

## HIGH-ORDER SCHEMES, ENTROPY INEQUALITIES, AND NONCLASSICAL SHOCKS\*

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**Abstract.** We are concerned with the approximation of undercompressive, regularization-sensitive, *nonclassical solutions* of hyperbolic systems of conservation laws by high-order accurate, conservative, and semidiscrete finite difference schemes. Nonclassical shock waves can be generated by diffusive and dispersive terms kept in balance. Particular attention is given here to a class of systems of conservation laws including the scalar equations and the system of nonlinear elasticity and to linear diffusion and dispersion in either the conservative or the entropy variables.

First, we investigate the existence and the properties of *entropy conservative* schemes—a notion due to Tadmor [*Math. Comp.*, 49 (1987), pp. 91–103]. In particular we exhibit a new five-point scheme which is *third-order* accurate, at least.

Second, we study a class of *entropy stable* and *high-order accurate* schemes satisfying a single *cell entropy inequality*. They are built from any high-order entropy conservative scheme by adding to it a mesh-independent, numerical viscosity, which preserves the order of accuracy of the base scheme. These schemes can only converge to solutions of the system of conservation laws satisfying the entropy inequality. These entropy stable schemes exhibit mild oscillations near shocks and, interestingly, may converge to classical or nonclassical entropy solutions, depending on the sign of their dispersion coefficient.

Then, based on a third-order, entropy conservative scheme, we propose a general scheme for the numerical computation of nonclassical shocks. Importantly, our scheme satisfies a cell entropy inequality. Following Hayes and LeFloch [*SIAM J. Numer. Anal.*, 35 (1998), pp. 2169–2194], we determine numerically the *kinetic function* which uniquely characterizes the dynamics of nonclassical shocks for each regularization of the conservation laws. Our results compare favorably with previous analytical and numerical results.

Finally, we prove that there exists no fully discrete and entropy conservative scheme and we investigate the entropy stability of a class of fully discrete, Lax–Wendroff type schemes.

**Key words.** hyperbolic, conservation law, entropy, difference scheme, shock wave, nonclassical, diffusion, dispersion

**AMS subject classifications.** 35L65, 65M12, 76L05

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**1. Introduction.** We are interested in discontinuous solutions of hyperbolic systems of conservation laws

$$(1.1) \quad \partial_t u + \partial_x f(u) = 0, \quad u(x, t) \in \mathbb{R}^N,$$

and their approximation by high-order accurate, conservative, and semidiscrete finite difference schemes. We consider systems of conservation laws endowed with an entropy-entropy flux pair  $(U, F) : \mathbb{R}^N \rightarrow \mathbb{R}^2$ . As is customary, the weak solutions of (1.1) are constrained by the entropy inequality

$$(1.2) \quad \partial_t U(u) + \partial_x F(u) \leq 0.$$

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By definition,  $\nabla F(u) = \nabla U(u) \cdot Df(u)$ , which implies that  $\nabla^2 U Df$  is a symmetric  $N \times N$  matrix. The function  $U(u)$  is strictly convex at those values  $u$  where the system (1.1) is strictly hyperbolic. The latter means that the Jacobian matrix  $A(u) = Df(u)$  of the flux  $f : \mathbb{R}^N \rightarrow \mathbb{R}^N$  has real and distinct eigenvalues and a basis of eigenvectors. For hyperbolic-elliptic systems, the entropy  $U$  is not convex everywhere.

The present paper is aimed at extending the recent work of Hayes and LeFloch [17, 18, 19] concerning (undercompressive, regularization-sensitive) nonclassical entropy solutions generated by diffusive-dispersive approximations of strictly hyperbolic systems of conservation laws. The main question we will address here is how to design difference schemes for the numerical computation of the *limit* of zero diffusion-dispersion approximations like

$$(1.3) \quad \partial_t u^\varepsilon + \partial_x f(u^\varepsilon) = \partial_x R(\varepsilon u_x^\varepsilon, \varepsilon^2 u_{xx}^\varepsilon, \dots).$$

The regularization term  $R$  is assumed to be *compatible* with the given entropy  $U$  of (1.1) in the sense that any limit  $\bar{u} := \lim_{\varepsilon \rightarrow 0} u^\varepsilon$  satisfies the fundamental entropy inequality (1.2). Such limits are relevant for many models arising in material science and magnetohydrodynamics. The scalar conservation law with cubic flux supplemented with linear diffusion and dispersion provides a useful model:

$$(1.4) \quad \partial_t u^\varepsilon + \partial_x (u^\varepsilon)^3 = \varepsilon u_{xx}^\varepsilon + \alpha \varepsilon^2 u_{xxx}^\varepsilon,$$

where  $\alpha$  is a “material” parameter presumably given by physical modeling.

The main difficulties in studying (1.3)–(1.4) are as follows:

- (1) The limits  $\bar{u}$  may contain *undercompressive, nonclassical shocks* which do not satisfy the standard entropy criteria of Lax [27, 28] and Liu [35]. These waves are admissible in the sense that they are associated with a diffusive-dispersive traveling wave. For undercompressive shocks, the traveling wave is in the generic case a connection between two saddle equilibrium points. Furthermore, in the model (1.4), for instance, Jacobs, McKinney, and Shearer [23] pointed out that the *sign* of the dispersion coefficient  $\alpha$  is critical. For  $\alpha < 0$  the solutions of (1.4) converge to classical entropy solutions, while if  $\alpha > 0$  the limits may contain nonclassical shocks.
- (2) The Cauchy problem (1.1)–(1.2) may not have a unique solution and a further admissibility condition—the *kinetic relation*—is necessary, which constrains the *entropy dissipation* of nonclassical shocks. Note that for *undercompressive* waves, the number of characteristics impinging on the discontinuity is less than what is required for linearized stability. See Abeyaratne and Knowles [1, 2], LeFloch [32], and Truskinovsky [46, 47].

We refer the reader to Hayes and LeFloch [17, 18, 19] and to [33] for a review.

The numerical approximation of the limit  $\bar{u}$  is an extremely challenging problem. First of all, for scalar conservation laws, say, nonclassical solutions violate the standard TVD (total variation diminishing) property. This excludes, for our purpose, the whole class of modern, shock-capturing TVD schemes. More importantly, nonclassical shocks turn out to be driven by the physical dissipation terms in the right-hand side of (1.3)–(1.4), which we must mimic at the numerical level. Otherwise, the artificial numerical diffusion which is effectively present in any finite difference scheme (the Glimm scheme [11] and the front tracking scheme [12, 6] being exceptions) would drive the propagation of the shocks. The situation is reminiscent of what was observed earlier by Hou and LeFloch [20] for nonconservative schemes. Wrong propagation speeds may be observed in these contexts.

In fluid dynamics and in material science, the dynamics of phase transitions has received a lot of attention. The model problem there is a hyperbolic-elliptic system of two conservation laws supplemented with a viscosity term and a dispersive-like capillarity term, similar to (1.4); see Slemrod [41]. See also [25, 40, 9] for early activity on the subject. The numerical analysis of this model was initiated in the papers [42, 3, 26, 8]. In particular, Cockburn and Gau [8] introduced a finite difference scheme satisfying a global entropy inequality and taking into account small parameter-dependent viscosity and capillarity terms.

The complex wave phenomena studied here also arise in non-strictly hyperbolic models, which have received a lot of attention. We refer to Azevedo et al. [4], Canic [7], Isaacson, Marchesin, and Plohr [24], and the many references cited therein.

In the present article, following [17, 18, 19], we mainly focus on the effect of *dispersive terms* in hyperbolic equations. We aim at understanding the fundamental properties of undercompressive shock waves and rigorously assessing the accuracy of approximation schemes. Our analytical results in sections 2 to 4 will be valid for both hyperbolic and hyperbolic-elliptic systems. All of the numerical experiments in this paper will be performed on scalar conservation laws with either quadratic ( $f(u) = u^2$ ) or cubic ( $f(u) = u^3$ ) flux-functions.

We consider approximation schemes that, after Lax [27, 28], Harten, Hyman, and Lax [15] and Lax and Wendroff [31], are in *conservative form* and satisfy a discrete form of the *entropy inequality* (1.2). Furthermore, for regularization-sensitive shocks, it is necessary that the numerical entropy dissipation of the discrete scheme mimic the one of the continuous model (1.3). This led Hayes and LeFloch in [19] to use the second-order accurate, entropy conservative scheme introduced earlier by Tadmor [44, 45], for the discretization of the flux term  $\partial_x f(u)$  in (1.1). Recall that this notion was introduced by Tadmor to derive a large class of schemes consistent with the entropy inequality (1.2). For the computation of nonclassical shocks, the entropy conservative schemes are particularly interesting since they minimize the effect of spurious numerical entropy dissipation.

In sections 2 and 3, we focus attention on the approximation of (1.1)–(1.2) by *entropy conservative schemes*. We discover in section 3 a new five-point, third-order accurate (at least) and entropy conservative scheme—which will play a central role in the numerical section 5. For a class of systems of conservation laws, we establish a striking parallel between the properties of this new entropy conservative scheme and its continuum equivalent equation.

Numerical results with entropy conservative schemes show that their behavior is dispersive in nature. As they possess so many analytical properties (see Theorems 2.5 and 3.6), it would be interesting to study these schemes for their own sake, along the lines of the works by Lax and Levermore [30], Goodman and Lax [13], and Lax [29].

Next, in section 4 we introduce a class of *high-order and entropy stable schemes*, which as we prove can only converge toward a weak solution of (1.1)–(1.2). The schemes are built by adding a mesh-independent, high-order, numerical viscosity to an entropy conservative scheme. The artificial numerical viscosity is an old concept for which we refer, to mention just a few names, to Von Neumann and Richtmyer [48], Lax and Wendroff [31], Harten and Zwas [16], and Majda and Osher [36]. (See also the references cited therein.) Our purpose is solely to point out the striking fact that a (actually singular) *mild numerical viscosity* is sufficient to drastically tame out the oscillations observed in entropy conservative schemes. We note that only a *weak* a priori estimate is available on the numerical *entropy dissipation* of the class of

entropy stable schemes under consideration.

Section 5 is built upon the results obtained in sections 2 to 4, especially upon the higher order entropy conservative scheme found in section 3. Generalizing the approach of Hayes and LeFloch [19] we design a scheme adapted to the numerical computation of nonclassical shocks. We consider both (1.4) and a *new model equation* of interest for the study of nonclassical shocks. As in (1.4) the flux is taken to be a cubic but now the diffusion and the dispersion are *linear in the flux variable*, i.e.,

$$(1.5) \quad \partial_t u^{\alpha,\varepsilon} + \partial_x f(u^{\alpha,\varepsilon}) = \varepsilon f(u^{\alpha,\varepsilon})_{xx} + \alpha\varepsilon^2 f(u^{\alpha,\varepsilon})_{xxx}, \quad f(u) = u^3,$$

and  $\alpha$  is a given parameter. We stress that  $f(u)$  is also the *entropy variable* associated with the entropy

$$(1.6) \quad U(u) = \int^u f(s) ds = \frac{u^4}{4}.$$

This convex entropy will play a role throughout the discussion in this paper. We will see that the limiting solutions generated by (1.5) contain nonclassical shocks as (1.4) does. We exhibit in section 5 qualitative differences between the two models. To investigate the properties of nonclassical shocks, we determine Hayes and LeFloch's kinetic function, which uniquely characterizes their dynamics. Our numerical results extend those obtained in [19]. For the model (1.5) we find that the kinetic function is globally very well approximated, even for *shock waves with large amplitude*.

In conclusion, we show that the higher-order entropy conservative schemes derived here provide an efficient computational method for a systematic study of nonclassical shocks in the physical sciences.

Other approaches for the numerical computation of regularization-sensitive, non-classical shock waves include the Glimm scheme [32, 49], the wave front tracking algorithm [49, 22, 5], and Osher–Sethian's level set method [21].

In section 6, we consider fully-discrete schemes—in which both the time and the space variables are discretized. We prove that there exists no fully discrete and entropy conservative scheme. Next the entropy stability of fully discrete, Lax–Wendroff type schemes is investigated. We provide analytical and numerical evidence for the conjecture that, for scalar equations with increasing flux  $f$ , the special entropy (1.6) yields an entropy inequality. We recall that Majda and Osher [36] were able to establish an entropy inequality but for a modified version of the Lax–Wendroff scheme.

**2. A second-order entropy conservative scheme.** This section discusses the second-order, entropy conservative scheme introduced by Tadmor in [44, 45] (also see [43] for an earlier related work). For a class of systems of conservation laws, including the  $2 \times 2$  system of nonlinear elasticity, we point out that the scheme has a simple form and additional properties can be derived. To begin with, we recall below Tadmor's definition of entropy conservative schemes.

Call  $v(u) = \nabla U(u)$  the entropy variable associated with  $U$ . When the entropy is strictly convex, this defines a change of variable [10] and one can set

$$(2.1) \quad g(v) := f(u), \quad G(v) := F(u), \quad B(v) := Dg(v).$$

The matrix  $B$  is symmetric since  $Dg(v) = Df(u)D^2U(u)^{-1}$ . There exists a scalar-valued function  $\psi = \psi(v)$  such that  $g = \nabla\psi$ ; in fact

$$(2.2) \quad \psi(v) = v \cdot g(v) - G(v),$$

uniquely defined up to a constant. To deal with examples when  $U$  is not convex everywhere, we make from now on the following *assumption* on the flux  $f(u)$ :

$$(2.3) \quad f(u) \text{ can be written as a function of } v;$$

that is, (2.1) holds for some functions  $g$  and  $G$ . Then again  $\psi$  can be defined by (2.2). Several examples will be of particular interest.

*Example 2.1.* For the scalar conservation laws ( $N = 1$ ) with increasing flux  $f$ , choose the (convex) entropy

$$(2.4) \quad U(u) = \int^u f(s) ds.$$

Interestingly, the flux  $g(v) = v$  is then a linear function of the entropy variable.

*Example 2.2.* Consider the system of nonlinear elasticity

$$(2.5) \quad \begin{aligned} \partial_t w - \partial_x V &= 0, \\ \partial_t V - \partial_x \sigma(w) &= 0, \end{aligned}$$

where  $V$  is the velocity,  $w$  is the stress, and the stress-strain function  $w \mapsto \sigma(w)$  depends on the material under study. Choose the entropy to be

$$(2.6) \quad U(w, V) = \int^w \sigma(s) ds + \frac{V^2}{2}, \quad F(w, V) = -\sigma(w) V.$$

We stress here that, without any assumption on  $\sigma$ , the flux can be written in terms of the entropy variables,  $(\sigma, V)$ , and—as in Example 2.1—is a linear function. Note in passing that when  $\sigma'(w) > 0$ , the system is hyperbolic and the entropy strictly convex, while otherwise it is elliptic and the entropy is neither convex nor concave.

*Example 2.3.* The symmetric systems for which the matrix  $Df$  is symmetric yields a general class—although not so relevant from the physical standpoint—of (not necessarily strictly) hyperbolic systems. The function

$$U(u) = |u|^2$$

is a strictly convex entropy for these systems, and the entropy variable  $v = u$  coincides with the conservative variable.

Let  $x_j = jh$ ,  $j \in \mathbf{Z}$ , be a regular mesh, where  $h > 0$  denotes the mesh length. Consider the following class of  $(2p + 1)$ -point, conservative, semidiscrete schemes

$$(2.7) \quad u'_j = -\frac{1}{h} \left( g_{j+1/2}^* - g_{j-1/2}^* \right),$$

where  $u_j = u_j(t)$  is an approximation of the value  $u(x_j, t)$  of a solution of (1.2). The numerical flux

$$g_{j+1/2}^* = g^*(v_{j-p+1}, \dots, v_{j+p}), \quad v_j = \nabla U(u_j),$$

is assumed to be consistent with the exact flux  $g$  (and, thus, with  $f$ ) in the sense that

$$g^*(v_{-p+1}, \dots, v_p) = g(v) \quad \text{when } v_{-p+1} = \dots = v_p = v.$$

Tadmor in [43] focused on *essentially three-point schemes*, for which

$$(2.8) \quad g^*(v_{-p+1}, \dots, v_p) = g(v) \quad \text{when } v_0 = v_1 = v.$$

As we will see in section 3, this restriction must be relaxed for third-order schemes, however.

The numerical flux (2.9) below was discovered by Tadmor, together with the cell entropy equality (2.10)–(2.11).

**THEOREM 2.4.** *Suppose that either the entropy  $U$  is strictly convex or (more generally) the assumption (2.3) holds. Consider the two-point numerical flux*

$$(2.9) \quad g^*(v_0, v_1) = \int_0^1 g(v_0 + s(v_1 - v_0)) ds, \quad v_0, v_1 \in \mathbb{R}^N.$$

(1) *Then the scheme (2.7)–(2.9) satisfies the cell entropy equality*

$$(2.10) \quad U(u_j)' + \frac{1}{h} \left( G_{j+1/2}^* - G_{j-1/2}^* \right) = 0,$$

where the numerical entropy flux is defined for every  $v_0, v_1 \in \mathbb{R}^N$  by

$$(2.11) \quad G^*(v_0, v_1) = \frac{G(v_0) + G(v_1)}{2} + \frac{(v_0 + v_1)}{2} g^*(v_0, v_1) - \frac{1}{2} \left( v_0 \cdot g(v_0) + v_1 \cdot g(v_1) \right).$$

(2) *The scheme is second-order accurate and its equivalent equation up to second-order has a conservative form*

$$(2.12) \quad \partial_t u + \partial_x f(u) = \frac{h^2}{6} \partial_x \left( -g(v)_{xx} + \frac{1}{2} v_x \cdot \partial_x Dg(v) \right), \quad v = \nabla U(u).$$

We stress that the equivalent equation of a *conservative* scheme, obtained through a formal Taylor expansion in any smooth region of the solution, is usually *not* in a conservative form. The conservative form (2.12) is a special property of the entropy conservative scheme (2.9).

*Proof.* The entropy inequality (2.10)–(2.11) is established in [44, 45] under the assumption that  $U$  is strictly convex. The proof easily extends to *nonconvex entropies*  $U$  as well, provided the entropy variables allow one to rewrite the system (1.1) in a symmetric form, as is assumed by (2.3). For completeness and since this will be useful for section 3, we revisit here the proof of Tadmor.

Multiply (2.7) by  $v_j = \nabla U(u_j)$  so that

$$U(u_j)' = -\frac{1}{h} v_j \cdot \left( g_{j+1/2}^* - g_{j-1/2}^* \right).$$

In the obvious identity

$$\begin{aligned} v_j \cdot \left( g_{j+1/2}^* - g_{j-1/2}^* \right) &= \frac{(v_j + v_{j+1})}{2} \cdot g_{j+1/2}^* - \frac{(v_{j-1} + v_j)}{2} \cdot g_{j-1/2}^* \\ &\quad - \frac{1}{2} \left( (v_{j+1} - v_j) \cdot g_{j+1/2}^* + (v_j - v_{j-1}) \cdot g_{j-1/2}^* \right), \end{aligned}$$

the first term on the right-hand side is already in a conservative form, and we deduce that a scheme is entropy conservative, i.e., (2.10) holds iff there exists

$$\psi_{j+1/2}^* = \psi^*(v_{j-p+1}, \dots, v_{j+p})$$

such that

$$(2.13) \quad \frac{1}{2} (v_{j+1} - v_j) \cdot g_{j+1/2}^* + \frac{1}{2} (v_j - v_{j-1}) \cdot g_{j-1/2}^* = \psi_{j+1/2}^* - \psi_{j-1/2}^*.$$

Then the entropy equality (2.10) would hold with

$$(2.14) \quad G_{j+1/2}^* = \frac{(v_j + v_{j+1})}{2} \cdot g_{j+1/2}^* - \psi_{j+1/2}^*.$$

In particular, returning to the choice made in (2.9) and using  $g = \nabla\psi$ , we see that

$$\frac{1}{2}(v_{j+1} - v_j) \cdot g_{j+1/2}^* = \frac{1}{2} \int_0^1 (v_{j+1} - v_j) \cdot g(v_j + s(v_{j+1} - v_j)) ds = \frac{1}{2} (\psi(v_{j+1}) - \psi(v_j)).$$

Since

$$\frac{1}{2} (\psi(v_{j+1}) - \psi(v_j)) + \frac{1}{2} (\psi(v_j) - \psi(v_{j-1})) = \frac{1}{2} (\psi(v_{j+1}) + \psi(v_j)) - \frac{1}{2} (\psi(v_j) + \psi(v_{j-1})),$$

we deduce from (2.13) that

$$\psi_{j+1/2}^* = \frac{1}{2} (\psi(v_{j+1}) + \psi(v_j)).$$

In view of (2.14), the corresponding entropy flux is

$$G_{j+1/2}^* = \frac{1}{2} (v_j + v_{j+1}) g_{j+1/2}^* - \frac{1}{2} (\psi(v_{j+1}) + \psi(v_j)),$$

which in view of (2.2) is in agreement with (2.11).

To determine the accuracy of the scheme, we calculate its equivalent equation via a formal Taylor expansion. From (2.7)–(2.9), we find

$$\partial_t u + \partial_x f(u) = -\frac{h^2}{12} v_x \cdot (\partial_x D^2 g(v)) \cdot v_x - \frac{h^2}{3} v_{xx} \cdot \partial_x Dg(v) - \frac{h^2}{6} Dg(v) \cdot v_{xxx}.$$

The right-hand side contains only terms of order 3, that is, having three derivatives in space. By easy manipulations, the conservative form (2.12) follows.  $\square$

It was observed in [43] that an essentially three-point scheme admits the following *viscous form*:

$$(2.15) \quad u'_j = -\frac{1}{2h} (g(v_{j+1}) - g(v_{j-1})) + \frac{1}{2h} (Q_{j+1/2}^* (v_{j+1} - v_j) - Q_{j-1/2}^* (v_j - v_{j-1})),$$

where the numerical viscosity matrix

$$Q_{j+1/2}^* = Q^*(v_{j-p+1}, \dots, v_{j+p})$$

is determined from the flux  $g^*$  by the condition

$$g_{j+1/2}^* = \frac{1}{2} (g(v_{j+1}) + g(v_j)) - \frac{1}{2} Q_{j+1/2}^* (v_{j+1} - v_j).$$

Clearly (2.8) is a necessary condition for  $Q^*$  to exist. Then considering any essentially three-point scheme, observe that for  $v_{-p+1}, \dots, v_p \in \mathbf{R}^N$ ,

$$g(v_1) - g^*(v_{-p+1}, \dots, v_p) = \int_0^1 \frac{\partial g^*}{\partial v_0} (v_{-p+1}, \dots, v_{-1}, v_0 + s(v_1 - v_0), v_1, \dots, v_p) ds (v_1 - v_0),$$

and thus

$$\begin{aligned}
 Q^*(v_{-p+1}, \dots, v_p) (v_1 - v_0) &= \int_0^1 \frac{\partial g^*}{\partial v_0}(v_{-p+1}, \dots, v_{-1}, v_0 + s(v_1 - v_0), v_1, \dots, v_p) ds (v_1 - v_0) \\
 &\quad - \int_0^1 \frac{\partial g^*}{\partial v_1}(v_{-p+1}, \dots, v_0, v_0 + s(v_1 - v_0), v_2, \dots, v_p) ds (v_1 - v_0).
 \end{aligned}$$

A rather natural (but *not* unique) choice for  $Q^*$  is thus

$$\begin{aligned}
 (2.16) \quad Q^*(v_{-p+1}, \dots, v_p) &= \int_0^1 \frac{\partial g^*}{\partial v_0}(v_{-p+1}, \dots, v_{-1}, v_0 + s(v_1 - v_0), v_1, \dots, v_p) ds \\
 &\quad - \int_0^1 \frac{\partial g^*}{\partial v_1}(v_{-p+1}, \dots, v_0, v_0 + s(v_1 - v_0), v_2, \dots, v_p) ds.
 \end{aligned}$$

To calculate a viscous form of the scheme (2.9), we rely on the general formula (2.16). Using the notation  $B(v) = Dg(v)$ , we get

$$\begin{aligned}
 (2.17) \quad Q^*(u_0, u_1) &= \int_0^1 B(v_0 + s(v_1 - v_0))(1 - s) ds - \int_0^1 B(v_0 + s(v_1 - v_0))s ds \\
 &= \int_0^1 B(v_0 + s(v_1 - v_0))(1 - 2s) ds,
 \end{aligned}$$

which is symmetric since the matrix  $B(v) = \nabla^2 U(u) Df(u)$  is symmetric. Clearly  $Q^*$  need not be nonnegative. Furthermore, using any norm of the matrix  $Q^*$ , we have

$$(2.18) \quad |Q^*(v_0, v_1)| = \left| \int_0^1 (B(v_0 + s(v_1 - v_0)) - B(v_0))(1 - 2s) ds \right| \leq C |v_1 - v_0|$$

for some constant  $C > 0$  and all  $v_0, v_1$  in a bounded set of  $\mathbb{R}^N$ .

We stress that the second-order entropy conservative schemes can be identified with their numerical viscosity coefficient,  $Q^*$ . The following formula was noticed by Tadmor [44, Theorem 2.1]:

$$Q^*(v_0, v_1) = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} (\xi^2 + \eta^2) D^2 g(2\xi\eta + 1/2) d\eta d\xi (v_1 - v_0),$$

which implies immediately the inequality above,  $|Q^*(v_0, v_1)| \leq C |v_1 - v_0|$ . This yields yet another proof for the second-order accuracy of Tadmor’s entropy conservative scheme.

Observe that, in general, the numerical viscosity  $Q^*$  of an entropy conservative scheme does not have any distinguished property. We now exhibit a class of systems of conservation laws of interest for which the numerical viscosity of Tadmor’s scheme is *identically zero* and the scheme has a simple form, allowing us to derive additional properties.

Due to an observation made earlier in Examples 2.1–2.2, the theorem below applies to the scalar conservation laws endowed with the entropy (2.4) and to the (hyperbolic or hyperbolic-elliptic) system of elasticity endowed with the entropy (2.6).



THEOREM 2.5. Consider any system of conservation laws endowed with a (convex or nonconvex) entropy function  $U$  such that

(2.19) the flux-function is a linear function of the entropy variable  $v$ .

(1) Then the numerical viscosity of the scheme (2.7)–(2.9) vanishes identically:

$$Q^* \equiv 0.$$

(2) The scheme coincides with the semidiscrete, second-order, centered scheme,

$$(2.20) \quad u'_j = -\frac{1}{2h} (g(v_{j+1}) - g(v_{j-1})), \quad v_j = \nabla U(u_j).$$

(3) Its equivalent equation is conservative up to any order of approximation, indeed,

$$(2.21) \quad \partial_t u + \partial_x f(u) = -\sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+1)!} \partial_x^{2n+1} f(u).$$

(4) The equation (2.21) is entropy conservative for the entropy  $U$ , in the sense that

$$(2.22) \quad \begin{aligned} &\partial_t U(u) + \partial_x F(u) \\ &= \partial_x \sum_{n=1}^{\infty} \left( \frac{(-1)^{n+1}}{2} \partial_x^n v \cdot \partial_x^n f(u) + \sum_{m=0}^{n-1} (-1)^m \partial_x^m v \cdot \partial_x^{2n-m} f(u) \right) \frac{h^{2n}}{(2n+1)!}, \end{aligned}$$

in which  $v = \nabla U(u)$ .

For instance, the equivalent equation (2.21) at the second-order contains a linear dispersion in the flux variable

$$(2.23) \quad \partial_t u + \partial_x f(u) = -\frac{h^2}{6} f(u)_{xxx},$$

and (2.22) yields

$$(2.24) \quad \partial_t U(u) + \partial_x F(u) = \frac{h^2}{2} ((v \cdot f(u))_{xx} - 3 v_x \cdot f(u)_x)_x, \quad v = \nabla U(u).$$

Theorem 2.5 establishes a striking parallel between the properties of the scheme (2.20)—which is conservative in the sense of Lax–Wendroff and entropy conservative in the sense of Tadmor—and the properties of its equivalent equation (2.21)—which is conservative and entropy conservative in the “continuous” sense. Under the assumption (2.19), no entropy dissipation can be “measured” at both the continuous and the discrete level. These properties will justify a reliance on the equivalent equation when designing a scheme adapted to nonclassical shocks in section 5.

*Proof.* The first two statements follow from (2.17) and (2.15). To show (2.21), we expand the approximate solution  $v_j(t) \approx v(x_j, t)$  in the neighborhood of a point  $(x_j, t) = (0, 0)$ . Evaluating all functions at  $(0, 0)$ , we find

$$v_{j+1} = \sum_{n=0}^{\infty} \partial_x^n v \frac{h^n}{n!}$$

and

$$\begin{aligned} u_t &= -\frac{1}{2h} Dg \sum_{n=0}^{\infty} \frac{\partial_x^n v}{n!} (h^n - (-h)^n) \\ &= -Dg \sum_{n=0}^{\infty} \partial_x^{2n+1} v \frac{h^{2n}}{(2n+1)!} = -g(v)_x - \sum_{n=1}^{\infty} \partial_x^{2n+1} g(v) \frac{h^{2n}}{(2n+1)!}. \end{aligned}$$

This yields (2.21) for the scheme (2.20).

To derive the entropy equality, we multiply (2.21) by  $\nabla U(u) = v$ . We obtain

$$\partial_t U(u) + \partial_x F(u) = - \sum_{n=1}^{\infty} v \cdot \partial_x^{2n+1} g(v) \frac{h^{2n}}{(2n+1)!}.$$

Using the fact that  $g(v) = Dg v$  and  $Dg$  is a symmetric matrix, we arrive at

$$\begin{aligned} &\partial_t U(u) + \partial_x F(u) \\ &= - \sum_{n=1}^{\infty} v \cdot Dg \partial_x^{2n+1} v \frac{h^{2n}}{(2n+1)!} \\ &= - \sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+1)!} ((v \cdot Dg \partial_x^{2n} v)_x - (v_x \cdot Dg \partial_x^{2n-1} v)_x + (v_{xx} \cdot Dg \partial_x^{2n-2} v)_x \\ &\quad - \dots + (-1)^{n-1} (\partial_x^{n-1} v \cdot Dg \partial_x^{n+1} v)_x + (-1)^n \partial_x^n v \cdot Dg \partial_x^{n+1} v). \end{aligned}$$

To treat the last term, still written in a nonconservative form, we observe that since  $Dg$  is symmetric,

$$\partial_x^n v Dg \partial_x^{n+1} v = \frac{1}{2} (\partial_x^n v Dg \partial_x^n v)_x.$$

The conservative form (2.22) follows.  $\square$

Observe that any entropy conservative scheme admits the two time-invariants

$$\sum_{j=-\infty}^{\infty} u_j(t) = \sum_{j=-\infty}^{\infty} u_j(0) \text{ and } \sum_{j=-\infty}^{\infty} U(u_j(t)) = \sum_{j=-\infty}^{\infty} U(u_j(0)).$$

Therefore, it cannot converge to a weak solution of (1.1) having discontinuities. The behavior of Tadmor’s scheme for scalar conservation laws is illustrated numerically below.

**Numerical experiments.** In Figure 2.1 we plot the numerical solution obtained by the second-order entropy conservative scheme (2.9), using entropy variables as described in Example 2.1, i.e.,  $U' = f$  and here  $f(u) = u^2/2$ . The initial datum is  $u_0(x) = 0.5 \sin(2\pi(x + 0.05)) + 0.5$  and the mesh contains 300 points. Here and in all subsequent numerical calculations, we use a higher order Runge–Kutta time discretization as proposed in [39]. We observe a train of oscillations with large amplitude (of the order of the shock strength) near shocks. As expected, the scheme does not converge in a strong norm when the mesh is refined.

**3. High-order entropy conservative schemes.** We now turn to investigating more general entropy conservative schemes, being especially interested in constructing higher-order schemes. A new class of such schemes is derived.

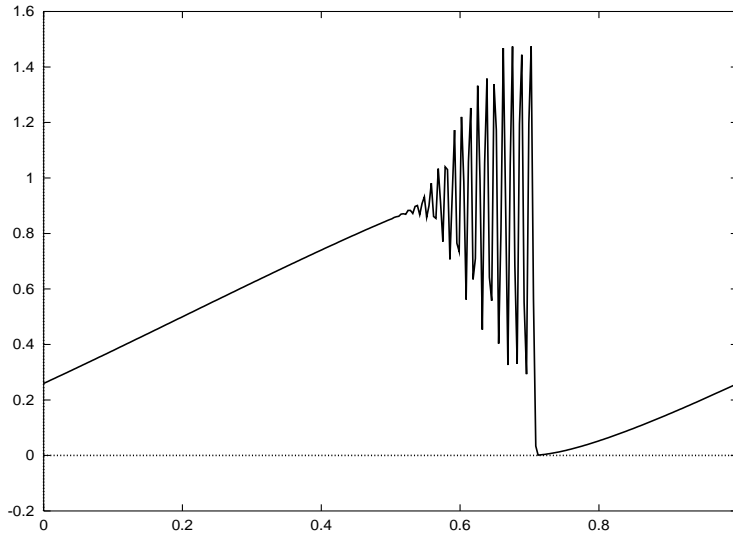


FIG. 2.1. Second-order entropy conservative scheme with  $f(u) = u^2/2$ .

**THEOREM 3.1.** Consider the system of conservation laws (1.1) together with the entropy inequality (1.2). Consider the numerical scheme

$$(3.1) \quad u'_j = -\frac{1}{h} \left( g_{j+1/2}^* - g_{j-1/2}^* \right), \quad g_{j+1/2}^* = g^*(v_{j-p+1}, \dots, v_{j+p})$$

for the class of numerical fluxes  $g^*$  defined by

$$(3.2) \quad \begin{aligned} &g^*(v_{-p+1}, \dots, v_p) \\ &= \int_0^1 g(v_0 + s(v_1 - v_0)) ds \\ &\quad - \frac{1}{12} ((v_2 - v_1) \cdot B^*(v_{-p+2}, \dots, v_p) - (v_0 - v_{-1}) \cdot B^*(v_{-p+1}, \dots, v_{p-1})), \end{aligned}$$

where the  $N \times N$  matrices  $B^*(v_{-p+2}, \dots, v_p)$  are symmetric.

- (1) The  $(2p + 1)$ -point scheme (3.1)–(3.2) is entropy conservative in the sense of Tadmor. Indeed the cell entropy equality (2.10) holds where the numerical entropy flux is now given by

$$(3.3) \quad \begin{aligned} G^*(v_{-p+1}, \dots, v_p) &= \frac{(v_0 + v_1)}{2} \cdot g^*(v_{-p+1}, \dots, v_p) \\ &\quad - \frac{1}{2} (\psi^*(v_{-p+2}, \dots, v_p) + \psi^*(v_{-p+1}, \dots, v_{p-1})), \end{aligned}$$

$$\psi^*(v_{-p+2}, \dots, v_p) = v_1 \cdot g(v_1) - G(v_1) + \frac{1}{12} (v_1 - v_0) \cdot B^*(v_{-p+2}, \dots, v_p) (v_1 - v_2).$$

- (2) When, for instance,  $p = 2$ , the five-point scheme is third-order accurate, at least, provided  $B^*$  satisfies

$$(3.4) \quad B^*(v, v, v) = B(v) (= Dg(v)).$$

The choice  $p = 2$  and

$$(3.5) \quad B^*(v_0, v_1, v_2) = Dg(v_1)$$

yields the entropy conservative scheme to be used in section 5 for computing nonclassical shocks.

*Remark 3.2.* We stress that (3.2) is generally not an essentially three-point scheme. So in general (3.2) does not admit a viscous form like (2.15).

*Proof.* The entropy conservative schemes are found by solving (2.13), i.e.,

$$(3.6) \quad \begin{aligned} (v_1 - v_0) \cdot g^*(v_{-p+1}, \dots, v_p) + (v_0 - v_{-1}) \cdot g^*(v_{-p}, \dots, v_{p-1}) \\ = 2(\psi^*(v_{-p+1}, \dots, v_p) - \psi^*(v_{-p}, \dots, v_{p-1})). \end{aligned}$$

To simplify the notation, we derive the scheme (3.2) on scalar equations, first. It is *sufficient* to find a function  $\varphi$  such that

$$(3.7) \quad \begin{aligned} (v_1 - v_0) \cdot g^*(v_{-p+1}, \dots, v_{-1}, v_0, v_1, v_2, \dots, v_p) \\ = \varphi(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) - \varphi(v_{-p+1}, \dots, v_{-1}, v_0, v_1, \dots, v_{p-1}). \end{aligned}$$

Namely, we can then set

$$(3.8) \quad \begin{aligned} \psi^*(v_{-p+1}, \dots, v_{-1}, v_0, v_1, v_2, \dots, v_p) \\ = \frac{1}{2}(\varphi(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) + \varphi(v_{-p+1}, \dots, v_{-1}, v_0, v_1, \dots, v_{p-1})) \end{aligned}$$

and (3.6) follows.

Choosing  $v_0 = v_1 = v$  in (3.7) we see that

$$(3.9) \quad \varphi(v_{-p+2}, \dots, v_{-1}, v, v, v_2, \dots, v_p) = \varphi(v_{-p+1}, \dots, v_{-1}, v, v, v_2, \dots, v_{p-1}).$$

This shows that for each  $v$  the functions

$$(v_{-p+2}, \dots, v_{-1}, v_2, \dots, v_p) \mapsto \varphi(v_{-p+2}, \dots, v_{-1}, v, v, v_2, \dots, v_p)$$

and

$$(v_{-p+1}, \dots, v_{-1}, v_2, \dots, v_{p-1}) \mapsto \varphi(v_{-p+1}, \dots, v_{-1}, v, v, v_2, \dots, v_{p-1})$$

are constant and equal to, say,  $\alpha(v)$ . Thus there exists a function  $H$  such that

$$\varphi(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) = \alpha(v_1) + (v_1 - v_0) H(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p).$$

Taking  $v_1 = v_2 = v$  and using (3.9) once more, we get

$$\alpha(v) = \alpha(v) + (v - v_0) H(v_{-p+2}, \dots, v_0, v, v, v_3, \dots, v_p).$$

Therefore  $H(v_{-p+2}, \dots, v_0, v, v, v_3, \dots, v_p) = 0$  and there exists a function  $B^*$  such that

$$H(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) = -\frac{1}{12}(v_2 - v_1) B^*(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p),$$

where the factor 1/12 is introduced to simplify the subsequent calculations. We have

$$\begin{aligned}
 & \varphi(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) \\
 (3.10) \quad & = \alpha(v_1) - \frac{1}{12} (v_1 - v_0) (v_2 - v_1) B^*(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p).
 \end{aligned}$$

Combining (3.10) with (3.7) we obtain

$$\begin{aligned}
 & g^*(v_{-p+1}, \dots, v_{-1}, v_0, v_1, v_2, \dots, v_p) \\
 (3.11) \quad & = \frac{\alpha(v_1) - \alpha(v_0)}{v_1 - v_0} - \frac{1}{12} (v_2 - v_1) B^*(v_{-p+2}, \dots, v_0, v_1, v_2, \dots, v_p) \\
 & \quad + \frac{1}{12} (v_0 - v_{-1}) B^*(v_{-p+1}, \dots, v_{-1}, v_0, v_1, \dots, v_{p-1}).
 \end{aligned}$$

To ensure the consistency property  $g^*(v, \dots, v) = g(v)$ , one must have  $\alpha(v) = \psi(v)$ . The formula (3.11) then defines an entropy conservative scheme for any choice of the function  $B^*$ .

Assuming  $p = 2$ , we now determine conditions on the function  $B^*$  for the scheme to be third-order accurate. A tedious calculation leads us to the equivalent equation

$$\begin{aligned}
 (3.12) \quad \partial_t u + \partial_x f(u) = & -\frac{1}{12} \left( 2h^2 g(v)_{xxx} - h^2 (v_x \partial_x g'(v))_x \right. \\
 & - h^2 (B''_{11} + B''_{22} + B''_{33} + 2 (B''_{12} + B''_{23} + B''_{31})) v_x^3 \\
 & \left. + 4h^2 (B'_1 + B'_2 + B'_3) v_x v_{xx} + 2h^2 B v_{xxx} \right),
 \end{aligned}$$

where  $B_{kl} = B_{kl}(v, v, v)$ , etc., and we write  $B$  instead of  $B^*$ . It follows that the scheme is third-order accurate iff

$$\begin{aligned}
 B''_{11} + B''_{22} + B''_{33} + 2 (B''_{12} + B''_{23} + B''_{31}) & = g''' , \\
 B'_1 + B'_2 + B'_3 & = g'' , \\
 B & = g' .
 \end{aligned}$$

A necessary and sufficient condition on  $B^*$  is thus

$$(3.13) \quad B^*(v, v, v) = g'(v).$$

For systems, the generalization is immediate. In the formula (3.2),  $B^*$  is now a (symmetric, for simplicity) matrix. The condition (3.13) now reads as (3.4). It is an exercise to check that (3.2) defines a third-order accurate scheme even for systems. The expression of the numerical entropy flux follows immediately from (2.14)–(2.13)–(2.14).  $\square$

In the following result, we restrict attention to essentially three-point schemes. In particular it is shown that it is not possible to construct essentially three-point schemes which are of third or even higher order and entropy conservative.

**THEOREM 3.3.** *Consider the system of conservation laws (1.1) together with the entropy inequality (1.2).*

*When  $N = 1$ , Tadmor’s flux (2.9) yields the unique, entropy conservative, three-point, semidiscrete scheme. This scheme is second-order accurate.*

For systems of  $N \geq 1$  equations, suppose that the flux-function  $f$  is not identically constant and the entropy  $U$  is not a linear function on any interval. Then any entropy conservative, essentially three-point, semidiscrete scheme is exactly second-order accurate.

*Proof.* First suppose  $N = 1$  and  $p = 1$ . Using  $v_{-1} = v_0 = v$  in (3.6), we obtain

$$(v_1 - v) \cdot g^*(v, v_1) = 2 (\psi^*(v, v_1) - \psi^*(v, v)),$$

while using  $v_0 = v_1 = v$  in (3.6) yields

$$(v - v_{-1}) \cdot g^*(v_{-1}, v) = 2 (\psi^*(v, v) - \psi^*(v_{-1}, v)).$$

Replacing  $(v_{-1}, v)$  with  $(v, v_1)$  in the latter and comparing with the former, we arrive at the identity

$$2 (\psi^*(v, v_1) - \psi^*(v, v)) = 2 (\psi^*(v_1, v_1) - \psi^*(v, v_1)),$$

which gives an explicit expression for  $\psi^*$ ,

$$(3.14) \quad \psi^*(v, v_1) = \frac{1}{2} (\psi^*(v_1, v_1) + \psi^*(v, v)).$$

The numerical flux then reads

$$g^*(v_0, v_1) = \frac{\psi^*(v_1, v_1) - \psi^*(v_0, v_0)}{v_1 - v_0},$$

where for consistency one must have

$$\psi^*(v, v) = \psi(v).$$

This leads us exactly to the numerical flux (2.9) and shows that scalar conservation laws admit a unique, entropy conservative, and three-point scheme.

For systems, several entropy conservative fluxes can be defined. Let us first consider *any*  $(2p + 1)$ -point numerical flux  $g^*$ . A straightforward but rather tedious calculation yields the equivalent equation of the scheme, at the third order,

(3.15)

$$\begin{aligned} & \partial_t u + \partial_x f(u) \\ &= \frac{h}{2} \sum_{i=-p+1}^p ((i-1)^2 - i^2) g_i \cdot v_{xx} + \frac{h}{2} \sum_{i,j=-p+1}^p ((i-1)(j-1) - ij) g_{ij} \cdot (v_x, v_x) \\ &+ h^2 \sum_{i=-p+1}^p ((i-1)^3 - i^3) g_i \cdot v_{xxx} \\ &+ \frac{h^2}{4} \sum_{i,j=-p+1}^p ((i-1)^2(j-1) + (i-1)(j-1)^2 - i^2j - ij^2) g_{ij} \cdot (v_{xx}, v_x) \\ &+ \frac{h^3}{6} \sum_{i,j,k=-p+1}^p ((i-1)(j-1)(k-1) - ijk) g_{ijk} \cdot (v_x, v_x, v_x). \end{aligned}$$

Here  $g_i = \partial g(v, \dots, v) / \partial v_i$ , etc.

If the scheme is essentially three-point, we can get

$$(3.16) \quad g_i = 0 \quad \text{for all } i \neq 0, 1$$

and

$$g_{ij} = 0, \quad \text{except if at least one } i, j \neq 0, 1.$$

It follows that the scheme is second-order accurate iff we have

$$(3.17) \quad \frac{\partial g}{\partial v_0}(v, \dots, v) = \frac{\partial g}{\partial v_1}(v, \dots, v).$$

On the other hand, for third-order accuracy one found the necessary condition

$$\frac{\partial g}{\partial v_0}(v, \dots, v) = -\frac{\partial g}{\partial v_1}(v, \dots, v),$$

which is not compatible with (3.17) (except in the trivial case  $g = \text{constant}$ ). This implies the well-known property that any essentially three-point scheme is at most second-order accurate.

It remains to check that any entropy conservative scheme satisfies the condition (3.17) for second-order accuracy. To this end we return to the general condition (3.6). Taking there  $v_{-1} = v_0$ , differentiating with respect to both  $v_0$  and  $v_1$ , and finally letting  $v_{-p} = \dots = v_p$ , we arrive at the identity

$$(3.18) \quad \frac{1}{2} \frac{\partial g}{\partial v_0}(v, \dots, v) - \frac{1}{2} \frac{\partial g}{\partial v_1}(v, \dots, v) = \frac{\partial^2 \psi^*}{\partial v_0 \partial v_1}(v, \dots, v),$$

where we also used (3.16). On the other hand, taking  $v_0 = v_1$ , differentiating with respect to both  $v_{-1}$  and  $v_0$ , and finally letting  $v_{-p} = \dots = v_p$ , we arrive now at

$$(3.19) \quad \frac{1}{2} \frac{\partial g}{\partial v_0}(v, \dots, v) - \frac{1}{2} \frac{\partial g}{\partial v_1}(v, \dots, v) = -\frac{\partial^2 \psi^*}{\partial v_0 \partial v_1}(v, \dots, v).$$

Comparing (3.18)–(3.19) yields (3.17), which completes the proof.  $\square$

As in Theorem 2.5 of section 2 we now focus on a particular class of systems.

**THEOREM 3.4.** *Consider any system of conservation laws endowed with a (convex or nonconvex) entropy function  $U$  such that the property (2.19) holds.*

(1) *Then the scheme (3.2)–(3.5) takes the form*

$$(3.20) \quad g^*(v_{-1}, \dots, v_2) = \frac{1}{2} (g(v_0) + g(v_1)) + \frac{1}{12} (-g(v_{-1}) + g(v_0) + g(v_1) - g(v_2)),$$

and thus

$$(3.21) \quad u'_j = -\frac{1}{2h} (g(v_{j+1}) - g(v_{j-1})) - \frac{1}{12h} (-g(v_{j+2}) + 2g(v_{j+1}) - 2g(v_{j-1}) + g(v_{j-2})).$$

(2) *It is fourth-order accurate.*

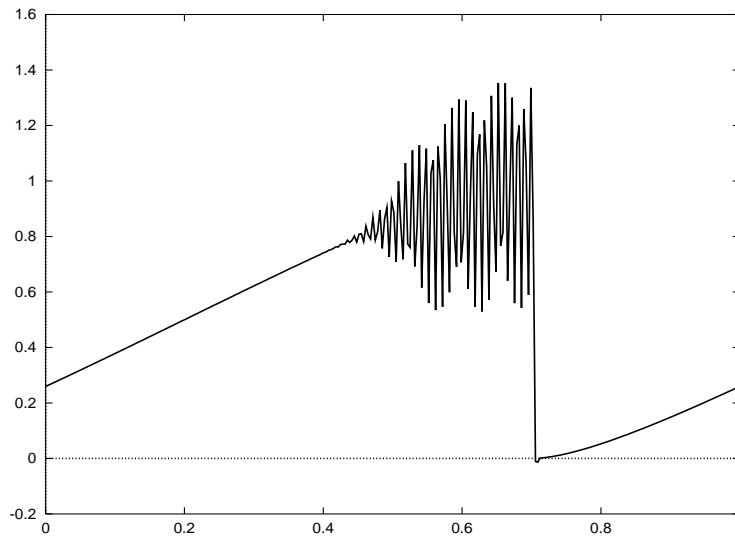


FIG. 3.1. Third-order entropy conservative scheme for  $f(u) = u^2/2$ .

(3) Its equivalent equation is conservative up to any order of approximation:

$$(3.22) \quad \partial_t u + \partial_x f(u) = \frac{4}{3} \sum_{n=2}^{\infty} (2^{2n-2} - 1) \frac{h^{2n}}{(2n+1)!} \partial_x^{2n+1} f(u).$$

(4) The equation (3.22) is entropy conservative for the entropy  $U$ , i.e.,

$$(3.23) \quad \begin{aligned} & \partial_t U(u) + \partial_x F(u) \\ &= \frac{4}{3} \partial_x \sum_{n=2}^{\infty} \left( \frac{(-1)^{n+1}}{2} \partial_x^n v \cdot \partial_x^n f(u) \right. \\ & \quad \left. + \sum_{m=0}^{n-1} (-1)^m \partial_x^m v \partial_x^{2n-m} f(u) \right) \frac{(2^{2n-2} - 1) h^{2n}}{(2n+1)!}, \end{aligned}$$

where  $v = \nabla U(u)$ .

*Proof.* The proof of the first two assertions follows via Taylor expansion as in the proof of Theorem 2.5. Note that the terms under the sum on the right-hand side of (3.22) are equal to the corresponding terms in (2.21) up to the factor  $(2^{2n-2} - 1)$ . Consequently (3.23) follows from (2.22).  $\square$

*Remark 3.5.* Surprisingly, the entropy conservative scheme found in (3.21) turns out to be identical with the one used—for scalar equations and the system of elasticity—by [19] without realizing the properties we obtain here in Theorem 3.4. Interestingly, in the case of phase transitions, we can also recover a scheme used earlier in [8].

*Remark 3.6.* Under the assumption (2.19), if we search for a *linear scheme*, then the matrix  $B^*$  in (3.2) is a constant. If  $B^* = 0$  we recover Tadmor’s second-order scheme in the form (2.20) pointed out in Theorem 2.5. The choice  $B^* = B$  gives the new five-point, fourth-order scheme. Other values of  $B^*$  lead to second-order entropy conservative schemes. Therefore, under the assumption (2.19), there exists no entropy conservative and “linear in the entropy variable” scheme of accuracy strictly higher than four.



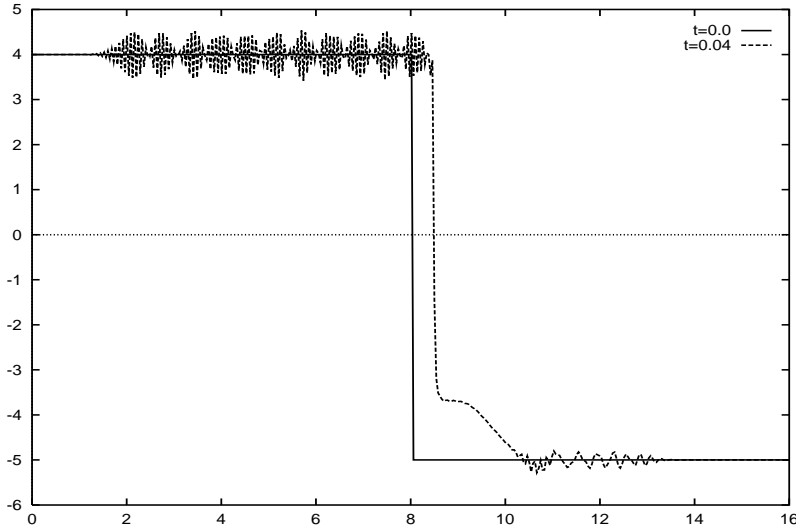


FIG. 3.2. A second-order entropy conservative scheme for  $f(u) = u^3$ .

*Remark 3.7.* As we demonstrate at the end of this section and of section 4, the choices  $B^* = 0$  and  $B^* = B$  provide schemes that generate only *classical shock waves*, while the choice  $B^* = 2B$ , say, yields a scheme which may generate *nonclassical shocks*. This can be explained in view of the equivalent equation (3.12) and from the observations in [23] and [19] concerning the *critical* role of the *sign* of the dispersion coefficient.

**Numerical experiments.** Figure 3.1 displays the numerical solution of the entropy conservative scheme (3.21) for the scalar equation in Example 2.1 with  $U' = f$  and  $f(u) = u^2/2$ . The initial datum is  $u_0(x) = 0.5 \sin(2.0\pi(x + 0.05)) + 0.5$ , the mesh contains 300 points, and time is  $t = 0.5$ . The support of the oscillations is larger, which is due to the larger stencil (5 points) of the scheme. Observe also that the oscillations appear to have some “structure.” According to Remark 3.7 we then perform a calculation for  $f(u) = u^3$  using the scheme with  $B^* = 5.0 \cdot B$ . As initial data we choose  $u_l = 4.0$  and  $u_r = -5.0$ ; a mesh of 400 points was used. The results are shown in Figure 3.2.

Although oscillations are still present the nonclassical behavior is obvious by the development of a middle state between the nonclassical shock and the rarefaction. Note again the characteristic oscillation pattern following the shock.

**4. A class of high-order, entropy stable schemes.** In [44, 45], Tadmor proves that a scheme that contains more numerical viscosity than an entropy conservative one satisfies a discrete entropy inequality. His analysis is based on the viscosity form of the schemes. We extend here Tadmor’s result to schemes of arbitrary order, for which the viscous form need not exist, and to mathematical entropies that need not be convex. We also establish a new consistency and convergence result.

Let  $g^*$  be any entropy conservative flux of order  $m^*$ , consistent with the exact flux  $g(v) = f(u)$  of (1.1). Consider the semidiscrete scheme

$$(4.1) \quad u'_j = -\frac{1}{h} (g_{j+1/2}^* - g_{j-1/2}^*) + \frac{1}{2h} (\tilde{Q}_{j+1/2} (v_{j+1} - v_j) - \tilde{Q}_{j-1/2} (v_j - v_{j-1})),$$

where  $v_j = \nabla U(u_j)$ . The *additional numerical viscosity*  $\tilde{Q}(v_{-p+1}, \dots, v_p)$  is assumed to be a symmetric matrix.

The initial data in  $L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$  are discretized to preserve the order of accuracy and the natural  $L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$  bounds.

THEOREM 4.1. *Assume that the matrix  $\tilde{Q}$  satisfies for some exponents  $0 \leq \alpha \leq \beta$*

$$(4.2) \quad (C_1 |v_1 - v_0|^{2+\beta}) Id \leq \tilde{Q}(v_{-p+1}, \dots, v_p) \leq \left( C_2 \sum_{i=-p+1}^{p-1} |v_{i+1} - v_i|^{2+\alpha} \right) Id$$

for all  $v_{-p+1}, \dots, v_p$  in any given, bounded set of  $\mathbb{R}^N$  and for some  $C_1, C_2 > 0$ .

- (1) *The scheme (4.1) is at least second-order accurate if  $m^* = 2$  and  $\alpha \geq 0$  and third-order accurate if  $m^* = 3$  and  $\alpha \geq 1$ .*
- (2) *It satisfies the cell entropy inequality*

$$(4.3) \quad \begin{aligned} U(u_j)' + \frac{1}{h} \left( \tilde{G}_{j+1/2}^* - \tilde{G}_{j-1/2}^* \right) \\ = -\frac{1}{2h} \left( (v_{j+1} - v_j) \cdot \tilde{Q}_{j+1/2} (v_{j+1} - v_j) \right. \\ \left. + (v_j - v_{j-1}) \cdot \tilde{Q}_{j-1/2} (v_j - v_{j-1}) \right) \leq 0, \end{aligned}$$

where the numerical entropy flux is

$$(4.4) \quad \tilde{G}_{j+1/2}^* := G_{j+1/2}^* - \frac{v_{j+1}}{2} \cdot \tilde{Q}_{j+1/2} (v_{j+1} - v_j),$$

$G^*$  being the entropy flux of the entropy conservative scheme.

- (3) *In particular, the scheme is entropy stable and has uniformly bounded entropy dissipation, i.e., for all  $t$*

$$(4.5) \quad \sum_{j=-\infty}^{\infty} U(u_j(t)) + \frac{C_1}{h} \int_0^t \sum_{j=-\infty}^{\infty} |v_{j+1}(s) - v_j(s)|^{4+\beta} ds \leq \sum_{j=-\infty}^{\infty} U(u_j(0)).$$

- (4) *Assume that the scheme is  $L^\infty$  stable and denote by  $\nu_{x,t}$  an associated Young measure. Then  $\nu$  satisfies the system of conservation laws (1.1) and the entropy inequality (1.2). (See (4.10)–(4.11) below.)*
- (5) *If the scheme is  $L^\infty$  stable and converges a.e., then the limiting function satisfies (1.1)–(1.2).*

Remark 4.2. Observe that our dissipation bound (4.5) is *weaker* than the one known for first-order schemes and for the standard viscosity method. It resembles the one obtained by the standard energy method for the equation with degenerate diffusion

$$\partial_t u^\varepsilon + \partial_x f(u^\varepsilon) = \varepsilon^{3+\beta} (|v_x^\varepsilon|^{2+\beta} v_x^\varepsilon), \quad v^\varepsilon = \nabla U(u^\varepsilon),$$

that is,

$$\varepsilon^{3+\beta} \int \int_{\mathbb{R} \times \mathbb{R}_+} |v_x^\varepsilon(x, t)|^{4+\beta} dx dt \leq C \int_{\mathbb{R}} |u^\varepsilon(x, 0)| dx.$$

(Compare with (4.6) below.)

*Remark 4.3.* Note that the entropy  $U$  need not be convex in Theorem 4.1 and the flux  $g^*$  and the viscosity  $Q^*$  need not be essentially three-point functions. Thus the result applies to the class of entropy conservative schemes found in Theorem 3.1.

*Proof.* Consider the case  $\alpha \geq 0$ . To determine the equivalent equation via formal Taylor expansion, we write

$$v_{j+1} - v_j = h v_x + \text{h.o.t.}$$

and also expand  $\tilde{Q}_{j+1/2}$ . Using the upper bound in (4.2) we see that

$$\tilde{Q}(v_{-p+1}, \dots, v_p) \leq C_2(2p - 1) h^2 |v_x|^2 + \text{h.o.t.}$$

To the equivalent equation of the entropy conservative scheme, one should add a term of order

$$\frac{1}{h} C_2(2p - 1) h^2 |v_x|^2 h |v_x| - \frac{1}{h} C_2(2p - 1) h^2 |v_x|^2 (-h) |v_x| + \text{h.o.t.} = O(h^2).$$

This shows that the scheme is second-order accurate when  $\alpha \geq 0$  and  $m^* = 2$ . The same argument applies to  $m^* = 3$  and  $\alpha \geq 1$ .

To derive the entropy inequality (4.3), we multiply (4.1) by  $v_j$ . The first term in the right-hand side takes a conservative form since  $g^*$  is entropy conservative. We obtain

$$\begin{aligned} U(u_j)' + \frac{1}{h} (G_{j+1/2}^* - G_{j-1/2}^*) &= \frac{v_j}{2h} \cdot \tilde{Q}_{j+1/2} (v_{j+1} - v_j) - \frac{v_j}{2h} \cdot \tilde{Q}_{j-1/2} (v_j - v_{j-1}) \\ &= \frac{1}{2h} (v_j - v_{j+1}) \cdot \tilde{Q}_{j+1/2} (v_{j+1} - v_j) - \frac{1}{2h} (v_j - v_{j-1}) \cdot \tilde{Q}_{j-1/2} (v_j - v_{j-1}) \\ &\quad + \frac{v_{j+1}}{2h} \cdot \tilde{Q}_{j+1/2} (v_{j+1} - v_j) - \frac{v_{j-1}}{2h} \cdot \tilde{Q}_{j-1/2} (v_j - v_{j-1}). \end{aligned}$$

This proves that the entropy inequality (4.3) holds with the numerical entropy flux given in (4.4). Then (4.5) follows by summation of (4.3) over  $j$  and integration in  $t$ , using the lower bound in (4.2).

Denote by  $u^h(x, t)$  the piecewise constant approximate solutions generated by the scheme

$$u^h(x, t) = u_j(t), \quad x \in (x_{j-1/2}, x_{j+1/2}),$$

where  $x_{j+1/2} := h(j + 1/2)$  and set also  $v^h(x, t) := \nabla U(u^h(x, t))$ . The entropy dissipation bound in (4.5) implies

$$(4.6) \quad \int_0^\infty \int_{\mathbb{R}} |v_x^h|^{4+\beta} dx dt = h^{-3-\beta} \int_0^\infty \sum_{j=-\infty}^\infty |v_{j+1} - v_j|^{4+\beta} dt \leq C h^{-2-\beta}.$$

Consider a Young measure  $\nu_{x,t}$  representing all weak-star limits of the functions  $u^h$  as  $h \rightarrow 0$ . That is,

$$(4.7) \quad \langle \nu_{x,t}, \varphi \rangle = \lim_{h \rightarrow 0} \varphi(u^h)$$

in the sense of distributions for all continuous functions  $\varphi$  having compact support. Similarly consider a Young measure  $\nu_{x,t}^\sharp$  associated with  $v^h$ . It is easily checked that

$$(4.8) \quad \langle \nu_{x,t}^\sharp, \psi \rangle = \langle \nu_{x,t}, \psi \circ \nabla U \rangle$$

for all continuous functions  $\psi$  with compact support.

Take a test-function  $\theta$  and set  $\theta_j(t) = \theta(x_j, t)$ . Multiply (4.1) by  $\theta_j$ , sum in  $j$ , integrate in  $t$ , and finally estimate each term successively. Observe first that

$$\sum_j \int_{\mathbb{R}_+} \theta_j(t) u'_j(t) dt \longrightarrow - \int \int_{\mathbb{R} \times \mathbb{R}_+} \partial_t \theta \langle \nu, u \rangle dx dt$$

by the definition (4.7) of the Young measure. On the other hand, we have

$$(4.9) \quad \begin{aligned} & - \int_{\mathbb{R}_+} \sum_{j \in \mathbf{Z}} \frac{\theta_j(t)}{h} \left( g_{j+1/2}^*(t) - g_{j-1/2}^*(t) \right) dt \\ &= \int_{\mathbb{R}_+} \sum_{j \in \mathbf{Z}} \frac{\theta_{j+1}(t) - \theta_j(t)}{h} g_{j+1/2}^*(t) dt \\ &= \int_{\mathbb{R}_+} \sum_{j \in \mathbf{Z}} \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \left( g_{j+1/2}^*(t) - g(v_j(t)) \right) dt \\ & \quad + \int_{\mathbb{R}_+} \sum_{j \in \mathbf{Z}} \frac{\theta_{j+1}(t) - \theta_j(t)}{h} g(v_j(t)) dt. \end{aligned}$$

The latter term converges, by definition of the Young measure, toward

$$\int \int_{\mathbb{R} \times \mathbb{R}_+} \partial_t \theta \langle \nu^\sharp, g \rangle dx dt.$$

Since the numerical flux  $g^*$  is consistent with the exact flux  $g$ , we have

$$|g_{j+1/2}^* - g(v_j)| \leq C \sum_{i=-p+1}^{p-1} |v_{j+i+1} - v_{j+i}|.$$

Using the notation  $\text{supp } \theta \subset [-R, R] \times [0, T]$ , we have

$$\begin{aligned} & \left| \int_{\mathbb{R}_+} \sum_{j \in \mathbf{Z}} \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \left( g_{j+1/2}^*(t) - g(v_j(t)) \right) dt \right| \\ & \leq C \int_0^T \sum_{-R-1 \leq jh \leq R+1} \left| \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \right| \sum_{i=-p+1}^{p-1} |v_{j+i+1} - v_{j+i}| dt \\ & \leq C' \left( \int_0^T \sum_{-R-1 \leq jh \leq R+1} \left| \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \right|^{\frac{4+\beta}{3+\beta}} dt \right)^{\frac{3+\beta}{4+\beta}} \\ & \quad \times \left( \int_0^T \sum_{-R-2 \leq jh \leq R+2} |v_{j+1} - v_j|^{4+\beta} dt \right)^{\frac{1}{4+\beta}} \\ & \leq C'' h^{\frac{1}{4+\beta}} \|\theta_x\|_{L_{x,t}^{\frac{4+\beta}{3+\beta}}} \longrightarrow 0, \end{aligned}$$

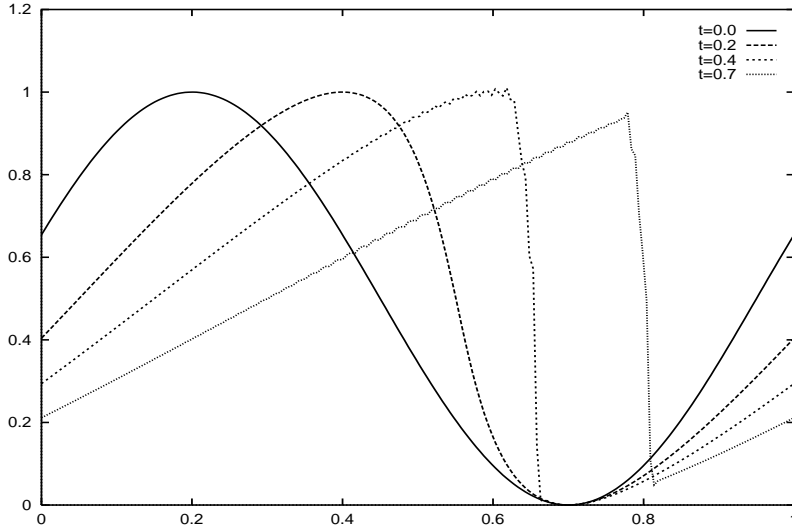


FIG. 4.1. Entropy stable scheme with  $f(u) = u^2/2$  and 200 points.

where we used the dissipation bound (4.6).

To treat the term containing  $\tilde{Q}_{j+1/2}$ , we observe that

$$\left| \int_0^T \sum_{j \in \mathbf{Z}} \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \tilde{Q}_{j+1/2} \cdot (v_{j+1} - v_j) dt \right| \leq C \int_0^T \sum_{j \in \mathbf{Z}} \left| \frac{\theta_{j+1}(t) - \theta_j(t)}{h} \right| |v_{j+1} - v_j| dt$$

and proceed as for the flux term above. We conclude that the Young measure satisfies

$$\partial_t \langle \nu, u \rangle + \partial_x \langle \nu^\sharp, g(v) \rangle = 0;$$

that is, by (4.8),

$$(4.10) \quad \partial_t \langle \nu, u \rangle + \partial_x \langle \nu, f(u) \rangle = 0.$$

The consistency of  $\nu$  with the entropy inequality is checked in a similar fashion. One uses that the entropy flux is bounded by

$$|G_{j+1/2}^* - G(v_j)| \leq C \sum_{i=-p+1}^{p-1} |v_{j+i+1} - v_{j+i}|$$

and that there is a favorable sign on the right-hand side of (4.3). This leads us to the inequality

$$(4.11) \quad \partial_t \langle \nu, U(u) \rangle + \partial_x \langle \nu, F(u) \rangle \leq 0$$

and completes the proof of Theorem 4.1.  $\square$

**Numerical experiments.**

- (1) In Figure 4.1, we display the numerical solutions for the scheme (3.21) with added numerical viscosity. As flux we have Burgers' flux; for the mesh we use 200 points. The initial datum is again  $u_0(x) = 0.5 \sin(2.0\pi(x + 0.05)) + 0.5$ .

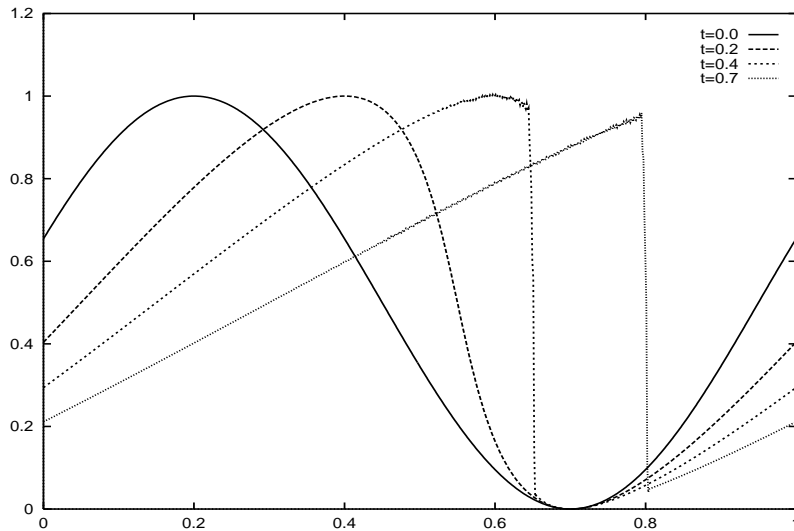


FIG. 4.2. Entropy stable scheme:  $f(u) = u^2/2$  and 800 points.

Each curve corresponds to successive times:  $t = 0.0, 0.2, 0.4, 0.7$ . Figure 4.2 shows the same results but now with 800 points. The strong convergence of the scheme is obvious if we compare with Figures 2.1–3.1. The additional numerical viscosity actually used here is given by

$$(4.12) \quad \tilde{Q}_{j+1/2} = 40.0 \left( (v_{j+2} - v_{j+1})^2 + (v_{j+1} - v_j)^2 + (v_j - v_{j-1})^2 \right).$$

- (2) Next we tested the entropy stable scheme for the cubic conservation law, having  $f(u) = u^3$  and initial data  $u_l = 4.0$ ,  $u_r = -5.0$ . The additional term in this case is chosen to be

$$(4.13) \quad \tilde{Q}_{j+1/2} = (v_{j+1} - v_j)^2.$$

The numerical solution exhibits classical behavior, i.e., the solution consists of a shock with an attached rarefaction (cf. Figure 4.3 with the result for  $t = 0.075$ ). Note that almost no visible oscillations arise even if the additional numerical viscosity (4.13) is very mild compared to (4.12).

- (3) The numerical experiments in section 3 demonstrate that we can produce nonclassical shocks with the scheme (3.1)–(3.2) by variation of  $B^*$ . The next test shows that the oscillations in Figure 3.2 can be dramatically damped if we stabilize the method using (4.13). For the results in Figure 4.4 we took  $f(u) = u^3$ ,  $B^* = 5.0 \cdot B$  and initial data  $u_l = 4.0$ ,  $u_r = -5.0$ . The numerical solution at time  $t = 0.1$  is displayed. We stress the fact that nevertheless this procedure doesn't destroy the development of nonclassical shock waves.

The numerical results for the scheme presented here clearly show that the numerical viscosity drastically tames the oscillations observed earlier with the entropy conservative schemes.

**5. A shock-capturing method for nonclassical shocks.** In this section, we use the high-order, entropy conservative scheme derived in section 3 to compute nonclassical solutions generated by vanishing diffusion-dispersion approximations. We

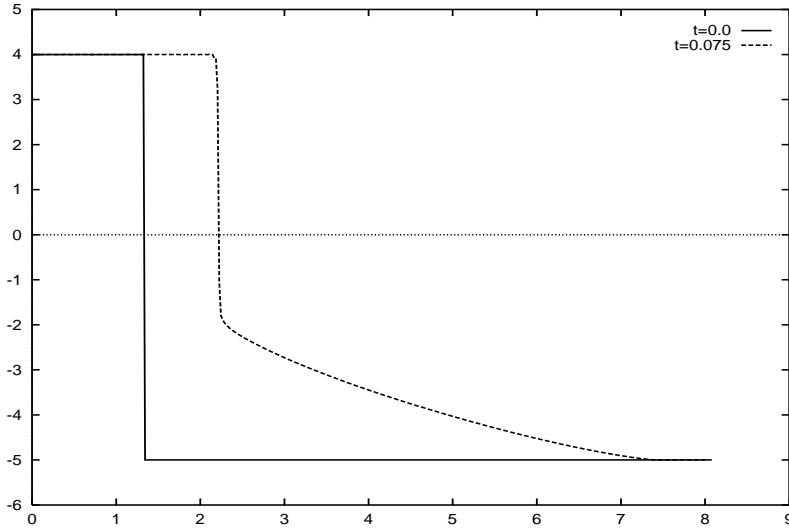


FIG. 4.3. Entropy stable scheme and classical solution:  $f(u) = u^3$  and 400 points.

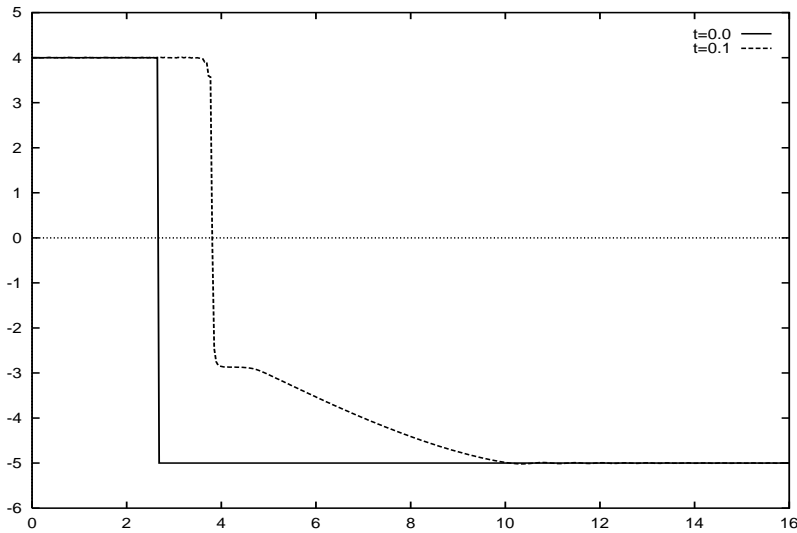


FIG. 4.4. Entropy stable scheme and nonclassical solution:  $f(u) = u^3$  and 400 points.

consider here two different models, one having *linear* regularization in the conservative variable and the other having *linear* regularization in the entropy variable. We use the entropy (2.4) whose interest was pointed out in section 2. We recall from [17] that to each regularization one may associate a kinetic function, say

$$u_+ = \varphi(u_-),$$

which provides the *right state*  $u_+$  across a nonclassical shock as a function of its left state  $u_-$ . The kinetic function will be determined here for several numerical schemes.

Our purpose is to design a computational method to capture nonclassical shocks. As such shocks are known to be regularization-sensitive one must be particularly

cautious when discretizing higher-order terms. The numerical experiments will deal both with the linear regularization

$$(5.1) \quad \partial_t u^{\alpha,\varepsilon} + \partial_x f(u^{\alpha,\varepsilon}) = \varepsilon u_{xx}^{\alpha,\varepsilon} + \alpha \varepsilon^2 u_{xxx}^{\alpha,\varepsilon}$$

and the following model:

$$(5.2) \quad \partial_t u^{\alpha,\varepsilon} + \partial_x f(u^{\alpha,\varepsilon}) = \varepsilon f(u^{\alpha,\varepsilon})_{xx} + \alpha \varepsilon^2 f(u^{\alpha,\varepsilon})_{xxx},$$

which has a regularization term that is linear in the flux variable. Some initial data are given at  $t = 0$  and  $\alpha$  are a fixed parameter.

The limit

$$u^\alpha := \lim_{\varepsilon \rightarrow 0} u^{\alpha,\varepsilon}$$

may differ [23, 17, 18] drastically from the classical solution—corresponding to the choice  $\alpha = 0$  in (5.1)–(5.2); that is, in general,

$$u^0 \neq u^\alpha \quad \text{for } \alpha \neq 0.$$

However, certain conditions are necessary for this to happen: the flux  $f$  should be nongenuinely nonlinear (nonconvex or nonconcave when  $N = 1$ ) and the parameter  $\alpha$  should lie in some range of values depending on the behavior of the flux. For instance, nonclassical shocks are observed for both models (5.1) and (5.2) when

$$(5.3) \quad N = 1 \quad \text{and} \quad f(u) = u^3, \quad \alpha > 0.$$

When  $f(u) = -u^3$ , one needs instead  $\alpha < 0$ .

For simplicity, the rest of the discussion is presented on the model (5.2), assuming that the linearity assumption (2.19) holds. Our discussion therefore includes the scalar equation (Example 2.1) and the system of elasticity (Example 2.2). We want to calculate the limit  $u^\alpha$  using a conservative and semidiscrete difference scheme:

$$(5.4) \quad u'_j(t) = -\frac{1}{h} \left( g_{j+1/2}(t) - g_{j-1/2}(t) \right).$$

We define the following numerical flux composed of two parts:

$$(5.5) \quad g(v_{-1}, \dots, v_2) = g^*(v_{-1}, \dots, v_2) + \tilde{g}(v_{-1}, \dots, v_2).$$

Here  $g^*$  is chosen to

- (1) either Tadmor's second-order flux, or
- (2) the new fourth-order entropy conservative scheme discovered in Theorem 3.4.

The flux  $\tilde{g}$  is defined to be a discretization of the regularization

$$(5.6) \quad \tilde{g}(v_{-1}, v_0, v_1, v_2) = -\frac{\beta}{2}(u_1 - u_0) - \frac{\gamma}{6}(u_2 - u_1 - u_0 + u_{-1}), \quad u = u(v),$$

in case (5.1) and

$$(5.7) \quad \tilde{g}(v_{-1}, v_0, v_1, v_2) = -\frac{\beta}{2}(v_1 - v_0) - \frac{\gamma}{6}(v_2 - v_1 - v_0 + v_{-1})$$

for (5.2). Here  $\beta$  and  $\gamma$  are two numerical constants to be chosen in agreement with the physical parameter  $\alpha$ . (See Theorem 5.1 below.)



Calling  $u^{(\beta,\gamma),h}$  the numerical solution and calling

$$u^{(\beta,\gamma)} := \lim_{h \rightarrow 0} u^{(\beta,\gamma),h}$$

the limit obtained by one of the above schemes, we stress that in general

$$(5.8) \quad u^{\beta,\gamma} \neq u^\alpha.$$

The kinetic relations determined numerically below allow us to estimate precisely the discrepancy between the analytical solution  $u^\alpha$  and the numerical solution  $u^{(\beta,\gamma)}$ . We will see below that only the ratio  $\gamma/\beta^2$  is relevant. We are particularly interested in pointing out any qualitative differences between the two models (7.1)–(7.2).

Let us make some notes on model (5.2). For the cubic flux  $f(u) = u^3$  and the entropy defined by  $U'(u) = 3u^3/4$ , i.e.,

$$U(u) = u^4,$$

we can describe the set of nonclassical shocks issuing from the left state  $u_l > 0$ . The right states must satisfy the Rankine–Hugoniot relation

$$\sigma = u^2 + u u_l + u_l^2$$

and the entropy inequality

$$-\sigma(u^4 - u_l^4) + 2(u^6 - u_l^6) \leq 0.$$

We find that

$$(u - u_l)^2(u^2 + u u_l + u_l^2)(u^2 - u_l^2) \leq 0.$$

Therefore, since the values  $u \in (u_l/2, u_l)$  correspond to classical Oleinik-entropy discontinuities, the interval for nonclassical shocks is

$$(5.9) \quad u \in (-u_l, -u_l/2).$$

Interestingly, this is exactly the same interval found in [17] for the quadratic entropy  $U(u) = u^2$ .

Finally we observe that the scheme satisfies a cell entropy inequality.

**THEOREM 5.1.** *The above scheme (5.5), (5.7) satisfies the cell entropy inequality*

$$(5.10) \quad U(u_j)'(t) + \frac{1}{h}(G_{j+1/2}(t) - G_{j-1/2}(t)) \leq 0,$$

where the numerical entropy flux is composed of two parts,

$$(5.11) \quad G_{j+1/2}(t) = G_{j+1/2}^*(t) + \tilde{G}_{j+1/2}(t).$$

Here  $G^*$  is defined by (3.3) and

$$(5.12) \quad \tilde{G}_{j+1/2}(t) = -\frac{\beta}{2}v_j(v_{j+1} - v_j) - \frac{\gamma}{6}(v_{j-1}v_{j+1} + v_jv_{j+2} - 2v_jv_{j+1}).$$

If, moreover,

$$(5.13) \quad \frac{\gamma}{\beta^2} = \frac{3}{4}\alpha,$$

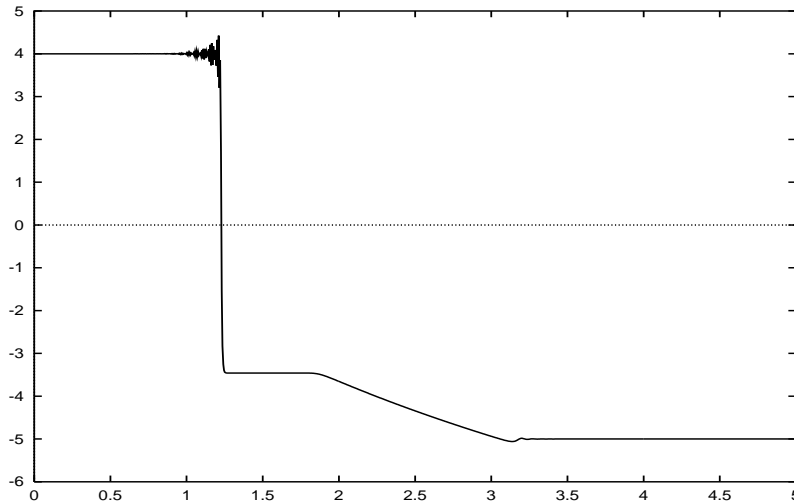


FIG. 5.1. Nonclassical shock + Nonattached rarefaction for model (5.1).

its equivalent equation up to third-order included coincides with the continuous model (7.2),

$$(5.14) \quad \partial_t u + \partial_x f(u) = \frac{\beta}{2} \left( h f(u)_{xx} + \alpha h^2 f(u)_{xxx} \right).$$

Of course the constant  $3/4$  in (5.13) can be scaled out in the definition of  $\beta, \gamma$ .

*Proof.* It is straightforward to calculate that

$$U(u_j)'(t) + \frac{1}{h} (G_{j+1/2}(t) - G_{j-1/2}(t)) = -D_j(t),$$

where

$$D_j(t) = \frac{\beta}{2} |v_j(t) - v_{j-1}(t)|^2 \geq 0.$$

The second part is also an easy calculation from the definitions.  $\square$

#### Numerical experiments for model (5.1).

- (1) We start with numerical calculations for single Riemann problems using the method (2.9) where the entropy conservative flux is given by (3.9). The physical and numerical coefficients are chosen to be  $\beta = 5.0$  and  $\gamma = 37.5$ .

In Figure 5.1 we see the result at time  $t = 0.03$  obtained for the initial data  $u_l = 4.0$  and  $u_r = -5.0$ . The solution consists of a shock and a fast rarefaction with a constant middle state in between which identifies the shock to be nonclassical. If we choose  $u_l = 4.0$  and  $u_r = -3.0$  we get a two-shock solution. The slow shock is of nonclassical type while the fast wave is classical (cf. Figure 5.2). Time is  $t = 0.03$ . These two different pictures are representative for all Riemann solutions of the scalar problem involving nonclassical waves.

For both calculations we used a grid of 400 points. Let us remark that in either case visible oscillations are only observed after the slow and before the fast wave.

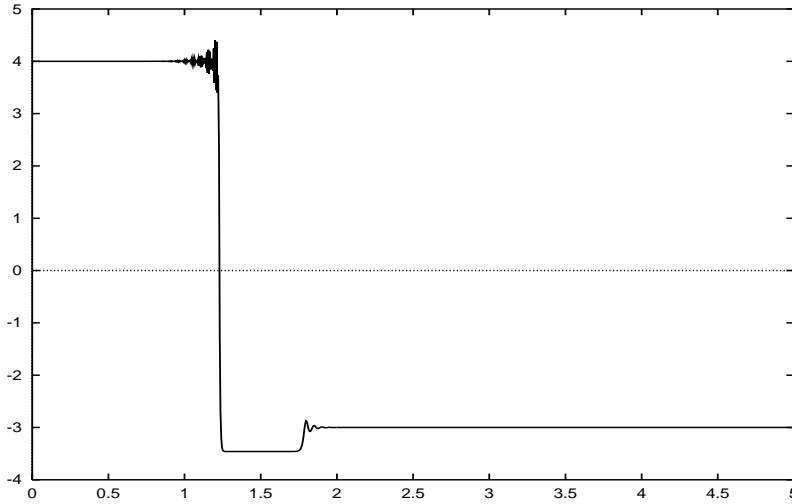


FIG. 5.2. Nonclassical shock + Classical shock for model (5.1).

- (2) The next numerical test is devoted to the comparison of results obtained by the numerical scheme for a specific choice of  $\beta, \gamma, h$  and the corresponding limit  $\lim_{\varepsilon \rightarrow 0} u^{\varepsilon, \alpha}$ ,  $\alpha > 0$  of the model problem (5.1). We let  $\alpha = 1.0$  and choose the parameters according to

$$\beta = 5.0, \quad \gamma = 18.75, \quad h = 0.005.$$

This choice agrees with (5.13) above. From our analytical observation on the equivalent scheme, then, the results should be close to  $\lim_{\varepsilon \rightarrow 0} u^{\varepsilon, \alpha}$  in model problem (5.1).

The test will be done by the computation of a series of Riemann problems that lead to nonclassical shocks, following the paper of LeFloch and Hayes [19]. We consider the Riemann problems to initial data  $u_l > 0$  and  $u_r = -1.25u_l$  for  $u_l$  taking values in  $[1.0, 15.0]$ . The solution consists of a shock connecting  $u_l$  and a middle state  $u_m$  which goes over to  $u_r$  by a separated rarefaction. From the analysis in [23, 17] we know the exact state  $u_m$  for  $\alpha = 1.0$ . In Figure 5.3 we plotted the calculated middle states together with the exact states, the classical states ( $u_m = -u_l/2$ , directly attached rarefaction) and the extreme nonclassical solution ( $u_m = u_l$ ), and the traveling-wave solution. If we take for  $g^*$  the second-order entropy conservative flux we obtain a reasonable approximation for small values of  $u_l$  as expected. For bigger values the calculated middle state becomes more classical and is nearly identical with the classical solution for  $u_l > 12.5$ . The approximation behavior for the scheme (5.4) is somewhat better. We note that even for big values the middle state indicates a nonclassical solution.

To compare the quality of approximation further we have calculated the entropy dissipation  $\phi$  for the nonclassical shock depending on the shock speed  $s$ . The result is displayed in Figure 5.4. Note that the function  $\phi(s)$  is scaled by  $s^2$ .

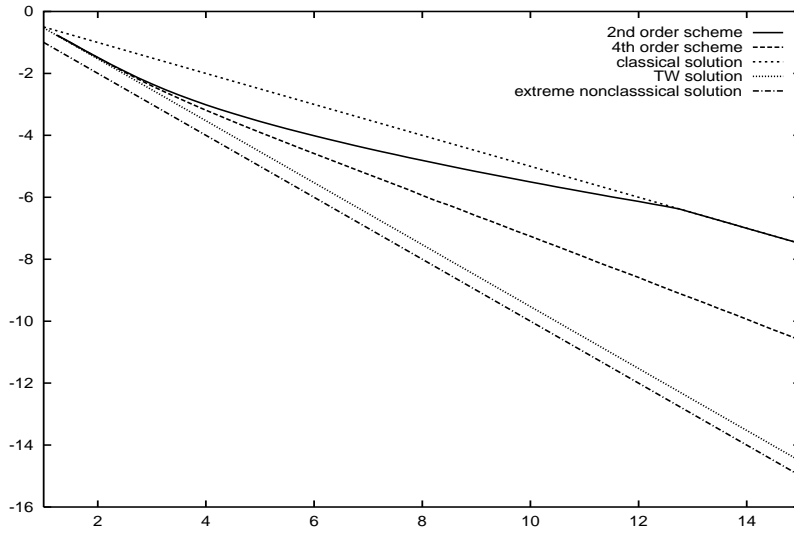


FIG. 5.3. Middle state versus left state for the first model.

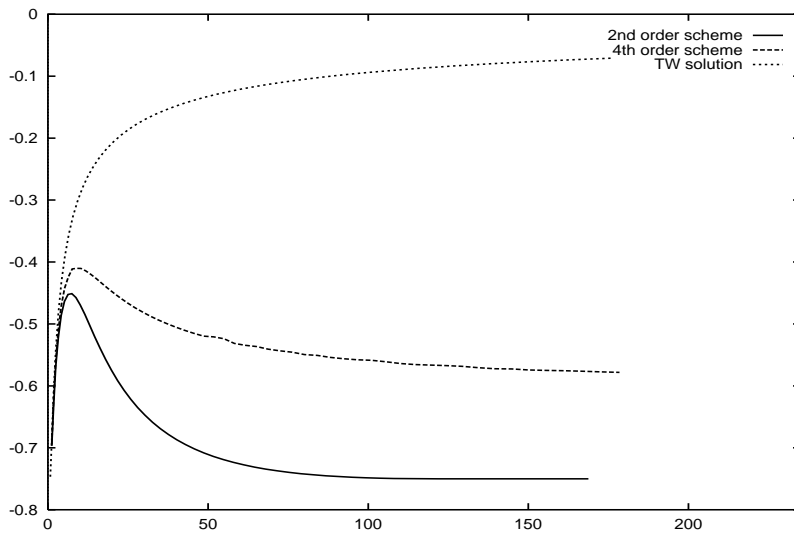


FIG. 5.4. Entropy dissipation versus shock speed for the first model.

**Numerical experiments for model (5.2).** Finally we present numerical calculations for the model equation (5.2). In Figure 5.5 one can see the result that we obtained choosing  $g_{j+1/2}^*$  to be the higher-order flux (3.3). Initial data are  $u_l = 75.0$  and  $u_r = 93.75$ . We used 1600 mesh points and  $t$  is equal to 0.0004. Note that the scheme does not produce visible oscillations in contrast to the tests for (5.1) even for such a big jump. Figure 5.6 exhibits a nonclassical shock followed by a classical shock. The initial data were taken to be the sine function. We used 5000 points for the mesh. Let us remark that typically the resolution of the nonclassical shock is much better than for the fast classical shock. Compare also Figure 5.2.

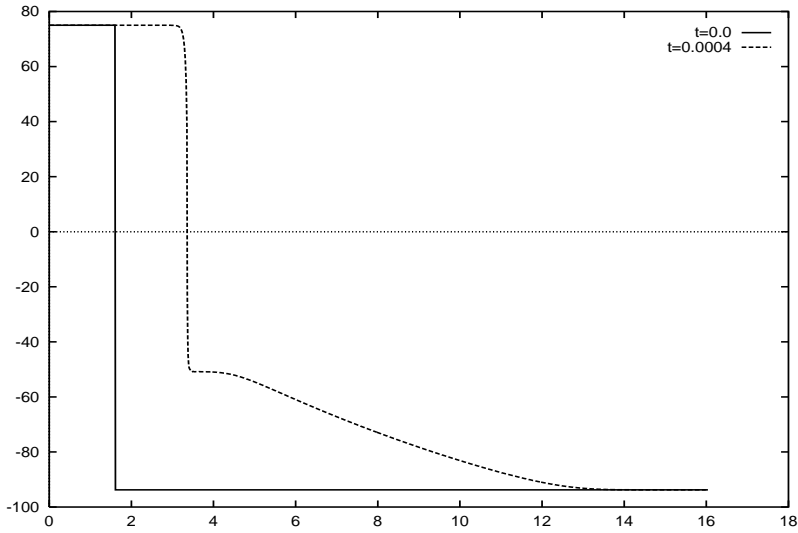


FIG. 5.5. *Nonclassical shock + nonattached rarefaction for the second model.*

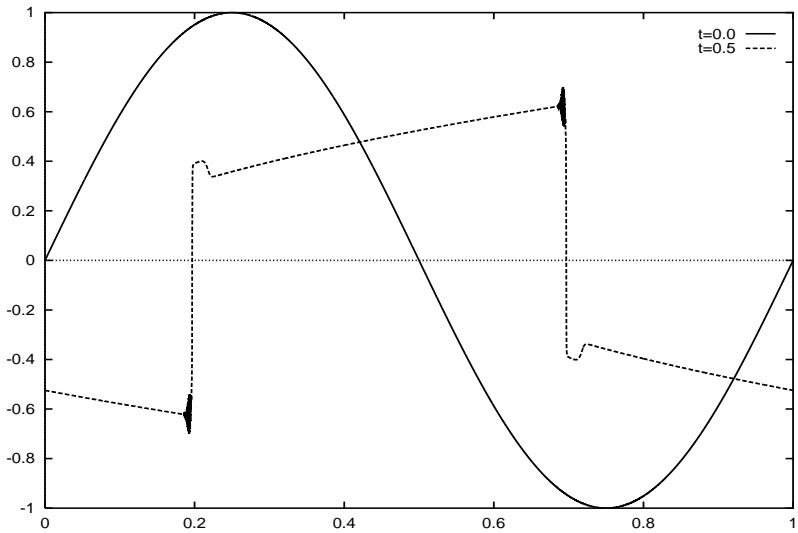


FIG. 5.6. *Nonclassical shock + classical shock for the second model.*

As in the case of (5.1) we tested how well the schemes capture nonclassical shocks. To this end we choose exactly the same setting of parameters as for (5.1). But for the states  $u_l$  we took values from the even larger interval  $[5.0, 150.0]$ . The results can be seen in Figure 5.7. Both schemes do *not* collapse to the classical solution and provide nearly the same middle states. A close view of the numerical data shows that the third-order scheme produces a somewhat more nonclassical solution. This is demonstrated with Figure 5.8 where we plot the difference between the two middle states.

**6. Fully-discrete Lax–Wendroff type schemes.** In this section we turn to fully-discrete schemes, focusing for simplicity on scalar conservation laws. Theorem

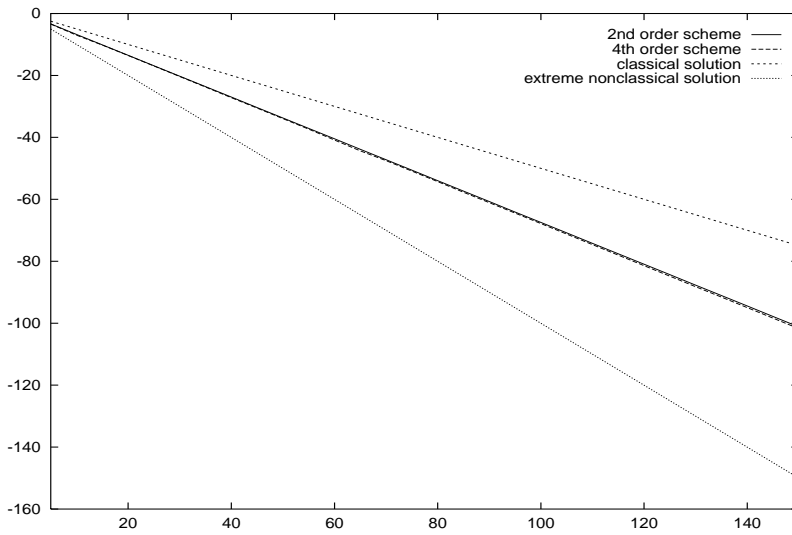


FIG. 5.7. Middle state versus left state for the second model.

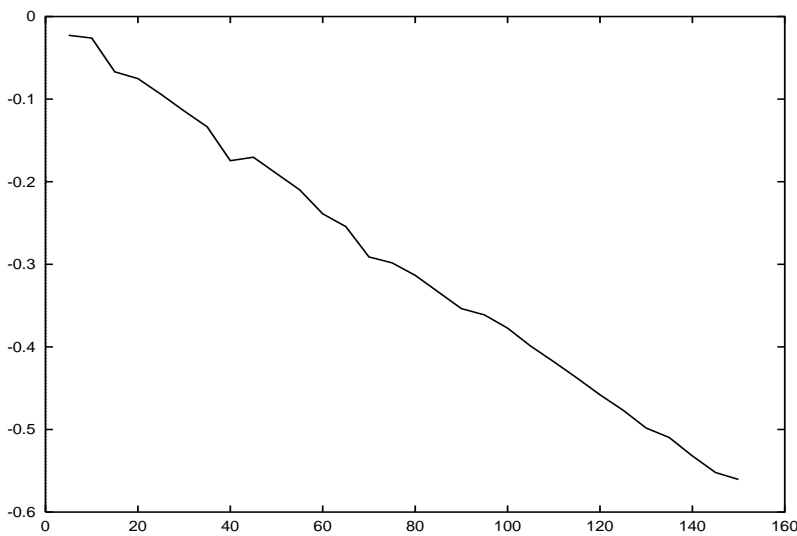


FIG. 5.8. Difference between the middle states for the two schemes.

6.1 below shows that the framework developed for semidiscrete schemes *cannot* be generalized to fully-discrete schemes. This leads us to study directly whether the Lax–Wendroff scheme—a typical second-order and fully discrete scheme closely related to the entropy conservative and semidiscrete schemes considered earlier—is entropy consistent, making along the way a striking connection with the results of the previous sections.

Denote by  $h$  and  $k$  the space and time mesh lengths and set

$$x_j = j h, \quad j \in \mathbf{Z}; \quad t_n = n k, \quad n \in \mathbf{N}, \quad \lambda = \frac{k}{h}.$$

We deal here with  $(2p+1)$ -point, fully discrete and conservative schemes of the general form

$$(6.1) \quad u_j^{n+1} = u_j^n - \lambda (g_{j+1/2}^n - g_{j-1/2}^n),$$

where  $g_{j+1/2}^n = g(u_{j-p+1}^n, \dots, u_{j+p}^n)$  is a numerical flux consistent with the exact flux  $f$ .

First, we prove the nonexistence of entropy conservative schemes.

**THEOREM 6.1.** *Consider a scalar conservation law together with a strictly convex entropy  $U$ . Suppose there exists a fully discrete scheme of the form (6.1) that is also entropy conservative in the sense*

$$(6.2) \quad U(u_j^{n+1}) - U(u_j^n) + \lambda (G_{j+1/2}^n - G_{j-1/2}^n) = 0$$

for some function  $G_{j+1/2}^n = G(u_{j-p+1}^n, \dots, u_{j+p}^n)$ . Assume that  $\lambda$  satisfies the stability condition

$$(6.3) \quad \lambda \max_{j \in \mathbf{Z}, n \in \mathbf{N}} \left| \frac{\partial g_{j+1/2}^n}{\partial v_j} \right| \leq 1, \quad \lambda \max_{j \in \mathbf{Z}, n \in \mathbf{N}} \left| \frac{\partial g_{j+1/2}^n}{\partial v_{j+1}} \right| \leq 1.$$

Then  $f$  is an affine function and the scheme is the upwinding scheme with moreover  $\lambda |f'| \equiv 1$ .

Our condition (6.3) is a variant of the standard Courant–Friedrichs–Lewy (CFL) condition

$$(6.4) \quad \lambda \max_{j \in \mathbf{Z}, n \in \mathbf{N}} |f'(u_j^n)| \leq 1.$$

*Remark 6.2.* Observe that no assumption is put on the order of accuracy of the scheme and that the function  $G$  is not explicitly assumed to be consistent with the entropy flux associated with  $U$ .

*Remark 6.3.* Recall that in [37], Schonbek proved (for systems of conservation laws) that if a *fully discrete* and *three-point* scheme satisfies a cell entropy inequality, then it is at most first-order accurate.

*Proof.* To simplify the presentation, we give the proof for a three-point scheme. It is straightforward to generalize inductively the forthcoming argument to deal with any  $2p + 1$ -point scheme.

Consider the function

$$H(u_0, u_1, u_2) = U(u_1 - \lambda (g(u_1, u_2) - g(u_0, u_1))) - U(u_1) + \lambda (G(u_1, u_2) - G(u_0, u_1)),$$

which by assumption vanishes identically. Compute the derivative  $\partial_{u_0} \partial_{u_2}$ :

$$0 = U''(u_1 - \lambda (g(u_1, u_2) - g(u_0, u_1))) \lambda g'_0(u_0, u_1) (-\lambda) g'_1(u_1, u_2).$$

Since  $U'' > 0$ , we have either

$$g'_0(u_0, u_1) \equiv 0 \text{ or } g'_1(u_1, u_2) \equiv 0.$$

In the first case,  $g'_0 \equiv 0$ , we obtain

$$H(u_1, u_2) = U(u_1 - \lambda (g(u_2) - g(u_1))) - U(u_1) + \lambda (G(u_1, u_2) - G(u_0, u_1)).$$

Since only  $G(u_0, u_1)$  may possibly depend on the variable  $u_0$ , we deduce that in fact the function  $G$  depends only on its second argument too. Then computing  $\partial_{u_1} \partial_{u_2}$  yields

$$g'(u_2) \left(1 - \lambda g'(u_1)\right) = 0$$

for all  $u_1, u_2$ . Therefore  $g \equiv \text{const}$  and  $f \equiv \text{const}$  or else  $g$  and  $f$  are linear function and  $\lambda g' \equiv 1$ .

In the second case,  $g'_1 \equiv 0$ , we obtain

$$H(u_1, u_2) = U\left(u_1 - \lambda(g(u_1) - g(u_0))\right) - U(u_1) + \lambda\left(G(u_1, u_2) - G(u_0, u_1)\right),$$

and therefore the entropy flux is also independent of its second argument. Computing now the derivative  $\partial_{u_0} \partial_{u_1}$  yields

$$g'(u_0) \left(1 - \lambda g'(u_1)\right) = 0,$$

and we reach the same conclusion. The proof is completed.  $\square$

In the rest of this section, we investigate the entropy stability of Lax–Wendroff type schemes [31].

Introduce a “numerical speed”  $a_{j+1/2}^n \in \mathbb{R}$  (for each  $j \in \mathbf{Z}$ ) that is consistent with  $f'(u_j^n)$ . Later on, we will make a more specific choice for  $a_{j+1/2}^n$ . Define the initial discretization  $u_j^0$  for  $j \in \mathbf{Z}$  via the initial data which are assumed to be in  $L^1(\mathbf{R}) \cap L^\infty(\mathbf{R})$ .

The fully-discrete Lax–Wendroff scheme takes the form  $n = 1, 2, \dots, j \in \mathbf{Z}$ ,

(6.5)

$$\begin{aligned} u_j^{n+1} &= u_j^n - \frac{\lambda}{2} (f(u_{j+1}^n) - f(u_{j-1}^n)) \\ &\quad + \frac{\lambda^2}{2} \left( a_{j+1/2}^n (f(u_{j+1}^n) - f(u_j^n)) - a_{j-1/2}^n (f(u_j^n) - f(u_{j-1}^n)) \right). \end{aligned}$$

Using the notation

$$g_{j+1/2}^n = \frac{1}{2} (f(u_{j+1}^n) + f(u_j^n)) - \frac{\lambda}{2} a_{j+1/2}^n (f(u_{j+1}^n) - f(u_j^n)),$$

we can rewrite the scheme in the conservation form (6.1). The scheme is second-order in space and time when  $a_j^n$  is consistent with  $f'(u_j^n)$ .

For the sake of making comparisons, we also consider a semidiscrete version of the Lax–Wendroff scheme: For  $j \in \mathbf{Z}$ , the function  $u_j : [0, \infty) \rightarrow \mathbb{R}$  satisfies

(6.6)

$$\begin{aligned} u_j'(t) &= -\frac{1}{2h} \left( f(u_{j+1}(t)) - f(u_{j-1}(t)) \right) \\ &\quad + \frac{\lambda}{2h} \left( a_{j+1/2}(t) \left( f(u_{j+1}(t)) - f(u_j(t)) \right) - a_{j-1/2}(t) \left( f(u_j(t)) - f(u_{j-1}(t)) \right) \right), \end{aligned}$$

where  $\lambda$  is here a given parameter and  $a_{j+1/2}$  satisfies

$$(6.7) \quad a_{j+1/2}(t) = \frac{f'(u_j(t)) + f'(u_{j+1}(t))}{2} + O\left(u_{j+1}(t) - u_j(t)\right)^2.$$



Observe that this scheme is only first-order accurate.

To establish the entropy stability of the Lax–Wendroff scheme, we should determine a convex function  $U$  such that

$$(6.8) \quad \sum_{j=-\infty}^{\infty} U(u_j^{n+1}) \leq \sum_{j=-\infty}^{\infty} U(u_j^n)$$

holds for all  $n \in \mathbf{N}$ . In the rest of this section we will provide analytical and numerical evidence for the following.

*Conjecture.* Consider an increasing flux function  $f$  and the convex entropy  $U$  defined by

$$(6.9) \quad U(u) := \int^u f(s) ds.$$

Then, for  $\lambda$  sufficiently small, the fully-discrete Lax–Wendroff type scheme (6.5) satisfies the entropy inequality (6.8).

To deal with decreasing fluxes, one should use  $U' = -f$  instead. It is interesting to note that the choice (6.9) was already proposed earlier, in the context of semidiscrete schemes. This is explained as follows. In the situation of Theorem 2.5, Tadmor’s second-order, entropy conservative scheme coincides with the centered scheme. The latter is also the dominant part of the scheme (6.5) when  $\lambda$  approaches zero. Therefore it is natural to use here also the same entropy function (6.9).

**THEOREM 6.4.** *Consider an increasing flux function  $f$  and the entropy  $U$  defined by (6.9). Consider the Lax–Wendroff scheme (6.5) with  $a_{j+1/2}^n$  given by*

$$(6.10) \quad a_{j+1/2}^n = \frac{f'(u_{j+1}^n) + f'(u_j^n)}{2} + O(\lambda) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^2.$$

*If the scheme is  $L^\infty$  stable, then it satisfies the entropy inequality*

$$(6.11) \quad \begin{aligned} & \sum_{j=-\infty}^{\infty} U(u_j^{n+1}) - \sum_{j=-\infty}^{\infty} U(u_j^n) \\ & \leq -\frac{\lambda^2}{4} \sum_{j=-\infty}^{\infty} f_j^n \left( f(u_{j+1}^n) - 2f(u_j^n) + f(u_{j-1}^n) \right)^2 + O(\lambda^3) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^3. \end{aligned}$$

*Remark 6.5.* Majda and Osher [36] have introduced a modified version of the Lax–Wendroff scheme, based a nonlinear, artificial diffusion term. It is also shown therein through a concrete example that the original Lax–Wendroff scheme is not  $L^p$ -stable for Burgers’ equation whenever the data change sign, i.e., when a sonic point arises.

*Proof.* For simplicity we omit the upper index  $n$  throughout and let  $f_j = f(u_j)$ . Using a Taylor expansion in  $\lambda$  in the (consistent and essentially three-point) scheme (6.1), we find

$$\begin{aligned} U(u_j^{n+1}) &= U\left(u_j - \lambda\left(g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}\right)\right) \\ &= U_j - \lambda U_j' \left(g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}\right) + \frac{\lambda^2}{2} U_j'' \left(g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}\right)^2 \\ &\quad + O(\lambda^3) \left(|u_j^n - u_{j-1}^n|^3 + |u_{j+1}^n - u_j^n|^3\right). \end{aligned}$$

For the Lax–Wendroff scheme (6.5) we deduce

$$\begin{aligned}
 (6.12) \quad U(u_j^{n+1}) &= U_j - U'_j \frac{\lambda}{2} (f_{j+1} - f_{j-1}) \\
 &\quad + U'_j \frac{\lambda^2}{2} \left( a_{j+1/2} (f_{j+1} - f_j) - a_{j-1/2} (f_j - f_{j-1}) \right) \\
 &\quad + U''_j \frac{\lambda^2}{8} (f_{j+1} - f_{j-1})^2 + O(\lambda^3) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^3.
 \end{aligned}$$

We sum up with respect to  $j \in \mathbf{Z}$  and get for the terms in (6.12) of order less than three

$$\sum_{j=-\infty}^{\infty} U(u_j^{n+1}) - \sum_{j=-\infty}^{\infty} U(u_j^n) = \sum_{j=-\infty}^{\infty} \left( R_1^j + R_2^j + R_3^j \right) + O(\lambda^3) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^3,$$

with obvious notation. Using the special choice  $U' = f$  leads for  $R_1^j$  to

$$(6.13) \quad -\frac{\lambda}{2} \sum_{j=-\infty}^{\infty} U'_j (f_{j+1} - f_{j-1}) = -\frac{\lambda}{2} \sum_{j=-\infty}^{\infty} f_j f_{j+1} - f_{j-1} f_j = 0.$$

For  $R_2^j$  and  $R_3^j$  we obtain

$$\begin{aligned}
 \sum_{j=-\infty}^{\infty} R_1^j + R_2^j &= \frac{\lambda^2}{2} \sum_{j=-\infty}^{\infty} U'_j \left( a_{j+1/2} (f_{j+1} - f_j) - a_{j-1/2} (f_j - f_{j-1}) \right) + \frac{1}{4} U''_j (f_{j+1} - f_{j-1})^2 \\
 &= \frac{\lambda^2}{8} \sum_{j=-\infty}^{\infty} f'_j (f_{j+1} - f_{j-1})^2 - 2 a_{j+1/2} (f_{j+1} - f_j)^2 - 2 a_{j-1/2} (f_j - f_{j-1})^2 \\
 &= \frac{\lambda^2}{8} \sum_{j=-\infty}^{\infty} (f'_j - 2 a_{j+1/2}) (f_{j+1} - f_j)^2 + (f'_j - 2 a_{j-1/2}) (f_j - f_{j-1})^2 \\
 &\quad + 2 f'_j (f_{j+1} - f_j) (f_j - f_{j-1}).
 \end{aligned}$$

For the last equality we used the identity

$$(f_{j+1} - f_{j-1})^2 = (f_{j+1} - f_j)^2 + 2(f_{j+1} - f_j)(f_j - f_{j-1}) + (f_j - f_{j-1})^2.$$

We proceed using (6.10) and get

$$\begin{aligned}
 (6.14) \quad &\sum_{j=-\infty}^{\infty} R_1^j + R_2^j \\
 &= \frac{\lambda^2}{8} \sum_{j=-\infty}^{\infty} \left( -f'_{j+1} (f_{j+1} - f_j)^2 - f'_{j-1} (f_j - f_{j-1})^2 + 2f'_j (f_{j+1} - f_j) (f_j - f_{j-1}) \right) \\
 &\quad + O(\lambda^3) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^3 \\
 &= -\frac{\lambda^2}{8} \sum_{j=-\infty}^{\infty} f'_j \left( f_{j+1} - 2f_j + f_{j-1} \right)^2 + O(\lambda^3) \sum_{j=-\infty}^{\infty} |u_{j+1}^n - u_j^n|^3.
 \end{aligned}$$

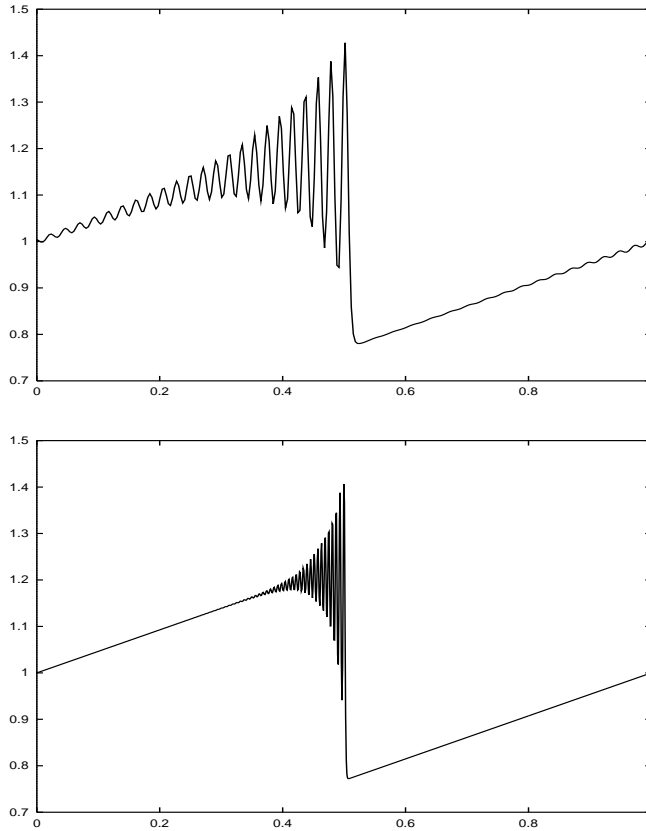


FIG. 6.1. Lax–Wendroff scheme with 200 and 1000 points.

Combining (6.13) and (6.14) gives the statement.  $\square$

Exactly the same arguments can be used to show the entropy stability of the semidiscrete Lax–Wendroff scheme (6.6), again for the choice (6.10). In this case *all* terms are handled. Note that in this case due to the multiplication of (6.6) with  $U'(u_j(t))$  no Taylor expansion is necessary and consequently no higher-order terms arise. We state without proof the following theorem.

**THEOREM 6.6.** *Consider an increasing flux function  $f$  and the entropy  $U$  defined by (6.9). Consider the Lax–Wendroff scheme (6.6) with  $a_{j+1/2}(t)$  given by*

$$(6.15) \quad a_{j+1/2}(t) = \frac{f'(u_{j+1}(t)) + f'(u_j(t))}{2}.$$

*Then we have the entropy inequality*

$$(6.16) \quad \frac{d}{dt} \sum_{j=-\infty}^{\infty} U(u(t)) \leq -\frac{\lambda^2}{4} \sum_{j=-\infty}^{\infty} f'_j(t) \left( f_{j+1}(t) - 2f_j(t) + f_{j-1}(t) \right)^2.$$

**Numerical experiments.** Figure 6.1 demonstrates numerically that the Lax–Wendroff scheme converges to the classical entropy solution for Burgers' equation. One can see the results for numerical calculations with 200 and 1000 mesh points at time  $t = 2.0$ . The initial datum was  $u_0(x) = \sin(2.0\pi x) + 1.0$ .

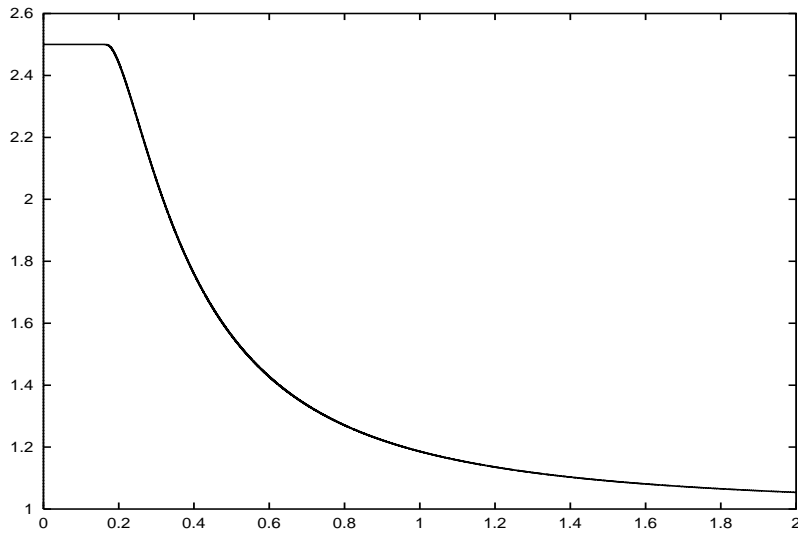


FIG. 6.2. Total entropy  $\sum_j U_1(u_j)$  versus time.

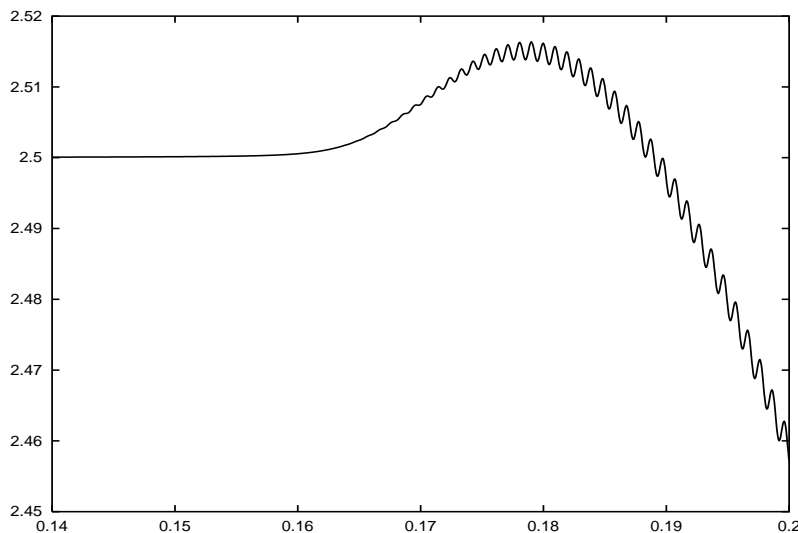


FIG. 6.3. Total entropy  $\sum_j U_2(u_j)/5.775$  versus time.

This periodic test case is now used to calculate the behavior of some entropy functional  $\sum_j U(u_j(t))$  in time. We have done numerical tests that support the conjecture that the entropy stability should hold for  $\lambda$  sufficiently small with the choice of entropy  $U_1(u_j(t)) = (u_j(t))^3/6$  which corresponds to  $U' = f$ . Figure 6.2 shows that  $\sum_j U_1(u_j(t))$  is decreasing in time. In contrast to  $U_1$  the entropy  $U_2(u_j(t)) = (u_j(t))^6$  leads to a nondecreasing functional which is displayed in Figure 6.3 for part of the time interval. Note that the kink in the graphs corresponds to the shock arising for  $t = 1/2\pi \approx 0.16$ . We performed both calculations with 1000 mesh points and a CFL-number of 0.1.

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