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Monotonicity and positivity preservation in Large Time Step methods

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Abstract We study the positivity preserving property of Large Time Step (LTS) finite volume methods. Herein, LTS denotes explicit methods stable for Courant numbers greater than one. LTS-Godunov and LTS-Roe schemes have been developed by LeVeque [*SIAM J. Numer. Anal.*, 22 (1985), pp. 1051–1073], while LTS extensions of the HLL (Harten-Lax-van Leer) and HLLC (HLL-Contact) schemes have recently been developed by Prebeg et al. [submitted, 2017]. In this paper, we determine the monotonicity conditions for LTS methods, and show that they are stronger than in standard (3-point) methods. We show that conditions for positivity preservation in LTS methods are also stronger than in standard methods. In particular, we show that the LTS-HLLE scheme is not positivity preserving and that the LTS-Lax-Friedrichs scheme is positivity preserving. We apply LTS methods to the one-dimensional Euler equations and consider the double rarefaction, LeBlanc's shock tube and the Sedov blast-wave problem. We numerically demonstrate that robustness of LTS methods can be increased by adding numerical diffusion.

Keywords Large Time Step · HLL · Positivity preservation · Euler equations · Riemann solver

Mathematics Subject Classification (2000) 65M08 · 35L65 · 65Y20

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1 Introduction

We consider a hyperbolic system of conservation laws:

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0, \qquad x \in \mathbb{R}, t \in \mathbb{R}^+, \tag{1.1a}$$

$$\mathbf{U}(x,0) = \mathbf{U}_0(x), \tag{1.1b}$$

where $\mathbf{U} \in \mathbb{R}^N$ is a vector of conserved variables, $\mathbf{F}(\mathbf{U}) : \mathbb{R}^N \to \mathbb{R}^N$ is a flux function and $\mathbf{U}_0$ is the initial data. We are interested in solving (1.1) with an explicit finite volume methods not limited by the CFL (Courant–Friedrichs–Lewy) condition, and we focus on the positivity preserving property of such methods.

When we use conservation laws to describe the real world, the conserved variables are representing some particular measurable properties of the nature. In addition to being conserved, these properties may have additional requirements imposed upon then. For example, when we solve the Euler equations it is required that the density is positive at all times:

$$\rho(x,t) > 0 \quad \forall x \in \mathbb{R}, t \in \mathbb{R}^+. \tag{1.2}$$

Does the numerical method ensure that the condition (1.2) is always satisfied on a discrete level? Namely, does the scheme enforce that:

$$\rho_j^n > 0 \quad \forall j, n. \tag{1.3}$$

To tackle this question, we start by considering a scalar conservation law. In this paper, we follow a common approach of treating monotonicity as a scalar counterpart of positivity preserving property [50]. Consider a one-dimensional initial value problem for the scalar conservation law:

$$u_t + f(u)_x = 0, \qquad x \in \mathbb{R}, t \in \mathbb{R}^+, \tag{1.4a}$$

$$u(x,0) = u_0(x), \tag{1.4b}$$

where $u \in \mathbb{R}$ is a conserved variable a $f(u) : \mathbb{R} \to \mathbb{R}$ is the flux function. A unique weak solution of (1.4) satisfies a strict *maximum principle*. Namely, if:

$$m = \min_x \left(u_0(x)\right), \quad M = \max_x \left(u_0(x)\right), \tag{1.5}$$

then:

$$u(x,t) \in [m, M] \quad \forall \quad x, t. \tag{1.6}$$

We want the numerical scheme to enforce this property on a discrete level. Define:

$$m = \min_j(u_j^0), \quad M = \max_j(u_j^0). \tag{1.7}$$

If the numerical scheme ensures that:

$$u_j^n \in [m, M] \quad \forall \quad j, n, \tag{1.8}$$

we say that the scheme is *maximum-principle-satisfying*. When we discuss systems of equations, it may be unreasonable to require that a certain variable remains bounded between its initial values at all time, but it might be necessary to require that a conserved variable remains bounded in some specific sense, such as for

example the positivity of the density and internal energy in the Euler equations. We then say that the scheme is *positivity preserving*.

The development of positivity preserving schemes has been an ongoing topic for many years now. For the standard methods, Einfeldt et al. [11] showed that the Godunov and the HLLE (HLL-Einfeldt) schemes are positivity preserving, while the Roe scheme is not. Batten et al. [3] showed that the HLLC (HLL-Contact) [44] scheme is positivity preserving with an appropriate choice of wave velocity estimates, and Bouchut [5] determined wave velocities estimates such that the HLLC scheme can also handle vacuum. Further, Perthame and Shu [33] established a general framework to achieve high-order positivity preserving methods for the Euler equations in one and two dimensions. Areas of interest include the Euler equations (Calgaro et al. [6], Hu et al. [16], Li et al. [23], Zhang and Shu [49–51]), shallow water equations [39,18,46,1], magnetohydrodynamics [2,17,12], multiphase flows (Chen and Shu [8]), unstructured meshes (Berthon [4]) and flux-vector splitting methods (Gressier et al. [13]), to name just a few. These papers consider standard methods and mostly tackle issues with positivity preservation that arise in high-order methods. This paper takes a different route and considers the issues with positivity preservation in Large Time Step (LTS) methods.

The LTS methods have been introduced by LeVeque [19–21], where the Godunov and Roe schemes were extended to the LTS-Godunov and LTS-Roe schemes, respectively, and applied to scalar conservation laws and the Euler equations. These ideas have been applied in different fields, including the shallow water equations (Murillo, Morales-Hernández and co-workers [32,28,31,29,30] and Xu et al. [47]), 3D Euler equations (Qian and Lee [37]), high speed combustion waves (Tang et al. [41]), Maxwell's equations (Makwana and Chatterjee [27]) and multiphase flows (Lindqvist and Lund [25] and Prebeg et al. [36]). Lindqvist et al. [24] studied the TVD properties of LTS methods and developed the LTS-Lax-Friedrichs scheme, while Prebeg et al. [35] developed an LTS extension of the HLL [15] and HLLC [44] schemes and applied them to the one-dimensional Euler equations. Prebeg [34] also used the modified equation analysis to show that the LTS-HLLE scheme yields entropy satisfying solutions.

The positivity preserving in the LTS-Roe scheme for the shallow water equations with source terms has been addressed by Morales-Hernández and co-workers [28,29], where they suggested to handle loss of positivity by reducing the Courant number when the it is likely to happen. In this paper, we focus on the LTS-HLLE scheme and consider scalar conservation laws and the Euler equations. Our first result are conditions on the numerical flux function of an LTS method that guarantees that the method is monotone. We show that the LTS-HLLE scheme is not monotone, and that the LTS-Lax-Friedrichs scheme is monotone. Next, we consider the Euler equations and the classical result by Einfeldt et al. [11] that states that the exact or approximate Riemann solver is positivity preserving if and only if the intermediate states generated by the Riemann solver are physically real. Our second result is showing that in the LTS framework this condition is necessary, but not sufficient for the positivity preservation. We then show that the LTS-HLLE scheme is not positivity preserving, and that the LTS-Lax-Friedrichs scheme is positivity preserving.

This paper is structured as follows. In section 2 we outline the problem we solve and the numerical methods we use. In order to investigate the monotonicity, we will interpret the HLL scheme as a numerical method for scalar conservation

laws. Extension to systems of equations is then obtained by a classical field-by-field decomposition. In section 3 we consider scalar conservation laws and how is monotonicity lost in LTS methods. In section 4 we move to systems of equations and investigate different ways how is positivity lost in the LTS-HLLE scheme when applied to the Euler equations. Section 5 presents numerical results, while section 6 closes with conclusions.

2 Preliminaries

2.1 Problem outline

As an example of (1.1) we consider the Euler equations. They can be written in the form (1.1) by defining:

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho v \\ E \end{bmatrix}, \qquad \mathbf{F}(\mathbf{U}) = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ v(E+p) \end{bmatrix}, \tag{2.1}$$

where ρ, v, E, p denote the density, velocity, total energy density and pressure, respectively. The system is closed by the relation for the total energy density, $E = \rho e + \rho v^2/2$, an equation of state for perfect gas, $e = p/(\rho(\gamma - 1))$, and $\gamma > 1$ (we use $\gamma = 1.4$ for air). We can write (1.1) in a quasilinear form as:

$$\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = 0, \qquad \mathbf{A}(\mathbf{U}) = \partial\mathbf{F}(\mathbf{U})/\partial\mathbf{U}. \tag{2.2}$$

We assume that the system of equations (2.2) is hyperbolic, i.e. the Jacobian matrix $\mathbf{A}$ has real eigenvalues and linearly independent eigenvectors. The eigenvalues of the Euler equations (2.1) are:

$$\lambda^1 = v - a, \quad \lambda^2 = v, \quad \lambda^3 = v + a, \tag{2.3}$$

where a is the speed of sound:

$$a = \sqrt{\gamma p/\rho}. \tag{2.4}$$

2.2 Numerical methods

We start by presenting the standard HLL and the LTS-HLL schemes for scalar conservation laws, and then generalize them to systems of equations.

2.2.1 Standard (3-point) methods

We discretize (1.4) by the explicit Euler method in time and the finite volume method in space:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right), \tag{2.5}$$

where u_j^n is a piecewise constant approximation of u in the cell with center at x_j at time level n, and $F_{j+1/2}^n$ is a numerical approximation of the flux function at the cell interface $x_{j+1/2}$ at time level n. In the case that the numerical flux depends

only on the neighboring cell values, we can with no loss of generality write the scheme in the numerical viscosity form [14,40]:

$$F_{j+1/2} = \frac{1}{2}\left(f_j + f_{j+1}\right) - \frac{1}{2}Q_{j+1/2}\left(u_{j+1} - u_j\right), \tag{2.6}$$

where $f_j = f\left(u_j\right)$, $Q_{j+1/2}$ is the numerical viscosity coefficient and the temporal index n is from now on omitted because we consider only explicit methods. The choice of the numerical viscosity coefficient uniquely determines the choice of the numerical method. For the HLL scheme [15], the numerical viscosity coefficient is (see [10]):

$$Q_{\mathrm{HLL},j+1/2} = \frac{\left|S_{\mathrm{R}}\right|\left(\lambda - S_{\mathrm{L}}\right) + \left|S_{\mathrm{L}}\right|\left(S_{\mathrm{R}} - \lambda\right)}{S_{\mathrm{R}} - S_{\mathrm{L}}}, \tag{2.7}$$

where λ is the shock speed determined by the Rankine–Hugoniot condition, and S_{L} and S_{R} are the wave velocity estimates to be determined later.

An alternative way to discretize (1.4) is with the flux-difference splitting form:

$$u_j^{n+1} = u_j - \frac{\Delta t}{\Delta x}\left(A^+_{j-1/2}\left(u_j - u_{j-1}\right) + A^-_{j+1/2}\left(u_{j+1} - u_j\right)\right), \tag{2.8}$$

where $A^{\pm}_{j-1/2}$ are the flux-difference splitting coefficients. The choice of the method in this form is determined by the choice of the flux-difference splitting coefficients, where for the HLL scheme we have:

$$A^{\pm}_{\mathrm{HLL},j-1/2} = \frac{S^{\pm}_{\mathrm{R}}\left(\lambda - S_{\mathrm{L}}\right) + S^{\pm}_{\mathrm{L}}\left(S_{\mathrm{R}} - \lambda\right)}{S_{\mathrm{R}} - S_{\mathrm{L}}}, \tag{2.9}$$

where $S^+_{\mathrm{R}} = \max(0, S_{\mathrm{R}})$ and $S^-_{\mathrm{R}} = \min(0, S_{\mathrm{R}})$.

A third way to discretize (1.4) is the wave propagation form that will be used in this paper:

$$u_j^{n+1} = u_j - \frac{\Delta t}{\Delta x}\left(\sum_{p=1}^{m} S^{p,+}_{j-1/2}\mathcal{W}^p_{j-1/2} + \sum_{p=1}^{m} S^{p,-}_{j+1/2}\mathcal{W}^p_{j+1/2}\right), \tag{2.10}$$

where we replaced the discontinuity in the conserved variable by m waves. For the HLL scheme $m = 2$, and we define the velocities S^p as:

$$S^1_{j-1/2} = S_{\mathrm{L},j-1/2}, \quad S^2_{j-1/2} = S_{\mathrm{R},j-1/2}, \tag{2.11}$$

and the waves $\mathcal{W}^p$ as:

$$\mathcal{W}^1_{j-1/2} = u^{\mathrm{HLL}}_{j-1/2} - u_{j-1}, \quad \mathcal{W}^2_{j-1/2} = u_j - u^{\mathrm{HLL}}_{j-1/2}, \tag{2.12}$$

where $u^{\mathrm{HLL}}_{j-1/2}$ is the intermediate state determined from the integral form of the conservation law (3.17) (see [15,43]):

$$u^{\mathrm{HLL}}_{j-1/2} = \frac{S_{\mathrm{R}}u_j - S_{\mathrm{L}}u_{j-1} + f_{j-1} - f_j}{S_{\mathrm{R}} - S_{\mathrm{L}}}. \tag{2.13}$$

We refer to [15,9–11,3,43] for a more detailed derivation of the HLL scheme.

2.2.2 Large Time Step methods

For the standard methods above, the size of time step in discretizations (2.5), (2.8) and (2.10) is limited by the CFL condition:

$$C = \max_{p,x,t} |\lambda^p(x,t)| \frac{\Delta t}{\Delta x} \leq 1, \tag{2.14}$$

where λ is $\partial f(u)/\partial u$ if we consider (1.4), and the eigenvalues of $\mathbf{A}(\mathbf{U})$ (eq. (2.2)) if we consider (1.1). In this paper, we consider explicit Large Time Step (LTS) methods that are not limited by the condition (2.14), i.e. we relax the CFL condition so that:

$$C = \max_{p,x,t} |\lambda^p(x,t)| \frac{\Delta t}{\Delta x} \leq k, \quad k \in \mathbb{Z}^+. \tag{2.15}$$

Following Lindqvist et al. [24], the LTS extension of the numerical viscosity formulation (2.6) is:

$$F_{j+1/2} = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2}\sum_{i=-\infty}^{\infty} Q^i_{j+1/2+i} \Delta u_{j+1/2+i}, \tag{2.16}$$

and the LTS extension of the flux-difference splitting formulation (2.8) is:

$$u_j^{n+1} = u_j - \frac{\Delta t}{\Delta x}\sum_{i=0}^{\infty}\left(A^{i+}_{j-1/2-i}\Delta u_{j-1/2-i} + A^{i-}_{j+1/2+i}\Delta u_{j+1/2+i}\right), \tag{2.17}$$

where we introduced the notation $\Delta u_{j-1/2} = u_j - u_{j-1}$ and the convention:

$$Q^{\pm i} = A^{i\pm} = 0 \quad \text{for} \quad i \geq k. \tag{2.18}$$

The LTS extension of the wave formulation (2.10) is:

$$u_j^{n+1} = u_j - \frac{\Delta t}{\Delta x}\sum_{i=0}^{\infty}\left(\sum_{p=1}^{m} S^{p,i+}_{j-1/2-i}\mathcal{W}^p_{j-1/2-i} + \sum_{p=1}^{m} S^{p,i-}_{j+1/2+i}\mathcal{W}^p_{j+1/2+i}\right). \tag{2.19}$$

We note that (2.16) differs from [24] in a sense that we scale Q^i by $\Delta x/\Delta t$. The newly introduced upper indices denote relative cell interfaces. For instance, $Q^i_{j+1/2+i}$ describes the contribution of the numerical viscosity coefficient Q from the cell interface $x_{j+1/2+i}$ to the numerical flux function $F_{j+1/2}$ which is $|i|$ cells away. From now on, we will suppress the subscript and our definition of Q will simply tell us how much does the numerical viscosity coefficient Q from an arbitrary interface contributes to the numerical flux function $|i|$ cells away. The same reasoning applies to the flux-difference splitting coefficients A and wave velocities S.

Lindquist et al. [24] determined the numerical viscosity and flux-difference splitting coefficients of the LTS-Godunov, LTS-Roe and LTS-Lax-Friedrichs schemes.

Prebeg et al. [35] determined the numerical viscosity coefficients of the LTS-HLL scheme as:

$$Q^{0}_{\mathrm{HLL}} = \frac{|S_{\mathrm{R}}|\,(\lambda - S_{\mathrm{L}}) + |S_{\mathrm{L}}|\,(S_{\mathrm{R}} - \lambda)}{S_{\mathrm{R}} - S_{\mathrm{L}}}, \tag{2.20a}$$

$$\begin{aligned} Q^{\mp i}_{\mathrm{HLL}} =& 2\frac{\lambda - S_{\mathrm{L}}}{S_{\mathrm{R}} - S_{\mathrm{L}}} \max\left(0, \pm S_{\mathrm{R}} - i\frac{\Delta x}{\Delta t}\right) \\ &+ 2\frac{S_{\mathrm{R}} - \lambda}{S_{\mathrm{R}} - S_{\mathrm{L}}} \max\left(0, \pm S_{\mathrm{L}} - i\frac{\Delta x}{\Delta t}\right) \quad \text{for} \quad i > 0, \end{aligned} \tag{2.20b}$$

and the flux-difference splitting coefficients of the LTS-HLL scheme as:

$$\begin{aligned} A^{i\pm}_{\mathrm{HLL}} =& \pm \frac{\lambda - S_{\mathrm{L}}}{S_{\mathrm{R}} - S_{\mathrm{L}}} \max\left(0, \min\left(\pm S_{\mathrm{R}} - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right) \\ &\pm \frac{S_{\mathrm{R}} - \lambda}{S_{\mathrm{R}} - S_{\mathrm{L}}} \max\left(0, \min\left(\pm S_{\mathrm{L}} - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right). \end{aligned} \tag{2.21}$$

The wave velocities in an arbitrary LTS method given by (2.19) are:

$$S^{p,i\pm} = \pm \max\left(0, \min\left(\pm S^{p} - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right). \tag{2.22}$$

The derivation and a detailed analysis of equations (2.16) and (2.17) can be found in [24], while the derivation of (2.20) and (2.21) can be found in [35].

2.2.3 Systems of equations

In order to apply the methods discussed above to systems of equations, we follow the standard approach of applying the scalar method to a field-by-field decomposition obtained through the Roe linearization [38]. We refer to the books by LeVeque [22] and Toro [43] for the standard theory, and to Lindqvist et al. [24] and Prebeg et al. [35] for LTS methods considered in this paper.

The LTS extensions of the numerical viscosity (2.16), flux-difference splitting (2.17) and wave formulation (2.19) for systems of equations are:

$$\mathbf{F}_{j+1/2} = \frac{1}{2}\left(\mathbf{F}_{j} + \mathbf{F}_{j+1}\right) - \frac{1}{2}\sum_{i=-\infty}^{\infty} \mathbf{Q}^{i}_{j+1/2+i} \Delta \mathbf{U}_{j+1/2+i}, \tag{2.23}$$

for the numerical viscosity,

$$\mathbf{U}^{n+1}_{j} = \mathbf{U}_{j} - \frac{\Delta t}{\Delta x}\sum_{i=0}^{\infty}\left(\hat{\mathbf{A}}^{i+}_{j-1/2-i}\Delta \mathbf{U}_{j-1/2-i} + \hat{\mathbf{A}}^{i-}_{j+1/2+i}\Delta \mathbf{U}_{j+1/2+i}\right), \tag{2.24}$$

for the flux-difference splitting, and:

$$\mathbf{U}^{n+1}_{j} = \mathbf{U}_{j} - \frac{\Delta t}{\Delta x}\sum_{i=0}^{\infty}\left(\sum_{p=1}^{m} S^{p,i+}_{j-1/2-i}\mathcal{W}^{p}_{j-1/2-i} + \sum_{p=1}^{m} S^{p,i-}_{j+1/2+i}\mathcal{W}^{p}_{j+1/2+i}\right), \tag{2.25}$$

for the wave formulation. For the LTS-HLL scheme [35], the partial viscosity matrices $\mathbf{Q}^i$ are defined through their eigenvalues by diagonalizing them as:

$$\mathbf{Q}^i_{j+1/2} = (\hat{\mathbf{R}}\mathbf{\Omega}^i\hat{\mathbf{R}}^{-1})_{j+1/2}, \tag{2.26}$$

where $\hat{\mathbf{R}}$ is matrix of eigenvectors of the Roe scheme [38], and $\mathbf{\Omega}^i$ is the diagonal matrix with the eigenvalues:

$$\omega^0_{\mathrm{HLL}} = \frac{|S_{\mathrm{R}}|\,(\lambda - S_{\mathrm{L}}) + |S_{\mathrm{L}}|\,(S_{\mathrm{R}} - \lambda)}{S_{\mathrm{R}} - S_{\mathrm{L}}}, \tag{2.27a}$$

$$\begin{aligned}\omega^{\mp i}_{\mathrm{HLL}} =& 2\frac{\lambda - S_{\mathrm{L}}}{S_{\mathrm{R}} - S_{\mathrm{L}}}\max\left(0, \pm S_{\mathrm{R}} - i\frac{\Delta x}{\Delta t}\right)\\ &+2\frac{S_{\mathrm{R}} - \lambda}{S_{\mathrm{R}} - S_{\mathrm{L}}}\max\left(0, \pm S_{\mathrm{L}} - i\frac{\Delta x}{\Delta t}\right) \quad \text{for } i > 0,\end{aligned} \tag{2.27b}$$

and the flux-difference splitting matrices $\hat{\mathbf{A}}^{i\pm}$ are defined through their eigenvalues by diagonalizing them as:

$$\hat{\mathbf{A}}^{i\pm}_{j+1/2} = (\hat{\mathbf{R}}\hat{\mathbf{\Lambda}}^{i\pm}\hat{\mathbf{R}}^{-1})_{j+1/2}, \tag{2.28}$$

where $\hat{\mathbf{\Lambda}}^{i\pm}$ is the diagonal matrix with the eigenvalues:

$$\begin{aligned}\lambda^{i\pm}_{\mathrm{HLL}} =& \pm\frac{\lambda - S_{\mathrm{L}}}{S_{\mathrm{R}} - S_{\mathrm{L}}}\max\left(0, \min\left(\pm S_{\mathrm{R}} - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right)\\ &\pm\frac{S_{\mathrm{R}} - \lambda}{S_{\mathrm{R}} - S_{\mathrm{L}}}\max\left(0, \min\left(\pm S_{\mathrm{L}} - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right).\end{aligned} \tag{2.29}$$

For the wave formulation, the wave velocities are the same as in (2.22):

$$S^{p,i\pm} = \pm\max\left(0, \min\left(\pm S^p - i\frac{\Delta x}{\Delta t}, \frac{\Delta x}{\Delta t}\right)\right). \tag{2.30}$$

We refer to [35] for the detailed derivation of (2.27) and (2.29).

3 Scalar conservation law

We consider the scalar conservation law (1.4) and we want to construct an LTS method that will guarantee that the numerical solution respects the strict maximum principle (1.8). The condition (1.8) is guaranteed if the numerical method is monotone. We can determine if the scheme is monotone by the following result:

Lemma 1 (Trangenstein [45]) *Suppose that:*

$$u^{n+1}_j = \mathcal{H}(u_{j-k}, \ldots, u_{j+k}; \Delta x, \Delta t), \tag{3.1}$$

is a monotone scheme and that it is differentiable in each of its u_l arguments for $j - k \le l \le j + k$. Then:

$$\frac{\partial \mathcal{H}}{\partial u_l} \ge 0, \quad \forall \quad j - k \le l \le j + k. \tag{3.2}$$

Conversely, if:

$$\frac{\partial \mathcal{H}}{\partial u_l} \ge 0, \quad \forall \quad j - k \le l \le j + k, \tag{3.3}$$

then (3.1) *is monotone scheme.*

For standard methods, monotonicity can be also shown by considering the numerical flux function (2.6):

$$F(a,b) = \frac{1}{2}\left(f(a)+f(b)\right) - \frac{1}{2}Q(a,b)\left(b-a\right). \tag{3.4}$$

The standard numerical method is monotone if the numerical flux function $F(a,b)$ is non-decreasing in its first argument, non-increasing in its second argument and the CFL condition (2.14) holds. Our first result is a set of conditions on the numerical flux function of an LTS method that yields a monotone scheme.

Proposition 1 *Suppose that an explicit* $(2k+1)$*-point scheme:*

$$u_j^{n+1} = \mathcal{H}\left(u_{j-k},\ldots,u_{j+k};\Delta x,\Delta t\right), \tag{3.5}$$

can be written in conservation form:

$$\begin{aligned} u_j^{n+1} = u_j + \frac{\Delta t}{\Delta x}\big(&F_{j-1/2}\big(u_{j-k},u_{j-k+1},\ldots,u_{j+k-1}\big) \\ &-F_{j+1/2}\big(u_{j-k+1},\ldots,u_{j+k-1},u_{j+k}\big)\big), \end{aligned} \tag{3.6}$$

where:

$$F = F\left(u^1,\ldots,u^{2k}\right), \tag{3.7}$$

is a Lipschitz continuous numerical flux function of $2k$ *arguments. The numerical method* (3.5) *is monotone if:*

$$\frac{\partial F}{\partial u^p} = \begin{cases} \dfrac{\partial F}{\partial u^p} \geq \dfrac{\partial F}{\partial u^{p-1}} \geq 0 & \text{for} \quad 1 < p \leq k, \\ \dfrac{\partial F}{\partial u^{p-1}} \leq \dfrac{\partial F}{\partial u^p} \leq 0 & \text{for} \quad k+1 < p \leq 2k; \end{cases} \tag{3.8}$$

and the condition:

$$\frac{\Delta t}{\Delta x}\left(\left|\frac{\partial F}{\partial u^k}\right| + \left|\frac{\partial F}{\partial u^{k+1}}\right|\right) \leq 1, \tag{3.9}$$

holds.

Remark 1 We note that we use lower indices to denote the absolute index position, $l \in [j-k,\ldots,j+k]$ for the numerical method $\mathcal{H}$ and the numerical flux function F, and upper indices to denote the relative (local) index position: $p \in [1,\ldots,2k+1]$ for the numerical method $\mathcal{H}$, and $p \in [1,\ldots,2k]$ for the numerical flux function F.

Proof We recall Lemma 1 and note that the scheme (3.5) is monotone iff:

$$\frac{\partial \mathcal{H}}{\partial u^p} \geq 0, \quad \forall \quad 1 \leq p \leq 2k+1. \tag{3.10}$$

By differentiating $\mathcal{H}$ with respect to its arguments u^p we obtain:

$$\frac{\partial \mathcal{H}}{\partial u^p} = \begin{cases} (a) & \frac{\Delta t}{\Delta x}\frac{\partial F}{\partial u^1} & \text{for} & p = 1, \\ (b) & \frac{\Delta t}{\Delta x}\left(\frac{\partial F}{\partial u^p} - \frac{\partial F}{\partial u^{p-1}}\right) & \text{for} & 1 < p \leq k, \\ (c) & 1 + \frac{\Delta t}{\Delta x}\left(\frac{\partial F}{\partial u^p} - \frac{\partial F}{\partial u^{p-1}}\right) & \text{for} & p = k+1, \\ (d) & \frac{\Delta t}{\Delta x}\left(\frac{\partial F}{\partial u^p} - \frac{\partial F}{\partial u^{p-1}}\right) & \text{for} & k+1 < p \leq 2k, \\ (e) & -\frac{\Delta t}{\Delta x}\frac{\partial F}{\partial u^{2k}} & \text{for} & p = 2k+1; \end{cases} \tag{3.11}$$

We now show that (3.8) implies that all conditions (a–e) are ≥ 0.

– Conditions (a) and (e): Condition (a) is satisfied by (3.8) because $\partial F/\partial u^p \geq 0$ when $p = 1$. In the same manner, condition (e) is satisfied by (3.8) because $\partial F/\partial u^p \leq 0$ when $p = 2k$.
– Conditions (b) and (d):

$$\left(\frac{\partial F}{\partial u^p} - \frac{\partial F}{\partial u^{p-1}}\right) \geq 0, \tag{3.12}$$

can be satisfied by any of the following:

$$\frac{\partial F}{\partial u^p} \geq \frac{\partial F}{\partial u^{p-1}} \geq 0, \tag{3.13a}$$

$$\frac{\partial F}{\partial u^{p-1}} \leq \frac{\partial F}{\partial u^p} \leq 0. \tag{3.13b}$$

However, conditions (a) and (e) require that F is non-decreasing in its first argument and non-increasing in its last argument. Therefore, only condition (3.13a) holds for $1 < p \leq k$, which is satisfied by (3.8); and only condition (3.13b) holds for $k + 1 < p \leq 2k$, which is satisfied by (3.8).
– Condition (c) can be written as:

$$1 + \frac{\Delta t}{\Delta x}\left(\frac{\partial F}{\partial u^{k+1}} - \frac{\partial F}{\partial u^k}\right) \geq 0, \tag{3.14}$$

and since for $p = k+1$ we have $\partial F/\partial u^p \leq 0$, and for $p = k$ we have $\partial F/\partial u^p \geq 0$, we may rewrite this as:

$$\frac{\Delta t}{\Delta x}\left(\left|\frac{\partial F}{\partial u^k}\right| + \left|\frac{\partial F}{\partial u^{k+1}}\right|\right) \leq 1, \tag{3.15}$$

which is the condition (3.9). □

It was already pointed out by LeVeque [20] that the LTS-Godunov scheme is not monotone for $C > 1$. We now use LeVeque's argument to show that the LTS-HLLE scheme is not monotone by constructing a counter-example. The LTS-HLLE scheme is obtained by defining the wave velocity estimates S_{L} and S_{R} according to Einfeldt [10]:

$$S_{\mathrm{L},j+1/2} = \min\left(f'\left(u_j\right), \lambda_{j+1/2}\right), \tag{3.16a}$$

$$S_{\mathrm{R},j+1/2} = \max\left(\lambda_{j+1/2}, f'\left(u_{j+1}\right)\right). \tag{3.16b}$$

Consider the initial value problem for the inviscid Burgers equations with the initial data:

$$u_i^0 = \begin{cases} 1 & \text{if} \quad i = j, \\ 0 & \text{if} \quad i \neq j. \end{cases} \tag{3.17}$$

We can see that for the initial data (3.17):

$$S_{\mathrm{R},j-1/2} = u_j > S_{\mathrm{R},j+1/2} = \lambda_{j+1/2}, \tag{3.18}$$

hence the wave from $x_{j-1/2}$ can pass the wave from $x_{j+1/2}$ at some finite time (see Fig. 1). Given enough time and a large enough Courant number, there will be a cell z in front of the shock such that (2.19) reduces to:

$$u_z^{n+1} = u_z - \frac{\Delta t}{\Delta x} S_{\mathrm{R},j-1/2} \mathcal{W}_{j-1/2}^2 = -\frac{\Delta t}{\Delta x} S_{\mathrm{R},j-1/2}\left(u_j - u_{j-1/2}^{\mathrm{HLLE}}\right) < 0. \tag{3.19}$$

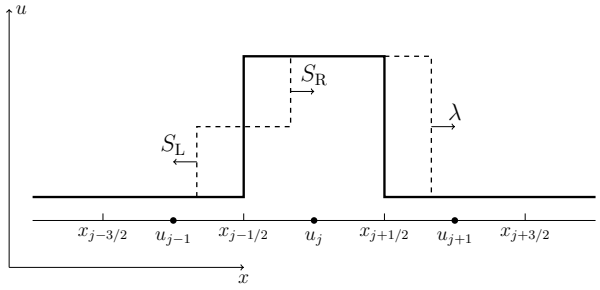

Fig. 1: Transport of initial data (3.17) with the LTS-HLLE scheme in the wave formulation (2.19)

Remark 2 We point out that both the LTS-Godunov and LTS-HLLE schemes are TVD (total variation diminishing). It is sometimes stated that the TVD methods are maximum-principle-satisfying, which we believe is due to the fact that authors implicitly assume standard methods. To the best of our knowledge, standard TVD methods are indeed maximum-principle-satisfying. However, as we showed above, that is not the case for the LTS TVD methods.

We now show that the LTS-Lax-Friedrichs scheme of Lindqvist et al. [24] is maximum-principle-satisfying by showing that it is monotone.

Proposition 2 *The LTS-Lax-Friedrichs scheme by Lindqvist et al. [24]:*

$$u_j^{n+1} = \mathcal{H}\left(u_{j-k}, u_{j+k}\right) = \frac{1}{2}\left(u_{j-k} + u_{j+k}\right) - \frac{\Delta t}{2k\Delta x}\left(f\left(u_{j+k}\right) - f\left(u_{j-k}\right)\right), \quad (3.20)$$

is monotone under the CFL condition:

$$C = \max_{x,t} |f'(u(x,t))| \frac{\Delta t}{\Delta x} \leq k. \quad (3.21)$$

Proof By differentiating (3.20) we have that:

$$\frac{\partial \mathcal{H}}{\partial u_l} = \begin{cases} \frac{1}{2}\left(1 + \frac{\Delta t}{k\Delta x} f'\left(u_{j-k}\right)\right) & l = j-k, \\ \frac{1}{2}\left(1 - \frac{\Delta t}{k\Delta x} f'\left(u_{j+k}\right)\right) & l = j+k, \\ 0 & \text{otherwise;} \end{cases} \quad (3.22)$$

which satisfies (3.3) if (3.21) holds. □

4 Systems of conservation laws

We begin by restating some existing results on positivity preservation in standard methods. We then move to LTS methods and outline how the loss of positivity occurs there.

4.1 Positivity preservation

We start by considering the existing result for positivity preserving properties of standard methods:

Definition 1 A class of schemes that always generate physical solutions from physical data is denoted as positivity preserving schemes.

This definition is due to Einfeldt et al. [11], where it is shown that the Godunov and HLLE schemes are positivity preserving, while the Roe scheme is not. Herein we outline the main points that will be used onwards. Consider a standard exact or approximate Riemann solver and note that the numerical algorithm may be seen as:

- (a) Solve the Riemann problem exactly or approximately to obtain the intermediate states in the Riemann fan.
- (b) Update the solution according to:

$$\mathbf{U}_j^{n+1} = \frac{1}{\Delta x}\int_0^{\frac{\Delta x}{2}} \widetilde{\mathbf{U}}_{j-1/2}\left(x/\Delta t\right)\mathrm{d}x + \frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{0} \widetilde{\mathbf{U}}_{j+1/2}\left(x/\Delta t\right)\mathrm{d}x, \quad (4.1)$$

where $\widetilde{\mathbf{U}}_{j\mp 1/2}(x/\Delta t)$ is the exact or approximate solution to the Riemann problem at the cell interface $x_{j\mp 1/2}$.

Einfeldt et al. [11] showed that if and only if step (a) generates physical states, then the scheme is positivity preserving. This is due to the fact that, given the physically admissible solutions to Riemann problems, the integration in (4.1) yields physical solutions. We have the following classical result:

Lemma 2 (Einfeldt et al. [11]) *An approximate Riemann solver leads to a positively conservative scheme if and only if all the states generated are physically real.*

Therefore, step (a) is the necessary and sufficient condition for the positivity preserving property of the scheme. Next, consider an exact or approximate LTS Riemann solver and note that the numerical algorithm may be seen as:

- (a) Solve the Riemann problem exactly or approximately to obtain the intermediate states in the Riemann fan
- (b) Update the solution according to:

$$\mathbf{U}_j^{n+1} = \frac{\Delta t}{\Delta x}\sum_{i=-\infty}^{\infty}\int_{(i-1)\frac{\Delta x}{\Delta t}}^{i\frac{\Delta x}{\Delta t}} \widetilde{\mathbf{U}}_{j-1/2-i}\left(\zeta_i\right)\mathrm{d}\zeta_i - \sum_{l=-\infty}^{\infty}\mathbf{U}_l, \quad (4.2)$$

where $\widetilde{\mathbf{U}}_{j-1/2}(\zeta_i)$ is the exact or approximate solution to the Riemann problem at the cell interface $x_{j-1/2-i}$ and $\zeta_i = (x - x_{j-1/2-i})/(t - t^n)$ (see [21,24] for details on (4.2)).

We observe that step (a) is the same for standard and LTS methods. We will show that in the LTS framework step (a) is only a necessary condition, i.e. (4.2) may yield non-physical states even when the solutions to the Riemann problems are physically real. In particular, we will show that:

Claim (1) The LTS-HLLE scheme is not positivity preserving.

Claim (2) The LTS-Lax-Friedrichs scheme is positivity preserving.

We will show that the LTS-HLLE is not positivity preserving by using the wave formulation (2.25) and by constructing a counter-example. General updating formula for an LTS method (4.2) can be rewritten as (2.23), (2.24) and (2.25). A nice feature of the wave formulation (2.25) is that we can decompose it to updating component by component. Since the wave velocity estimates are scalars, and the waves $\mathcal{W}$ are vectors, (2.25) allows us to treat the updating field-by-field as:

$$\theta_j^{n+1} = \theta_j^p - \frac{\Delta t}{\Delta x} \sum_{i=0}^{\infty} \left(\sum_{p=1}^{m} S^{p,i+}_{j-1/2-i} \theta^p_{j-1/2-i} + \sum_{p=1}^{m} S^{p,i-}_{j+1/2+i} \theta^p_{j+1/2+i} \right), \quad (4.3)$$

where θ is an arbitrary conserved variable from (2.1), and θ^p is the value of θ in the wave $\mathcal{W}^p$.

4.2 Loss of positivity with LTS-HLLE scheme in the Euler equations

We now consider two different ways how positivity can be lost in the Euler equations. The goal of this section is not to cover all possible ways how positivity can be lost. Instead, we aim to show that the LTS-HLLE scheme is not positivity preserving by constructing a counter-example, and we wish to illustrate the mechanism behind the loss of positivity. In particular, we consider only a class of initial data with the initial velocity:

$$v_0(x) = 0. \quad (4.4)$$

Further, we assume a special type of initial data where the perturbation of the data is limited to a single cell. Finally, the wave velocity estimates S_{L} and S_{R} in the HLLE scheme [10] are determined as the approximations to the smallest and the largest eigenvalues:

$$S_{\mathrm{L}} = \min\left(\lambda^1_j, \lambda^1_{j+1/2}\right), \quad (4.5a)$$

$$S_{\mathrm{R}} = \max\left(\lambda^3_{j+1/2}, \lambda^3_{j+1}\right), \quad (4.5b)$$

which for the one-dimensional Euler equations carry the indices 1 and 3, and where $\lambda^{1,3}_{j+1/2}$ are the Roe averaged eigenvalues [38].

4.2.1 Local collapse in density

Consider the initial data with a density spike in a single cell:

$$(\rho, v, p)^0_i = \begin{cases} (\rho_j, 0, 1) & \text{if} \quad i = j; \\ (\rho_0, 0, 1) & \text{if} \quad i \neq j, \end{cases} \quad (4.6)$$

with $\rho_j > \rho_0$. By using (2.3) and (2.4), the hierarchy of the eigenvalues in the neighborhood of the cell j is:

$$\lambda^1_{j-1} < \lambda^1_{j-1/2} < \lambda^1_j, \quad (4.7a)$$

$$\lambda^3_{j-1} > \lambda^3_{j-1/2} > \lambda^3_j, \quad (4.7b)$$

at the interface $x_{j-1/2}$ and:

$$\lambda_j^1 > \lambda_{j+1/2}^1 > \lambda_{j+1}^1, \tag{4.8a}$$

$$\lambda_j^3 < \lambda_{j+1/2}^3 < \lambda_{j+1}^3, \tag{4.8b}$$

at the interface $x_{j+1/2}$. For the density in the cell j, the LTS-HLLE scheme (4.3) yields:

$$\rho_j^{n+1} = \rho_j - \frac{\Delta t}{\Delta x}\left(S_{R,j-1/2}^{0+}\left(\rho_j - \rho_{j-1/2}^{\mathrm{HLLE}}\right) + S_{L,j+1/2}^{0-}\left(\rho_{j+1/2}^{\mathrm{HLLE}} - \rho_j\right)\right), \tag{4.9}$$

where we note that for the initial data (4.6) we have $\rho_{j-1/2}^{\mathrm{HLLE}} = \rho_{j+1/2}^{\mathrm{HLLE}}$ and $\rho_{j\mp1} = \rho_0$.

Lemma 3 *For the initial data* (4.6)*, the LTS-HLLE scheme preserves the positivity of the density in the cell j if:*

$$\rho_{j-1/2}^{HLLE} > \frac{1}{2}\rho_j. \tag{4.10}$$

Proof Both waves updating (4.9) reduce the density in the cell j. The decrease in the density is greatest when the Courant number C is large enough that (2.30) yields:

$$S_{R,j-1/2}^{0+} = \frac{\Delta x}{\Delta t}, \quad S_{L,j+1/2}^{0-} = -\frac{\Delta x}{\Delta t}. \tag{4.11}$$

Then (4.9) reduces to:

$$\rho_j^{n+1} = 2\rho_{j-1/2}^{\mathrm{HLLE}} - \rho_j, \tag{4.12}$$

which is positive when (4.10) holds. □

Lemma 4 *For the initial data* (4.6)*, the condition* (4.10) *holds for:*

$$\rho_j < b\rho_0, \tag{4.13}$$

where:

$$b = \frac{2}{3}\left(4 + \sqrt[3]{19 - 3\sqrt{33}} + \sqrt[3]{19 + 3\sqrt{33}}\right) \approx 5.6786. \tag{4.14}$$

Proof For the initial data (4.6), the intermediate state $\rho_{j-1/2}^{\mathrm{HLLE}}$ is determined by (2.13):

$$\rho_{j-1/2}^{\mathrm{HLLE}} = \frac{S_{\mathrm{R}}\rho_j - S_{\mathrm{L}}\rho_0}{S_{\mathrm{R}} - S_{\mathrm{L}}}. \tag{4.15}$$

By using (4.7) in (4.5) we have that at $x_{j-1/2}$:

$$S_{\mathrm{L}} = \lambda_0^1 = -a_0 = -\sqrt{\gamma p/\rho_0}, \tag{4.16a}$$

$$S_{\mathrm{R}} = \lambda_{j-1/2}^3 = a_{j+1/2} = \sqrt{\gamma p/\sqrt{\rho_0\rho_j}}, \tag{4.16b}$$

where $a_{j-1/2}$ is the Roe averaged speed of the sound (see for instance [22]). The intermediate state (4.15) now becomes:

$$\rho_{j-1/2}^{\mathrm{HLLE}} = \frac{\sqrt{\frac{1}{\sqrt{\rho_0\rho_j}}}\rho_j + \sqrt{\frac{1}{\rho_0}}\rho_0}{\sqrt{\frac{1}{\sqrt{\rho_0\rho_j}}} + \sqrt{\frac{1}{\rho_0}}}. \tag{4.17}$$

Then we can rewrite the condition (4.10) as:

$$\frac{1}{2}\rho_j\sqrt{\frac{1}{\sqrt{\rho_0\rho_j}}}-\sqrt{\frac{1}{\rho_0}}\left(\frac{1}{2}\rho_j-\rho_0\right)>0. \tag{4.18}$$

We know that $\rho_0<\rho_j$, i.e. we may write $\rho_j=b\rho_0$, $b>1$. By using this in (4.18) we obtain:

$$b^{3/4}-b+2>0, \tag{4.19}$$

which is a decreasing function of $b\in(1,\infty)$ and becomes negative when b exceeds the condition (4.14). □

4.2.2 Local collapse in internal energy

Consider the initial data with a pressure spike in a single cell:

$$(\rho,v,p)_i^0=\begin{cases}(1,0,p_j) & \text{if} \quad i=j;\\ (1,0,p_0) & \text{if} \quad i\neq j,\end{cases} \tag{4.20}$$

with $p_j>p_0$. By using (2.3) and (2.4), the hierarchy of the eigenvalues in the neighborhood of the cell j is:

$$\lambda^1_{j-1}>\lambda^1_{j-1/2}>\lambda^1_j, \tag{4.21a}$$
$$\lambda^3_{j-1}<\lambda^3_{j-1/2}<\lambda^3_j, \tag{4.21b}$$

at the interface $x_{j-1/2}$ and:

$$\lambda^1_j<\lambda^1_{j+1/2}<\lambda^1_{j+1}, \tag{4.22a}$$
$$\lambda^3_j>\lambda^3_{j+1/2}>\lambda^3_{j+1}, \tag{4.22b}$$

at the interface $x_{j+1/2}$. For the total energy density in the cell j, the LTS-HLLE scheme (4.3) yields:

$$E_j^{n+1}=E_j-\frac{\Delta t}{\Delta x}\left(S^{0+}_{R,j-1/2}\left(E_j-E^{\mathrm{HLLE}}_{j-1/2}\right)+S^{0-}_{L,k+1/2}\left(E^{\mathrm{HLLE}}_{j+1/2}-E_j\right)\right). \tag{4.23}$$

By using the following relations (superscript denotes the time step):

$$E_j^0=\rho_j^0e_j^0+\frac{1}{2}\rho_j^0[v_j^0]^2=\rho_j^0e_j^0, \tag{4.24a}$$
$$E_j^1=\rho_j^1e_j^1+\frac{1}{2}\rho_j^1[v_j^1]^2, \tag{4.24b}$$
$$\rho_j^1=\rho_j^0, \quad \forall j, \tag{4.24c}$$

we can obtain from (4.23) that the internal energy is:

$$\begin{aligned}e_j^{n+1}=&e_j-\frac{\Delta t}{\Delta x}\left(S^{0+}_{R,j-1/2}\left(e_j-e^{\mathrm{HLLE}}_{j-1/2}\right)+S^{0-}_{L,k+1/2}\left(e^{\mathrm{HLLE}}_{j+1/2}-e_j\right)\right)\\ &-\frac{1}{2}\left[v_j-\frac{\Delta t}{\Delta x}\left(S^{0+}_{R,j-1/2}\left(v_j-v^{\mathrm{HLLE}}_{j-1/2}\right)+S^{0-}_{L,k+1/2}\left(v^{\mathrm{HLLE}}_{j+1/2}-v_j\right)\right)\right]^2.\end{aligned} \tag{4.25}$$

We note that for the initial data (4.20) we have $e^{\mathrm{HLLE}}_{j-1/2}=e^{\mathrm{HLLE}}_{j+1/2}$, $v^{\mathrm{HLLE}}_{j-1/2}=-v^{\mathrm{HLLE}}_{j+1/2}$ and $p_{j\mp1}=p_0$.

Lemma 5 *For the initial data* (4.20)*, the LTS-HLLE scheme preserves the positivity of the internal energy in the cell* j*.*

Proof Both waves associated with the internal energy and the term associated with the kinetic energy reduce the internal energy in the cell j, eq. (4.25). The decrease in the internal energy is greatest when the Courant number C is large enough that (2.30) yields:

$$S^{0+}_{R,j-1/2} = \frac{\Delta x}{\Delta t}, \quad S^{0-}_{L,j+1/2} = -\frac{\Delta x}{\Delta t}. \tag{4.26}$$

Then (4.25) reduces to:

$$e_j^{n+1} = 2e^{\text{HLLE}}_{j-1/2} - e_j - \frac{1}{2}\left[v^{\text{HLLE}}_{j-1/2} + v^{\text{HLLE}}_{j+1/2}\right]^2 = 2e^{\text{HLLE}}_{j-1/2} - e_j, \tag{4.27}$$

which is always positive, as we will show next. For the initial data (4.20), the intermediate state $e^{\text{HLLE}}_{j-1/2}$ is:

$$e^{\text{HLLE}}_{j-1/2} = \frac{S_{\text{R}} e_j - S_{\text{L}} e_0}{S_{\text{R}} - S_{\text{L}}}. \tag{4.28}$$

By using (4.21) in the (4.5) we have that at $x_{j-1/2}$:

$$S_{\text{L}} = \lambda^1_{j-1/2} = -a_{j-1/2} = -\sqrt{\gamma\left(p_0 + p_j\right)/\left(2\rho\right)}, \tag{4.29a}$$

$$S_{\text{R}} = \lambda^3_j = a_j = \sqrt{\gamma p_j/\rho}. \tag{4.29b}$$

The intermediate state (4.28) now becomes:

$$e^{\text{HLLE}}_{j-1/2} = \frac{1}{\gamma - 1}\frac{\sqrt{p_j}p_j + \sqrt{\frac{p_0+p_j}{2}}p_0}{\sqrt{p_j} + \sqrt{\frac{p_0+p_j}{2}}}. \tag{4.30}$$

We wish to show that (4.27) is always positive, i.e. $e^{\text{HLLE}}_{j-1/2} > \frac{1}{2}e_j$ always holds:

$$\frac{1}{\gamma - 1}\frac{\sqrt{p_j}p_j + \sqrt{\frac{p_0+p_j}{2}}p_0}{\sqrt{p_j} + \sqrt{\frac{p_0+p_j}{2}}} > \frac{1}{2}\frac{p_j}{\gamma - 1},$$

$$\frac{1}{2}p_j\sqrt{p_j} + \sqrt{\frac{p_0+p_j}{2}}\left(p_0 - \frac{1}{2}p_j\right) > 0. \tag{4.31}$$

We know that $p_0 < p_j$, i.e. we may write $p_j = bp_0$, $b > 1$. By using this in (4.31) we obtain:

$$\frac{1}{2}b\sqrt{b} + \sqrt{\frac{1+b}{2}}\left(1 - \frac{1}{2}b\right) > 0, \tag{4.32}$$

which is an increasing function of $b \in (1, \infty)$, hence the inequality (4.27) always holds. □

4.2.3 Nonlocal collapse in density

In the section above we described how positivity can be lost in the cell where there is a spike in the initial data. We now show that a spike in the initial data in one cell can also cause loss of positivity in other cells as well. Such collapse will be denoted as a *nonlocal collapse*. It is this type of loss of positivity that in a system of equations is equivalent to the loss of monotonicity described in section 3.

Consider the initial data with a density spike in a single cell:

$$(\rho, v, p)_i^0 = \begin{cases} (\rho_j, 0, 1) & \text{if} \quad i = j; \\ (\rho_0, 0, 1) & \text{if} \quad i \neq j, \end{cases} \tag{4.33}$$

with $\rho_j > \rho_0$. The hierarchy of the eigenvalues in the neighborhood of cell j is the same as earlier, see (4.7) and (4.8). We note that the problem is symmetric and focus on the right side. There is a cell z to the right of cell j such that $z > j$ for which the LTS-HLLE scheme (4.3) yields:

$$\rho_z^{n+1} = \rho_z - \frac{\Delta t}{\Delta x}\left(S_{R,j-1/2}^{(z-j)+}\left(\rho_j - \rho_{j-1/2}^{\text{HLLE}}\right) + S_{R,j+1/2}^{(z-j-1)+}\left(\rho_{j+1} - \rho_{j+1/2}^{\text{HLLE}}\right)\right), \tag{4.34}$$

where we note that for the initial data (4.33) we have $\rho_{j-1/2}^{\text{HLLE}} = \rho_{j+1/2}^{\text{HLLE}}$ and $\rho_{j\mp1} = \rho_z = \rho_0$.

Lemma 6 *For the initial data* (4.33) *the LTS-HLLE scheme preserves the positivity of the density in the cell z if:*

$$\rho_{j-1/2}^{HLLE} > \frac{1}{2}\rho_j. \tag{4.35}$$

Proof We consider (4.34) and note that the wave from $x_{j-1/2}$ decreases the density in the cell z, while the wave from $x_{j+1/2}$ increases the density in the cell z. By using (4.7) and (4.8) in (4.5) we find out that the waves are moving with velocities:

$$S_{\text{R},j-1/2} = \lambda_{j-1/2}^3 = \lambda_{j+1/2}^3 < S_{\text{R},j+1/2} = \lambda_{j+1}^3, \tag{4.36}$$

hence the waves updating (4.34) cannot pass each other. The critical case is when the Courant number C is large enough that (2.30) yields:

$$S_{R,j-1/2}^{(z-j)+} = \frac{\Delta x}{\Delta t}, \qquad S_{R,j+1/2}^{(z-j-1)+} = \frac{\Delta x}{\Delta t}. \tag{4.37}$$

Then (4.34) reduces to:

$$\rho_z^{n+1} = 2\rho_{j-1/2}^{\text{HLLE}} - \rho_j, \tag{4.38}$$

which is positive when (4.35) holds. □

We note that the condition (4.35) holds under the same condition as in Lemma 4.

4.2.4 Nonlocal collapse in internal energy

Consider the initial data with a pressure spike in a single cell:

$$(\rho, v, p)_i^0 = \begin{cases} (1, 0, p_j) & \text{if} \quad i = j; \\ (1, 0, p_0) & \text{if} \quad i \neq j, \end{cases} \tag{4.39}$$

with $p_j > p_0$. The hierarchy of the eigenvalues in the neighborhood of cell j is the same as earlier, see (4.21) and (4.22). We note that the problem is symmetric and focus on the right side. There is a cell z to the right of cell j such that $z > j$ for which the LTS-HLLE scheme (4.3) yields:

$$E_z^{n+1} = E_z - \frac{\Delta t}{\Delta x}\left(S_{R,j-1/2}^{(z-j)+}\left(E_j - E_{j-1/2}^{\text{HLLE}}\right) + S_{R,j+1/2}^{(z-j-1)+}\left(E_{j+1} - E_{j+1/2}^{\text{HLLE}}\right)\right). \tag{4.40}$$

By using the relations given in (4.24), we can obtain from (4.40) that the internal energy is:

$$\begin{aligned} e_z^{n+1} =& e_z - \frac{\Delta t}{\Delta x}\left(S_{R,j-1/2}^{(z-j)+}\left(e_j - e_{j-1/2}^{\text{HLLE}}\right) + S_{R,j+1/2}^{(z-j-1)+}\left(e_{j+1} - e_{j+1/2}^{\text{HLLE}}\right)\right) \\ & -\frac{1}{2}\left[v_z - \frac{\Delta t}{\Delta x}\left(S_{R,j-1/2}^{(z-j)+}\left(v_j - v_{j-1/2}^{\text{HLLE}}\right) + S_{R,j+1/2}^{(z-j-1)+}\left(v_{j+1} - v_{j+1/2}^{\text{HLLE}}\right)\right)\right]^2. \end{aligned} \tag{4.41}$$

We note that for the initial data (4.39) we have $e_{j-1/2}^{\text{HLLE}} = e_{j+1/2}^{\text{HLLE}}$, $v_{j-1/2}^{\text{HLLE}} = -v_{j+1/2}^{\text{HLLE}}$ and $p_{j\mp1} = p_0$.

Lemma 7 *For the initial data* (4.39)*, the LTS-HLLE scheme preserves positivity of the internal energy in the cell z if:*

$$e_{j-1/2}^{HLLE} > e_j - e_0 + \frac{1}{2}[v_{j-1/2}^{HLLE}]^2. \tag{4.42}$$

Proof We consider (4.41) and note that the wave from $x_{j-1/2}$ decreases the internal energy in cell z, the wave from $x_{j+1/2}$ increases the internal energy in the cell z, and the term corresponding to kinetic energy decreases the internal energy in the cell z. By using (4.21) and (4.22) in (4.5) we find out that the waves are moving with velocities:

$$S_{\text{R},j-1/2} = \lambda_j^3 > S_{\text{R},j+1/2} = \lambda_{j+1/2}^3, \tag{4.43}$$

hence the waves updating (4.40) can pass each other. The critical case is when the Courant number C is such that (2.30) yields:

$$S_{R,j-1/2}^{(z-j)+} = \frac{\Delta x}{\Delta t}, \qquad S_{R,j+1/2}^{(z-j-1)+} = 0, \tag{4.44}$$

i.e. the wave decreasing the internal energy completely passes through the cell z, and the wave increasing the internal energy does not reach the cell z. Then (4.41) reduces to:

$$e_z^{n+1} = e_0 - e_j + e_{j-1/2}^{\text{HLLE}} - \frac{1}{2}[v_{j-1/2}^{\text{HLLE}}], \tag{4.45}$$

which is positive when (4.42) holds. □

Lemma 8 *For the initial data* (4.39)*, the condition* (4.42) *holds for:*

$$p_j < 3.09224 p_0. \tag{4.46}$$

Proof For the initial data (4.39), the intermediate state $e^{\mathrm{HLLE}}_{j-1/2}$ was already defined in (4.30), while the intermediate state $v^{\mathrm{HLLE}}_{j-1/2}$ can be determined in a similar manner as:

$$v^{\mathrm{HLLE}}_{j-1/2} = \frac{p_0 - p_j}{\sqrt{\gamma p_0} + \sqrt{\gamma \frac{p_0+p_j}{2}}}. \tag{4.47}$$

Then we can rewrite the condition (4.42) as:

$$\frac{1}{\gamma-1}\frac{\sqrt{p_j}p_j + \sqrt{\frac{p_0+p_j}{2}}p_0}{\sqrt{p_j} + \sqrt{\frac{p_0+p_j}{2}}} + \frac{p_0}{\gamma-1} - \frac{p_j}{\gamma-1} - \frac{1}{2}\left[\frac{p_0 - p_j}{\sqrt{\gamma p_0} + \sqrt{\gamma \frac{p_0+p_j}{2}}}\right]^2 > 0 \tag{4.48}$$

We know that $p_0 < p_j$, i.e. we may write $p_j = b p_0$ and $b > 1$. By using that we have:

$$\sqrt{\frac{1+b}{2}}(2-b) + \sqrt{b} - \frac{\gamma-1}{2\gamma}\left(\frac{1-2b+b^2}{b + 2\sqrt{b}\sqrt{\frac{(1+b)}{2}} + \frac{(1+b)}{2}}\right)\left(\sqrt{b} + \sqrt{\frac{1+b}{2}}\right) > 0. \tag{4.49}$$

This is a decreasing function of $b \in (1, \infty)$ and becomes negative when $b = 3.09224$. □

We showed four different examples how positivity of density and internal energy can be lost when we use the LTS-HLLE scheme. We note that these examples are limited to very special types of the initial data, and it is reasonable to expect that arbitrary initial data might lead to more ways to lose positivity, especially if the velocity differences between the cells would be very large.

We now proceed to show that the LTS-Lax-Friedrichs scheme by Lindqvist et al. [24] is positivity preserving.

4.3 LTS-Lax-Friedrichs scheme for the Euler equations

Proposition 3 *The LTS-Lax-Friedrichs scheme by Lindqvist et al. [24]:*

$$\mathbf{U}^{n+1}_j = \frac{1}{2}\left(\mathbf{U}_{j-k} + \mathbf{U}_{j+k}\right) - \frac{\Delta t}{2k\Delta x}\left(\mathbf{F}_{j+k} - \mathbf{F}_{j-k}\right), \tag{4.50}$$

is positivity preserving for the one-dimensional Euler equations under the CFL condition:

$$C = \max_{p,x,t} |\lambda^p(x,t)| \frac{\Delta t}{\Delta x} \leq k, \quad k \in \mathbb{Z}^+. \tag{4.51}$$

Our proof is based on the paper by Zhang and Shu [49] where it is shown that the standard Lax-Friedrichs scheme is positivity preserving for the Euler equations under the standard CFL condition (2.14). We follow their proof and generalize it to hold under the relaxed CFL condition (4.51). We start with the following result:

Lemma 9 (Zhang and Shu [49]) *Define the set of admissible states by:*

$$G = \left\{ \mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} \middle| \rho > 0, \quad \text{and} \quad p = (\gamma - 1)\left(E - \tfrac{1}{2}\rho v^2\right) > 0 \right\}, \tag{4.52}$$

then G is a convex set.

Proof (Proposition 3) We can rewrite (4.50) as:

$$\mathbf{U}_j^{n+1} = \frac{1}{2}\left(\mathbf{U}_{j-k} + \frac{\Delta t}{k\Delta x}\mathbf{F}_{j-k}\right) + \frac{1}{2}\left(\mathbf{U}_{j+k} - \frac{\Delta t}{k\Delta x}\mathbf{F}_{j+k}\right). \tag{4.53}$$

We assume that $\mathbf{U}_{j-k}$ and $\mathbf{U}_{j+k}$ are in the set G, and we want to show that $\mathbf{U}_j^{n+1} \in G$ under the CFL condition (4.51). We start by observing that $\mathbf{U}_j^{n+1}$ is a convex combination of vectors:

$$\mathbf{U}_{j-k} + \frac{\Delta t}{k\Delta x}\mathbf{F}_{j-k}, \quad \text{and} \quad \mathbf{U}_{j+k} - \frac{\Delta t}{k\Delta x}\mathbf{F}_{j+k}. \tag{4.54}$$

Therefore, we only need to show that these vectors are in the set G. For the first component of $\mathbf{U}$ (the density) we obtain:

$$\left(1 \pm \frac{\Delta t}{k\Delta x} v_{j\mp k}\right) \rho_{j\mp k} > 0, \tag{4.55}$$

which is satisfied when (4.51) holds. The next step is showing the positivity of pressure. By dropping subscripts, the pressure ($p = (\gamma - 1)\rho e$) can be written as a function of conserved variables:

$$\begin{aligned} p\left(\mathbf{U} \pm \frac{\Delta t}{k\Delta x}\mathbf{F}\right) =& p\left(\left[\rho \pm \frac{\Delta t}{k\Delta x}\rho v, \rho v \pm \frac{\Delta t}{k\Delta x}(\rho v^2 + p), E \pm \frac{\Delta t}{k\Delta x} v(E+p)\right]^{\mathrm{T}}\right) \\ =& p\left(1 \pm \frac{\Delta t}{k\Delta x} v\right)\left(1 - \frac{p}{\rho}\frac{\gamma - 1}{2\left(\frac{k\Delta x}{\Delta t} \pm v\right)^2}\right). \end{aligned} \tag{4.56}$$

The first bracket is positive since it is equal to the bracket in (4.55), while the second bracket can be rewritten as:

$$\left(1 - \frac{p}{\rho}\frac{\gamma - 1}{2\left(\frac{k\Delta x}{\Delta t} \pm v\right)^2}\right) > 0 \quad \longrightarrow \quad \sqrt{\frac{2\gamma}{\gamma - 1}}\left(\frac{k\Delta x}{\Delta t} \pm v\right) > \sqrt{\gamma\frac{p}{\rho}}, \tag{4.57}$$

which always holds under the CFL condition (4.51). □

4.4 Towards a positivity preserving LTS method

In the existing literature, two main ways to tackle the loss of positivity are:

– Constructing an unconditionally positivity preserving scheme (see references in section 1). This approach is currently available only for standard methods, and at the moment it seems unattainable for a wide class of LTS methods because of lack of full understanding of all possible ways the positivity can be lost. Currently, the LTS-Lax-Friedrichs scheme is the only known positivity preserving LTS method.

– Reducing the Courant number. This approach works for LTS methods as well, and it has been exploited by Morales-Hernández and co-workers [28,29]. The straightforward way to do this is by repeating the time step with a reduced Courant number when the positivity is lost, while more sophisticated approaches include determining if the loss of positivity is likely to happen at the beginning of each time step.

Herein, we propose a very general way to increase the robustness of the LTS method and its ability to preserve positivity by adding numerical diffusion. We start by observing that by defining the wave velocity estimates as $S_{\mathrm{L}} = -k\Delta x/\Delta t$ and $S_{\mathrm{R}} = k\Delta x/\Delta t$ in the LTS-HLL scheme we recover the LTS-Lax-Friedrichs scheme of Lindquist et al. [24]. Since the LTS-Lax-Friedrichs scheme is positivity preserving, we propose to parametrize the wave velocity estimates as a convex combination between the HLLE and Lax-Friedrichs schemes:

$$S_{\mathrm{L}} = (1-\beta)\, S_{\mathrm{L}}^{\mathrm{E}} + \beta S_{\mathrm{L}}^{\mathrm{LxF}}, \qquad S_{\mathrm{R}} = (1-\beta)\, S_{\mathrm{R}}^{\mathrm{E}} + \beta S_{\mathrm{R}}^{\mathrm{LxF}}, \tag{4.58}$$

where $S_{\mathrm{L,R}}^{\mathrm{E}}$ are the wave velocity estimates according to Einfeldt (4.5). We will denote this method as the LTS-HLLEβ.

5 Numerical results

In this section we present numerical results for three test cases commonly used to test the robustness of numerical methods. The input discretization parameters are the Courant number C and Δx. Then, the time step Δt is evaluated at each time step according to:

$$\Delta t = \frac{C\Delta x}{\max\limits_{p,j} |\lambda_j^p|}\ . \tag{5.1}$$

5.1 Double rarefaction

As the first test case we consider the double rarefaction test case already considered by Prebeg [34], with initial data $\mathbf{V}(x,0) = (\rho, v, p)^{\mathrm{T}}$:

$$\mathbf{V}(x,0) = \begin{cases} (1,-2,0.4)^{\mathrm{T}} & \text{if} \quad x < 0, \\ (1,2,0.4)^{\mathrm{T}} & \text{if} \quad x > 0, \end{cases} \tag{5.2}$$

where the solution is evaluated at $t = 0.05$ on a grid with 100 cells in the interval $[-0.2, 0.2]$. Figure 2 shows that the LTS-HLLE scheme successfully resolves problem (5.2) at the Courant number $C = 5$. Further, we observe that the LTS-HLLEβ scheme yields smoother profiles of all variables. We note that the LTS-HLLE scheme preserves positivity for the problem (5.2) for all Courant numbers we tried.

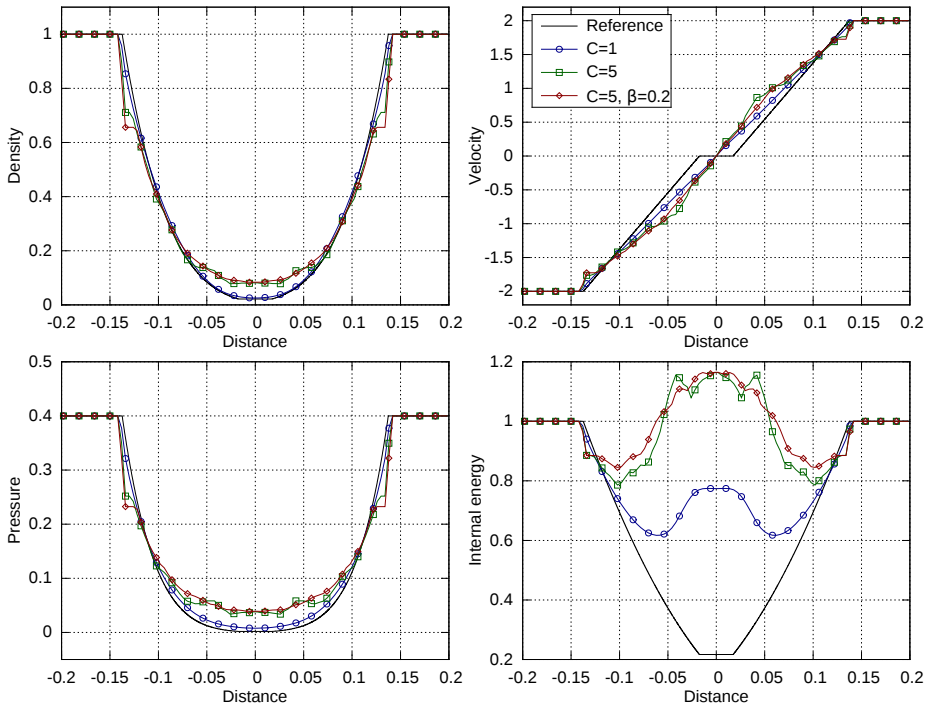

Fig. 2: The HLLE and LTS-HLLE(β) schemes for the problem (5.2)

5.2 LeBlanc's shock tube

As the second test case we consider LeBlanc's shock tube with initial data $\mathbf{V}(x,0) = (\rho, v, p)^{\mathrm{T}}$:

$$\mathbf{V}(x,0) = \begin{cases} (1, 0, (2/3)0.1)^{\mathrm{T}} & \text{if} \quad x < 3, \\ (0.001, 0, (2/3)10^{-7})^{\mathrm{T}} & \text{if} \quad x > 3, \end{cases} \tag{5.3}$$

and $\gamma = 5/3$, where the solution is evaluated at $t = 6$ on a grid with 600 cells in the interval $[0, 9]$. Figure 3 shows that both LTS-HLLE(β) schemes perform better than the LTS-Roe scheme. This becomes even more notable as we increase the Courant number, and the LTS-Roe scheme losses positivity and crashes for $C \geq 10$, while the LTS-HLLE(β) schemes preserve positivity for all Courant numbers we tried. Introducing numerical diffusion smoothened the profiles, but also calculated position of the right shock even further to the right. We note that large errors observed in velocity and internal energy (even with the standard methods) have been reported by other authors as well, see for instance [26, 7, 48].

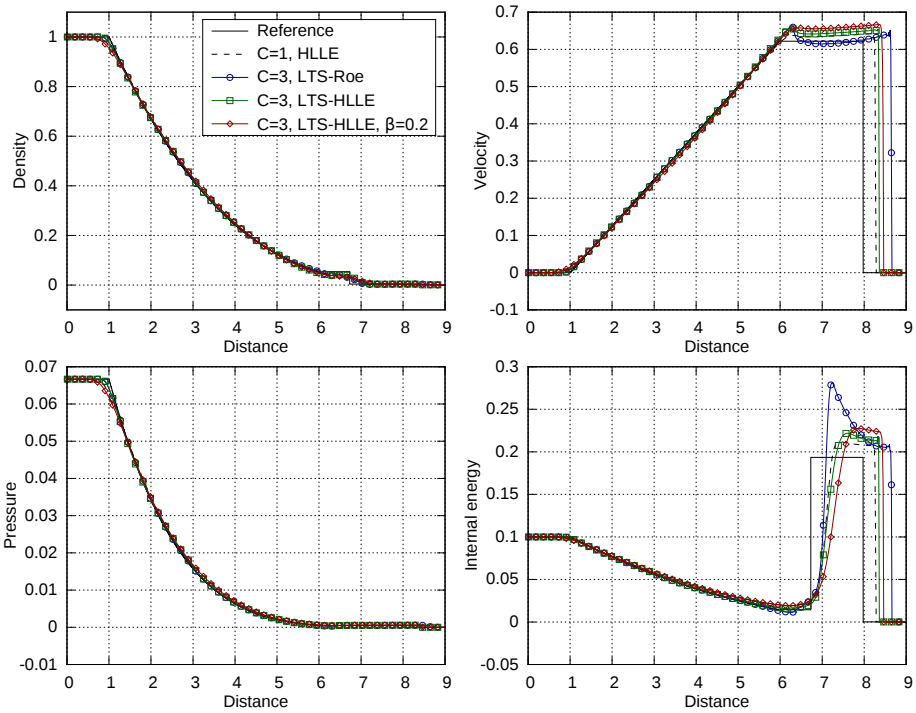

Fig. 3: The HLLE, LTS-Roe and LTS-HLLE(β) schemes for the problem (5.3)

5.3 Sedov blast-wave

As the last test case we consider the planar Sedov blast-wave problem with the initial data $\mathbf{V}(x,0) = (\rho, v, p)^{\mathrm{T}}$:

$$\mathbf{V}(x,0) = \begin{cases} (1, 0, 4 \times 10^{-13}) & \text{if} \quad -2 < x < -0.5\Delta x, \quad 0.5\Delta x < x < 2 \\ (1, 0, 2.56 \times 10^{8}) & \text{if} \quad -0.5\Delta x < x < 0.5\Delta x, \end{cases} \tag{5.4}$$

where the solution is evaluated at $t = 10^{-3}$ on a grid with 800 cells in the interval $[-2, 2]$. The exact solution is obtained with free software [42]. In the previous two test cases, the LTS-HLLE scheme preserved positivity for any Courant number we tried. For the Sedov blast-wave, the LTS-HLLE scheme loses positivity for $C > 4$, but we were able to use $C > 4$ by adding numerical diffusion, see Fig. 4. The loss of positivity for the LTS-HLLE scheme is expected because the initial data (5.4) closely resembles the initial data studied in section 4.

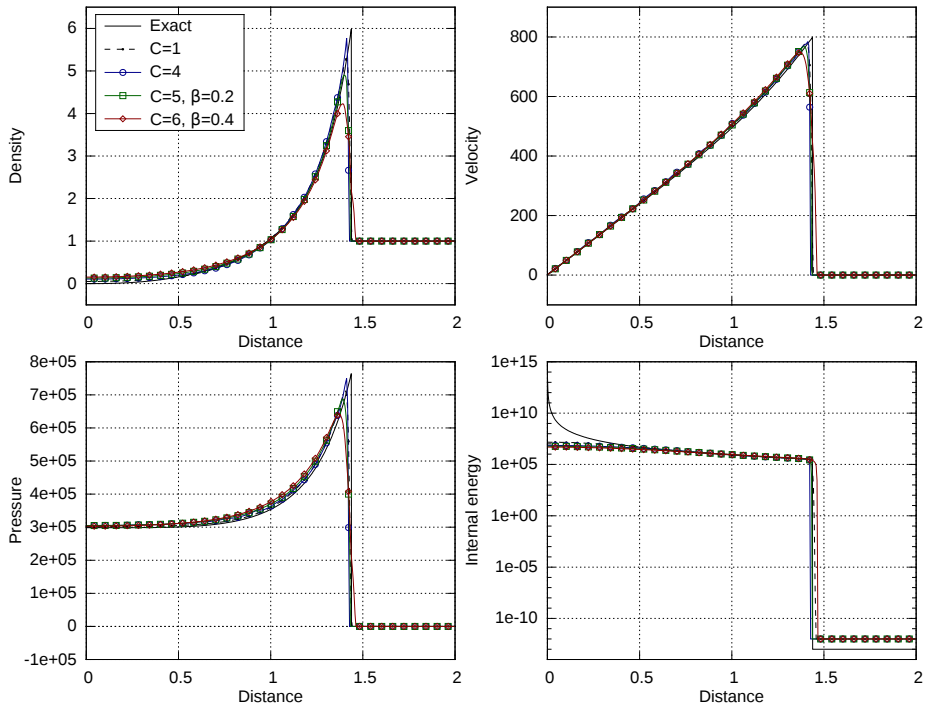

Fig. 4: The HLLE and LTS-HLLE(β) schemes for the problem (5.4)
(the solution is symmetric and only the right half of the domain is shown)

6 Conclusions

We have investigated the monotonicity and positivity preserving properties in LTS methods, with a special focus on the LTS-HLLE scheme for the Euler equations. In particular, we have determined the monotonicity conditions on the numerical flux function of the LTS method for scalar conservation laws (Proposition 1), and we showed that the LTS-HLLE scheme is not positivity preserving. Further, we showed that the LTS-Lax-Friedrichs scheme for scalar conservation laws is monotone (Proposition 2) and that the LTS-Lax-Friedrichs scheme for the Euler equations is positivity preserving (Proposition 3).

We applied the LTS-HLLE(β) schemes to three test cases commonly used to test the positivity preserving property. Even though the LTS-HLLE scheme is not positivity preserving, numerical investigations suggest that it always preserves positivity for the double rarefaction and LeBlanc's shock tube. The LTS-HLLE scheme lost positivity for the Sedov blast-wave when we increased the Courant number above certain values. We proposed a very simple way to make the schemes more robust by adding numerical diffusion, which allowed us to increase the Courant number used for the Sedov blast-wave. Unfortunately, increased robustness obtained by adding numerical diffusion results in less accurate solutions.

We believe that the decrease in accuracy due to additional diffusion can be reduced by more sophisticated ways of introducing numerical diffusion. In our

investigations the parameter β is constant across the whole domain and at all time steps. By selectively introducing numerical diffusion we could introduce a minimal amount of numerical diffusion required to ensure positivity preservation, while keeping the solution as sharp as possible. The development of such methods requires further insight into the ways positivity is lost, and at the moment it remains outside the scope of this paper.

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