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Numerical analysis / Analyse numérique

The positive entropy production property for augmented nonlinear hyperbolic models

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Abstract. Given a first-order nonlinear hyperbolic system of conservation laws endowed with a convex entropy-entropy flux pair, we consider the class of weak solutions containing shock waves depending upon some small scale parameters. In this Note, after introducing a notion of *positive entropy production property* that involves test-functions (rather than solutions), we define and derive several classes of entropy-dissipating augmented models, as we call them, which involve (possibly nonlinear) second- and third-order augmentation terms. Such terms typically arise in continuum physics and model viscosity and other high-order effects in a fluid. By introducing a new notion of positive entropy production that concerns general functions rather than solutions, we can easily check the entropy-dissipating property for a broad class of augmented models. The weak solutions associated with the corresponding zero-limit may contain (nonclassical undercompressive) shocks whose selection is determined from these high-order effects, for instance by using traveling wave solutions. Having a *classification* of the underlying models, as we propose, is essential for developing a general shock wave theory.

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1. Continuum physics modeling from small-scales to macro-scales

Many models in continuum physics involve augmentation terms containing small parameters such as the viscosity, heat conduction, relaxation effects, etc. These terms are typically modeled by second- or third-order derivatives which are taken into account in the fundamental conservation principles of continuum physics. For instance in a compressible fluid, when the viscosity effects are dominant, no region with a sharp gradient can form. On the other hand, when the third-order effects are dominant, highly oscillating patterns are observed near sharp gradients of the solutions. In the present Note, the regime we are interested in is the one when the second-

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and third-order effects are small while being kept *in balance* with each other [9]. It is natural to assume that the orders of magnitude of the physical coefficients (which depend on the fluid or solid material under consideration) arising in (for instance) a combination of terms like (see below) $v u_{xx} + \kappa u_{xxx}$ are such that the ratio $\xi = \kappa/v^2$ is of order 1. We can then write these terms (for some η, ε) as $v u_{xx} + \kappa u_{xxx} = \eta \varepsilon u_x^\varepsilon + \xi \eta^2 \varepsilon^2 u_{xx}^\varepsilon$.

We are still assuming that the hyperbolic aspects of the flow are dominant, and the secondand third-order terms are relevant only in a neighborhood of large gradients of the solutions. In the theory of nonclassical shocks one is interested in describing the macro-scale features, that is, only the *limit* $\varepsilon \rightarrow 0$ and to do so we need to extract some "information" from the small-scales. Importantly, for the present Note, the global dynamics of the shocks turn out to depend upon the small-scale physical modeling, and it is our aim here to provide a framework in which general classes of interest can be derived and analyzed. We build here upon many earlier works on this subject, especially [1–15].

Our main purpose in this Note is to provide a working notion of "positive entropy production" (which is not solution-dependent), together with a methodology in order to derive sufficient and necessary conditions ensuring that the augmentation terms are compatible with a given entropy. We postpone to the last section of this Note several motivations and implications of our results. So, we directly introduce our key definition in the one-dimension context in Definition 1, below.

2. Augmented models with linear terms

2.1. Systems endowed with an entropy

While our results hold in several space dimensions, they are easier to present in one space dimension, so we restrict attention here to

$$u_t + f(u)_x = 0, \qquad u = u(t, x) \in \mathscr{U} \subset \mathbb{R}^N, \tag{1}$$

with unknown $u = (u_a) = (u_1, ..., u_N) \in \mathcal{U}$ (an open subset of \mathbb{R}^N). We assume this system to be endowed with a convex entropy-entropy flux pair (U, F), and we impose the entropy inequality

$$U(u)_t + F(u)_x \le 0. \tag{2}$$

In the entropy variable $v = v_{\sharp}(u) := \nabla U(u)$ after performing the change of variable $u \in \mathcal{U} \mapsto v \in \nabla U(\mathcal{U}) \subset \mathbb{R}^N$ we have

$$u_{\sharp}(v)_{t} + f_{\sharp}(v)_{x} = 0, \tag{3}$$

and observing that

$$v^{T} u_{\sharp}(v)_{t} = U_{\sharp}(v)_{t}, \qquad v^{T} f_{\sharp}(v)_{x} = F_{\sharp}(v)_{x}, \tag{4}$$

we obtain

$$U_{\sharp}(\nu)_t + F_{\sharp}(\nu)_x \le 0. \tag{5}$$

It is natural to express the high-order contributions in terms of v and we now proceed by listing classes of augmented models of increasing difficulty. For simplicity in the presentation, we often suppress the subscript ε except when emphasis is necessary.

It will be useful to have a short-hand notation for the "total" flux and entropy flux, that is, we will write the augmented model in the form

$$u_{\sharp}[\nu]_{t} + f^{\sharp \text{Tot}}[\nu]_{x} = 0, \tag{6a}$$

and its entropy balance law in the form

$$U_{\sharp}[v]_{t} + F^{\sharp \operatorname{Tot}}[v]_{x} = D_{\sharp}[v], \tag{6b}$$

in which the following expressions can be determined for each model of interest:

$$f^{\text{\#Tot}}[v] = f_{\sharp}(v) + f^{\text{\#Diff}}[v] + f^{\text{\#Disp}}[v], \qquad F^{\text{\#Tot}}[v] = F_{\sharp}(v) + F^{\text{\#Diff}}[v] + F^{\text{\#Disp}}[v].$$
(6c)

2.2. Linear second- and third-order terms

We begin with augmentation terms that are linear in v_x and v_{xx} with constant coefficients. Namely, we consider

$$\iota_{\sharp}(\nu)_{t} + f_{\sharp}(\nu)_{x} = \varepsilon B_{\sharp} \nu_{xx} + \varepsilon^{2} K_{\sharp} \nu_{xxx} = \left(S_{\sharp} \left[\nu^{\varepsilon} \right] \right)_{x}, \tag{7}$$

in which B_{\sharp} and K_{\sharp} are given $(N \times N)$ -matrices. We propose the following novel notion of positivity, which involves general functions rather than solutions.

Definition 1. A nonlinear expression $S[w^{\varepsilon}]$ of a sequence of functions $w^{\varepsilon} : \mathbb{R} \to \mathcal{U}_{\sharp} \subset \mathbb{R}^{N}$ involving a function w^{ε} and its (rescaled) derivatives $\varepsilon \partial_{x} w^{\varepsilon}$ and $\varepsilon^{2} \partial_{xx} w^{\varepsilon}$ is said to enjoy the positive entropy production property *if*

$$\liminf_{\varepsilon \to 0} \int_{\mathbb{R}} \partial_x w^{\varepsilon} \cdot S_{\sharp} \left[w^{\varepsilon} \right] \theta \, dx \ge 0 \tag{8}$$

for all test-functions $\theta = \theta(x) \ge 0$ and for any sequence of bounded functions $w^{\varepsilon} = w^{\varepsilon}(x)$ with bounded total dissipation

$$\limsup_{\varepsilon \to 0} \|w^{\varepsilon}\|_{L^{\infty}(\mathbb{R})} + \limsup_{\varepsilon \to 0} \int_{\mathbb{R}} \varepsilon |\partial_x w^{\varepsilon}|^2 dx < +\infty.$$
(9)

Our sign condition (8) is equivalent to saying

$$\liminf_{\varepsilon \to 0} \int_{\mathbb{R}} \left(w_x^{\varepsilon} \right)^T \left(\varepsilon B_{\sharp} w_x^{\varepsilon} + \varepsilon^2 K_{\sharp} w_{xx}^{\varepsilon} \right) \theta dx \ge 0$$
 (10)

for all test-functions $\theta = \theta(x) \ge 0$ and all sequences $w^{\varepsilon} : \mathbb{R} \to \mathcal{U}_{\sharp} \subset \mathbb{R}^{N}$ satisfying (9).

Proposition 2 (Linear second- and third-order terms). A necessary condition for the onedimensional augmented model (7) to satisfy the positive entropy production property in Definition 1 (see (10)) is:

$$B_{\sharp}^{I} + B_{\sharp}$$
 is a non-negative matrix, K_{\sharp} is a symmetric matrix. (11)

Moreover, the entropy inequality holds as follows:

$$U_{\sharp}(\nu)_{t} + F^{\sharp \operatorname{Tot}}[\nu]_{x} = D_{\sharp}[\nu] = -\frac{1}{2} \varepsilon \nu_{x}^{T} \left(B_{\sharp} + B_{\sharp}^{T} \right) \nu_{x} \le 0,$$
(12a)

where (together with (6c))

$$F^{\sharp\text{Diff}}[v] = -\varepsilon v^T B_{\sharp} v_x, \quad F^{\sharp\text{Disp}}[v] := \frac{\varepsilon^2}{2} \Big(3 v_x^T K_{\sharp} v_x - \big(v^T K_{\sharp} v \big)_{xx} \Big).$$
(12b)

Proof. We will analyze the second- and third-order terms successively. It is important to distinguish between a solution and an arbitrary function w^{ε} (in the notation of Definition 1) and we thus consider a sequence w^{ε} satisfying the bounds (9). For simplicity we write $w = w^{\varepsilon}$ and $\mathscr{D}[w^{\varepsilon}] := \int_{\mathbb{R}} \varepsilon |\nabla w^{\varepsilon}|^2 dx$.

1. First of all, for the diffusion we have

$$w^{T}B_{\sharp}w_{xx} = (w^{T}B_{\sharp}w_{x})_{x} - w_{x}^{T}B_{\sharp}w_{x} = (w^{T}B_{\sharp}w_{x})_{x} - \frac{1}{2}w_{x}^{T}(B_{\sharp}^{T} + B_{\sharp})w_{x}.$$

For the latter term we have

$$-\frac{\varepsilon}{2}\int_{\mathbb{R}}w_x^T\left(B_{\sharp}^T+B_{\sharp}\right)w_x\theta\,dx$$

which is non-positive as required, provided $B_{\sharp}^{T} + B_{\sharp}$ is a non-negative matrix. On the other hand, if $B_{\sharp}^{T} + B_{\sharp}$ admits a direction $z \in \mathbb{R}^{N}$ such that $z^{T}(B_{\sharp}^{T} + B_{\sharp})z < 0$ we can always choose a function w which has w_{x} parallel to z in some small interval of \mathbb{R} , more precisely

$$w^{\varepsilon}(x) = z \, \chi\left(\frac{x}{\varepsilon^{b}}\right),\tag{13}$$

where b > 0 is a parameter and $\chi : \mathbb{R} \to [0, 1]$ is a function with compact support (to be specified). We compute

$$w_x^{\varepsilon}(x) = \frac{z}{\varepsilon^b} \chi'\left(\frac{x}{\varepsilon^b}\right),\tag{14}$$

thus by choosing $\theta = \theta_0(x/\varepsilon^b)$ (in order to localize the integral at the origin x = 0)

$$-\int_{\mathbb{R}}^{r}\sqrt{\varepsilon}w_{x}^{T}\left(B_{\sharp}^{T}+B_{\sharp}\right)\sqrt{\varepsilon}w_{x}\theta\,dx=-z^{T}\left(B_{\sharp}^{T}+B_{\sharp}\right)z\Omega^{\varepsilon},$$

with

$$\Omega^{\varepsilon} := \int_{\mathbb{R}} \left(\frac{1}{\varepsilon^{b-1/2}} \chi' \left(\frac{x}{\varepsilon^{b}} \right) \right)^{2} \theta_{0} \left(x/\varepsilon^{b} \right) dx.$$

It remains to choose *b* so that Ω^{ε} tends to a finite and positive value and, simultaneously, the condition (9) holds along the sequence w^{ε} . We consider (by performing an obvious change of variable)

$$\int_{\mathbb{R}} \frac{1}{\varepsilon^{2b-1}} \chi' \left(\frac{x}{\varepsilon^{b}}\right)^{2} \theta_{0} \left(x/\varepsilon^{b}\right) dx = \varepsilon^{-b+1} \int_{\mathbb{R}} \chi'(y)^{2} \theta_{0}(y) dy = 1,$$

provided b = 1 and $\int_{\mathbb{R}} \chi'(y)^2 dy = 1$. For instance we can take $\chi(y) = (1 - y^2)/2$ within the interval $y \in [-1,1]$ and $\chi(y)$ vanishing outside this interval, and on the other hand we choose the (compactly supported) function θ_0 to be identically 3/2 within the support of the function χ . Therefore, we have found a sequence of functions w^{ε} such that

$$\lim_{\varepsilon \to 0} -\frac{\varepsilon}{2} \int_{\mathbb{R}} \left(w_x^{\varepsilon} \right)^T \left(B_{\sharp}^T + B_{\sharp} \right) w_x^{\varepsilon} \theta \, dx = -z^T \left(B_{\sharp}^T + B_{\sharp} \right) z > 0$$

which also clearly satisfies (9). In conclusion, the positivity of the matrix $(B_{\sharp}^{T} + B_{\sharp})$ is a necessary and sufficient condition for the first term in (10) to provide a non-negative contribution.

2. Next, for the third-order terms we compute

$$w^{T} K_{\sharp} w_{xxx} = (w^{T} K_{\sharp} w_{xx})_{x} - w_{x}^{T} K_{\sharp} w_{xx}$$
$$= (w^{T} K_{\sharp} w_{xx})_{x} - \frac{1}{2} (w_{x}^{T} K_{\sharp} w_{x})_{x} + \frac{1}{2} w_{x}^{T} (K_{\sharp}^{T} - K_{\sharp}) w_{xx}$$

therefore

$$\varepsilon^{2} \int_{\mathbb{R}} w_{x}^{T} K_{\sharp} w_{xxx} \theta dx$$
$$= -\varepsilon^{2} \int_{\mathbb{R}} w^{T} K_{\sharp} w_{xx} \theta_{x} dx + \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}} w_{x}^{T} K_{\sharp} w_{x} \theta_{x} dx + \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}} w_{x}^{T} \left(K_{\sharp}^{T} - K_{\sharp} \right) w_{xx} \theta dx.$$

Since

$$w^{T}K_{\sharp}w_{xx} = (w^{T}K_{\sharp}w_{x})_{x} - w^{T}_{x}K_{\sharp}v_{x} = (w^{T}K_{\sharp}w_{x})_{x} - \frac{1}{2}w^{T}_{x}(K^{T}_{\sharp} + K_{\sharp})v_{x},$$

we obtain

$$\varepsilon^{2} \int_{\mathbb{R}} w_{x}^{T} K_{\sharp} w_{xxx} \theta dx = -\varepsilon^{2} \int_{\mathbb{R}} \left(\left(w^{T} K_{\sharp} w_{x} \right)_{x} - \frac{1}{2} w_{x}^{T} \left(K_{\sharp}^{T} + K_{\sharp} \right) w_{x} \right) \theta_{x} dx + \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}} w_{x}^{T} K_{\sharp} w_{x} \theta_{x} dx + \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}} w_{x}^{T} \left(K_{\sharp}^{T} - K_{\sharp} \right) w_{xx} \theta dx,$$

therefore

$$\varepsilon^{2} \int_{\mathbb{R}} w_{x}^{T} K_{\sharp} w_{xxx} \theta dx$$
$$= \varepsilon^{2} \int_{\mathbb{R}} w^{T} K_{\sharp} w_{x} \theta_{xx} dx + \frac{3\varepsilon^{2}}{4} \int_{\mathbb{R}} w_{x}^{T} \left(K_{\sharp}^{T} + K_{\sharp} \right) w_{x} \theta_{x} dx + \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}} w_{x}^{T} \left(K_{\sharp}^{T} - K_{\sharp} \right) w_{xx} \theta dx.$$
(15)

Clearly, if K_{\sharp} is symmetric, the third term in the right-hand side of (15) vanishes identically. Obviously, $K_{\sharp}^{T} - K_{\sharp}$ is anti-symmetric, so this term $w_{x}^{T}(K_{\sharp}^{T} - K_{\sharp})w_{xx}$ can never be a total *x*-derivative (unless $K_{\sharp}^{T} - K_{\sharp}$ vanishes).

On the other hand, if $(K_{\sharp}^T - K_{\sharp}) \neq 0$ we can choose a direction $z \in \mathbb{R}^N$ such that $z^T (K_{\sharp}^T - K_{\sharp}) z \neq 0$ (where the sign now cannot be chosen!), and we proceed as follows in order to exhibit a wrong sign as far as (10) is concerned.

Using the same sequence of functions v^{ε} as defined in (13) and with a test-function $\theta = \theta_0(x/\varepsilon^b)$ as before, we can also compute the second-order derivative:

$$w_{xx}^{\varepsilon}(x) = \frac{z}{\varepsilon^{2b}} \chi''\left(\frac{x}{\varepsilon^{b}}\right),\tag{16}$$

and together with (14)

$$\varepsilon^{2} \int_{\mathbb{R}} \left(w_{x}^{\varepsilon} \right)^{T} \left(K_{\sharp}^{T} - K_{\sharp} \right) w_{xx}^{\varepsilon} \theta dx = w^{T} \left(K_{\sharp}^{T} - K_{\sharp} \right) z \Omega^{\varepsilon},$$

with

$$\Omega^{\varepsilon} := \varepsilon^2 \int_{\mathbb{R}} \frac{1}{\varepsilon^b} \chi'\left(\frac{x}{\varepsilon^b}\right) \frac{1}{\varepsilon^{2b}} \chi''\left(\frac{x}{\varepsilon^b}\right) \theta_0\left(\frac{x}{\varepsilon^b}\right) dx$$
$$= \varepsilon^{2-2b} \int_{\mathbb{R}} \chi'(y) \chi''(y) \theta_0(y) dy = -\frac{1}{2} \varepsilon^{2-2b} \int_{\mathbb{R}} \chi'(y)^2 \theta'_0(y) dy =: -\frac{1}{2} \Omega_*.$$

We take again b = 1. By properly choosing¹ the functions χ and θ_0 we can always ensure that Ω_* is non-vanishing and has the same sign as $z^T (K_{\sharp}^T - K_{\sharp}) z$:

$$\Omega_* = \begin{cases} 1, & z^T \left(K_{\sharp}^T - K_{\sharp} \right) z > 0, \\ -1, & z^T \left(K_{\sharp}^T - K_{\sharp} \right) z < 0. \end{cases}$$
(17)

We recall that both functions must have compact support while θ_0 must be *non-negative* and χ has no specific sign. For instance we again take $\chi(y) = (1 - y^2)/2$ within the interval $y \in [-1, 1]$ and $\chi(y)$ vanishing outside this interval. On the other hand we choose the (compactly supported) function θ_0 to be 3(1 - |y + 1|) within the interval [-2, 0] and zero outside this interval. In turn, we obtain $\int_{-1}^{1} \chi'(y)^2 \theta_0(y) dy = -1$. A different choice of θ_0 is required for the positive sign, for instance θ_0 to be 3(1 - |y - 1|) within the interval [0, 2] and zero outside this interval.

3. Augmented models with nonlinear terms

3.1. Nonlinear second- and third-order terms. Sufficient conditions

We proceed by successive generalizations of the augmentation terms and we now consider a nonlinear version of (7), that is,

$$u_{\sharp}(v)_{t} + f_{\sharp}(v)_{x} = \varepsilon \left(B_{\sharp}(v) v_{x} \right)_{x} + \varepsilon^{2} \left(\nabla h_{\sharp}(v)^{T} H h_{\sharp}(v)_{xx} \right)_{x} = \varepsilon \left(S_{\sharp} \left[v^{\varepsilon} \right] \right)_{x},$$
(18)

in which $B_{\sharp} = B_{\sharp}(v)$ is a given $(N \times N)$ -matrix-valued mapping and $h_{\sharp} = h_{\sharp}(v)$ is an *N*-vectorvalued mapping, while *H* is a constant matrix. The choice of this structure will be further motivated below; at this stage, we consider (18) as an interesting broad class of models.

Our sign condition for the entropy dissipation now takes the form

$$\limsup_{\varepsilon \to 0} \int_{\mathbb{R}} \left(w_x^{\varepsilon} \right)^T \left(\varepsilon B_{\sharp} \left(w^{\varepsilon} \right) w_x^{\varepsilon} + \varepsilon^2 \nabla h_{\sharp} \left(w^{\varepsilon} \right)^T H h_{\sharp} \left(w^{\varepsilon} \right)_{xx} \right) \theta \, dx \ge 0$$
(19)

¹Observe that we need now to properly choose the *derivative* θ'_0 .

for all test-functions $\theta = \theta(x) \ge 0$ and all sequences $w^{\varepsilon} : \mathbb{R} \to \mathcal{U}_{\sharp} \subset \mathbb{R}^{N}$ satisfying (9). It is convenient to introduce the notation $u_{\sharp}(v)_{t} + (f^{\sharp \text{Tot}}[v])_{x} = 0$ where we now have

$$f^{\sharp \text{Tot}}[v] = f^{\sharp \text{Tot}}\left(v, \varepsilon v_x, \varepsilon^2 v_{xx}\right) := f_{\sharp}(v) + f^{\sharp \text{Diff}}(v, \varepsilon v_x) + f^{\sharp \text{Disp}}\left(v, \varepsilon v_x, \varepsilon^2 v_{xx}\right),$$
(20a)

with

$$f^{\sharp \text{Diff}}[\nu] = f^{\sharp \text{Diff}}(\nu, \varepsilon \nu_x) := \varepsilon B_{\sharp}(\nu) \nu_x,$$
(20b)

and

$$f^{\sharp \text{Disp}}[\nu) = f^{\sharp \text{Disp}}(\nu, \varepsilon \nu_{x}, \varepsilon^{2} \nu_{xx}) := -\varepsilon^{2} \nabla h_{\sharp}(\nu)^{T} H h_{\sharp}(\nu)_{xx}$$
$$= -\varepsilon^{2} \nabla h_{\sharp}(\nu)^{T} H \nabla h_{\sharp}(\nu) \nu_{xx} - \varepsilon^{2} \nabla h_{\sharp}(\nu)^{T} H \nabla^{2} h_{\sharp}(\nu) (\nu_{x}, \nu_{x}).$$
(20c)

Proposition 3 (Nonlinear second- and third-order terms.). Provided the following properties hold:

$$B_{\sharp}(\nu)^{T} + B_{\sharp}(\nu) \quad is \ a \ non-negative \ matrix,$$

$$H \qquad is \ a \ symmetric \ matrix,$$
(21)

the augmented model (18) satisfies the positive entropy production property in Definition 7 (see (19)) and, furthermore, the entropy inequality holds as follows:

$$U_{\sharp}(v)_{t} + \left(F^{\sharp \text{Tot}}[v]\right)_{x} = D_{\sharp}[v] = -\frac{1}{2}\varepsilon v_{x}^{T}\left(B_{\sharp}(v) + B_{\sharp}^{T}(v)\right)v_{x} \le 0,$$
(22a)

where

$$F^{\sharp\text{Tot}}[\nu] = F_{\sharp}(\nu) + F^{\sharp\text{Diff}}[\nu] + F^{\sharp\text{Disp}}[\nu], \qquad F^{\sharp\text{Diff}}[\nu] = -\varepsilon \nu^{T} B_{\sharp}(\nu) \nu_{x},$$

$$F^{\sharp\text{Disp}}[\nu] := -\nu^{T} \nabla h_{\sharp}(\nu)^{T} H_{\sharp} h_{\sharp}(\nu)_{xx} + \frac{1}{2} h_{\sharp}(\nu)_{x} H h_{\sharp}(\nu)_{x}$$

$$= \frac{\varepsilon^{2}}{2} \left(3\nu_{x}^{T} K_{\sharp}(\nu) \nu_{x} - \left(\nu^{T} K_{\sharp}(\nu) \nu\right)_{xx} \right) + \varepsilon^{2} \nabla^{2} h_{\sharp}(\nu, \nu_{x})^{T} H_{\sharp} h_{\sharp}(\nu)_{x}$$

$$= -\frac{\varepsilon^{2}}{2} \left(\nu^{T} K_{\sharp}(\nu) \nu \right)_{xx} + \varepsilon^{2} \nu_{x}^{T} L_{\sharp}(\nu) \nu_{x}, \qquad (22b)$$

and

$$K_{\sharp}(\nu) := \nabla h_{\sharp}(\nu)^{T} H_{\sharp} \nabla h_{\sharp}(\nu), \quad L_{\sharp}(\nu) := \frac{3}{2} K_{\sharp}(\nu) + \nabla^{2} h_{\sharp}(\nu, \cdot)^{T} H \nabla h_{\sharp}(\nu).$$
(22c)

Observe that $K_{\sharp}(v)$ is automatically a symmetric matrix when H is symmetric. Note also that the model (18) reduces to (7) if $h_{\sharp}(v)$ is chosen to be v. Observe that $F^{\sharp\text{Disp}}[v]$ is the sum of a term in a divergence form and a quadratic term, while $F^{\sharp\text{Diff}}[v] = -\varepsilon v^T B_{\sharp}(v) v_x$ would also have a divergence form if we restrict attention to diffusion matrices deriving from a scalar potential b_{\sharp} of the form $v^T B_{\sharp} = \nabla b_{\sharp}$ and thus $F^{\sharp\text{Diff}}[v] = -\varepsilon b_{\sharp}(v)_x$. In the applications, the quadratic term related to $B_{\sharp}(v)^T + B_{\sharp}(v)$ will indeed have the required sign, while the third-order contribution from $L_{\sharp}(v)$ will also often be non-negative.

3.2. Necessary conditions

We will now discuss the question of whether the term $\nabla h_{\sharp}(v)^T H h_{\sharp}(v)_{xx}$ is the most general diffusive term ensuring a good entropy structure. For clarity in the discussion we restrict attention to scalar equations with a quadratic entropy, that is, with F' := u f'

$$u_t + f(u)_x = 0, \quad \frac{1}{2}(u^2)_t + F(u)_x \le 0.$$
 (23)

Proposition 4 (Necessary conditions. I). Consider the conservation law with quadratic entropy (23). Given some continuous functions B = B(u), $k_1 = k_1(u)$, and $k_2 = k_2(u)$, the augmentation terms in the diffusive-dispersive model

$$u_t + f(u)_x = \varepsilon \left(B(u)u_x \right)_x + \varepsilon^2 \left(k_1(u) \left(k_2(u)u_x \right)_x \right)_x = \left(S \left[u, \varepsilon u_x, \varepsilon^2 u_{xx} \right] \right)_x$$
(24)

satisfy the positive entropy dissipation property in Definition 7 if and only if the functions satisfy

$$B(u) \ge 0, \qquad k_1(u) = c \, k_2(u), \qquad u \in \mathbb{R},$$
 (25)

where c is an arbitrary constant. This is precisely the structure already analyzed in Proposition 3.

We complete our discussion by analyzing the most general diffusive term that is linear with respect to the highest derivative. An example ensuring the favorable signs below is $S_1(u, v) = b_1(u) v^{2p+1}$ and $S_2(u, v) = b_2(u) v^{2q+1}$ provided $b_1 \ge 0$ and $b'_2 \le 0$.

Proposition 5 (Necessary conditions. II). Consider the conservation law with quadratic entropy (23). Given some functions $S_1 = S_1(u, \varepsilon u_x)$ and $S_2 = S_2(u, \varepsilon u_x)$, assumed to be analytic in their arguments, the augmentation terms in the diffusive-dispersive model

$$u_t + f(u)_x = \left(S_1(u,\varepsilon u_x) + \varepsilon^2 u_{xx} S_2(u,\varepsilon u_x)\right)_x \tag{26}$$

satisfy the positive entropy dissipation property (in Definition 7) if and only if

$$vS_1(u,v) - v^3 \partial_1 \overline{S}_2(u,v) \ge 0, \quad u,v \in \mathbb{R},$$
(27)

where

$$\overline{S}_{2}(u,v) := \int_{0}^{1} \int_{0}^{1} S_{2}(u,v(1+m(s-1)))(1-s) \, ds \, dm.$$
(28)

The corresponding entropy balance law then reads

$$\frac{1}{2}(u^2)_t + \left(F^{\sharp \text{Tot}}[u]\right)_x = D_{\sharp}[u] = -u_x S_1(u, \varepsilon u_x) + \varepsilon^2 u_x^3 \partial_1 \overline{S}_2(u, \varepsilon u_x) \le 0,$$
(29a)

where

$$F^{\sharp\text{Diff}}[v] := uS_1(u,\varepsilon u_x), \quad F^{\sharp\text{Disp}}[v] := -\varepsilon^2 u_{xx} uS_2(u,\varepsilon u_x) - \varepsilon^2 u_x^2 \overline{S}_2(u,\varepsilon u_x).$$
(29b)

4. Applications, implications, and generalizations

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4.1. The Euler–Navier–Stokes–Korteweg model in Lagrangian variables

The ideas in the present paper can be applied to other classes of systems and we illustrate this with the model of viscous-capillarity fluids. We can model a fluid or elastic material by the following system of three conservation laws for the mass, momentum, and total energy of a fluid flow, which we state here in Lagrangian coordinates:

$$v_t - u_x = 0,$$

$$u_t - \varepsilon_v (v, S)_x = (v \, u_x)_x - (\mu \, v_x)_{xx} + \frac{1}{2} (\mu_v \, v_x^2)_x,$$

$$E_t - (\varepsilon_v (v, S) \, u)_x = (v \, u \, u_x)_x + (\frac{\mu_v}{2} u \, v_x^2 - u \, (\mu \, v_x)_x)_x + (\mu \, u_x \, v_x)_x.$$
(30a)

The main unknowns are the specific volume v > 0, the fluid velocity u, and the specific entropy S > 0. The total energy E of the flow is defined as

$$E = \varepsilon(v, S) + \frac{u^2}{2},$$
(30b)

in which we must also prescribe the internal energy $\varepsilon = \varepsilon(v, S)$. Moreover, the coefficients v = v(v, S) and $\mu = \mu(v, S)$ are non-negative functions of the specific volume and the specific entropy, representing the viscosity and capillarity coefficients of the fluid, respectively.

We will be interested in the situation where the first-order Lagrangian fluid system

$$\begin{aligned}
\nu_t - u_x &= 0, \\
u_t - \varepsilon_v (v, S)_x &= 0, \\
E_t - (\varepsilon_v (v, S) u)_x &= 0,
\end{aligned}$$
(30c)

is a hyperbolic-elliptic type, a typical example of interest being given by the (nonconvex) equation of state of van der Waals fluids:

$$\varepsilon(\nu, S) = \frac{8a}{3} (3\nu - 1)^{-1/a} e^{3S/(8a)} - \frac{3}{\nu},$$
(30d)

where *a* is some positive parameter. Note that this equation if state requires the lower bound on the specific volume v > 1/3.

4.2. A class of models with space-derivatives generating time-derivatives

Building upon our study above, we now introduce another class of models which *contains the Navier–Stokes–Korteweg system above* as a special case. We consider

$$u_{\sharp}(v)_{t} + f_{\sharp}(v)_{x} = \varepsilon B_{\sharp} v_{xx} + \varepsilon^{2} \kappa K_{1} k_{\sharp}(v)_{xxx}$$
(31)

in which B_{\sharp} is constant $(N \times N)$ -matrix $k_{\sharp} = k_{\sharp}(v)$ is a *N*-vector-valued mapping, and K_0, K_1 are constant matrices and we assume the following structure condition on the system

There exists a constant matrix K_0

This condition can be expressed in a purely algebraic form, as follows:

$$K_0^T D_v k_{\sharp}(v) \left(-f_{\sharp}(v)_x + \varepsilon B v_{xx} + \varepsilon^2 \kappa K_1 k_{\sharp}(v)_{xxx} \right) - K_1^T v_x = 0.$$

such that every solution to (31) also satisfies $K_0^T k_{\sharp}(v)_t - K_1^T v_x = 0$.

Since first-, second-, and third-order derivatives can be chosen independently (say at some initial time), we deduce that all three contributions above vanish:

$$K_0^T D_v k_{\sharp}(v) D_v f_{\sharp}(v) + K_1^T = 0,$$

$$K_0^T D_v k_{\sharp}(v) B = 0,$$

$$K_0^T D_v k_{\sharp}(v) K_1 k_{\sharp}(v)_{xxx} = 0.$$

It is straightforward to extend Definition 1 to the class (31).

Proposition 6. A necessary and sufficient condition for the augmented model (31) to satisfy the positive entropy production property is:

$$B_{\sharp}^{T} + B_{\sharp} \quad is \ a \ non-negative \ matrix,$$

$$K_{0}^{T} + K_{0} \quad is \ a \ non-negative \ matrix.$$
(33)

Moreover, the entropy inequality holds as follows:

$$U^{\sharp \text{Tot}}[\nu]_t + F^{\sharp \text{Tot}}[\nu]_x = D_{\sharp}[\nu] = -\frac{1}{2}\varepsilon \nu_x^T \left(B_{\sharp} + B_{\sharp}^T\right) \nu_x \le 0,$$
(34)

where

$$U^{\sharp \text{Tot}}[v] = U_{\sharp}(v) + \frac{1}{2} \varepsilon^{2} \kappa k(v)_{x}^{T} K_{0} k_{\sharp}(v)_{x},$$

$$F^{\sharp \text{Tot}}[v] = F_{\sharp}(v) + F^{\sharp \text{Diff}}[v] + F^{\sharp \text{Disp}}[v],$$

$$F^{\sharp \text{Diff}}[v] = -\varepsilon v^{T} B_{\sharp} v_{x},$$

$$F^{\sharp \text{Disp}}[v] := \varepsilon^{2} \kappa \left(v^{T} K_{1}(v) k_{\sharp}(v)_{xx} \right)_{x} - \varepsilon^{2} \kappa \left(k(v)_{t}^{T} K_{0} k_{\sharp}(v)_{x} \right)_{x} s.$$
(35)

Proof. We only sketch the proof

$$\varepsilon^{2} \kappa v^{T} \left(K_{1} k_{\sharp}(v)_{xx} \right)_{x} = \varepsilon^{2} \kappa \left(v^{T} K_{1} k_{\sharp}(v)_{xx} \right)_{x} - \varepsilon^{2} \kappa v_{x}^{T} K_{1} k_{\sharp}(v)_{xx}$$

$$= \varepsilon^{2} \kappa \left(v^{T} K_{1} k_{\sharp}(v)_{xx} \right)_{x} - \varepsilon^{2} \kappa k(v)_{t}^{T} K_{0} k_{\sharp}(v)_{xx}$$

$$= \varepsilon^{2} \kappa \left(v^{T} K_{1} k_{\sharp}(v)_{xx} \right)_{x} - \varepsilon^{2} \kappa \left(k(v)_{t}^{T} K_{0} k_{\sharp}(v)_{x} \right)_{x} - \varepsilon^{2} \kappa k(v)_{tx}^{T} K_{0} k_{\sharp}(v)_{xx}$$

$$(36)$$

in which

$$\varepsilon^{2} \kappa k(v)_{tx}^{T} K_{0} k_{\sharp}(v)_{x} = \frac{1}{2} \varepsilon^{2} \kappa \left(k(v)_{x}^{T} K_{0} k_{\sharp}(v)_{x} \right)_{t}$$

This completes the argument.

4.3. Application

The elastodynamics model is easily recovered since $w_t - v_x = 0$ is equivalent to saying

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}_t - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \sigma(w) \\ v \end{pmatrix}_x = \begin{pmatrix} 0 \\ w_t - v_x \end{pmatrix},$$

while we express the diffusion term $(w_{xx})_x$ in the matrix form

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \nu \\ w \end{pmatrix}_{xx} = \begin{pmatrix} 0 \\ w_{xx} \end{pmatrix},$$

4.4. Global entropy balance law

Denoting now the solution by v^{ε} and integrating in space over \mathbb{R} , we find (provided the solution decays appropriately at infinity)

$$\frac{d}{dt}\int_{\mathbb{R}}U_{\sharp}\left(v^{\varepsilon}\right)dx = \int_{\mathbb{R}}D^{\sharp\mathrm{Diff}}\left(v^{\varepsilon},\varepsilon\,v^{\varepsilon}_{x}\right)dx \leq 0,$$

and in particular $t \ge 0 \mapsto \int_{\mathbb{R}} U_{\sharp}(v^{\varepsilon}(t,x)) dx$ is non-increasing. We conclude our discussion in the present section with the following observation. Note that the diffusion and dispersion coefficients and matrices may well be degenerate. Finally, we make the following important observation. For every model we introduced, if the sequence of initial data $v^{\varepsilon}(0, \cdot)$ has uniformly bounded entropy and the solutions v^{ε} remain uniformly bounded in sup-norm, i.e. $\limsup_{\varepsilon \to 0} \|v^{\varepsilon}\|_{L^{\infty}(\mathbb{R})} < +\infty$ and converge almost everywhere to some limit v, i.e. $v := \lim_{\varepsilon \to 0} v^{\varepsilon}$, then one has

 $f^{\sharp \text{Tot}}[\nu] - f_{\sharp}(\nu) \to 0 \text{ and } F^{\sharp \text{Tot}}[\nu] - F_{\sharp}(\nu) \to 0 \text{ in the sense of distributions,}$

 $\mathscr{D}[v^{\varepsilon}]$ is a sequence of locally uniformly bounded non-negative measures,

and, moreover, the limit is a weak solution satisfying the entropy inequality, that is,

$$u_{\sharp}(v)_t + f_{\sharp}(v)_x = 0, \qquad U_{\sharp}(v)_t + F_{\sharp}(v)_x \le 0.$$

We also emphasize that specific models from nonlinear elasticity and phase transition dynamics are found to fit within our setting. For further results and examples we refer to [13].

For the equations derived here, we have also developed adapted numerical schemes that are "structure-preserving" [13]. For nonlinear hyperbolic problems, many strategies have been proposed in recent years in order to discretize certain algebraic or differential properties. A distinct feature of diffusive-dispersive shocks is the richer variety of waves that are observed, yet these standard structure-preserving techniques are relevant for dealing with the more involved models introduced in the present Note.

4.5. A broad class of augmented systems with diffusion and dispersion

Our results apply in a much wider context, including systems of the form

$$\partial_t u + \sum_{j=1}^d \partial_j f^j(u) = 0, \qquad u = u(t, x) \in \mathcal{U} \subset \mathbb{R}^N, \quad t \ge 0, \, x \in \mathbb{R}^d, \tag{37}$$

with unknown $u = (u_a) = (u_1, ..., u_N) \in \mathcal{U}$ (an open subset of \mathbb{R}^N containing 0). We assume such a system to be endowed with a convex entropy-entropy flux pair (U, F) satisfying, by definition,

 $D^2U > 0$ and $DF^j = (DU)^T Df^j$, and normalized so that U(0) = 0, as well as f(0) = 0 and F(0) = 0. By definition, physically meaningful solutions, also called entropy solutions, must satisfy the entropy inequality

$$\partial_t U(u) + \sum_{j=1}^d \partial_j F^j(u) \le 0, \qquad t \ge 0, \ x \in \mathbb{R}^d.$$
(38)

The so-called entropy variable defined by

$$v = v_{\sharp}(u) := \nabla U(u) \in \mathscr{U}_{\sharp} := v_{\sharp}(\mathscr{U}), \qquad u = u_{\sharp}(v) := (\nabla U)^{-1}(v), \tag{39}$$

will play a fundamental role in our approach. Performing the change of variable $u \in \mathcal{U} \mapsto v \in \nabla U(\mathcal{U}) \subset \mathbb{R}^N$ and setting

$$f^{j}_{\sharp}(\nu) := f^{j}(u), \quad U_{\sharp}(\nu) := U(u), \quad F_{\sharp}^{j}(\nu) := F^{j}(u),$$
(40)

we rewrite (37) and (38) in the form:

$$\partial_t u_{\sharp}(\nu) + \sum_{j=1}^d \partial_j f_{\sharp}^j(\nu) = 0, \qquad \partial_t U_{\sharp}(\nu) + \sum_{j=1}^d \partial_j F_{\sharp}^j(\nu) \le 0, \qquad t \ge 0, \ x \in \mathbb{R}^d.$$
(41)

Many systems in fluid and solid dynamics fit into the above class. In order to fully describe the dynamics of small-scale sensitive shocks, augmentation terms are required, as follows. The relevant physical models read

$$\partial_t u^{\varepsilon} + \sum_{j=1}^d \partial_j f^j \left(u^{\varepsilon} \right) = \sum_{j=1}^d \partial_j S^j \left[u^{\varepsilon} \right], \qquad u^{\varepsilon} = u^{\varepsilon}(t, x), \tag{42}$$

in which $\varepsilon > 0$ is a small parameter and $S^{j}[u^{\varepsilon}]$ depends on (suitably scaled) first- and higher-order derivatives $\varepsilon \partial_{j} u^{\varepsilon}$ and $\varepsilon^{2} \partial_{j} \partial_{k} u^{\varepsilon}$. We assume the normalization that if $u^{\varepsilon} = u^{\varepsilon}(x)$ is a constant function then $S^{j}[u^{\varepsilon}]$ vanishes identically.

The fundamental requirement we want to impose on the higher-order terms is the following *sign condition*:

$$\limsup_{\varepsilon \to 0} \iint_{\mathbb{R}^+ \times \mathbb{R}^N} \sum_{j=1}^d \nabla U(u^{\varepsilon})^T \partial_j S^j [u^{\varepsilon}] \theta dx dt \le 0$$
(43)

for *every solution* u^{ε} to (42) and every (smooth and compactly supported) test-function $\theta = \theta(t, x) \ge 0$. Clearly, if the condition (43) holds, then we deduce from the augmented model (42) that the limiting solution $u := \lim u^{\varepsilon}$ (if it exists in a suitable functional space) satisfies the entropy inequality (38). However, the condition (43) is *not explicit* enough to be useful in practice, for instance for numerical discretization. We are going to present suitable classes of models that are, both, physically relevant and numerically tractable, and enjoy a *positive entropy production property*. Our notion guides us in identifying the interesting classes of models (and later designing the schemes adapted to these models).

It is important to handle the condition (43) in the entropy variable, that is, to write

$$\partial_t u_{\sharp} \left(v^{\varepsilon} \right) + \sum_{j=1}^d \partial_j f^j_{\sharp} \left(v^{\varepsilon} \right) = \sum_{j=1}^d \partial_j S^j_{\sharp} \left[v^{\varepsilon} \right], \qquad v^{\varepsilon} = v^{\varepsilon}(t, x), \qquad t \ge 0, \, x \in \mathbb{R}^d, \tag{44}$$

together with the sign condition

$$\limsup_{\varepsilon \to 0} \iint_{\mathbb{R}^+ \times \mathbb{R}^N} \sum_{j=1}^d \left(v^{\varepsilon} \right)^T \partial_j S^j_{\sharp} \left[v^{\varepsilon} \right] \theta \, dx \, dt \le 0.$$
(45)

Here, we have set $S^j_{\sharp}[v^{\varepsilon}] := S^j[u^{\varepsilon}]$ and (45) is required for all test-functions $\theta = \theta(t, x) \ge 0$ and all solutions $v^{\varepsilon} = v^{\varepsilon}(x)$ to (44).

4.6. The positive entropy production property for augmentation terms

We proceed by suppressing the time integral in the dissipation bound that arises from (43) and we propose the following notion which, importantly, *no longer refers* to the PDE under consideration, but imposes a condition on the augmentation terms for *general functions* rather than solutions.

Definition 7. A nonlinear expression $S[w^{\varepsilon}] = (S^{j}[w^{\varepsilon}])_{1 \le j \le d}$ of a sequence of functions $w^{\varepsilon} : \mathbb{R}^{d} \to \mathcal{U}_{\sharp} \subset \mathbb{R}^{N}$ involving w^{ε} and its (rescaled) derivatives $\varepsilon \partial_{j} w^{\varepsilon}$ and $\varepsilon^{2} \partial_{j} \partial_{k} w^{\varepsilon}$ has the positive entropy production property if (8) holds with now ∂_{x} replaced by ∇ and $\nabla w^{\varepsilon} \cdot S_{\sharp}[w^{\varepsilon}] := \sum_{j=1}^{N} \partial_{j} w_{\varepsilon}^{T} S_{\sharp}^{j}[w^{\varepsilon}]$ for all test-functions $\theta = \theta(x) \ge 0$ and for any sequence of bounded functions $w^{\varepsilon} = w^{\varepsilon}(x)$ with bounded total dissipation

$$\limsup_{\varepsilon \to 0} \|w^{\varepsilon}\|_{L^{\infty}(\mathbb{R}^{N})} + \limsup_{\varepsilon \to 0} \int_{\mathbb{R}^{d}} \varepsilon |\nabla w^{\varepsilon}|^{2} dx < +\infty.$$
(46)

We can prove that if the augmentation terms satisfy the positive entropy production property, then the dissipation bound in (46) follows from the sole assumption that the total entropy is bounded. More generally, the augmentation terms could also depend on time-derivatives, but such a generalization is more involved since the time variable must be handled by using the equation [13].

Consider any nonlinear expression $S[w^{\varepsilon}] = (S^a[w^{\varepsilon}])_{1 \le a \le d}$, having the positive entropy production property (cf. Definition 7) and depending upon a sequence of functions $w^{\varepsilon} : \mathbb{R}^d \to \mathbb{R}^N$ and its (rescaled) derivatives $\varepsilon \partial_a w^{\varepsilon}$ and $\varepsilon^2 \partial_a \partial_b w^{\varepsilon}$ with a, b = 1, ..., d. Assuming the usual bound

$$\limsup_{\varepsilon \to 0} \|w^{\varepsilon}\|_{L^{\infty}(\mathbb{R}^{N})} + \limsup_{\varepsilon \to 0} \int_{\mathbb{R}^{d}} \varepsilon |\nabla w^{\varepsilon}|^{2} dx < +\infty,$$
(47)

we can associate to $w = (w^{\varepsilon})$ a locally bounded measure μ_w defined over \mathbb{R}^N so that for every test-function $\theta = \theta(x) \ge 0$

$$\langle \mu_{w}, \theta \rangle := \liminf_{\varepsilon \to 0} \int_{\mathbb{R}^{d}} \varepsilon \nabla w^{\varepsilon} \cdot S_{\sharp} \left[w^{\varepsilon} \right] \theta \, dx \ge 0.$$
(48)

This measure depends upon the choice of the sequence. As far as classical shocks are concerned, the positivity of this measure implies that the physically meaningful shock wave is selected by our augmented model. However, the actual values of this measure are required for selecting of nonclassical (undercompressive) shocks.

To conclude, we point out that the proposed methodology provides one with a guideline in order to select and discretize augmented terms. Higher-order terms may be added to the entropy function, so that our approach is sufficiently general in order to encompass many models of physical interest. In particular, it is applicable to equations arising in quantum fluid dynamics and phase transition dynamics [2, 4, 5], and allows us to characterize dissipation and dispersive mechanisms that are compatible with the underlying entropy of these equations.

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