FULLY DISCRETE, ENTROPY CONSERVATIVE SCHEMES OF ARBITRARY ORDER[*]

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Abstract. We consider weak solutions of (hyperbolic or hyperbolic-elliptic) systems of conservation laws in one-space dimension and their approximation by finite difference schemes in conservative form. The systems under consideration are endowed with an entropy-entropy flux pair. We introduce a general approach to construct *second and third order accurate, fully discrete* (in both space and time) *entropy conservative schemes.* In general, these schemes are fully nonlinear implicit, but in some important cases can be explicit or linear implicit. Furthermore, semidiscrete entropy conservative schemes of *arbitrary order* are presented. The entropy conservative schemes are used to construct a numerical method for the computation of weak solutions containing nonclassical regularization-sensitive shock waves. Finally, specific examples are investigated and tested numerically. Our approach extends the results and techniques by Tadmor [in *Numerical Methods for Compressible Flows—Finite Difference, Element and Volume Techniques,* ASME, New York, 1986, pp. 149–158], LeFloch and Rohde [*SIAM J. Numer. Anal.,* 37 (2000), pp. 2023–2060].

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1. Introduction. In this paper, we are interested in the numerical approximation of discontinuous solutions of general systems of conservation laws of the form

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

endowed with a smooth entropy-entropy flux pair $(U, F) : \mathbb{R}^N \to \mathbb{R}^2$. In (1.1), the flux-function $f : \mathbb{R}^N \to \mathbb{R}^N$ is a smooth given mapping. As is well known, we should seek solutions satisfying the entropy inequality

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

understood in the sense of distributions.

From the numerical standpoint, following Lax and Wendroff [12], it is natural to search for (fully discrete in space and time) conservative schemes associated with (1.1) which, furthermore, satisfy a discrete version of the inequality (1.2). Whenever the Cauchy problem for (1.1)–(1.2) is well-posed (for instance, when (1.1) is a scalar conservation law with convex flux) such a scheme can converge only to the (so-called) entropy solution of interest.

Weak (entropy) solutions of (1.1) can be considered as limits of solutions of higher order systems with vanishing regularization terms. The physical meaning of these terms comes from viscosity, heat conduction, or capillarity usually leading to a smooth

solution that satisfies (1.2) in the pointwise sense. In some situations it is necessary to control explicitly the rate of dissipation that one introduces (in the continuous as well as in the discrete setting).

In this context it has been suggested that the numerical approximation of (1.1) should be based on schemes satisfying (1.2) as an *equality* (cf. [10]), that is

$$(1.3) \qquad \partial_t U(u) + \partial_x F(u) = 0.$$

High order terms such as viscosity, heat conduction, capillarity, etc., should then be added to such an *entropy conservative scheme* in a way to get an *entropy dissipative scheme*, i.e., satisfying a discrete (consistent) version of (1.2). The notion of *entropy conservative* schemes for conservation laws was introduced first and investigated in a pioneering work by Tadmor [24, 25] when constructing semidiscrete difference schemes satisfying a discrete form of (1.2). For another approach we refer to [21]. In a close context, linear implicit, fully discrete, *energy conservative* schemes were designed in Aregba-Driollet and Mercier [4] (in the spirit of a fully nonlinear scheme introduced by Strauss and Vasquez [22]) to study solutions of semilinear hyperbolic systems satisfying an *energy conservation*, i.e., satisfying (1.3) for a (possibly nonconvex) energy U.

In the light of the above work, attention in the present paper is focused precisely on constructing fully discrete, conservative, and entropy conservative schemes for conservation laws, consistent with both (1.1) and (1.3).

The investigation of semidiscrete schemes (keeping the time variable continuous) was completed only recently. A second order entropy conservative scheme was discovered by Tadmor [24, 25] who introduced this notion in order to construct schemes satisfying a discrete form of (1.2). Next, the notion was further investigated by LeFloch and Rohde [16], who discovered a class of third order entropy conservative schemes.

The study of fully discrete schemes for diffusive-dispersive conservation laws was initiated by Chalons and LeFloch [5]. The authors made a direct use of the semidiscrete numerical fluxes proposed in the earlier papers. By enforcing a suitable CFL stability condition, the entropy inequality (1.2) holds, provided diffusive terms are taken into account in the right-hand side of (1.1).

Our motivation to construct entropy conservative schemes was to study systems of conservation laws that either have nonconvex modes or are of hyperbolic-elliptic type. In this paper we will focus on two representative examples: the first is the cubic scalar conservation law, a nonconvex hyperbolic equation, for which dynamics is well understood and which is used as a test model. The second is a p-system that models adiabatic phase transition dynamics, a hyperbolic-elliptic system; see Truskinovsky [26], Abeyaratne and Knowles [2, 3], and LeFloch [13] for related results in the linearly degenerate case, and see Mercier and Piccoli [18] and references therein for the genuinely nonlinear case. The main difficulty of a nonconvex hyperbolic or hyperbolic-elliptic system of conservation laws is that the single entropy inequality (1.2) does not characterize a unique solution of the system and further selection mechanisms must be added, specifically the so-called *kinetic relation*. For general nonconvex systems, we refer to Hayes and LeFloch [9], LeFloch and Thanh [17], and LeFloch [14].

Kinetic relations can be determined in several situations from physics. From the mathematical point of view they can be exhibited from regularization terms. Kinetic regularizations associated with difference schemes were numerically determined and

compared with analytical kinetic relations in [10]. The dependence of the kinetic relation upon physical and numerical parameters was discussed therein.

An important point is that capillarity terms require high order schemes (at least third order). Thus our first aim is to derive a general approach to construct finite difference schemes for systems of conservation laws that are

(1) fully discrete in space and time,
(2) conservative in the sense of Lax and Wendroff [12],
(3) entropy conservative in the sense of Tadmor [23, 24],
(4) and high order accurate (at least third order).

This program will be carried out in sections 2 and 3. First, we propose a general approach for the construction of such schemes in section 2. Next, in section 3, several classes of second and third order schemes are identified, which can be fully implicit, linear implicit, or explicit methods. This is certainly not a straightforward task. Recall that, for nonaffine f, there are no two time-level, fully discrete, *explicit,* and conservative schemes with smooth numerical flux satisfying a discrete version of the entropy equality; see [16].

In section 4 we return to the investigation of semidiscrete schemes. We will present entropy conservative schemes of *arbitrarily high order*. This can be transferred to the fully discrete case, however, only for a weaker form of entropy conservation.

Finally in section 5, adding appropriate dissipative terms, we will obtain schemes for the above mentioned model problems. Numerical experiments presented in particular in section 6 underline their good performance.

We emphasize that the techniques developed in this paper also apply to other types of evolution equations for which an energy conservation or dissipation is available, such as the heat, Schrödinger, or wave equations. A first result in this direction is given in the second part of subsection 5.2 (Theorem 5.2). Furthermore, these techniques, considered in the one dimensional case, apply straightforwardly to higher dimensions when using Cartesian grids.

2. A general approach to construct entropy conservative schemes. In this section we propose a general method to construct fully discrete, conservative, and entropy conservative schemes.

We follow the notation in Tadmor [24] and LeFloch and Rohde [16]. Call $v(u) = \nabla U(u)$ the *entropy variable* associated with the given entropy U. When the entropy is strictly convex, $v \mapsto v(u)$ is a one-to-one mapping. This can be used as a change of variable (Friedrichs and Lax [7]); that is, we can set

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

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

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

uniquely defined up to a constant.

Furthermore, to deal with examples when U is not globally convex, the following assumption on the flux-function of (1.1) is made:

$$(2.3) \qquad f(u) \text{ and } F(u) \text{ can be expressed as functions of the entropy variable } v;$$

that is, (2.1) holds for some functions g and G. Then, again, ψ can be defined by (2.2). The assumption (2.3), which we make from now on, is motivated by several examples of interest; see [16] and section 5 below. We stress that (2.3) holds in $\mathbb{R}^N$ when U is strictly convex.

For mesh parameters $h, \tau > 0$, let $x_j = j\,h$, $j \in \mathbb{Z}$, and $t_n = n\,\tau$, $n \in \mathbb{N}_0$. We set $\lambda \equiv \tau/h$ and start discussing the (multilevel) time discretization. For $q \in \mathbb{N}$, choose a locally Lipschitz continuous mapping

$$u^* : \left(u^{-q+1}, \ldots, u^0\right) \in \mathbb{R}^{qN} \mapsto u^*\left(u^{-q+1}, \ldots, u^0\right) \in \mathbb{R}^N$$

consistent with the conservative variable u in the sense that

$$u^*\left(u, \ldots, u\right) = u, \quad u \in \mathbb{R}^N.$$

It will be called the *discrete conservative variable* in what follows. The integer q indicates the number of time-levels used by the scheme and is related to the order of accuracy in time. Setting $u_j^{*n} = u^*(u_j^{n-q+1}, \ldots, u_j^n)$, we approximate the continuous derivative $\partial_t u$ in (1.1) by the following discrete derivative:

$$\frac{u_j^{*n+1} - u_j^{*n}}{\tau}.$$

To guarantee that the difference equation is solvable in terms of the conservative variable u_j^{n+1}, we assume that

(2.4)   the mapping $u \mapsto u^*\left(u^{n-q+1}, \ldots, u^n, u\right)$ is smoothly invertible
for all $u^{n-q+1}, \ldots, u^n \in \mathbb{R}^N$.

Next, choose some locally Lipschitz continuous mapping

$$U^* : \left(u^{-q+1}, \ldots, u^0\right) \in \mathbb{R}^{qN} \mapsto U^*\left(u^{-q+1}, \ldots, u^0\right) \in \mathbb{R}$$

consistent with the continuous entropy; i.e.,

$$U^*\left(u, \ldots, u\right) = U\left(u\right), \quad u \in \mathbb{R}^N.$$

It will be called the *discrete entropy function*. Also set $U_j^{*n} = U^*(u_j^{n-q+1}, \ldots, u_j^n)$.

As we will see below the two functions u^* and U^* cannot be chosen arbitrarily from each other. We make the following assumption.

Assumption 2.1. There exists a continuous mapping $v^* : \mathbb{R}^{(N+1)q} \to \mathbb{R}^N$ with the properties

(i) $v^*(u, \ldots, u) = v(u) \qquad (v \in \mathbb{R}^N)$,

(2.5)   (ii) $U^*\left(u^{-q+1}, \ldots, u^0\right) - U^*\left(u^{-q}, \ldots, u^{-1}\right)$
$$= \left(u^*\left(u^{-q+1}, \ldots, u^0\right) - u^*\left(u^{-q}, \ldots, u^{-1}\right)\right) \cdot v^*\left(u^{-q}, \ldots, u^0\right).$$

v^* is called a discrete entropy variable.

Finally, we also set

$$v_j^{*n+1} = v^*\left(u_j^{n-q+1}, \ldots, u_j^{n+1}\right).$$

The validity of Assumption 2.1 will be discussed later on for specific examples.

We now turn to discuss the space discretization, based on a discrete flux

$$g^* : (v_{-p+1}, \ldots, v_p) \in \mathbb{R}^{2pN} \mapsto g^* (v_{-p+1}, \ldots, v_p) \in \mathbb{R}^N,$$

consistent with the continuous flux-function $g(v)$; i.e.,

$$g^* (v, \ldots, v) = g(v), \quad v \in \mathbb{R}^N.$$

Observe that now we rely directly on the entropy variable v. Here the integer p indicates that the scheme uses $2p + 1$ space-levels and is related to the order of accuracy in space: setting

$$g_{j+1/2}^{*n+1} = g^* \left(v_{j-p+1}^{*n+1}, \ldots, v_{j+p}^{*n+1} \right),$$

we are led to a space discretization by replacing the continuous derivative $\partial_x g(v) = \partial_x f(u)$ in (1.1) with

$$\frac{g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1}}{h}.$$

Our approach relies on entropy conservative discrete fluxes. Recall from [25] that a discrete flux g^* (expressed in the entropy variable v) is *entropy conservative* if there exists a *discrete entropy flux*

$$G^* : (v_{-p+1}, \ldots, v_p) \in \mathbb{R}^{2pN} \mapsto G^* (v_{-p+1}, \ldots, v_p) \in \mathbb{R}$$

consistent with the entropy flux $G(v)$ such that

$$(2.6) \quad \begin{aligned} v_0 \cdot & \left(g^* (v_{-p+1}, \ldots, v_p) - g^* (v_{-p}, \ldots, v_{p-1}) \right) \\ &= \quad G^* (v_{-p+1}, \ldots, v_p) - G^* (v_{-p}, \ldots, v_{p-1}). \end{aligned}$$

Finally, also set

$$G_{j+1/2}^{*n+1} = G^* \left(v_{j-p+1}^{*n+1}, \ldots, v_{j+p}^{*n+1} \right).$$

The existence of such entropy conservative fluxes will be discussed below. First we state the central result of this section, providing a general approach to construct classes of fully discrete schemes.

THEOREM 2.2. *Consider a hyperbolic or hyperbolic-elliptic system of conservation laws (1.1) endowed with an entropy-entropy flux pair (U, F) satisfying condition (2.3). Consider a discrete conservative variable u^* and a discrete entropy function U^* such that Assumption 2.1 holds. For $n \in \mathbb{N}$ fixed, let the sequence $\{u_j^n\}_{j \in \mathbb{Z}}$ in $\mathbb{R}^N$ be given.*

Then, for any entropy conservative discrete flux g^* and $0 < \lambda \ll 1$, the $(q+1) \times (2p+1)$-point difference equation

$$(2.7) \qquad u_j^{*n+1} - u_j^{*n} + \lambda \left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1} \right) = 0 \qquad (j \in \mathbb{Z})$$

has a unique solution $u_j^{n+1} \in \mathbb{R}^N$.

The associated scheme is entropy conservative with respect to U^* in the sense that

$$(2.8) \qquad U_j^{*n+1} - U_j^{*n} + \lambda \left(G_{j+1/2}^{*n+1} - G_{j-1/2}^{*n+1} \right) = 0 \qquad (n \in \mathbb{N}, j \in \mathbb{Z}).$$

Proof. The result follows from the discussion preceding the theorem. Indeed, in view of (2.4) and (2.5) and by applying the inverse function theorem, there exists $0 < \lambda \ll 1$ for which (2.7) determines a unique solution u_j^{n+1}. Next, multiplying (2.7) by v_j^{*n+1}, we obtain

$$\left(u_j^{*n+1} - u_j^{*n}\right) \cdot v_j^{*n+1} = \lambda \left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1}\right) \cdot v_j^{*n+1}.$$

The conservative form (2.8) is a direct consequence of the definitions of discrete entropy variable (2.5) and entropy conservative discrete flux (2.6). □

It is the main goal of the following sections to show precisely that the framework in Theorem 2.2 covers a variety of situations of practical interest.

NOTE 2.3.

(1) *The key points for using Theorem* 2.2 *are an appropriate choice of the functions* u^*, U^* *such that Assumption* 2.1 *holds and entropy conservative discrete fluxes* g^* *exist. The choice of the functions* u^*, U^* *will be discussed in section* 3. *A second order entropy conservative discrete flux has been designed in* [25]. *Third order entropy conservative fluxes have been derived in* [16]. *In section* 4 *below, we will return to constructing even higher order entropy conservative fluxes.*

(2) *The entropy equality* (2.8) *implies the following nonlinear stability property:*

$$\sum_{j=-\infty}^{\infty} U_j^{*n} = \text{const.}$$

Depending on the properties of the discrete entropy U^*, *this may provide us with some a priori bound on the discrete solution. For instance, if* U^* *is strictly convex, essentially we recover the* L^2-*stability of the scheme. In general,* (2.7) *is a fully nonlinear implicit scheme. As we have an implicit scheme we may expect to have stability for large CFL-numbers. However, convergence of an iterative method for solving the nonlinear system might enforce a stricter CFL-like condition.*

(3) *In general, the schemes* (2.7) *are fully implicit. However, in some situations of interest we obtain linear implicit or even explicit schemes (section* 3).

3. Two and three time-level entropy conservative schemes. In this section we give first applications of Theorem 2.2. We start investigating the simplest case of a two time-level discretization. We will see that such schemes are always fully nonlinear, except in the case of linear systems of conservation laws. Next we investigate three time-level schemes, for which there exists more freedom in choosing a convenient discretization of the entropy. We use this freedom to construct explicit or linear implicit schemes of third order.

We will rely on the consistent entropy conservative numerical flux-function g_2^* that has been constructed by Tadmor [25]; i.e.,

(3.1) $$g_2^*(v_0, v_1) = \int_0^1 g(v_0 + s(v_1 - v_0))\, ds, \qquad v_0, v_1 \in \mathbb{R}^N.$$

The associated numerical entropy flux reads as

(3.2) $$G_2^*(v_0, v_1) = \frac{G(v_0) + G(v_1)}{2} + \frac{(v_0 + v_1)}{2} \cdot g_2^*(v_0, v_1)$$
$$-\frac{1}{2}\left(v_0 \cdot g(v_0) + v_1 \cdot g(v_1)\right).$$

3.1. A class of two time-level entropy conservative schemes. We first consider schemes based on two time-levels only and on two-point discrete fluxes. Consider the following discretization

$$(3.3) \qquad u_j^{n+1} = u_j^n - \lambda \left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1} \right)$$

corresponding to the simple choice $q = 1$:

$$u^* \left(u^0 \right) = u^0.$$

For schemes with $q = 1$ the only consistent entropy is $U^* (u) = U (u)$. The only two-point entropy conservative flux is the one proposed by Tadmor. We get the following result from Theorem 2.2.

THEOREM 3.1. *Let $u^* (u) = u$, $U^* (u) = U (u)$. Let Assumption 2.1 be valid. Then the scheme (3.3) considered with Tadmor flux (3.1) is entropy conservative with respect to the entropy U^*. Furthermore, this scheme is second order accurate in space and time in the sense that its equivalent equation is*

$$\partial_t u(x_j, t^{n+1/2}) + \partial_x g(v(x_j, t^{n+1/2})) = \mathcal{O}(h^2).$$

To satisfy Assumption 2.1 we can choose v^* to be

$$(3.4) \qquad v^*(u^0, u^1) = \int_0^1 v(su^*(u^1) + (1 - s)u^*(u^0))\, ds.$$

Note that—at least in the linear case and with $U(u) = u^2/2$—the time discretization in (3.3) is exactly the Crank–Nicholson time discretization.

In general, (3.3) with (3.4) is fully nonlinear in u_j^{n+1}. To obtain an at least linear implicit scheme, g_2^* has to be linear, and $v^* = v^*(u^0, u^1)$ has to be linear with respect to u^1. The latter is true if and only if U is quadratic. By definition, the Tadmor flux g_2^* is linear if and only if g is linear. With U to be quadratic we obtain that the flux f has to be linear. In the next section we will provide explicit and linear implicit entropy conservative schemes.

Example 3.2. For the sake of illustration of the scheme (3.3) we present a numerical experiment. We consider the scalar case

$$f(u) = U(u) = \frac{u^2}{2}.$$

This leads to the scheme

$$(3.5) \qquad \begin{aligned} u_j^{n+1} = u_j^n - \frac{\lambda}{24} \Big(&(u_j^n + u_j^{n+1})(u_{j+1}^n + u_{j+1}^{n+1} - u_{j-1}^n - u_{j-1}^{n+1}) \\ &+ (u_{j+1}^n + u_{j+1}^{n+1})^2 - (u_{j-1}^n + u_{j-1}^{n+1})^2 \Big). \end{aligned}$$

For each time step, the nonlinear difference equation (3.5) is solved by a fixed-point iteration method which is stopped if the L^1-relative difference between two succeeding approximate solutions is less than a threshold. This fixed-point iteration approach will be used throughout this paper for all numerical experiments. Results for initial data $u_0(x) = \sin(2\pi x) + 1$ at different times are shown in the left picture of Figure 3.1. The computational domain is $[0, 1]$ with periodic boundary conditions. Here we chose 250 cells, and the CFL-number to be 0.25. As expected for a central scheme, the method leads to a highly oscillating wave pattern after formation of the shock wave, indicating that the method will not converge in any strong topology when refining the grid. We note that by adding artificial dissipation the oscillations can be suppressed (cf. section 5 for examples with nonclassical shocks).
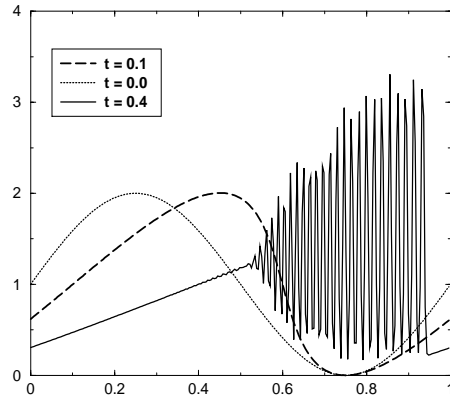
FIG. 3.1. *Numerical approximation of weak solutions of Burgers' equation with a two time-level entropy conservative scheme.*

3.2. A class of three time-level entropy conservative schemes. We consider three time-level schemes of the type

$$(3.6) \qquad u_j^{*n+1} = u_j^{*n} - \lambda \left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1} \right),$$

where the discrete conservative variable u^* is defined by

$$(3.7) \qquad u^* \left(u^0, u^1 \right) = \alpha u^0 + (1 - \alpha) u^1 \qquad (\alpha \in \mathbb{R}).$$

Straightforwardly we get the following theorem.

THEOREM 3.3. *Let $U^* \left(u^0, u^1 \right)$ be chosen such that Assumption 2.1 is satisfied for some entropy variable $v^* = v^* \left(u^{-1}, u^0, u^1 \right)$.*

Then the scheme (3.6) considered with Tadmor flux (3.1) is a three time-level entropy conservative scheme with respect to the entropy $U^* \left(u^0, u^1 \right)$.

To satisfy Assumption 2.1 we can always choose U^* and v^* as

$$
(3.8) \qquad
\begin{aligned}
U^*(u^0, u^1) &= U(u^*(u^0, u^1)), \\
v^*(u^{-1}, u^0, u^1) &= \int_0^1 v(su^*(u^0, u^1) + (1 - s)u^*(u^{-1}, u^0)) \, ds.
\end{aligned}
$$

If the entropy U is nonnegative, another possible choice for the discrete entropy is $U^* \left(u^0, u^1 \right) = \sqrt{U \left(u^1 \right) U \left(u^0 \right)}$, together with the entropy variable v^* as above.

3.3. Explicit three time-level schemes for quadratic entropies. Symmetric systems yield a general class of hyperbolic systems. For these systems, we can design three time-level explicit entropy conservative schemes. Let B be any constant positive symmetric matrix. For symmetric systems, the function

$$U(u) = u \cdot B \, u$$

is a strictly convex entropy for which the entropy variable is $v(u) = Bu$.

Let u^* be given by (3.7) for the special choice $\alpha = 1/2$, and choose the discrete entropy function

$$U^* \left(u^0, u^1 \right) = \frac{1}{2} \, u^0 \cdot B \, u^1.$$

To satisfy Assumption 2.1 define

$$(3.9) \qquad v^* \left(u^{-1}, u^0, u^1 \right) = B \, u^0.$$

The Tadmor flux gives an *explicit* scheme.

PROPOSITION 3.4. *Suppose that Df is symmetric. Choose $U^* \left(u^0, u^1 \right) = \frac{1}{2} u^0 \cdot B \, u^1$ and Tadmor's flux (3.1). With v^* from (3.9) the scheme (3.6) is an explicit scheme, entropy conservative with respect to the entropy U^*.*

3.4. Linear implicit three time-level schemes. As pointed out in section 3.2, the three-point conservative scheme (3.6) allows different choices for the entropy U^*. Here we consider scalar conservation laws and highlight a choice of U^* that leads to a *linear implicit* scheme.

Consider the case $N = 1$ with the flux $f(u) = u^3$ and entropy

$$U(u) = \int_0^u f(s) \, ds = \frac{u^4}{4}.$$

The flux written in the entropy variable is $g(v) = v$. Consider the discrete entropy

$$U_j^{*n} = U^{*n} \left(u_j^n, u_j^{n-1} \right) = \frac{1}{4} \left(u_j^n u_j^{n-1} \right)^2.$$

Assumption 2.1 is satisfied if the discrete entropy variable v^* is defined to be

$$v_j^{*n+1} = v^* (u_j^{n-1}, u_j^n, u_j^{n+1}) = \frac{1}{2} (u_j^n)^2 (u_j^{n+1} + u_j^{n-1}).$$

For the flux we take

$$g_{j+1/2}^{*,n+1} = g_2^* \left(v_j^{*n+1}, v_j^{*n+1} \right) = \frac{1}{4} \left((u_j^n)^2 (u_j^{n-1} + u_j^{n+1}) + (u_{j+1}^n)^2 (u_{j+1}^{n-1} + u_{j+1}^{n+1}) \right).$$

The resulting three time-level scheme (3.6) is linear implicit:

$$(3.10) \qquad u_j^{n+1} = u_j^{n-1} - \frac{\lambda}{2} \left(\left(u_{j+1}^{n+1} + u_{j+1}^{n-1} \right) \left(u_{j+1}^n \right)^2 - \left(u_{j-1}^{n+1} + u_{j-1}^{n-1} \right) \left(u_{j-1}^n \right)^2 \right).$$

Example 3.5. We present a numerical experiment for scheme (3.10). Consider the cubic scalar conservation law for $u_0(x) = \sin(2x/\pi)$ on $[0, 1]$ with periodic boundaries. The results for 250 cells and the CFL-number 0.25 are displayed in the right picture of Figure 3.2. Again we stress the fact that these schemes produce extreme oscillations after the shock has formed. When supplementing regularizing terms this effect will disappear.

3.5. Third order, three time-level entropy conservative schemes. Consider the following choice for the discrete entropy variable:

$$(3.11) \qquad u^* \left(u^0, u^1 \right) = \left(\frac{1}{2} - \frac{1}{\sqrt{2}} \right) u^0 + \left(\frac{1}{2} + \frac{1}{\sqrt{2}} \right) u^1.$$

THEOREM 3.6. *Consider a hyperbolic or hyperbolic-elliptic system of conservation laws (1.1) endowed with an entropy-entropy flux pair (U, F) satisfying condition (2.3). Consider the discrete conservative variable u^* from (3.11), $U^* \left(u^0, u^1 \right) = U \left(u^* \left(u^0, u^1 \right) \right)$, and v^* to be*

$$v^* \left(u^{-1}, u^0, u^1 \right) = \int_0^1 v \left(s u^* \left(u^0, u^1 \right) + (1 - s) \, u^* \left(u^{-1}, u^0 \right) \right) ds.$$
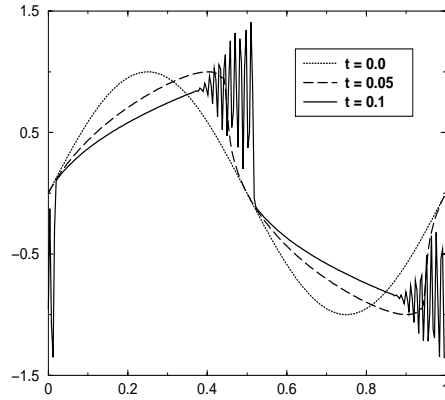
FIG. 3.2. *Numerical approximation of the cubic scalar conservation law with a three time-level entropy conservative scheme.*

For an entropy conservative flux g^* of order $2p$, $p \in \mathbb{N}$, the scheme

$$u_j^{*n+1} - u_j^{*n} + \lambda \left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1} \right) = 0$$

has a unique solution u_j^{n+1} if and only if λ is small enough. The scheme is entropy conservative and third order accurate in time; i.e., its equivalent equation is

$$\partial_t u \left(x_j, t^n + \frac{\tau}{\sqrt{2}} \right) + \partial_x g \left(v \left(x_j, t^n + \frac{\tau}{\sqrt{2}} \right) \right) = O\left(\tau^3 \right) + O\left(h^{2p} \right).$$

The order of accuracy of these scheme can be checked easily. See also section 4.2 for a constructive demonstration.

NOTE 3.7. *Using the Tadmor flux leads to a second order in space accurate conservative scheme ($p = 1$ in the previous formula). The next section provides the explicit construction of conservative fluxes of arbitrary higher order. A numerical example of this section is considered in section 5.*

4. Entropy conservative schemes of arbitrary order.

4.1. Semidiscrete entropy conservative schemes of arbitrary order. Consider the conservation law (1.1) with entropy-entropy flux pair (U, F). Let $x_j = jh$, $j \in \mathbb{Z}$, be a regular mesh, h denoting the grid point distance. For $v_j = \nabla U(u_j)$, we consider $(2p + 1)$-point semidiscrete schemes of type

(4.1)
$$\begin{aligned} u_j'(t) &= -\frac{1}{h} \left(g_{2p,j+1/2}^* - g_{2p,j-1/2}^* \right) \\ &= -\frac{1}{h} \left(g_{2p}^*(v_{j-p+1}, \ldots, v_{j+p}) - g_{2p}^*(v_{j-p}, \ldots, v_{j+p-1}) \right), \end{aligned}$$

where $u_j(t)$ approximates the solution u of (1.1) in (x_j, t) and $'$ denotes time derivation. In this section we show that there exist smooth numerical fluxes $g_{2p}^* : \mathbb{R}^{2pN} \to \mathbb{R}^N$ satisfying the following conditions for all $j \in \mathbb{Z}$, $p \in \mathbb{N}$ and all smooth enough

functions $v = \nabla U(u)$ (denoting $v_j = v(x_j, t)$):

(i) $g^*(v_j, \ldots, v_j) = g(v_j)$.

(ii) $\dfrac{g^*_{2p}(v_{j-p+1}, \ldots, v_{j+p}) - g^*_{2p}(v_{j-p}, \ldots, v_{j+p-1})}{h} = \partial_x g(v_j) + \mathcal{O}(h^{2p})$.

(iii)   There is a function $G^*_{2p} : \mathbb{R}^{2pN} \to \mathbb{R}$ consistent with G such that

$$U(u_j(t))' = -\frac{1}{h}\Big(G^*_{2p}(v_{j-p+1}, \ldots, v_{j+p}) - G^*_{2p}(v_{j-p}, \ldots, v_{j+p-1})\Big).$$

In other words, we will show that there exist consistent semidiscrete entropy conservative schemes (4.1) of arbitrary order. So far, only fluxes of order two [23] or three [16] have been available.

For $\alpha_{1,p}, \ldots, \alpha_{p,p} \in \mathbb{R}$, we make an ansatz for g^*_{2p} as a linear combination of Tadmor's flux g^*_2 (cf. (3.1)):

(4.2) $g^*_{2p}(v_{-p+1}, \ldots, v_p) = \displaystyle\sum_{i=1}^{p} \alpha_{i,p}\Big(g^*_2(v_0, v_i) + \cdots + g^*_2(v_{-i+1}, v_1)\Big).$

So the flux difference is given by

(4.3) $g^*_{2p}(v_{-p+1}, \ldots, v_p) - g^*_{2p}(v_{-p}, \ldots, v_{p-1}) = \displaystyle\sum_{i=1}^{p} \alpha_{i,p}\Big(g^*_2(v_0, v_i) - g^*_2(v_{-i}, v_0)\Big).$

NOTE 4.1 (linear entropy flux). *Assume that the function g can be written as an affine function, say $g(v) = Av + b$, $A \in \mathbb{R}^{N \times N}$, $b \in \mathbb{R}^N$ (cf. sections 3.4, 3.5). Then the Tadmor flux difference is simply the centered difference $A(v_1 - v_{-1})/2$, and we get in our case*

(4.4) $g^*_{2p}(v_{-p+1}, \ldots, v_p) - g^*_{2p}(v_{-p}, \ldots, v_{p-1}) = A \displaystyle\sum_{i=1}^{p} \alpha_{i,p}(v_i - v_{-i}).$

We show first that the general ansatz (4.2) leads to a scheme satisfying (i), (iii).

PROPOSITION 4.2. *Let $p \in \mathbb{N}$. Consider the scheme (4.1) for g^*_{2p} from (4.2) and $\alpha_{1,p}, \ldots, \alpha_{p,p} \in \mathbb{R}$ satisfying*

(4.5) $2\displaystyle\sum_{i=1}^{p} i\alpha_{i,p} = 1.$

Then (i) *and* (iii) *are satisfied for*

(4.6) $G^*_{2p} = G^*_{2p}(v_{-p+1}, \ldots, v_p) = \displaystyle\sum_{i=1}^{p} \alpha_{i,p}\Big(G^*_2(v_0, v_i) + \cdots + G^*_2(v_{-i+1}, v_1)\Big),$

where G^*_2 is given by (3.2).

Proof. Using (4.3) and Tadmor entropy fluxes $G^*_2(v_0, v_1)$, we get

$$v_0 \cdot \Big(g^*_{2p}(v_{-p+1}, \ldots, v_p) - g^*_{2p}(v_{-p}, \ldots, v_{p-1})\Big)$$

$$= v_0 \cdot \sum_{i=1}^{p} \alpha_{i,p}\Big(g^*_2(v_0, v_i) - g^*_2(v_{-i}, v_0)\Big)$$

$$= \sum_{i=1}^{p} \alpha_{i,p}\Big(G^*_2(v_0, v_i) - G^*_2(v_{-i}, v_0)\Big).$$

The last line equals $G_{2p}^*(v_{-p+1},\ldots,v_p) - G_{2p}^*(v_{-p},\ldots,v_{p-1})$, which proves (iii). The consistency of g_{2p}^*, G_{2p}^* with g, G follows from (4.5). $\quad\square$

Next, we fix the up-to-now free coefficients $\alpha_{1,p},\ldots,\alpha_{p,p}$ to provide a high-order scheme.

PROPOSITION 4.3. *For $p \in \mathbb{N}$, assume that $\alpha_{1,p},\ldots,\alpha_{p,p}$ solve the p linear equations*

$$(4.7) \qquad 2\sum_{i=1}^{p} i\alpha_{i,p} = 1, \quad \sum_{i=1}^{p} i^{2s-1}\alpha_{i,p} = 0 \quad (s = 2,\ldots,p).$$

Then the flux g_{2p}^* given by formula (4.2) satisfies (ii); i.e., for smooth enough function v we have

$$(4.8) \qquad \frac{g_{2p}^*(v_{j-p+1},\ldots,v_{j+p}) - g_{2p}^*(v_{j-p},\ldots,v_{j+p-1})}{h} = \partial_x g(v_j) + \mathcal{O}(h^{2p}).$$

Here we used $C_{2p} = \sum_{i=1}^{p} \frac{\alpha_{i,p} i^{2p+1}}{(2p+1)!}$ and $v_j = v(x_j)$ for $j \in \mathbb{Z}$.

Proof. By Taylor expansion around x_0 we obtain for $i = 1,\ldots,p$

$$g_2^*(v_0, v_i) - g_2^*(v_{-i}, v_0) = 2\sum_{k=0}^{p} \frac{(ih)^{2k+1}}{(2k+1)!} \partial_x^{(2k+1)} g(v_0) + \mathcal{O}(h^{2p+2}).$$

This leads by (4.3) to the expression

$$g_{2p}^*(v_{-p+1},\ldots,v_p) - g_{2p}^*(v_{-p},\ldots,v_{p-1})$$
$$= 2\sum_{i=1}^{p} \alpha_{i,p}\left(\sum_{k=0}^{p} \frac{(ih)^{2k+1}}{(2k+1)!} \partial_x^{(2k+1)} g(v_0)\right) + \mathcal{O}(h^{2p+2}).$$

The definition of $\alpha_{1,p},\ldots,\alpha_{p,p}$ in (4.7) gives the statement of the proposition. $\quad\square$

Note that the first equation in (4.7) equals (4.5) and ensures consistency. We summarize Proposition 4.2 and 4.3 in the following theorem.

THEOREM 4.4. *Consider a hyperbolic or hyperbolic-elliptic system of conservation laws (1.1) with an entropy-entropy flux pair (U, F). Assume that $\alpha_{i,1},\ldots,\alpha_{i,p}$ solve (4.7).*

Then the flux g_{2p}^* given by formula (4.2) satisfies the conditions (i), (ii), (iii).

The scheme (4.1) is an entropy conservative semidiscrete scheme with respect to U which is of order $2p$.

4.2. Fully discrete entropy conservative schemes of arbitrary order. In this section we present fully discrete schemes of arbitrary order verifying a weaker form of entropy conservation. For an integer $q \geq 1$, the schemes will use $q + 1$ time-levels and be of order $q + 1$ in time.

Let $j \in \mathbb{Z}$ and $n \in \mathbb{N}$. We approximate the continuous derivative $\partial_t u$ in (1.1) by

$$(4.9) \qquad \frac{u_j^{*n} - u_j^{*n-1}}{\tau} := \sum_{i=0}^{q} \beta_{i,q}^t u_j^{n-q+i}.$$

In the formula above, $\beta_{0,q}^t,\ldots,\beta_{q,q}^t \in \mathbb{R}$ are parameters that have to be chosen according to the desired $(q + 1)$st order of accuracy; i.e., for smooth enough function u, we

have the following expansion around a time $\bar{t}^q > 0$ to be determined:

$$(4.10) \qquad \sum_{i=0}^{q} \beta_{i,q}^t u_j^{n-q+i} = \partial_t u\left(x_j, \bar{t}^n\right) + O\left(\tau^{q+1}\right).$$

Consider the $q+1$ linear equations

$$(4.11)$$
$$\sum_{i=0}^{q}(t^{n-q+i} - \bar{t}^n)\beta_{i,q}^t = 1, \quad \sum_{i=0}^{q}(t^{n-q+i} - \bar{t}^n)^s \beta_{i,q}^t = 0 \quad (s = 0, \ldots, q, \ s \neq 1).$$

This last system is a Vandermonde system. If $\bar{t}^n$ does not belong to the set of time grid points $\{t^n\}_{n \geq 0}$, it also is nondegenerate. In this last case, the unique solutions $\beta_{0,q}^t, \ldots, \beta_{q,q}^t \in \mathbb{R}$ of (4.11) provides via (4.9) an approximation of $\partial_t u(x_j, \bar{t}^n)$ with at least order q, as a straightforward Taylor expansion of $u(x_j, t^{n-q}), \ldots, u(x_j, t^n)$ around $(x_j, \bar{t}^n)$ shows. Note that we are left with one degree of freedom, namely to choose $\bar{t}^n$. There exists a choice that allows us to gain one order of accuracy in time and obtain (4.10): choose $\bar{t}^n$ satisfying (4.11) and

$$(4.12) \qquad \sum_{i=0}^{q}(t^{n-q+i} - \bar{t}^n)^{s+1}\beta_{i,q}^t = 0.$$

To prove the existence of such an intermediate solution, we introduce the following polynomial

$$P(t) = \sum_{i=0}^{q} \frac{(-1)^i \prod_{\substack{0 \leq l \leq q \\ l \neq i}} \left(t^{n-l} - t\right)^2}{\prod_{\substack{0 \leq l \leq i \\ l \neq i}} |t^{n-i} - t^{n-l}|}.$$

One can check, using the explicit solution of the Vandermonde system (4.11), that any root of the previous polynomial provides a solution of (4.11), (4.12). It can be easily seen that this polynomial has q solutions, the ith solution $(i = 0, \ldots, q-1)$ lying in $[t^{n-i}, t^{n-i-1}]$. For stability reasons we always take the solution in $[t^{n-1}, t^n]$. For instance, in the case $q = 1$ we get $\bar{t}^n = \frac{t^{n-1}+t^n}{2}$, that is the Crank–Nicholson choice. For $q = 2$, we get $\bar{t}^n = t^n - \frac{\tau}{\sqrt{2}}$, that is, a third order scheme as considered in section 3.5. For $q > 2$, we compute numerically the solution that belongs to $[t^{n-1}, t^n]$.

In a similar way, define the coefficients $\beta_{0,q}^u, \ldots, \beta_{q,q}^u \in \mathbb{R}$ to be such that the expansion

$$(4.13) \qquad \sum_{i=0}^{q} \beta_{i,q}^u u_j^{n-q+i} = u\left(x_j, \bar{t}^q\right) + \mathcal{O}\left(\tau^{q+1}\right)$$

holds, that is, solving the equations

$$(4.14) \qquad \sum_{i=0}^{q}\beta_{i,q}^u = 1, \quad \sum_{i=0}^{q}(t^{n-q+i} - \bar{t}^n)^s \beta_{i,q}^u = 0 \quad (s = 1, \ldots, q).$$

The entropy variable being $v(u)$, define the discrete entropy variable $v_{q+1}^{*n} : \mathbb{R}^{(q+1)N} \to \mathbb{R}^N$ to be

$$(4.15) \qquad v_{q+1}^{*n}\left(u_j^{n-q}, \ldots, u_j^n\right) = v\left(\sum_{i=0}^{q} \beta_{i,q}^u u_j^{n-q+i}\right),$$

and denote $v_{q+1,j}^{*n+1} := v_{q+1}^{*n+1}\left(u_j^{n-q},\ldots,u_j^n\right)$. Now using the high order entropy conservative numerical fluxes constructed in the preceding section, we obtain arbitrarily high order fully discrete schemes, however, only satisfying a weaker form of entropy conservation.

THEOREM 4.5. *Consider a hyperbolic or hyperbolic-elliptic system of conservation laws (1.1) endowed with an entropy-entropy flux pair (U, F) satisfying condition (2.3). Let u_{q+1}^{*n} be a discrete conservative variable defined with (4.9)–(4.10) and a discrete entropy variable v_{q+1}^* satisfying (4.13). For a 2p-point numerical flux g_{2p}^* from Theorem 4.4, consider the following $(2p+1) \times (q+1)$-point scheme:*

$$u_j^{*n+1} = u_j^{*n} - \lambda\left(g_{j+1/2}^{*n+1} - g_{j-1/2}^{*n+1}\right).$$

Then, for λ small enough, there exists an unique solution u_j^{n+1}. The scheme is entropy conservative in the sense

(4.16) $$\left(u_j^{*n+1} - u_j^{*n}\right)v_{q+1,j}^{*n+1} + \lambda\left(G_{j+1/2}^{*n+1} - G_{j-1/2}^{*n+1}\right) = 0.$$

Furthermore, it is of order $(q+1)$ in time and 2p in space in the sense that its equivalent equation is

$$\partial_t u\left(x_j, \bar{t}^n\right) + \partial_x g\left(v\left(u\left(x_j, \bar{t}^n\right)\right)\right) = \mathcal{O}\left(h^{2p}\right) + \mathcal{O}\left(\tau^{q+1}\right).$$

Proof. The weak entropy conservation (4.16) follows from multiplying the scheme difference equation by $v_{q+1}^{*n+1}\left(u_j^{n-q},\ldots,u_j^n\right)$ and using property (2.6) for g_{2p}^*.

The equivalent equation comes from (4.13) and Theorem 4.4. □

NOTE 4.6. *For $q=1$ (Crank–Nicholson choice) and $q=2$, the discrete entropy variable constructed above, i.e., satisfying (4.13), also verifies Assumption 2.1 for U. It follows that these schemes are entropy conservative in the sense*

$$U_j^{*n+1} - U_j^{*n} + \lambda\left(G_{j+1/2}^{*n+1} - G_{j-1/2}^{*n+1}\right) = 0 \qquad (n \in \mathbb{N}, j \in \mathbb{Z})$$

with $U_j^{*n+1} = U\left(u_j^{*n+1}\right)$.

We illustrate this section with a fully discrete, fourth order accurate entropy scheme for the system of nonlinear elasticity.

For a stress-strain function $w \mapsto \sigma(w)$, consider the system

(4.17) $$\partial_t w - \partial_x V = 0, \qquad \partial_t V - \partial_x \sigma(w) = 0.$$

Here V is the particle velocity and w is the stress, collected in $u := (w, V)$. The mathematical entropy pair is

$$(U(u), F(u)) = \left(\int_0^w \sigma(s)\,ds + \frac{V^2}{2},\ \sigma(w)V\right).$$

We choose the stress-strain function σ given by

$$\sigma\left(w\right) = w^3 - w.$$

Then (4.17) represents a model for phase transitions in shape memory alloys. Note that, for $w \in [-1/\sqrt{3}, 1/\sqrt{3}]$, the problem is elliptic, and hyperbolic outside this interval. The flux in (4.17) can be written in terms of the entropy variable $v = $
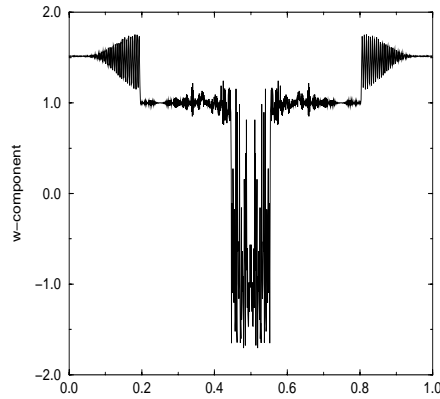
FIG. 4.1. *A fourth order in time, fourth order in space conservative scheme for the p-system (w-component).*

$(v_1, v_2)^T = (\sigma, V)^T$ and—as in the scalar case of section 3.4—is a linear function: $g(v_1, v_2) = -(v_2, v_1)^T$.

To discretize this system we design a four time-level scheme using the construction given in Theorem 3.6. We compute the values of the parameters $\beta_{0,q}^{t/u}, \dots, \beta_{q,q}^{t/u}$ and $\bar{t}^n$ as described above. Define

$$v_j^{*n+1} = \left(v_{1,j}^{*n+1}, v_{2,j}^{*n+1}\right)^T = \left(\sum_{i=0}^{3} \beta_{i,3}^u V_j^{n-3+i}, \sigma\left(\sum_{i=0}^{3} \beta_{i,3}^u w_j^{n-3+i}\right)\right)^T.$$

Consider now the fourth order conservative flux (cf. (4.2))

$$g_{j+1/2}^{*n+1} = g\left(\frac{2}{3}\left(v_j^{*n+1} + v_{j+1}^{*n+1}\right) - \frac{1}{12}\left(v_{j-1}^{*n+1} + \cdots + v_{j+2}^{*n+1}\right)\right).$$

The resulting scheme is, denoting componentwise $g_{j+1/2}^{*n+1} = (g_{1,j+1/2}^{*n+1}, g_{2,j+1/2}^{*n+1})^T$,

$$(4.18) \qquad \begin{cases} w_j^{*n+1} - w_j^{*n} + \lambda\left(g_{1,j+1/2}^{*n+1} - g_{1,j-1/2}^{*n+1}\right) &= 0, \\ V_j^{*n+1} - V_j^{*n} + \lambda\left(g_{2,j+1/2}^{*n+1} - g_{2,j-1/2}^{*n+1}\right) &= 0 \end{cases} \qquad (j \in \mathbb{Z}).$$

Such a scheme is a fully nonlinear fourth order scheme. The numerical experiment takes place in the interval $[0,5]$ with periodic boundaries. Choose initial data

$$(4.19) \qquad u_0(x) = \begin{cases} (1,-1)^T : x \in [0, 2.5), \\ (1,1)^T \ \ : x \in [2.5, 5). \end{cases}$$

For such Riemann initial data, an intermediate middle state lying in the opposite phase, i.e., $\{w \in \mathbb{R} \mid w \leq -1/\sqrt{3}\}$, must evolve for positive time [18]. The results for 1000 cells and the CFL-number 0.25 at time 0.1 are displayed in Figure 4.1.

5. Computation of regularization-sensitive weak solutions.

5.1. Analytical background and the basic numerical scheme. In the physical context the conservation law (1.1) is embedded into a higher order regularized but singularly perturbed model. For a small perturbation parameter $\varepsilon > 0$ and $D_2, D_3 : \mathbb{R}^N \to \mathbb{R}^{N \times N}$, let us consider systems of equations involving spatial derivatives up to order three:

$$(5.1) \qquad \partial_t u^\varepsilon + \partial_x f(u^\varepsilon) = \varepsilon \partial_x \Big(D_2(u^\varepsilon) \partial_x u^\varepsilon \Big) + \varepsilon^2 \partial_x \Big(D_3(u^\varepsilon) \partial_{xx} u^\varepsilon \Big).$$

We are interested in weak solutions u of (1.1) that arise as limits of a sequence of smooth solutions $\{u^\varepsilon\}_{\varepsilon > 0}$ of (5.1) for vanishing regularization parameter ε. While the second order derivatives in (5.1) correspond to physical effects like fluid viscosity or heat conduction, the third order term models capillarity phenomena [11, 15, 26].

A very interesting property of these *viscosity-capillarity* approximations u^ε is the fact that the limit solution u can contain undercompressive regularization-sensitive shock waves. Changing D_2, D_3 can produce a different weak solution; in other words, the limit function depends crucially on the entropy dissipation.

The numerical approximation of such weak solutions is a big challenge since also for the discrete counterpart the numerical entropy dissipation has to be tuned exactly. To overcome these difficulties Hayes and Lefloch suggested using *entropy conservative* numerical fluxes as a building block for finite difference schemes. To approximate the weak solution $u = \lim_{\varepsilon \to 0} u^\varepsilon$ of (1.1) they consider the following class of schemes (written down in the semidiscrete version, for simplicity):

$$(5.2) \qquad \begin{aligned} u_j'(t) &= -\frac{1}{h} \left(\tilde{g}^*_{2p, j+1/2} - \tilde{g}^*_{2p, j+1/2} \right), \\ \tilde{g}^*_{2p, j+1/2} &:= g^*_{2p, j+1/2} - f^{2*}_{j+1/2} - f^{3*}_{j+1/2}. \end{aligned}$$

Here g^*_{2p} is the smooth entropy conservative numerical flux from (4.2), and

$$f^{2/3*}_{j+1/2} = f^{2/3*}(u_{j-r+1}, \ldots, u_{j+r}) \quad (r \in \mathbb{N}),$$

where $f^{2/3*} : \mathbb{R}^{2rN} \to \mathbb{R}^N$ are smooth and satisfy for all smooth enough functions u (denoting $u_j = u(x_j, t)$)

$$\frac{f^{2*}(u_{j-r+1}, \ldots, u_{j+r}) - f^{2*}(u_{j-r}, \ldots, u_{j+r-1})}{h} = h \partial_x \Big(D_2(u_j) \partial_x u_j \Big) + \mathcal{O}(h^3),$$

$$\frac{f^{3*}(u_{j-r+1}, \ldots, u_{j+r}) - f^{3*}(u_{j-r}, \ldots, u_{j+r-1})}{h} = h^2 \partial_x \Big(D_3(u_j) \partial_{xx} u_j \Big) + \mathcal{O}(h^3).$$

Then we obtain the following equivalent equation for the scheme (5.2):

$$(5.3)$$
$$u_j'(t) + \partial_x f(u_j(t))$$
$$= h \partial_x \Big(D_2(u_j(t)) \partial_x u_j(t) \Big) + h^2 \partial_x \Big(D_3(u_j(t)) \partial_{xx} u_j(t) \Big) + \mathcal{O}(h^{2p}) + \mathcal{O}(h^3).$$

We observe that the equivalent equation mimics (5.1) provided we have $p \geq 2$. This is precisely the motivation for considering (5.2) with *high order* fluxes. While in

[9, 16] only semidiscrete entropy conservative schemes were available, here we have constructed fully discrete high order entropy conservative schemes.

In what follows we will consider numerical experiments. Furthermore, in a special case this construction allows us to consider a discrete counterpart for the entropy inequality.

5.2. Regularizations that are linear in the entropy variable. In this section we consider in this section a regularization mechanism of (1.1) in which the dissipative terms are *linear* functions of the entropy variable v:

(5.4) $$\partial_t u^\varepsilon + \partial_x f(u^\varepsilon) = \varepsilon B_2 \partial_{xx} v + \varepsilon^2 B_3 \partial_{xxx} v^\varepsilon.$$

Here we assume that

(5.5) $$B_2, B_3 \text{ are } (N \times N) \text{ constant matrices,}$$

and we make the hypothesis

(5.6) $$B_2 \text{ is positive definite and } B_3 \text{ is symmetric.}$$

The advantage of this particular choice is the following. Multiplying (5.4) by v^ε and performing integration by parts, the hypothesis (5.6) leads immediately to the entropy stability estimate

(5.7) $$\frac{d}{dt} \int_\mathbb{R} U\left(u^\varepsilon\left(x\right)\right) dx \leq 0.$$

In what follows we assume that there is a classical solution of the Cauchy problem for (5.4) and a weak solution u of the Cauchy problem for (1.1) such that $\lim_{\varepsilon \to 0} u^\varepsilon = u$. As we are interested in the numerical approximation of the function u we consider on the (semi)discrete level the scheme (5.2) together with smooth fluxes $f_{j+1/2}^{2/3*} : \mathbb{R}^{2rN} \to \mathbb{R}^N$, $r \in \mathbb{N}$, that are *linear* in v and satisfy for all smooth enough functions u,

$$\frac{f^{2*}(u_{j-r+1}, \ldots, u_{j+r}) - f^{2*}(u_{j-r}, \ldots, u_{j+r-1})}{h} = hB_2\partial_x^2 v_j + \mathcal{O}(h^3),$$

$$\frac{f^{3*}(u_{j-r+1}, \ldots, u_{j+r}) - f^{3*}(u_{j-r}, \ldots, u_{j+r-1})}{h} = h^2 B_3 \partial_{xxx} v_j + \mathcal{O}(h^3).$$

NOTE 5.1. *Since the estimate (5.7) is the immediate and natural a priori bound for u^ε, it should be also possible to prove a discrete entropy dissipation property for the approximate solution. For a result in a particular case we refer to [16, Theorem 5.1] and [6].*

Independent of these analytical issues, the numerical experiments in section 6.2 below clearly demonstrate the benefits of the linear regularization.

In the rest of this subsection we will focus on a somewhat different but strongly related issue: We consider special high order discretizations for smooth solutions of (5.4) (and not for weak solutions of (1.1) that arise as vanishing dissipation limits of (5.4)).

We introduce a discrete version of (5.7): a form $\tilde{g}^*(v_{-p+1}, \ldots, v_p)$ is entropy dissipative if, for any compactly supported sequence $(v_j)_{j \in \mathbb{Z}}$ in $\mathbb{R}^N$,

(5.8) $$\sum_{j \in \mathbb{Z}} v_j \cdot (g^*(v_{-p+j+1}, \ldots, v_{p+j}) - g^*(v_{-p+j}, \ldots, v_{p+j-1})) \leq 0.$$

Note that a conservative form $\tilde{g}^* = \tilde{g}^* (v_{-p+j+1}, \ldots, v_{p+j})$ (i.e., a form satisfying (2.6)) verifies (5.8) as an equality.

To provide a $2p$ order discretization of the capillarity term $\partial_x^3 v$, let us introduce the coefficients $\alpha_{i,1}^{(3)}, \ldots, \alpha_{i,p}^{(3)}$ as the solutions of the p linear equations:

$$(5.9) \qquad 2 \sum_{i=1}^{p} i^3 \alpha_{i,p} = 1, \quad \sum_{i=1}^{p} i^{2s-1} \alpha_{i,p}^{(3)} = 0 \quad (s = 1, \ldots, p, s \neq 2).$$

As for (4.7), the previous system is a Vandermonde system and thus has an unique solution. Let us introduce the form $v_{2p}^{(3)*}$, defined by

$$(5.10) \qquad v_{2p}^{(3)*} (v_{-p+1}, \ldots, v_p) = \sum_{i=1}^{p} \alpha_{i,p}^{(3)} (v_i + v_{i-1} + \cdots + v_{-i+1}),$$

Here v_i stands for $v(x_i)$, v being any smooth enough vector-valued function $v(x) \in \mathbb{R}^N$. As for (4.7), the difference

$$(5.11) \qquad v_{2p}^{(3)*} (v_{-p+1}, \ldots, v_p) - v_{2p}^{(3)*} (v_{-p}, \ldots, v_{p-1}) = \sum_{i=1}^{p} \alpha_{i,p}^{(3)} (v_i - v_{-i})$$

provides a formula of order $2p$ for $\partial_x^3 v_0$. This is straightforward from Taylor expansions of order $2p$ around v_0. Also note that such a form is conservative in the sense of (2.6), because the structure exhibited in (5.11) corresponds to the special form exhibited in (4.4).

Now we turn to a $2p$ order discretization of the viscous term $\partial_x^2 v$. Let us introduce the coefficients $\alpha_{i,1}^{(2)}, \ldots, \alpha_{i,p}^{(2)}$ as the solutions of the p linear equations

$$(5.12) \qquad \sum_{i=1}^{p} \alpha_{i,p}^{(2)} = 1, \quad \sum_{i=1}^{p} i^{2s} \alpha_{i,p}^{(2)} = 0 \quad (s = 1, \ldots, p-1).$$

We also introduce the form $v_{2p}^{(2)}$ defined by

$$(5.13) \qquad v_{2p}^{(2)*} (v_{-p+1}, \ldots, v_p) = \sum_{i=1}^{p} \alpha_{i,p}^{(2)} (v_i + \cdots + v_1 - v_0 - \cdots - v_{-i+1}).$$

Straightforwardly from Taylor expansions around v_0, the difference

$$(5.14) \qquad v_{2p}^{(2)*} (v_{-p+1}, \ldots, v_p) - v_{2p}^{(2)*} (v_{-p}, \ldots, v_{p-1}) = \sum_{i=1}^{p} \alpha_{i,p}^{(2)} (v_i + v_{-i} - 2v_0)$$

provides a $2p$ order discretization of $\partial_x^2 v_0$.

To provide a discretization for the whole equation (5.4), denote

$$(5.15) \qquad \widetilde{g}_{2p}^* = g_{2p}^* - v_{2p}^{(2)*} - v_{2p}^{(3)*},$$

where g_{2p}^* is defined in the previous section (see formula (4.2)). Set $\widetilde{g}_{2p,j+1/2}^{*n+1} = \widetilde{g}_{2p}^* (v_{j-p+1}^{*n+1}, \ldots, v_{j+p}^{*n+1})$. The main theorem of this section follows.

THEOREM 5.2. *Consider the system of conservation laws* (5.4) *together with an entropy pair* (U, F) *and the compatibility conditions* (5.6). *Let* $p > 1$ *and consider the semidiscrete scheme*

$$u'_j(t) = -\frac{1}{h}\left(\widetilde{g}^*_{2p,j+1/2} - \widetilde{g}^*_{2p,j-1/2}\right), \qquad t > 0.$$

The equivalent equation of this scheme is the system (5.4) *evaluated in* (x_j, t) *up to a term of order* $2p$ *in space.*

Assume that $u_j(t)$ *vanishes for* $|j|$ *big enough for all* $t > 0$. *Then the scheme is entropy decreasing:*

(5.16) $$\sum_{j \in \mathbb{Z}} U'(u_j(t)) \leq 0, \qquad t > 0.$$

NOTE 5.3. *We could also have stated a fully discrete version of the previous theorem using the time discretization exhibited in Theorem* 4.5*: let* $q + 1$ *as defined in Theorem* 4.5 *be the number of time-levels used by the scheme. Then we are able to construct a fully discrete scheme of order* $q + 1$ *in time,* $2p$ *in space with respect to* (5.4) *It satisfies the entropy dissipation property*

$$\sum_{j \in \mathbb{Z}} \left(u^{*n+1}_j - u^{*n+1}_j\right) v^{*n+1}_j \leq 0.$$

We notice also that, using an entropy variable satisfying Assumption 2.1*, we are led to a scheme verifying the strongest entropy dissipation property*

(5.17) $$\sum_{j \in \mathbb{Z}} U\left(u^{*n+1}_j\right) \leq 0.$$

In particular, consider the third order accurate conservative scheme described in section 3.5*. Following the guidelines described above, we are able to construct fully discrete schemes of accuracy order* 3 *in time,* $2p$ *in space with respect to* (5.4)*, satisfying the entropy dissipation property* (5.17)*.*

Proof of Theorem 5.2. It is enough to prove the dissipation property.

$$\sum_{i \in \mathbb{Z}} \left(\widetilde{g}^*_{2p,j+1/2} - \widetilde{g}^*_{2p,j-1/2}\right) v_j \leq 0.$$

Since g^*_{2p} and $v^{(3)*}_{2p}$ are entropy conservative fluxes (i.e., they satisfy a stronger version of (5.8)), the only point is to show the statement for $v^{(2)*}_{2p}$.

Note that the elementary forms $(v_{-i} + v_i - 2v_0)$ are the building block of (5.14). We compute

$$(v_{-i} + v_i - 2v_0)\, v_0 = -(v_i - v_0)^2 + v_i^2 - v_i v_0 - \left(v_0^2 - v_0 v_{-i}\right).$$

Denoting $G^{(2)*}_2(v_0, v_i) = v_i^2 - v_i v_0$ and $G^{(2)*}_{2p,j+1/2} = \sum_{l=0}^{j-1} G^{(2)*}_2(v_{-l}, v_{j-l})$, we have

$$(v_{-i} + v_i - 2v_0)\, v_0 = -(v_i - v_0)^2 + G^{(2)*}_2(v_0, v_i) - G^{(2)*}_2(v_{-i}, v_0)$$

$$= -(v_i - v_0)^2 + \sum_{l=0}^{i-1} G^{(2)*}_2(v_{-l}, v_{i-l}) - \sum_{l=0}^{i-1} G^{(2)*}_2(v_{-l-1}, v_{i-l-1})$$

$$= -(v_i - v_0)^2 + \left(G^{(2)*}_{2p,i+1/2} - G^{(2)*}_{2p,i-1/2}\right).$$

This proves that

$$\sum_{j\in\mathbb{Z}}\left(v_j\left(v^{(2)}_{2p,j+1/2}-v^{(2)}_{2p,j-1/2}\right)\right)+\sum_{i=1}^{p}\alpha^{(2)}_{i,p}\sum_{j\in\mathbb{Z}}\frac{(v_{i+j}-v_j)^2}{2}=0.$$

The last sum in the last equation can be estimated from below by a sum independent of i. Therefore $\sum_{i=1,\dots,p}\alpha^{(2)}_{i,p}=1$ from (5.12) shows that $v^{(2)}_{2p}$ is entropy decreasing. □

Further results on the discrete Laplace operator in this context can be found in [1], for instance.

6. Numerical experiments.

6.1. A shock-capturing method for the scalar cubic problem. For $\gamma > 0$ fixed and some initial data $u_0 : \mathbb{R}\to\mathbb{R}$, consider as a model problem the (regularized) scalar Cauchy problem

(6.1)
$$\begin{aligned}u^{\gamma,\epsilon}_t+\left((u^{\gamma,\epsilon})^3\right)_x&=\epsilon\,u^{\gamma,\epsilon}_{xx}+\gamma\epsilon^2\,u^{\gamma,\epsilon}_{xxx},\\u^{\gamma,\epsilon}(.,0)&=u_0\end{aligned}$$

corresponding to (5.1).

It is well known [20] that there exists a weak solution u^γ of the hyperbolic conservation law, i.e., (6.1) with $\epsilon=0$, which is the L^1-limit of a sequence of solutions $\{u^{\gamma,\epsilon}\}_{\epsilon>0}$ for vanishing ϵ. In particular for Riemann problem initial data u_0, the function u^γ might contain undercompressive shock waves which depend on u_0 and the coefficient γ [11, 8].

Following subsection 5.1, we choose our viscosity and capillarity fluxes according to

$$\begin{aligned}f^{2*}(u_{j-1},\dots,u_{j+2})&=\frac{\beta}{2}\left(u_{j+1}-u_j\right),\\f^{3*}(u_{j-1},\dots,u_{j+2})&=\frac{\delta}{6}\left(u_{j+2}-u_{j+1}-u_j+u_{j-1}\right).\end{aligned}$$

To satisfy (5.3) assume $\delta/\beta^2=3\gamma/4$ for $\beta,\delta>0$. With the entropy of choice $U(u)=u^4/4$ the basic entropy conservative schemes are given by either

> I   scheme (3.6) with $\alpha=1/2$ and $p=1$ or
>
> II   scheme (3.6) with $\alpha=1/2-1/\sqrt{2}$ and $p=2$.

In both cases we use $U^*\left(u^0,u^1\right)=U\left(u^*\left(u^0,u^1\right)\right)$ and v^* to be

$$\begin{aligned}v^*\left(u^{-1},u^0,u^1\right)&=\int_0^1 v\left(su^*\left(u^0,u^1\right)+(1-s)\,u^*\left(u^{-1},u^0\right)\right)ds\\&=\frac{1}{4}\left(u^*(u^0,u^1)+u^*(u^{-1},u^0)\right)\left(u^*(u^0,u^1)^2+u^*(u^{-1},u^0)^2\right).\end{aligned}$$

The basic entropy conservative scheme in case I (II) is of second (third) order in space and time.

In all numerical experiments described below, the viscosity and capillarity fluxes for fluxes $f^{2/3}_{j+1/2}$ are evaluated in $u^{n+1}_{j-1},\dots,u^{n+1}_{j+2}$, i.e., we treat them implicitly.
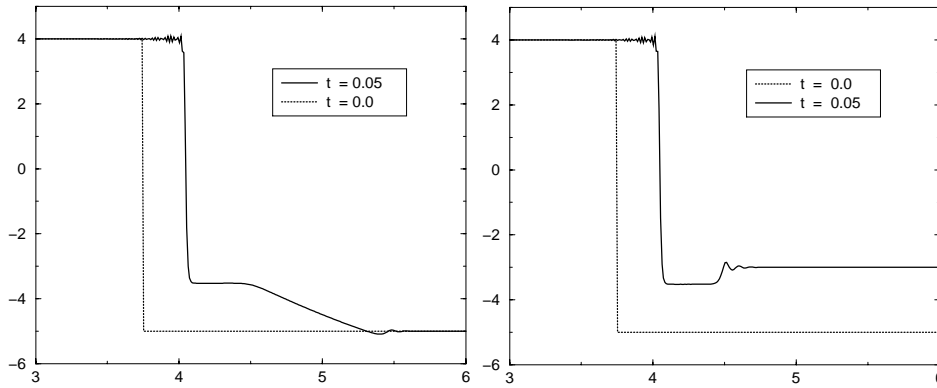
FIG. 6.1. *Typical wave patterns involving nonclassical shock waves. Results for scheme* II *are displayed.*

In Figure 6.1 we present the numerical results for two different choices of the initial data:

$$(6.2) \qquad u_0^1(x) = \begin{cases} 4 : x < 0, \\ -5 : x > 0, \end{cases} \qquad u_0^2(x) = \begin{cases} 4 : x < 0, \\ -3 : x > 0. \end{cases}$$

For $\gamma = 2$ and initial data u_0^1, the weak solution u^γ consists of a slow nonclassical shock and a fast rarefaction, while u_0^2 enforces a slow nonclassical shock followed by a fast Lax shock. The numerical results have been performed with the discretization parameters

$$(6.3) \qquad\qquad \beta = 5.0, \qquad \delta = 37.5, \qquad h = 0.005.$$

The figures demonstrate the ability of the scheme to reproduce nonclassical shock waves arising in Riemann problems together with shock and rarefaction waves. We approximately obtained the value -3.52 for the middle constant state in the second experiment with nonclassical and classical shock. This is better than the values obtained in [10, 16]. However, the correct value of the exact solution u^γ is $-11/3$.

To present a quantitative comparison we run the following experiment. We fix $\gamma = 2$ and choose the parameters according to (6.3). Now we compute the approximate solutions for both schemes I, II with the initial data

$$u_0(x) = \begin{cases} u_l : x < 0, \\ -\dfrac{5}{4} u_l : x > 0. \end{cases}$$

For $u_l > 1$, the exact solution u^γ consists of a nonclassical shock and a rarefaction connected by a middle state u_m as described above. In Figure 6.2 the approximate values of the middle state u_m obtained by schemes I and II are displayed for several values of $u_l \in [1, 11]$. The graphs describing the exact value $u_m = u_m(u_\gamma)$ in the cases $\gamma = 0, \gamma = 2, \gamma = \infty$ are also presented. The cases $\gamma = 0, \gamma = \infty$ give the exact middle value for the classical case, respectively, the extreme nonclassical case. We observe for small values of u_l a good approximation of the exact solution while bigger values of u_l lead to wrong solutions. The approximation of scheme II with the higher order
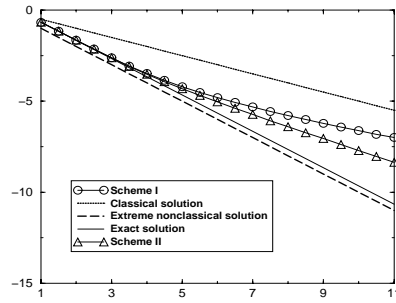
FIG. 6.2. *The (approximate) middle state u_m versus the state u_l.*

basic entropy flux is always better than the approximation by scheme I. We conclude by saying that our method seems to be reliable for computing nonclassical shocks at least for small amplitude initial data.

6.2. The "linear" shock capturing method for the scalar cubic problem. We now present numerical data for schemes approximating nonclassical weak solutions of the scalar cubic problem that are based on the regularization that is linear in the entropy variable $v = U'(u) = f(u) = u^3$ (while in subsection 6.1 the regularization was linear in the conservative variable u). Therefore, instead of (6.1), we consider

$$(6.4) \qquad \begin{aligned} u_t^{\gamma,\epsilon} + f(u^{\gamma,\epsilon})_x &= \epsilon f(u^{\gamma,\epsilon})_{xx} + \gamma\epsilon^2 f(u^{\gamma,\epsilon})_{xxx}, \\ u^{\gamma,\epsilon}(.,0) &= u_0. \end{aligned}$$

This leads to the following choice for the viscosity and capillarity fluxes:

$$\begin{aligned} f^{2*}(u_{j-1},\ldots,u_{j+2}) &= \frac{\beta}{2}\Big(f(u_{j+1}) - f(u_j)\Big), \\ f^{3*}(u_{j-1},\ldots,u_{j+2}) &= \frac{\delta}{6}\Big(f(u_{j+2}) - f(u_{j+1}) - f(u_j) + f(u_{j-1})\Big). \end{aligned}$$

As the basic entropy scheme we take (corresponding to scheme II in subsection 6.1) scheme (3.6) with $\alpha = 1/2 - 1/\sqrt{2}$ and $p = 2$. For the numerical parameters, let β, γ to be 37.5, respectively, 1. In Figure 6.3 we present computations for the Riemann initial data

$$u_0^1(x) = \begin{cases} 50 : x < 5, \\ -62.5 : x > 5, \end{cases} \qquad u_0^2(x) = \begin{cases} 100 : x < 5, \\ -125 : x > 5. \end{cases}$$

The calculations have been performed with discretization width $h = 0.005$. In the specific cases considered here we obtain a configuration with a slow nonclassical shock and a fast rarefaction.

Note that these type of schemes allow the stable computation of nonclassical shocks, even for *very large* amplitude data. This was not possible for the discretization based on (6.1).

6.3. The p-system with phase transition: A shape memory material. In this section, we perform long-time computations for the p-system (4.17). We consider
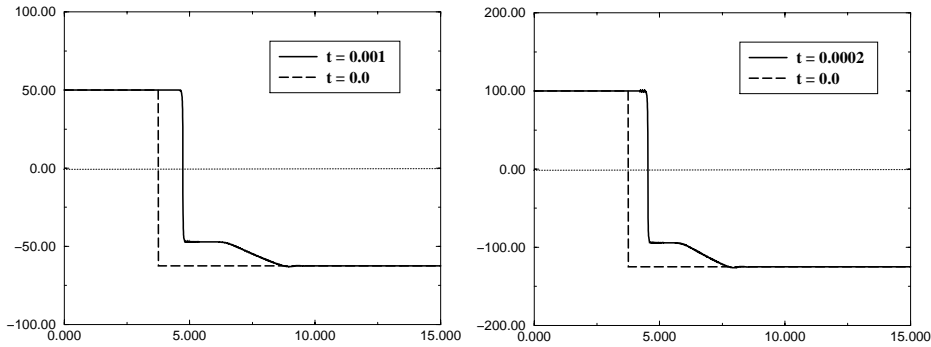
FIG. 6.3. *Stable computation of nonclassical shocks for large initial data $u_0^{1/2}$.*

the weak solution that is obtained as the limit (as $\varepsilon \to 0$) of classical solutions of the p-system with linear viscous regularization in the entropy variable:

$$
\begin{aligned}
\partial_t w^\varepsilon - \partial_x V^\varepsilon &= \varepsilon \partial_{xx} \sigma(w^\varepsilon), \\
\partial_t V^\varepsilon - \partial_x \sigma(w^\varepsilon) &= \varepsilon \partial_{xx} V^\varepsilon.
\end{aligned}
$$
(6.5)

The scheme that we consider here is the fourth order entropy conservative scheme (4.18) to which we add a viscous flux of fourth order. Following the notations introduced for scheme (4.18), we define the complete numerical flux by

$$
\widetilde{g}_4^* = g_4^* - v_4^{(2)*},
$$

where the entropy conservative flux g_4^* is given by

$$
g_4^* \left(v_{j-1}, \ldots, v_{j+2} \right) = g \left(\frac{2}{3} \left(v_j + v_{j+1} \right) - \frac{1}{12} \left(v_{j-1} + \cdots + v_{j+2} \right) \right),
$$

whereas the viscous flux is defined by

$$
v_4^{(2)*} \left(v_{j-1}, \ldots, v_{j+2} \right) = \frac{2h}{3} \left(v_{j+1} - v_j \right) - \frac{h}{24} \left(v_{j+1} + v_{j+2} - v_j - v_{j-1} \right).
$$

Taylor expansion shows that this flux is of fourth order with respect to $h\partial_{xx}v$. The resulting scheme is, denoting $\widetilde{g}_{j+1/2}^{*n+1} = (\widetilde{g}_{1,j+1/2}^{*n+1}, \widetilde{g}_{2,j+1/2}^{*n+1})^T$,

$$
\begin{cases}
w_j^{*n+1} - w_j^{*n} + \lambda \left(\widetilde{g}_{1,j+1/2}^{*n+1} - \widetilde{g}_{1,j-1/2}^{*n+1} \right) &= 0, \\
V_j^{*n+1} - V_j^{*n} + \lambda \left(\widetilde{g}_{2,j+1/2}^{*n+1} - \widetilde{g}_{2,j-1/2}^{*n+1} \right) &= 0
\end{cases}
\qquad (j \in \mathbb{Z}).
$$

We present two computations with periodic boundaries. The results have been obtained on a grid of 1000 cells and with CFL-number 0.25.

The first experiment deals with the same initial Riemann data as in the previous example (cf. (4.19)). We illustrate the effect of artificial viscous regularization on the results plotted in Figure 4.1. The numerical experiment is performed in the interval $[0, 1]$, with initial data

$$
u_0(x) = \begin{cases}
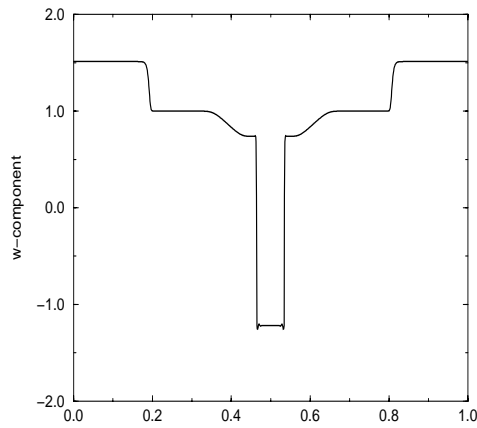(1, 1)^T & : x \in [0, 0.5), \\
(1, -1)^T & : x \in [0.5, 1).
\end{cases}
$$

FIG. 6.4. *Numerical approximation of the p-system with artificial viscosity.*
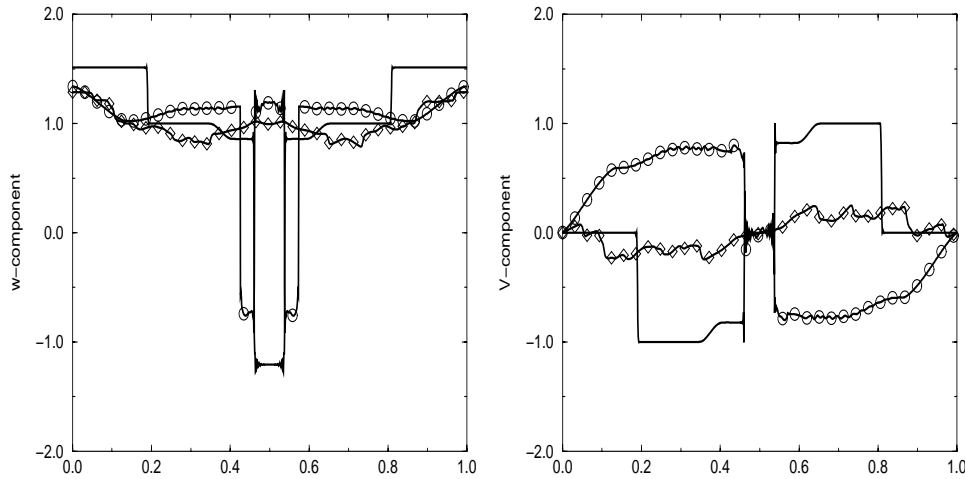

FIG. 6.5. *Time evolution of a diphasic stressed material for short time range (no symbols), intermediate time range (circles), and long time range (diamonds).*

Note that the computed solution (Figure 6.4) corresponds to the four wave "classical" pattern described by Shearer [19].

The second experiment corresponds to the same initial data, but now we performed a longer time computation. We illustrate the property of these materials to come back to their initial configuration at rest, i.e., the constant solution $(w, V) = (1, 0)$. During the computations, numerous phase transitions were created and canceled out. The evolution in time of the approximate solution is displayed in Figure 6.5 for different times. The left figure shows the w-component, and the right figure the V-component.

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