

ASC Report No. 22/2019

When do cross-diffusion systems have an entropy structure ?

X. Chen and A. Jüngel

Most recent ASC Reports

- 21/2019 *M. Innerberger and D. Praetorius*
Instance-optimal goal-oriented adaptivity
- 20/2019 *C.-M. Pfeiler and D. Praetorius*
Dörfler marking with minimal cardinality is a linear complexity problem
- 19/2019 *A. Jüngel, O. Leingang, and S. Wang*
Vanishing cross-diffusion limit in a Keller-Segel system with additional cross-diffusion
- 18/2019 *D. Praetorius, M. Ruggeri, and E.P. Stephan*
The saturation assumption yields optimal convergence of two-level adaptive BEM
- 17/2019 *G. Di Fratta and A. Fiorenza*
BMO-type seminorms from Escher-type tessellations
- 16/2019 *R. Pruckner, H. Woracek*
Limit behaviour of Nevanlinna functions
- 15/2019 *G. Di Fratta, C. Muratov, F. Rybakov, and V. Slastikov*
Variational principles of micromagnetics revisited
- 14/2019 *E. Davoli, G. Di Fratta*
Homogenization of chiral magnetic materials - A mathematical evidence of Dzyaloshinskii's predictions on helical structures
- 13/2019 *J.M. Melenk, A. Rieder*
On superconvergence of Runge-Kutta convolution quadrature for the wave equation
- 12/2019 *J.M. Melenk, A. Rieder*
 hp -FEM for the fractional heat equation

Institute for Analysis and Scientific Computing
Vienna University of Technology
Wiedner Hauptstraße 8–10
1040 Wien, Austria

E-Mail: admin@asc.tuwien.ac.at
WWW: <http://www.asc.tuwien.ac.at>
FAX: +43-1-58801-10196

ISBN 978-3-902627-00-1

© Alle Rechte vorbehalten. Nachdruck nur mit Genehmigung des Autors.



WHEN DO CROSS-DIFFUSION SYSTEMS HAVE AN ENTROPY STRUCTURE?

XIUQING CHEN AND ANSGAR JÜNGEL

ABSTRACT. Necessary and sufficient conditions for the existence of an entropy structure for certain classes of cross-diffusion systems with diffusion matrix $A(u)$ are derived, based on results from matrix factorization. The entropy structure is important in the analysis for such equations since $A(u)$ is typically neither symmetric nor positive definite. In particular, the normal ellipticity of $A(u)$ for all u and the symmetry of the Onsager matrix implies its positive definiteness and hence an entropy structure. If A is constant or nearly constant in a certain sense, the existence of an entropy structure is equivalent to the normal ellipticity of A . Several applications and examples are presented, including the n -species population model of Shigesada, Kawasaki, and Teramoto, a volume-filling model, and a fluid mixture model with partial pressure gradients. Furthermore, the normal ellipticity of these models is investigated and some extensions are discussed.

1. INTRODUCTION

Cross-diffusion systems are systems of quasilinear parabolic equations in which the gradient of one variable induces a flux of another variable. They arise naturally in multicomponent systems from physics, chemistry, and biology and describe, for instance, segregation in population species, ion transport through nanopores, or dynamics of gas mixtures (see [18]). A characteristic feature of most of these systems arising from applications is that the diffusion matrix is generally neither symmetric nor positive definite which significantly complicates the mathematical analysis. However, it turns out that there might exist a transformation of variables (called entropy variables) such that the transformed diffusion matrix becomes positive definite and sometimes even symmetric. This is an important ingredient in the global existence analysis of the equations. The question is under which conditions does such a transformation exist? In this paper, we will give some necessary and sufficient conditions for the existence of entropy variables for certain classes of cross-diffusion systems.

Date: August 16, 2019.

2000 Mathematics Subject Classification. 35K40, 35K55, 35Q92, 35Q79, 15A23, 15A24.

Key words and phrases. Cross diffusion, entropy method, normal ellipticity, matrix factorization, Lyapunov equation, population model, volume-filling model, fluid mixture model.

The first author acknowledges support from the National Natural Science Foundation of China (NSFC), grant 11471050. The second author acknowledges partial support from the Austrian Science Fund (FWF), grants P30000, W1245, and F65.

The setting. We consider the equations

$$(1) \quad \partial_t u_i = \operatorname{div} \left(\sum_{j=1}^n A_{ij}(u) \nabla u_j \right) \quad \text{in } \Omega, \quad t > 0, \quad i = 1, \dots, n,$$

subject to the initial and no-flux boundary conditions

$$(2) \quad u_i(0) = u_i^0 \quad \text{in } \Omega, \quad \sum_{j=1}^n A_{ij}(u) \nabla u_j \cdot \nu = 0 \quad \text{on } \partial\Omega, \quad t > 0, \quad i = 1, \dots, n,$$

where $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain, $u_i : \Omega \times (0, \infty) \rightarrow \mathbb{R}$ are the unknowns (for instance, densities or concentrations), $A_{ij}(u) \in \mathbb{R}$ are the diffusion coefficients, and ν is the exterior unit normal vector to $\partial\Omega$. More general equations, where $A_{ij}(u)$ are matrices, will be briefly discussed in Section 8. We may add reaction terms to (1), but we concentrate in this paper on the diffusion operator.

Typically, $A(u)$ is neither symmetric nor positive definite (see the examples below) such that even the local-in-time existence of solutions to (1)–(2) is nontrivial. Amann [1] has shown that there exist local classical solutions if the operator $\operatorname{div}(A(u)\nabla(\cdot))$ is normally elliptic, which means that all eigenvalues of $A(u)$ have positive real parts. By slightly abusing the notation, we call such matrices normally elliptic. This property is usually not sufficient for global-in-time existence. In many applications, there exists a transformation of variables $w = h'(u)$, where $h \in C^2(\mathcal{D})$ ($\mathcal{D} \subset \mathbb{R}^n$ being a domain) is called an entropy density and h' its derivative, such that (1) can be written as

$$(3) \quad \partial_t u_i(w) = \operatorname{div} \left(\sum_{j=1}^n B_{ij}(w) \nabla w_j \right) \quad \text{in } \Omega, \quad t > 0, \quad i = 1, \dots, n,$$

where $u(w) := (h')^{-1}(w)$, and $B(w) = A(u(w))h''(u(w))^{-1}$ is positive definite in the sense that $B(w) + B(w)^\top$ is symmetric positive definite. (We assume that the inverse functions exist.) In this situation, $t \mapsto \int_\Omega h(u(t))dx$ is a Lyapunov functional along the solutions to (1)–(2). Indeed, using $w = h'(u)$ as a test function in (1), a formal computation yields

$$\frac{d}{dt} \int_\Omega h(u)dx + \int_\Omega \nabla u : h''(u)A(u)\nabla u dx = 0,$$

where “:” denotes the Frobenius matrix product. Since $B(w)$ is assumed to be positive definite, so does $h''(u)A(u)$, which shows that $t \mapsto \int_\Omega h(u(t))dx$ is nonincreasing. Moreover, the second integral generally provides gradient estimates which are essential in the existence analysis. We say that (1) possesses an entropy structure if there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that $B(w)$ or, equivalently, $h''(u)A(u)$ is positive definite.

The aim of this paper is to explore under which conditions there exists an entropy structure and how the corresponding entropy density can be constructed. Furthermore, we will explore the connection between normal ellipticity and the existence of an entropy structure.

Examples. In the literature, an entropy structure has been found for specific classes of cross-diffusion systems. For instance, segregating population species can be modeled by equations (1) with the diffusion coefficients

$$A_{ij}(u) = \delta_{ij}p_i(u) + u_i\partial p_i/\partial u_j, \quad i, j = 1, \dots, n,$$

where $p_i(u)$ are transition rates originating from the lattice model from which these equations can be formally derived [28, Appendix A]. This model was suggested by Shigesada, Kawasaki, and Teramoto [27] for $p_i(u) = a_{i0} + \sum_{j=1}^n a_{ij}u_j$ and $n = 2$. The n -species model with linear or nonlinear functions $p_i(u)$ was analyzed in [9, 11, 17, 22], and the existence of global weak solutions was proved. Equations (1) with diffusion coefficients associated to linear functions p_i ,

$$(4) \quad A_{ij}(u) = \delta_{ij} \left(a_{i0} + \sum_{k=1}^n a_{ik}u_k \right) + a_{ij}u_i, \quad i, j = 1, \dots, n,$$

where $a_{i0} \geq 0$, $a_{ij} \geq 0$, are called the SKT model. It has an entropy structure if there exist numbers $\pi_1, \dots, \pi_n > 0$ such that $\pi_i a_{ij} = \pi_j a_{ji}$ for all $i \neq j$ holds. This assumption can be recognized as the detailed-balance condition for the Markov chain generated by (a_{ij}) . Moreover, the function $h(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$ is an entropy density, and $h''(u)A(u)$ is positive definite for all $u \in \mathcal{D} = \mathbb{R}_+^n$.

A second example are volume-filling models which describe multi-species systems which take into account the finite size of the species and are given by (1) with the diffusion coefficients

$$(5) \quad A_{ij}(u) = \delta_{ij}p_i(u)q_i(u_0) + u_i p_i(u) q_i'(u_0) + u_i q_i(u_0) \partial p_i / \partial u_j,$$

where p_i and q_i are transition rates (again, see [28, Appendix A] for a formal derivation) and $u_0 := 1 - \sum_{i=1}^n u_i$ is the volume fraction of “free space” (in the context of biological models) or the solvent concentration (in the context of fluid mixtures). The concentration vector $u = (u_1, \dots, u_n)$ is an element of $\mathcal{D} = \{u \in \mathbb{R}_+^n : \sum_{i=1}^n u_i < 1\}$, the so-called Gibbs simplex. The existence of global weak solutions to system (1) with $q_i = q$ in (5) was proved in [28]. If there exists a convex function χ such that $\partial \chi / \partial u_i = \log p_i$ for $i = 1, \dots, n$, then the function

$$h(u) = \sum_{i=1}^n u_i (\log u_i - 1) + \int_a^{u_0} \log q(s) ds + \chi(u), \quad u \in \mathcal{D},$$

is an entropy density, and $h''(u)A(u)$ is positive definite for $u \in \mathcal{D}$.

A third example are equations for fluid mixtures driven by partial pressure gradients,

$$(6) \quad \partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad i = 1, \dots, n,$$

where u_i is the density of the i th fluid component and p_i is the i th partial pressure. This model follows from the mass continuity equation $\partial_t u_i + \operatorname{div}(u_i v_i) = 0$ if the partial velocities v_i are related to the partial pressures via Darcy’s law, $v_i = -\nabla p_i(u)$. This system was derived from an interacting particle system in the mean-field limit in [8]. The entropy

structure of this system is unknown up to now. We determine conditions on the pressures p_i under which (6) has an entropy structure.

Main results. We sketch some of our main results. For details, we refer to the following sections.

- Section 2: If a matrix $A \in \mathbb{R}^{n \times n}$ can be decomposed as the product $A_1 A_2$ with a symmetric positive definite square matrix A_1 , the normal ellipticity or diagonalizability of A can be proved subject to properties of the square matrix A_2 . We collect known results from matrix factorization theory and prove a new result characterizing the normal ellipticity of A . We apply these findings in Sections 3–6.
- Section 3: Any cross-diffusion system with entropy structure has a normally elliptic diffusion matrix. Thus, the normal ellipticity is a necessary condition. Under this condition, if there exists a strictly convex function $h \in C^2(\mathcal{D})$ ($\mathcal{D} \subset \mathbb{R}^n$ being a domain) such that $h''(u)A(u)$ is symmetric in \mathcal{D} , then $h''(u)A(u)$ is positive definite in \mathcal{D} . The symmetry requirement may be used to determine $h(u)$, and we present some examples in this direction.
- Section 4: If the diffusion matrix A is constant, then its normal ellipticity is equivalent to the existence of an entropy structure. Even if the normally elliptic constant matrix A is perturbed by a bounded nonlinear matrix, (1) has an entropy structure. Such a structure also exists if $h''(u)A(u)$ is symmetric up to a bounded nonlinear perturbation.
- Section 5: If the entropy density is the sum of single-valued functions and $h''(u)A(u)$ is symmetric, the positive definiteness of $h''(u)A(u)$ is equivalent to the positivity of the leading principal minors of $A(u)$. This avoids the computation of the eigenvalues of $A(u)$ to check its normal ellipticity. The idea allows us to construct entropies in some situations, for instance for a general class of 2×2 diffusion matrices.
- Section 6: If the matrix $(\partial p_i / \partial u_j)$ is normally elliptic in \mathcal{D} and the detailed-balance condition

$$\pi_i \frac{\partial p_i}{\partial u_j}(u) = \pi_j \frac{\partial p_j}{\partial u_i}(u) \quad \text{for all } u \in \mathcal{D}, \quad i \neq j,$$

holds, then the fluid mixture model (6) has an entropy structure with a Boltzmann-type entropy density. Surprisingly, there exists a *second* entropy density, which is of quadratic type. It is derived from the Poincaré lemma for closed differential forms by interpreting the detailed-balance condition as the curl-freeness of the vector-field $(\pi_1 p_1, \dots, \pi_n p_n)$. These results are new.

- Section 7: We prove that the diffusion matrix (4) of the SKT model is normally elliptic. Surprisingly, this property has not been proved in the literature so far (except for the easy case $n = 2$). Furthermore, we investigate the normal ellipticity of the diffusion matrix (5) of the volume-filling model and (6) of the fluid mixture model. Also these results are new.

Finally, we discuss in Section 8 some connections with results of other authors and some extensions.

Definitions and notation. We consider only real matrices $A \in \mathbb{R}^{n \times n}$ with coefficients A_{ij} . The coefficients of a vector $u \in \mathbb{R}^n$ are denoted by u_1, \dots, u_n . The set $\sigma(A)$ signifies the spectrum of A . We say that the (possibly nonsymmetric) matrix A is positive definite if $z^\top A z > 0$ for all $z \in \mathbb{R}^n$, $z \neq 0$, or, equivalently, if $A + A^\top$ is positive definite. The matrix A is normally elliptic if $\operatorname{Re}(\lambda) > 0$ for all $\lambda \in \sigma(A)$. In stability theory, this property is sometimes called positive stability. We say that A is diagonalizable if there exists a nonsingular matrix $P \in \mathbb{R}^{n \times n}$ such that $A = P\Lambda P^{-1}$ and $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n) \in \mathbb{R}^{n \times n}$, where $\lambda_i \in \sigma(A)$ for $i = 1, \dots, n$. In particular, the eigenvalues of diagonalizable matrices are (here) real. We denote by $I \in \mathbb{R}^{n \times n}$ the identity matrix.

Let $\mathcal{D} \subset \mathbb{R}^n$ be a domain. We say that (1) has an entropy structure if there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that $h''(u)A(u)$ is positive definite for all $u \in \mathcal{D}$. The matrix $A(u)h''(u)^{-1}$ is called the Onsager matrix and it is symmetric and/or positive definite if and only if $h''(u)A(u)$ is symmetric and/or positive definite, respectively. The integral $\mathcal{H}(u) = \int_{\Omega} h(u) dx$ is called an entropy and $-d\mathcal{H}/dt$ the entropy production. Finally, we set $\mathbb{R}_+ = (0, \infty)$ and $\mathbb{C}_+ = \{y \in \mathbb{C} : \operatorname{Re}(y) > 0\}$.

2. FACTORIZATION OF MATRICES

In this section, we collect some results concerned with the factorization of a normally elliptic or diagonalizable matrix $A \in \mathbb{R}^{n \times n}$. Some of these results are new. We will apply them to the diffusion matrix $A(u)$ from (1). The factorization is based on the Lyapunov theorem for matrix equations; see, e.g., [15, Theorems 2.2.1 and 2.2.3].

Theorem 1 (Lyapunov). (i) *If $A \in \mathbb{R}^{n \times n}$ is normally elliptic then for any given $G \in \mathbb{R}^{n \times n}$, there exists a unique matrix $H \in \mathbb{R}^{n \times n}$ such that $HA + A^\top H = G$.*

(ii) *The matrix $A \in \mathbb{R}^{n \times n}$ is normally elliptic if and only if for a given symmetric positive definite matrix $G \in \mathbb{R}^{n \times n}$, there exists a symmetric positive definite matrix $H \in \mathbb{R}^{n \times n}$ such that $HA + A^\top H = G$.*

We are analyzing factorizations $A = A_1 A_2$ or $A = A_2 A_1$ such that A_1 is symmetric positive definite. We will determine properties of A when A_2 is symmetric or positive definite and vice versa.

Proposition 2 (Positive definite factorization). *The matrix $A \in \mathbb{R}^{n \times n}$ is normally elliptic if and only if there exists a symmetric positive definite matrix A_1 and a positive definite matrix A_2 such that $A = A_1 A_2$ (or $A = A_2 A_1$).*

Proof. Let $A \in \mathbb{R}^{n \times n}$ be normally elliptic. By the Lyapunov theorem, there exists a symmetric positive definite matrix H such that $HA + A^\top H = I$. Then $A_1 = H^{-1}$ is symmetric positive definite and $A_2 = HA$ satisfies $A_2 + A_2^\top = I$, i.e., A_2 is positive definite. This yields the desired factorization $A = A_1 A_2$. Furthermore, since A^\top is normally elliptic, the same argument shows that there exists a symmetric positive definite matrix A_1 and a positive definite matrix B such that $A^\top = A_1 B$. We conclude that $A = A_2 A_1$ with $A_2 := B^\top$.

Assume that $A = A_1 A_2$, where A_1 is symmetric positive definite and A_2 is positive definite. Set $H := A_1^{-1}$. Then $A_2 = HA$ and $HA + A^\top H = A_2 + A_2^\top$ is positive definite.

By the Lyapunov theorem, A is normally elliptic. If $A = A_2A_1$, the same argument can be applied to $A^\top = A_1A_2^\top$. \square

The first part of the following result is proved in [5, Theorem 6].

Proposition 3 (Symmetric factorization). (i) *The matrix $A \in \mathbb{R}^{n \times n}$ is diagonalizable if and only if there exists a symmetric positive definite matrix A_1 and a symmetric matrix A_2 such that $A = A_1A_2$ (or $A = A_2A_1$).*

(ii) *If $A = A_1A_2$ or $A = A_2A_1$ is normally elliptic with A_1 being symmetric positive definite and A_2 being symmetric, then A_2 is also positive definite.*

Proof. It remains to prove part (ii). Indeed, we have $A_1^{-1} = A_2A^{-1}$ and hence $A_2A^{-1} + (A^{-1})^\top A_2 = A_1^{-1} + (A_1^{-1})^\top = 2A_1^{-1}$. Since A^{-1} is normally elliptic and $2A_1^{-1}$ is symmetric positive definite, we conclude from the Lyapunov theorem that there exists a unique symmetric positive definite matrix H such that $HA^{-1} + (A^{-1})^\top H = 2A_1^{-1}$. The uniqueness of H implies that $H = A_2$, showing that A_2 is positive definite. The same argument can be made for $A = A_2A_1$. \square

Remark 4 (Eigenvalues of A). If $A = A_1A_2$ factorizes in a symmetric positive definite matrix A_1 and a symmetric matrix A_2 , Proposition 3 implies in particular that the eigenvalues of A are real. We can say a bit more: By the inertia theorem of Sylvester [7, Section 1], the inertia of A_1A_2 and A_2 are the same, which means that the number of positive, negative, and vanishing eigenvalues of A and A_2 , respectively, are the same. In particular, if A_2 has only positive eigenvalues, A is normally elliptic. The eigenvalues of A can be bounded from below (or above) by the product of the eigenvalues of A_1 and A_2 ; see, e.g., [23, Theorem 2.2] for details. \square

Remark 5 (Compatibility of factorizations). Let $A = A_1A_2$ or $A = A_2A_1$ be a matrix factorization with a symmetric positive definite matrix A_1 . Proposition 3 (ii) states that if A is normally elliptic and A_2 is symmetric then A_2 is positive definite. We may ask whether the diagonalizability of A and positive definiteness of A_2 imply symmetry of A_2 . The answer is no. A counter-example is given as follows. Let

$$A = \begin{pmatrix} 1 & 2 \\ 0 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}.$$

Then $A = P\Lambda P^{-1}$ is diagonalizable and positive definite. The matrix $A_1 = I$ is symmetric positive definite, $A_2 = A$ is positive definite, and $A = A_1A_2 = A_2A_1$. However, A_2 is not symmetric. Still, we can factorize $A = A_1A_2$ with two symmetric positive definite matrices

$$A_1 = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & -2 \\ -2 & 6 \end{pmatrix}.$$

This motivates the following proposition. \square

Proposition 6 (Symmetric positive definite factorization). *The matrix $A \in \mathbb{R}^{n \times n}$ is normally elliptic and diagonalizable if and only if it is a product of two symmetric positive definite matrices.*

Note that $A \in \mathbb{R}^{n \times n}$ is normally elliptic and diagonalizable if and only if A is diagonalizable with positive eigenvalues. Thus, the proposition is the same as [5, Theorem 7], but our proof is new.

Proof. The sufficiency follows from Propositions 2 and 3, while the necessity is a consequence of Proposition 3. \square

Table 1 summarizes the factorization results.

TABLE 1. Types of factorization. PD = positive definite, S = symmetric, NE = normally elliptic, D = diagonalizable.

Factorization	Prop.	A	$\sigma(A)$	A_1	A_2
Positive definite	2	NE	\mathbb{C}_+	S+PD	PD
Symmetric	3	D	\mathbb{R}	S+PD	S
Symmetric positive definite	6	NE+D	\mathbb{R}_+	S+PD	S+PD

3. NECESSARY CONDITIONS FOR AN ENTROPY STRUCTURE

We use the matrix factorization results to characterize the entropy structure of (1).

Theorem 7. *Let $A(u) \in \mathbb{R}^{n \times n}$ with $u \in \mathcal{D}$.*

- (i) *If (1) has an entropy structure then $A(u)$ is normally elliptic for all $u \in \mathcal{D}$.*
- (ii) *If $A(u)$ is normally elliptic for all $u \in \mathcal{D}$ and there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that $h''(u)A(u)$ is symmetric for all $u \in \mathcal{D}$, then $h''(u)A(u)$ is positive definite for all $u \in \mathcal{D}$, i.e., (1) has an entropy structure.*
- (iii) *If (1) has an entropy structure such that $h''(u)A(u)$ is symmetric for all $u \in \mathcal{D}$, then $A(u)$ is diagonalizable with positive eigenvalues.*

Proof. The theorem follows from Propositions 2, 3 (ii), and 6. We factorize $A(u) = A_1A_2$ with $A_1 = h''(u)^{-1}$, which is symmetric positive definite, and $A_2 = h''(u)A(u)$.

(i) By assumption, A_2 is positive definite, so the result follows from Proposition 2. Another more elementary proof is given in [19, Lemma 3.2].

(ii) As the matrix A_2 is assumed to be symmetric, Proposition 3 (ii) shows that A_2 is positive definite.

(iii) Proposition 6 implies that $A(u)$ is normally elliptic and diagonalizable, which is equivalent to $A(u)$ being diagonalizable and having only positive eigenvalues. \square

Remark 8 (Consequences). The theorem can be used to determine whether an entropy structure exists.

(i) By Amann’s result [1, Section 1], the normal ellipticity of $A(u)$ is a natural minimal condition for the local-in-time existence of smooth solutions. If $A(u)$ is not normally elliptic, we cannot expect any entropy structure.

(ii) If $h''(u)A(u)$ is symmetric, so does the Onsager matrix $A(u)h''(u)^{-1}$. The symmetry of the Onsager matrix is a natural condition imposed in general systems consisting of irreversible thermodynamic processes. If the application behind system (1) should satisfy this

principle, we may calculate the entropy density by exploiting the symmetry of $h''(u)A(u)$; see the examples below.

(iii) A simple check whether an entropy structure for (1) exists with a symmetric Onsager matrix is to compute the eigenvalues of $A(u)$. According to Theorem 7, if the diffusion matrix $A(u)$ is not diagonalizable with positive eigenvalues, we cannot expect such a structure. \square

We consider the following cases to detect an entropy structure. Let $A(u) = A_1A_2$ or $A(u) = A_2A_1$, where A_1 is always symmetric positive definite.

Case 1.1. Let $A(u) = A_1A_2$ and let A_2 be positive definite. (According to Proposition 2, $A(u)$ is normally elliptic.) If we are able to find a function $h \in C^2(\mathcal{D})$ such that $h''(u) = A_1^{-1}$ (implying that h is strictly convex), then $A_2 = h''(u)A(u)$ is positive definite, and (1) has an entropy structure.

As an example, we consider the Keller–Segel system with additional cross-diffusion:

$$(7) \quad \partial_t u_1 = \operatorname{div}(\nabla u_1 - u_1 \nabla u_2), \quad \partial_t u_2 = \Delta u_1 + \delta \Delta u_2 + u_1 - u_2 \quad \text{in } \Omega \subset \mathbb{R}^2,$$

together with the initial and boundary conditions (2). The variables u_1 and u_2 denote the cell density and the concentration of the chemical signal, respectively. The parameter $\delta > 0$ describes the strength of the additional cross-diffusion. The classical parabolic-parabolic Keller–Segel model is obtained when $\delta = 0$. It is well known that this model has solutions that blow up in finite time if $d \geq 2$ and the total mass is sufficiently large [6, 10]. System (7) was suggested in [14] to allow for global-in-time solutions for any initial data.

The eigenvalues of $A(u)$ are $\lambda = 1 \pm i\sqrt{\delta u_1}$, so $A(u)$ is normally elliptic. We can factorize $A(u) = A_1A_2$ with

$$A_1 = \begin{pmatrix} u_1 & 0 \\ 0 & \delta \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1/u_1 & -1 \\ 1 & 1/\delta \end{pmatrix},$$

where A_1 is symmetric positive definite and A_2 is positive definite for $u_1 > 0$. Then $h''(u) = A_1^{-1}$ and hence, $A_2 = h''(u)A(u)$ is positive definite. We can solve

$$h''(u) = \begin{pmatrix} 1/u_1 & 0 \\ 0 & 1/\delta \end{pmatrix}$$

explicitly. Since $\partial^2 h / \partial u_1 \partial u_2 = 0$, the entropy density is the sum of $h_1(u_1)$ and $h_2(u_2)$ such that $h_1''(u_1) = 1/u_1$, $h_2''(u_2) = 1/\delta$. This gives $h(u) = u_1(\log u_1 - 1) + u_2^2/(2\delta)$.

Case 1.2. Let $A(u) = A_1A_2$ and let A_2 be symmetric. (According to Proposition 3, $A(u)$ is diagonalizable.) If we are able to find a function $h \in C^2(\mathcal{D})$ such that $h''(u) = A_1^{-1}$, then $A_2 = h''(u)A(u)$ is symmetric. Thus, if $A(u)$ is normally elliptic, Theorem 7 (ii) implies that (1) has an entropy structure, i.e., $h''(u)A(u)$ is positive definite.

To illustrate this result, we consider the n -species population model (1) with diffusion matrix (4). The existence of global weak solutions was proved in [9] under the detailed-balance condition, i.e., there exist $\pi_1, \dots, \pi_n > 0$ such that

$$\pi_i a_{ij} = \pi_j a_{ji} \quad \text{for all } i \neq j.$$

Under this condition, there exists a symmetric factorization $A(u) = A_1 A_2$ with

$$(A_1)_{ij} = \frac{u_i}{\pi_i} \delta_{ij}, \quad (A_2)_{ij} = \frac{\pi_i}{u_i} \delta_{ij} \left(a_{i0} + \sum_{k=1}^n a_{ik} u_k \right) + \pi_i a_{ij},$$

where $i, j = 1, \dots, n$. Clearly, A_1 is symmetric positive definite if $u_i > 0$, while A_2 is symmetric. We set $h''(u) = A_1^{-1}$ and $A_2 = h''(u)A(u)$. We prove in Section 7 that $A(u)$ is normally elliptic. Then Theorem 7 (ii) shows that $h''(u)A(u)$ is positive definite, and (1) has an entropy structure. Clearly, the positive definiteness of $h''(u)A(u)$ can be also verified directly; see [9, Lemma 4]. We solve $h''(u) = A_1^{-1}$ by observing that $\partial^2 h / \partial u_i \partial u_j = 0$ for $i \neq j$ (so, $h(u)$ is the sum of some functions $h_i(u_i)$), and it follows that $h''_i(u_i) = \pi_i / u_i$. We infer that $h(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$, which is the entropy density suggested in [9].

Case 2.1. Let $A(u) = A_2 A_1$ and let A_2 be positive definite (thus, $A(u)$ is normally elliptic). If $A_1 = h''(u)$ and $A_2 = A(u)h''(u)^{-1}$ then (1) has an entropy structure.

For instance, we wish to determine the entropy structure of the following system:

$$(8) \quad \partial_t u_1 = \frac{1}{2} \Delta(u_1^2 + u_3^2), \quad \partial_t u_2 = \frac{1}{2} \Delta(u_1^2 + u_2^2), \quad \partial_t u_3 = \frac{1}{2} \Delta(u_2^2 + u_3^2),$$

together with the no-flux boundary conditions in (2). This system is of the form $\partial_t u = \Delta F(u)$, where $F : \mathcal{D} \rightarrow \mathbb{R}^3$. The example was not considered in the literature before. The diffusion matrix is given by

$$A(u) = \begin{pmatrix} u_1 & 0 & u_3 \\ u_1 & u_2 & 0 \\ 0 & u_2 & u_3 \end{pmatrix}.$$

Then $A(u) = A_2 A_1$, where

$$A_1 = \begin{pmatrix} u_1 & 0 & 0 \\ 0 & u_2 & 0 \\ 0 & 0 & u_3 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

The matrix A_2 is positive definite and A_1 is symmetric positive definite if $u_i > 0$ for $i = 1, 2, 3$. Then $h''(u) = A_1$, and $A_2 = A(u)h''(u)^{-1}$ is positive definite, which provides the entropy structure. The equation $h''(u) = A_1$ can be solved explicitly and leads to the entropy density $h(u) = (u_1^3 + u_2^3 + u_3^3)/6$. Indeed, a formal computation shows that along solutions to (8),

$$\frac{d}{dt} \int_{\Omega} h(u) dx + \frac{1}{2} \sum_{i=1}^3 \int_{\Omega} |\nabla u_i^2|^2 dx = 0.$$

Case 2.2. Let $A(u) = A_2 A_1$ and A_2 be symmetric (then $A(u)$ is diagonalizable). If $h''(u) = A_1$, then $A_2 = A(u)h''(u)^{-1}$ is symmetric. If $A(u)$ is also normally elliptic, then $A(u)h''(u)^{-1}$ and consequently $h''(u)A(u)$ is positive definite, by Proposition 6. We infer that (1) has an entropy structure.

As an example, consider the volume-filling model with diffusion matrix $q_i = q$ in (5). We assume that $q > 0$, $q' > 0$ and there exists a convex function χ such that $p_i = \exp(\partial\chi/\partial u_i)$ for $i = 1, \dots, n$. Then $\partial p_i/\partial u_j = p_i \partial^2 \chi / \partial u_i \partial u_j$ and consequently,

$$A_{ij}(u) = u_i p_i(u) q(u_0) \left(\frac{\delta_{ij}}{u_i} + \frac{q'(u_0)}{q(u_0)} + \frac{\partial^2 \chi}{\partial u_i \partial u_j} \right),$$

recalling that $u_0 = 1 - \sum_{i=1}^n u_i$. We can decompose $A(u) = A_2 A_1$, where

$$(A_2)_{ij} = u_i p_i(u) q(u_0) \delta_{ij}, \quad (A_1)_{ij} = \frac{\delta_{ij}}{u_i} + \frac{q'(u_0)}{q(u_0)} + \frac{\partial^2 \chi}{\partial u_i \partial u_j}(u).$$

Both A_1 and A_2 are symmetric positive definite for $u \in \mathcal{D}$. The entropy density can be computed from

$$\frac{\partial^2 h}{\partial u_i \partial u_j}(u) = \frac{\delta_{ij}}{u_i} + \frac{q'(u_0)}{q(u_0)} + \frac{\partial^2 \chi}{\partial u_i \partial u_j}(u)$$

by integration, which leads, up to unimportant linear terms, to

$$h(u) = \sum_{i=1}^n u_i (\log u_i - 1) + \int_a^{u_0} \log q(s) ds + \chi(u), \quad u \in \mathcal{D},$$

where $a > 0$. This is the same entropy density as used in [28].

4. APPLICATION: PERTURBATIONS

We show some applications of Propositions 2 and 3 (ii). In particular, we analyze perturbations of symmetric Onsager matrices and of constant diffusion matrices.

Proposition 9 (Perturbation of $h''(u)A(u)$). *Let $A(u)$ be normally elliptic uniformly in \mathcal{D} and diagonalizable. Assume that there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that $h''(u)A(u) = S(u) + \varepsilon N(u)$, where $S(u)$ is symmetric, $\varepsilon > 0$, and N is bounded in \mathcal{D} . We also suppose that the eigenvalues of S are bounded in \mathcal{D} and the condition number $\|A(u)\| \|A(u)^{-1}\|$ and $\|h''(u)^{-1}N(u)\|$ are bounded in \mathcal{D} , where the matrix norm is induced by the absolute norm in \mathbb{C}^n . Then there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, (1) has an entropy structure.*

Proof. Since $A(u)$ is diagonalizable, we can apply the Bauer–Fike theorem [16, Theorem 6.3.2]: Let $\lambda(u)$ be an eigenvalue of $A(u)$ and $\mu(u)$ be an eigenvalue of $h''(u)^{-1}S(u)$. Then

$$\operatorname{Re}(\lambda(u)) - \operatorname{Re}(\mu(u)) \leq |\lambda(u) - \mu(u)| \leq \varepsilon \|A(u)\| \|A(u)^{-1}\| \|h''(u)^{-1}N(u)\| \leq \varepsilon C_1,$$

where $C_1 > 0$ does not depend on $u \in \mathcal{D}$. By assumption, there exists $\lambda^* > 0$ such that $\operatorname{Re}(\lambda(u)) \geq \lambda^*$. Therefore, we have $\operatorname{Re}(\mu(u)) \geq \lambda^*/2$ for all $0 < \varepsilon < \varepsilon_1 = \lambda^*/(2C_1)$. Thus, $h''(u)^{-1}S(u)$ is normally elliptic. Moreover, we can decompose $h''(u)^{-1}S(u) = A_1 A_2$, where $A_1 = h''(u)^{-1}$ is symmetric positive definite and $A_2 = S(u)$ is symmetric. We deduce from Proposition 3 (ii) that $S(u)$ is positive definite. By assumption on the eigenvalues of S , there exists $\kappa > 0$ such that for all $z^\top S(u) z \geq \kappa |z|^2$. Thus, for all $z \in \mathbb{R}^n$,

$$z^\top h''(u)A(u)z = z^\top S(u)z + \varepsilon z^\top N(u)z \geq (\kappa - \varepsilon K)|z|^2,$$

where $K = \|N(u)\|$. Thus, if $0 < \varepsilon < \varepsilon_2 < \kappa/K$, the matrix $h''(u)A(u)$ is positive definite, and the proof is finished after setting $\varepsilon_0 = \min\{\varepsilon_1, \varepsilon_2\} > 0$. \square

Remark 10. In cross-diffusion systems with volume filling, $h''(u)^{-1}$ may be uniformly bounded. As an example, let $h(u) = \sum_{i=1}^3 u_i(\log u_i - 1)$, where $u \in \mathcal{D} = \{u \in \mathbb{R}_+^2 : \sum_{i=1}^2 u_i < 1\}$ and $u_3 = 1 - u_1 - u_2$. Then

$$h''(u)^{-1} = \begin{pmatrix} u_1(u_2 + u_3) & -u_1u_2 \\ -u_1u_2 & u_2(u_1 + u_3) \end{pmatrix}$$

is indeed bounded in \mathcal{D} . Consequently, if $N(u)$ is bounded, so does $h''(u)^{-1}N(u)$, which is one of the assumptions in Proposition 9. \square

For a constant diffusion matrix, normal ellipticity and the existence of an entropy structure are equivalent.

Proposition 11 (Constant diffusion matrix). *If $A \in \mathbb{R}^{n \times n}$ is normally elliptic then (1) has an entropy structure and vice versa.*

Proof. By Theorem 7 (i), an entropy structure implies that A is normally elliptic. Conversely, if A is normally elliptic, by Proposition 2, there exists a symmetric positive definite matrix A_1 and a positive definite matrix A_2 such that $A = A_1A_2$. Defining the entropy density $h(u) = \frac{1}{2}u^\top Hu$ with $H := A_1^{-1}$, we infer that $h''(u)A = HA = A_2$ is positive definite. \square

Remark 12 (Explicit formula for H). The matrix H appearing in the entropy density $h(u) = \frac{1}{2}u^\top Hu$ can be constructed explicitly. By the Lyapunov theorem, there exists a unique symmetric positive definite matrix $H \in \mathbb{R}^{n \times n}$ such that $HA + A^\top H = I$. Then $HA + (HA)^\top = HA + A^\top H = I$ is symmetric positive definite, i.e., $h''(u)A = HA$ is positive definite. According to [15, Problem 9, Section 2.2], it follows that

$$H = \int_0^\infty e^{-A^\top t} e^{-At} dt.$$

An interesting consequence from this formula is that

$$\det H = \int_0^\infty \det(e^{-At}) \det(e^{-A^\top t}) dt = \int_0^\infty \det(e^{-2At}) dt = \int_0^\infty e^{-2\operatorname{tr}(A)t} dt = \frac{1}{2\operatorname{tr}(A)},$$

where we used the property $\det(e^{-2At}) = e^{-2\operatorname{tr}(A)t}$ [13, Theorem 2.12]. \square

Proposition 11 can be slightly generalized to the sum of a constant matrix and a nonlinear perturbation. Note that we do not assume that $A(u)$ is diagonalizable.

Proposition 13 (Perturbations of constant diffusion matrices). *Let $A_0 \in \mathbb{R}^{n \times n}$ be a constant normally elliptic matrix.*

(i) *Let $A(u) = A_0 + p(u)I$, where $p(u)$ is a positive scalar function. Then (1) has an entropy structure.*

(ii) *Let $A(u) = A_0 + \varepsilon A_1(u)$, where $A_1(u)$ is a bounded matrix in \mathcal{D} and $\varepsilon > 0$. Then there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, (1) has an entropy structure.*

Proof. (i) By Proposition 11, there exists a symmetric positive definite matrix $H \in \mathbb{R}^{n \times n}$ such that $h''(u)A_0$ is positive definite, where $h(u) = \frac{1}{2}u^\top H u$. Then $h''(u)A(u) = HA_0 + p(u)H$ is positive definite as the sum of two positive definite matrices.

(ii) We know from part (i) that HA_0 is positive definite, where H is symmetric positive definite. Thus, there exists $\lambda > 0$ such that $z^\top HA_0 z \geq \lambda|z|^2$ for all $z \in \mathbb{R}^n$. Since $A_1(u)$ is bounded, there exists $M > 0$ such that $\|HA_1(u)\| \leq M$ for all $u \in \mathcal{D}$. We conclude that $z^\top h''(u)A(u)z \geq (\lambda - \varepsilon M)|z|^2$ for $z \in \mathbb{R}^n$, and the positive definiteness follows after choosing $0 < \varepsilon < \varepsilon_0 < \lambda/M$. \square

5. APPLICATION: SUM OF SINGLE-SPECIES ENTROPY DENSITIES

When the entropy density $h(u)$ can be written as the sum of functions depending on u_i , we can give an easy criterion for the positive definiteness of $h''(u)A(u)$, avoiding the computation of the eigenvalues of $A(u)$ in order to check the normal ellipticity.

Proposition 14. *If there exists a strictly convex function $h(u) = \sum_{i=1}^n h_i(u_i)$ for some functions $h_i \in C^2(\mathcal{D})$ such that $h''(u)A(u)$ is symmetric, then $h''(u)A(u)$ is positive definite if and only if all leading principal minors of $A(u)$ are positive.*

Proof. It holds that $h''(u)A(u) = (h''_i(u_i)A_{ij}(u)) \in \mathbb{R}^{n \times n}$. Let M_k be the k th leading principal minor of $h''(u)A(u)$ and let $A_k \in \mathbb{R}^{k \times k}$ be the leading principal submatrix of order k of $A(u)$. Then

$$M_k = \prod_{i=1}^k h''_i(u_i) \det(A_k).$$

Thus, if $h''(u)A(u)$ is symmetric positive definite, then $M_k > 0$ for all $k = 1, \dots, n$, by Sylvester's criterion and hence $\det(A_k) > 0$ for all $k = 1, \dots, n$. On the other hand, if $\det(A_k) > 0$ then $M_k > 0$ for all $k = 1, \dots, n$, and we conclude from the symmetry of $h''(u)A(u)$, by Sylvester's criterion again, that $h''(u)A(u)$ is positive definite. \square

The symmetry of $h''(u)A(u)$ implies that $h''_i(u_i)A_{ij}(u) = h''_j(u_j)A_{ji}(u)$ for all $i \neq j$. Since $h''_i(u_i) > 0$, this shows that both $A_{ij}(u)$ and $A_{ji}(u)$ are positive, negative, or zero for any $i \neq j$. We apply Proposition 14 to various examples.

Construction of entropies in two-species systems. We construct convex entropy densities $h(u) = h_1(u_1) + h_2(u_2)$ for (1) with the diffusion matrix

$$A(u) = \begin{pmatrix} a_{11}(u) & b_1(u_1)b_2(u_2) \\ c_1(u_1)c_2(u_2) & a_{22}(u) \end{pmatrix},$$

where $a_{11} > 0$, $b_1 b_2 c_1 c_2 > 0$, and $\det A > 0$ in \mathcal{D} . The symmetry of $h''(u)A(u)$ is equivalent to $b_1 b_2 h''_1 = c_1 c_2 h''_2$ or $b_1 h''_1 / c_1 = c_2 h''_2 / b_2$. The left-hand side depends only on u_1 , the right-hand side only on u_2 . Thus, both sides are constant and, say, equal to $k \in \mathbb{R}$. Since h''_1 and h''_2 are positive, we may set $k = \text{sign}(b_1(u)c_1(u))|k|$. (Note that the sign of $b_1(u)c_1(u)$ must be the same for all $u \in \mathcal{D}$.) Then

$$h_1(u_1) = |k| \int_{u_1^*}^{u_1} \int_{v_1^*}^{v_1} \left| \frac{c_1(s)}{b_1(s)} \right| ds dv_1, \quad h_2(u_2) = |k| \int_{u_2^*}^{u_2} \int_{v_2^*}^{v_2} \left| \frac{b_2(s)}{c_2(s)} \right| ds dv_2,$$

at least if these integrals exist. Without loss of generality, we may choose $|k| = 1$. Our assumptions imply that the leading principal minors of $A(u)$, namely $a_{11}(u)$ and $\det(A(u))$, are positive. Thus, by Proposition 14, $h''(u)A(u)$ is positive definite, and (1) has an entropy structure.

Construction of entropies in n -species systems. The idea for two-species systems can be extended to $n \times n$ matrices. To simplify, we consider entropy densities $h(u) = \sum_{i=1}^n h_i(u_i)$ and diffusion matrices of the form

$$(9) \quad A(u) = \begin{pmatrix} a_{11}(u) & a_{12}u_1 & a_{13}u_1 & \cdots & a_{1n}u_1 \\ a_{21}u_2 & a_{22}(u) & a_{23}u_2 & \cdots & a_{2n}u_2 \\ a_{31}u_3 & a_{32}u_3 & a_{33}(u) & & a_{3n}u_3 \\ \vdots & \vdots & & \ddots & \vdots \\ a_{n1}u_n & a_{n2}u_n & a_{n3}u_n & \cdots & a_{nn}(u) \end{pmatrix},$$

where $a_{ij} \in \mathbb{R}$ and $u \in \mathbb{R}_+^n$. We assume that both a_{ij} and a_{ji} are positive, negative, or zero for any $i \neq j$ and that the leading principal minors of $A(u)$ are positive. Matrices like (9) appear, for instance, in diffusive population dynamics; see (4). The matrix $h''(u)A(u)$ is symmetric if and only if

$$h''_i(u_i)u_i a_{ij}(u) = h''_j(u_j)u_j a_{ji}(u) \quad \text{for all } u \in \mathcal{D}, \quad i, j = 1, \dots, n.$$

Hence, there exist constants $k_{ij} \in \mathbb{R}$ such that

$$h''_i(u_i)u_i a_{ij} = h''_j(u_j)u_j a_{ji} = k_{ij} = \text{sign}(a_{ij})|k_{ij}|.$$

Case 1. Let $a_{ij}a_{ji} > 0$ for any $1 \leq i < j \leq n$. Then

$$h''_i(u_i) = \frac{k_{ij}}{a_{ij}u_i} = \frac{|k_{ij}|}{|a_{ij}|u_i} \quad \text{for } i + 1 \leq j \leq n,$$

$$h''_j(u_j) = \frac{k_{ij}}{a_{ji}u_j} = \frac{|k_{ij}|}{|a_{ji}|u_j} \quad \text{for } 1 \leq i \leq j - 1.$$

We introduce the numbers $\pi_i = |k_{ij}|/|a_{ij}|$ for $i + 1 \leq j \leq n$ and $\pi_j = |k_{ij}|/|a_{ji}|$ for $1 \leq i \leq j - 1$. Then it holds that $\pi_i > 0$ for $i = 1, \dots, n$ and $\pi_i|a_{ij}| = \pi_j|a_{ji}|$ for $1 \leq i < j \leq n$. Since we assume that $a_{ij}a_{ji} > 0$ for $i < j$, this yields the detailed-balance condition

$$\pi_i a_{ij} = \pi_j a_{ji} \quad \text{for } i \neq j,$$

which has been already imposed in [9] (but we allow for negative values of a_{ij} and a_{ji}). This shows that $h''_i(u_i) = \pi_i/u_i$ and hence, the entropy density becomes

$$h(u) = \sum_{i=1}^n h_i(u_i) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1).$$

Note that the detailed-balance condition is equivalent to the symmetry of $h''(u)A(u)$.

Case 2. To simplify the presentation, we assume that there exists only one couple of indices (i_0, j_0) with $1 \leq i_0 < j_0 \leq n$ such that $a_{i_0 j_0} = a_{j_0 i_0} = 0$. Case 1 applies to all indices $(i, j) \neq (i_0, j_0)$, while for $(i, j) = (i_0, j_0)$, we have

$$\begin{aligned}\pi_{i_0} &= \frac{|k_{i_0 j}|}{|a_{i_0 j}|}, & j &= i_0 + 1, \dots, j_0 - 1, j_0 + 1, \dots, n, \\ \pi_{j_0} &= \frac{|k_{i j_0}|}{|a_{i j_0}|}, & i &= 1, \dots, i_0 - 1, i_0 + 1, \dots, j_0 - 1.\end{aligned}$$

The detailed-balance condition $\pi_{i_0} a_{i_0 j_0} = \pi_{j_0} a_{j_0 i_0}$ is automatically satisfied since $a_{i_0 j_0} = a_{j_0 i_0} = 0$. For example, if $n = 3$ and $a_{12} = a_{21} = 0$, the detailed-balance condition reduces to the identities $\pi_1 a_{13} = \pi_3 a_{31}$ and $\pi_2 a_{23} = \pi_3 a_{32}$, while $\pi_1 a_{12} = \pi_2 a_{21}$ is no longer needed.

6. APPLICATION: FLUID MIXTURE AND POPULATION MODELS

We construct entropy densities for diffusive fluid mixture and population systems.

Fluid models with partial pressure gradients. Let us consider the fluid mixture model (6) which has the diffusion matrix $A_{ij}(u) = u_i \partial p_i / \partial u_j$ for $i, j = 1, \dots, n$. Essential for the analysis of is the following detailed-balance condition: There exist numbers $\pi_1, \dots, \pi_n > 0$ such that

$$(10) \quad \pi_i \frac{\partial p_i}{\partial u_j} = \pi_j \frac{\partial p_j}{\partial u_i} \quad \text{in } \mathcal{D} \text{ for all } i \neq j,$$

and we assume that $\mathcal{D} \subset \mathbb{R}_+^n$.

Proposition 15. *Assume that the matrix $Q = (\partial p_i / \partial u_j)$ is normally elliptic and that the detailed-balance condition (10) holds. Then (6) has an entropy structure with the entropy density $h(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$.*

Proof. The normally elliptic matrix Q factorizes according to $Q = A_1 A_2$, where $A_1 = \text{diag}(\pi_1^{-1}, \dots, \pi_n^{-1})$ is symmetric positive definite and $A_2 = (\pi_i \partial p_i / \partial u_j)$ is symmetric. Therefore, Proposition 3 (ii) shows that $h''(u)A(u) = A_2$ is positive definite. \square

Remark 16 (Alternative proof). We claim that the normal ellipticity of $A(u)$ is equivalent to that of Q . Then Proposition 15 is an immediate consequence of Theorem 7 (ii) since $h''(u)A(u) = (\pi_i \partial p_i / \partial u_j)$ is assumed to be symmetric. We use the inertia theorem of Sylvester [7, Section 1]: If A_1 is symmetric positive definite and A_2 is symmetric, then the inertia of $A_1 A_2$ and A_2 coincide. As a consequence, $A_1 A_2$ and A_2 have the same number of eigenvalues with positive real parts. We apply this result to $A_1 = \text{diag}(\pi_1^{-1}, \dots, \pi_n^{-1})$ and $A_2 = (\pi_i \partial p_i / \partial u_j)$ to infer that $A_1 A_2 = Q$ and A_2 have the same number of eigenvalues with positive real parts. The same argument applied to $\tilde{A}_1 = \text{diag}(u_1 \pi_1^{-1}, \dots, u_n \pi_n^{-1})$ and A_2 shows that also $\tilde{A}_1 A_2 = A(u)$ and A_2 have the same number of eigenvalues with positive part. This implies that the number of eigenvalues with real parts of $A(u)$ and Q coincide, proving the result. \square

Interestingly, there exists a second entropy density.

Proposition 17 (Second entropy). *Let $p_1, \dots, p_n \in C^1(\mathcal{D})$ be defined on the simply connected set $\mathcal{D} \subset \mathbb{R}_+^n$ and assume that the detailed-balance condition (10) holds. If $Q = (\partial p_i / \partial u_j)$ is invertible on \mathcal{D} then (1) has an entropy structure with an entropy density $h(u)$ satisfying $\partial h / \partial u_i = \pi_i p_i$ for $i = 1, \dots, n$.*

Proof. The proof is based on the Poincaré lemma for closed differential forms. Since $(\pi_i p_i)$ defines a curl-free vector field in the sense $\partial(\pi_i p_i) / \partial u_j = \partial(\pi_j p_j) / \partial u_i$ for all $i \neq j$, there exists a function $h \in C^2(\mathcal{D})$ such that $\partial h / \partial u_i = \pi_i p_i$ for $i = 1, \dots, n$. It follows from the detailed-balance condition that for all $z \in \mathbb{R}^n$,

$$\begin{aligned} z^\top h''(u) A(u) z &= \sum_{i,j,k=1}^n \pi_i \frac{\partial p_i}{\partial u_k} u_k \frac{\partial p_k}{\partial u_j} z_i z_j = \sum_{i,j,k=1}^n \pi_k u_k \frac{\partial p_k}{\partial u_i} \frac{\partial p_k}{\partial u_j} z_i z_j \\ &= \sum_{k=1}^n \pi_k u_k \left(\sum_{j=1}^n \frac{\partial p_k}{\partial u_j} z_j \right)^2 \geq 0. \end{aligned}$$

Assume that $z^\top h''(u) A(u) z = 0$ for $z \neq 0$. Since $u_k > 0$, it follows that $Qz = 0$. However, Q is invertible which implies that $z = 0$, contradiction. Thus, $z^\top h''(u) A(u) z > 0$ for $z \neq 0$. \square

Note that if the matrix $(\partial p_i / \partial u_j)$ is normally elliptic then it is invertible. As an example, consider $p_i(u) = \sum_{j=1}^n a_{ij} u_j$ with coefficients $a_{ij} \geq 0$. Then the Jacobian of (p_1, \dots, p_n) equals the matrix (a_{ij}) . Thus, if this matrix is invertible (and the detailed-balance condition holds), Proposition 17 applies, and (6) with this choice has an entropy structure. The entropy density can be constructed explicitly from $\partial h / \partial u_i = \pi_i \sum_{j=1}^n a_{ij} u_j$ leading to

$$h(u) = \frac{1}{2} \sum_{i,j=1}^n \pi_i a_{ij} u_i u_j.$$

If u is a (smooth) solution to (2), (6) and $\partial h / \partial u_i = \pi_i p_i$ for $i = 1, \dots, n$, it follows that

$$\frac{d}{dt} \int_{\Omega} h(u) dx + \int_{\Omega} \sum_{i=1}^n \pi_i u_i |\nabla p_i(u)|^2 dx = 0,$$

which yields slightly better integrability than the Boltzmann-type entropy density from Proposition 15.

Population models. We have considered the n -species SKT population model with diffusion matrix (4) already in Section 3. Here, we study a more general version, given by

$$(11) \quad \partial_t u_i = \Delta(u_i p_i(u)) = \operatorname{div}(u_i \nabla p_i(u) + p_i(u) \nabla u_i), \quad i = 1, \dots, n,$$

where $p_i(u) > 0$ are transition rates from the underlying lattice model [28, Appendix A]. In the classical SKT model (4), we have $p_i(u) = a_{i0} + \sum_{j=1}^n a_{ij} u_j$. Generally, the diffusion matrix has the elements $A_{ij}(u) = \delta_{ij} p_i(u) + u_i \partial p_i / \partial u_j$. Compared to the fluid model (6), system (11) contains the additional term $p_i(u)$ on the diagonal of the diffusion matrix. Therefore, we have the same result as in Proposition 15.

Corollary 18 (General SKT model). *Let $p_1, \dots, p_n : \mathcal{D} \rightarrow \mathbb{R}_+$ be defined on the simply connected set $\mathcal{D} \subset \mathbb{R}_+^n$, let the matrix $Q = (\partial p_i / \partial u_j)$ be normally elliptic, and let the detailed-balance condition (10) hold. Then (11) has an entropy structure with entropy density $h(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$ for $u \in \mathcal{D}$.*

Proof. The matrix $h''(u)A(u)$ is the sum of the diagonal matrix with positive entries $\pi_i u_i^{-1} p_i$ and the matrix $(\pi_i \partial p_i / \partial u_j)$. Since it follows from Proposition 15 that both matrices are symmetric positive definite, so does $h''(u)A(u)$. \square

This idea can be generalized to cross-diffusion systems of the form

$$(12) \quad \partial_t u_i = \Delta F_i(u), \quad i = 1, \dots, n.$$

The diffusion matrix is given by the elements $A_{ij}(u) = \partial F_i / \partial u_j$ for $i, j = 1, \dots, n$. We recover (11) for $F_i(u) = u_i p_i(u)$.

Proposition 19. *Let $F_1, \dots, F_n \in C^1(\mathcal{D})$ be defined on the simply connected set $\mathcal{D} \subset \mathbb{R}^n$, let the Jacobian of (F_1, \dots, F_n) be invertible and let the detailed-balance condition (10) with p_i replaced by F_i hold. Then (12) has an entropy structure.*

Proof. By assumption, $(\pi_1 F_1, \dots, \pi_n F_n)$ is curl-free. Hence, we deduce from the Poincaré lemma for closed differential forms the existence of a function $h : \mathcal{D} \rightarrow \mathbb{R}$ such that $\partial h / \partial u_i = \pi_i F_i$ for $i = 1, \dots, n$. This implies for all $z \in \mathbb{R}^n$, $z \neq 0$ that

$$z^\top h''(u)A(u)z = \sum_{i,j,k=1}^n \pi_i \frac{\partial F_i}{\partial u_k} \frac{\partial F_k}{\partial u_j} z_i z_j = \sum_{i,j,k=1}^n \pi_k \frac{\partial F_k}{\partial u_i} \frac{\partial F_k}{\partial u_j} z_i z_j = \sum_{k=1}^n \pi_k \left(\sum_{j=1}^n \frac{\partial F_k}{\partial u_j} z_j \right)^2.$$

Since $(\partial F_k / \partial u_j)$ is invertible, we infer as in the proof of Proposition 17 that the previous expression is positive for all $z \neq 0$. \square

7. NORMAL ELLIPTICITY

We prove the normal ellipticity of the diffusion matrices associated to the three models introduced in the introduction.

SKT model. The normal ellipticity of the two-species SKT model with diffusion matrix (4) was proved in [2, Section 17.1]. Surprisingly, this property is not known for the n -species model. Under the detailed-balance condition $\pi_i a_{ij} = \pi_j a_{ji}$ for $i \neq j$, the existence of an entropy structure was shown in [9, Lemma 4], so that in this case $A(u)$ is normally elliptic by Theorem 7 (i). In the following, we prove that this property also holds when the detailed-balance condition is not valid.

Lemma 20. *Define the matrix $A(u) \in \mathbb{R}^{n \times n}$ by (4), i.e.*

$$A_{ii}(u) = a_{i0} + 2a_{ii}u_i + \sum_{j \neq i} a_{ij}u_j, \quad A_{ij} = a_{ij}u_i \quad \text{for } i \neq j.$$

If $a_{i0} \geq 0$, $a_{ij} \geq 0$ with $a_{i0} + a_{ii} > 0$ for $i, j = 1, \dots, n$, then $A(u)$ is normally elliptic for any $u \in \mathbb{R}_+^n$.

Proof. We reformulate the matrix $A(u)$ by setting $B_{ii} = a_{i0} + 2a_{ii}u_i$ and $B_{ij} = a_{ij}u_j$ for $i \neq j$. Then $A_{ii} = \sum_{j=1}^n B_{ij}$ and $A_{ij} = B_{ij}$ for $i \neq j$. We define the matrix

$$\tilde{A} = \begin{pmatrix} A_{11} & a_{12}u_2 & \cdots & a_{1n}u_n \\ a_{21}u_1 & A_{22} & & a_{2n}u_n \\ \vdots & & \ddots & \\ a_{n1}u_1 & a_{n2}u_2 & & A_{nn} \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^n B_{1j} & B_{12} & \cdots & B_{1n} \\ B_{21} & \sum_{j=1}^n B_{2j} & & B_{2n} \\ \vdots & & \ddots & \\ B_{n1} & B_{n2} & & \sum_{j=1}^n B_{nj} \end{pmatrix}.$$

Then $A(u)$ and \tilde{A} are similar since $\tilde{A} = U^{-1}A(u)U$, where $U = \text{diag}(u_1, \dots, u_n)$, and thus they have the same eigenvalues. Since $B_{ii} = a_{i0} + 2a_{ii} > 0$ by assumption, the matrix \tilde{A} is strictly diagonally dominant. It follows from [16, Theorem 6.1.10] that all eigenvalues of \tilde{A} have a positive real parts and so does $A(u)$. This means that $A(u)$ is normally elliptic. \square

This result can be generalized to population models of the form (11), where $A_{ij}(u) = p_i(u)\delta_{ij} + u_i\partial p_i/\partial u_j$. Indeed, if $\partial p_i/\partial u_j \geq 0$ and $p_i(u) > \sum_{k \neq i} u_k \partial p_i/\partial u_k$ for $u \in \mathcal{D}$ and $i, j = 1, \dots, n$ then $A(u)$ is normally elliptic. For instance, if

$$p_i(u) = a_{i0} + \sum_{j=1}^n a_{ij}u_j^s, \quad i = 1, \dots, n,$$

this condition is satisfied if $0 < s < 1$, $a_{i0} \geq 0$, $a_{ij} \geq 0$, and $a_{i0} + a_{ii} > 0$.

Another generalization concerns the condition $a_{i0} + a_{ii} > 0$. It is not necessary to conclude the normal ellipticity of $A(u)$. By applying the Routh–Hurwitz stability criterion [15, Section 2.3] (or the stability criterion of Liénard–Chipart [12, Theorem 11, p. 221]), we may allow for $a_{i0} + a_{ii} = 0$. To avoid too many technicalities, we restrict ourselves to the case $n = 3$. Then the Routh–Hurwith criterion reads as follows: The roots of the polynomial $\lambda^3 + b_2\lambda^2 + b_1\lambda + b_0$ have negative real parts if and only if $b_i > 0$ for $i = 0, 1, 2$ and $b_2b_1 > b_0$.

Lemma 21. *Let $a_{i0} \geq 0$, $a_{ij} \geq 0$ for $i, j = 1, 2, 3$ and set $b_{ij} = a_{ij}$ for $i \neq j$ and $b_{ii} = a_{i0} + a_{ii}$. Assume that there exists a tripel $(i, j, k) \in \{1, 2, 3\}^3$ such that*

$$(i, j) \neq (2, 1), \quad (i, k) \neq (3, 1), \quad (j, k) \neq (3, 2), \quad \text{and} \quad b_{1i}b_{2j}b_{3k} > 0.$$

Then $A(u)$ is normally elliptic for any $u \in \mathbb{R}_+^3$.

Proof. The characteristic polynomial $p(\lambda) = \det(A(u) - \lambda I)$ equals $q(\lambda) = p(-\lambda) = \lambda^3 + b_2\lambda^2 + b_1\lambda + b_0$, where

$$b_0 = \det A, \quad b_1 = \sum_{1 \leq i < j \leq 3} \det \begin{pmatrix} A_{ii} & A_{ij} \\ A_{ji} & A_{jj} \end{pmatrix}, \quad b_2 = \text{trace } A.$$

According to the Routh–Hurwitz criterion, we need to verify that $b_i > 0$ for $i = 0, 1, 2$ and $b_2b_1 - b_0 > 0$ to deduce the normal ellipticity of $A(u)$. To this end, we recall the definition of B_{ij} from the proof of Lemma 20: $B_{ii} = a_{i0} + 2a_{ii}u_i$ and $B_{ij} = a_{ij}u_j$ for $i \neq j$. Then

$A_{ii} = \sum_{j=1}^3 B_{ij}$ and for $u \in \mathbb{R}_+^3$,

$$\begin{aligned} b_2 &= \sum_{i,j=1}^3 B_{ij} > 0, \\ b_1 &= \sum_{1 \leq i < j \leq 3} (A_{ii}A_{jj} - B_{ij}B_{ji}) = \sum_{1 \leq i < j \leq 3} \sum_{(k,\ell) \neq (j,i)} B_{ik}B_{j\ell} > 0, \\ b_0 &= A_{11}A_{22}A_{33} + B_{12}B_{23}B_{31} + B_{13}B_{32}B_{21} \\ &\quad - A_{11}B_{23}B_{32} - A_{22}B_{13}B_{31} - A_{33}B_{12}B_{21} \\ &= \sum_{(i,j,k)} B_{1i}B_{2j}B_{3k} + B_{12}B_{23}B_{31} + B_{13}B_{32}B_{21} > 0, \end{aligned}$$

where the sum is over all $(i, j, k) \in \{1, 2, 3\}^3$ such that $(i, j) \neq (2, 1)$, $(i, k) \neq (3, 1)$, and $(j, k) \neq (3, 2)$. Finally, we have

$$b_2b_1 - b_0 \geq 2 \sum_{i,j,k=1}^3 B_{1i}B_{2j}B_{3k} - B_{12}B_{23}B_{31} - B_{13}B_{32}B_{21} \geq \sum_{i,j,k=1}^3 B_{1i}B_{2j}B_{3k} > 0$$

for $u \in \mathbb{R}_+^3$, finishing the proof. \square

For instance, the matrix

$$A(u) = \begin{pmatrix} u_3 & 0 & u_1 \\ u_2 & u_1 & 0 \\ 0 & u_3 & u_2 \end{pmatrix}$$

satisfies the conditions of Lemma 21 with $(i, j, k) = (1, 2, 3)$. Note that the detailed-balance condition is *not* satisfied for this matrix, but Lemma 21 states that it is normally elliptic. It is an open question whether (1) with this diffusion matrix has an entropy structure.

Volume-filling models. We show the normal ellipticity of the diffusion matrix (5) associated to the volume-filling models in a special case.

Lemma 22. *Let $A(u)$ be defined by*

$$A_{ij}(u) = \delta_{ij}p_i(u_i)q_i(u_0) + u_i p_i(u_i) q_i'(u_0) + \delta_{ij} u_i q_i(u_0) \frac{\partial p_i}{\partial u_i}(u_i), \quad i, j = 1, \dots, n,$$

for $i = 1, \dots, n$, $u \in \mathcal{D} = \{u \in \mathbb{R}_+^n : \sum_{i=1}^n u_i < 1\}$, and we recall that $u_0 = 1 - \sum_{i=1}^n u_i$. We assume that p_i , q_i , and q_i' are positive functions. Then $A(u)$ is normally elliptic (and diagonalizable).

Proof. Since we can write

$$A_{ij}(u) = (\delta_{ij} u_i p_i q_i) \left(\delta_{ij} \left(\frac{1}{u_i} + \frac{p_i'}{p_i} \right) + \frac{q_i'}{q_i} \right),$$

we can decompose $A(u) = A_1 A_2$, where

$$(A_1)_{ij} = \delta_{ij} u_i p_i q_i \left(\prod_{k \neq i} \frac{q'_k}{q_k} \right)^{-1}, \quad (A_2)_{ij} = \delta_{ij} \left(\frac{1}{u_i} + \frac{p'_i}{p_i} \right) \prod_{k \neq i} \frac{q'_k}{q_k} + \prod_{k=1}^n \frac{q'_k}{q_k}.$$

Setting $V := \prod_{k=1}^n q'_k/q_k$ and $R_i := (1/u_i + p'_i/p_i) \prod_{k \neq i} q'_k/q_k$, the matrix A_2 becomes

$$A_2 = \begin{pmatrix} R_1 + V & V & \cdots & V \\ V & R_2 + V & & V \\ \vdots & & \ddots & \\ V & V & & R_n + V \end{pmatrix}.$$

This matrix is symmetric positive definite since the leading principle minors are positive,

$$\prod_{k=1}^i R_k \left(1 + V \sum_{k=1}^i \frac{1}{R_k} \right) > 0, \quad i = 1, \dots, n$$

(or since $z^\top A_2 z = \sum_{i=1}^n R_i z_i^2 + (\sum_{i=1}^n z_i)^2 V > 0$ for $z \neq 0$). We infer from Proposition 6 that $A(u)$ is normally elliptic and diagonalizable. \square

Fluid mixture model governed by partial pressure gradients. The diffusion matrix $A(u)$ of the fluid mixture model (6) is given by $A_{ij}(u) = u_i \partial p_i / \partial u_j$. We consider the case of linear pressures, $p_i(u) = \sum_{j=1}^n a_{ij} u_j$ with $a_{ij} \geq 0$. Then $A_{ij}(u) = u_i a_{ij}$, and $A(u)$ can be decomposed according to $A(u) = A_1 A_2$ with $A_1 = \text{diag}(u_1, \dots, u_n)$ and $A_2 = (a_{ij})$. The matrix A_1 is clearly symmetric positive definite. Thus, $A(u)$ is normally elliptic if (a_{ij}) is positive definite (but not necessarily symmetric).

This condition is sufficient but not necessary. Indeed, if $n = 2$ and $a_{ij} \geq 0$, $A(u)$ is normally elliptic in \mathcal{D} if and only if $\det A_2 = a_{11} a_{22} - a_{12} a_{21} > 0$, and in this case, the eigenvalues of $A(u)$ are positive. On the other hand, (a_{ij}) is positive definite if and only if $\det A_2 > \frac{1}{4}(a_{12} - a_{21})^2$, which is more restrictive than $\det A_2 > 0$ except if A_2 is symmetric.

8. CONNECTIONS AND EXTENSIONS

More general cross-diffusion systems. Amann [2, Section 4] considered a more general class of cross-diffusion equations:

$$(13) \quad \partial_t u_i = \sum_{j=1}^n \sum_{k,\ell=1}^d \frac{\partial}{\partial x_k} \left(A_{ij}^{k\ell}(u) \frac{\partial u_j}{\partial x_\ell} \right), \quad i = 1, \dots, n.$$

These equations reduce to (1) if $A_{ij}^{k\ell}(u) = \delta_{k\ell} A_{ij}(u)$. Amann calls the differential operator on the right-hand side normally elliptic if all the eigenvalues of its principal part $A_\pi(u, z)$ have positive real parts, where

$$A_\pi(u, z) = \sum_{k,\ell=1}^d A^{k\ell}(u) z_k z_\ell, \quad u \in \mathcal{D}, \quad z \in \mathbb{R}^n.$$

If $A_{ij}^{k\ell}(u) = \delta_{k\ell}A_{ij}(u)$, this coincides with our definition. We say that (13) has an entropy structure if there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that

$$(14) \quad \sum_{k,\ell=1}^d h''(u)A^{k\ell}(u)z_kz_\ell$$

is positive definite for all $u \in \mathcal{D}$, $z \in \mathbb{R}^n$. Our results can be extended in a straightforward way to this situation. For instance, if $A_\pi(u, z)$ is normally elliptic and there exists a strictly convex function $h \in C^2(\mathcal{D})$ such that $h''(u)A^{k\ell}(u)$ is symmetric for all $u \in \mathcal{D}$ and $k, \ell = 1, \dots, d$ then (13) has an entropy structure. This follows from the fact that $A_\pi(u, z) = A_1A_2$, where $A_1 = h''(u)^{-1}$ is symmetric positive definite and $A_2 = \sum_{k,\ell=1}^d h''(u)A^{k\ell}(u)z_kz_\ell$ is symmetric. So, the claim follows from Proposition 3 (ii).

Symmetrization by Kawashima and Shizuta. The entropy structure of (13) has been explored by Kawashima and Shizuta [21], also including first-order terms. They call $h \in C^2(\mathcal{D})$ an entropy for (13) if h is strictly convex, the Onsager matrix $A^{k\ell}(u)h''(u)^{-1}$ is symmetric, and (14) is symmetric positive semidefinite for all $u \in \mathcal{D}$ and $k, \ell = 1, \dots, d$. In our situation, this is equivalent to the symmetry and positive semidefiniteness of $h''(u)A(u)$. It is shown in [21] that if an entropy exists then system (13) can be symmetrized in the sense that it can be written as

$$(15) \quad \partial_t u_i(w) = \sum_{j,k,\ell=1}^n \frac{\partial}{\partial x_j} \left(B_{ij}^{k\ell}(w) \frac{\partial u_j}{\partial x_\ell} \right), \quad i = 1, \dots, n,$$

where $B^{k\ell}(w) = A^{k\ell}(u(w))u'(w)$ is symmetric positive semidefinite and $u(w) := (h')^{-1}(w)$. Conversely, if there exists a diffeomorphism $w \mapsto u(w)$ such that the Jacobian $(\partial w_i / \partial u_j)$ is symmetric and $B^{k\ell}(w)$ is symmetric positive semidefinite then there exists an entropy. Indeed, by Poincaré's lemma for closed differential forms and the symmetry $\partial w_i / \partial u_j = \partial w_j / \partial u_i$, there exists a function g such that $\partial g / \partial w_i = w_i$. Then $h(u) = u \cdot w(u) - g(w(u))$ is an entropy for (13).

In the presence of first-order terms, we obtain hyperbolic-parabolic balance laws:

$$\partial_t u_i + \sum_{j=1}^d \frac{\partial f_{ij}}{\partial x_j}(u) = \sum_{j=1}^n \sum_{k,\ell=1}^d \frac{\partial}{\partial x_k} \left(A_{ij}^{k\ell}(u) \frac{\partial u_j}{\partial x_\ell} \right),$$

and the existence of an entropy requires the additional condition $h'(u)f'_j(u) = q'_j(u)$ for some real-valued smooth functions q_j , where $f_j = (f_{1j}, \dots, f_{nj})$ and $j = 1, \dots, d$. The first-order terms do not modify the entropy production. We refer to [21, Theorem 2.1] for details. Such systems have been also studied in [26], including rank deficient Onsager matrices. The extension of our results to such situations is a future work. An example are Maxwell–Stefan systems whose diffusion matrix has rank $n - 1$; see [4, 20]. The symmetrizability property of the Euler equations was first observed by Gudonov and later by Friedrichs and Lax and extended by Boillat to general hyperbolic systems; see, e.g., [3]. Note that our definition of entropy does not need the symmetry of the Onsager matrix; see Case 1.1 in Section 3.

Gradient-flow structure. The entropy structure of (1) is strongly related to the gradient-flow formulation of Mielke and co-workers [24, 25]. Let M be a manifold, $H : M \rightarrow \mathbb{R}$ be differentiable, and $K(u) : T_u^*M \rightarrow T_uM$ be symmetric positive definite for all $u \in M$, where T_uM is the tangent space at $u \in M$ and T_u^*M its cotangent space. Physically, elements of T_uM are the thermodynamic fluxes and elements of T_u^*M are the driving forces (here: entropy variables). Then Mielke et al. call a solution $u : [0, T] \rightarrow M$ to

$$\partial_t u = -K(u)H'(u), \quad t > 0,$$

a gradient flow. The positive definiteness of $K(u)$ implies that

$$\frac{dH}{dt} = \langle H'(u), \partial_t u \rangle = -\langle H'(u), K(u)H'(u) \rangle \leq 0,$$

and we can interpret H as an entropy. Here, $\langle \cdot, \cdot \rangle$ is the dual pairing between T_u^*M and T_uM . In the special case $K(u) = -\operatorname{div}(B(w(u))\nabla(\cdot))$ and identifying $H'(u)$ with $h'(u)$, we recover (1) since $K(u)H'(u) = \operatorname{div}(B(w(u))\nabla h'(u)) = \operatorname{div}(A(u)\nabla u)$, where $B(w(u)) = A(u)h''(u)^{-1}$. Note that the mapping $\xi \mapsto K(u)\xi$ is linear. This framework was generalized to nonlinear mappings $\xi \mapsto K(u, \xi)\xi$ in [25]. Physically, this means that the thermodynamics fluxes depend nonlinearly on the driving forces. Then the gradient-flow equation reads as

$$\partial_t u = \partial_\xi \Psi(u, -H'(u)), \quad t > 0,$$

where $\Psi^* : TM \rightarrow \mathbb{R}$ is convex in its second argument and $\partial_\xi \Psi^*$ is the partial derivative with respect to the second argument. This equation is by Legendre–Fenchel theory equivalent to

$$\Psi(u, \partial_t u) + \Psi^*(u, -H'(u)) + \langle H'(u), u \rangle = 0.$$

An example is $\Psi^*(u, \xi) = \frac{1}{2}\langle \xi, K(u)\xi \rangle$. The function $H(u)$ is an entropy in the sense

$$\frac{dH}{dt} = \langle H'(u), \partial_t u \rangle = -\Psi(u, \partial_t u) - \Psi^*(u, -H'(u)) \leq 0,$$

since $\Psi \geq 0$ and $\Psi^* \geq 0$ (see [25] for details). It is an open question to what extent the results of this paper can be extended to this case.

REFERENCES

- [1] H. Amann. Dynamic theory of quasilinear parabolic equations. II. Reaction-diffusion systems. *Diff. Int. Eqs.* 3 (1990), 13–75.
- [2] H. Amann. Nonhomogeneous linear and quasilinear elliptic and parabolic boundary value problems. In: H.J. Schmeisser and H. Triebel (editors), *Function Spaces, Differential Operators and Nonlinear Analysis*, pp. 9–126. Teubner, Stuttgart, 1993.
- [3] G. Boillat, C. Dafermos, P. Lax, and T.-P. Liu. *Recent Mathematical Methods in Nonlinear Wave Propagation*. Lect. Notes Math. 1640. Springer, Berlin, 1996.
- [4] D. Bothe. On the Maxwell–Stefan equations to multicomponent diffusion. In: J. Escher et al. (eds.), *Parabolic Problems. Progress in Nonlinear Differential Equations and their Applications*, pp. 81–93. Springer, Basel, 2011.
- [5] A. Bosch. Note on the factorization of a square matrix into two Hermitian or symmetric matrices. *SIAM Review* 29 (1987), 463–468.

- [6] V. Calvez and L. Corrias. The parabolic-parabolic Keller–Segel model in \mathbb{R}^2 . *Commun. Math. Sci.* 6 (2008), 417–447.
- [7] D. Carlson and H. Schneider. Inertia theorems for matrices: the semi-definite case. *J. Math. Anal. Appl.* 6 (1963), 430–446.
- [8] L. Chen, E. Daus, and A. Jüngel. Rigorous mean-field limits and cross-diffusion. *Z. Angew. Math. Phys.* 70 (2019), no. 122, 21 pages.
- [9] X. Chen, E. Daus, and A. Jüngel. Global existence analysis of cross-diffusion population systems for multiple species. *Arch. Ration. Mech. Anal.* 227 (2018), 715–747.
- [10] L. Corrias, B. Perthame, and H. Zaag. Global solutions of some chemotaxis and angiogenesis systems in high space dimensions. *Milan J. Math.* 72 (2004), 1–28.
- [11] L. Desvillettes, T. Lepoutre, A. Moussa, and A. Trescases. On the entropic structure of reaction-cross diffusion systems. *Commun. Partial Diff. Eqs.* 40 (2015), 1705–1747.
- [12] F. R. Gantmacher. *The Theory of Matrices*. Volume 2. Chelsea Publishing Company, New York, 1959.
- [13] B. Hall. *Lie Groups, Lie Algebras, and Representations*. Second edition. Springer, Cham, 2015.
- [14] S. Hittmeir and A. Jüngel. Cross diffusion preventing blow up in the two-dimensional Keller–Segel model. *SIAM J. Math. Anal.* 43 (2011), 997–1022.
- [15] R. Horn and C. Johnson. *Topics in Matrix Analysis*. First edition. Cambridge University Press, Cambridge, 1991.
- [16] R. Horn and C. Johnson. *Matrix Analysis*. Second edition. Cambridge University Press, Cambridge, 2013.
- [17] A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. *Nonlinearity* 28 (2015), 1963–2001.
- [18] A. Jüngel. *Entropy Methods for Diffusive Partial Differential Equations*. SpringerBriefs in Mathematics, Springer, 2016.
- [19] A. Jüngel. Cross-diffusion systems with entropy structure. In: K. Mikula, D. Ševčovič, and J. Urbán (eds.). *Proceedings of Equadiff 2017 Conference*, Spektrum Stu Publishing, Bratislava, 2017, pp. 181–190.
- [20] A. Jüngel and I. Stelzer. Existence analysis of Maxwell–Stefan systems for multicomponent mixtures. *SIAM J. Math. Anal.* 45 (2013), 2421–2440.
- [21] S. Kawashima and Y. Shizuta. On the normal form of the symmetric hyperbolic-parabolic systems associated with the conservation laws. *Tohoku Math. J.* 40 (1988), 449–464.
- [22] T. Lepoutre and A. Moussa. Entropic structure and duality for multiple species cross-diffusion systems. *Nonlin. Anal.* 159 (2017), 298–315.
- [23] L.-Z. Lu and C. E. M. Pearce. Some new bounds for singular values and eigenvalues of matrix products. *Ann. Oper. Research* 98 (2000), 141–148.
- [24] M. Liero and A. Mielke. Gradient structures and geodesic convexity for reaction-diffusion systems. *Phil. Trans. Royal Soc. A.* 371 (2005), 20120346, 28 pages, 2013.
- [25] A. Mielke, M. Peletier, and D. Renger. A generalization of Onsager’s reciprocity relations to gradient flows with nonlinear mobility. *J. Non-Equil. Thermodyn.* 41 (2016), 141–149.
- [26] D. Serre. The structure of dissipative viscous system of conservation laws. *Physica D* 239 (2000), 1381–1386.
- [27] N. Shigesada, K. Kawasaki, and E. Teramoto. Spatial segregation of interacting species. *J. Theor. Biol.* 79 (1979), 83–99.
- [28] N. Zamponi and A. Jüngel. Analysis of degenerate cross-diffusion population models with volume filling. *Ann. Inst. H. Poincaré – Anal. non lin.* 34 (2017), 1–29. (Erratum: 34 (2017), 789–792.)

SCHOOL OF MATHEMATICS (ZHUHAI), SUN YAT-SEN UNIVERSITY, ZHUHAI 519082, GUANGDONG PROVINCE, CHINA

E-mail address: `buptxchen@yahoo.com`

INSTITUTE FOR ANALYSIS AND SCIENTIFIC COMPUTING, VIENNA UNIVERSITY OF TECHNOLOGY, WIEDNER HAUPTSTRASSE 8-10, 1040 WIEN, AUSTRIA

E-mail address: `juengel@tuwien.ac.at`