i.e.,

$$\rho_i^{n+1} \geq 0 \quad \text{and} \quad T_i^{n+1} \geq 0$$

Proof: Equation (2.2) is the first order update formula for LSKUM. given by,

$$\begin{aligned}
U_i^{n+1} &= U_i^n - \Delta t \left(\frac{F_i^+}{l_i} - \frac{F_i^-}{r_i} \right) + \frac{\Delta t}{l_i} \sum_{j \in \mathcal{L}_i} F_j^+ \frac{|\Delta x_{ji}|}{S_{l_i}} + \frac{\Delta t}{r_i} \sum_{j \in \mathcal{R}_i} (-F_j^-) \frac{\Delta x_{ji}}{S_{r_i}} \\
&\succeq U_i^n - \Delta t \left(\frac{F_i^+}{l_i} - \frac{F_i^-}{r_i} \right) \\
&= U_i^n - \frac{\Delta t}{h_i} \left(\frac{r_i F_i^+ + l_i |F_i^-|}{r_i + l_i} \right) \\
&\succeq U_i^n - \frac{\Delta t}{h_i} |F_i| \\
&\succeq U_i^n - \frac{\Delta t \lambda_i^n}{h_i} U_i^n \\
&\succeq 0
\end{aligned}$$

and hence the theorem is proved.

Definition: [Stability]
The numerical scheme

$$U_i^{n+1} = \mathbb{F}(U_i^n; U_j^n), \quad j \in \mathcal{C}_i$$

is said to be stable in the norm $\|\cdot\|$ if

$$\|U\|^{n+1} \leq K \|U\|^n$$

for some constant K, $0 \leq K < \infty$.

Definition: [Norm]
The norm that will be used in the stability analysis is defined as

$$\|\phi\|_L = \sum_i h_i |\phi_i| \tag{4.7}$$

Definition: [Connectivity Number, ϖ]
Let

$$\varpi_i = \sum_{\substack{\text{all } j \\ i \in \mathcal{C}_j}} 1$$

Then, the connectivity number ϖ is defined as

$$\varpi = \max_i \varpi_i$$

Lemma 4 *If $\rho \geq 0$ and $T \geq 0$, then*

$$\Phi^+ \geq 0 \quad \textit{and} \quad \Phi^- \leq 0 \tag{4.8}$$

for $-\infty < M < \infty$ and $1 < \gamma \leq 3$.

Proof: The proof follows obviously from the definition of the kinetic split fluxes.

Lemma 5 *Under the conditions of lemma (4) and $|\Phi|$ as defined by equation (2.6), we have,*

$$\begin{aligned} |\Phi| &= \Phi^+, \quad u \geq 0 \\ &= -\Phi^-, \quad u \leq 0 \end{aligned}$$

Proof: We note that

$$\Phi^+ - (-\Phi^-) = \Phi^+ + \Phi^- = \Phi = \begin{bmatrix} \rho \\ e+p \end{bmatrix} u$$

so that

$$\begin{aligned} \Phi^+ - (-\Phi^-) &\geq 0, \quad u \geq 0 \\ &\leq 0, \quad u \leq 0 \end{aligned}$$

and hence the lemma is proved.

Lemma 6 *For $1 < \gamma \leq 2$*

$$|\Phi| \leq \lambda(U) W \tag{4.9}$$

Proof: Consider the case $u \geq 0$. Then, by lemma (5),

$$\begin{aligned} |F_\rho| &= F_\rho^+ \\ &= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v(vf) \\ &= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v(Cf) + u \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v(f) \\ &= \int_0^\infty \mathrm{d}I \int_{-u}^\infty \mathrm{d}C(Cf) + \frac{\rho u}{2} \\ &= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C(Cf) + \int_0^\infty \mathrm{d}I \int_{-u}^0 \mathrm{d}C(Cf) + \frac{\rho u}{2} \\ &\leq \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C(Cf) + \rho u \\ &\leq \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C(Cf) + \rho u \\ &= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C(Cf) + \rho u \\ &= \left(u + \sqrt{\frac{RT}{2\pi}} \right) \rho \\ &\leq \lambda(U) \rho \end{aligned}$$

Similarly,

$$\begin{aligned}
F_e^+ &\le \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C(I+|C+u|^2/2)(Cf) + u\int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v(I+v^2/2)(f) \\
&= \sqrt{\frac{RT}{2\pi}}\left[\frac{\gamma+1}{2(\gamma-1)}p + \frac{\rho u^2}{2}\right] + \frac{pu}{2} + \frac{eu}{2} \\
&\le \frac{\gamma+1}{2}\sqrt{\frac{RT}{2\pi}}\left[\frac{p}{\gamma-1} + \frac{\rho u^2}{2}\right] + ue, \quad \text{since } p \le e \text{ and } (\gamma+1)/2 \ge 1 \\
&= \left(u + \frac{\gamma+1}{2}\sqrt{\frac{RT}{2\pi}}\right)e \\
&\le \lambda(U)e
\end{aligned}$$

If $u \le 0$, then

$$|\Phi| = -\Phi^- = \Phi^+(-u) \le \left(-u + \frac{\gamma+1}{2}\sqrt{\frac{RT}{2\pi}}\right)W$$

and hence the lemma is proved.

Theorem 2 *Under the conditions of theorem (1), the first order LSKUM is stable in the norm* $\|\cdot\|_L$ *and*

$$\max_{\mathcal{G}} h_i W_i^{n+1} \le 2\max_{\mathcal{G}} h_i W_i^n \tag{4.10}$$

Proof:

$$\begin{aligned}
W_i^{n+1} &= W_i^n - \Delta t\left(\frac{\Phi_i^+}{l_i} - \frac{\Phi_i^-}{r_i}\right) + \frac{\Delta t}{l_i}\sum_{j\in\mathcal{L}_i}\Phi_j^+\frac{|\Delta x_{ji}|}{S_{l_i}} + \frac{\Delta t}{r_i}\sum_{j\in\mathcal{R}_i}(-\Phi_j^-)\frac{\Delta x_{ji}}{S_{r_i}} \\
&\le W_i^n - \frac{\Delta t}{h_i}\left(\frac{r_i\Phi_i^+ + l_i|\Phi_i^-|}{r_i+l_i}\right) + \frac{\Delta t}{l_i}\max_{j\in\mathcal{L}_i}\Phi_j^+ + \frac{\Delta t}{r_i}\max_{j\in\mathcal{R}_i}(-\Phi_j^-) \\
&\le W_i^n + \frac{\Delta t}{l_i}\max_{j\in\mathcal{L}_i}\Phi_j^+ + \frac{\Delta t}{r_i}\max_{j\in\mathcal{R}_i}(-\Phi_j^-) \\
&= W_i^n + \frac{\Delta t}{l_i}\Phi_{i_l}^+ + \frac{\Delta t}{r_i}(-\Phi_{i_r}^-) \\
&\le W_i^n + \frac{\Delta t}{l_i}|\Phi_{i_l}| + \frac{\Delta t}{r_i}|\Phi_{i_r}| \\
&\le W_i^n + \frac{\Delta t}{h_i}|\Phi_i^*|
\end{aligned}$$

In the above equations, $i_l \in \mathcal{L}_i$ and $i_r \in \mathcal{R}_i$, and

$$\Phi_{i_l}^+ = \max_{j\in\mathcal{L}_i}\Phi_j^+, \qquad (-\Phi_{i_r}^-) = \max_{j\in\mathcal{R}_i}(-\Phi_j^-)$$

and

$$|\Phi_i^*| = \max\{|\Phi_{i_l}|, |\Phi_{i_r}|\}$$

From this we have,

$$\begin{aligned}
h_i W_i^{n+1} &\le h_i W_i^n + \Delta t|\Phi_i^*| \\
&\le h_i W_i^n + \frac{\Delta t\lambda(U_i^*)}{h_i^*}h_i^* W_i^* \\
&\le h_i W_i^n + h_i^* W_i^*
\end{aligned}$$

We immediately obtain,

$$\max_{\mathcal{G}} h_i W_i^{n+1} \leq 2 \max_{\mathcal{G}} h_i W_i^n$$

Also,

$$\begin{aligned} \|W\|_L^{n+1} &= \sum_i h_i W_i^{n+1} \\ &< \sum_i h_i W_i^n + \sum_i h_i^* W_i^* \\ &\leq \|W\|_L^n + \varpi \sum_i h_i W_i^n \\ &= (1+\varpi)\|W\|_L^n \end{aligned}$$

Finally, we have

$$\begin{aligned} |\rho u| &= \left(\rho(\rho u^2)\right)^{1/2} \\ &\leq (2\rho e)^{1/2} \\ &\leq |\rho| + |e| \end{aligned}$$

so that

$$\|\rho u\|_L \leq \|\rho\|_L + \|e\|_L$$

and hence the theorem is proved.

<u>Remark</u>: [Weighted Least Squares]
All the above results are valid for weighted least squares with positive weights, except that equations (1.1)-(1.2) must be modified as follows.

$$D_{l_i} = \sum_{j \in \mathcal{L}_i} w_{ji} \Delta x_{ji}^2, \quad D_{r_i} = \sum_{j \in \mathcal{R}_i} w_{ji} \Delta x_{ji}^2 \tag{4.11}$$

$$S_{l_i} = -\sum_{j \in \mathcal{L}_i} w_{ji} \Delta x_{ji}, \quad S_{r_i} = \sum_{j \in \mathcal{R}_i} w_{ji} \Delta x_{ji} \tag{4.12}$$

5 Some Terminalogy in 2-D

Consider a two dimensional grid $\mathcal{G}$, the coordinates of the points being $\{(x_i, y_i) \mid i \in \mathcal{G}\}$. For each $i \in \mathcal{G}$, there exist a set of points $\mathcal{C}_i = \{j \mid j \in \mathcal{G}\}$ which are said to be in the connectivity of point i. Further, each $\mathcal{C}_i$ is divided into $\mathcal{L}_i, \mathcal{R}_i, \mathcal{U}_i$ and $\mathcal{D}_i$, so that $\mathcal{C}_i = \mathcal{L}_i \cup \mathcal{R}_i = \mathcal{U}_i \cup \mathcal{D}_i$, and

$$\begin{aligned} \mathcal{L}_i &= \{j \in \mathcal{C}_i \mid \Delta x_{ji} \leq 0\} \\ \mathcal{R}_i &= \{j \in \mathcal{C}_i \mid \Delta x_{ji} \geq 0\} \\ \mathcal{D}_i &= \{j \in \mathcal{C}_i \mid \Delta y_{ji} \leq 0\} \\ \mathcal{U}_i &= \{j \in \mathcal{C}_i \mid \Delta y_{ji} \geq 0\} \end{aligned}$$

Let $\mathcal{S}_i$ denote one of these half-stencils. We also define the following quantities.

$$\mathrm{X}_j(\mathcal{S}_i) = \left(\sum_k \Delta y_{ki}^2\right) \Delta x_{ji} - \left(\sum_k \Delta x_{ki} \Delta y_{ki}\right) \Delta y_{ji}, \quad j, k \in \mathcal{S}_i$$

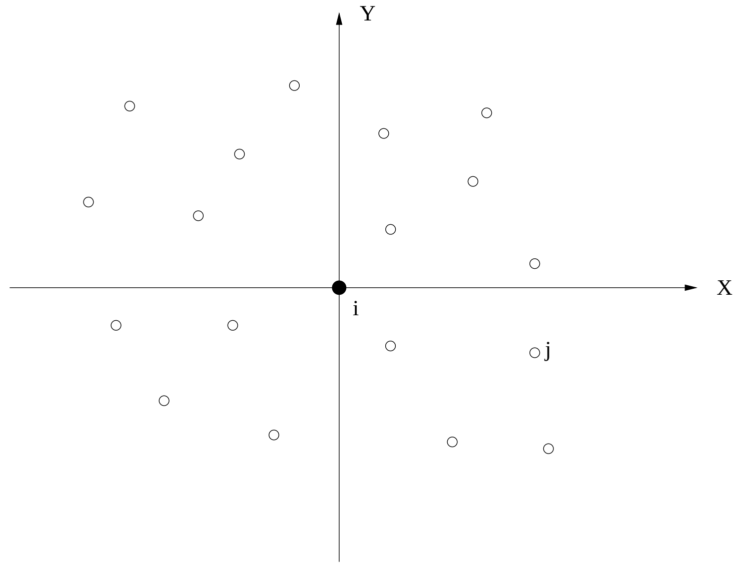

Figure 2: Typical stencil for 2-D LSKUM

$$\mathrm{Y}_j(\mathcal{S}_i) = \left(\sum_k \Delta x_{ki}^2\right)\Delta y_{ji} - \left(\sum_k \Delta x_{ki}\Delta y_{ki}\right)\Delta x_{ki}, \quad j,k \in \mathcal{S}_i$$

$$\mathrm{D}(\mathcal{S}_i) = \left(\sum \Delta x_{ji}^2\right)\left(\sum \Delta y_{ji}^2\right) - \left(\sum \Delta x_{ji}\Delta y_{ji}\right)^2, \quad j \in \mathcal{S}_i$$

By Cauchy-Schwarz inequality,

$$\mathrm{D}(\mathcal{S}_i) \geq 0$$

6 First order LSKUM in Two-Dimensions

Consider the Boltzmann equation in two-dimension without the collision term,

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x} + v_2 \frac{\partial f}{\partial y} = 0$$

The above equation can be rewritten after splitting the molecular velocities v_1 and v_2 into positive and negative parts,

$$\frac{\partial f}{\partial t} + \frac{v_1 + |v_1|}{2}\frac{\partial f}{\partial x} + \frac{v_1 - |v_1|}{2}\frac{\partial f}{\partial x} + \frac{v_2 + |v_2|}{2}\frac{\partial f}{\partial y} + \frac{v_2 - |v_2|}{2}\frac{\partial f}{\partial y} = 0$$

Using least squares for the derivatives, we obtain the first order update formula for f as,

$$f_i^{n+1} = f_i^n - \Delta t\left[v_1^+\left(\frac{\delta f_i}{\delta x}\right)_{\mathcal{L}_i}^n + v_1^-\left(\frac{\delta f_i}{\delta x}\right)_{\mathcal{R}_i}^n + v_2^+\left(\frac{\delta f_i}{\delta y}\right)_{\mathcal{D}_i}^n + v_2^-\left(\frac{\delta f_i}{\delta y}\right)_{\mathcal{U}_i}^n\right]$$

where

$$\frac{\delta f_i}{\delta x} = \frac{\left(\sum \Delta y_{ji}^2\right)\left(\sum \Delta x_{ji}\Delta f_{ji}\right) - \left(\sum \Delta x_{ji}\Delta y_{ji}\right)\left(\sum \Delta y_{ji}\Delta f_{ji}\right)}{\left(\sum \Delta x_{ji}^2\right)\left(\sum \Delta y_{ji}^2\right) - \left(\sum \Delta x_{ji}\Delta y_{ji}\right)^2}$$

$$\frac{\delta f_i}{\delta y} = \frac{\left(\sum \Delta x_{ji}^2\right)\left(\sum \Delta y_{ji}\Delta f_{ji}\right) - \left(\sum \Delta x_{ji}\Delta y_{ji}\right)\left(\sum \Delta x_{ji}\Delta f_{ji}\right)}{\left(\sum \Delta x_{ji}^2\right)\left(\sum \Delta y_{ji}^2\right) - \left(\sum \Delta x_{ji}\Delta y_{ji}\right)^2}$$

The conserved variables are obtained by taking ψ-moments of f_i^{n+1},

$$U^{n+1} = \int_{\mathbb{R}^2\times\mathbb{R}^+} \psi f^{n+1} \mathrm{d}\vec{v}\mathrm{d}I = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ e \end{bmatrix}$$

where

$$\psi = \begin{bmatrix} 1 \\ v_1 \\ v_2 \\ I + \vec{v}^2/2 \end{bmatrix}$$

The update equation for U is

$$U_i^{n+1} = U_i^n - \Delta t \left[\left(\frac{\delta F_i^+}{\delta x}\right)_{\mathcal{L}_i}^n + \left(\frac{\delta F_i^-}{\delta x}\right)_{\mathcal{R}_i}^n + \left(\frac{\delta G_i^+}{\delta y}\right)_{\mathcal{D}_i}^n + \left(\frac{\delta G_i^-}{\delta y}\right)_{\mathcal{U}_i}^n \right] \tag{6.1}$$

where

$$F^{\pm} = \int v_1^{\pm} \psi f \mathrm{d}\vec{v}\mathrm{d}I$$

$$G^{\pm} = \int v_2^{\pm} \psi f \mathrm{d}\vec{v}\mathrm{d}I$$

Similar to the 1-D case, we define the following quantities.

$$\Phi = \begin{bmatrix} F_\rho \\ F_e \end{bmatrix}$$

$$\Psi = \begin{bmatrix} G_\rho \\ G_e \end{bmatrix}$$

with obvious definitions for $\Phi^{\pm}$ and $\Psi^{\pm}$. Finally,

$$|\Phi| = \max\{\Phi^+, -\Phi^-\}, \quad |\Psi| = \max\{\Psi^+, -\Psi^-\}$$

The solution space is

$$\mathcal{W} = \{U \in \mathbb{R}^4 : U_1 \geq 0, U_4 \geq (U_2^2 + U_3^2)/(2U_1)\} \subset \mathbb{R}^4$$

<u>Definition</u> [Genuine Connectivity]
The connectivity $\mathcal{C}_i$ is said to be genuine if, $\forall j \in \mathcal{C}_i$,

$$\begin{array}{rcl} \mathrm{X}_j(\mathcal{L}_i) & \leq & 0 \\ \mathrm{X}_j(\mathcal{R}_i) & \geq & 0 \\ \mathrm{Y}_j(\mathcal{D}_i) & \leq & 0 \\ \mathrm{Y}_j(\mathcal{U}_i) & \geq & 0 \end{array} \tag{6.2}$$

and strict inequality holds for atleast one j in each of the four stencils[2]

[2] This implies that $\mathrm{D}(\mathcal{S}_i) > 0$ for each of the four stencils.

Definition [Genuine Grid]
A grid, all of whose nodes have genuine connectivity is said to be a genuine grid.

Definition
For a genuine connectivity, we define the following lengths.

$$\begin{aligned}
L(\mathcal{L}_i) &= -\frac{\mathrm{D}(\mathcal{L}_i)}{\sum \mathrm{X}_j(\mathcal{L}_i)} \\
L(\mathcal{R}_i) &= \frac{\mathrm{D}(\mathcal{R}_i)}{\sum \mathrm{X}_j(\mathcal{R}_i)} \\
L(\mathcal{D}_i) &= -\frac{\mathrm{D}(\mathcal{D}_i)}{\sum \mathrm{Y}_j(\mathcal{D}_i)} \\
L(\mathcal{U}_i) &= \frac{\mathrm{D}(\mathcal{U}_i)}{\sum \mathrm{Y}_j(\mathcal{U}_i)}
\end{aligned} \tag{6.3}$$

Note that all the above quantities are positive. We define three more lengths based on the above.

$$H_i = \frac{L(\mathcal{L}_i)L(\mathcal{R}_i)}{L(\mathcal{L}_i) + L(\mathcal{R}_i)} \tag{6.4}$$

$$V_i = \frac{L(\mathcal{D}_i)L(\mathcal{U}_i)}{L(\mathcal{D}_i) + L(\mathcal{U}_i)} \tag{6.5}$$

$$h_i = \min\{H_i, V_i\} \tag{6.6}$$

Theorem 3 *For a genuine grid and* $1 < \gamma \le 3$*, the first order LSKUM is positivity preserving under the CFL condition,*

$$\sigma^n \le \frac{1}{2}$$

Proof: The first order update formula for U can be written as,

$$\begin{aligned}
U_i^{n+1} &= U_i^n - \Delta t \left(\frac{F_i^+}{L(\mathcal{L}_i)} - \frac{F_i^-}{L(\mathcal{R}_i)} \right) - \Delta t \left(\frac{G_i^+}{L(\mathcal{D}_i)} - \frac{G_i^-}{L(\mathcal{U}_i)} \right) \\
&\quad + \Delta t \left[\frac{\sum F_j^+ |\mathrm{X}_j(\mathcal{L}_i)|}{\mathrm{D}(\mathcal{L}_i)} + \frac{\sum (-F_j^-) \mathrm{X}_j(\mathcal{R}_i)}{\mathrm{D}(\mathcal{R}_i)} + \frac{\sum G_j^+ |\mathrm{Y}_j(\mathcal{D}_i)|}{\mathrm{D}(\mathcal{D}_i)} + \frac{\sum (-G_j^-) \mathrm{Y}_j(\mathcal{U}_i)}{\mathrm{D}(\mathcal{U}_i)} \right] \\
&\succeq U_i^n - \Delta t \left(\frac{F_i^+}{L(\mathcal{L}_i)} - \frac{F_i^-}{L(\mathcal{R}_i)} \right) - \Delta t \left(\frac{G_i^+}{L(\mathcal{D}_i)} - \frac{G_i^-}{L(\mathcal{U}_i)} \right) \\
&\succeq U_i^n - \frac{\Delta t}{H_i} |F_i| - \frac{\Delta t}{V_i} |G_i| \\
&\succeq U_i^n - \frac{\Delta t \lambda(U_i^n)}{H_i} U_i^n - \frac{\Delta t \lambda(U_i^n)}{V_i} U_i^n \\
&\succeq U_i^n - \frac{2 \Delta t \lambda(U_i^n)}{h_i} U_i^n \\
&\succeq 0
\end{aligned}$$

Lemma 7 *If $\rho \geq 0,\ T \geq 0,$ then for $1 < \gamma \leq 3$,*

$$\Phi^+ \geq 0, \qquad \Phi^- \leq 0$$

and

$$\Psi^+ \geq 0, \qquad \Psi^- \leq 0$$

Proof: The proof follows obviously from the definition of the kinetic split fluxes.

Lemma 8 *For $1 < \gamma \leq 2$,*

$$|\Phi| \leq \lambda(U)W, \qquad |\Psi| \leq \lambda(U)W$$

Proof: Consider the case $u_1 \geq 0$. Then,

$$\begin{aligned}
|F_\rho| &= F_\rho^+ \\
&= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v_1 \int_{-\infty}^\infty \mathrm{d}v_2 (v_1 f) \\
&= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v_1 \int_{-\infty}^\infty \mathrm{d}v_2 (C_1 f) + u_1 \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v_1 \int_{-\infty}^\infty \mathrm{d}v_2 (f) \\
&= \int_0^\infty \mathrm{d}I \int_{-u_1}^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \frac{\rho u_1}{2} \\
&= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \int_0^\infty \mathrm{d}I \int_{-u_1}^0 \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \frac{\rho u_1}{2} \\
&\leq \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \frac{\rho u_1}{2} \\
&\leq \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \rho u_1 \\
&= \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (C_1 f) + \rho u_1 \\
&= \left(u_1 + \sqrt{\frac{RT}{2\pi}} \right) \rho \\
&\leq \lambda(U)\rho
\end{aligned}$$

Similarly,

$$\begin{aligned}
F_e^+ &\leq \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}C_1 \int_{-\infty}^\infty \mathrm{d}C_2 (I + |\vec{C} + \vec{u}|^2/2)(C_1 f) \\
&\quad + u_1 \int_0^\infty \mathrm{d}I \int_0^\infty \mathrm{d}v_1 \int_{-\infty}^\infty \mathrm{d}v_2 (I + |\vec{v}|^2/2)(f) \\
&= \sqrt{\frac{RT}{2\pi}} \left[\frac{\gamma+1}{2(\gamma-1)} p + \frac{\rho |\vec{u}|^2}{2} \right] + \frac{p u_1}{2} + \frac{e u_1}{2} \\
&\leq \frac{\gamma+1}{2} \sqrt{\frac{RT}{2\pi}} \left[\frac{p}{\gamma-1} + \frac{\rho |\vec{u}|^2}{2} \right] + e u_1 \\
&= \left(u_1 + \frac{\gamma+1}{2} \sqrt{\frac{RT}{2\pi}} \right) e \\
&\leq \lambda(U) e
\end{aligned}$$

If $u_1 \leq 0$, then

$$|F| = -F^- = F^+(-u_1) \leq \lambda(U)W$$

The proof for Ψ is also similar and hence the lemma is proved.

Theorem 4 *Under the conditions of theorem (3), the first order LSKUM is stable in the norm* $\|\cdot\|_L$ *and*

$$\max_{\mathcal{G}} h_i W_i^{n+1} \leq 2 \max_{\mathcal{G}} h_i W_i^n \tag{6.7}$$

Proof:

$$\begin{aligned}
W_i^{n+1} &\leq W_i^n + \frac{\Delta t \sum \Phi_j^+ |\mathrm{X}_j(\mathcal{L}_i)|}{\mathrm{D}(\mathcal{L}_i)} + \frac{\Delta t \sum (-\Phi_j^-)\mathrm{X}_j(\mathcal{R}_i)}{\mathrm{D}(\mathcal{R}_i)} \\
&\quad + \frac{\Delta t \sum \Psi_j^+ |\mathrm{Y}_j(\mathcal{D}_i)|}{\mathrm{D}(\mathcal{D}_i)} + \frac{\Delta t \sum (-\Psi_j^-)\mathrm{Y}_j(\mathcal{U}_i)}{\mathrm{D}(\mathcal{U}_i)} \\
&= W_i^n + \frac{\Delta t}{L(\mathcal{L}_i)} \frac{\sum \Phi_j^+ |\mathrm{X}_j(\mathcal{L}_i)|}{\sum_k |\mathrm{X}_k(\mathcal{L}_i)|} + \frac{\Delta t}{L(\mathcal{R}_i)} \frac{\sum (-\Phi_j^-)\mathrm{X}_j(\mathcal{R}_i)}{\sum_k \mathrm{X}_k(\mathcal{R}_i)} \\
&\quad + \frac{\Delta t}{L(\mathcal{D}_i)} \frac{\sum \Psi_j^+ |\mathrm{Y}_j(\mathcal{D}_i)|}{\sum_k |\mathrm{Y}_k(\mathcal{D}_i)|} + \frac{\Delta t}{L(\mathcal{U}_i)} \frac{\sum (-\Psi_j^-)\mathrm{Y}_j(\mathcal{U}_i)}{\sum_k \mathrm{Y}_k(\mathcal{U}_i)} \\
&\leq W_i^n + \frac{\Delta t}{L(\mathcal{L}_i)} \max_{j\in\mathcal{L}_i} \Phi_j^+ + \frac{\Delta t}{L(\mathcal{R}_i)} \max_{j\in\mathcal{R}_i} (-\Phi_j^-) + \frac{\Delta t}{L(\mathcal{D}_i)} \max_{j\in\mathcal{D}_i} \Psi_j^+ \\
&\quad + \frac{\Delta t}{L(\mathcal{U}_i)} \max_{j\in\mathcal{U}_i} (-\Psi_j^-) \\
&= W_i^n + \frac{\Delta t}{L(\mathcal{L}_i)} \Phi_{i_1}^+ + \frac{\Delta t}{L(\mathcal{R}_i)} (-\Phi_{i_2}^-) + \frac{\Delta t}{L(\mathcal{D}_i)} \Psi_{i_3}^+ + \frac{\Delta t}{L(\mathcal{U}_i)} (-\Psi_{i_4}^-) \\
&\leq W_i^n + \frac{\Delta t}{L(\mathcal{L}_i)} |\Phi_{i_1}| + \frac{\Delta t}{L(\mathcal{R}_i)} |\Phi_{i_2}| + \frac{\Delta t}{L(\mathcal{D}_i)} |\Psi_{i_3}| + \frac{\Delta t}{L(\mathcal{U}_i)} |\Psi_{i_4}| \\
&\leq W_i^n + \frac{\Delta t}{H_i} |\Phi_i^*| + \frac{\Delta t}{V_i} |\Psi_i^{**}| \\
&\leq W_i^n + \frac{\Delta t}{h_i} |\Phi_i^*| + \frac{\Delta t}{h_i} |\Psi_i^{**}|
\end{aligned}$$

In the above, we have defined,

$$\Phi_{i_1}^+ = \max_{j\in\mathcal{L}_i} \Phi_j^+, \quad (-\Phi_{i_2}^-) = \max_{j\in\mathcal{R}_i} (-\Phi_j^-)$$

$$\Psi_{i_3}^+ = \max_{j\in\mathcal{D}_i} \Psi_j^+, \quad (-\Psi_{i_4}^-) = \max_{j\in\mathcal{U}_i} (-\Psi_j^-)$$

$$|\Phi_i^*| = \max\{|\Phi_{i_1}|, |\Phi_{i_2}|\}, \quad |\Psi_i^{**}| = \max\{|\Phi_{i_3}|, |\Phi_{i_4}|\}$$

From this we obtain,

$$\begin{aligned}
h_i W_i^{n+1} &\leq h_i W_i^n + \Delta t |\Phi_i^*| + \Delta t |\Psi_i^{**}| \\
&\leq h_i W_i^n + \frac{1}{2} \left(h_i^* W_i^* + h_i^{**} W_i^{**} \right)
\end{aligned}$$

so that

$$
\begin{aligned}
\|W\|_L^{n+1} &= \sum_i h_i W_i^{n+1} \\
&\leq \sum_i h_i W_i^n + \frac{1}{2}\left(\sum_i h_i^* W_i^* + \sum_i h_i^{**} W_i^{**}\right) \\
&\leq \|W\|_L^n + \frac{1}{2}\left(2\varpi \|W\|_L^n\right) \\
&= (1+\varpi)\|W\|_L^n
\end{aligned}
$$

Finally, we have

$$
\begin{aligned}
|\rho u_1| &= \left(\rho(\rho u_1^2)\right)^{1/2} \\
&\leq (2\rho e)^{1/2} \\
&\leq |\rho| + |e|
\end{aligned}
$$

so that

$$\|\rho u_1\|_L \leq \|\rho\|_L + \|e\|_L$$

and similarly

$$\|\rho u_2\|_L \leq \|\rho\|_L + \|e\|_L$$

Condition (6.7) follows similar to theorem (1).

7 Numerical Results

The higher order version of LSKUM known as q-LSKUM [1] has the same structure as LSKUM and hence is expected to inherit the positivity and stability properties of LSKUM. This method is applied to a problem with a large expansion which was suggested by Sjogreen [7]. The initial conditions of the problem are given in table (1).

ρ_l	p_l	u_l	ρ_r	p_r	u_r
1.0	0.4	-2.0	1.0	0.4	2.0

Table 1: Initial conditions for the one-dimensional problem.

A uniform grid of 1001 points was used. The q-derivatives used in the algorithm were limited by a min-max limiter. For all the derivatives, a weight of r^{-2} was used. Based on the CFL number (4.5), we were able to use a CFL of upto 1.5, beyond which the program gave negative pressures. The density and pressure obtained at $t = 0.15$ are shown in figures (3) and (4) in a semilog plot. Figure (5) shows negative pressure obtained for CFL=1.6

8 Summary

The positivity property of first order LSKUM has been established under a CFL-like condition. Based on the positivity condition, some stability bounds have been derived. New length scales are obtained in the definition of the CFL number which are less restrictive than Δx_i. Numerical experiments using q-LSKUM on a problem involving a large expansion show that the same CFL condition works well.

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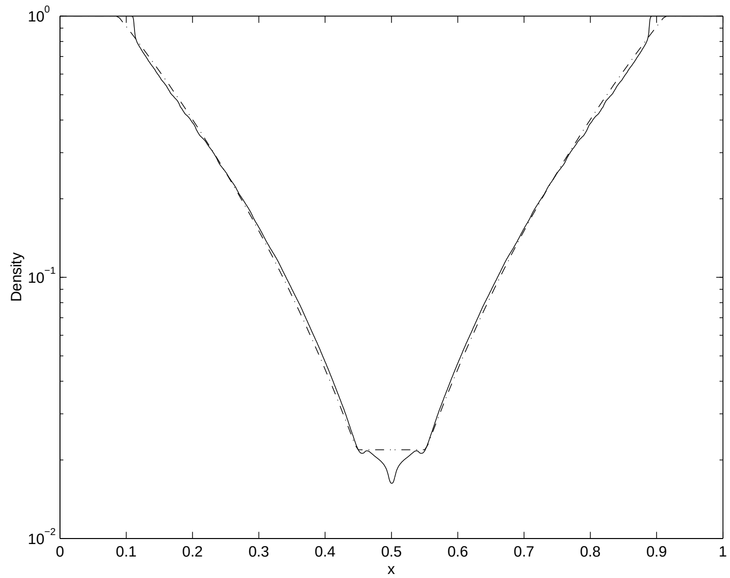

Figure 3: One-dimensional problem using q-LSKUM and CFL=1.5

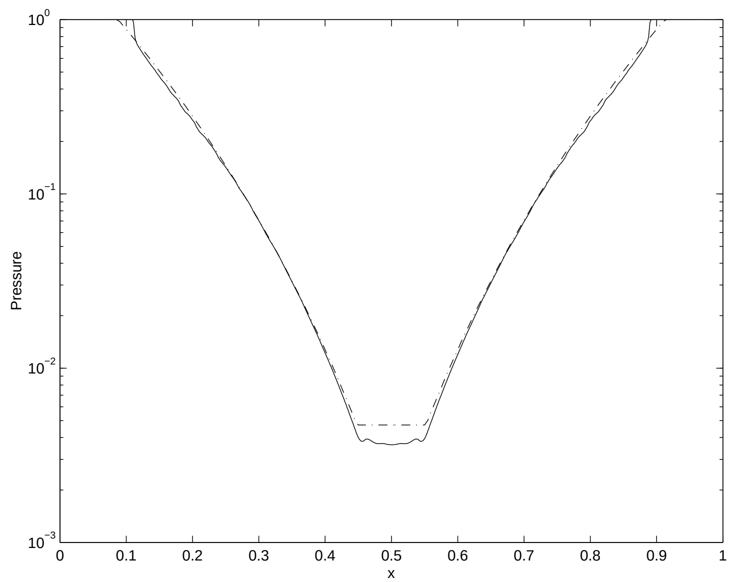

Figure 4: One-dimensional problem using q-LSKUM and CFL=1.5

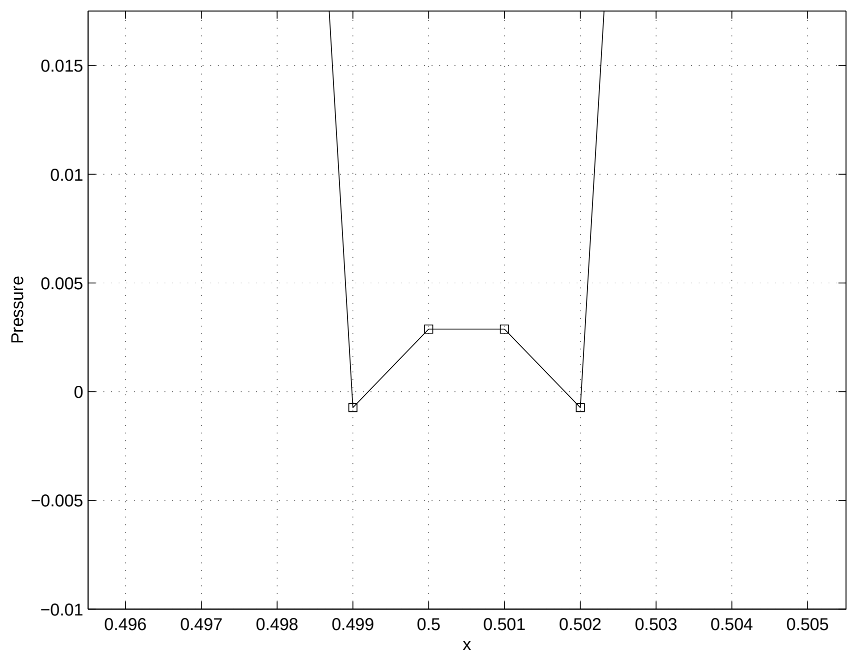

Figure 5: One-dimensional problem using q-LSKUM and CFL=1.6; loss of positivity.