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Entropy stable schemes for initial-boundary-value conservation laws

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Abstract. We consider initial-boundary-value problems for systems of conservation laws and design entropy stable finite difference schemes to approximate them. The schemes are shown to be entropy stable for a large class of systems that are equipped with a symmetric splitting, derived from the entropy formulation. Numerical examples for the Euler equations of gas dynamics are presented to illustrate the robust performance of the proposed method.

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1. Introduction

We consider systems of conservation laws in one space dimension:

$$\begin{aligned} u_t + f(u)_x &= 0, \quad x \in (0,1) \\ u(x,0) &= u^0(x), \\ L_b(u) &= (g_l(t), g_r(t))^\top. \end{aligned} \tag{1}$$

Here, $u = (u_1, \ldots, u_n)^\top$ is the vector of unknowns and the fluxes $f = (f_1, f_2, \ldots, f_n)^\top$ are Lipschitz continuous functions of u. The expression L_b is an operator that enforces boundary conditions (weakly) at $x = 0, 1$ using data $g_{l,r}(t)$. The precise action of this operator will be specified later.

A prototypical example for the system of conservation laws (1) is provided by the Euler equations of gas dynamics:

$$\begin{aligned} u_t + f(u)_x &= 0 \\ u &= (\rho, m, E)^{\mathrm{T}} \\ f(u) &= (m, \rho q^2 + P, (E+P)q)^{\mathrm{T}} \\ P &= (\gamma - 1)\left(E - \frac{1}{2}\rho q^2\right). \end{aligned} \tag{2}$$

ρ, q, P and E are the density, velocity, pressure and total energy of a gas. The momentum is denoted as $m = \rho q$ and γ the ratio of the specific heats.

Solutions to (1) generally have to be interpreted in a weak sense. A weak solution of the conservation law (1) is defined below.

Definition. A locally integrable function u is defined as a weak solution to (1) if it satisfies the following integral identity for all $\varphi \in C_0^\infty((0,1) \times R_+)$,

$$\int_{R_+} \int_0^1 u \cdot \varphi_t + f(u) \cdot \varphi_x \mathrm{d}x\mathrm{d}t + \int_0^1 u_0(x) \cdot \varphi(x,0)\mathrm{d}x = 0. \tag{3}$$

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Weak solutions are not unique, and to single out the physically relevant solution, an extra, so-called entropy condition, is necessary. We will use the following form of the entropy condition,

Definition. Let (E, F) be any pair of smooth functions such that E is strictly convex and $F_u = E_u f_u$. Such a pair of functions is defined as an *entropy-entropy flux* pair. Then, $u \in L^1_{\text{loc}}((0,1) \times R_+)$ is an entropy solution of (1) if for all entropy-entropy flux pairs, (E, F), and for all $0 \leq \varphi \in C_0^\infty((0,1) \times R_+)$, the following inequality holds,

$$\int\limits_{R_+} \int\limits_0^1 E(u)\varphi_t + F(u)\varphi_x \mathrm{d}x\mathrm{d}t \geq 0. \tag{4}$$

Stability and convergence of numerical approximations to (systems of) conservation laws has been the subject of intensive study for decades, but generally applicable results for systems remain elusive. From the numerical perspective, stability (in a sufficiently strong sense) is the single most important aspect for the reliability of numerical results. Stability is also the key to prove convergence of numerical solutions.

For Cauchy problems, there are several successful schemes that guarantee convergence of scalar conservation laws. They include the so-called E-schemes for scalar conservation laws (see for example [16]). The stability of E-schemes for scalar conservation laws originates from a locally satisfied entropy inequality, valid for all possible entropy pairs. Scalar conservation laws are equipped with an infinite number of entropy pairs which can be used to prove a sufficiently strong stability result such that convergence follows. Systems, however, generally lack this richness of entropies, and the E-scheme requirement is less natural. Nevertheless, there have been efforts to generalize E-schemes to systems of conservation laws, [1].

A less restrictive way to construct schemes, for scalar equations or systems, is to make them satisfy a local entropy inequality for one particular entropy. Such schemes are termed *entropy stable.* (See [16].) For the canonical example, the Euler equations of gas dynamics (2), entropy stability implies an L^2 bound on the solution as long as the density ρ remains positive.

Most rigorous results on the stability and convergence of numerical schemes for conservation laws are available for the Cauchy problem. For the initial-boundary-value problem corresponding to (1), stability and convergence results for monotone (first-order) numerical schemes approximating scalar conservation laws in several space dimensions were obtained by Coquel et al. [3]. The authors heavily used the monotonicity of the corresponding solution operator in their analysis. Our aim in this paper is to obtain stability results for a system of conservation laws. As the solution operator is not necessarily monotone, the arguments of [3] are no longer applicable. Before describing stable numerical schemes for the initial-boundary-value problem for systems, we discuss some theoretical results below.

In DuBois and Le Floch [2], the continuous problem (1) was studied and, under sufficiently strong stability assumptions, the following *boundary entropy inequality* was obtained.

$$F(u_0) - F(g) - E_u(g)(f(u_0) - f(g)) \leq 0 \tag{5}$$

where g is the boundary data at $x = 0$ and u_0 the solution at the same point. Any numerical scheme devised for the initial-boundary-value problem should converge to a solution satisfying this inequality. However, this result sheds no light on how such a solution can be generated.

In Olsson and Oliger [11], the initial-boundary-value problem was analyzed. They used the so-called *canonical splitting* (later termed *entropy splitting*) in order to obtain energy estimates (or global entropy estimates), but at the expense of sacrificing the conservative form. To this end, they demand the flux function to satisfy a so-called *cone condition*, which can be verified in certain important cases. For scalar conservation laws, this technique resulted in standard L^p estimates for the solution variable. For systems, however, the estimate requires the assumption that the signal speeds of the in-going characteristics are bounded by data. It is difficult to see that this assumption is valid in general. Another slight drawback is that the entropies they adopt do not symmetrize the heat flux in the Navier–Stokes equations. In a series of papers, Olsson and Gerritsen use this form, discretized with Summation-by-parts finite difference schemes and a boundary projection method for imposing boundary conditions. As a result, they obtain stable schemes for the Euler equations including the boundaries, although not on conservative form. (See [5,6,9,10].)

The entropy splitting used by the above authors introduces a non-conservative term that causes problem when discontinuous solutions are sought. In Hou and Le Floch [7], it was shown that a non-conservative term generates a Borel measure source term at discontinuities. This source term produces an error that grows linearly in time and causes the shock location to drift (independent of the grid resolution).

Our aim is to design a conservative scheme and prove a global entropy bound including the boundaries. We will also require that local entropy inequalities are satisfied and that the converged limit solution satisfies Du Bois and Le Floch's boundary entropy inequality. To achieve this, we start with the results by Olsson and Oliger since these are the only global stability results available for an initial-boundary-value problem for systems of conservation laws. In Sect. 3, we will derive a suitable weak imposition of characteristic-type boundary conditions and show that a bound on the entropy is achieved without the cone condition or any assumption on the signal speed. The key to these proofs is to utilize the specific entropy pair used in [6,11].

Our main result is the derivation of a *conservative entropy stable scheme on a bounded domain.* We exploit the specific entropy pair from [6,11] and show that the diffusion needed for entropy stability in the Cauchy case is sufficient to obtain a global bound. Furthermore, we prove that the numerical solution satisfies local entropy inequalities and test numerically that Du Bois and Le Floch's boundary entropy inequality is satisfied.

To the best of our knowledge, these are the first stability results for a numerical scheme approximating systems of conservation laws on a bounded domain.

2. The entropy pair

The key to obtain a global estimate, as observed in [11], is the use of a specific entropy pair, and in this section, we will introduce this entropy and derive a few auxiliary relations.

Mock [8] showed that a conservation law can be symmetrized by its entropy pair. The conservation law

$$u_t + f(u)_x = 0 \tag{6}$$

turns into

$$u_w w_t + G(w)_x = 0 \tag{7}$$

where u_w is symmetric positive definite and $G_w(w)$ is symmetric. We will use entropy (canonical) splitting proposed in [11], which is based on a well-known one-thirds rule for Burgers' equation.

We begin by stating standard results for entropy solutions. For the entropy pair (E, F), we have that $E_t = E_u^{\mathrm{T}} u_t$ and $E_u^{\mathrm{T}} f_u = F_u$ by definition. Furthermore, the entropy variables are defined as $E_u = w$ and $f(u) = G(w)$ such that G_w is symmetric. Hence, we multiply (6), or equivalently (7), by $E_u^{\mathrm{T}} = w^{\mathrm{T}}$ such that

$$E_t + w^{\mathrm{T}} G(w)_x = 0. \tag{8}$$

Here, we use the idea put forward in [11]. G_w is symmetric and we can define

$$\mathcal{G}(w) = \int_0^1 G(\theta w) \mathrm{d}\theta \tag{9}$$

which satisfies

$$G_x = (G - \mathcal{G})_x + \mathcal{G}_x = (\mathcal{G}_w w)_x + \mathcal{G}_w w_x \tag{10}$$

which they term the "canonical splitting". The symmetry of G' implies symmetry of $\mathcal{G}'$. Furthermore, for any flux that satisfies $G' = G'^{\mathrm{T}}$ and

$$G'w = pG, \quad p \in \mathbf{R} \tag{11}$$

the following relations hold

$$\mathcal{G} = \frac{1}{p+1}G, \quad \mathcal{G}' = \frac{1}{p+1}G'. \tag{12}$$

Unfortunately, the above does not hold for the Euler equations (2) unless very specific entropy variables are used. (See [4], and for completeness, we include their results in "Appendix I".) In addition to the above relations, this particular entropy pair also implies

$$u_w w = pu. \tag{13}$$

2.1. Auxiliary relations

From now on, we will only consider entropy pairs that satisfy (11) and (13). In particular, we will assume that $p = 1$ although this requirement is strictly not necessary.

Lemma 2.1. *Let $F(w)$ denote the entropy flux and w the entropy variables that make the flux function $G(w)$ homogeneous of order 1 (i.e., (11) with $p = 1$). Then,*

$$F(b) - F(a) = \frac{1}{2} w^{\mathrm{T}} G_w w|_a^b$$

Proof. By the definition of an entropy flux, $F_x = w^{\mathrm{T}} G_x$, but $w^{\mathrm{T}} G_x = w^{\mathrm{T}}(\mathcal{G}_w w)_x + w^{\mathrm{T}} \mathcal{G}_w w_x$. Then,

$$\int_a^b F_x \,\mathrm{d}x = \int_a^b w^{\mathrm{T}}(\mathcal{G}_w w)_x + w^{\mathrm{T}} \mathcal{G}_w w_x \,\mathrm{d}x$$

$$F(b) - F(a) = w^{\mathrm{T}} \mathcal{G}_w w|_a^b = \frac{1}{2} w^{\mathrm{T}} G_w w|_a^b$$

□

Lemma 2.2. *Let $F(w)$ denote the entropy flux, $\Psi(w) = \langle w, f \rangle - F(w)$ the entropy potential and w the entropy variables that make the flux function $G(w)$ homogeneous of order 1. Then,*

$$\Psi(w) = \frac{1}{2} w^{\mathrm{T}} G_w(w) w,$$
$$F(w) = \frac{1}{2} w^{\mathrm{T}} G_w(w) w.$$

Proof.

$$\begin{aligned}
\Psi(a) &= \Psi(a) - (\Psi(b) - \Psi(b)) \\
&= \Psi(a) - (w^{\mathrm{T}}(b) G_w(b) w(b) - F(b) - \Psi(b)) \\
&= w^{\mathrm{T}}(a) G_w(a) w(a) - F(a) - (w^{\mathrm{T}}(b) G_w(b) w(b) - F(b) - \Psi(b)) \\
&= \frac{1}{2}(w^{\mathrm{T}}(a) G_w(a) w(a) - w^{\mathrm{T}}(b) G_w(b) w(b)) + \Psi(b))
\end{aligned}$$

In the last equality, we use Lemma 2.1. The final expressions are a sum of two functions. One only depending on a, and the other only on b. Hence, we are forced to conclude that

$$\Psi(a) = \frac{1}{2} w^{\mathrm{T}}(a) G(a) w(a),$$
$$-\frac{1}{2} w^{\mathrm{T}}(b) G_w(b) w(b) + \Psi(b) = 0,$$

which proves the first relation in the lemma. The second part follows directly from the identity $\Psi = w^{\mathrm{T}}G - F$. $\square$

3. Stable boundary conditions

Equipped with the particular entropy pair described above, we will derive a *formal* global entropy estimate for smooth solutions where the skew-symmetric splitting can be used. The purpose of this analysis is to derive a stable form of boundary conditions for a nonlinear conservation law.

Since the solution is assumed to be smooth, we may use (10) in (8), which yields

$$\begin{aligned}\int_0^1 E_t \mathrm{d}x &= -\int_0^1 w^{\mathrm{T}} \left((\mathcal{G}_w w)_x + \mathcal{G}_w w_x \right) \mathrm{d}x \\ &= -\int_0^1 w^{\mathrm{T}} \left((\mathcal{G}_w w)_x + \mathcal{G}_w w_x \right) \mathrm{d}x = -w^{\mathrm{T}} \mathcal{G}_w w|_0^1 = -\frac{1}{2} w^{\mathrm{T}} G_w w|_0^1 \end{aligned} \tag{14}$$

To obtain a bound on the boundary terms, we must introduce the boundary conditions appropriately. To this end, we introduce $G_w = A = R^{\mathrm{T}}\Lambda R$, where Λ is the diagonal eigenvalue matrix, with $\lambda_i \in \mathbb{R}$ and $R^{\mathrm{T}}R = I$ due to the symmetry of G_w. Furthermore, we denote $A^+ = R^{\mathrm{T}}\Lambda^+ R$ where Λ^+ contains only the positive entries of Λ. We will also use the notation $|A| = R^{\mathrm{T}}|\Lambda|R$ and the specific case $G_w(g) = A_g = R_g^{\mathrm{T}}\Lambda_g R_g$.

For simplicity, we focus on the quarter-plane problem and ignore the right boundary by considering the following modification of (1):

$$u_t + f_x = \sigma\delta_0(x) A^+(w)(w - w_g) \quad 0 \leq x < \infty \tag{15}$$

where δ_0 denotes the Dirac delta function with its mass at $x = 0$, and $w_g = w(g)$ is the entropy variables with respect to the boundary data $g(t)$ at $x = 0$.

We remark that the addition of a measure source term at the boundary is a way to weakly impose the boundary condition in (1) at the left boundary. We also assume that the initial conditions have compact support.

Theorem 3.1. *If u is a continuously differentiable solution, then Eq. (15) satisfies a global entropy estimate with $\sigma = -1$. Moreover, the correct number of boundary conditions, as dictated by the linearized equation, is enforced.*

Proof. Changing variables to the entropy form, multiplying by w^{T}, utilizing the canonical splitting and $\sigma = -1$, we arrive at

$$\int_0^\infty E_t \mathrm{d}x - \frac{1}{2} w^{\mathrm{T}} G_w w|_0 = -w^{\mathrm{T}} \tilde{A}^+ (w - w_g)|_0$$

Dropping the index since all boundary terms are at $x = 0$, we need to prove that

$$\widehat{BT} = \frac{1}{2} w^{\mathrm{T}} G_w w - w^{\mathrm{T}} A_0^+ (w - w_g) \tag{16}$$

is bounded. We use the notation $G_w(w(0,t)) = A_0$. Rewriting (16),

$$\begin{aligned}\widehat{BT} &= \frac{1}{2}w^{\mathrm{T}}A_0 w - w^{\mathrm{T}}A_0^+(w-w_g)\\ &= \frac{1}{2}w^{\mathrm{T}}A_0^- w - \frac{1}{2}w^{\mathrm{T}}A_0^+ w + w^{\mathrm{T}}A_0^+ w_g\\ &= \frac{1}{2}w^{\mathrm{T}}A_0^- w - \frac{1}{2}(w-w_g)^{\mathrm{T}}A_0^+(w-w_g) + \frac{1}{2}w_g^{\mathrm{T}}A_0^+ w_g \end{aligned} \tag{17}$$

In the last expression, the first two terms are negative and do not imply a growth of w_0. The requirement for stability is that BT has an upper bound. Before treating the general case, we note that in 3 cases, a bound on BT, and hence stability, follows immediately. 1) If A_0^+ is bounded (as in the linear case), the last term implies a finite growth (which is acceptable). 2) A bound is also readily obtained for a nonlinear system, if $w_g = 0$. 3) In the scalar case, a direct calculation shows that

$$-\frac{1}{2}(w-w_g)^{\mathrm{T}}A_0^+(w-w_g) + \frac{1}{2}w_g^{\mathrm{T}}A_0^+ w_g < \text{Constant} \tag{18}$$

for all $|w|$ large enough.

Next, we prove the result in the general case of a system of conservation laws. We need to show that there is a constant $C > 0$ such that for all w with $|w| > C$, there exists a constant $\widehat{C} = \widehat{C}(C, w_g)$ such that

$$BT(w, w_g) = -\frac{1}{2}(w-w_g)^{\mathrm{T}}A^+(w-w_g) + \frac{1}{2}w_g^{\mathrm{T}}A^+ w_g < \widehat{C}. \tag{19}$$

Here, we have suppressed the subscript 0 for the matrices for notational convenience.

Recall that $A = R\Lambda R^{\mathrm{T}}$ is an orthogonal eigendecomposition of the symmetric matrix $A = G_w(w_0)$ with $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ and $R = [r_1|\cdots|r_n]$ with λ_i and r_i being the ith eigenvalue and eigenvector, respectively.

Without loss of generality, let λ_1 be the growing eigenvalue, that is,

$$|\lambda_1(w)| \to \infty \quad \text{as} \quad |w| \to \infty.$$

Furthermore, we assume that other eigenvalues are bounded. The argument below is easy to generalize to the case where some or all the eigenvalues satisfy the above growth condition.

Denote

$$\Lambda_1 = \operatorname{diag}(\lambda_1, 0, \ldots, 0).$$

We decompose A as $A = \tilde{A} + A_1$ with $A_1 = R\Lambda_1 R^{\mathrm{T}}$ and denote

$$\begin{aligned} BT_1 &= -\frac{1}{2}(w-w_g)^{\mathrm{T}}A_1^+(w-w_g) + \frac{1}{2}w_g^{\mathrm{T}}A_1^+ w_g,\\ \tilde{BT} &= -\frac{1}{2}(w-w_g)^{\mathrm{T}}\tilde{A}(w-w_g) + \frac{1}{2}w_g^{\mathrm{T}}\tilde{A}w_g. \end{aligned}$$

From (19), we obtain that $BT = BT_1 + \widetilde{BT}$.

From our assumptions, $\tilde{A}$ is bounded as $|w| \to \infty$. Therefore, it is easy to check that there exists a constant $\tilde{C}$ such that

$$\widetilde{BT} < \tilde{C}, \tag{20}$$

for all w such that $|w| > C$. The estimate (20) follows as the negative term in $\widetilde{BT}$ grows quadratically where as the positive term is bounded.

Next, we consider the term BT_1. A direct calculation with the definitions of A_1 shows that

$$\begin{aligned} BT_1 &= -\frac{1}{2}(w-w_g)^{\mathrm{T}}A_1^+(w-w_g)+\frac{1}{2}w_g^{\mathrm{T}}A_1^+w_g, \\ &= -\frac{1}{2}(w-w_g)^{\mathrm{T}}R\Lambda_1R^{\mathrm{T}}(w-w_g)+\frac{1}{2}w_g^{\mathrm{T}}R\Lambda_1R^{\mathrm{T}}w_g. \end{aligned} \tag{21}$$

Assuming that BT_1 grows unboundedly implies that the condition

$$\left|r_1^{\mathrm{T}}(w)(w-w_g)\right| < \left|r_1^{\mathrm{T}}w_g\right|. \tag{22}$$

must be satisfied. For otherwise, the first term of (21) will dominate the second and $BT1$ will be bounded, contrary to the assumption.

However, as the eigenvectors are normalized, $r_1(w)$ is bounded. Hence, the condition (22) is violated when $|w|$ grows such that $|r_1^{\mathrm{T}}w| \to \infty$ as the left hand side in (22) grows linearly, whereas the right-hand side is bounded. However, if $|r_1^{\mathrm{T}}w|$ is actually bounded, it means that BT_1 is bounded. A contradiction to the assumption, and hence $BT1$ is always bounded. A growth in any other direction than r_1 appears in $\widetilde{BT}$ and is hence bounded by (20). (Under the assumption that the remaining eigenvalues are bounded. If not, we isolate the growing eigenvalues and repeat the argument above.) In summary, we conclude that (19) is satisfied.

Finally, we note that the boundary conditions for the in-going characteristics are enforced, which is consistent with linear theory for well-posedness. □

Most existing codes for the Euler equations use the conservative variables as opposed to the entropy variables. Hence, we will connect the two forms and state the scheme in the conservative form.

$$u_t + f_x = \sigma\delta_0(x)\mathbb{A}^+(u-g) \quad 0 \le x < \infty \tag{23}$$

where $\mathbb{A}$ is the Jacobian matrix for the conservative variables and $\mathbb{A}^+$ its positive part determined from the eigenvalues.

Theorem 3.2. *Under the same conditions as in Theorem 3.1, (23) satisfies a global entropy bound (with the correct number of boundary conditions).*

Proof. First, a few auxiliary relations found in [16]. Denote $u_w = H, f_u = \mathbb{A}$ and $\mathbb{B} = G_w$ such that $G_w = \mathbb{B} = \mathbb{A}H = f_u u_w$. With our particular entropy pair, we have $H^{-1}u = w$. Since B and H are symmetric, it follows that

$$H^{-1/2}\mathbb{A}H^{1/2} = H^{-1/2}\mathbb{B}H^{-1/2} \tag{24}$$

is symmetric.

Furthermore, denote by λ_k the kth eigenvalue of A and r_k its eigenvector, such that $Ar_k = \lambda_k r_k$. Clearly, the following holds

$$H^{-1/2}\mathbb{A}H^{1/2}(H^{-1/2}r_k) = \lambda_k H^{-1/2}r_k \tag{25}$$

such that after normalization $(\lambda_k, H^{-1/2}r_k)$ becomes the eigensystem of $H^{-1/2}\mathbb{A}H^{1/2}$.

Next, we turn to (23) and multiply by w^{T}. Jumping a few steps similar to the previous proof, we must bind

$$\begin{aligned} \mathbb{K} &= w^{\mathrm{T}}G_w w - 2w^{\mathrm{T}}\mathbb{A}^+(u-g) \\ &= w^{\mathrm{T}}G_w w - 2w^{\mathrm{T}}\mathbb{A}^+HH^{-1}(u-g) \\ &= w^{\mathrm{T}}G_w w - 2w^{\mathrm{T}}\mathbb{A}^+H^{1/2}H^{1/2}(w-H^{-1}g)) \end{aligned}$$

We introduce $\tilde{w} = H^{1/2}w$ and $\tilde{g} = H^{-1/2}g$, and we recall that $H^{-1/2} = H^{-1/2}(w_0)$. Furthermore, u, w and $\tilde{w}$ represent solution values at $x = 0$. Further manipulations yield

$$\mathbb{K} = w^{\mathrm{T}}H^{1/2}H^{-1/2}\mathbb{B}H^{-1/2}H^{1/2}w - 2w^{\mathrm{T}}H^{1/2}H^{-1/2}\mathbb{A}^+H^{1/2}(\tilde{w}-\tilde{g}))$$

Introduce $Z = H^{-1/2}\mathbb{A}H^{1/2}$ and by (25), the eigenvalues of $\mathbb{A}$ and Z coincide (up to a normalization) such that $H^{-1/2}\mathbb{A}^{+}H^{1/2} = Z^{+}$ follows. Hence,

$$\mathbb{K} = \tilde{w}^{\mathrm{T}}Z\tilde{w} - 2\tilde{w}^{\mathrm{T}}Z^{+}(\tilde{w} - \tilde{g}) \tag{26}$$

The expression (26) has the same form as (16), and the rest of the proof is identical. □

4. The conservative scheme

Throughout this article, we assume that $G(w)$ is homogeneous of order 1, that is, $p = 1$ in (11), in order not to clutter the article with excessive notation, but the theory is readily extended to flux functions homogeneous of a different order.

Discretize the interval $[0, 1]$ with $N + 1$ equidistant points and $h = 1/N$. We will use the standard second-order accurate Summation-by-parts (SBP) operator.

$$D = \frac{1}{2h}\begin{pmatrix} -2 & 2 & 0 & \dots & & \\ -1 & 0 & 1 & 0 & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & -1 & 0 & 1 \\ & & \dots & 0 & -2 & 2 \end{pmatrix} \tag{27}$$

with the property that

$$PD = Q, \qquad Q + Q^{\mathrm{T}} = \mathrm{diag}(-1, 0, \dots, 0, 1) = B \tag{28}$$

when $P = h \cdot \mathrm{diag}(\frac{1}{2}, 1, \dots, 1, \frac{1}{2})$. We will also use the row-vector $\bar{p}$ with components $(\bar{p})_i = p_i = [P]_{ii}$. We arrange the unknowns as $u^{\mathrm{T}} = (u_0, u_1, \dots, u_N)$ and similarly for f. For notational convenience, we will carry out the analysis for a scalar equation.

Denote $G_w(w_i) = a_i$ and note that $G_i = G(w_i) = a_i w_i$. Furthermore, let $A = \mathrm{diag}(a_0, \dots a_N)$.

Next, we will state the key result that will enable us to prove stability. We will need the undivided difference operator.

$$D_- = \begin{pmatrix} 0 & 0 & 0 & \\ -1 & 1 & 0 & \\ 0 & -1 & 1 & \\ & & & \ddots \end{pmatrix}.$$

Let $F(w)$ denote the entropy flux, $\Psi(w)$ the entropy potential and $f_i = f(u_i)$. Define the following consistent numerical fluxes

$$\begin{aligned} f_{i+1/2} &= \frac{f_{i+1} + f_i}{2} \\ g^*_{i+1/2} &= f_{i+1/2} - D^*_{i+1/2}(w_{i+1} - w_i) \end{aligned} \tag{29}$$

$g^*_{i+1/2}$ is the entropy conservative flux that satisfies

$$(w_{i+1} - w_i)g^*_{i+1/2} - (\Psi_{i+1} - \Psi_i) = 0 \tag{30}$$

where $\Psi_i = \Psi(w_i)$. Furthermore, $D^*_{i+1/2}$ is the diffusion coefficient specifically chosen such that (30) holds. (It need not be positive.) Furthermore, the numerical entropy flux associated with the entropy conservative flux is

$$F^*_{j+1/2} = \frac{1}{2}(w_{i+1} + w_i)g^*_{i+1/2} - \frac{1}{2}(\Psi_{i+1} + \Psi_i). \tag{31}$$

It was shown in [16] that for a three-point stencil, the entropy conservative flux can always be stated as in (29). It should be noted, however, that obtaining analytical expressions for $D^*_{i+1/2}$ may be difficult and we use it here only as a theoretical tool. The main idea in the entropy stability framework is to find analytically expressible diffusion coefficients greater than the entropy conservative choice. For the Cauchy problem, we define a flux

$$g_{j+1/2} = f_{i+1/2} - D_{i+1/2}(w_{i+1} - w_i). \tag{32}$$

If $D_{j+1/2} \geq |D^*_{j+1/2}|$, then (32) is an entropy stable flux that satisfies,

$$\frac{1}{2}\left((w_{i+1} - w_i)g_{i+1/2} - (\Psi_{i+1} - \Psi_i)\right) \leq 0.$$

From this, it follows that the scheme satisfies a local entropy inequality,

$$(E_i)_t + \frac{F_{i+1/2} - F_{i+1/2}}{h} \leq 0,$$

where $F_{i+1/2} = \frac{1}{2}(w_{i+1} + w_i)g_{i+1/2} - \frac{1}{2}(\Psi_{i+1} + \Psi_i)$. For an extensive explanation of the entropy stability framework, we refer the reader to [16]. Furthermore, in [15], a thorough accuracy analysis of entropy stable schemes is found.

Lemma 4.1. *Let w the entropy variables that make the flux function $G(w)$ homogeneous of order 1. Denote by $P^{-1}Q$ the second-order central SBP operator defined in (27). Then,*

$$w^{\mathrm{T}}Qf = \frac{1}{2}w^{\mathrm{T}}Bf + \frac{1}{2}w^{\mathrm{T}}D_-^{\mathrm{T}}AD_-w \tag{33}$$

where $A = diag(0, D^*_{1/2}, D^*_{3/2}, \ldots, D^*_{N+1/2})$.

Proof. Consider

$$u_t + P^{-1}Qf = 0 \tag{34}$$

We begin by rephrasing (34) to flux form. For a grid with $N+1$ points, we obtain

$$\begin{aligned} (u_0)_t + \frac{f_{1/2} - f_0}{h/2} &= 0, \\ (u_i)_t + \frac{f_{i+1/2} - f_{i-1/2}}{h} &= 0, \quad i = 1\ldots, N-1 \\ (u_N)_t + \frac{f_N - f_{N-1/2}}{h/2} &= 0. \end{aligned} \tag{35}$$

Next, we note that by (29), the following identity holds,

$$f_{i+1/2} = g^*_{i+1/2} + D^*_{i+1/2}(w_{i+1} - w_i). \tag{36}$$

Then, consider the following scheme

$$\begin{aligned} (u_0)_t + \frac{g^*_{1/2} - g^*_{-1/2}}{h/2} &= 0, \\ (u_i)_t + \frac{g^*_{i+1/2} - g^*_{i-1/2}}{h} &= 0, \quad i = 1\ldots, N-1 \\ (u_N)_t + \frac{g^*_{N+1/2} - g^*_{N-1/2}}{h/2} &= 0, \end{aligned} \tag{37}$$

which, by (36) is equivalent to

$$u_t + P^{-1}Qf = P^{-1}D_-^{\mathrm{T}}AD_-w \tag{38}$$

We will proceed and analyze (37). To this end, we will carry out the operations corresponding to multiplying (38) by $w^{\mathrm{T}}P$ on the component form (37). Recalling the $p_0 = p_N = h/2$ and all other $p_i = h$, we multiply the second line by $w_i h$.

$$h(E_i)_t + F^*_{i+1/2} - F^*_{i-1/2} = \frac{1}{2}\left((w_{i+1} - w_i)g^*_{i+1/2} - (\Psi_{i+1} - \Psi_i)\right) + \frac{1}{2}\left((w_i - w_{i-1})g^*_{i-1/2} - (\Psi_i - \Psi_{i-1})\right) = 0 \tag{39}$$

(See [16] for details.) The right-hand side equals 0 due to the entropy conservative relation (30). Next, we derive the corresponding expressions for the boundary scheme.

$$(u_0)_t + \frac{g^*_{1/2} - g^*_{-1/2}}{h/2} = 0$$

Here $g^*_{1/2} = g^*(u_0, u_1)$ is defined as above, and we let $g^*_{-1/2} = f_0$. Multiply the boundary scheme in (37) by $w_0 h/2$.

$$\frac{h}{2}(E_0)_t + w_0(g^*_{1/2} - g^*_{-1/2}) = 0.$$

Then, the boundary scheme can be transformed into

$$\frac{h}{2}(E_0)_t + F^*_{1/2} - F^*_{-1/2} = \frac{1}{2}\left((w_1 - w_0)g^*_{1/2} - (\Psi_1 - \Psi_0)\right), \tag{40}$$

with

$$F^*_{-1/2} = w_0 f_0 - \Psi_0.$$

The numerical entropy fluxes above are consistent. With our particular entropy pair and by Lemma 2.2, we deduce that

$$F^*_{-1/2} = \frac{1}{2} w_0 f_0. \tag{41}$$

For the boundary at x_N, we obtain in a similar way

$$\begin{aligned} F^*_{N+1/2} &= \frac{1}{2} w_N f_N \\ \frac{h}{2}(E_N)_t + F^*_{N+1/2} - F^*_{N-1/2} &= 0. \end{aligned} \tag{42}$$

Summing (40), (42) and (39) over i results in

$$\bar{p}\bar{E}_t - F^*_{-1/2} + F^*_{N+1/2} = 0 \tag{43}$$

where $\bar{E} = (E_0, E_1, \ldots, E_N)^{\mathrm{T}}$. Using (38), we can write (43) as

$$w^{\mathrm{T}}Pu_t + w^{\mathrm{T}}Qf - w^{\mathrm{T}}D_-^{\mathrm{T}}AD_-w = -F^*_{-1/2} + F^*_{N+1/2} = \frac{1}{2}w^{\mathrm{T}}Bf$$

and the Lemma follows. □

Next, we introduce $\Sigma_0 = (1, 0, 0, \ldots, 0)^{\mathrm{T}}$ and $\Sigma_N = (0, 0, \ldots, 0, N)^{\mathrm{T}}$ and consider the conservative scheme

$$u_t + P^{-1}Qf = P^{-1}D_-^{\mathrm{T}}\Lambda D_-w - P^{-1}\Sigma_0 A^+(w_0 - g_0) + P^{-1}\Sigma_N A^-(w_N - g_N) \tag{44}$$

or equivalently on component form

$$\begin{aligned}(u_0)_t + \frac{\bar{f}_{1/2} - f_0}{h/2} &= -\mathbb{S}_0 \\ (u_i)_t + \frac{\bar{f}_{i+1/2} - \bar{f}_{i-1/2}}{h} &= 0, \quad i = 1, \dots, N-1 \\ (u_N)_t + \frac{f_N - \bar{f}_{N-1/2}}{h/2} &= \mathbb{S}_N\end{aligned} \tag{45}$$

with

$$\bar{f}_{i+1/2} = \frac{f_{i+1} + f_i}{2} - \frac{\lambda_{i+1/2}}{2}(w_{i+1} - w_i). \tag{46}$$

and

$$\begin{aligned}\mathbb{S}_0 &= [P^{-1}]_0 A^+ (w_0 - g_0), \\ \mathbb{S}_N &= [P^{-1}]_N A^- (w_N - g_N).\end{aligned} \tag{47}$$

$\lambda_{j+1/2}$ is the diffusion coefficient. As outlined above, for entropy stability of the Cauchy problem, we would choose it greater than the entropy conservative choice, $D^*_{j+1/2}$. It turns out that this is the appropriate choice for the initial-boundary value problem as well. This will be stated in the theorem below.

Associated with this scheme is the numerical entropy flux,

$$\begin{aligned}\mathbb{F}_{j+1/2} &= \frac{1}{2}(w_{i+1} + w_i)\bar{f}_{i+1/2} - \frac{1}{2}(\Psi_{i+1} + \Psi_i) \\ \mathbb{F}_{-1/2} &= w_0 f_0 - \Psi_0 - \bar{p}_0 w_0 \mathbb{S}_0 \\ \mathbb{F}_{N+1/2} &= w_N f_N - \Psi_N - \bar{p}_N w_N \mathbb{S}_N\end{aligned}$$

Next, we will introduce the notion strong entropy stability.

Definition. The scheme is called *strongly entropy stable*, if it satisfies a local entropy inequality, along with a global entropy estimate for non-homogeneous boundary data, that is, $\sum_{i=0}^{N} \bar{p}_i (E_i)_t <$ Constant.

Now, we will state the main result of this paper.

Theorem 4.2. *The scheme (44)–(47) approximating (23) satisfies a global entropy estimate if* $\lambda_{i+1/2} \geq |D^*_{i+1/2}|, i = 0 \dots N-1$. *Furthermore, the scheme also satisfies the local entropy inequalities*

$$(E_t)_i + \frac{\mathbb{F}_{i+1/2} - \mathbb{F}_{i-1/2}}{p_i} \leq 0, \quad i = 0 \dots N, \tag{48}$$

and hence the scheme is strongly entropy stable.

Proof. Multiply (44) by $w^{\mathrm{T}} P$. Using Lemma 4.1, we obtain

$$\begin{aligned}w^{\mathrm{T}} P u_t + w^{\mathrm{T}} Q f - \frac{1}{2} w^{\mathrm{T}} B f &= w^{\mathrm{T}} D_-^{\mathrm{T}} (A + \Lambda) D_- w \\ &\quad + \sigma_0 w_0^{\mathrm{T}} A_0^+ (w_0 - g_0) + \sigma_N w_0^{\mathrm{T}} A_N^- (w_N - g_N).\end{aligned}$$

The quadratic diffusion is indefinite and can be bounded by choosing $\lambda_{i+1/2} \geq |D^*_{i+1/2}|$. The boundary terms are bounded by the the RHS source terms, and the proof is the same as in (17) (extended to cover both the left and right boundaries).

The condition $\lambda_{i+1/2} \geq |D^*_{i+1/2}|$ is coincides exactly with the condition for entropy stability as defined in [16], which in turn implies that a local entropy estimate is satisfied. (This also follows from (40).) □

As a remark, we stress that although the derivations are carried out for a scalar conservation law, it is merely a matter of notation to generalize it to the case of a scheme. In fact, as the scheme is stated in (45), u and f can be vectors and $\lambda_{i+1/2}$ positive definite matrices, in which case it would approximate a system of conservation laws. Clearly, the proof is still valid, and the scheme is *strongly entropy stable.*

Remark. The above scheme is conservative and is well adapted to computing solutions with shocks. For smooth flows (like in subsonic flow situations with the Euler equations), we suggest a non-conservative scheme of the form

$$u_t + \frac{1}{2}(DA + AD)w = \mathbb{S} \tag{49}$$

where $\mathbb{S}$ is a source term that will contain the Simultaneous Approximation Terms (SAT) that enforce the boundary conditions. $\mathbb{S}_0$ and $\mathbb{S}_N$ are defined above and $\mathbb{S}_i = 0$ for other i's can be used. Analysis of this scheme is carried out in "Appendix II". This scheme is highly desirable for approximating smooth flows as it can be easily extended to higher order of accuracy.

5. Computations

We will demonstrate the robustness of this scheme for a number of standard cases. In all test cases, we will use the entropy-fixed Roe scheme for the internal diffusion. The diffusion will be localized with the limiter derived in [12] where it was shown to not interfere with the proofs of entropy stability. In these computations, however, we will also use the entropy stable boundary conditions implemented for the standard Jacobian matrix on conservative form. Hence, the scheme is stated entirely with the conservative variables and the entropy variables are not explicitly used. We also use the standard fourth-order Runge–Kutta scheme to march in time.

The governing equations in all the tests are the one-dimensional Euler equations for a polytropic gas.

$$\begin{aligned} u_t + f(u)_x &= 0 \\ u &= (\rho, m, E)^{\mathrm{T}} \\ f(u) &= qu + (0, P, qP)^{\mathrm{T}} \\ P &= (\gamma - 1)\left(E - \frac{1}{2}\rho q^2\right). \end{aligned}$$

ρ, q, P and E are the density, velocity, pressure and total energy. $m = \rho q$ is the momentum and γ the ratio of the specific heats. The eigenvalues of the Jacobian matrix $A(u) = \frac{\partial f}{\partial u}$ are, $q - c, q, q + c$, where $c = \sqrt{\gamma P/\rho}$ is the speed of sound.

5.0.1. Shock/entropy wave interaction. The first example is the one-dimensional prototype for shock-turbulence interaction proposed in [13]. It is an entropy wave interacting with a strong shock. The initial conditions used in [13] on the domain $-5 \leq x \leq 5$ are

$$\begin{aligned} (\rho, q, P) &= (3.857143, 2.629369, 10.33333) \quad \text{for } x < -4, \\ (\rho, q, P) &= (1 + \epsilon \sin(5x), 0, 1) \quad \text{for } x \geq -4, \end{aligned}$$

with $\epsilon = 0.2$.

The quality of the solution in the interior is as expected for a second-order scheme with localized diffusion. (See [12].) The focusof these experiments is mainly to test the robustness of the boundary conditions. Initially, the waves will travel toward the left boundary, and a bad boundary implementation can cause the solution to explode.

As an example, we tried to overwrite the solution with data at each time step (so-called injection), which is a commonly used technique in practice. The solution is a Mach 3 shock wave, and hence all characteristics are in-going and the procedure do not over-specify the boundary. Indeed, the numerical solution explodes immediately. Possibly one could stabilize the solution with more diffusion, but needless to say, any such effort would degrade the accuracy.

With our proposed technique, the solution stays bounded and the solution at $T = 1.8, 2.5, 4.0$ computed with 200 grid points can be viewed in Fig. 1. The results are very similar to those reported in [12]. The initial disturbances hitting the left boundary do not cause any stability problems.

We also note that the shock is leaving the domain and the boundary appears to be quite transparent. Furthermore, the boundary entropy inequality (5) was evaluated numerically, and the maximal and minimal value of were found to be $(3.7512e{-}05, -4.2864e{-}15)$ (for 200 points and $(1.2260e{-}05, -3.2642e{-}15)$ for 400 points).

5.0.2. Shock tube. The next example found in [13] and originally in [14] is the Euler equations with initial data

$$(\rho, q, P) = (1, 0, 1)\ x \leq 0,$$
$$(\rho, q, P) = (0.125, 0, 0.1)\ x \geq 0,$$

on the domain $-5 \leq x \leq 5$. These initial data will develop a rarefaction wave, a shock and a contact discontinuity.

In [13], 100 grid points were used and we will follow their example. The results at two different times are shown in Fig. 2.

Again, we note that the discontinuities leave the domain smoothly. In this case, maximum and minimum of (5) were $(9.8608e - 32, -0.0088384)$, respectively. (For 200 points the values are $(1.9722e - 31, -0.0064286)$.)

5.1. Woodward-Colella

In this case, both boundaries are walls and shocks will impinge on them. A severe test of robustness. We construct boundary data ($g_{x=-5}(t)$ and $g_{x=5}(t)$) by taking the solution $u(\{-5, 5\}, t)$ and setting $q = 0$. (Formally, the stability proof is not valid since $g_{x=-5,5}$ is not bounded functions but depend on the solution.)

The initial data are as follows for $0 < x < 0.1$: $(\rho, q, P) = (1, 0, 1000)$; for $0.1 < x < 0.9 (\rho, q, P) = (1, 0, 0.01)$; and for $0.9 < x < 1.0 (\rho, q, P) = (1, 0, 0, 100)$.

The solution was computed with 400 grid points, and the boundary entropy $F_0 - F_g - w_g(f_0 - f_g)$ varied between $-2.1849e - 14$ and $6.2530e - 12$. (For 200 points: $(-2.9049e - 14, 6.2539e - 12)$.) The solution at $T = 0.05$ and $T = 0.4$ is shown in Fig. 3

6. Conclusions

In this article, we have addressed the problem of imposing boundary conditions on systems of conservation laws. The most important tool in this endeavor was the specific entropy pair introduced in [11]. This allowed us to weakly impose characteristic-based boundary conditions and obtain a global entropy estimate.

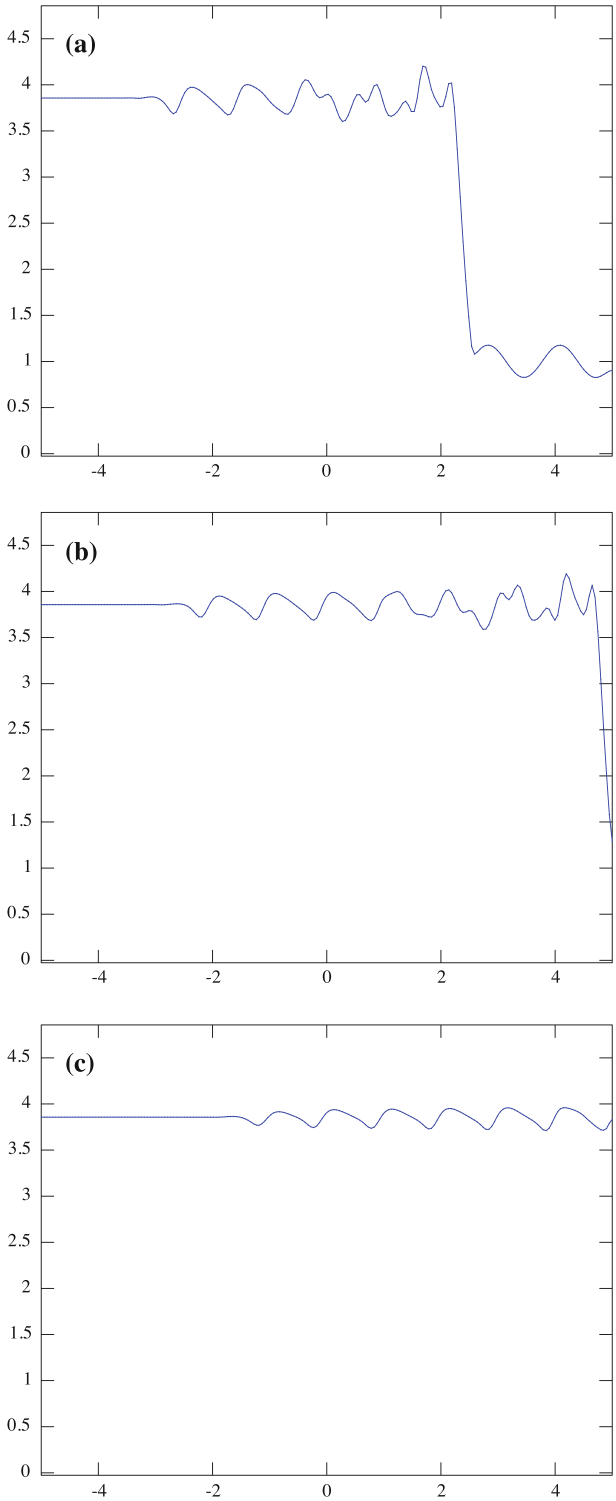

FIG. 1. Plots of ρ solution with 400 grid points. **a** $T = 1.8$. **b** $T = 2.5$. **c** $T = 4.0$

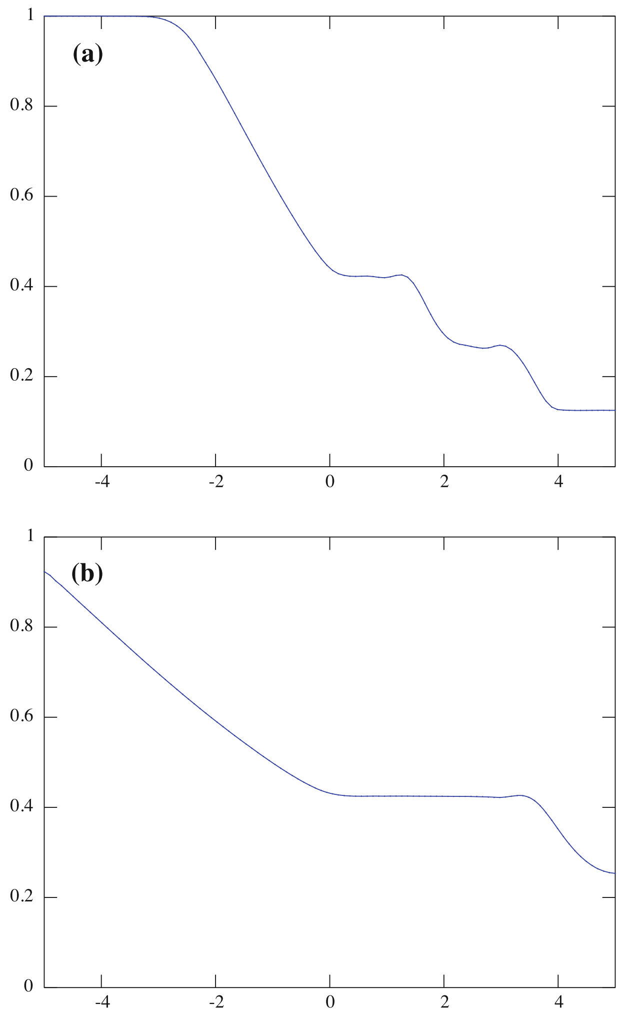

FIG. 2. The solution is computed with 100 grid points. The ρ solution with a rarefaction wave and two contact discontinuities. **a** $T = 2.0$. **b** $T = 4.0$

Our main result is an entropy stable *conservative* scheme on a bounded domain. Again, the key analytical tool was the specific entropy pair. Using this entropy pair, we showed that by augmenting the scheme with a numerical diffusion that guarantees entropy stability in the Cauchy case, it will retain a summation-by-parts property and we could use a weak enforcement of boundary conditions to derive a global bound on the entropy. Furthermore, we have shown that the numerical solution satisfies local entropy inequalities.

Finally, we demonstrated the robustness of the numerical scheme in a series of examples for the Euler equations of gas dynamics. The first two used characteristic boundary conditions, which were shown to be transparent to nonlinear waves and very robust. In the third case, the robustness of a wall boundary condition was tested. Furthermore, we evaluated the boundary entropy inequality (5), and in all cases, the maximal value was 0, if not to round-off errors, so to well within the numerical accuracy, a strong indication that our proposed boundary scheme satisfies the boundary inequality as well.

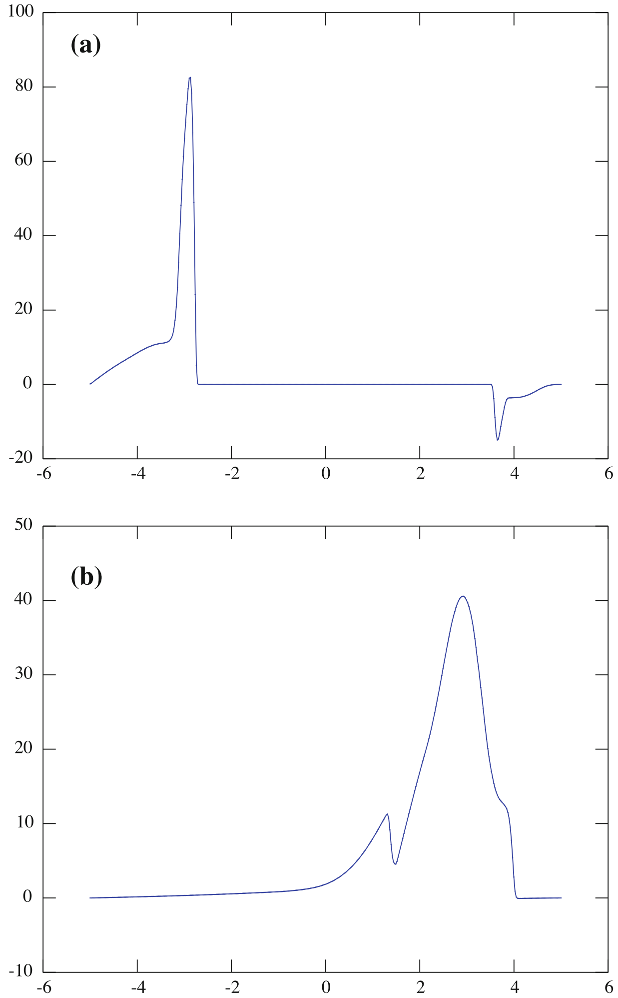

Fig. 3. The solution is computed with 400 grid points. The momentum ρq is depicted. **a** $T = 0.05$. **b** $T = 0.4$

Appendix I: Homogeneity for the Euler equations

We will give a specific example from [4]. (In particular, this is the case with $\alpha = 1 - 2\gamma$ and $\beta = 1$.)

If $G(\theta w) = \theta^\beta g(w)$, then $G_w w = \beta w$ which is what we want. We will now list all the variables, fluxes and entropies for the case $\beta = 1$. Beginning with the entropy:

$$E(u) = \rho h(S)$$
$$h(S) = K \exp(\kappa S) = K(p\rho^{-\gamma})^\kappa$$
$$\kappa = \frac{1}{1-\gamma}$$

where K is an arbitrary constant. Furthermore,

$$p^* = \frac{\gamma - 1}{1 - 2\gamma}\left(w_1 - \frac{1}{2}\frac{w_2^2}{w_3}\right)$$
$$p = (-K)^{-1}\left((p^*)^{1-2\gamma} w_3^\gamma\right)^{1/(1-\gamma)}$$

In the particular case of air, with $\gamma = 7/5$, the following relations appear

$$\frac{p^*}{p} = -K\left(\frac{p}{\rho}\right)^{-7/2}$$
$$\frac{p}{p^*} = (-K)^{-1}(p^*/w_3)^{7/2}.$$

Returning to a general γ, the variables and fluxes are

$$\begin{aligned} w^{\mathrm{T}} &= \frac{p^*}{p}\left(u_3 + \frac{-2\gamma}{\gamma-1}p,\, -u_2,\, u_1\right)^{\mathrm{T}} \\ u^{\mathrm{T}} &= \frac{p}{p^*}\left(w_3,\, -w_2,\, w_1 - \frac{-2\gamma}{\gamma-1}p^*\right)^{\mathrm{T}} \\ g(w)^{\mathrm{T}} &= \frac{p}{p^*}\left(-w_2,\, \frac{w_2^2}{w_3} + p^*,\, -\frac{w_2}{w_3}(w_1 + \frac{3\gamma-1}{\gamma-1}p^*)\right)^{\mathrm{T}} \end{aligned}$$

Finally, we have

$$G_w = \begin{pmatrix} a\rho u & a\rho u^2 - p & u(\frac{a\rho u^2}{2} - bp) \\ & u(a\rho u^2 - 3p) & -\frac{bp^2}{\rho} + cpu^2 + \frac{a\rho u^4}{2} - \frac{1}{2}pu^2 \\ \text{symm} & & u(bc\frac{p^2}{\rho} + cpu^2 + \frac{a}{4}\rho u^4) \end{pmatrix} \tag{50}$$

where

$$\begin{aligned} a &= \gamma/(1-2\gamma) \\ b &= \gamma/(\gamma-1) \\ c &= (1-2\gamma)/(\gamma-1) \end{aligned}$$

Appendix II: A non-conservative scheme

In this section, we analyze the non-conservative scheme (49). We remark that this scheme is essentially the same as in Gerritsen and Olsson [5]. It differs only in the way boundary conditions are enforced.

Like in the continuous case, we multiply (49) by the entropy variables scaled with the P matrix to utilize the SBP property of the difference operators.

$$w^{\mathrm{T}}Pu_t + w^{\mathrm{T}}P(DA + AD) = w^{\mathrm{T}}P\mathbb{S} \tag{51}$$

and

$$\bar{p}E_t + \frac{1}{2}\left(w^{\mathrm{T}}QAw + w^{\mathrm{T}}AQw\right) = w^{\mathrm{T}}P\mathbb{S} \tag{52}$$

Using $Q = B - Q^{\mathrm{T}}$ and by the symmetry of A, we obtain

$$\bar{p}E_t + \frac{1}{2}w^{\mathrm{T}}ABw = w^{\mathrm{T}}P\mathbb{S} \tag{53}$$

Definition. A numerical scheme for the initial-boundary-value problem (1) with inhomogeneous boundary data is said to be *globally entropy stable*, if $\bar{p}E_t \leq$ Constant.

To prove stability, we must choose $\mathbb{S}$ suitably by utilizing the boundary conditions derived in the previous section. We must ensure

$$-\frac{1}{2}w^{\mathrm{T}}ABw + w^{\mathrm{T}}P\mathbb{S} < \text{Constant}, \tag{54}$$

and hence we choose the vector $\mathbb{S}$ as

$$\mathbb{S}_0 = -[P^{-1}]_0 A^{+}\left(w_0 - g_0\right),$$
$$\mathbb{S}_N = [P^{-1}]_N A^{-}\left(w_N - g_N\right),$$

and all other $\mathbb{S}_i = 0$. The proof of stability is exactly the same as the proof of Theorem 3.1. We summarize the results in the following proposition.

Proposition 6.1. *For a flux function f and an entropy pair that makes $G(w)$ homogeneous of order 1, the approximation (49) of (23) with boundary conditions imposed by (47) is globally entropy stable.*

Remark. Since the equation is nonlinear, Lax-Richtmyer's equivalence theorem does not hold and solutions of a stable and consistent scheme (like (49)) does not necessarily converge. Nevertheless, stability will certainly be a necessary requirement in any convergence theory.

An important property of the scheme (49) is that it is trivially generalized to high-order accuracy, by exchanging the SBP operator (27) with a high-order counterpart. It is straightforward to see that the stability proof still holds (keeping in mind that the P matrix in (47) will also change). The important property for the stability proof is (28).

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