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Entropy production in second-order three-point schemes*

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Summary. We discuss semi-discrete three-point finite difference methods for the numerical solution of systems of conservation laws which are second order accurate in space in the sense of truncation error. Particular discretizations of the numerical entropy flux associated with such schemes are studied clarifying the importance of this discretization with regard to the production of numerical entropy. Using a numerical entropy flux constructed in a canonical way we prove that a wide class of finite difference methods cannot satisfy a discrete entropy inequality. Together with a well known result of Schonbek concerning Lax-Wendroff type schemes our result indicates a strong relationship between entropy production and oscillations in numerical solutions.

Mathematics Subject Classifikation (1991): 65M06, 65M12, 65M20

1 Introduction

Let $D := \{(x, t) \in \mathbb{R} \times \mathbb{R}_0^+\}$ be a half plane in $\mathbb{R}^2$ and $\Omega \subset \mathbb{R}^m$ an open set which will be called state space. If $u_0 \in [BV_{\mathrm{loc}} \cap L^\infty](\mathbb{R}; \Omega)$ then $u \in [BV_{\mathrm{loc}} \cap L^\infty](D; \Omega)$ is called a weak solution of the Cauchy problem

(1) $$\partial_t u + \partial_x f(u) = 0$$

(2) $$u(x, 0) = u_0(x), \quad x \in \mathbb{R}$$

if

(3) $$\forall \Phi \in C_0^1(D; \Omega): \int_D \{u^{\mathrm{T}} \partial_t \Phi + f(u)^{\mathrm{T}} \partial_x \Phi\}\, dx\, dt +$$

(4) $$+ \int_{\mathbb{R}} \{u_0(x)^{\mathrm{T}} \Phi(x, 0)\}\, dx = 0\,.$$

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In the case of solutions containing only jump discontinuities this definition is equivalent to the celebrated Rankine-Hugoniot condition encountered in gas dynamics [14].

Equations of the form (1) are called conservation laws, since the integral of u_0 with respect to the x-coordinate is conserved in time. The function f is called the flux function which is assumed to be nonlinear but of class $C^2(\Omega; \mathbb{R}^m)$. We always assume hyperbolicity of the problem in the sense of Friedrichs, i.e. the Jacobian matrix $\Omega \ni s \overset{\nabla_u f}{\mapsto} \nabla_u f(s) \in \mathbb{R}^{m \times m}$ of f exhibits exactly m real eigenvalues $\zeta_1(s) \leqq \zeta_2(s) \leqq \ldots \leqq \zeta_m(s)$ and m linearly independent eigenvectors $r_k: \forall k = 1(1)m$: $\nabla_u f(s) r_k(s) = \zeta_k(s) r_k(s)$.

Some structural properties of weak solutions are worth mentioning. For a detailed account the reader is referred to [2]. For $1 \leqq k \leqq m$ the k-th characteristic wave field consists of the curves $\frac{dx}{dt} = \zeta_k(u(x, t))$. It is called genuinely nonlinear if for all $s \in \Omega$: $(\nabla_u \zeta_k(s))^T r_k(s) \neq 0$, otherwise it is called linearly degenerate. In the case of a genuinely nonlinear field the normalization $(\nabla_u \zeta_k(s))^T r_k(s) = 1$ is assumed. A continuously differentiable function $\Omega \ni s \overset{R}{\mapsto} R(s) \in \mathbb{R}$ is called a k-th Riemann invariant if for all $s \in \Omega$: $r_k(s)^T \nabla_u R(s) = 0$. If $u \in [C^1](G; \Omega)$ is a solution of (1) in a domain $G \subset D$ and if all k-th Riemann invariants are constant in G, then u is called a k-simple wave or k-rarefaction wave. A k-rarefaction wave is called centered at $(x_0, t_0) \in G$ if $u(x, t) = u\left(\frac{x - x_0}{t - t_0}\right)$.

For further reference we cite an important theorem concerning the existence of a parametrization of genuinely nonlinear wave fields. The proof of this theorem can be found in [14].

Theorem 1. *Let the k-th characteristic wave field be genuinely nonlinear in Ω and normalized. Let $u_L \in \Omega$. Then there exists a one-parameter family of states*

$$\mathbb{R} \supset [0, a] \ni \varepsilon \overset{u}{\mapsto} u(\varepsilon) \in \Omega \tag{5}$$

for an $a > 0$ each member of which can be connected with u_L by a centered k-rarefaction wave. Furthermore the expressions

$$u(0) = u_L \tag{6}$$

$$\left. \frac{du(\varepsilon)}{d\varepsilon} \right|_{\varepsilon = 0} = r_k(u_L) \tag{7}$$

are valid.

Most of the problems concerning existence of weak solutions to (1), (2) are still open, except in the case of systems exhibiting genuinely nonlinear wave fields exclusively [4]. It is well known [14] that weak solutions are not uniquely determined. We recall the following definition [6]:

Definition 1. A pair of functions $\Omega \ni s \overset{\eta}{\mapsto} \eta(s) \in \mathbb{R}$, $\Omega \ni s \overset{q}{\mapsto} q(s) \in \mathbb{R}$ is called an entropy pair for the conservation law (1) if

1. η is strictly convex, and
2. the fundamental compatibility relation

$$\forall s \in \Omega : \nabla_u \eta(s)^{\mathrm{T}} \nabla_u f(s) = \nabla_u q(s)^{\mathrm{T}} \tag{8}$$

holds. The function η is called entropy while q is called entropy flux.

The compatibility relation (8) follows easily from the quasilinear form of (1) multiplied by $\nabla_u \eta(u)^{\mathrm{T}}$:

$$\partial_t \eta(u) + \nabla_u \eta(u)^{\mathrm{T}} \nabla_u f(u) \partial_x u = 0 \, .$$

and the assumption that entropy is conserved where u is smooth, i.e.:

$$\partial_t \eta(u) + \partial_x q(u) = 0 \, .$$

Examining viscous perturbation $\partial_t u^\delta + \partial_x f(u^\delta) = \delta \partial_x^2 u^\delta$ in the limit $\delta \to 0$ leads to [6]:

Definition 2. A weak solution u is called admissible, if for all entropy pairs (η, q) the entropy inequality

$$\partial_t \eta(u) + \partial_x q(u) \leqq 0 \tag{9}$$

holds in the weak sense.

Remark 1. Instead of considering weak solutions and weak entropy inequalities one may consider the conservation law (1) and the entropy inequality in the space of Radon measures, since, by assumption, $u \in BV_{\mathrm{loc}}(D; \Omega)$. Then

$$\Theta_u := \partial_t \eta(u) + \partial_x q(u) \tag{10}$$

is a Radon measure supported at the discontinuities γ of u. If $B \subset \mathbb{R}^2$ is a Borel set containing exactly one discontinuity of u then the application of the theorem of Gauss-Green-Federer [3] yields

$$\Theta_u(\gamma) = \int_\gamma \{ n_t(\eta(u_{\mathrm{L}}) - \eta(u_{\mathrm{R}})) + n_x(q(u_{\mathrm{L}}) - q(u_{\mathrm{R}})) \} \, dH^1 \tag{11}$$

where $(n_t, n_x)^{\mathrm{T}}$ is the normal to γ, u_{L} and u_R the left and right limit, respectively, and H^1 the one-dimensional Hausdorff measure. Thus, (11) is a Rankine-Hugoniot-like condition for the entropy.

Remark 2. As was pointed out by Sever [13] quite recently, an admissible solution is not necessarily unique even in the case of a genuinely nonlinear system.

An important feature of entropies is their property to transform any hyperbolic system (1) into a symmetric hyperbolic system while not changing the set of solutions. This symmetrization is due to Mock [8]. Let $\Omega \ni s \overset{v}{\mapsto} v(s) = \nabla_u \eta(s) \in \hat{\Omega}$ be the entropy variables and $\hat{\Omega}$ the transformed state space. Then the following theorem is valid.

Theorem 2. *The matrix* $\nabla_v u(v)$ *is positive definite and* $\nabla_v f(u(v))$ *is symmetric. Furthermore* u *is a weak solution of* (1) *if and only if it is weak solution of the symmetric hyperbolic system*

$$\partial_t u(v) + \partial_x \hat{f}(v) = 0 \tag{12}$$

where $\hat{f}(v) := f(u(v))$.

In the sequel we will make extensive use of this symmetrization.

For the numerical solution of systems of conservation laws (1) we consider conservative semi-discrete three-point schemes

$$\frac{du_i(t)}{dt} = -\frac{1}{\Delta x}(h(w,z) - h(z,v)) \tag{13}$$

where $v = u_{i-1}(t)$, $z = u_i(t)$, $w = u_{i+1}(t)$ and $u_i(t) := u(i\Delta x, t)$, $i \in \mathbb{Z}$ on a grid with mesh size $\Delta x > 0$ in space direction. The function h is called the numerical flux and is assumed to be consistent with the flux f in the sense of $\forall s \in \Omega$: $h(s, s) = f(s)$. The discrete solution constitutes a piecewise constant grid function u^Δ by means of

$$u^\Delta(x,t) := u_i(t); \quad t \geqq 0, (i - \tfrac{1}{2})\Delta x < x \leqq (i + \tfrac{1}{2})\Delta x\,. \tag{14}$$

To characterize admissible numerical solutions we define the discrete entropy inequality to be

$$\frac{d\eta(u_i(t))}{dt} \leqq -\frac{1}{\Delta x}(H(w,z) - H(z,v)) \tag{15}$$

with a numerical entropy flux H consistent with the entropy flux q in the sense of $\forall s \in \Omega$: $H(s,s) = q(s)$. A numerical method (13) yielding solutions which fulfil a discrete entropy inequality (15) is called entropy stable. If only equality occurs in (15) the scheme is called entropy conservative. Since the choice of H is by no means obvious once a scheme is given we insist to call entropy stable schemes *entropy stable with respect to the numerical entropy flux H.*

The numerical flux of any three-point scheme can be expressed uniquely in the viscosity form

$$h(w,z) = \tfrac{1}{2}(f(w) + f(z)) - Q(w,z)(w - z) \tag{16}$$

where the matrix $\Omega \times \Omega \ni (w,z) \overset{Q}{\mapsto} Q(w,z) \in \mathbb{R}^{m\times m}$ is the numerical viscosity coefficient (see [18]). Clearly, if $Q \equiv 0$ the resulting flux difference $h(w,z) - h(z,v)$ turns out to be the unstable central difference not exhibiting any dissipative features.

We define now the notion of order of a difference scheme.

Definition 3. A conservative three-point scheme is purely p-th order in space if

$$\frac{1}{\Delta x}(h(w,z) - h(z,v)) = \partial_x f(u)|_{u=z} + \mathcal{O}(\Delta x)^p\,. \tag{17}$$

Obviously only the values $p \in \{0, 1, 2\}$ are possible. Schemes with $p = 0$ are inconsistent and therefore not very interesting. If the simple time stepping

$$\frac{du_i(t)}{dt} = \frac{u_i((n+1)\Delta t) - u_i(n\Delta t)}{\Delta t} + \mathcal{O}(\Delta t), \quad n \in \mathbb{N}_0 \tag{18}$$

is used, the case $p = 1$ covers such successful methods as Godunov's and the Lax-Friedrichs scheme. A satisfying theory of entropy production of such schemes was developed by Tadmor [16, 17], Osher [9] and Osher et al. [10] and later summarized and enlarged by Tadmor and Osher [11]. It is important to note that all these first order schemes satisfying a discrete entropy inequality have the favourable property of being total variation diminishing (TVD) schemes, thus exhibiting nice monotonicity properties. No oscillations will occur before or after shocks.

The remaining interesting cases are methods of purely 2nd order in space. To point out the meaning of Definition 3 we note that the celebrated Lax-Wendroff scheme does not belong to this class. This point will be discussed more detailed in the following section.

2 The order of difference schemes and Merriam's conjecture

The notion of order used in finite difference methods is based on Taylor expansions. The following theorem characterizes the methods of purely 2nd order in space with respect to their numerical viscosity coefficients.

Theorem 3. *A conservative three-point scheme is of purely* 2nd *order in space if and only if for the numerical viscosity coefficient the null consistency*

$$Q(z, z) = 0 \tag{19}$$

as well as the anti-symmetry consistency

$$\nabla_w Q(w, z)|_{w=z} = -\nabla_v Q(z, v)|_{v=z} \tag{20}$$

holds for all $z \in \Omega$.

Proof. Choose the k-th component h_k of the numerical flux function h. Let $w = z + \Delta_1$, $v = z + \Delta_2$. Taylor expansion yields

$$h_k(w, z) = f_k(z) + \Delta_1^{\mathrm{T}} \nabla_w h_k(w, z)|_{w=z} + \tfrac{1}{2} \Delta_1^{\mathrm{T}} \nabla_w^2 h_k(w, z)|_{w=z} \Delta_1 + \mathcal{O}(|\Delta_1|^3)$$

$$h_k(z, v) = f_k(z) + \Delta_2^{\mathrm{T}} \nabla_v h_k(z, v)|_{v=z} + \tfrac{1}{2} \Delta_2^{\mathrm{T}} \nabla_v^2 h_k(z, v)|_{v=z} \Delta_2 + \mathcal{O}(|\Delta_2)|^3) .$$

The derivatives of the flux function are given by

$$\nabla_w h_k(w, z)|_{w=z} = \tfrac{1}{2} \nabla_u f_k(z) - Q_k(z, z)$$

$$\nabla_u h_k(z, v)|_{v=z} = \tfrac{1}{2} \nabla_u f_k(z) + Q_k(z, z)$$

$$\nabla_w^2 h_k(w, z)|_{w=z} = \tfrac{1}{2} \nabla_u^2 f_k(z) - \nabla_w Q_k(w, z)|_{w=z} - (\nabla_w Q_k(w, z)|_{w=z})^{\mathrm{T}}$$

$$\nabla_v^2 h_k(z, v)|_{v=z} = \tfrac{1}{2} \nabla_u^2 f_k(z) + \nabla_v Q_k(z, v)|_{v=z} + (\nabla_v Q_k(z, v)|_{v=z})^{\mathrm{T}} ,$$

where Q_k denotes the k-th row in the matrix of the numerical viscosity coefficient. Expansion of the increments Δ_1, Δ_2 leads to

$$\begin{aligned}\Delta_1 &= w - z = u_{i+1} - u_i \\ &= \Delta x \partial_x u|_{x=x_i} + \frac{(\Delta x)^2}{2} \partial_x^2 u|_{x=x_i} + \mathcal{O}(\Delta x)^3 \\ \Delta_2 &= v - z = u_{i-1} - u_i \\ &= -\Delta x \partial_x u|_{x=x_i} + \frac{(\Delta x)^2}{2} \partial_x^2 u|_{x=x_i} + \mathcal{O}(\Delta x)^3 .\end{aligned}$$

Insertion of these terms yields

$$\begin{aligned}h_k(w, z) = f_k(z) &+ \tfrac{1}{2}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) - \Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &+ \tfrac{1}{4}(\Delta x)^2 (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) - \tfrac{1}{2}(\Delta x)^2 (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &+ \tfrac{1}{4}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u^2 f_k(z) \Delta x \partial_x u|_{x=x_i} \\ &- \tfrac{1}{2}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} T_1 \Delta x \partial_x u|_{x=x_i} + \mathcal{O}(\Delta x)^3 \\ h_k(z, v) = f_k(z) &- \tfrac{1}{2}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) - \Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &+ \tfrac{1}{4}(\Delta x)^2 (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) + \tfrac{1}{2}(\Delta x)^2 (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &+ \tfrac{1}{4}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u^2 f_k(z) \Delta x \partial_x u|_{x=x_i} \\ &+ \tfrac{1}{2}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} T_2 \Delta x \partial_x u|_{x=x_i} + \mathcal{O}(\Delta x)^3 ,\end{aligned}$$

where

$$\begin{aligned}T_1 &:= \nabla_w Q_k(w, z)|_{w=z} + (\nabla_w Q_k(w, z)|_{w=z})^{\mathrm{T}} =: T_{01} + T_{01}^{\mathrm{T}} \\ T_2 &:= \nabla_v Q_k(z, v)|_{v=z} + (\nabla_v Q_k(z, v)|_{v=z})^{\mathrm{T}} =: T_{02} + T_{02}^{\mathrm{T}} .\end{aligned}$$

Therefore the difference of the numerical flux can be calculated to give

$$\begin{aligned}h_k(w, z) - h_k(z, v) &= \Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) - (\Delta x)^2 (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &\quad - (\Delta x)^2 (\partial_x u|_{x=x_i})^{\mathrm{T}} [T_1 + T_2] \partial_x u|_{x=x_i} + \mathcal{O}(\Delta x)^3 .\end{aligned}$$

Division by Δx and insertion of $(\partial_x u|_{x=x_i})^{\mathrm{T}} \nabla_u f_k(z) = \partial_x f_k(z)$ leads to

$$\begin{aligned}(21)\quad \frac{1}{\Delta x}(h_k(w, z) - h_k(z, v)) &= \partial_x f_k(z) - \Delta x(\partial_x^2 u|_{x=x_i})^{\mathrm{T}} Q_k(z, z) \\ &\quad - \tfrac{1}{2}\Delta x(\partial_x u|_{x=x_i})^{\mathrm{T}} [T_1 + T_2] \partial_x u|_{x=x_i} + \mathcal{O}(\Delta x)^2 .\end{aligned}$$

Writing $(\partial_x u)^{\mathrm{T}} [T_1 + T_2] \partial_x u =: \langle \partial_x u, [T_1 + T_2] \partial_x u \rangle$ it follows that

$$\begin{aligned}\langle \partial_x u, [T_1 + T_2] \partial_x u \rangle &= \langle \partial_x u, T_1 \partial_x u \rangle + \langle \partial_x u, T_2 \partial_x u \rangle \\ &= \langle \partial_x u, T_{01} \partial_x u \rangle + \langle \partial_x u, T_{01}^{\mathrm{T}} \partial_x u \rangle \\ &\quad + \langle \partial_x u, T_{02} \partial_x u \rangle + \langle \partial_x u, T_{02}^{\mathrm{T}} \partial_x u \rangle\end{aligned}$$

and since for any $a \in \mathbb{R}^m$ and $A \in \mathbb{R}^{m \times m}$ always $\langle a, Aa \rangle = \langle a, A^{\mathrm{T}} a \rangle$, the expression $\langle \partial_x u, [T_1 + T_2] \partial_x u \rangle = 2 \langle \partial_x u, [T_{01} + T_{02}] \partial_x u \rangle$ holds. Thus (21) can be expressed as

$$\frac{1}{\Delta x}(h_k(w, z) - h_k(z, v)) = \partial_x f_k(z) - \Delta x (\partial_x^2 u|_{x=x_i})^{\mathrm{T}} Q_k(z, z)$$
$$- \Delta x (\partial_x u|_{x=x_i})^{\mathrm{T}} [T_{01} + T_{02}] \partial_x u(x)|_{x=x_i} + \mathcal{O}(\Delta x)^2 .$$

If the method is of purely 2nd order in space then $Q_k(z, z)$ and the sum enclosed in square brackets have to vanish for all k. If on the other hand these terms vanish, the method is of purely 2nd order space. □

Remark 3. The Lax-Wendroff method is based on the Taylor expansion

$$u(x, t + \Delta t) = u(x, t) + \Delta t \partial_t u(x, t) + \frac{(\Delta t)^2}{2} \partial_t^2 u(x, t) + \mathcal{O}(\Delta t)^3 , \tag{22}$$

where the time derivatives are replaced by space derivatives using the conservation law. Central differencing of the resulting space derivatives yields the final formula defined by the numerical viscosity coefficient $Q^{\mathrm{LW}}(w, z) = \frac{\lambda}{4}((\nabla_u f(w))^2 + (\nabla_u f(z))^2)$, where $\lambda = \frac{\Delta t}{\Delta x}$. Separating the time stepping (18) leads to

$$\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \partial_t u(x, t) + \frac{(\Delta t)}{2} \partial_t^2 u(x, t) + \mathcal{O}(\Delta t)^2$$

and the remaining Δt is the reason for the exclusion of this method from the class of methods of purely 2nd order in space.

There is a relation between the notion of order and some properties of numerical solutions of finite difference schemes. As was shown by Harten [5] a three-point method which does not produce oscillations (a TVD scheme) is necessarily first order accurate. This implies that solutions of second-order three-point schemes usually exhibit oscillations before or after shocks and this is in fact observed in practice.

In [7] Merriam argued that there may also be an intimate relation between monotonicity properties (monotone or TVD schemes) and entropy production in the sense of the discrete entropy inequality (15). The crucial point in all discussions concerning discrete entropy inequalities is the choice of the numerical entropy flux H. Since $\forall s \in \Omega : H(s, s) = q(s)$ is the only a priori requirement we are led to the following dilemma:

Every numerical entropy flux taken from the set $\{H : H(w, z) = \frac{1}{2}(q(w) + q(z)) - K(w, z), K(s, s) = 0 \forall s \in \Omega\}$ *is a consistent numerical entropy flux for any three-point method.*

Merriam discusses schemes of the form

$$\frac{du_i(t)}{dt} = -\frac{1}{\Delta x}(f(u_{i+\frac{1}{2}}) - f(u_{i-\frac{1}{2}}))$$

where $u_{i+\frac{1}{2}} = \phi(w, z)$, $u_{i-\frac{1}{2}} = \phi(z, v)$ are interpolants at cell boundaries. He defines a numerical entropy flux to be proper, if the same interpolants are used to build the discrete entropy inequality, i.e.

$$\frac{d\eta(u_i(t))}{dt} \leqq -\frac{1}{\Delta x}(q(u_{i+\frac{1}{2}}) - q(u_{i-\frac{1}{2}}))\,.$$

Due to his experiences with second order schemes he formulated the following

Conjecture 1 (Merriam). *If the solutions of a second-order three-point scheme satisfy the discrete entropy inequality with a proper numerical entropy flux, then these solutions exhibit nice monotonicity properties.*

As Merriam we are also not able to prove this conjecture, but we shall prove a related theorem. We show that no three-point method which is purely 2nd order in space (and thus exhibits oscillations) can satisfy a discrete entropy inequality in which a proper numerical entropy flux is used.

3 Entropy and three-point schemes

As already mentioned there is a well known theory of entropy production of first order methods. It turns out that this theory allows statements which are quite similar to Merriam's conjecture. Lax [6] was the first to prove entropy stability of a scheme applied to a system of conservation laws when he showed that the Lax-Friedrichs scheme

$$h^{\mathrm{LF}}(w, z) = \tfrac{1}{2}(f(w) + f(z)) - \frac{1}{2\lambda}(w - z) \tag{23}$$

satisfies a discrete entropy inequality with respect to the numerical entropy flux

$$H^{\mathrm{LF}}(w, z) = \tfrac{1}{2}(q(w) + q(z)) - \frac{1}{2\lambda}(\eta(w) - \eta(z))\,. \tag{24}$$

Note that this numerical entropy flux is choosen quite close to what Merriam called a proper flux.

In the case of the second order Lax-Wendroff method there is a negative result by Schonbek [12] dating back to 1985:

Theorem 4 (Schonbek). *The Lax-Wendroff method is not entropy stable, regardless what numerical entropy flux is used.*

As described above the Lax-Wendroff method is not of purely 2nd order in space, since it is based on a Taylor expansion in time. Therefore $Q(s, s) \neq 0$ in general. Since Schonbeck extended her proof to the case where the numerical flux of the Lax-Wendroff method is perturbed by arbitrary $(\Delta x)^2$ terms, it is also easily extendable to all three-point second-order methods with $Q(s, s) \neq 0$. Moreover, Böing and Jeltsch [1] extended Schonbek's theorem to the case of $(2k + 1)$-point Lax-Wendroff-type schemes, $k \in \mathbb{N}$, showing that such a method is only first order accurate if a discrete entropy inequality is required to hold.

The interesting question whether there are methods of purely 2nd order in space which are entropy stable with respect to some numerical entropy flux was answered by Tadmor [18].

3.1 *The Tadmor theory*

We now switch to entropy variables leading to the symmetric system

$$\partial_t u(v) + \partial_x \hat{f}(v) = 0 \tag{25}$$

where $\hat{f}(v) := f(u(v))$. The transformed entropy inequality then reads as

$$\partial_t \hat{\eta}(v) + \partial_x \hat{q}(v) \leqq 0 \tag{26}$$

where $\hat{\eta}(v) := \eta(u(v))$ and $\hat{q}(v) := q(u(v))$. Three-point schemes now take the form

$$\frac{d}{dt} u(v_i) = -\frac{1}{\Delta x}(\hat{h}(\hat{w}, \hat{z}) - \hat{h}(\hat{z}, \hat{v})) \tag{27}$$

$$\hat{h}(\hat{w}, \hat{z}) = \tfrac{1}{2}(\hat{f}(\hat{w}) + \hat{f}(\hat{z})) - \hat{Q}(\hat{w}, \hat{z})(\hat{w} - \hat{z}) \tag{28}$$

and discrete entropy inequalities are written as

$$\frac{d}{dt}\hat{\eta}(v_i) + \frac{1}{\Delta x}(\hat{H}(\hat{w}, \hat{z}) - \hat{H}(\hat{z}, \hat{v})) \leqq 0 \tag{29}$$

$$\forall s \in \hat{\Omega} : \hat{H}(s, s) = \hat{q}(s) .$$

The following theorem summarizes the results in [18].

Theorem 5 (Tadmor). *Let a three-point scheme be given, defined by its numerical viscosity coefficient $\hat{Q}^1$. This method is entropy stable with respect to the numerical entropy flux*

$$\hat{H}^{\bullet}(\hat{w}, \hat{z}) := \tfrac{1}{2}(\hat{q}(\hat{w}) + \hat{q}(\hat{z})) - \tfrac{1}{2}(\hat{w}^{\mathrm{T}}\hat{f}(\hat{w}) + \hat{z}^{\mathrm{T}}\hat{f}(\hat{z})) + \tfrac{1}{2}(\hat{w} + \hat{z})^{\mathrm{T}}[\hat{h}^1(\hat{w}, \hat{z}) - \tfrac{1}{2}(\hat{Q}^1(\hat{w}, \hat{z}) - \hat{Q}^*(\hat{w}, \hat{z}))(\hat{w} - \hat{z})] \tag{30}$$

if and only if

$$(\hat{w} - \hat{z})^{\mathrm{T}}(\hat{Q}^1(\hat{w}, \hat{z}) - \hat{Q}^*(\hat{w}, \hat{z}))(\hat{w} - \hat{z}) > 0 \quad (\hat{w} - \hat{z}) \neq 0 . \tag{31}$$

Here, $\hat{Q}^*$ is the numerical viscosity coefficient

$$\hat{Q}^*(\hat{w}, \hat{z}) := \tfrac{1}{2}\int_0^1 (2\xi - 1)\nabla_v \hat{f}(\hat{z} + \xi(\hat{w} - \hat{z}))\, d\xi , \tag{32}$$

of a method called Tadmor scheme. This scheme is entropy conservative with respect to the numerical entropy flux

$$\hat{H}^*(\hat{w}, \hat{z}) := \tfrac{1}{2}(\hat{q}(\hat{w}) + \hat{q}(\hat{z})) + \tfrac{1}{2}(\hat{w} - \hat{z})^{\mathrm{T}}\hat{h}(\hat{w}, \hat{z}) - \tfrac{1}{2}(\hat{w}^{\mathrm{T}}\hat{f}(\hat{w}) + \hat{z}^{\mathrm{T}}\hat{f}(\hat{z})) . \tag{33}$$

Remark 4. Note that in the case $\hat{Q}^1 = \hat{Q}^*$ the numerical entropy flux $\hat{H}^\bullet$ reduces to $\hat{H}^*$. Both numerical entropy fluxes are consistent but by no means proper in any sense similar to Merriam's requirements. It is easily seen that Tadmor's scheme is of purely 2nd order in space.

A scheme fulfilling (31) is said to contain more numerical viscosity than the Tadmor scheme.

3.2 The discrete dissipation function

Since $\frac{d\eta_i}{dt} = (\nabla_u \eta(z))^{\mathrm{T}} \frac{du_i}{dt}$ the definition of a three-point scheme yields

$$\frac{d\eta_i}{dt} = -\frac{(\nabla_u \eta(z))^{\mathrm{T}}}{\Delta x}(h(w, z) - h(z, v)) .$$

Thus, if a discrete entropy inequality is required to hold we conclude

$$-(\nabla_u \eta(z))^{\mathrm{T}}(h(w, z) - h(z, v)) \leqq -(H(w, z) - H(z, v)) .$$

To measure the entropy production we therefore use

Definition 4. The mapping

$$\Omega \times \Omega \times \Omega \ni (v, z, w) \overset{\Gamma}{\mapsto} \Gamma(v, z, w) \in \mathbb{R}$$

defined by

$$\Gamma(v, z, w) := H(w, z) - H(z, v) - (\nabla_u \eta(z))^{\mathrm{T}}(h(w, z) - h(z, v)) \tag{34}$$

is called the discrete dissipation function. Entropy stable schemes are characterized by $\Gamma \leqq 0$, entropy conservative ones by $\Gamma \equiv 0$.

If the discrete dissipation function exhibits a maximum at $(v, z, w) = (z, z, z)$ the corresponding scheme is entropy stable (at least in a neighborhood of (z, z, z)) and vice versa. Therefore we conclude

Proposition 1. *Let* $h \in [C^2](\Omega \times \Omega, \mathbb{R}^n)$, $H \in [C^2](\Omega \times \Omega, \mathbb{R})$ *and* (z, z, z) *root of* Γ *in a neighborhood* $\mathscr{U}(z, z, z) \subset \Omega \times \Omega \times \Omega$. *If*

$$\begin{bmatrix} \nabla_v \Gamma \\ \nabla_w \Gamma \end{bmatrix}(v, z, w)\big|_{v=w=z} = 0$$

and if the Hessian matrix

$$\nabla^2_{v,w}\Gamma(v, z, w)\big|_{v=w=z} = \begin{bmatrix} [\partial_{v_i}\partial_{v_j}\Gamma]_{i,j=1(1)m} & [\partial_{v_i}\partial_{w_j}\Gamma]_{i,j=1(1)m} \\ [\partial_{w_i}\partial_{v_j}\Gamma]_{i,j=1(1)m} & [\partial_{w_i}\partial_{w_j}\Gamma]_{i,j=1(1)m} \end{bmatrix}\Bigg|_{v=w=z}$$

is negative definite, then the method defined by the numerical flux h is entropy stable. If the Hessian matrix is indefinite, then the method certainly is not entropy stable.

3.3 C-consistency

Since entropy stability can be characterized by maxima of the discrete dissipation function at constant states the value (z, z, z) should be a critical point of Γ. As necessary conditions we identify

$$\nabla_w \Gamma(v, z, w)|_{v=w=z} = -((\nabla_u \eta(z))^T \nabla_w h(w, z) - \nabla_w H(w, z))|_{w=z} \stackrel{!}{=} 0$$

and the similar expression for the v-derivative. If on the other hand consistency of a numerical entropy flux with the compatibility condition (8) is required, we are led to

Definition 5. A numerical entropy flux H satisfying the conditions

(35) $$\forall s \in \Omega : (\nabla_u \eta(s))^T \nabla_v h(s, v)|_{v=s} = \nabla_v H(s, v)|_{v=s}$$

(36) $$\forall s \in \Omega : (\nabla_u \eta(s))^T \nabla_w h(w, s)|_{w=s} = \nabla_w H(w, s)|_{w=s}$$

is called c-consistent (compatibility consistent) with respect to h.

Comparing this consistency requirement with the necessary condition for Γ to exhibit a maximum at constant states we conclude

Proposition 2. *A numerical entropy flux H is c-consistent with respect to h if and only if (z, z, z) is critical point of the discrete dissipation function Γ.*

Furthermore the rate of entropy production is already fixed with c-consistent numerical entropy fluxes:

Proposition 3. *Let H be a c-consistent numerical entropy flux. Then the expression*

(37) $$\Gamma(v, z, w) = \mathcal{O}(|w - z|^2 + |z - v|^2)\,,$$

holds.

The proof of this lemma follows directly by means of Taylor expansions. An inspection of the numerical entropy fluxes $\hat{H}^{\bullet}$ and $\hat{H}^*$ used in the Tadmor theory shows that both are c-consistent. But there is another characterization of proper numerical entropy fluxes which we shall discuss in the sequel.

3.4 Lax-consistency

Since three-point schemes are uniquely determined by their numerical viscosity coefficients it seems natural to carry the viscosity form over to the definition of a proper numerical entropy flux. This corresponds to the selection of the numerical entropy flux used by Lax to prove the entropy stability of the Lax-Friedrichs scheme (compare with (24)). Thus, a proper numerical entropy flux should have the form

(38) $$H(w, z) = \tfrac{1}{2}(q(w) + q(z)) - \tilde{Q}(w, z)(\eta(w) - \eta(z))$$

with a mapping $\Omega \times \Omega \ni (w, z) \overset{\tilde{Q}}{\mapsto} \mathbb{R}$ to be specified. In order to be c-consistent such a numerical entropy flux has to fulfill the condition

$$\nabla_u \eta(z) \tilde{Q}(z, z) = (\nabla_u \eta(z))^T Q(z, z) \tag{39}$$

which on the left is a vector times a scalar while on the right we have a vector times matrix operation. Since the numerical entropy flux Lax used in the case of the Lax-Friedrichs scheme satisfies conditions (38) and (39) we give the following definition.

Definition 6. A numerical entropy flux is called Lax-consistent if it can be written in the form (38) with a dissipation coefficient $\tilde{Q}$. If the dissipation coefficient satisfies condition (39) the numerical entropy flux is called Lax-c-consistent.

Remark 5. In [15] the following suggestion is made to construct Lax-consistent numerical entropy fluxes: Let $\mathbf{1} \in \mathbb{R}^m$. By means of

$$A(u) := \eta(u)\, \mathbf{1}$$
$$B(u) := q(u)\, \mathbf{1}$$

an entropy vector and an entropy flux vector are defined. The system

$$\partial_t A(u) + \partial_x B(u) \leqq 0 \tag{40}$$

therefore consists of m identical copies of the entropy inequality. A numerical entropy flux vector Ψ is defined to be

$$\Psi(w, z) = \tfrac{1}{2}(B(w) + B(z)) - \tilde{\mathcal{Q}}(w, z)(A(w) - A(z)) \tag{41}$$

where $\tilde{\mathcal{Q}}$ is a matrix. By means of this notion we are able to give the following recipe: Let the matrix $\tilde{\mathcal{Q}}$ be constructed from Q by means of the substitution rule

$$\forall i, j = 1(1)m : \tilde{\mathcal{Q}}_{ij} = Q_{ij} \begin{pmatrix} \text{const.} \mapsto \text{const.} \\ \text{id}(\cdot) \mapsto \eta(\cdot) \\ f(\cdot) \mapsto q(\cdot) \\ \partial_{u_k}^{p_1} \partial_{u_l}^{p_2} f_s(\cdot) \mapsto \partial_{u_k}^{p_1} \partial_{u_l}^{p_2} q(\cdot) \end{pmatrix}$$

where $p_1, p_2 \in \mathbb{N}$; $k, l, s \in \{1, \ldots, m\}$. (Take the elements of the numerical viscosity coefficient and replace solution values by entropy values, fluxes by entropy fluxes and derivatives of fluxes by the corresponding derivatives of the entropy flux).

The required scalar dissipation coefficient is then constructed by means of

$$\frac{1}{m} (\mathbf{1})^T \Psi(w, z) =: H(w, z) .$$

In the representation

$$H(w, z) = \tfrac{1}{2}(q(w) + q(z)) - \tilde{Q}(w, z)(w - z)$$

the dissipation coefficient is therefore given by

$$\tilde{Q}(w, z) = \frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{m} \tilde{\mathcal{Q}}_{ij}(w, z) . \tag{42}$$

Here, $\tilde{\mathcal{Q}}_{ij}$ are the elements of the matrix $\tilde{\mathcal{Q}}$.

3.5 Order and discrete entropy

With the notion of Lax-consistent numerical entropy fluxes the discretization of the flux functions are carried over to the discretization of the entropy fluxes. Therefore it would seem natural if Lax-consistent numerical entropy fluxes would exhibit the same order of accuracy as the scheme itself.

Definition 7. Let a three-point scheme defined by the numerical flux h be of purely 2nd order in space. A numerical entropy flux H is called order preserving, if

$$\frac{1}{\Delta x}(H(w, z) - H(z, v)) = \partial_x q(z) + \mathcal{O}(\Delta x)^2 .$$

The following theorem indicates the importance of Lax-consistent numerical entropy fluxes.

Theorem 6. *Let a three-point scheme defined by the numerical flux h be of purely 2nd order in space. If the numerical entropy flux H is Lax-c-consistent with respect to h then H is order preserving.*

Proof. In the definition of c-consistency (35) the k-th ($1 \leqq k \leqq m$) components are

(43) $$\sum_{i=1}^{m} \partial_{u_i}\eta(s)\partial_{w_k}h_i(w, s)|_{w=s} = \partial_{w_k}H(w, s)|_{w=s}$$

(44) $$\sum_{i=1}^{m} \partial_{u_i}\eta(s)\partial_{v_k}h_i(s, v)|_{v=s} = \partial_{v_k}H(s, v)|_{v=s} .$$

From the i-th components of the viscosity forms

$$h_i(w, z) = \tfrac{1}{2}(f_i(w) + f_i(z)) - \sum_{l=1}^{m} Q_{il}(w, z)(w_l - z_l)$$

$$h_i(z, v) = \tfrac{1}{2}(f_i(z) + f_i(v)) - \sum_{l=1}^{m} Q_{il}(z, v)(z_l - v_l)$$

with $(Q_{ij}(w, z))_{i,j=1(1)m} = Q(w, z)$ and $(Q_{ij}(z, v))_{i,j=1(1)m} = Q(z, v)$ we conclude

$$\partial_{w_k}h_i(w, s)|_{w=s} = \tfrac{1}{2}\partial_{u_k}f_i(s) - Q_{ik}(s, s)$$

$$\partial_{v_k}h_i(s, v)|_{v=s} = \tfrac{1}{2}\partial_{u_k}f_i(s) + Q_{ik}(s, s) .$$

Since H is Lax-consistent by assumption the representation

$$H(w, z) = \tfrac{1}{2}(q(w) + q(z)) - \tilde{Q}(w, z)(\eta(w) - \eta(z))$$

$$H(z, v) = \tfrac{1}{2}(q(z) + q(v)) - \tilde{Q}(z, v)(\eta(z) - \eta(v))$$

exists from which

$$\partial_{w_k} H(w,s)|_{w=s} = \tfrac{1}{2}\partial_{u_k} q(s) - \partial_{u_k}\eta(s)\tilde{Q}(s,s)$$
$$\partial_{v_k} H(s,v)|_{v=s} = \tfrac{1}{2}\partial_{u_k} q(s) + \partial_{u_k}\eta(s)\tilde{Q}(s,s)$$

follows. The difference of the conditions (43) and (44) reads as

$$\sum_{i=1}^{m} \partial_{u_i}\eta(s)(\partial_{w_k} h_i(w,s)|_{w=s} - \partial_{v_k} h_i(s,v)|_{v=s}) = \partial_{w_k} H(w,s)|_{w=s} - \partial_{v_k} H(s,v)|_{v=s}\,,$$

which, after insertion of the derivatives, leads to

$$\beta_k(s) := -2\sum_{i=1}^{m} \partial_{u_i}\eta(s) Q_{ik}(s,s) + 2\partial_{u_k}\eta(s)\tilde{Q}(s,s) = 0\,.$$

Consider $\nabla_s \beta_k(s)$:

$$\text{(45)}\qquad \nabla_s\beta_k(s) = -2\sum_{i=1}^{m} \partial_{u_i}(\nabla_u \eta(s)) Q_{ik}(s,s) - 2\sum_{i=1}^{m} \partial_{u_i}\eta(s)\nabla_s Q_{ik}(s,s)$$
$$+ 2\partial_{u_k}(\nabla_u\eta(s))\tilde{Q}(s,s) + 2\partial_{u_k}\eta(s)\nabla_s\tilde{Q}(s,s) = 0\,.$$

Since $\nabla_s Q_{ik}(s,s) = \nabla_w Q_{ik}(w,s)|_{w=s} + \nabla_v Q_{ik}(z,v)|_{v=s}$ and $\nabla_s \tilde{Q}(s,s) = \nabla_w \tilde{Q}(w,s)|_{w=s} + \nabla_v \tilde{Q}(s,v)|_{v=s}$ it follows

$$\text{(46)}\qquad -2\partial_{u_k}(s)(\nabla_w \tilde{Q}(w,s)|_{w=s} + \nabla_v \tilde{Q}(s,v)_{v=s}$$
$$= -2\sum_{i=1}^{m} \partial_{u_i}(\nabla_u\eta(s))Q_{ik}(s,s) + 2\partial_{u_k}\,(\nabla_u\eta(s))\tilde{Q}(s,s)$$
$$-2\sum_{i=1}^{m} \partial_{u_i}\eta(s)(\nabla_w Q_{ik}(w,s)|_{w=s}$$
$$\text{(47)}\qquad + \nabla_v Q_{ik}(s,v)|_{v=s})\,.$$

Since the scheme under consideration was assumed to be of purely 2nd order in space it follows from Theorem 3 that the null consistency (19) as well as the antisymmetric consistency (20) of the numerical viscosity coefficient holds. Since the numerical entropy flux was assumed to be Lax-c-consistent it follows from condition (39) together with the null consistency (19) that $\tilde{Q}(s,s) = 0$. Therefore (46) boils down to

$$2\partial_{u_k}\eta(s)(\nabla_w\tilde{Q}(w,s)|_{w=s} + \nabla_v\tilde{Q}(s,v)|_{v=s}) = 0$$

showing the antisymmetric consistency

$$\nabla_w\tilde{Q}(w,s)|_{w=s} = -\nabla_v\tilde{Q}(s,v)|_{v=s}$$

of the dissipation coefficient. Following Theorem 3 we conclude

$$\frac{1}{\Delta x}(H(w,z) - H(z,v)) = \partial_x q(z) + \mathcal{O}(\Delta x)^2$$

and thus H is order preserving. □

In order to be Lax-consistent a numerical entropy flux has to satisfy the condition (39). In the scalar case this means $\tilde{Q}(z, z) = Q(z, z)$. Looking again at the numerical entropy fluxes used in the Tadmor theory we now show that $\hat{H}^*$ defined in (33) is not Lax-consistent in the scalar case. Without loss of generality assume that $\hat{z} = 0$ and $\hat{q}(0) = 0$. Then (33) reads as

$$\hat{H}^*(\hat{w}, 0) = \tfrac{1}{2}\,\hat{q}(\hat{w}) + \tfrac{1}{2}\,\hat{w}\hat{h}(\hat{w}, 0) - \tfrac{1}{2}(\hat{w}\hat{f}(\hat{w}))\,.$$

Assuming this numerical entropy flux to be a proper one the representation (38) compared with $\hat{H}^*$ yields

$$\tilde{\hat{Q}}(\hat{w}, 0) = \frac{\frac{1}{2}\hat{w}\hat{f}(\hat{w}) - \frac{1}{2}\hat{w}\hat{h}(\hat{w}, 0)}{\hat{\eta}(\hat{w})}\,.$$

Let now be $\hat{\eta}(s) = \frac{1}{2}s^2$. Then $\tilde{\hat{Q}}(\hat{w}, 0) = \frac{1}{\hat{w}}(\hat{f}(\hat{w}) - \hat{h}(\hat{w}, 0))$ and application of the Bernoulli l'Hospital rule shows $\tilde{\hat{Q}}(0, 0) = \nabla_u \hat{f}(0)$ and thus $\tilde{\hat{Q}}(0, 0) \neq \hat{Q}(0, 0) = 0$. Therefore this numerical entropy flux is not Lax-consistent. The argument in the vector case is similar.

4 The entropy barrier

We examine now the behavior of general methods of purely 2nd order in space with respect to Lax-c-consistent numerical entropy fluxes. The following considerations are based on the use of the entropy variables already defined. Following Theorem 1 there is a parametrization of genuinely nonlinear k-th characteristic wave fields. On such a wave field we fix $\hat{z} \in \hat{\Omega}$. The parametrization is used for the left state $\hat{v}$ as well as for the right state $\hat{w}$ and is given by

(48) $$\mathbb{R} \supset [0, a_1] \ni \varepsilon \overset{\hat{v}}{\mapsto} \hat{v}(\varepsilon)$$

with

(49) $$\hat{v}(0) = \hat{z}$$

(50) $$\frac{d}{d\varepsilon}\,\hat{v}(0) = r_k(\hat{z})$$

and

(51) $$\mathbb{R} \supset [0, a_2] \ni \delta \overset{\hat{w}}{\mapsto} \hat{w}(\delta)$$

with

(52) $$\hat{w}(0) = \hat{z}$$

(53) $$\frac{d}{d\delta}\,\hat{w}(0) = r_k(\hat{z})$$

for sufficiently small $a_1 > 0$, $a_2 > 0$. Let the parametrized discrete dissipation function be the mapping

(54) $$\hat{\Gamma}(\varepsilon, \delta) := \Gamma(\hat{v}(\varepsilon), \hat{z}, \hat{w}(\delta))\,.$$

Without proof we state two Propositions concerning the derivatives of the parametrized dissipation function, numerical flux functions and numerical entropy fluxes. Both proofs are straight forward standard calculations.

Proposition 4. *The derivatives of the parametrized dissipation function* $\acute{\Gamma}$ *at the point* $(\varepsilon, \delta) = (0, 0)$ *are given by*

(55) $$\partial_\varepsilon \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \{(\nabla_{\hat{v}} \Gamma(\hat{v}, \hat{z}, \hat{w}))^{\mathrm{T}} r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}} = \{[-(\nabla_{\hat{v}} \hat{H}(\hat{z}, \hat{v}))^{\mathrm{T}} + \nabla_{\hat{v}} \hat{h}(\hat{z}, \hat{v})\hat{z}] r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}}$$

(56) $$\partial_\delta \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \{(\nabla_{\hat{w}} \Gamma(\hat{v}, \hat{z}, \hat{w}))^{\mathrm{T}} r_k(\hat{z}) = [(\nabla_{\hat{w}} \hat{H}(\hat{w}, \hat{z}))^{\mathrm{T}} - \nabla_{\hat{w}} \hat{h}(\hat{w}, \hat{z})\hat{z}] r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}}$$

(57) $$\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \{r_k^{\mathrm{T}}(\hat{z}) \nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w}) r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}} + \left\{(\nabla_{\hat{v}} \Gamma(\hat{v}, \hat{z}, \hat{w}))^{\mathrm{T}} \frac{d^2}{d\varepsilon^2} \hat{v}(0)\right\}_{\hat{v}=\hat{w}=\hat{z}}$$

(58) $$\partial_\delta^2 \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \left\{r_k^{\mathrm{T}}(\hat{z}) \nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w}) r_k(\hat{z}) + (\nabla_{\hat{w}} \Gamma(\hat{v}, \hat{z}, \hat{w}))^{\mathrm{T}} \frac{d^2}{d\varepsilon^2} \hat{w}(0)\right\}_{\hat{v}=\hat{w}=\hat{z}}$$

(59) $$\partial_\varepsilon \partial_\delta \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = 0 .$$

The Hessian matrices of the parametrized dissipation function at the point $(\hat{v}, \hat{z}, \hat{w}) = (\hat{z}, \hat{z}, \hat{z})$ *read as*

(60) $$\nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} = \left\{-\nabla_{\hat{v}}^2 \hat{H}(\hat{z}, \hat{v}) + \sum_{i=1}^m \hat{z}_i \nabla_{\hat{v}}^2 \hat{h}_i(\hat{z}, \hat{v})\right\}_{\hat{v}=\hat{z}}$$

(61) $$\nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} = \left\{\nabla_{\hat{w}}^2 \hat{H}(\hat{w}, \hat{z}) - \sum_{i=1}^m \hat{z}_i \nabla_{\hat{w}}^2 \hat{h}_i(\hat{w}, \hat{z})\right\}_{\hat{w}=\hat{v}} .$$

Proposition 5. *Let a method of purely 2nd order in space defined by its numerical flux function* $\hat{h}$ *be given. Let the numerical entropy flux* $\hat{H}$ *defined by its dissipation coefficient* $\hat{Q}$ *be Lax-c-consistent. For the i-th* $(1 \leqq i \leqq m)$ *components of the numerical flux the expressions*

(62) $$\nabla_{\hat{v}} \hat{h}_i(\hat{z}, \hat{v})|_{\hat{v}=\hat{z}} = \tfrac{1}{2} \nabla_v \hat{f}_i(\hat{z})$$

(63) $$\nabla_{\hat{v}}^2 \hat{h}_i(\hat{z}, \hat{v})|_{\hat{v}=\hat{z}} = [\{\tfrac{1}{2} \partial_{v_k} \partial_{v_l} \hat{f}_i(\hat{z}) + \partial_{\hat{v}_k} \hat{Q}_{il}(\hat{z}, \hat{v}) + \partial_{\hat{v}_l} \hat{Q}_{ik}(\hat{z}, \hat{v})\}_{\hat{v}=\hat{z}}]_{k,l=1(1)m}$$

(64) $$\nabla_{\hat{w}} \hat{h}_i(\hat{w}, \hat{z})|_{\hat{w}=\hat{z}} = \tfrac{1}{2} \nabla_v \hat{f}_i(\hat{z})$$

(65) $$\nabla_{\hat{w}}^2 \hat{h}_i(\hat{w}, \hat{z})|_{\hat{w}=\hat{z}} = [\{\tfrac{1}{2} \partial_{v_k} \partial_{v_l} \hat{f}_i(\hat{z}) - \partial_{\hat{w}_k} \hat{Q}_{il}(\hat{w}, \hat{z}) + \partial_{\hat{w}_l} \hat{Q}_{ik}(\hat{w}, \hat{z})\}_{\hat{w}=\hat{z}}]_{k,l=1(1)m}$$

are valid and for the numerical entropy flux

(66) $$\nabla_{\hat{v}} \hat{H}(\hat{z}, \hat{v})|_{\hat{v}=\hat{z}} = \tfrac{1}{2} \nabla_v \hat{q}(\hat{z})$$

(67) $$\nabla_{\hat{v}}^2 \hat{H}(\hat{z}, \hat{v})|_{\hat{v}=\hat{z}} = [\{\tfrac{1}{2}\partial_{v_k}\partial_{v_l}\hat{q}(\hat{z}) + \partial_{\hat{v}_l}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_k}\hat{\eta}(\hat{z}) + \partial_{\hat{v}_k}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_l}\hat{\eta}(\hat{z})\}_{\hat{v}=\hat{z}}]_{k,l=1(1)m}$$

(68) $$\nabla_{\hat{w}}\hat{H}(\hat{w}, \hat{z})|_{\hat{w}=\hat{z}} = \tfrac{1}{2}\nabla_v \hat{q}(\hat{z})$$

(69) $$\nabla_{\hat{w}}^2 \hat{H}(\hat{w}, \hat{z})|_{\hat{w}=\hat{z}} = [\{\tfrac{1}{2}\partial_{v_k}\partial_{v_l}\hat{q}(\hat{z}) - \partial_{\hat{w}_l}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_k}\hat{\eta}(\hat{z}) - \partial_{\hat{w}_k}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_l}\hat{\eta}(\hat{z})\}_{\hat{w}=\hat{z}}]_{k,l=1(1)m}$$

hold.

The following Proposition describes consequences of the transformed compatibility condition.

Proposition 6. 1. *The derivatives of the transformed entropy are given by*

(70) $$\forall k = 1(1)m : \partial_{v_k}\hat{\eta}(\hat{z}) = \sum_{j=1}^{m} \hat{z}_j \partial_{v_k} u_j(\hat{z}) .$$

2. *The expression*

(71) $$\nabla_v u = [\nabla_u^2 \eta(u(v))]^{-1} .$$

is valid.

3. *The second derivatives of the transformed entropy flux are*

(72) $$\forall k, l = 1(1)m : \partial_{v_k}\partial_{v_l}\hat{q}(v) = \sum_{j=1}^{m} v_j \partial_{v_k}\partial_{v_l}\hat{f}_j(v) + \partial_{v_k}\hat{f}_l(v) .$$

Proof.
1. If $k = 1(1)m$ then:

$$\partial_{v_k}\hat{\eta}(v) = \partial_{v_k}\eta(u(v)) = (\nabla_u \eta(u(v)))^T \partial_{v_k} u(v) = \sum_{j=1}^{m} v_j^T \partial_{v_k} u_j(v) .$$

2. Due to strict convexity of η the mapping $u \overset{v}{\mapsto} v(u) = \nabla_u \eta(u)$ is invertible. Differentiating the identity $v(u(v)) = \nabla_u \eta(u(v))$ with respect to v yields

$$I = \nabla_u^2 \eta(u(v)) \nabla_v u .$$

3. The k-th component of the transformed compatibility relation is given by

$$\partial_{v_k}\hat{q}(v) = \sum_{j=1}^{m} v_j \partial_{v_k}\hat{f}_j .$$

Differentiating again with respect to a v_l shows (72). □

We are now able to state and prove the following theorem concerning the entropy production of purely 2nd order three-points methods with respect to Lax-c-consistent numerical entropy fluxes.

Theorem 7. *No three-point scheme which is purely 2nd order in space is entropy stable with respect to a Lax-c-consistent numerical entropy flux.*

Proof. If a method under consideration is entropy stable then $\acute{\Gamma}(\varepsilon, \delta)$ exhibits a maximum at the point $(\varepsilon, \delta) = (0, 0)$. Since we are concerned with Lax-c-consistent numerical entropy fluxes this point is also a critical point of $\acute{\Gamma}$ as can be seen from Proposition 2. We prove that

$$\{\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta)\partial_\delta^2 \acute{\Gamma}(\varepsilon, \delta) - (\partial_\varepsilon \partial_\delta \acute{\Gamma}(\varepsilon, \delta))^2\}_{\varepsilon=\delta=0} < 0$$

and

$$\{\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta) + \partial_\delta^2 \acute{\Gamma}(\varepsilon, \delta)\}_{\varepsilon=\delta=0} = 0 \,,$$

such that at $(\varepsilon, \delta) = (0, 0)$ certainly no extremum occurs in $\acute{\Gamma}$.

Since $(\varepsilon, \delta) = (0, 0)$ is critical point of $\acute{\Gamma}$ (or equivalently $(\hat{z}, \hat{z}, \hat{z})$ is critical point of Γ) the second derivatives of the parametrized dissipation function boil down to

$$\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \{r_k(\hat{z})^{\mathrm{T}} \nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w}) r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}} \tag{73}$$

$$\partial_\delta^2 \acute{\Gamma}(\varepsilon, \delta)|_{\varepsilon=\delta=0} = \{r_k(\hat{z})^{\mathrm{T}} \nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w}) r_k(\hat{z})\}_{\hat{v}=\hat{w}=\hat{z}} \,. \tag{74}$$

From (60) and (61) with the help of (62), (65), (67) and (69) we get expressions for the Hessian matrices of the parametrized dissipation function.

$$\nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}=} = \Bigg[\Bigg\{ -\tfrac{1}{2}\partial_{v_k}\partial_{v_l}\hat{q}(\hat{z}) - \partial_{\hat{v}_l}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_k}\hat{\eta}(\hat{z}) - \partial_{\hat{v}_k}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_l}\hat{\eta}(\hat{z}) + \frac{1}{2}\sum_{i=1}^{m} \hat{z}_i \partial_{v_k}\partial_{v_l}\hat{f}_i(\hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{v}_k}\hat{Q}_{il}(\hat{z}, \hat{v}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{v}_l}\hat{Q}_{ik}(\hat{z}, \hat{v}) \Bigg\}_{\hat{v}=\hat{z}}\Bigg]_{k,l=1(1)m} \tag{75}$$

$$\nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} = \Bigg[\Bigg\{ \frac{1}{2}\partial_{v_k}\partial_{v_l}\hat{q}(\hat{z}) - \partial_{\hat{w}_l}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_k}\hat{\eta}(\hat{z}) - \partial_{\hat{w}_k}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_l}\hat{\eta}(\hat{z}) - \frac{1}{2}\sum_{i=1}^{m} \hat{z}_i \partial_{v_k}\partial_{v_l}\hat{f}_i(\hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_k}\hat{Q}_{il}(\hat{w}, \hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_l}\hat{Q}_{ik}(\hat{w}, \hat{z}) \Bigg\}_{\hat{w}=\hat{z}}\Bigg]_{k,l=1(1)m} \tag{76}$$

Insertion of the second derivatives of the transformed entropy flux (72) yields

$$\nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{z}=\hat{w}} = \Bigg[\Bigg\{ -\frac{1}{2}\partial_{v_k}\hat{f}_l(\hat{z}) - \partial_{\hat{v}_l}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_k}\hat{\eta}(\hat{z}) - \partial_{\hat{v}_k}\tilde{\hat{Q}}(\hat{z}, \hat{v})\partial_{v_l}\hat{n}(\hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{v}_k}\hat{Q}_{il}(\hat{z}, \hat{v}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{v}_l}\hat{Q}_{ik}(\hat{z}, \hat{v}) \Bigg\}_{\hat{v}=\hat{z}}\Bigg]_{k,l=1(1)m}$$

$$\nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} = \Bigg[\Bigg\{ \frac{1}{2}\partial_{v_k}\hat{f}_l(\hat{z}) - \partial_{\hat{w}_l}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_k}\hat{\eta}(\hat{z}) - \partial_{\hat{w}_k}\tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_l}\hat{\eta}(\hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_k}\hat{Q}_{il}(\hat{w}, \hat{z}) + \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_l}\hat{Q}_{ik}(\hat{w}, \hat{z}) \Bigg\}_{\hat{w}=\hat{z}}\Bigg]_{k,l=1(1)m}$$

Since the methods are of purely 2nd order in space by assumption, from Theorem 3 follows the antisymmetric consistency of the numerical viscosity coefficient. Since the entropy flux is assumed to be Lax-c-consistent the antisymmetric consistency carries over to the dissipation coefficient by means of Definition 6, yielding

$$\nabla_{\hat{v}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} = -\nabla_{\hat{w}}^2 \Gamma(\hat{v}, \hat{z}, \hat{w})|_{\hat{v}=\hat{w}=\hat{z}} .$$

Let the real number on the right side of (73) be denoted by Ψ. Thus

$$\{\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta)\partial_\delta^2 \acute{\Gamma}(\varepsilon, \delta) - (\partial_\varepsilon \partial_\delta \acute{\Gamma}(\varepsilon, \delta))^2\}_{\varepsilon=\delta=0} = -\Psi^2 \leqq 0 ,$$

since the mixed derivative vanishes according to Proposition 4. Furthermore

$$\{\partial_\varepsilon^2 \acute{\Gamma}(\varepsilon, \delta) + \partial_\delta^2 \acute{\Gamma}(\varepsilon . \delta)\}_{\varepsilon=\delta=0} = 0 ,$$

holds, so that both second derivatives can be never be positive simultaneously. Furthermore we have $\Psi = 0$ if and only if for the Jacobian matrix of the flux function the expression

$$\tfrac{1}{2}[\partial_{v_k} \hat{f}_l(\hat{z})]_{k,l=1(1)m} = \Bigg[\Bigg\{\partial_{\hat{w}_l} \tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_k} \hat{\eta}(\hat{z}) + \partial_{\hat{w}_k} \tilde{\hat{Q}}(\hat{w}, \hat{z})\partial_{v_l} \hat{\eta}(\hat{z})$$
$$- \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_k} \hat{Q}_{il}(\hat{w}, \hat{z}) - \sum_{i=1}^{m} \hat{z}_i \partial_{\hat{w}_l} \hat{Q}_{ik}(\hat{w}, \hat{z})\Bigg\}_{\hat{w}=\hat{z}}\Bigg]_{k,l=1(1)m}$$

is valid. The value of the Jacobian at the point $\hat{z}$ on the left of this equation is independent of any numerical scheme, the right hand side depends on the method used. Therefore in general $\Psi \neq 0$. □

5 Conclusion

The inability of three-point methods of purely 2nd order in space to satisfy a discrete entropy inequality with a proper numerical entropy flux was shown. The requirement of 2nd order accuracy in space by means of a three-point stencil and simultaneous satisfaction of a proper discrete entropy inequality can thus not be met. It is interesting to note that in the case of Lax-Wendroff type methods (in the sense that $Q(z, z) \neq 0$) no entropy stability can be achieved, while in the class of methods of purely 2nd order in space there are numerical entropy fluxes indicating entropy stability (see Tadmor theory). Only if a Lax-c-consistent numerical entropy flux is used these methods are also not entropy stable.

It would be interesting to study second order schemes which use a wider stencil, for example 5-point TVD schemes. Unfortunately the viscosity form is then no longer the unique representation of such schemes so that additional problems occur. If it would be possible to prove that some 5-point TVD methods are entropy stable with respect to a proper discrete entropy inequality we would be much closer to a proof of Merriams conjecture.

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References

1. Böing, H., Jeltsch, R. (1987): On the numerical entropy and explicit difference schemes for conservation laws. Institut für Geometrie und Praktische Mathematik der RWTH Aachen, Bericht Nr. 48
2. DiPerna, R. (1976): Singularities of solutions of nonlinear hyperbolic systems of conservation laws. Arch. Ration. Mech. Anal. **60**, 75–100
3. Federer, H. (1969): Geometric measure theory. Springer, Berlin Heidelberg New York
4. Glimm, J. (1965): Solutions in the large for nonlinear hyperbolic systems of equations. Commun. Pure Appl. Math. **18**, 697–715
5. Harten, A. (1983): High resolution schemes for hyperbolic conservation laws. J. Comput. Phys. **49**, 357–393
6. Lax, P.D. (1971): Shock waves and entropy. In: E.H. Zarantonello, ed., Contributions to Nonlinear Functional Analysis. Academic Press, New York San Francisco London
7. Merriam, M.L. (1989): An entropy based approach to nonlinear stability. NASA Technical Memorandum 101086, NASA Ames
8. Mock, M.S. (1980): Systems of conservation laws of mixed type. J. Differ. Equations **37**, 70–88
9. Osher, S. (1984): Riemann solvers, the entropy condition, and difference approximations. SIAM J. Numer. Anal. **21**, 217–235
10. Osher, S., Chakravarty, S. (1984): High resolution schemes and the entropy condition. SIAM J. Numer. Anal. **21**, 955–984
11. Osher S., Tadmor E. (1988): On the convergence of difference approximations to scalar conservation laws. Math. Comput. **50**, 19–51
12. Schonbek, M.E. (1985): Second order conservative schemes and the entropy condition. Math. Comput. **44**, 31–38
13. Sever, M. (1989): Uniqueness failure for entropy solutions of hyperbolic systems of conservation laws. Commun. Pure Appl. Math. **42**, 173–183
14. Smoller, J. (1983): Shock waves and reaction diffusion equations. Springer Berlin Heidelberg New York
15. Sonar, T. (1991): Nichtlineare Dissipationsmodelle und Entropie-Produktion in finiten Differenzenverfahren. Dissertation, Universität Stuttgart
16. Tadmor, E. (1984): The large-time behaviour of the scalar, genuineley nonlinear Lax-Friedrichs sceme. Math. Comput. **43**, 353–368
17. Tadmor, E. (1984): Numerical viscosity and the entropy condition for conservative difference schemes. Math. Comput. **43**, 369–381
18. Tadmor, E. (1987): The numerical viscosity of entropy stable schemes for systems of conservation laws. I. Math. Comput. **49**, 91–103