Cross-diffusion systems with entropy structure

Lecture Notes

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CHAPTER 1

Introduction

1.1. What are cross-diffusion systems?

Diffusion is a physical process that models many real-life situations from natural sciences, economics, data science, and social sciences. A particle or substance or individual undergoing diffusion spreads out from a location at which there is a higher concentration of that particle or substance or individual. Although diffusion is considered to be an equilibrating process, it may lead to counterintuitive phenomena. For instance, constant equilibria that are stable in ordinary differential equations may become unstable if spatial diffusion is added (Turing instability [24]). This is not necessarily a negative effect: It gives rise to pattern formation in reaction-diffusion equations, modeling, for instance, spatio-temporal periodic structures in chemical reactions, wind pattern formed in sand, or pattern on animal skins.

The situation is more complex for systems of diffusion equations. First, substances in multicomponent systems may flow in the direction of lower concentrations due to the influence of the other substances. This phenomenon is called *uphill diffusion*. The first experimental evidence of uphill diffusion in fluids dates back to Hartley [13], followed by experiments on solids by Darken [6]. This phenomenon can be understood as a result of the competition between the density gradients of each component. We refer to the review [16] for more details. Second, a species may segregate completely from another species. Particle segregation may appear due to different particle sizes in sheared granular mixtures [10, 12] or in hyperbolic–parabolic diffusion systems from population dynamics [3, 4].

Both phenomena – uphill diffusion and segregation – typically occur in the presence of cross diffusion. Cross diffusion refers to the phenomenon in which a flux of one fluid component is induced by the gradient of another component. The experimental investigation of binary mixtures started already in 1850 [11], while cross terms in multicomponent models were suggested in 1932 [19]. The experiment of Duncan and Toor [7] has shown that standard diffusion is not able to describe the experimental results, and cross diffusion needs to be taken into account.

Cross-diffusion systems are generally quasilinear parabolic equations of the form

$$\partial_t u_i - \sum_{j=1}^n \sum_{k,\ell=1}^d \frac{\partial}{\partial x_k}\left(A_{ij}^{k\ell}(x,u)\frac{\partial u_j}{\partial x_\ell}\right) = r_i(u) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{1.1}$$

describing the dynamics of, for instance, the densities or concentrations $u_i(x,t)$ of the ith component of a mixture in a bunded domain $\Omega \subset \mathbb{R}^d$ ($d \geq 1$). Here, $u = (u_1,\ldots,u_n)$ is the density vector, $A_{ij}^{k\ell}(u)$ are the diffusion coefficients, and $r_i(u)$ are reaction terms. Cross-diffusion equations may also be of elliptic type, but we consider only the parabolic case in this book. We

impose the initial conditions

$$u_i(x,0) = u_i^0(x) \quad \text{for } x \in \Omega,\ i = 1,\ldots,n, \tag{1.2}$$

and the boundary conditions can be of Dirichlet, Neumann, mixed Dirichlet–Neumann, Robin, or no-flux type. For simplicity, we consider the no-flux conditions

$$\sum_{j=1}^n \sum_{k,\ell=1}^d \nu_k A_{ij}^{k\ell}(x,u)\frac{\partial u_j}{\partial x_\ell} = 0 \quad \text{on } \partial\Omega,\ t > 0,\ i = 1,\ldots,n, \tag{1.3}$$

where $\nu = (\nu_1,\ldots,\nu_d)$ is the exterior unit normal vector to the boundary $\partial\Omega$. This corresponds to the situation that the mixture cannot leave the domain Ω. When mixed Dirichlet–Neumann boundary conditions are prescribed, the particle densities are fixed at the Dirichlet boundary, while the remaining Neumann boundary models isolating boundary parts.

In many applications, the diffusion coefficients $A_{ij}^{k\ell}(x,u)$ simplify to $A_{ij}^{k\ell}(x,u) = A_{ij}(u)\delta_{k\ell}$, where $\delta_{k\ell}$ denotes the Kronecker symbol. In this book, (almost) only this case is considered. Then the initial-boundary value problem (1.1)–(1.3) reduces to

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j\right) = r_i(u), \quad \text{in } \Omega,\ t > 0,\ i = 1,\ldots,n, \tag{1.4}$$

$$u_i(\cdot,0) = u_i^0 \quad \text{in } \Omega, \quad \sum_{j=1}^n A_{ij}(u)\nabla u_j \cdot \nu = 0 \quad \text{on } \partial\Omega,\ t > 0. \tag{1.5}$$

It is convenient to write equations (1.4) more compactly in vector form:

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = r(u),$$

where $A(u) = (A_{ij}(u))_{i,j=1,\ldots,n}$ and $r(u) = (r_i(u))_{i=1,\ldots,n}$.

The mathematical analysis of cross-diffusion systems is very delicate. First, the very useful maximum principle cannot generally be applied to diffusion systems such that the proof of $L^\infty(\Omega)$ bounds for the solutions is not clear. Second, there does not exist a regularity theory like for scalar parabolic equations, and solutions may develop singularities in finite time [21].

To ensure the solvability of problem (1.4)–(1.5), we need some notion of parabolicity. Uniform positive definiteness of the diffusion matrix $A(u)$ is in principle sufficient to conclude at least local-in-time solvability. Unfortunately, many cross-diffusion systems arising in applications have a diffusion matrix that is neither symmetric nor positive definite. In fact, this is not needed: Amann has shown [1] that *normal ellipticity*of the associated elliptic operator is sufficient, meaning that the real parts of the eigenvalues of $A(u)$ are positive. This condition only ensures *local* solvability, and some regularity conditions on the solutions (basically Hölder continuity) are required to conclude *global* solvability. However, this regularity property is generally very difficult to prove. This motivates us to consider only a subclass of cross-diffusion systems, namely those that possess a certain structure inherited from the underlying thermodynamic model. It turns out that such a structure is provided by the free energy or entropy. It leads to a priori estimates that are the key step to prove global solvability. For this reason, we analyze the class of *cross-diffusion systems with entropy structure*.

1.2. What is an entropy structure?

As mentioned in the previous subsection, additional conditions need to be imposed on cross-diffusion systems to ensure global solvability. We claim that such a condition (plus possibly additional assumptions) is provided by the entropy structure. In this subsection, we detail this notion and explain relations to thermodynamics and hyperbolic conservation laws.

We assume that there exists a strictly convex functional

$$\mathcal{H}(u) = \int_\Omega h(u)\mathrm{d}x$$

for suitable functions $u : \Omega \times (0,T) \to \mathcal{D}$, where $\mathcal{D} \subset \mathbb{R}^n$ is an open set, such that equations (1.4) can be written in gradient-flow form with a positive definite diffusion matrix. More precisely, we suppose that (1.4) can be written as

$$\partial_t u - \operatorname{div}\big(B(u)\nabla h'(u)\big) = r(u) \quad \text{in } \Omega,\ t>0, \tag{1.6}$$

where $B(u) \in \mathbb{R}^{n\times n}$ is a positive definite matrix for all $u \in \mathcal{D}$ and h' is the derivative of h. This formulation is related to a gradient-flow structure in the sense that (1.6) can be written in operator form as

$$\partial_t u + K(u)\mathrm{D}\mathcal{H}(u) = r(u), \quad t>0,$$

where $K(u)\xi = -\operatorname{div}(B(u)\nabla\xi)$ is the so-called *Onsager operator* and $\mathrm{D}\mathcal{H}(u)$ is the variational derivative of $\mathcal{H}$ at u (which can be identified with $h'(u)$ by the Riesz representation theorem). Gradient flows can be defined in Hilbert spaces and even in metric spaces [2, 17]. We do not define this notion here, since we only need the algebraic structure expressed in (1.6). Introducing the *entropy variable* $w := h'(u)$, we can formulate (1.6) also as

$$\partial_t u - \operatorname{div}(B(u)\nabla w) = r(u), \quad B(u) = A(u)h''(u)^{-1}. \tag{1.7}$$

Here, $h'' : \mathcal{D} \to \mathbb{R}^{n\times n}$ is the Hessian matrix of h and the new unknown $w = w(x,t)$ is a vector-valued function. The set $\mathcal{D}$ may equal $(0,\infty)^n$ in the case of densities or be a subset of $(0,1)^n$ in the case of mass fractions. In formulation (1.6), we interpret u as a function of w by means of $u(w) := (h')^{-1}(w)$. (We suppose that the inverses of h' and h'' exist.) The matrix $B(u)$ is called the *mobility matrix* or *Onsager matrix*. Then (1.7) is understood as an evolution equation in the variable w, and the density vector $u = u(w)$ is computed a posteriori.

Definition 1.1 (Entropy structure)**.** *If there exists a strictly convex functional $h(u)$, called the entropy density, such that $B(u) = A(u)h''(u)^{-1}$ is positive definite for all $u \in \mathcal{D}$, we call equations (1.4) a cross-diffusion system with entropy structure.*

We stress the fact that we do *not* suppose the positive definiteness on $\overline{\mathcal{D}}$, since in many applications, the matrix $B(u)$ is only positive semidefinite on this set. As the positive definiteness may fail on $\partial\mathcal{D}$, our definition of entropy structure includes degenerate and singular equations; see Chapter 2 for examples. In particular, standard parabolic theory cannot be applied to such situations.

The functional $\mathcal{H}(u) = \int_\Omega h(u)\mathrm{d}x$ is called an entropy, since it corresponds to the physical entropy (up to the sign) in nonequilibrium thermodynamics; see Remark 1.4.

The entropy structure has two important consequences. First, if $r(u) = 0$, it implies that the entropy $t \mapsto \mathcal{H}(u(t))$ is decreasing along trajectories of (1.7):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(u) = -\int_\Omega \nabla u^T h''(u) A(u) \nabla u \mathrm{d}x = -\int_\Omega \nabla w^T B(u) \nabla w \mathrm{d}x \le 0,$$

where we used the no-flux boundary conditions. This justifies in some sense the notion of gradient flow. Second, the entropy structure leads to $L^\infty(\Omega)$ bounds if the inverse of h (if it exists) has a bounded codomain. Indeed, let $\mathcal{D} \subset \mathbb{R}^n$ be a bounded open set and let $h' : \mathcal{D} \to \mathbb{R}^n$ be invertible. Furthermore, let w be a solution to (1.7). Then the values of the function $u(x,t) := u(w(x,t)) = (h')^{-1}(u(x,t))$ lie in the bounded set $\mathcal{D}$. Thus, the solution u to (1.6) is automatically bounded, without the use of any maximum principle. Clearly, since we did not specify the solution spaces, this statement is only formal here.

Example 1.2 (Bounded solutions)**.** An example for a function satisfying the previous properties is given by

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + u_0(\log u_0 - 1) \quad \text{with} \quad u_0 = 1 - \sum_{i=1}^n u_i,$$

defined on the open simplex

$$\mathcal{D} = \left\{ u = (u_1, \dots, u_n) \in \mathbb{R}^n : u_i > 0 \text{ for all } i, \ \sum_{i=1}^n u_i < 1 \right\}.$$

The function $h(u)$ corresponds to the Boltzmann–Shannon entropy density for a mixture with mass fractions $u_1, \dots, u_n$ and the solvent fraction u_0. The entropy variables are

$$w_i = \frac{\partial h}{\partial u_i} = \log \frac{u_i}{u_0}, \quad i = 1, \dots, n. \tag{1.8}$$

The Hessian $H := h''(u)$ has the entries $H_{ij} = \delta_{ij}/u_i + 1/u_0$, and its inverse H^{-1} has the coefficients $\delta_{ij}u_i - u_i u_j$ for $i, j = 1, \dots, n$. Relations (1.8) can be inverted:

$$u_i(w) = \frac{\exp w_i}{1 + \sum_{j=1}^n \exp w_j}, \quad i = 1, \dots, n,$$

showing that $u_i(w) > 0$, $\sum_{i=1}^n u_i(w) < 1$, and consequently $u(w) \in \mathcal{D}$ for any $w \in \mathbb{R}^n$. Applications which can be described by cross-diffusion systems with this entropy structure are detailed in Chapter 2. The solutions for these models are bounded. □

Example 1.3 (Degenerate and singular systems)**.** The dynamics of two population species can be described by cross-diffusion systems (1.4) with the diffusion matrix

$$A(u) = \begin{pmatrix} a_{10} + (s+1)a_{11}u_1^s + a_{12}u_2^s & s a_{12} u_1 u_2^{s-1} \\ s a_{21} u_1^{s-1} u_2 & a_{20} + (s+1)a_{22}u_2^s + a_{21}u_1^s \end{pmatrix},$$

where $a_{i0} > 0$, $a_{ij} \ge 0$ for $i, j = 1, 2$, and $s > 1$. We choose the entropy density

$$h(u) = \frac{1}{s(s-1)}(a_{21}u_1^s + a_{12}u_2^s) \quad \text{for } u = (u_1, u_2) \in \mathcal{D} = (0, \infty)^2.$$

Then the matrix $B(u) = A(u)h''(u)^{-1}$ is symmetric. Under the conditions $\min\{a_{11}/a_{21}, a_{22}/a_{12}\} \geq s/(s+1)$, a computation shows that, for $z \in \mathbb{R}^2$,

$$z^T B(u)z \geq \frac{a_{10}}{a_{21}} u_1^{2-s} z_1^2 + \frac{a_{20}}{a_{12}} u_2^{2-s} z_2^2 + s(u_1 z_1 + u_2 z_2)^2.$$

This shows that the matrix $B(u)$ is positive definite on $\mathcal{D}$, but not uniformly in u and only positive semidefinite on $\overline{\mathcal{D}}$ if $1 < s < 2$. In fact, we may interpret equations (1.7) as degenerate in this case and singular at $u_1 = 0$ or $u_2 = 0$ if $s > 2$.

The novelty of the entropy approach is that we can handle nonstandard *degenerate* or *singular* diffusion (see Chapter 2) and that we obtain in some cases *bounded* weak solutions. In fact, the assumption that the domain $\mathcal{D}$ is bounded, can be relaxed. For instance, the entropy density $h(u) = \sum_{i=1}^n u_i(\log u_i - 1)$ is defined on $\mathcal{D} = (0,\infty)^n$. Then the entropy variables are $w_i = \log u_i$ with inverse $u_i = \exp(w_i) > 0$. This yields nonnegative solutions, but they may have no upper bound.

Remark 1.4 (Relation to thermodynamics)**.** The transformation of cross-diffusion systems to the form (1.6) is not surprising from a thermodynamic viewpoint, and the entropy variables are related to the chemical potentials. To make this statement more specific, consider an isothermal ideal gas mixture consisting of $n+1$ components with partial mass (or volume) fractions $u_0, \ldots, u_n$. By definition, the total mass fraction is constant, $\sum_{i=0}^n u_i = 1$. Let the Helmholtz free energy F be given. The chemical potential μ_i of the ith species is defined in thermodynamics as the partial derivative $\mu_i = \partial F/\partial u_i$. Actually, the free energy density F equals $F = U - \theta S$, where U is the internal energy density, θ is the temperature of the mixture, and η is the physical entropy. As the mixture is assumed to be ideal and isothermal, the internal energy is constant. Thus, normalizing the temperature to one, $\theta = 1$, the chemical potential becomes $\mu_i = -\partial\eta/\partial u_i$. Since $u_0 = 1 - \sum_{i=1}^n u_i$, we introduce the mathematical entropy density as a function of $u_1, \ldots, u_n$:

$$h(u) = -\eta\left(1 - \sum_{i=1}^n u_i, u_1, \ldots, u_n\right), \quad \text{where } u = (u_1, \ldots, u_n).$$

With this notation, the entropy variables become

$$w_i = \frac{\partial h}{\partial u_i} = -\frac{\partial \eta}{\partial h_i} + \frac{\partial \eta}{\partial u_0} = \mu_i - \mu_0, \quad i = 1, \ldots, n.$$

These relations relate entropy variables and chemical potentials. The entropy of ideal gas mixtures equals $\eta = -\sum_{i=0}^n u_i(\log u_i - 1)$ such that the chemical potentials become $\mu_i = \log u_i$. Then

$$w_i = \log\frac{u_i}{u_0}, \quad i = 1, \ldots, n,$$

which corresponds to (1.8). This transformation of variables is well known in thermodynamics; see, e.g., [9].

Observe that the mathematical and physical entropy differ by the sign. The reason is that the physical entropy is always nondecreasing in thermodynamics, by the second law of thermodynamics, while it is preferred in mathematics to work with a nonincreasing quantity, the mathematical entropy, which is nonincreasing along the corresponding trajectories. □

1.3. When do cross-diffusion systems have an entropy structure?

The question how to determine the entropy structure for a given cross-diffusion system, if it exists, is delicate. Often, the entropy is related to the free energy of the system if it has a thermodynamic origin, which may be used as a mathematical entropy. In this section, we only show some properties which may help to understand whether an entropy structure exists.

Necessary conditions for an entropy structure can be determined from matrix factorization theory. We proceed as in [5] and consider cross-diffusion systems of the type

$$\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j\right) \quad \text{in } \Omega,\ t>0, \tag{1.9}$$

where $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain. An important result that relates the entropy structure to Amann's normal ellipticity is as follows. Let $\mathcal{D} \subset \mathbb{R}^n$ be any open set. We recall that equations (1.9) have 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 $u \in \mathcal{D}$.

Theorem 1.5. *Let $A(u) \in \mathbb{R}^{n\times n}$ be defined for $u \in \mathcal{D}$. If (1.9) has an entropy structure then the operator $u \mapsto \operatorname{div}(A(u)\nabla u)$, defined for suitable functions u, is normally elliptic. If $A(u)$ is a constant matrix, the existence of an entropy structure and the normal ellipticity are equivalent.*

Before we prove the theorem, we comment this result. If there is an eigenvalue of $A(u)$ with a negative real part, the operator $u \mapsto \operatorname{div}(A(u)\nabla u)$ is not normally elliptic. In this case, we cannot expect any entropy structure. The proof of Theorem 1.5 is based on matrix factorization theory (and Lyapunov's theorem on matrix equations). We only state the results and refer to [5, Sec. 2] for the proof and references therein.

We say that a matrix $A(u)$ is *positively stable* if the real part of any eigenvalue of $A(u)$ is positive, and we say that $A(u)$ is *positive definite* if its symmetric part $A(u) + A(u)^T$ is positive definite. If $A(u)$ is positively stable, the operator $u \mapsto \operatorname{div}(A(u)\nabla u)$ is normally elliptic by definition.

Proposition 1.6 (Matrix factorization)**.** *Let $A \in \mathbb{R}^{n\times n}$ be a matrix.*

(i) *The matrix A is positively stable if and only if there exist a symmetric positive definite matrix A_1 and a positive definite matrix A_2 such that $A = A_1A_2$ (or $A = A_2A_1$).*
(ii) *The matrix A is positively stable and diagonalizable if and only if it is the product of two symmetric positive definite matrices.*
(iii) *If A is positively stable and $A = A_1A_2$ or $A = A_2A_1$ with A_1 being symmetric positive definite and A_2 being symmetric, then A_2 is also positive definite.*

Proof of Theorem 1.5. For fixed $u \in \mathcal{D}$, we factorize $A(u) = A_1A_2$, where $A_1 = h''(u)^{-1}$ and $A_2 = h''(u)A(u)$. Let equations (1.9) have an entropy structure, i.e., A_2 is positive definite. Since $h(u)$ is strictly convex, A_1 is symmetric positive definite, and Proposition 1.6 (i) implies that $A(u)$ is positively stable. Next, let $A = A(u)$ be constant and positively stable. By Proposition 1.6 (i) again, there exist a symmetric positive definite matrix A_1 and a positive definite matrix A_2 such that $A = A_1A_2$. Defining the entropy density $h(u) = \frac{1}{2}u^TA_1^{-1}u$, we

infer that $h''(u)A = A_1^{-1}A = A_2$ is positive definite and thus, equations (1.9) have an entropy structure. □

The matrix $H := A_1^{-1}$ appearing in the entropy density $h(u) = \frac{1}{2}u^THu$ for constant and positively stable matrices A can be constructed explicitly, namely $H = \int_0^\infty \mathrm{e}^{-A^Tt}\mathrm{e}^{-At}\mathrm{d}t$ [14, Problem 9, Sec. 2.2].

The symmetry of the mobility matrix is a natural condition for irreversible thermodynamic processes. Interestingly, the symmetry of the mobility matrix implies its positive definiteness (but not vice versa as there exist counterexamples).

Proposition 1.7. *If $A(u) \in \mathbb{R}^{n\times n}$ is positively stable for all $u \in \mathcal{D} \subset \mathbb{R}^n$ 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 equations (1.9) have an entropy structure. Moreover, if equations (1.9) have 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. For fixed $u \in \mathcal{D}$, we again factorize $A(u) = A_1A_2$, where $A_1 = h''(u)^{-1}$ and $A_2 = h''(u)A(u)$. By assumption, A_1 is symmetric positive definite and A_2 is symmetric. Proposition 1.6 (iii) shows that A_2 is positive definite, proving the first claim. Next, let A_2 be symmetric positive definite. We infer from Proposition 1.6 (ii) that $A(u)$ is positively stable and diagonalizable, which implies that $A(u)$ has only positive eigenvalues. □

Theorem 1.5 states that if $A = A(u)$ is a constant positively stable matrix, then equations (1.9) have an entropy structure. This statement is stable under bounded perturbations.

Proposition 1.8. *Let $A_0 \in \mathbb{R}^{n\times n}$ be positively stable and let $A(u) = A_0 + \varepsilon A_*(u)$, where $A_*(u)$ is a bounded matrix in $\mathcal{D}$ and $\varepsilon > 0$. Then there exists $\varepsilon_0 > 0$ such that equations (1.9) have an entropy structure for all $0 < \varepsilon < \varepsilon_0$.*

Proof. By Proposition 1.6 (i), we can factorize $A_0 = A_1A_2$ with a symmetric positive definite matrix A_1 and a positive definite matrix A_2. Then $H := A_1^{-1}$ is symmetric positive definite and $HA_0 = A_2$ is positive definite. Thus, there exists $\lambda > 0$ such that $z^THA_0z \ge \lambda|z|^2$ for all $z \in \mathbb{R}^n$. Since $A_*(u)$ is bounded, there exists $M > 0$ such that $\|HA_*(u)\| \le M$ for all $u \in \mathcal{D}$ for some (submultiplicative) matrix norm. Let $h(u) = \frac{1}{2}u^THu$. We infer that $z^Th''(u)A(u)z = z^T(HA_0 + \varepsilon HA_*(u))z \ge (\lambda - \varepsilon M)|z|^2$. The claim follows after choosing $\varepsilon_0 := \lambda/(2M)$. □

Example 1.9 (Fluid mixture models)**.** We consider the equations

$$\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n D_{ij}(u)\nabla p_j(u)\right), \quad i = 1,\ldots,n, \tag{1.10}$$

together with initial and no-flux boundary conditions. Here, u_i is the density of the ith fluid component, p_i is the ith partial pressure, and $D_{ij}(u)$ are diffusion coefficients. This model describes a fluid micture that is driven by all the partial pressures. If $D_{ij}(u) = \delta_{ij}u_i$, we recover the model discussed in detail in Section 2.1.2. We assume that (the symmetric part of) $(D_{ij}(u))$

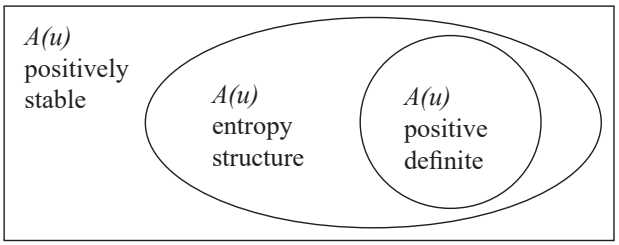

FIGURE 1. Cross-diffusion systems with an entropy structure form a subset of all systems with a positively stable diffusion matrix $A(u)$.

is positive semidefinite and that p_i satisfies the symmetry condition

$$\frac{\partial p_i}{\partial u_j}(u) = \frac{\partial p_j}{\partial u_i}(u) \quad \text{for all } i \neq j,\ u \in \mathcal{D}. \tag{1.11}$$

Furthermore, we suppose that $\mathcal{D} \subset (0,\infty)^n$ is star-shaped. Since $(p_1,\ldots,p_n)$ defines a curl-free vector field on the star-shaped set $\mathcal{D}$ in the sense of (1.11), it is conservative, by the Poincaré lemma for closed differential forms. This means that there exists $h \in C^2(\mathcal{D})$ such that $\partial h/\partial u_i = p_i$ for $i = 1,\ldots,n$. This shows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h(u)\mathrm{d}x = \sum_{i=1}^n \int_\Omega \partial_t u_i p_i(u)\mathrm{d}x = -\int_\Omega \sum_{i,j=1}^n D_{ij}(u)\nabla p_j(u)\cdot\nabla p_i(u)\mathrm{d}x \le 0,$$

since $(D_{ij}(u))$ is assumed to be positive semidefinite. Hence, $u \mapsto \int_\Omega h(u)\mathrm{d}x$ is an entropy along solutions to (1.10). □

We can illustrate the sets of matrices, which are positively stable, or which induce an entropy structure, or which are positive definite, in Figure 1. If $A(u)$ is positively stable, the Lyapunov theorem [14, Theorem 2.2.1] implies the existence of a symmetric positive definite matrix $H(u) \in \mathbb{R}^{n\times n}$ such that $H(u)A(u) + A(u)^T H(u) = 2I$, where I is the unit matrix. This means that $\frac{1}{2}(H(u)A(u) + A(u)^T H(u))$ is symmetric positive definite and consequently, $H(u)A(u)$ is positive definite. If $H(u)$ is induced by the Hessian of a function $h \in C^2(\mathcal{D})$, $H(u) = h''(u)$ for $u \in \mathcal{D}$, we obtain an entropy structure, and $A(u)$ is positively stable. If $H(u)$ is the unit matrix, $A(u)$ is positive definite. The entropy structure is given by the quadratic entropy density $h(u) = \frac{1}{2}|u|^2$. The determination of an entropy, if is exists, for a given cross-diffusion system is a delicate issue and a general strategy is missing.

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CHAPTER 2

Examples from physics and biology

Many applications in physics, chemistry, and biology describe systems with multiple components like gas mixtures, competing population species, and reacting chemical substances. Therefore, it is natural to model the multicomponent applications on the macroscopic level by reaction-diffusion equations with cross-diffusion terms. In this chapter, we give some examples from the literature showing the variety of applications.

Generally, the cross-diffusion systems under consideration are of the type

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j + D_i(u)\nabla\Phi\right) = r_i(u) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{2.1}$$

where $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain, $u_i = u_i(x,t)$ are representing particle densities, mass concentrations, or mass fractions of the ith component, $A_{ij}(u)$ are the diffusion coefficients, $D_i(u)$ is the drift term, $\Phi : \Omega \to \mathbb{R}$ is a (e.g. electric or environmental) potential, and $r_i(u)$ is the reaction rate. The initial conditions are given by $u_i(0) = u_i^0$ in Ω. To simplify the presentation and the computations, we generally impose the no-flux boundary conditions

$$\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j + D_i(u)\nabla\Phi\right)\cdot\nu = 0 \quad \text{on } \partial\Omega,\ i=1,\ldots,n,$$

where ν denotes the exterior unit normal vector to $\partial\Omega$, which is assumed to exist. Setting $A(u) = (A_{ij}(u))_{i,j=1}^n$, $D(u) = (D_i(u))_{i=1}^n$, and $r(u) = (r_i(u))_{i=1}^n$, we can write equation (2.1) in compact form as

$$\partial_t u - \operatorname{div}(A(u)\nabla u + D(u)\nabla\Phi) = r(u) \quad \text{in } \Omega,\ t>0.$$

We present in the following some examples of cross-diffusion systems.

2.1. Population dynamics

2.1.1. Shigesada–Kawasaki–Teramoto model. The possibly best known cross-diffusion system is the population model suggested by Shigesada, Kawasaki, and Teramoto in [103], called the SKT model. The authors assume that two population species prefer the same environment but avoid the other species, which means that they have the tendency to segregate from each other. The evolution of the densities of the population species u_1 and u_2 is given by (2.1) with $n = 2$ and the diffusion matrix

$$A(u) = \begin{pmatrix} a_{10} + 2a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + 2a_{22}u_2 \end{pmatrix}, \tag{2.2}$$

where $u = (u_1, u_2)$, a_{ij} are nonnegative parameters, and the drift vector has the components $D_i(u) = u_i$. The parameters a_{12} and a_{21} are called *cross-diffusion coefficients*, and a_{11} and a_{22} are the *self-diffusion coefficients*, since the diffusivity $a_{ii}u_i$ ($i = 1, 2$) depends on the density itself. Observe that without linear diffusion, $a_{10} = a_{20} = 0$, equations (2.1) with (2.2) are of degenerate type since they contain the diffusion $\operatorname{div}(2a_{ii}u_i\nabla u_i)$, which vanishes if $u_i = 0$. This corresponds to a porous-medium equation with quadratic nonlinearity. The potential Φ models areas where the environmental conditions are more or less favorable. The reaction terms are of Lotka–Volterra type:

$$r_i(u) = u_i(b_{i0} - b_{i1}u_1 - b_{i2}u_2), \quad i = 1, 2,$$

with $b_{ij} \geq 0$. For nonnegative functions u_i, these terms grow at most linearly and are quasi-positive, i.e. for all $(u_1, \ldots, u_n) \in \mathbb{R}^n_+ := [0, \infty)^n$,

$$r_i(u_1, \ldots, u_{i-1}, 0, u_{i+1}, \ldots, u_n) \geq 0.$$

The above model (without drift and reaction) can be derived from an on-lattice model in the diffusion limit (Example 3.3) or from moderately interacting particle systems in the mean-field limit.

The matrix $A(u)$ is generally neither symmetric nor positive definite, but it has positive eigenvalues. This means that the associated differential operator is normally elliptic, which is a minimal condition for local solvability. By the minimum principle, the densities u_i are nonnegative (use $u_i^- = \min\{0, u_i\}$ as a test function in (2.1) and exploit the quasi-positivity of r_i). However, the derivation of a priori estimates is delicate. Therefore, the global existence of solutions under general assumptions was an open problem for some decades.

The first global existence result seems to be due to Kim [84], who considered the one-dimensional case, neglected self-diffusion ($a_{11} = a_{22} = 0$) and assumed equal coefficients ($a_{ij} = 1$). Deuring [42] generalized this result to any space dimension and allowing for $a_{10} \neq a_{20}$, but with sufficiently small cross-diffusion parameters a_{12} and a_{21}. Again some years later, Yagi [109] proved an existence theorem under the assumption that the diffusion matrix is positive definite ($a_{12} < 8a_{11}$, $a_{21} < 8a_{22}$, and $a_{12} = a_{21}$). The tridiagonal case was investigated by several authors. Amann [1] proved local solvability in two space dimensions and global solvability if the local solution is bounded in a Hölder norm. Lou, Ni, and Wu [91] were able to show the existence of global solutions in $C^0([0, \infty); W^{1,p}(\Omega))$ for $p > 2$ in the two-dimensional case. More recently, Desvillettes and Trescases [41] revisited the triangular system with general reaction terms (possibly being nonquadratic).

Major progress was made by Amann [1]. He reduced the question whether a local solution exists globally in time to the problem of finding a priori estimates in the $W^{1,p}(\Omega)$ norm with $p > d$. Unfortunately, the derivation of such a bound is difficult. The first global existence result without any restriction on the diffusion coefficients a_{ij} (except positivity) was achieved in [52] in one space dimension and in [30, 31] in several space dimensions.

From a biological viewpoint, model (2.1)–(2.2) has some interesting properties. For instance, under certain conditions on the parameters, there exist nonconstant steady states, which represents pattern formation. It turns out that large diffusion coefficients a_{10}, a_{20} tend to eliminate any pattern, while large cross-diffusion coefficents a_{12}, a_{21} help to create pattern. The interplay

between diffusion and cross-diffusion was explored in detail by, e.g., Lou and Ni [90]. We also refer to the review [95].

Equations (2.1) with (2.2) can be formulated as

$$\partial_t u_i - \Delta(u_i p_i(u)) = r_i(u), \quad p_i(u) = a_{i0} + \sum_{k=1}^2 a_{ik}u_k.$$

This formulation allows one to derive higher-integrability bounds by means of the so-called duality method [39]. Furthermore, it motivates the following generalization of the SKT model to an arbitrary number $n \in \mathbb{N}$ of species:

$$\partial_t u_i - \Delta(u_i p_i(u)) = r_i(u), \quad p_i(u) = a_{i0} + \sum_{k=1}^n a_{ik}u_k. \tag{2.3}$$

The associated diffusion matrix has the entries

$$A_{ij}(u) = \delta_{ij}\left(a_{i0} + \sum_{k=1}^n a_{ik}u_k\right) + a_{ij}u_i, \quad i,j = 1,\ldots,n. \tag{2.4}$$

A global existence result was proved in [107] assuming that $A(u)$ is positive definite. Without this condition, the analysis of (2.3) for $n \geq 3$ is much more involved than the two-species case. The existence of local solutions follows from [2]; the delicate point is the global solvability.

It was shown in [33, Theorem 1] that there exists a global weak solution to (2.3) (with initial and no-flux boundary conditions) under the *detailed-balance condition*: There exist $\pi_1,\ldots,\pi_n > 0$ such that

$$\pi_i a_{ij} = \pi_j a_{ji} \quad \text{for all } i,j = 1,\ldots,n. \tag{2.5}$$

If $n = 2$, this condition is always fulfilled with, for instance, $\pi_1 = a_{21}$ and $\pi_2 = a_{21}$. However, it does not hold if, for instance,

$$A(u) = \begin{pmatrix} 0 & 0 & a_{13}u_3 \\ a_{21}u_1 & 0 & 0 \\ 0 & a_{32}u_2 & 0 \end{pmatrix}.$$

Condition (2.5) is *sufficient* but *not necessary* for global solvability of the SKT system. Global existence can also be shown if self-diffusion dominates cross-diffusion in a certain sense; see [33, Theorem 1] and [36, Theorem 1].

The key of the existence analysis is the entropy structure of (2.1)–(2.2). Indeed, let

$$h_B(u) = \sum_{i=1}^n \pi_i u_i(\log u_i - 1) \quad \text{for } u \in \mathbb{R}^n_+ \tag{2.6}$$

be the modified Boltzmann–Shannon entropy density, where the numbers $\pi_i > 0$ are defined in (2.5).

Lemma 2.1. *Let u be a smooth solution to (2.4) with no-flux boundary conditions and $r_i \equiv 0$ for $i = 1, \ldots, n$. Then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h_B(u)\mathrm{d}x + 4\sum_{i=1}^n \int_\Omega \pi_i p_i(u)|\nabla\sqrt{u_i}|^2\mathrm{d}x + \sum_{i,j=1}^n \int_\Omega \pi_i a_{ij}\nabla u_i\cdot\nabla u_j\mathrm{d}x = 0. \tag{2.7}$$

If the detailed-balance condition (2.5) holds, the matrix $(\pi_i a_{ij})_{ij}$ is positive definite, and the last term on the left-hand side is nonnegative, yielding $L^2(\Omega)$ bounds for ∇u_i.

Proof. We compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h_B(u)\mathrm{d}x &= \sum_{i=1}^n\int_\Omega \pi_i\partial_t u_i\log u_i\mathrm{d}x = -\sum_{i=1}^n\int_\Omega \pi_i(p_i(u)\nabla u_i + u_i\nabla p_i(u))\cdot\nabla\log u_i\mathrm{d}x \\ &= -\sum_{i=1}^n\int_\Omega \pi_i p_i(u)\frac{|\nabla u_i|^2}{u_i}\mathrm{d}x - \sum_{i=1}^n\int_\Omega \pi_i\nabla p_i(u)\cdot\nabla u_i\mathrm{d}x,\end{aligned}$$

and inserting the definition of $p_i(u)$ gives the entropy equality. If the detailed-balance condition holds, the matrix $(\pi_i a_{ij})$ is symmetric. Thus, we can decompose $A = (a_{ij}) = A_1A_2$, where $A_1 = \mathrm{diag}(\pi_i^{-1})$ is symmetric positive definite and $A_2 = (\pi_i a_{ij})$ is symmetric. By Proposition 1.6 (iii), A_2 is positive definite. □

The previous lemma provides $H^1(\Omega)$ bounds for $\sqrt{u_i}$ if $a_{i0} > 0$ and $H^1(\Omega)$ bounds for u_i if (2.5) holds. These estimates are the key for the global existence analysis. Here, the detailed-balance condition (2.5) is crucial. In fact, it has a further consequence: Property (2.5) is equivalent to the symmetry of the mobility matrix $B := A(u)h''(u)^{-1}$ [33, Prop. 19]. Then equations (2.1) write as

$$\partial_t u - \mathrm{div}(B\nabla w) = r(u), \quad w = h'(u) \quad \text{in } \Omega,\ t > 0,$$

where w is the entropy variable (see Remark 1.4). The equivalence of the symmetry of B and the detailed-balance condition is not surprising, since (2.5) means that $(\pi_1, \ldots, \pi_n)$ is a reversible measure of the Markov chain associated to (a_{ij}). In fact, time-reversibility of a thermodynamic system is equivalent to the symmetry of the so-called Onsager or mobility matrix B, so symmetry and reversibility are related mathematically and thermodynamically.

Remark 2.2 (Potential terms)**.** Originally, the SKT model included drift terms taking into account the influence of the given environmental potential Φ:

$$\partial_t u_i - \mathrm{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j + \mu_i u_i\nabla\Phi\right) = r_i(u), \quad i = 1, \ldots, n,$$

where $\mu_i > 0$ are so-called mobility constants. The article [33] only analyzed the SKT model with $\Phi = $ const. However, the analysis also works with nonconstant potentials. Indeed, to compute the entropy inequality (2.7), we use $\pi_i\log u_i$ as a test function in the evolution equation, and considering the drift term yields, after integrating by parts,

$$-\sum_{i=1}^n\int_\Omega \mu_i\pi_i u_i\nabla\Phi\cdot\nabla\log u_i\mathrm{d}x = \sum_{i=1}^n\int_\Omega \mu_i\pi_i u_i\Delta\Phi\mathrm{d}x - \sum_{i=1}^n\int_{\partial\Omega}\mu_i\pi_i u_i\nabla\Psi\cdot\nu\mathrm{d}s.$$

If $\Delta\Phi \in L^\infty(\Omega)$ and $\nabla\Psi\cdot\nu \ge 0$ on $\partial\Omega$, the right-hand side can be bounded from above by the entropy density (2.6), and we obtain the entropy inequality (2.7) on any finite time interval $(0,T)$, with a different constant on the right-hand side (depending on T), after applying a Gronwall argument. □

Remark 2.3 (Nonlinear functions $p_i(u)$)**.** In the literature, nonlinear functions $p_i(u)$ have been suggested, often using power-law nonlinearities [33, 40, 86],

$$p_i(u) = a_{i0} + \sum_{k=1}^n a_{ik}u_k^{s_k}, \quad \text{where } s_k > 0. \tag{2.8}$$

The exponents s_k do not necessarily have a biological interpretation but they can be used as fitting parameters to match experimental results [58]. The entropy structure for (2.3) with (2.8) is different compared to the affine functions $p_i(u)$. We define the entropy density

$$h(u) = \sum_{i=1}^n \frac{\pi_i u_i^s}{s(s-1)}, \quad u \in \mathbb{R}^n_+,$$

where we have set $s = s_k$ for all k to simplify. Assume that $\pi_i a_{ij} = \pi_j a_{ji}$ for all $i \ne j$ and for some $\pi_i > 0$. A computation shows that (see [33, Sec. 2] for a proof)

$$\text{if } 0 < s \le 1: \qquad z^T h''(u)A(u)z \ge \sum_{i=1}^n \pi_i(a_{i0} + (s+1)a_{ii}u_i^s)u_i^{s-2}z_i^2,$$

$$\text{if } s > 1: \qquad z^T h''(u)A(u)z \ge \sum_{i=1}^n \pi_i a_{i0}u_i^{s-2}z_i^2 + (s+1)\sum_{i=1}^n \eta_i\pi_i u_i^{2s-2}z_i^2,$$

where

$$\eta_i := a_{ii} - \frac{s}{2(s+2)}\sum_{j=1}^n \left(\sqrt{a_{ij}} - \sqrt{a_{ji}}\right)^2.$$

Thus, if $\eta_i \ge 0$, the matrix $h''(u)A(u)$ or equivalently $B = A(u)h''(u)^{-1}$ is positive definite on $(0,\infty)^n$. □

Remark 2.4 (Detailed balance and symmetry)**.** We may replace the detailed-balance condition (2.5) by the assumption that the matrix (a_{ij}) is symmetric. Indeed, transforming to the variables $v_i := \pi_i u_i$, we write (2.3) with $r_i = 0$ as

$$\partial_t v_i = \Delta(v_i\widetilde{p}_i(v)), \quad \widetilde{p}_i(v) = a_{i0} + \sum_{k=1}^n \frac{a_{ik}}{\pi_k}v_k,$$

and (2.5) means that the transformed matrix (a_{ik}/π_k) is symmetric. Thus, without loss of generality, we may assume that (a_{ij}) is symmetric. □

2.1.2. Generalized Busenberg–Travis model. The evolution of the ith species is driven in the SKT model by the diffusion coefficients $a_{ij}u_i$ and $p_i(u)$. As diffusion counteracts segregation and the SKT model is supposed to describe segregation, one may ask whether a model with less diffusion better describes the segregation behavior. This motivates us to drop the last term in the SKT model,

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

and to consider instead the population model

$$\partial_t u_i = \operatorname{div}(u_i\nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij}u_j \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{2.9}$$

together with initial and no-flux boundary conditions. This model, for functions p_i only depending on the sum $\sum_{j=1}^n u_j$, has been first suggested by Busenberg and Travis [24] in epidemiological modelling. Gurtin and Pipkin [62] have considered populations that disperse to avoid crowding by setting $p_i = k_i\sum_{j=1}^n u_j$, where k_i are some positive constants. This is a special case of equations (2.9) with $a_{ij} = k_i$. Models with general coefficients a_{ij} and two species were analyzed in [53] assuming positive definiteness for $(a_{ij}) \in \mathbb{R}^{2\times 2}$.

Model (2.9) can be derived from interacting particle systems in the many-particle limit [53] (the single case $n = 1$ is analyzed in [25]). A proof for multiple species, assuming moderate interactions and using a mean-field approach, can be found in [29].

There is some reason to believe that model (2.9) better describes the dynamics of segregating populations than the SKT model. First, it is the mean-field limit of a natural interacting particle system, where the coefficients a_{ij} measure the strength of the interaction potentials; see [29]. Also the SKT model is the mean-field limit of an interacting particle system, but requiring that the interaction potentials are part of the diffusion and not of the drift, which seems less natural [28].

Second, we may interpret (2.9) as a conservation law of the density of the ith species, where the partial velocity is given by $v_i := -\nabla p_i(u)$ [62]. Interpreting $p_i(u)$ as the pressure of the ith species, equation $v_i = -\nabla p_i(u)$ expresses Darcy's law. Thus, equations (2.9) have a thermodynamic interpretation. Third, under detailed balance, the SKT model possesses an entropy structure via the Boltzmann–Shannon entropy, while equations (2.9) allow for *two* entropies: the Boltzmann–Shannon entropy and the so-called Rao entropy, which measures the functional diversity of the species [98].

We detail the last statement. Recall the modified Boltzmann–Shannon entropy h_B, defined in (2.6), and the Rao entropy

$$h_R(u) = \frac{1}{2}\sum_{i,j=1}^n \pi_i a_{ij}u_i u_j \quad \text{for } u \in \mathbb{R}^n_+.$$

Assuming the detailed-balance condition (2.5) and computing along solutions to (2.9) yields [78, 81]

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h_B(u)\mathrm{d}x + \sum_{i,j=1}^n \int_\Omega \pi_i a_{ij}\nabla u_i\cdot\nabla u_j \mathrm{d}x = 0, \tag{2.10}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h_R(u)\mathrm{d}x + \sum_{i=1}^n \int_\Omega \pi_i u_i |\nabla p_i(u)|^2 \mathrm{d}x = 0. \tag{2.11}$$

Let the matrix (a_{ij}) be positively stable (i.e., all eigenvalues have a positive real part). The proof of Lemma 2.1 reveals that $(\pi_i a_{ij})$ is positive definite. Hence, identities (2.10) and (2.11) yield $H^1(\Omega)$ bounds for u_i and the regularity $\sqrt{u_i}\nabla p_i(u) \in L^2(\Omega)$. These estimates are the key for the existence analysis [78, Theorem 17]. We remark that an earlier existence result for $n = 2$ species was proved in [54].

The numerical results in [28, Sec. 7], performed on the level of the associated particle systems, indicate that the densities of (2.9) show a much clearer componentwise segregation behavior than those of the SKT model (2.3).

Interestingly, complete segregation (in the sense that the supports of the densities do not intersect) happens if the determinant of the matrix (a_{ij}) vanishes. Bertsch et al. seem to be the first who analyzed such a situation in [9] for the two-species system,

$$\partial_t u_i = \mathrm{div}(u_i\nabla p_i(u)), \quad p_i(u) = u_1 + u_2 \quad \text{in } \Omega,\ t > 0,\ i = 1, 2, \tag{2.12}$$

where $a > 0$. The one-dimensional situation of [9] was generalized to multiple space dimensions in [10]. The authors of [9] proved that if the initial data are segregated ($u_1(0)u_2(0) = 0$ in Ω) then the solutions are segregated for all time ($u_1(t)u_2(t) = 0$ in Ω for all $t > 0$). This behavior appears to be counterintuitive for parabolic systems, but in fact, (2.12) is a hyperbolic–parabolic system. This can be seen by introducing the change of variables

$$v_1 = u_1 + u_2, \quad v_2 = \frac{u_1}{u_1 + u_2}. \tag{2.13}$$

If (u_1, u_2) solves (2.12), then (v_1, v_2) is a solution to

$$\partial_t v_1 = \frac{1}{2}\Delta(v_1^2), \quad \partial_t v_2 - \nabla v_1 \cdot \nabla v_2 = 0 \quad \text{in } \Omega.$$

The first equation is the (parabolic) porous-medium equation with quadratic nonlinearity, while the second one is a (hyperbolic) transport equation. Using regularity theory for the porous-medium equation, Bertsch et al. [10] argued that the velocity field $-\nabla v_1$ is Hölder continuous and has a certain Sobolev regularity, which allows one to use DiPerna's and Lions' theory of renormalized solutions of transport equations for v_2 [43].

A discrete-time gradient-flow approach was suggested in [85, Theorem 1.1], where it is shown, in one space dimension and assuming complete segregation of the initial data, that the time-discrete solutions to a minimizing movement scheme converge to a (completely segregated) weak solution to (2.12). The existence of weak solutions of bounded variation for general initial data was shown in [26] by using a variational splitting scheme and optimal transport methods. The loss of regularity due to the hyperbolic character indicates that regularity better than bounded variation cannot be expected.

Another idea is to replace Darcy's law $v = -\nabla p_i(u) = -\nabla(u_1 + u_2)$ (here v is the fluid velocity) by Brinkman's law [21, (5)]

$$\partial_t u_i = \mathrm{div}(u_i\nabla w), \quad -\varepsilon\Delta w + w = -(u_1 + u_2) \quad \text{in } \Omega,\ t > 0.$$

The parameter $\varepsilon > 0$ can be interpreted as a viscosity, which is a way to represent friction between the particles. In the limit $\varepsilon \to 0$, we revover (2.12). The (inviscid) limit $\varepsilon \to 0$ was proved in [37, Theorem 1.3].

System (2.12) has been generalized in various directions. Assuming that the pressure is given as in fluid dynamics by $p(u) = \bar{u}^\gamma$, where $\bar{u} = u_1 + u_2$ is the total mass density and $\gamma > 2 - 4/d$, the existence of global weak solutions was proved in [63] (even with suitable reaction terms). A more general approach was studied in [74] via the duality $\bar{u}p(u) = g(\bar{u}) + g^*(\bar{u})$, where g is a convex function and g^* its convex dual.

The two-species model (2.12) can be generalized to n species by considering (2.9), i.e.

$$\partial_t u_i = \operatorname{div}(u_i p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j \quad \text{in } \Omega,\ t > 0,\ i = 1, \ldots, n, \tag{2.14}$$

but now assuming that the matrix (a_{ij}) has not full rank. The rank-one case is special in the sense that it provides a thermodynamical interpretation. Indeed, if $a_{ij} = a_j > 0$ for $i = 1, \ldots, n$, the function $p_i(u)$ is independent of the index i and may again be interpreted as the pressure of the mixture. It is shown in [48] that there exists a unique classical solution to (2.14) on the torus $\Omega = \mathbb{T}^d$ satisfying the initial conditions $u_i(0) = u_i^0$ in Ω. Equations (2.14) with pressures that depend nonlinearly on the density vector were analyzed in [47]. The idea is to transform equations (2.14) to a nonlinear parabolic equation and a symmetrizable hyperbolic system.

If the rank of the matrix is larger than one, $r := \operatorname{rank}(a_{ij}) \in \{1, \ldots, n-1\}$, we can transform (2.14) again to a symmetric hyperbolic–parabolic system, consisting of r parabolic equations and $n - r$ hyperbolic equations. Using an energy approach, such systems admit a unique local classical solution provided the initial data is sufficiently smooth and positive [48]. For integrable initial data, the existence of dissipative measure-valued solutions was shown in [67].

2.2. Fluid mixtures

The dynamics of gaseous mixtures can be described by the so-called Maxwell–Stefan equations, which model the diffusive transport of the components of the mixture. Applications arise in many fields like sedimentation, dialysis, respiratory airways, electrolysis, and chemical reactors [108]. We introduce this model by first assuming that the partial mass fractions $u_i(x,t)$ of the mixture are driven by the balance equations

$$\partial_t u_i + \operatorname{div}(u_i v + J_i) = r_i(u) \quad \text{in } \Omega,\ t > 0,\ i = 0, \ldots, n, \tag{2.15}$$

where v is the barycentric velocity, $J_i = u_i v_i$ are the partial fluxes with the partial velocities v_i, and r_i the reaction rates. We choose the initial and boundary conditions

$$u_i(0) = u_i^0 \quad \text{in } \Omega, \quad J_i \cdot \nu = 0 \quad \text{on } \partial\Omega,\ i = 0, \ldots, n.$$

To derive the Maxwell–Stefan equations, we impose four assumptions:

(1) The barycentric velocity $v := \bar{u}^{-1} \sum_{i=0}^n u_i v_i$ with the total mass fraction $\bar{u} = \sum_{i=0}^n u_i$ vanishes, $v = 0$, i.e., the mixture is not moving globally.
(2) The total reaction rate is zero, which means that no particles are created, $\sum_{i=0}^n r_i = 0$.
(3) The initial total mass fraction is constant, $\sum_{i=0}^n u_i^0 = 1$ in Ω.

(4) Spatial variations of the mass fractions arise from differences of the partial velocities,

$$\nabla u_i = -\sum_{j=0}^n d_{ij} u_i u_j (v_i - v_j), \quad i = 1, \ldots, n,$$

where $d_{ij} = d_{ji}$ are positive diffusion coefficients.

The first assumption implies that the total flux vanishes, $\sum_{i=0}^n J_i = 0$. Then, in view of the second assumption, the sum of (2.15) leads to the total mass conservation equation $\partial_t \bar{u} = -\operatorname{div}(\bar{u} v) = 0$. Thus, the total mass fraction $\bar{u}$ is constant in time and, because of the third assumption, equal to one, $\sum_{0=1}^n u_i = 1$ in Ω for all time. Finally, the fourth assumption shows that the dynamics of the partial mass fractions is given by

$$\partial_t u_i + \operatorname{div} J_i = r_i(u), \quad \nabla u_i = -\sum_{j=0}^n d_{ij}(u_j J_i - u_i J_j) \quad \text{in } \Omega,\ t > 0,\ i = 0, \ldots, n. \tag{2.16}$$

In this formulation, the fluxes are not explicitly given as linear combinations of the density gradients, but the density gradients are linear combination of the fluxes; we call this the Maxwell–Stefan formulation. If the fluxes are linear combinations of the density gradients, we call this the Fick–Onsager formulation. Both formulations are in fact equivalent in the sense detailed in [16].

Equations (2.16) are called the Maxwell–Stefan model. They were suggested in 1866 by James Maxwell [93] for dilute gases and in 1871 by Joseph Stefan [105] for fluids. In contrast to Fick's law, which predicts a linear dependence between ∇u_i and J_i, the flux J_i in the Maxwell–Stefan approach also depends on the gradients ∇u_j for $j \neq i$. This model is able to predict uphill diffusion (reverse diffusion in the direction of the gradient) or osmotic diffusion (diffusion with vanishing gradient) in multicomponent mixtures, which have been demonstrated experimentally by Duncan and Toor [49]. These phenomena can in principle be modeled by using the theory of nonequilibrium thermodynamics, where the fluxes are assumed to be linear combinations of the thermodynamic forces [38, Chap. 4]. However, this approach requires the knowledge of all binary diffusion coefficients, which are not always easy to determine, and the positive semidefiniteness of the diffusion matrix. The advantage of the Maxwell–Stefan approach is that it can describe uphill diffusion effects without assuming particular properties on the diffusivities (besides symmetry).

The Maxwell–Stefan equations can be derived from the multi-species Boltzmann equation in the diffusive approximation; see [19] for a formal derivation and [12, 20] for rigorous results. Another derivation starts from Euler equations with friction terms, and the high-friction limit rigorously gives the Maxwell–Stefan equations in the Fick–Onsager formulation [71]. The three-species Maxwell–Stefan model was obtained as a hydrodynamic limit of locally interacting Brownian motions in [101]. A formal derivation from thermodynamical principles can be found in [14, Sec. 14].

The existence of local-in-time solutions to the Maxwell–Stefan equations was shown in [13, 60, 64], while the existence of global-in-time weak solutions can be found in [80].

2.2.1. Fick–Onsager formulation. In the following, we explain how the Maxwell–Stefan equations can be written as a cross-diffusion system of the Fick–Onsager form (2.1). For this, we

need to invert the gradient–flux relation in (2.16). Let the matrix $D(u) = (D_{ij}(u))$ be given by

$$D_{ii}(u) = \sum_{j=0,\, j\neq i}^{n} d_{ij}u_j, \quad D_{ij}(u) = -d_{ij}\sqrt{u_i u_j} \quad \text{if } i \neq j,$$

for $i, j = 0, \dots, n$. Then the gradient–flux relation in (2.16) becomes

$$2\nabla\sqrt{u_i} = -\sum_{j=0}^{n} D_{ij}(u)\frac{J_j}{\sqrt{u_j}}, \quad i = 0, \dots, n. \tag{2.17}$$

This system has to be solved under the constraint $\sum_{i=0}^n J_i = 0$. Since (d_{ij}) is symmetric by assumption, we deduce from

$$0 = \sum_{i,j=1}^{n} D_{ij}(u)z_j = \sum_{j\neq i}^{n} d_{ij}u_j z_i - \sum_{j\neq i}^{n} d_{ij}\sqrt{u_i u_j}z_j = \sum_{j\neq i}^{n} d_{ij}\sqrt{u_j}(\sqrt{u_j}z_i - \sqrt{u_i}z_j)$$

that $z_i/\sqrt{u_i} = z_j/\sqrt{u_j}$ for all $i \neq j$ and hence $z_i = \sqrt{u_i}$ and $\ker D(u) = \operatorname{span}\{\sqrt{u}\}$, where $\sqrt{u} := (\sqrt{u_1}, \dots, \sqrt{u_n}\}$. Thus, $D(u)$ is *not* invertible. However, we can invert this matrix on a subspace.

For this, let $L = \{z \in \mathbb{R}^{n+1} : \sqrt{u} \cdot z = 0\}$ and let P_L and $P_{L^\perp}$ be the projections on L and $L^\perp$, respectively, given by

$$(P_L)_{ij} = \delta_{ij} - \sqrt{u_i u_j}, \quad (P_{L^\perp})_{ij} = \sqrt{u_i u_j} \quad \text{for } i, j = 0, \dots, n. \tag{2.18}$$

Then $\ker D(u) = L^\perp$, so $D(u)$ is invertible on L only. We claim that $D(u)P_L + P_{L^\perp}$ is invertible in $\mathbb{R}^n$.

Lemma 2.5. *Let $D \in \mathbb{R}^{(n+1)\times(n+1)}$ be a matrix satisfying $\ker D = L^\perp$. Then $DP_L + P_{L^\perp}$ is invertible in $\mathbb{R}^{n+1}$.*

Proof. We first show that $\ker(DP_L + P_{L^\perp}) = \ker(DP_L) \cap L$. Let $z \in \ker(DP_L + P_{L^\perp})$. Since $\operatorname{ran} D = L$, we have $DP_L = P_L DP_L$. Thus, if $0 = (DP_L + P_{L^\perp})z = P_L(DP_L z) + P_{L^\perp}z$, then $DP_L z = 0$ and $P_{L^\perp}z = 0$. It follows from $\ker P_{L^\perp} = L$ that $z \in \ker(DP_L) \cap L$. The other inclusion follows in a similar way. Next, we compute the kernel of DP_L. Any $z \in \ker(DP_L)$ satisfies $Dz = DP_{L^\perp}z + DP_L z = DP_L z = 0$ (since $\ker D = L^\perp$). We infer that $\ker(DP_L) = \ker D = L^\perp$. This shows that

$$\ker(DP_L + P_{L^\perp}) = \ker(DP_L) \cap L = L^\perp \cap L = \{0\},$$

and consequently, the matrix $DP_L + P_{L^\perp}$ is invertible. □

The set of solutions to $Dz = b$, $z \in L$ is the same as the set of solutions to $(DP_L + P_{L^\perp})z = b$, since $P_L z = z$ and $P_{L^\perp}z = 0$. Thus, the lemma shows that $z = (DP_L + P_{L^\perp})^{-1}b$ exists if $b \in L$.

The left-hand side of (2.17) satisfies $2\nabla\sqrt{u} \cdot \sqrt{u} = \sum_{i=0}^n \nabla u_i = 0$, so it is an element of L. Therefore, we can invert (2.17) by means of the so-called *Bott–Duffin inverse* [18]

$$D^{BD}(u) := P_L\big(D(u)P_L + P_{L^\perp}\big)^{-1}$$

(which is symmetric since $D(u)$ is symmetric), and

$$\frac{J_i}{\sqrt{u_i}} = -2\sum_{j=1}^n D_{ij}^{BD}(u)\nabla\sqrt{u_j}, \quad i=0,\ldots,n.$$

Giovangigli used in [59, Sec. 7.3.4] the group inverse to invert the gradient–flux relations (2.17). In fact, since the matrix (D_{ij}) is symmetric and $L = \operatorname{ran} D(u)$, the Bott–Duffin inverse and group inverse coincide [102, Lemma 2.2].

Consequently, the equations in (2.16) become

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=0}^n A_{ij}(u)\nabla u_j\right) = r_i(u), \tag{2.19}$$
$$\text{where } A_{ij}(u) = \sqrt{\frac{u_i}{u_j}}D_{ij}^{BD}(u),\ i,j=0,\ldots,n,$$

which corresponds to formulation (2.1) (with $D_i(u)=0$). We call equations (2.19) the Maxwell–Stefan system in Fick–Onsager form.

Example 2.6 (Fick–Onsager formulation for three species)**.** In the case $n=2$, we can invert equations (2.16) explicitly. Indeed, inserting $u_0 = 1-u_1-u_2$ and $J_0 = -J_1-J_2$ into (2.16) for $i=1,2$ and taking into account the symmetry of (d_{ij}), we find that

$$\begin{aligned}\nabla u_1 &= -\big(d_{01}+(d_{12}-d_{01})u_2\big)J_1 + (d_{12}-d_{01})u_1J_2,\\ \nabla u_2 &= (d_{12}-d_{02})u_2J_1 - \big(d_{02}+(d_{12}-d_{02})u_1\big)J_2.\end{aligned}$$

Multiplying the first equation by $d_{02}+(d_{12}-d_{02})u_1$ and the second one by $(d_{12}-d_{01})u_1$ and adding both equations to eliminate J_2 yields

$$\begin{aligned}&\big(d_{02}+(d_{12}-d_{02})u_1\big)\nabla u_1 + (d_{12}-d_{01})u_1\nabla u_2\\ &\quad = -J_1\big(d_{12}d_{01}u_1 + d_{12}d_{02}u_2 + d_{01}d_{02}(1-u_1-u_2)\big).\end{aligned}$$

In a similar way, we can eliminate J_1 to obtain an expression for J_2. Inserting J_1 and J_2 into (2.16) then leads to $\partial_t u - \operatorname{div}(A(u)\nabla u) = r(u)$ with

$$A(u) = \frac{1}{a(u)}\begin{pmatrix} d_{02}+(d_{12}-d_{02})u_1 & (d_{12}-d_{01})u_1\\ (d_{12}-d_{02})u_2 & d_{01}+(d_{12}-d_{01})u_2\end{pmatrix},$$
$$\text{where } a(u) = d_{01}d_{02}(1-u_1-u_2) + d_{01}d_{12}u_1 + d_{02}d_{12}u_2.$$

Notice that $a(u) \ge \min\{d_{01},d_{02},d_{12}\} > 0$. □

2.2.2. Entropy structure. Formulation (2.19) allows us to determine the entropy structure of the Maxwell–Stefan system. Introduce the n-dimensional simplex

$$\mathcal{D} := \left\{u=(u_1,\ldots,u_n)\in(0,1)^n : \sum_{i=1}^n u_i < 1\right\}. \tag{2.20}$$

We assume that

$$\sum_{i=0}^{n} r_i(u)\log u_i \le 0 \quad \text{for all } u\in\mathcal{D}\ u_0 = 1-\sum_{i=1}^{n} u_i. \tag{2.21}$$

Lemma 2.7. *There exists $c>0$, only depending on (d_{ij}), such that for all $u\in\mathbb{R}^{n+1}$ with $\sum_{i=0}^n u_i = 1$ and $z\in\mathbb{R}^{n+1}$ that*

$$z^T D^{BD}(u) z \ge c|P_L z|^2.$$

Proof. By [72, Lemma 4], the eigenvalues of $(D(u)P_L + P_{L^\perp})^{-1}$ are larger than or equal $c>0$, and this constant only depends on (d_{ij}). Moreover, we conclude from $(D(u)P_L + P_{L^\perp})P_{L^\perp} = P_{L^\perp}$ that $P_{L^\perp} = (D(u)P_L + P_{L^\perp})^{-1}P_{L^\perp}$ and hence

$$0 = P_L P_{L^\perp} = P_L(D(u)P_L + P_{L^\perp})^{-1}P_{L^\perp} = D^{BD}(u)P_{L^\perp}.$$

Conequently, $D^{BD}(u) = D^{BD}(u)(P_L + P_{L^\perp}) = D^{BD}(u)P_L$. This implies for all $u\in\mathbb{R}^{n+1}$ with $\sum_{i=0}^n u_i = 1$ and $z\in\mathbb{R}^{n+1}$ that

$$z^T D^{BD}(u) z = z^T P_L(D(u)P_L + P_{L^\perp})^{-1}P_L z \ge c|P_L z|^2,$$

ending the proof. □

Let the Boltzmann–Shannon entropy density be given by

$$h(u) = \sum_{i=1}^{n} u_i(\log u_i - 1) + u_0(\log u_0 - 1) \quad \text{for } u\in\mathcal{D}, \tag{2.22}$$

where $u_0 = 1-\sum_{i=1}^n u_i$. Then, along solutions to (2.19), integrating by parts, and taking into account (2.21),

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h(u)\mathrm{d}x &= \sum_{i=0}^{n}\int_\Omega \log u_i \partial_t u_i \mathrm{d}x \\ &= -4\sum_{i=0}^{n}\int_\Omega D_{ij}^{BD}(u)\nabla\sqrt{u_i}\cdot\nabla\sqrt{u_j}\mathrm{d}x + \sum_{i=0}^{n}\int_\Omega r_i(u)\log u_i \mathrm{d}x \\ &\le -4c\int_\Omega |P_L\nabla\sqrt{u}|^2\mathrm{d}x.\end{aligned} \tag{2.23}$$

First, this shows that $t\mapsto\int_\Omega h(u(t))\mathrm{d}x$ is nonincreasing. In fact, it is sufficient to find an upper bound for this function. This can be achieved under the weaker condition (compared to (2.21))

$$\sum_{i=0}^{n} r_i(u)\log u_i \le C(1+h(u)) \quad \text{for all } u\in\mathcal{D}.$$

Second, the entropy inequality (2.23) provides gradient bounds for $\sqrt{u_i}$ in $L^2(\Omega)$, since

$$|P_L\nabla\sqrt{u}|^2 = \sum_{i=0}^{n}\left|\sum_{j=0}^{n}(\delta_{ij}-\sqrt{u_i u_j})\nabla\sqrt{u_j}\right|^2 = \sum_{i=0}^{n}|\nabla\sqrt{u_i}|^2,$$

where we used the property $\sum_{j=0}^n \sqrt{u_j}\nabla\sqrt{u_j} = \frac{1}{2}\sum_{j=0}^n \nabla u_j = 0$. This implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h(u)\mathrm{d}x + 4c\sum_{i=0}^n |\nabla\sqrt{u_i}|^2\mathrm{d}x \le 0. \tag{2.24}$$

We note that the Maxwell–Stefan equations can also be written in terms of the entropy variables $w_i = \partial h/\partial u_i = \log(u_i/u_0)$:

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n M_{ij}(u)\nabla w_j\right) = r_i(u) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{2.25}$$

where the mobility matrix $M(u) = (M_{ij}(u)) \in \mathbb{R}^{n\times n}$ has the entries $M_{ij}(u) = \sqrt{u_iu_j}D_{ij}^{BD}(u)$. Since the Bott–Duffin inverse is symmetric [72, Lemma 15], the mobility matrix is symmetric too, which expresses Onsager's reciprocal relations. Observe that we have $n+1$ equations (2.19) in the variables $u_0,\ldots,u_n$ (one of which is superfluous) and n equations (2.25) in the variables $w_1,\ldots,w_n$.

The idea is first to find solutions $w = (w_1,\ldots,w_n)$ to (an approximate version of) (2.25) and then to define a posteriori the partial mass fractions $u_i = u_i(w)$ by inverting the relation $w_i = \log(u_i/\sum_{j=1}^n u_j)$ explicitly:

$$u_i = \frac{\exp w_i}{1+\sum_{j=1}^n \exp w_j}, \quad i=1,\ldots,n.$$

Then automatically $u = (u_1,\ldots,u_n) \in \mathcal{D}$ (defined in (2.20)), which proves lower and upper bounds of u_i without the use of an maximum principle. This strategy has been called in [75] the *boundedness-by-entropy method*, since the entropy implies the boundedness of the physical variables.

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CHAPTER 3

Derivation of cross-diffusion equations

Cross-diffusion equations can be derived from basic models by various techniques. In this section, we detail some of these methods, starting from random-walk lattices or kinetic equations. Other approaches include fast-diffusion limits [14], nonlocal-to-local limits [32], and relaxation limits by reaction-diffusion [23] or by elliptic regularization [2], but all of them start from diffusion equations. All derivations in this chapter are formal to highlight the ideas and to simplify the presentation. We will give references in the text for rigorous proofs.

3.1. Derivation from random-walk lattice models

Diffusion can be viewed as the continuum limit of a spatially discrete random walk process for a single species. If several species are involved, we show in this section that generally cross-diffusion terms appear.

3.1.1. Random walk on a lattice. We consider particles distributed over cells in one space dimension. The following arguments can be extended in a straightforward way to multi-dimensional lattices. The particles are allowed to move to one of the neighboring cells with a certain probability. We wish to derive the particle dynamics if the cell size tends to zero.

The lattice consists of cells with midpoints x_j ($j \in \mathbb{Z}$) with a uniform cell size $h = x_j - x_{j-1} > 0$ (see Figure 1). The particle density at time $t > 0$ is denoted by $u(x_j) = u(x_j, t)$, and the function $u(x)$ is supposed to be smooth. We assume that the particles move from cell j to cell $j+1$ with transition rate q and from cell j to cell $j-1$ with transition rate $1-q$. If $q = 1/2$, this corresponds to an unbiased random walk (no direction is preferred), while $q \neq 1/2$ is a biased random walk. In principle, the movement is done in each time step. Then the probability to find a particle at position x_j after N jumps is given by the binomial distribution. We prefer to work with a time-continuous movement, which makes the computations easier. The evolution of the density is given by the so-called *master equation* for a discrete-space random walk on $\mathbb{R}$:

$$\partial_t u(x_j) = qu(x_{j-1}) + (1-q)u(x_{j+1}) - (q + (1-q))u(x_j), \quad j \in \mathbb{Z},\ t > 0,$$

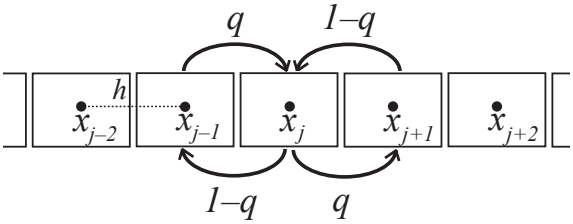

FIGURE 1. Random walk on a one-dimensional lattice.

with the initial condition $u(x_j,0)=u^0(x_j)$. The first two terms represent the gain from incoming particles from cell $j-1$ with transition rate q and from cell $j+1$ with transition rate $1-q$, and the last term describes the loss of particles that move to the neighboring cells $j\pm1$ with transition rates q and $1-q$, respectively.

To perform the limit $h\to 0$, we expand the densities around x_j according to

$$u(x_{j\pm1}) = u(x_j) \pm h\partial_x u(x_j) + \frac{h^2}{2}\partial_x^2 u(x_j) + O(h^3) \tag{3.1}$$

and insert this expansion into the master equation. To simplify the notation, we set $u^j := u(x_j)$. We obtain

$$\begin{aligned}\partial_t u^j &= q\left(u^j - h\partial_x u^j + \frac{h^2}{2}\partial_x^2 u^j\right) + (1-q)\left(u^j + h\partial_x u^j + \frac{h^2}{2}\partial_x^2 u^j\right) + O(h^3) - u^j \\ &= (1-2q)h\partial_x u^j + \frac{h^2}{2}\partial_x^2 u^j + O(h^3).\end{aligned} \tag{3.2}$$

In the naive limit $h\to 0$, the cell size becomes smaller and smaller and the size of the particle jumps tends to zero. Indeed, the limit $h\to 0$ in (3.2) leads to the trivial equation $\partial_t u^j = 0$, i.e., the densities do not change in time. To recover the dynamics in the limit, we consider the evolution on a longer time scale. This means that we change t by t/h^2 and correspondingly ∂_t by $h^2\partial_t$. After division by h^2 in (3.2), the first term on the right-hand side is unbounded when $h\to 0$. Therefore, we require that this term is also of order h^2 and set $(1-2q)h = vh^2$ for some number $v\in\mathbb{R}$. In other words, we choose the transition rate $q = 1/2 - vh/2$, i.e., our random walk is biased but asymptotically unbiased. Then, after dividing equation (3.2) by h^2 and performing the formal limit $h\to 0$ with $u^j = u(x_j)\to u(x)$ gives the diffusion equation

$$\partial_t u(x) = v\partial_x u(x) + \frac{1}{2}\partial_x^2 u(x), \quad x\in\mathbb{R},\ t>0. \tag{3.3}$$

The first term expresses the transport of the particles with velocity v and is a remainder of the slightly biased random walk, while the second term is a linear diffusion with coefficient $1/2$. On a multi-dimensional lattice, the diffusion limit leads to $\partial_t u = v\cdot\nabla u + \frac{1}{2}\Delta u$ in $\mathbb{R}^d$.

We may derive nonlinear diffusion terms if the transition rate depends on $u(x_j)$, $p^j = p(u(x_j))$. The master equation changes in the unbiased case to

$$h^2\partial_t u^j = p^{j-1}u^{j-1} + p^{j+1}u^{j+1} - 2p^j u^j. \tag{3.4}$$

where we included already the diffusion time scale. Here, we need to expand not only $u^{j\pm1}$ around x_j but also $p^{j\pm1}$:

$$\begin{aligned}p^{j\pm1} &= p(u^{j\pm1}) = p(u^j) + \partial_u p^j(u^{j\pm1}-u^j) + \frac{1}{2}\partial_u^2 p^j(u^{j\pm1}-u^j)^2 + \cdots \\ &= p^j \pm h\partial_u p^j\partial_x u^j + \frac{h^2}{2}\partial_u p^j\partial_x^2 u^j + \frac{1}{2}\partial_u^2 p^j(h\partial_x u^j)^2 + O(h^3),\end{aligned}$$

and we used expansion (3.1) in the last step. Next, we insert the previous expansion and (3.1) into the master equation. It turns out that the terms of order $O(1)$ and $O(h)$ cancel, and we end

up with

$$h^2\partial_t u = h^2 u^j\big(\partial_u p^j \partial_x^2 u^j + \partial_u^2 p^j (\partial_x u^j)^2\big) + 2\partial_u p^j (\partial_x u^j)^2 + p^j \partial_x^2 u^j + O(h^3).$$

We divide this equation by h^2 and perform the formal limit $h \to 0$:

$$\begin{aligned}\partial_t u &= u\partial_u p \partial_x^2 u + u\partial_u^2 p(\partial_x u)^2 + 2\partial_u p(\partial_x u)^2 + p\partial_x^2 u \\ &= \partial_x\big((p(u) + u\partial_u p(u))\partial_x u\big) \quad \text{in } \mathbb{R},\ t > 0.\end{aligned}$$

This is a nonlinear diffusion equation with coefficient $p(u) + u\partial_u p(u)$. If $p(u)$ is constant, we recover the linear equation (3.3) with $v = 0$, since we considered the unbiased case. The multi-dimensional equation reads as

$$\partial_t u = \operatorname{div}\big((p(u) + u\partial_u p(u))\nabla u\big) = \Delta(up(u)) \quad \text{in } \mathbb{R}^d,\ t > 0.$$

3.1.2. Population dynamics models. We generalize the technique from the previous subsection to multiple particle species, following the description in [33, 36]; also see [26, Sec. 4.2]. Again, we consider a one-dimensional lattice for simplicity. As before, the lattice consists of cells with midpoints x_j ($j \in \mathbb{Z}$) with the uniform cell size $h = x_j - x_{j-1} > 0$, and the particle density of the ith population at time $t > 0$ is denoted by $u_i(x_j) = u_i(x_j, t)$. We assume that the particles move from the jth cell to the neighboring cells $j \pm 1$ with the transition rate $R_i^{j,\pm}$. Conversely, the particles from the neighboring cells move to the jth cell with rate $R_i^{j-1,+}$ if they come from the $(j-1)$th cell and $R_i^{j+1,-}$ if they come from the $(j+1)$th cell. The time evolution is then given by the diffusion-scaled *master equation*

$$h^2\partial_t u_i(x_j) = R_i^{j-1,+}u_i(x_{j-1}) + R_i^{j+1,-}u_i(x_{j+1}) - (R_i^{j,+} + R_i^{j,-})u_i(x_j), \tag{3.5}$$

where $i = 1, \ldots, n$, $j \in \mathbb{Z}$, $t > 0$, supplemented by the initial condition $u_i(x_j, 0) = u_i^0(x_j)$. The first two terms represent the gain from incoming particles, the last two terms the loss from leaving particles.

If the departure cell is crowded or the neighboring cells are less populated, the particles tend to leave the cell, otherwise they prefer to stay. This suggests the multiplicative ansatz

$$R_i^{j,\pm} = p_i(u(x_j))q_i(u_0(x_{j\pm1})) \tag{3.6}$$

for some functions p_i and q_i. The function $u = (u_1, \ldots, n)$ is the vector of the species' densities and $u_0 = 1 - \sum_{i=1}^n u_i$ represents the void (no particles). We can interpret $u_1, \ldots, u_n$ also as the densities of some substances and u_0 as the solvent density. The mixture is then called saturated since $\sum_{i=0}^n u_i = 1$. Therefore, it is more precise to call u_i a *mass fraction* or a *volume fraction* (depending on the physical context). The quantities $p_i(u(x_j))$ and $q_i(u_0(x_{j\pm1}))$, respectively, measure the tendency of the ith species to leave the jth cell, or to move into the jth cell from one of the neighboring cells.

We claim that the master equations converge in the limit $h \to 0$ to a cross-diffusion system.

Theorem 3.1. *Let $(u_0, \ldots, u_n)$ be a smooth solution to the master equations (3.5) with transition rates (3.6). Then equations (3.5) converge in the limit $h \to 0$ formally to*

$$\partial_t u_i = \partial_x\left(\sum_{j=1}^n A_{ij}(u)\partial_x u_j\right) \quad \textit{in } \mathbb{R},\ t > 0,\ i = 1, \ldots, n, \tag{3.7}$$

with the diffusion coefficients

$$A_{ij}(u) = \delta_{ij} p_i(u) q_i(u_0) + u_i p_i(u) \frac{\mathrm{d}q_i}{\mathrm{d}u_0}(u_0) + u_i q_i(u_0) \frac{\partial p_i}{\partial u_j}(u), \tag{3.8}$$

and $u_0 := 1 - \sum_{i=1}^n u_i$.

Proof. We proceed as in [36]. To simplify the presentation, we abbreviate

$$u_i^j = u_i(x_j), \quad p_i^j = p_i(u(x_j)), \quad q_i^j = q_i(u_0(x_j)),$$
$$\partial_k p_i^j = \frac{\partial p_i}{\partial u_k}(u(x_j)), \quad \partial_0 q_i^j = \frac{\mathrm{d}q_i}{\mathrm{d}u_0}(u_0(x_j)).$$

This allow us to formulate the master equation (3.5) compactly as

$$h^2 \partial_t u_i^j = q_i^j \big(p_i^{j-1} u_i^{j-1} + p_i^{j+1} u_i^{j+1}\big) - p_i^j u_i^j \big(q_i^{j+1} + q_i^{j-1}\big). \tag{3.9}$$

We compute the Taylor expansions of p_i and q_i around $u(x_j)$ up to second order,

$$p_i^{j\pm1} = p_i^j + \sum_{k=1}^n \partial_k p_i^j (u_k^{j\pm1} - u_k^j) + \frac{1}{2} \sum_{k,\ell=1}^n \partial_{k\ell}^2 p_i^j (u_k^{j\pm1} - u_k^j)(u_\ell^{j\pm1} - u_\ell^j) + \cdots,$$
$$q_i^{j\pm1} = q_i^j + \partial_0 q_i^j (u_0^{j\pm1} - u_0^j) + \frac{1}{2} \partial_0^2 q_i^j (u_0^{j\pm1} - u_0^j)^2 + \cdots,$$

insert the Taylor expansion $u_k^{j\pm1} - u_k^j = \pm h \partial_x u_k^j + (h^2/2) \partial_x^2 u_k^j + O(h^3)$, and collect the terms up to second order:

$$\begin{aligned}
p_i^{j\pm1} &= p_i^j \pm h \sum_{k=1}^n \partial_k p_i^j \partial_x u_k^j + \frac{h^2}{2} \sum_{k=1}^n \partial_k p_i^j \partial_x^2 u_k^j + \frac{h^2}{2} \sum_{k,\ell=1}^n \partial_{k\ell}^2 p_i^j (\partial_x u_k^j)(\partial_x u_\ell^j) + O(h^3), \\
q_i^{j\pm1} &= q_i^j \pm h \partial_0 q_i^j \partial_x u_0^j + \frac{h^2}{2} \partial_0 q_i^j \partial_x^2 u_0^j + \frac{h^2}{2} \partial_0^2 q_i^j (\partial_x u_i^j)^2 + O(h^3), \\
&= q_i^j \mp h \partial_0 q_i^j \sum_{k=1}^n \partial_x u_k^j - \frac{h^2}{2} \partial_0 q_i^j \sum_{k=1}^n \partial_x^2 u_k^j + \frac{h^2}{2} \partial_0^2 q_i^j \sum_{k,\ell=1}^n (\partial_x u_k^j)(\partial_x u_\ell^j) + O(h^3),
\end{aligned} \tag{3.10}$$

where we replaced $\partial_x u_0^j$ by $-\sum_{k=1}^n \partial_x u_k^j$ in the last step. Then the terms of order $O(h)$ cancel out in the two sums in (3.9):

$$\begin{aligned}
-p_i^j u_i^j \big(q_i^{j+1} + q_i^{j-1}\big) &= -2 p_i^j u_i^j q_i^j + h^2(\cdots) + O(h^3), \\
q_i^j \big(p_i^{j-1} u_i^{j-1} + p_i^{j+1} u_i^{j+1}\big) &= q_i^j \bigg(p_i^j - h \sum_{k=1}^n \partial_k p_i^j \partial_x u_k^j + h^2(\cdots)\bigg) \bigg(u_i^j - h \partial_x u_i^j + \frac{h^2}{2} \partial_x^2 u_i^j\bigg) \\
&\quad + q_i^j \bigg(p_i^j + h \sum_{k=1}^n \partial_k p_i^j \partial_x u_k^j + h^2(\cdots)\bigg) \bigg(u_i^j + h \partial_x u_i^j + \frac{h^2}{2} \partial_x^2 u_i^j\bigg) + O(h^3) \\
&= 2 q_i^j p_i^j u_i^j + h^2(\cdots) + O(h^3).
\end{aligned}$$

Taking the sum, we see that also the term $2p_i^j q_i^j u_i^j$ cancels out, and there remain only terms of order $O(h^2)$. Rearranging these terms and dividing (3.9) by h^2, we end up, after some elementary computations, with

$$\begin{aligned}\partial_t u_i^j &= \sum_{k=1}^n \partial_x^2 u_k^j \big(p_i^j q_i^j \delta_{ik} + u_i^j q_i^j \partial_k p_i^j + u_i^j p_i^j \partial_0 q_i^j\big) \\ &\quad + \sum_{k,\ell=1}^n (\partial_x u_k^j)(\partial_x u_\ell^j)\big(2q_i^j \partial_k p_i^j \delta_{i\ell} + u_i^j q_i^j \partial_{k\ell}^2 p_i^j - u_i^j p_i^j \partial_0^2 q_i^j\big) + O(h).\end{aligned}$$

We pass to the limit $h \to 0$ and omit the superindex j in the previous equation:

$$\begin{aligned}\partial_t u_i &= \sum_{k=1}^n \partial_x^2 u_k \bigg(p_i q_i \delta_{ik} + u_i q_i \frac{\partial p_i}{\partial u_k} + u_i p_i \frac{\mathrm{d}q_i}{\mathrm{d}u_0}\bigg) \\ &\quad + \sum_{k,\ell=1}^n (\partial_x u_k)(\partial_x u_\ell)\bigg(2q_i \frac{\partial p_i}{\partial u_k}\delta_{i\ell} + u_i q_i \frac{\partial^2 p_i}{\partial u_k \partial u_\ell} - u_i p_i \frac{\mathrm{d}^2 q_i}{\mathrm{d}u_0^2}\bigg).\end{aligned}$$

A lengthy but straightforward computation shows that

$$\partial_x\bigg(p_i q_i \delta_{ik} + u_i q_i \frac{\partial p_i}{\partial u_k} + u_i p_i \frac{\mathrm{d}q_i}{\mathrm{d}u_0}\bigg) = \sum_{\ell=1}^n \partial_x u_\ell \bigg(2q_i \frac{\partial p_i}{\partial u_k}\delta_{i\ell} + u_i q_i \frac{\partial^2 p_i}{\partial u_k \partial u_\ell} - u_i p_i \frac{\mathrm{d}^2 q_i}{\mathrm{d}u_0^2}\bigg).$$

We infer that the differential equation for u_i becomes

$$\partial_t u_i = \sum_{k=1}^n \partial_x \bigg\{\bigg(p_i q_i \delta_{ik} + u_i q_i \frac{\partial p_i}{\partial u_k} + u_i p_i \frac{\mathrm{d}q_i}{\mathrm{d}u_0}\bigg)\partial_x u_k\bigg\},$$

which equals (3.7)–(3.8). □

Theorem 3.1 also holds in the multidimensional situation, and equations (3.7) become

$$\partial_t u_i = \operatorname{div}\bigg(\sum_{j=1}^n A_{ij}(u)\nabla u_j\bigg) \quad \text{in } \mathbb{R}^d,\ t>0,\ i=1,\ldots,n, \tag{3.11}$$

where the diffusion coefficients (3.8) stay unchanged. Interestingly, equations (3.11) can be reformulated as

$$\partial_t u_i = \operatorname{div}\bigg(q_i(u_0)^2 \nabla \frac{u_i p_i(u)}{q_i(u_0)}\bigg), \tag{3.12}$$

yielding a diagonal mobility matrix but more complicated variables. Indeed, it follows from $\sum_{j=1}^n u_j = 1 - u_0$ that

$$\begin{aligned}\sum_{j=1}^n A_{ij}(u)\nabla u_j &= p_i(u)q_i(u_0)\nabla u_i + u_i p_i(u)\frac{\mathrm{d}q_i}{\mathrm{d}u_0}\sum_{j=1}^n \nabla u_j + u_i q_i(u_0)\sum_{j=1}^n \frac{\partial p_i}{\partial u_j}(u)\nabla u_j \\ &= p_i(u)q_i(u_0)\nabla u_i - u_i p_i(u)\frac{\mathrm{d}q_i}{\mathrm{d}u_0}\nabla u_0 + u_i q_i(u_0)\nabla p_i(u)\end{aligned}$$

$$= q_i(u_0)^2\nabla\left(\frac{u_ip_i(u)}{q_i(u_0)}\right),$$

and inserting this expression into (3.11) yields (3.12).

The limit $h\to 0$ can be made rigorous; see, e.g., [13]. The idea is to write the master equation as a finite-difference scheme, to derive a discrete entropy inequality, and to apply compactness results to the linear interpolant of the finite-difference solution defined at the nodes x_j.

The cross-diffusion system (3.12) has an entropy structure [36] if $q(u_0) := q_i(u_0)$ for all $i=1,\ldots,n$ and if there exists a function $\chi:\mathcal{D}\to\mathbb{R}$ such that

$$p_i(u) = \exp\left(\frac{\partial\chi}{\partial u_i}(u)\right) \quad \text{for all } u\in\mathcal{D} := \left\{u\in(0,1)^n : \sum_{i=1}^n u_i < 1\right\}. \tag{3.13}$$

Notice that all functions q_i are the same and that p_i possesses a particular structure. It is unknown whether system (3.12) has an entropy structure under more general conditions. Introduce the entropy density

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + \int_a^{u_0}\log q(s)\mathrm{d}s + \chi(u) \tag{3.14}$$

for some $a\in(0,1)$. If $q(u_0)0u_0$ and $\chi(u)=1$, we recover, up to an additive constant, the Boltzmann-Shannon entropy density

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + u_(\log u_0 - 1) - a(\log a - 1) + 1.$$

The following result holds.

Lemma 3.2. *Let $q=q_i$ for all $i=1,\ldots,n$ and let (3.13) hold. Furthermore, let $(u_0,u_1,\ldots,u_n)$ be a smooth solution to (3.11) with (3.8). Then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} h(u)\mathrm{d}x + 4\sum_{i=1}^n\int_{\mathbb{R}^d} q(u_0)^2\left|\nabla\sqrt{\frac{u_ip_i(u)}{q(u_0)}}\right|^2\mathrm{d}x = 0.$$

Proof. We deduce from $\log p_i = \partial\chi/\partial u_i$ and $\partial u_0/\partial u_i = -1$ that

$$\frac{\partial h}{\partial u_i}(u) = \log u_i + \log q(u_0)\frac{\partial u_0}{\partial u_i} + \frac{\partial\chi}{\partial u_i} = \log\frac{u_ip_i(u)}{q(u_0)}$$

and therefore, after inserting (3.12) and integrating by parts,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} h(u)\mathrm{d}x = \sum_{i=1}^n\int_{\mathbb{R}^d}\frac{\partial h}{\partial u_i}\partial_t u_i\mathrm{d}x = -\sum_{i=1}^n\int_{\mathbb{R}^d} q(u_0)^2\nabla\frac{u_ip_i(u)}{q(u_0)}\cdot\nabla\log\frac{u_ip_i(u)}{q(u_0)}\mathrm{d}x,$$

which finishes the proof. □

The entropy production can be estimated from below by [36, Theorem 1]

$$4\sum_{i=1}^n\int_{\mathbb{R}^d} q(u_0)^2\left|\nabla\sqrt{\frac{u_ip_i(u)}{q(u_0)}}\right|^2\mathrm{d}x \ge C\int_\Omega\left(\sum_{i=1}^n q(u_0)^2|\nabla\sqrt{u_i}|^2 + |\nabla q(u_0)|^2\right)\mathrm{d}x,$$

which provides some gradient estimates. We consider some examples.

Example 3.3 (*Population dynamics models*)**.** We suppose that cells can be arbitrarily packed with particles, i.e., we discard the variable u_0 and set $q_i(u_0) = 1$. Then the transition rates only depend on the functions $p_i(u)$. The diffusion coefficients (3.8) simplify to $A_{ij}(u) = (\partial/\partial u_j)(u_i p_i(u))$, and we can write (3.7) (or equivalently (3.12)) as

$$\partial_t u_i = \Delta(u_i p_i(u)) \quad \text{in } \mathbb{R}^d, \ i = 1, \ldots, n. \tag{3.15}$$

Choosing $n = 3$ and the linear ansatz $p_i(u) = a_{i0} + a_{i1}u_1 + a_{i2}u_2$, we recover the Shigesada–Kawasaki–Teramoto population system introduced in Section 2.1.1. Clearly, the linear ansatz is just a choice; we may also choose a nonlinear dependence like

$$p_i(u) = a_{i0} + a_{1i}u_1^s + a_{i2}u_2^s, \quad i = 1, 2, \quad s > 0.$$

Such models have been analyzed in, e.g., [12, 18, 30]. The Laplacian structure of (3.15) is quite surprising. It allows for $L^2(\Omega)$ regularity for $u_i\sqrt{p_i(u)}$, by the duality method [17], instead of the usual $L^2(\Omega)$ regularity for u_i in bounded domains Ω. This improves the integrability of u_i. □

Example 3.4 (*Volume-filling models*)**.** The other extreme case is $p_i(u) = 1$ for all $i = 1, \ldots, n$. Then the diffusion coefficients (3.8) reduce to

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

where $q' = \mathrm{d}q/\mathrm{d}u_0$. Taking into account $\sum_{j=1}^n \nabla u_j = -\nabla u_0$, we obtain

$$\sum_{j=1}^n A_{ij}(u)\nabla u_j = q_i(u_0)\nabla u_i - u_i q_i'(u_0)\nabla u_0 = q_i(u_0)\nabla u_i - u_i \nabla q_i(u_0),$$

and equations (3.12) can be written as

$$\partial_t u_i = \operatorname{div}\big(q_i(u_0)\nabla u_i - u_i\nabla q(u_0)\big) = \operatorname{div}\left(u_i q_i(u_0)\nabla \log\frac{u_i}{q_i(u_0)}\right).$$

Unfortunately, we are unable to find a functional $h(u)$ that satisfies $\partial h/\partial u_i = \log(u_i/q_i(u_0))$ except in the case $q_i \equiv q$. Indeed, a necessary condition is that

$$\frac{\partial}{\partial u_j}\log\frac{u_i}{q_i(u_0)} = \frac{\partial}{\partial u_i}\log\frac{u_j}{q_j(u_0)} \quad \text{for } i \neq j,$$

which is equivalent to $(\log q_i(u_0))' = (\log q_j(u_0))'$. This seems to be possible only of $q_i \equiv q$ for all i. □

3.2. Derivation from kinetic equations

We first introduce some basic concepts of kinetic theory and then derive formally the Maxwell–Stefan systems from Boltzmann equations in the diffusion limit.

3.2.1. Basics of kinetic theory. The dynamics of N particles moving in $\mathbb{R}^d$ can in be described by Newton's laws of motion, which leads to $2dN$ differential equations in the phase space $\mathbb{R}^d \times \mathbb{R}^d$. The solution of these equations is computationally very costly if the number of particles N is large. Often, we are interested in the behavior of the particle *ensemble* instead of the behavior of the *individual* particles, such that is is reasonable to use a statistical description. This idea is made precise in kinetic theory: The system, composed of a large number of particles, is described by a distribution function $f(x,\xi,t)$, where $x \in \mathbb{R}^d$ is the position, ξ the velocity, and t the time of the ensemble. The function $f(x,\xi,t)$ is interpreted is a density in the sense that the integral $\int_B f(x,\xi,t)\mathrm{d}(x,\xi)$ is the number of particles in the phase-space domain $B \subset \mathbb{R}^d \times \mathbb{R}^d$ at time t. Observable macroscopic quantities like the particle density $u(x,t)$ and velocity $v(x,t)$ are given by moments (i.e. integrals of functions of ξ) with respect to the measure $f(x,\xi,t)\mathrm{d}\xi$:

$$u(x,t) = \int_{\mathbb{R}^d} f(x,\xi,t)\mathrm{d}\xi, \quad v(x,t) = \frac{1}{u(x,t)} \int_{\mathbb{R}^d} \xi f(x,\xi,t)\mathrm{d}\xi.$$

The second moment $\frac{1}{2}\int_{\mathbb{R}^d} |\xi|^2 f\mathrm{d}\xi$ is the energy density. By definition of the distribution function, and in the absence of collisions, $f(x,\xi,t)$ should be constant along trajectories of the particle ensemble. Denoting by $(x(t),\xi(t))$ the position and velocity of the particle ensemble at time t, respectively, and by $\partial_t x = v$ the velocity, we find that

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} f(x(t),\xi(t),t) = \partial_t f + v(t)\cdot\nabla_x f + \partial_t\xi\cdot\nabla_\xi f.$$

According to Newton's law, the acceleration $\partial_t\xi$ equals the force F divided by the particle mass m (which we normalize to one).This yields the *Vlasov equation*

$$\partial_t f + \xi\cdot\nabla_x f + F\cdot\nabla_v f = 0 \quad \text{in } \mathbb{R}^d\times\mathbb{R}^d,\ t>0.$$

This argument is very simplified, since we just considered the movement of the whole ensemble. Taking into account the evolution of each particle, we obtain generally a Vlasov equation for the distribution function $f(\boldsymbol{x},\boldsymbol{\xi},t)$ with the position variable $\boldsymbol{x} = (x^{(1)},\ldots,x^{(N)}) \in \mathbb{R}^{dN}$ and the velocity variable $\boldsymbol{\xi} = (\xi^{(1)},\ldots,\xi^{(N)}) \in \mathbb{R}^{dN}$. This equation in $\mathbb{R}^{dN}\times\mathbb{R}^{dN}$ is as complex as Newton's laws of motion. Under the so-called initial chaos assumption (which is a condition on the initial data), it is possible to show that the one-particle distribution function $f(x,\xi,t)$ with $(x,\xi)\in\mathbb{R}^{2d}$ contains the dynamics of the many-particle problem with distribution function $f(\boldsymbol{x},\boldsymbol{\xi},t)$; see, e.g., [10, Chap. 2] or [5, Sec. 3.2].

The Vlasov equation describes the dynamics of the particles without collisions. To include collisional effects, we include a collision operator $Q(f)$ on the right-hand side of the Vlasov equation,

$$\partial_t f + \xi\cdot\nabla_x f + F\cdot\nabla_v f = Q(f) \quad \text{in } \mathbb{R}^d\times\mathbb{R}^d,\ t>0. \tag{3.16}$$

This equation is called the *Boltzmann equation*, first formulated by Boltzmann in 1872 [3]. To determine the term $Q(f)$, we assume that

- collisions between particles are binary, i.e., we neglect collisions involving three or more particles, which is reasonable for dilute gases;
- collisions are local, as if the particles are billard balls;

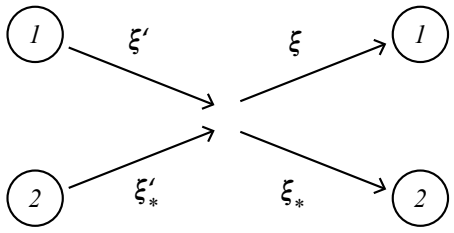

FIGURE 2. Precollisional velocities (ξ', ξ'_*) and postcollisional velocities (ξ, ξ_*) of a collision of two particles.

- collisions are elastic, which means that the total momentum and total kinetic energy are conserved by the collision process.

Let (ξ', ξ'_*) be the precollisional velocities of two particles and (ξ, ξ_*) be the postcollisional velocities, and assume that all particles have the same mass $m = 1$; see Figure 2. Then the conservation of total momentum and kinetic energy means that

$$m\xi' + m\xi'_* = m\xi + m\xi_*, \quad \frac{m}{2}|\xi'|^2 + \frac{m}{2}|\xi'_*|^2 = \frac{m}{2}|\xi|^2 + \frac{m}{2}|\xi_*|^2. \tag{3.17}$$

These equations allow us to express (ξ', ξ'_*) in terms of (ξ, ξ_*). Indeed, let $\sigma \in \mathbb{R}^d$ be such that $|\sigma| = 1$ and let $A \in \mathbb{R}$. Then we can write $A\sigma := \xi' - \xi$, which implies, by momentum conservation, that $\xi'_* - \xi_* = -A\sigma$ and consequently, $\xi' = \xi + A\sigma$, $\xi'_* = \xi_* - A\sigma$. We replace ξ' and ξ'_* in the energy conservation by these expressions and expand the squares to find that $A = (\xi_* - \xi) \cdot \sigma$. This shows that

$$\xi' = \xi + ((\xi_* - \xi) \cdot \sigma)\sigma, \quad \xi'_* = \xi_* - ((\xi_* - \xi) \cdot \sigma)\sigma. \tag{3.18}$$

Since $\sigma = (\xi' - \xi)/A$ is normalized, we have $\sigma = (\xi' - \xi)/|\xi' - \xi|$.

The collision term $Q(f)$ is the difference of the gain $f'f'_*$ and the loss ff_*, integrated over all velocities $\xi_* \in \mathbb{R}^d$ and directions $\sigma \in \mathbb{S}$, where we abbreviated $f' = f(x, \xi', t)$, $f_* = f(x, \xi_*, t)$, $f'_* = f(x, \xi'_*, t)$, and $\mathbb{S}$ is the d-dimensional unit sphere:

$$Q(f)(\xi) = \int_{\mathbb{R}^d} \int_{\mathbb{S}} B(\xi, \xi_*, \sigma)(f'f'_* - ff_*)\mathrm{d}\sigma\mathrm{d}\xi_*.$$

The collision kernel $B(\xi, \xi_*, \sigma) \geq 0$ is generally a function of $|\xi - \xi_*|$ and $|(\xi - \xi_*) \cdot \sigma|$. For more details on the Boltzmann collision operator, we refer to [9]. The following lemma shows that the collision term conserves the mass, momentum, and energy.

Lemma 3.5. *The conservation of mass, momentum, and energy, respectively, hold:*

$$\int_{\mathbb{R}^d} Q(f)\mathrm{d}\xi = 0, \quad \int_{\mathbb{R}^d} Q(f)\xi\mathrm{d}\xi = 0, \quad \frac{1}{2}\int_{\mathbb{R}^d} Q(f)|\xi|^2\mathrm{d}\xi = 0.$$

PROOF. Let $\phi(\xi)$ be a smooth function. We observe that the collision kernel B is invariant under the changes of variables $(\xi, \xi_*) \mapsto (\xi', \xi'_*)$ and $(\xi, \xi_*) \mapsto (\xi_*, \xi)$. Hence, we can reformulate the integral over $Q(f)\phi(\xi)$:

$$\int_{\mathbb{R}^d} Q(f)(\xi)\phi(\xi)\mathrm{d}\xi = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(f'f'_* - ff_*)\phi(\xi)\mathrm{d}\sigma\mathrm{d}\xi_*\mathrm{d}\xi \tag{3.19}$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(f_*'f' - f_*f)\phi(\xi_*)\mathrm{d}\sigma\mathrm{d}\xi_*\mathrm{d}\xi \\
&\quad \text{(swapping } \xi \text{ and } \xi_* \text{ and hence } \xi' \text{ and } \xi_*') \\
&= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(f'f_*' - ff_*)\big(\phi(\xi) + \phi(\xi_*)\big)\mathrm{d}\sigma\mathrm{d}\xi_*\mathrm{d}\xi \\
&\quad \text{(adding the last two lines)} \\
&= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(ff_* - f'f_*')\big(\phi(\xi') + \phi(\xi_*')\big)\mathrm{d}\sigma\mathrm{d}\xi_*\mathrm{d}\xi \\
&\quad \text{(swapping } (\xi,\xi_*) \text{ and } (\xi',\xi_*')) \\
&= \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(f'f_*' - ff_*)\big(\phi(\xi) + \phi(\xi_*) - \phi(\xi') - \phi(\xi_*')\big)\mathrm{d}\sigma\mathrm{d}\xi_*\mathrm{d}\xi. \\
&\quad \text{(adding the last two lines)}
\end{aligned}
$$

Choosing $\phi(\xi) = 1$ directly yields mass conservation. The choices $\phi(\xi) = \xi$ and $\phi(\xi) = \frac{1}{2}|\xi|^2$, together with properties (3.17), finish the proof. □

There is another consequence of (3.19). The choice $\phi(\xi) = \log f(\xi)$ leads to

$$
\int_{\mathbb{R}^d} Q(f)\log f\mathrm{d}\xi = -\frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B(f'f_*' - ff_*)\big(\log(f'f_*') - \log(ff_*)\big)\mathrm{d}\xi\mathrm{d}\xi_*\mathrm{d}\sigma \le 0,
$$

since the logarithm is monotone. Thus, introducing the *Boltzmann entropy*

$$
\mathcal{H}(f) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(\log f - 1)\mathrm{d}\xi\mathrm{d}x,
$$

a formal computation shows that

$$
\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(f) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \partial_t f\log f\mathrm{d}\xi\mathrm{d}x = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} Q(f)\log f\mathrm{d}\xi\mathrm{d}x \le 0.
$$

This property, which is called the *H-theorem*, has an important consequence. It is possible to show that $\mathrm{d}\mathcal{H}(f)/\mathrm{d}t = 0$ if and only if $\log f$ is at most quadratic in ξ with coefficients depending on (x,t) [**10**, Theorem 3.1.1],

$$
\log f(x,\xi,t) = A(x,t) + B(x,t)\cdot\xi + C(x,t)|\xi|^2.
$$

This can be written as

$$
f(\xi) = \exp\left(C\left|\xi + \frac{B}{2C}\right|^2 - \frac{|B|}{4C} + A\right).
$$

For $f(\xi)$ to be integrable, the constant C must be negative. Thus, choosing $C' := -C$, $B' := -B/(2C)$, and $A' := \exp(-|B|^2/(4C) + A)$, we have

$$
f(\xi) = A'\exp(-C'|\xi - B'|^2).
$$

Such distribution functions are called *local thermodynamic equilibria*. They can be equivalently formulated as

$$M(x,\xi,t) = \frac{u(x,t)}{(2\pi\theta(x,t))^{d/2}} \exp\left(-\frac{|\xi - v(x,t)|^2}{2\theta(x,t)}\right), \tag{3.20}$$

where the functions $u(x,t)$, $v(x,t)$, $\theta(x,t)$ have the physical meaning of a particle density, velocity, and temperature, respectively, since a computation, transforming $\eta = (\xi - v)/\sqrt{\theta}$, shows that

$$\begin{aligned}
\int_{\mathbb{R}^d} M\mathrm{d}\xi &= \frac{u}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}\mathrm{d}\eta = u, \\
\int_{\mathbb{R}^d} M\xi\mathrm{d}\xi &= \frac{u}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}(v+\sqrt{\theta}\eta)\mathrm{d}\eta = uv, \\
\frac{1}{2}\int_{\mathbb{R}^d} M|\xi|^2\mathrm{d}\xi &= \frac{u}{2(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}\big(|v|^2 + 2\sqrt{\theta}v\cdot\eta + \theta|\eta|^2\big)\mathrm{d}\eta = u\bigg(\frac{|v|^2}{2} + \frac{d}{2}\theta\bigg).
\end{aligned}$$

The expression in the brackets is the total energy density, being the sum of the kinetic and thermal energy.

3.2.2. Maxwell–Stefan equations. The aim of this section is the formal derivation of the Maxwell–Stefan equations introduced in Section 2.2. We proceed as in [7]. Let $\Omega \subset \mathbb{R}^d$ be a bounded position domain and consider a mixture of $n+1$ species, each of which is described by the Boltzmann equation

$$\partial_t f_i + v\cdot\nabla_x f_i = \sum_{j=0}^n Q_{ij}(f_i,f_j) \quad \text{in } \Omega\times\mathbb{R}^d,\ t>0, \quad f_i(\cdot,\cdot,0) = f_i^0,$$

where $i = 0,\ldots,n$. For simplicity, we have neglected the force F in (3.16) and we assume that the particles have the same mass; we refer to [7] for a mixture with different masses. The collision operators are given by

$$Q_{ij}(f_i,f_j) = \int_{\mathbb{R}^d}\int_{\mathbb{S}} B_{ij}(\xi,\xi_*,\sigma)(f_i'f_{j*}' - f_if_{j*})\mathrm{d}\sigma\mathrm{d}\xi_*, \tag{3.21}$$

where the collision kernels B_{ij} satisfy the conditions

$$B_{ij}(\xi,\xi_*,\sigma) = B_{ji}(\xi,\xi_*,\sigma), \quad B_{ij}(\xi,\xi_*,\sigma) = B_{ij}(\xi',\xi_*',\sigma),$$

which we have already assumed in the single-species case of Section 3.2.1. A generalization of Lemma 3.5 shows that these operators satisfy mass, momentum, and energy conservation in the sense [7, Sec. 3.3]

$$\begin{aligned}
\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)\mathrm{d}\xi &= 0, \\
\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)\xi\mathrm{d}\xi + \int_{\mathbb{R}^d} Q_{ji}(f_j,f_i)\xi\mathrm{d}\xi &= 0, \\
\frac{1}{2}\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)|\xi|^2\mathrm{d}\xi + \frac{1}{2}\int_{\mathbb{R}^d} Q_{ji}(f_j,f_i)|\xi|^2\mathrm{d}\xi &= 0 \quad \text{for } i\neq j,
\end{aligned} \tag{3.22}$$

and if $i=j$, Lemma 3.5 implies mass, momentum, and energy conservation for $Q_{ii}(f_i^\varepsilon, f_i^\varepsilon)$.

The Maxwell–Stefan equations are derived in the diffusion limit. For this, we impose the following assumptions:

(1) The time scale is large and the collisions dominate the dynamics.
(2) The initial functions are local Maxwellians with small initial velocity.
(3) The temperature is uniform in space and time, $\theta=1$.
(4) The collision kernels B_{ij} only depend on the collision angle σ.

The first condition means that the time t is replaced by t/ε for some $\varepsilon>0$ and $Q_{ij}(f_i,f_j)$ is replaced by $\varepsilon^{-1}Q_{ij}(f_i,f_j)$:

$$\varepsilon\partial_t f_i + v\cdot\nabla_x f_i = \frac{1}{\varepsilon}\sum_{j=0}^n Q_{ij}(f_i,f_j) \quad \text{in } \Omega\times\mathbb{R}^d,\ t>0. \tag{3.23}$$

According to (3.20), the second and third conditions mean that

$$f_i^0(x,\xi) = \frac{u_i^0(x)}{(2\pi)^{d/2}}\exp\left(-\frac{1}{2}|\xi-\varepsilon v_i^0(x)|^2\right) \quad \text{for } (x,\xi)\in\Omega\in\mathbb{R}^d,$$

where $u_i^0\ge 0$ and $v_i^0\in\mathbb{R}^d$ are given initial particle densities and velocities satisfying $\sum_{i=0}^n u_i^0=1$ in Ω. Finally, the fourth condition is used later to evaluate the integral of B_{ij} over σ.

We impose a further crucial assumption. We assume that the system keeps the distribution functions in the local Maxwellian state, i.e., there exist functions u_i^ε, v_i^ε such that

$$f_i^\varepsilon(x,\xi,t) = \frac{u_i^\varepsilon(x,t)}{(2\pi)^{d/2}}\exp\left(-\frac{1}{2}|\xi-\varepsilon v_i^\varepsilon(x,t)|^2\right) \quad \text{for } (x,\xi)\in\Omega\times\mathbb{R}^d,\ t>0. \tag{3.24}$$

The functions u_i^ε and v_i^ε can be interpreted as the particle densities and velocities since

$$\int_{\mathbb{R}^d} f_i^\varepsilon \mathrm{d}\xi = u_i^\varepsilon, \quad \int_{\mathbb{R}^d} f_i^\varepsilon\xi\mathrm{d}\xi = \varepsilon u_i^\varepsilon v_i^\varepsilon.$$

Now we are able to derive the Maxwell–Stefan equations. First, we integrate (3.23) over ξ, using (3.22),

$$0 = \varepsilon\partial_t\int_{\mathbb{R}^d} f_i^\varepsilon\mathrm{d}\xi + \operatorname{div}_x\int_{\mathbb{R}^d} f_i^\varepsilon\xi\mathrm{d}\xi = \varepsilon\partial_t u_i^\varepsilon + \varepsilon\operatorname{div}_x(u_i^\varepsilon v_i^\varepsilon), \tag{3.25}$$

which expresses the conservation of mass. Second, we multiply (3.23) by ξ and integrate over ξ:

$$\varepsilon\partial_t\int_{\mathbb{R}^d} f_i^\varepsilon\xi\mathrm{d}\xi + \operatorname{div}_x\int_{\mathbb{R}^d} f_i^\varepsilon\xi\otimes\xi\mathrm{d}\xi = \frac{1}{\varepsilon}\sum_{j=0}^n\int_{\mathbb{R}^d} Q_{ij}(f_i^\varepsilon,f_j^\varepsilon)\xi\mathrm{d}\xi. \tag{3.26}$$

Lemma 3.6. *It holds for $i,j=0,\dots,n$ that*

$$\varepsilon\partial_t\int_{\mathbb{R}^d} f_i^\varepsilon\xi\mathrm{d}\xi = \varepsilon^2\partial_t(u_i^\varepsilon v_i^\varepsilon),$$
$$\operatorname{div}_x\int_{\mathbb{R}^d} f_i^\varepsilon\xi\otimes\xi\mathrm{d}\xi = \nabla_x u_i^\varepsilon + \varepsilon^2\operatorname{div}_x(u_i^\varepsilon v_i^\varepsilon\otimes v_i^\varepsilon),$$

$$\frac{1}{\varepsilon}\int_{\mathbb{R}^d} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)\xi \mathrm{d}\xi = b_{ij}u_i^\varepsilon u_j^\varepsilon(v_i^\varepsilon - v_j^\varepsilon).$$

PROOF. We use the definition of f_i^ε and substitute ξ by $\eta = \xi - \varepsilon v_i^\varepsilon$ in the integral to find that

$$\int_{\mathbb{R}^d} f_i^\varepsilon \xi \mathrm{d}\xi = \frac{u_i^\varepsilon}{(2\pi)^{d/2}}\int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}(\eta + \varepsilon v_i^\varepsilon)\mathrm{d}\eta = \varepsilon u_i^\varepsilon v_i^\varepsilon.$$

In a similar way, we compute

$$\begin{aligned}\int_{\mathbb{R}^d} f_i^\varepsilon \xi\otimes\xi \mathrm{d}\xi &= \frac{u_i^\varepsilon}{(2\pi)^{d/2}}\int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}(\eta+\varepsilon v_i^\varepsilon)\otimes(\eta+\varepsilon v_i^\varepsilon)\mathrm{d}\eta \\ &= \frac{u_i^\varepsilon}{(2\pi)^{d/2}}\int_{\mathbb{R}^d} \mathrm{e}^{-|\eta|^2/2}\eta\otimes\eta\mathrm{d}\eta + \varepsilon^2\frac{u_i^\varepsilon}{(2\pi)^{d/2}} v_i^\varepsilon\otimes v_i^\varepsilon\int_{\mathbb{R}^d}\mathrm{e}^{-|\eta|^2/2}\mathrm{d}\eta \\ &= u_i^\varepsilon\mathbb{I} + \varepsilon^2 u_i^\varepsilon v_i^\varepsilon\otimes v_i^\varepsilon,\end{aligned}$$

where $\mathbb{I}$ is the unit matrix in $\mathbb{R}^{d\times d}$. Next, we insert definition (3.21) of $Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)$ and transform $\eta_i = \xi - \varepsilon v_i^\varepsilon$, $\eta_j = \xi - \varepsilon v_j^\varepsilon$ (observing that B_{ij} does not change):

$$\begin{aligned}\int_{\mathbb{R}^d} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)\xi\mathrm{d}\xi &= \frac{u_i^\varepsilon u_j^\varepsilon}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B_{ij}\mathrm{e}^{-(|\eta'|^2-|\eta_*'|^2)/2}(\eta_i+\varepsilon v_i^\varepsilon)\mathrm{d}\sigma\mathrm{d}\eta_*\mathrm{d}\eta \\ &\quad - \frac{u_i^\varepsilon u_j^\varepsilon}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}} B_{ij}\mathrm{e}^{-(|\eta|^2+|\eta_*|^2)/2}(\eta_j+\varepsilon v_j^\varepsilon)\mathrm{d}\sigma\mathrm{d}\eta_*\mathrm{d}\eta.\end{aligned}$$

The integrals over η_i and η_j vanish. The fourth condition imposed above implies that $b_{ij} := \int_{\mathbb{S}} B_{ij}\mathrm{d}\sigma$ is a number. Hence,

$$\int_{\mathbb{R}^d} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)\xi\mathrm{d}\xi = \varepsilon b_{ij}u_i^\varepsilon u_j^\varepsilon(v_i^\varepsilon - v_j^\varepsilon).$$

This ends the proof. □

We deduce from the previous lemma that (3.26) can be written as

$$\varepsilon^2\partial_t(u_i^\varepsilon v_i^\varepsilon) + \varepsilon^2\operatorname{div}_x(u_i^\varepsilon v_i^\varepsilon\otimes v_i^\varepsilon) + \nabla_x u_i^\varepsilon = \sum_{j=0}^n b_{ij}u_i^\varepsilon u_j^\varepsilon(v_i^\varepsilon - v_j^\varepsilon). \tag{3.27}$$

Assuming that $u_i^\varepsilon \to u_i$ and $v_i^\varepsilon \to v_i$ as $\varepsilon\to 0$, we can perform, in the third step, the formal limit $\varepsilon\to 0$ in (3.25) and (3.27), leading to the Maxwell–Stefan equations for $i = 0,\ldots,n$:

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad \nabla u_i = -\sum_{j=0}^n b_{ij}u_i u_j(v_j - v_i) \quad \text{in } \Omega,\ t>0. \tag{3.28}$$

Since $\int_{\mathbb{R}^d} f_i^0\mathrm{d}\xi = u_i^0$, the initial conditions become

$$u_i(0) = u_i^0 \quad \text{in } \Omega,\ i = 0,\ldots,n.$$

It remains to verify that $\sum_{i=0}^n u_i^0 = 1$ implies that $\sum_{i=0}^n u_i(t) = 1$. This does not directly follow from the mass conservation law, since we do not know whether $u_i v_i\cdot\nu = 0$ on $\partial\Omega$ (with

ν being the exterior normal unit vector to $\partial\Omega$). To this end, we multiply (3.23) by $|\xi|^2$, integrate over $\mathbb{R}^d$, and sum over $i=0,\ldots,n$:

$$\varepsilon\partial_t\sum_{i=0}^n\int_{\mathbb{R}^d}f_i^\varepsilon|\xi|^2\mathrm{d}\xi+\frac{1}{\varepsilon}\operatorname{div}_x\sum_{i=0}^n\int_{\mathbb{R}^d}f_i^\varepsilon|\xi|^2\mathrm{d}\xi=\frac{1}{\varepsilon^2}\sum_{i,j=0}^n\int_{\mathbb{R}^d}Q_{ij}(f_i^\varepsilon,f_j^\varepsilon)|\xi|^2\mathrm{d}\xi=0, \tag{3.29}$$

where we used properties (3.22) of Q_{ij}. The integrals on the left-hand side can be computed as in the proof of Lemma 3.6:

$$\sum_{i=0}^n\int_{\mathbb{R}^d}f_i^\varepsilon|\xi|^2\mathrm{d}\xi=du_i^\varepsilon+O(\varepsilon^2),\quad\sum_{i=0}^n\int_{\mathbb{R}^d}f_i^\varepsilon|\xi|^2\mathrm{d}\xi=\varepsilon(d+2)u_i^\varepsilon v_i^\varepsilon+O(\varepsilon^2),$$

where $O(\varepsilon^2)$ denotes terms of order ε^2. We insert these expressions into (3.29) and pass to the formal limit $\varepsilon\to 0$:

$$d\partial_t\sum_{i=0}^n u_i+(d+2)\operatorname{div}\sum_{i=0}^n u_iv_i=0.$$

Summing the mass conservation laws in (3.28) over $i=0,\ldots,n$, we find that

$$\partial_t\sum_{i=0}^n u_i+\operatorname{div}\sum_{i=0}^n u_iv_i=0.$$

Both equations can only hold if $\sum_{i=0}^n u_i=0$ and $\operatorname{div}\sum_{i=0}^n u_iv_i=0$. In particular, the total particle density $\sum_{i=0}^n u_i$ is constant in time. Since we assumed that initially $\sum_{i=1}u_i^0=1$, we conclude that $\sum_{i=1}^n u_i(t)=1$ for all $t\ge 0$, which shows the claim.

Summarizing, we have proved that the formal limit functions (u_i,v_i) solve equations (3.28), the initial conditions $u_i(0)=u_i^0$ for $i=1,\ldots,n$, and the side condition $\sum_{i=0}^n u_i=1$ in Ω, $t>0$. Equations (3.28) coincide with the Maxwell–Stefan equations of Section 2.2. Notice, however, that we have not derived any boundary conditions for u_i on $\partial\Omega$.

Remark 3.7 (Chapman–Enskog expansion)**.** An alternative way to derive Maxwell–Stefan-type equations is to use a variant of the Chapman–Enskog expansion [11], which is a perturbative approach. This allows for a rigorous mathematical derivation [6, 8]. The idea is to expand the solution f_i^ε to the scaled Boltzmann equation (3.23) around the global Maxwellian $M(\xi)=(2\pi)^{-d/2}\exp(-|\xi|^2/2)$ according to

$$f_i^\varepsilon(x,\xi,t)=u_i(x,t)M(\xi)+\varepsilon g_i(x,\xi,t),\quad i=0,\ldots,n,$$

which can be interpreted as the definition of $g_i(x,\xi,t)$. We insert this expansion into the scaled Boltzmann equation (3.23) and sort the terms in powers of ε:

$$\begin{aligned}&\xi\cdot\nabla_x(u_iM)+\varepsilon\big(\partial_t(u_iM)+\xi\cdot\nabla_x g_i\big)+\varepsilon^2\partial_t g_i\\&\quad=\frac{1}{\varepsilon}\sum_{j=0}^n Q_{ij}(u_iM,u_jM)+\sum_{j=0}^n\big(Q_{ij}(u_iM,g_j)+Q_{ij}(g_i,u_jM)\big)+\varepsilon\sum_{j=0}^n Q_{ij}(g_i,g_j).\end{aligned}$$

Observing that the energy conservation (3.17) implies that $Q_{ij}(u_iM, u_jM) = 0$, we identify the terms of order $O(1)$ and $O(\varepsilon)$:

$$\varepsilon^0: \quad M(\xi\cdot\nabla_x u_i) = \sum_{j=0}^n \big(Q_{ij}(u_iM, g_j) + Q_{ij}(g_i, u_jM)\big) =: L_i(g), \tag{3.30}$$

$$\varepsilon^1: \quad M\partial_t u_i + \xi\cdot\nabla_x g_i = \sum_{j=0}^n Q_{ij}(g_i, g_j). \tag{3.31}$$

First, we integrate (3.31) over $\xi\in\mathbb{R}^d$, observe that $\int_{\mathbb{R}^d} M\mathrm{d}\xi = 1$, and take into account that Q_{ij} conserves the total mass so that $\int_{\mathbb{R}^d} Q_{ij}(g_i,g_j)\mathrm{d}\xi = 0$:

$$\partial_t u_i + \mathrm{div}_x\, J_i = 0, \quad \text{where } J_i = \int_{\mathbb{R}^d} g_i\xi\mathrm{d}\xi. \tag{3.32}$$

Second, the flux J_i is determined by analyzing the zeroth-order equations (3.30). We split $L(g) = (L_1(g),\ldots,L_n(g))$ into two terms, $L_i(g) = (Kg)_i - \nu_i(\xi)g_i$, where $g = (g_1,\ldots,g_n)$ and

$$(Kg)_i = \sum_{j=0}^n Q_{ij}(u_iM, g_j) + \sum_{j=1}^n \int_{\mathbb{R}^d}\int_{\mathbb{S}} B_{ij} g_i' u_j M_*' \mathrm{d}\sigma\mathrm{d}\xi_*,$$

$$\nu_i(\xi) = \sum_{j=0}^n \int_{\mathbb{R}^d}\int_{\mathbb{S}} B_{ij}(\xi,\xi_*,\sigma) u_j M_* \mathrm{d}\sigma\mathrm{d}\xi_*.$$

The quantity ν_i can be interpreted as a collision frequency. It is proved in [6, Prop. 2] that the operator K, defined on a suitable space, is compact and that $(M\xi\cdot\nabla_x u_i)_{i=1}^n \in (\ker L^*)^\perp$, where L^* denotes the adjoint operator of L. Because of the compactness of K, the range of $L_i = K - \nu_i\mathbb{I}$ is closed. This shows that $(\ker L_i^*)^\perp = \overline{\mathrm{ran}\, L_i} = \mathrm{ran}\, L_i$. Consequently, there exists a function g such that $L_i(g) = W_i$, i.e.

$$g = L^{-1}(W), \quad \text{where } W_i = M\xi\cdot\nabla_x u_i,\ i = 0,\ldots,n,$$

and the flux becomes

$$J_i = \int_{\mathbb{R}^d} g_i\xi\mathrm{d}\xi = \int_{\mathbb{R}^d} L^{-1}(W)_i\xi\mathrm{d}\xi.$$

Using some properties of the linear operator L^{-1} (self-adjointness on $(\ker L^*)^\perp$), it is shown in [8, Sec. 4] that

$$J_i = -\sum_{j=1}^n u_i G_{ij}(u)\nabla u_j, \quad i = 0,\ldots,n,$$

where $G_{ij}(u) = \langle L^{-1}(w_i), w_j\rangle$, w_i is a vector depending on M, ξ, and $\ker L_i^*$, and $\langle\cdot,\cdot\rangle$ is a scalar product in some weighted $L^2(\mathbb{R}^d)$ space. This shows that the mass conservation law (3.32) can be written as the cross-diffusion system

$$\partial_t u_i - \mathrm{div}\left(\sum_{j=0}^n u_i G_{ij}(u)\nabla u_j\right) = 0, \quad i = 0,\ldots,n. \tag{3.33}$$

The matrix (G_{ij}) is symmetric, its kernel is spanned by the vector $(u_1,\ldots,u_n)$, and it has n positive eigenvalues as long as $\min_i u_i$ is positive [8, Sec. 5]. System (3.33) is called the Fick–Onsager formulation, which is linked to the Maxwell–Stefan formulation; see Section 2.2.1. We observe that equations (3.33) ressemble the generalized Busenberg–Travis model in Section 2.1.2, but in the latter model the matrix (G_{ij}) does not depend on u and has a trivial kernel. □

References for Chapter 3

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CHAPTER 4

Structure-preserving finite-volume approximations

In numerical simulations, it is desirable to design numerical schemes that preserve as many properties of the cross-diffusion systems as possible, in particular conservation or control of the total mass, nonnegativity of the densities, and preservation of the entropy structure. In this chapter, we introduce two-point flux approximation finite-volume methods for cross-diffusion systems, which preserve these properties at the discrete level. We start with a brief introduction of finite-volume methods and then detail structure-preserving finite-volume schemes for population cross-diffusion systems and volume-filling cross-diffusion systems.

4.1. Basics of finite-volume methods

We explain a special class of finite-volume techniques, the two-point flux approximation. We decompose the computational domain $\Omega \subset \mathbb{R}^d$ (typically, $d = 2$ or $d = 3$) in open polygonal control volumes $K \in \mathcal{T}$ such that the closure of the union of these volumes forms a partition of $\overline{\Omega}$, namely $\overline{\cup_{K\in\mathcal{T}} K} = \overline{\Omega}$, where $\mathcal{T}$ is the set of control volumes. Finite-volume methods are usually applied to differential equations in divergence form. The idea is to integrate the equation over each control volume and to apply the divergence theorem in order to convert the volume integral containing the divergence term to a surface integral. Finite-volume methods differ in the way they approximate the flux through the surface. We present here the two-point flux approximation. For detailed expositions of the finite-volume method, we refer to [8, 15].

The finite-volume method was introduced into the field of computational fluid dynamics (Euler equations) in the seventies [17, 18], but there are early approaches for convection-diffusion equations in the sixties; see, e.g., [21]. The mathematical analysis of finite-volume schemes started only in the nineties [8, 10].

Some advantages of finite-volume methods are:

- They are based on weak formulations of the equations and are independent of the domain geometry, like finite-element methods.
- They allow for the conservation of discrete physical quantities.
- They seem to be superior to finite-element methods in problems dealing with discontinuities.

Finite-volume methods usually use piecewise constant base functions, possibly with a higher-order interpolation scheme for the fluxes. This leads to methods that are first-order or second-order accurate. A drawback is that it is not straightforward to design higher-order methods, which is easier in finite-element methods. Another drawback is that the two-point approximations that we discuss below need an orthogonality condition which restricts the geometry of the meshes,

in particular in three space dimensions. A comparison between finite-volume schemes and so-called approximate gradient schemes, which include mass-lumping finite elements [5], mixed finite elements [3], and mimetic finite differences [16], is presented in [7].

4.1.1. Notation and numerical scheme. Consider the diffusion equation

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = f(x) \quad \text{in } \Omega, \quad A(u)\nabla u\cdot\nu = 0 \quad \text{on } \partial\Omega,\ t>0, \tag{4.1}$$

with the initial condition $u(\cdot,0)=u^0\ge 0$ in Ω. The function $A:[0,\infty)\to\mathbb{R}$ is assumed to be continuous and nonnegative. We integrate (4.1) over $K\in\mathcal{T}$ and use the divergence theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_K u\mathrm{d}x - \int_{\partial K} A(u)\nabla u\cdot\nu\mathrm{d}s = \int_K f(x)\mathrm{d}x.$$

Let $\mathcal{E}$ be the set of all edges (in two space dimensions) or faces (in three space dimensions). Denoting by $\mathcal{E}_K$ the set of all edges that are part of ∂K, we write the previous equation as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_K u\mathrm{d}x - \sum_{\sigma\in\mathcal{E}_K}\int_\sigma A(u)\nabla u\cdot\nu\mathrm{d}s = \int_K f(x)\mathrm{d}x. \tag{4.2}$$

Let $\Delta t>0$ be the (uniform) time step and $u^k(x)$ be an approximation of $u(x,k\Delta t)$. We introduce the space-time piecewise constant functions

$$u_K^k = \frac{1}{\mathrm{m}(K)}\int_K u^k(x)\mathrm{d}x, \quad f_K = \frac{1}{\mathrm{m}(K)}\int_K f(x)\mathrm{d}x, \quad K\in\mathcal{T},\ k\ge 0,$$

where $\mathrm{m}(K)$ denotes the measure of K. Replacing the time derivative by the implicit Euler scheme, equation (4.2) is approximated by

$$\frac{\mathrm{m}(K)}{\Delta t}(u_K^k - u_K^{k-1}) + \sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^k = \mathrm{m}(K)f_K. \tag{4.3}$$

The discrete flux $F_{\sigma,K}^k$ through the edge (or face) σ still needs to be defined. In the two-point flux approximation, we wish to replace the gradient by the finite difference $(u_L^k-u_K^k)/\mathrm{dist}(K,L)$, where K and L are the adjacent control volumes of the edge σ, written as $\sigma=K|L$, and $\mathrm{dist}(K,L)$ is some "distance between K and L". The question is how this distance can be defined, since u^k is piecewise constant and generally discontinuous through the edges. Therefore, we introduce a set of points $(x_K)_{K\in\mathcal{T}}$ associated to the control volumes such that the straight line $\overline{x_Kx_L}$ between two centers of neighboring cells is orthogonal to the edge $\sigma=K|L$; see Figure 1. We discuss below which meshes satisfy such a condition. The distance $\mathrm{dist}(K,L)$ is defined as the Euclidean distance $\mathrm{d}(K,L)$ between the points x_K and x_L. Then, if $\sigma=K|L$, the flux $F_{\sigma,K}$ can be approximated by

$$F_{K,\sigma}^k = -\mathrm{m}(\sigma)A(u_\sigma^k)\frac{u_L^k-u_K^k}{\mathrm{d}(x_K,x_L)},$$

where u_σ^k is a mean value of u^k at the edge σ, which still needs to be determined. If the boundary of the control volume is part of the boundary $\partial\Omega$, the flux vanishes because of the no-flux boundary conditions, and we set $F_{K,\sigma}^k=0$ if $\sigma\subset\partial\Omega$. To unify the notation, we introduce the set $\mathcal{E}_{\mathrm{int},K}$ of

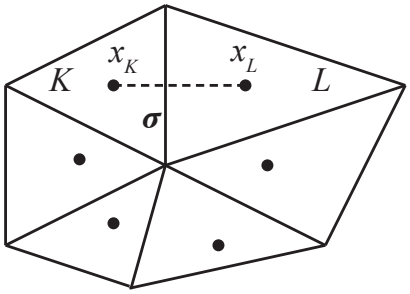

FIGURE 1. Cell-centered method.

edges contained in Ω and the set $\mathcal{E}_{\mathrm{ext},K}$ of edges σ satisfying $\sigma \subset \partial\Omega$. Then $\mathcal{E}_K = \mathcal{E}_{\mathrm{int},K} \cup \mathcal{E}_{\mathrm{ext},K}$ is the set of edges of K. We also define for $\sigma \in \mathcal{E}$ the distance

$$\mathrm{d}_\sigma = \begin{cases} \mathrm{d}(x_K, x_L) & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int},K}, \\ \mathrm{d}(x_K, \sigma) & \text{if } \sigma \in \mathcal{E}_{\mathrm{ext},K}. \end{cases}$$

With the notation

$$v_{K,\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int},K}, \\ v_K & \text{if } \sigma \in \mathcal{E}_{\mathrm{ext},K}, \end{cases}$$

we introduce the discrete operator

$$\mathrm{D}_{K,\sigma} v := v_{K,\sigma} - v_K \quad \text{for } \sigma = K|L, \tag{4.4}$$

which equals $\mathrm{D}_{K,\sigma} v = v_L - v_K$ if $\sigma = K|L$ and $\mathrm{D}_{K,\sigma} v = 0$ if $\sigma \in \mathcal{E}_{\mathrm{ext},K}$. Then the discrete flux becomes

$$F_{K,\sigma}^k = -\mathrm{m}(\sigma) A(u_\sigma^k) \frac{\mathrm{D}_{K,\sigma} u^k}{\mathrm{d}_\sigma}, \quad K \in \mathcal{T},\ \sigma \in \mathcal{E}. \tag{4.5}$$

We still need to define the value of u_σ^k at the edge σ. The choice depends on the desired properties of the scheme. Possible choices are, for instance

$$u_\sigma^k = \frac{1}{2}(u_L^k + u_K^k), \quad u_\sigma^k = \min\{u_L^k, u_K^k\} \quad \text{for } \sigma = K|L. \tag{4.6}$$

The first choice is an arithmetic average, the second one is called an *upwind scheme*. It defines the direction of the "upstream information" with respect to the location of σ. An advantage of the second option is that it preserves the nonnegativity of the solution if $f \le 0$; see Lemma 4.8. Both choices imply that the numerical fluxes $F_{K,\sigma}^k$ are consistent approximations of the exact fluxes through the edges, i.e. $F_{K,\sigma}^k + F_{L,\sigma}^k = 0$ for all $\sigma = K|L$.

We summarize our discussion. Introducing the so-called *transmissibility coefficient*,

$$\tau_\sigma = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}, \tag{4.7}$$

the recursive scheme (4.3) becomes

$$\frac{\mathrm{m}(K)}{\Delta t}(u_K^k - u_K^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma}^k = \mathrm{m}(K) f_K, \quad F_{K,\sigma}^k = -\tau_\sigma A(u_\sigma^k) \mathrm{D}_{K,\sigma} u^k \tag{4.8}$$

for all $K \in \mathcal{T}$. It remains to specify our assumptions on the mesh; see [8, Definition 9.1] for a more detailed definition.

Definition 4.1 (Admissible mesh)**.** *Let $\Omega \subset \mathbb{R}^d$ with $d = 2, 3$ be an open bounded polygonal set. An* admissible mesh *of Ω consists of*

- *a family $\mathcal{T}$ of open polygonal convex sets of Ω, called* control volumes*, which do not overlap and satisfy $\overline{\Omega} = \overline{\cup_{K\in\mathcal{T}} K}$;*
- *a family $\mathcal{E}$ of edges ($d = 2$) or faces ($d = 3$) of the control volumes with positive measure;*
- *a family of points $\mathcal{P} = (x_K)$ of Ω such that $x_K \in \overline{K}$ and the straight line $\overline{x_K x_L}$ between two centers of neighboring cells is orthogonal to the edge $\sigma = K|L$.*

Generally, the structure assumption on the mesh is rather restrictive. However, on non-admissible meshes, the numerical fluxes may not be consistent and the scheme may not converge to the solution to the continuous problem [9]. At least in two space dimension, the construction of admissible triangular meshes is not too difficult as shown by the following examples, which are taken from [8, Example 9.1].

Example 4.2 (Triangular meshes)**.** Let Ω be an open bounded polygonal subset of $\mathbb{R}^2$ and let $\mathcal{T}$ be a family if open triangular disjoint subsets of Ω. We suppose that (i) any two triangles K and L with the common edge $\sigma = K|L$ have two common vertices and (ii) all angles of the triangles are less than $\pi/2$. The latter condition implies that $x_K \in K$. Such a mesh is admissible. Condition (ii) can be relaxed to the so-called *strict Delaunay condition*, i.e., the closure of the circumscribed circle of each triangle does not contain any other triangle of the mesh. Another example of admissible meshes are Voronoï meshes [8, Example 9.2]. Voronoï meshes can be derived as dual grids of boundary-conforming Delaunay triangulations. The construction of Voronoï meshes can also be applied to non-polygonal domains. □

The weak formulation of equation (4.1),

$$\int_\Omega \partial_t u v \mathrm{d}x + \int_\Omega A(u)\nabla u \cdot \nabla v \mathrm{d}x = \int_\Omega f v \mathrm{d}x \quad \text{for } v \in H^1(\Omega)$$

is based on integration by parts. We need a similar property for the numerical scheme.

Lemma 4.3 (Discrete integration by parts)**.** *Let $F^k_{K,\sigma} + F^k_{L,\sigma} = 0$ for $\sigma = K|L$ and let (v_K) be a piecewise constant function. Then*

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F^k_{K,\sigma} v_K = -\sum_{\sigma=K|L\in\mathcal{E}_{\mathrm{int}}} F^k_{K,\sigma}(v_L - v_K),$$

where $\mathcal{E}_{\mathrm{int}} = \cup_{K\in\mathcal{T}} \mathcal{E}_{\mathrm{int},K}$.

Proof. In the sum over $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$, we count every edge twice. Therefore, since $F^k_{K,\sigma} = 0$ for $\sigma \in \mathcal{E}_{\mathrm{ext},K}$,

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F^k_{K,\sigma} v_K = \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma=K|L}} F^k_{K,\sigma} v_K + \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma=K|L}} F^k_{L,\sigma} v_L$$

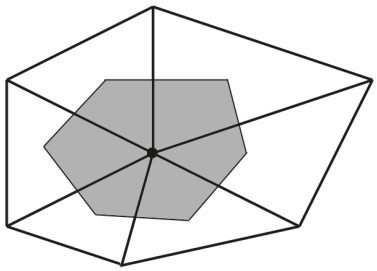

FIGURE 2. Vertex-centered method. The dual mesh consists of polygonal sets around the vertices. The gray area is one control volume.

$$= \sum_{\substack{\sigma\in\mathcal{E}_{\rm int}\\ \sigma=K|L}} F^k_{K,\sigma} v_K - \sum_{\substack{\sigma\in\mathcal{E}_{\rm int}\\ \sigma=K|L}} F^k_{K,\sigma} v_L = - \sum_{\sigma=K|L\in\mathcal{E}_{\rm int}} F^k_{K,\sigma}(v_L - v_K),$$

which proves the statement. □

We finish this subsection with some remarks.

Remark 4.4 (Cell centered versus vertex centered)**.** The presented finite-volume technique belongs to the class of *cell-centered methods*. Another class are *vertex-centered methods*. In cell-centered methods, the control volumes are formed by the mesh cells with the points x_K storing the average value in the control volume. In vertex-centered methods, the control volumes are centered around the vertices of the cells and form a dual mesh, while the vertices store the average value over the control volumes (see Figure 2). The edges of the control volumes are constructed within the cells rather than at the cell interfaces like in the cell-centered method. The cell-centered method is very efficient and requires matrices with low band width (which is equal to the number of cell neighbors plus one). However, the mesh topology is restricted due to the orthogonality requirement. The vertex-centered method is less efficient and requires more storage but the mesh topology does not have the same restrictions as the cell-centered method. □

Remark 4.5 (Comparison with finite differences)**.** Because of the flux definition by the finite difference $\mathrm{D}_{K,\sigma}u^k = u^k_L - u^k_K$ for $\sigma = K|L$, the finite-volume scheme looks like a generalization of the finite-difference method. However, as pointed out in [8, Sec. 5.2], the (finite-difference) truncation error associated to the finite-volume scheme generally does not tend to zero, while this is the case for the finite-difference scheme.

As an example, consider the one-dimensional diffusion equation $-u_{xx} = f$ in $\Omega = (0,1)$. An admissible mesh is given by the family $K_1,\dots,K_N$ such that $K_i = (x_{i-1/2}, x_{i+1/2})$and a family $(x_0,\dots,x_{N+1})$ such that $x_0 = 0$, $x_{N+1} = 1$, and $x_{i-1} < x_{i-1/2} < x_i$ for all $i = 1,\dots,N+1$. We set

$$h_i = \mathrm{m}(K_i) = x_{i+1/2} - x_{i-1/2}, \quad h_{i+1/2} = x_{i+1} - x_i;$$

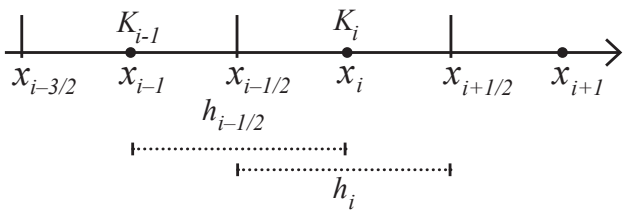

FIGURE 3. One-dimensional non-uniform mesh.

see Figure 3. Let $h = \max\{h_{i/2} : i = 1, \dots, 2N\}$. and $h_{i\pm1/2}/h_i \le C$ for some $C > 0$ independent of h (this condition only becomes relevant in the convergence analysis $h \to 0$). The discrete unknowns u_i for $i = 1, \dots, N$ are approximations of u in the control volume K_i, and we set $f_i = h_i^{-1} \int_{K_i} f(x)\mathrm{d}x$. The finite-volume scheme reads as

$$h_i f_i = \frac{1}{h_i}(F_{i+1/2} - F_{i-1/2}) = \frac{1}{h_i}\bigg(- \frac{u_{i+1} - u_i}{h_{i+1/2}} + \frac{u_i - u_{i-1}}{h_{i-1/2}}\bigg).$$

We wish to compute the finite-difference truncation error

$$T_i := \frac{1}{h_i}\bigg(- \frac{u(x_{i+1}) - u(x_i)}{h_{i+1/2}} + \frac{u(x_i) - u(x_{i-1})}{h_{i-1/2}}\bigg) - h_i f(x_i).$$

Assuming that the functions are sufficiently smooth, inserting the Taylor expansions

$$h_i f_i = \int_{K_i} (f(x_i) + h_i f_x(\xi))\mathrm{d}x = h_i f(x_i) + O(h^2),$$

$$u(x_{i\pm1}) = u(x_i) \pm h_{i\pm1/2} u_x(x_i) + \frac{1}{2} h_{i\pm1/2}^2 u_{xx}(x_i) + O(h^3),$$

and taking into account that $f(x_i) = u_{xx}(x_i)$, we arrive at

$$\begin{aligned} T_i &= \frac{1}{h_i}\bigg\{ - \Big(u_x(x_i) + \frac{1}{2} h_{i+1/2} u_{xx}(x_i)\Big) + \Big(u_x(x_i) - \frac{1}{2} h_{i-1/2} u_{xx}(x_i)\Big)\bigg\} - f(x_i) + O(h) \\ &= -\frac{h_{i+1/2} + h_{i-1/2}}{2h_i} u_{xx}(x_i) + u_{xx}(x_i) + O(h). \end{aligned}$$

If $h = h_i = h_{i\pm1/2}$, the truncation error becomes $T_i = O(h) \to 0$ as $h \to 0$. Generally, however, $(h_{i+1/2} + h_{i-1/2})/(2h_i) \ne 1$, and the truncation error does not tend to zero as $h \to 0$. Thus, the scheme is not consistent in the finite-difference sense (but it is consistent in the finite-volume sense).

The consistent finite-difference scheme is derived from

$$\begin{aligned} f(x_i) &= -u_{xx}(x_i) \\ &= \frac{2}{h_{i+1/2} + h_{i-1/2}}\bigg\{ - \Big(u_x(x_i) + \frac{1}{2} h_{i+1/2} u_{xx}(x_i)\Big) + \Big(u_x(x_i) - \frac{1}{2} h_{i-1/2} u_{xx}(x_i)\Big)\bigg\}, \end{aligned}$$

and reads as

$$\frac{2}{h_{i+1/2} + h_{i-1/2}}\bigg(- \frac{u_{i+1} - u_i}{h_{i+1/2}} + \frac{u_i - u_{i-1}}{h_{i-1/2}}\bigg) = f(x_i).$$

Because of the different prefactor $2/(h_{i+1/2} + h_{i-1/2})$, the truncation error becomes $T_i = -u_{xx}(x_i) + f(x_i) + O(h) = O(h)$, which converges to zero. This shows that the finite-difference and finite-volume schemes coincide for uniform mesh sizes, up to a different approximation of the source term $f(x)$. □

Remark 4.6 (Mixed Dirichlet–Neumann boundary conditions)**.** If the diffusion equation (4.1) is supplemented with the mixed boundary conditions

$$u = u^D \quad \text{on } \Gamma_D, \quad A(u)\nabla \cdot \nabla \nu = 0 \quad \text{on } \Gamma_N,$$

where ν is the exterior unit normal vector to $\partial\Omega = \Gamma_D \cup \Gamma_N$ and u^D is defined on Γ_D, the scheme slightly changes. We assume that each exterior edge is an element of either the Dirichlet or Neumann boundary, $\mathcal{E}_{\mathrm{ext},K} = \mathcal{E}^D_{\mathrm{ext},K} \cup \mathcal{E}^N_{\mathrm{ext},K}$ and $\mathcal{E}_{\mathrm{ext}} = \mathcal{E}^D_{\mathrm{ext}} \cup \mathcal{E}^N_{\mathrm{ext}}$. Then, setting $u^D_\sigma = \mathrm{m}(\sigma)^{-1} \int_\sigma u^D(x)\mathrm{d}x$, we introduce

$$u^k_{K,\sigma} = \begin{cases} u^k_L & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int}}, \\ u^D_\sigma & \text{if } \sigma \in \mathcal{E}^D_{\mathrm{ext},K}, \\ u^k_K & \text{if } \sigma \in \mathcal{E}^N_{\mathrm{ext},K}. \end{cases}$$

The numerical scheme (4.8) does not change but the discrete integration by parts becomes

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F^k_{K,\sigma} = -\sum_{\sigma\in\mathcal{E}} F^k_{K,\sigma} \mathrm{D}_{K,\sigma} u^k + \sum_{\sigma\in\mathcal{E}^D_{\mathrm{ext}}} F^k_{K,\sigma} u^k_{K,\sigma}.$$

We still have local conservation of the numerical fluxes, but they vanish on the Neumann boundary edges, $F^k_{K,\sigma} = 0$ for $\sigma \in \mathcal{E}^N_{\mathrm{ext},K}$. □

4.1.2. Structure preservation. The finite-volume scheme preserves many properties of the continuous diffusion equation, namely

- local conservation of the flux;
- conservation of the total mass if $f = 0$;
- preservation of nonnegativity if $f \le 0$ and $u^0 \ge 0$;
- preservation of the entropy structure.

We already mentioned that the numerical fluxes (4.5) with (4.6) are locally conserved, $F^k_{K,\sigma} + F^k_{L,\sigma} = 0$ for $\sigma = K|L$. This property is automatically satisfied if u_σ is symmetric in K and L. Also conservation of the total mass is an inherent property of the scheme.

Lemma 4.7 (Discrete conservation of the total mass)**.** *Let $f = 0$. Then*

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K) u^k_K = \sum_{K\in\mathcal{T}} \mathrm{m}(K) u^0_K,$$

recalling that $u^0_K = \mathrm{m}(K)^{-1} \int_K u^0(x)\mathrm{d}x$.

Proof. We sum scheme (4.8) over $K \in \mathcal{T}$ and use discrete integration by parts:

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\tau_\sigma}(u^k_K - u^{k-1}_K) = -\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F^k_{K,\sigma} = 2 \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma=K|L}} F^k_{K,\sigma} = \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma=K|L}} (F^k_{K,\sigma} + F^k_{L,\sigma}) = 0.$$

Thus, by recursion,

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K) u^k_K = \sum_{K\in\mathcal{T}} \mathrm{m}(K) u^{k-1}_K = \cdots = \sum_{K\in\mathcal{T}} \mathrm{m}(K) u^0_K,$$

which ends the proof. □

Lemma 4.8 (Preservation of nonnegativity)**.** *Let $A(z) = 0$ for $z \le 0$, $f_K \le 0$ and let $u^0_K \ge 0$ for all $K \in \mathcal{T}$. The value of u^k on the edge is given by the upwind scheme $u^k_\sigma = \min\{u^k_L, u^k_K\}$. Then the solution to (4.3), if it exists, satisfies $u^k_K \ge 0$ for all $K \in \mathcal{T}$.*

PROOF. We assume, by recursion, that $u_K^{k-1} \geq 0$ for all $K \in \mathcal{T}$ for some $k \geq 1$. If $k = 1$, this property is satisfied by assumption. The goal is show that $u_K^k \geq 0$. To this end, we multiply (4.8) by $(u_K^k)^- = \min\{0, u_K^k\}$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$\begin{aligned} 0 \geq \sum_{K\in\mathcal{T}} \mathrm{m}(K) f_K &= \sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(u_K^k - u_K^{k-1})(u_K^k)^- + \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^k (u_K^k)^- \\ &= \sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(u_K^k - u_K^{k-1})(u_K^k)^- - \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma = K|L}} F_{K,\sigma}^k \big((u_L^k)^- - (u_K^k)^-\big). \end{aligned}$$

The function $z \mapsto z^-$ is convex, which implies that $(z-y)z^- \geq \frac{1}{2}((z^-)^2 - (y^-)^2)$. Taking into account definition (4.5) of $F_{K,\sigma}^k$, we infer that

$$\frac{1}{2}\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}\big([(u_K^k)^-]^2 - [(u_K^{k-1})^-]^2\big) \leq -\sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}} \\ \sigma = K|L}} \tau_\sigma A(u_\sigma^k)(u_L^k - u_K^k)\big((u_L^k)^- - (u_K^k)^-\big). \tag{4.9}$$

If both $u_L^k \geq 0$ and $u_K^k \geq 0$, the right-hand side is nonpositive (since $A(u_\sigma^k) \geq 0$ by assumption). If $u_L^k < 0$ or $u_K^k < 0$, the upwind definition of u_σ implies that $u_\sigma^k = 0$. Since $A(z) = 0$ for $z \leq 0$, we have $A(u_\sigma^k) = 0$ in this case. Thus, the right-hand side of (4.9) is nonpositive or zero. Since our recursion assumption implies that $(u_K^{k-1})^- = 0$, we arrive at

$$\frac{1}{2}\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}[(u_K^k)^-]^2 \leq 0.$$

We conclude that $(u_K^k)^- = 0$ and thus $u_K^k \geq 0$ for $K \in \mathcal{T}$. □

Finally, we discuss the preservation of the entropy structure at the discrete level. Let $h \in C^1([0,\infty))$ be a convex function. We use the test function $h'(u)$ in the weak formulation of the continuous equation (4.1) with $f = 0$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h(u)\mathrm{d}x = \int_\Omega h'(u)\partial_t u \mathrm{d}x = -\int_\Omega A(u)h''(u)|\nabla u|^2 \mathrm{d}x, \tag{4.10}$$

and the right-hand side is nonpositive since $h''(u) \geq 0$ by assumption. Thus, any convex function is a Lyapunov functional (or entropy density) along the solutions to (4.1) with $f = 0$.

To translate this property to the discrete level, we multiply scheme (4.8) by $h'(u_K^k)$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$\begin{aligned} \sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(u_K^k - u_K^{k-1})h'(u_K^k) &= \sum_{K\in\mathcal{K}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma A(u_\sigma^k)\mathrm{D}_{K,\sigma}(u^k)h'(u_K^k) \\ &= -\sum_{\sigma = K|L\in\mathcal{E}_{\mathrm{int}}} \tau_\sigma A(u_\sigma^k)(u_L^k - u_K^k)(h'(u_L^k) - h'(u_K^k)). \end{aligned}$$

We deduce from the convexity of h that $(z-y)h'(z) \geq h(z)-h(y)$ for all $z, y \geq 0$, which yields

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(h(u_K^k) - h(_K^{k-1})) \leq -\sum_{\sigma\in\mathcal{E}_{\rm int}} \tau_\sigma A(u_\sigma^k)(u_L^k - u_K^k)(h'(u_L^k) - h'(u_K^k)).$$

By the mean-value theorem, we can define u_σ^k (if it exists) as the generalized *Stolarsky mean* [20]

$$h''(u_\sigma^k) = \frac{h'(u_L^k) - h'(u_K^k)}{u_L^k - u_K^k} \quad \text{for } \sigma = K|L,\ k\in\mathbb{N}.$$

This yields the discrete analog of (4.10):

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(h(u_K^k) - h(_K^{k-1})) \leq -\sum_{\sigma\in\mathcal{E}_{\rm int}} \tau_\sigma A(u_\sigma^k)h''(u_\sigma^k)(u_L^k - u_K^k)^2.$$

An example for an entropy density is $h(u) = u(\log u - 1)$. Then $h'(u) = \log u$, which shows that we need to be careful with the definition of u_σ^k if $u_K^k = 0$ or $u_L^k = 0$. Therefore, we define the mean value as

$$u_\sigma^k = \begin{cases} \widetilde{u}_\sigma^k & \text{if } u_K^k > 0,\ u_{K,\sigma}^k > 0, \text{ and } u_K^k \neq u_{K,\sigma}^k, \\ u_K^k & \text{if } u_K^k = u_{K,\sigma}^k > 0, \\ 0 & \text{else}, \end{cases} \tag{4.11}$$

where $\widetilde{u}_\sigma^k \in (0,\infty)$ is the unique solution to

$$h''(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma}u^k = \mathrm{D}_{K,\sigma}h'(u^k) \quad \text{for } K\in\mathcal{T},\ \sigma\in\mathcal{E}_K,\ i=1,\ldots,n. \tag{4.12}$$

This equation is the discrete version of the chain rule $h''(u)\nabla u = \nabla h'(u)$. Equation (4.12) is solvable by the mean-value theorem applied to the function h'. The solution $\widetilde{u}_\sigma^k$ is unique if h'' is strictly monotone.

The discrete chain rule (4.12) resembles the discrete-gradient method [11, Sec. V.5]. If h equals the Boltzmann entropy density $h(u) = u(\log u - 1)$, the discrete chain rule (4.12) becomes the *logarithmic mean*

$$\widetilde{u}_\sigma^k = \frac{u_L^k - u_K^k}{\log u_L^k - \log u_K^k} \quad \text{for } \sigma = K|L \text{ if } u_L^k > 0,\ u_K^k > 0.$$

The logarithmic mean is well-known in numerical analysis [2, (28)] and in gradient-flow Markov chains [19, (1.3)]. Property (4.12) can be also satisfied for the power-law entropy densities $h(u) = u^\alpha$ with $\alpha > 0$.

If $h(u) = u(\log u - 1)$, Definition (4.11) of u_σ^k is consistent with the discrete chain rule (4.12). Indeed, let $u_L^k > 0$ and $u_K^k \to 0$. Then $h'(u_K^k) = \log u_K^k \to -\infty$ and $h''(\widetilde{u}_\sigma^k)(u_L^k - u_K^k) = h'(u_L^k) - h'(u_K^k) \to \infty$. We deduce from $h''(\widetilde{u}_\sigma^k) = 1/\widetilde{u}_\sigma^k \to \infty$ that $\widetilde{u}_\sigma^k \to 0$, which is consistent with the definition $u_\sigma^k = 0$ if $u_K^k = 0$.

We summarize our results in the following lemma.

Lemma 4.9 (Preservation of the entropy structure)**.** *Let $h : [0,\infty) \to \mathbb{R}$ be a convex function such that h'' is strictly monotone and introduce the discrete entropy*

$$\mathcal{H}_d(u^k) = \sum_{K\in\mathcal{T}} \mathrm{m}(K) h(u_K^k), \quad k \ge 0.$$

Then the function $k \mapsto \mathcal{H}(u^k)$ is nonincreasing for $k \in \mathbb{N}$. Moreover, if u_σ^k is defined by (4.11), then the discrete analog of (4.10) holds:

$$\mathcal{H}_d(u^k) + \sum_{\sigma\in\mathcal{E}_{\rm int}} \tau_\sigma A(u_\sigma^k) h''(u_\sigma)(u_L^k - u_K^k)^2 \le \mathcal{H}_d(u^{k-1}), \quad k \in \mathbb{N}.$$

4.2. Finite volumes for population systems

The goal of this section is to design a structure-preserving finite-volume scheme for population cross-diffusion models. First, we present a general scheme and then apply it to some examples. We proceed as in [12].

4.2.1. General scheme.

We wish to discretize the cross-diffusion equations

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j\right) = r_i(u) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{4.13}$$

$$\sum_{j=1}^n A_{ij}(u)\nabla u_j\cdot\nu = 0 \quad \text{on } \partial\Omega,\ t>0, \quad u_i(0) = u_i^0 \quad \text{in } \Omega, \tag{4.14}$$

where $\Omega \subset \mathbb{R}^d$ ($d \ge 1$) is a bounded domain, $u = (u_1,\ldots,u_n)$ is the density vector, and ν is the exterior unit normal vector to $\partial\Omega$. We assume that this system has a weak solution that is nonnegative componentwise and an entropy structure in the sense that there exists an entropy density $h(u)$ such that $h''(u)A(u)$ is uniformly positive definite. Then the following entropy inequality holds:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h(u)\mathrm{d}x &= \int_\Omega \partial_t u\cdot h'(u)\mathrm{d}x = -\int_\Omega \nabla u^T h''(u)A(u)\nabla u\mathrm{d}x + \int_\Omega f(u)\cdot h'(u)\mathrm{d}x \\ &\le -c\int_\Omega |\nabla u|^2\mathrm{d}x + \int_\Omega f(u)\cdot h'(u)\mathrm{d}x,\end{aligned}$$

where $c > 0$ is the smallest eigenvalue of $h''(u)A(u)$ and $f(u) = (f_1(u),\ldots,f_n(u))$.

The goal is to design a finite-volume scheme that preserves this structure and the nonnegativity of the solutions. This is a nontrivial task because of the cross-diffusion terms. Our main assumption is that the entropy density is the sum of the single-species entropy densities $h_i(u_i)$. A more general entropy density is considered in Section 4.3.

Let $(\mathcal{T},\mathcal{E},\mathcal{P})$ be an admissible mesh (see Definition 4.1) with the mesh size $\Delta x := \max_{K\in\mathcal{T}}\operatorname{diam}(K)$. We denote for some given end time $T > 0$ by $\Delta t = T/N$ for $N \in \mathbb{N}$ the time step size and set $t_k = k\Delta t$ for $k = 0,\ldots,N$. The space of spatially piecewise constant

functions is defined by

$$V_{\Delta x} = \left\{ v : \Omega \to \mathbb{R} : \exists (v_K)_{K\in\mathcal{T}} \subset \mathbb{R},\ v(x) = \sum_{K\in\mathcal{T}} v_K 1_K(x) \right\},$$

where 1_K is the characteristic function on K.

We introduce the numerical scheme for the cross-diffusion model (4.13)–(4.14). The initial functions are approximated by

$$u_{i,K}^0 = \frac{1}{\mathrm{m}(K)} \int_K u_i^0(x)\mathrm{d}x \quad \text{for } K\in\mathcal{T},\ i=1,\ldots,n.$$

Let $u^{k-1} = (u_1^{k-1},\ldots,u_n^{k-1}) \in V_{\Delta x}^n$ be given. The values $u_{i,K}^k$ are determined from the implicit Euler finite-volume scheme

$$\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}^k - u_{i,K}^{k-1}) + \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k = \mathrm{m}(K) r_i(u_K^k), \quad i=1,\ldots,n, \tag{4.15}$$

where the fluxes $F_{i,K,\sigma}^k$ are given by

$$F_{i,K,\sigma}^k = -\sum_{j=1}^n \tau_\sigma A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_j^k \quad \text{for } K\in\mathcal{T},\ \sigma\in\mathcal{E}_K, \tag{4.16}$$

recalling definition (4.7) of τ_σ and definition (4.4) of $\mathrm{D}_{K,\sigma}$.

It remains to determine the values u_σ^k on the edges. We suppose that h is convex and that h'' is strictly monotone. We wish to choose this value in such a way that the discrete analog $h''(\widetilde{v}_\sigma)(v_L - v_K) = h'(v_L) - h'(v_K)$ for $v\in V_{\Delta x}$ of the chain rule $h''(u)\nabla u = \nabla h'(u)$ holds. The difficulty is that the mean-value theorem for vector-valued functions can be formulated only as

$$\left(\int_0^1 h''(\theta v_L + (1-\theta)v_K)\mathrm{d}\theta\right)(v_L - v_K) = h'(v_L) - h'(v_K),$$

and generally a mean vector $\widetilde{v}_\sigma$ cannot be found. Therefore, we assume that the entropy density is the sum of the single-species entropy densities, $h(u) = \sum_{i=1}^n h_i(u_i)$. Then the Hessian h'' is diagonal, and the standard mean-value theorem can be applied *componentwise* like in the previous section.

More precisely, we define for $i=1,\ldots,n$ the mean value

$$u_{i,\sigma}^k = \begin{cases} \widetilde{u}_{i,\sigma}^k & \text{if } u_{i,K}^k > 0,\ u_{i,K,\sigma}^k > 0, \text{ and } u_{i,K}^k \neq u_{i,K,\sigma}^k, \\ u_{i,K}^k & \text{if } u_{i,K}^k = u_{i,K,\sigma}^k > 0, \\ 0 & \text{else,} \end{cases} \tag{4.17}$$

where $\widetilde{u}_{i,\sigma}^k \in (0,\infty)$ is the unique solution to

$$h_i''(\widetilde{u}_{i,\sigma}^k)\mathrm{D}_{K,\sigma}u_i^k = \mathrm{D}_{K,\sigma}h_i'(u_i^k) \quad \text{for } K\in\mathcal{T},\ \sigma\in\mathcal{E}_K,\ i=1,\ldots,n. \tag{4.18}$$

As shown in the previous section, this equation is uniquely solvable. Moreover, $\widetilde{u}_{i,\sigma}^k$ lies between $u_{i,K}^k$ and $u_{i,L}^k$ if $\sigma = K|L$. Hence,

$$\min\{u_{i,K}^k, u_{i,K,\sigma}^k\} \le \widetilde{u}_{i,\sigma}^k \le \max\{u_{i,K}^k, u_{i,K,\sigma}^k\} \quad \text{for } K \in \mathcal{T},\ \sigma \in \mathcal{E}_K,\ i = 1, \ldots, n.$$

Before verifying the preservation of the entropy structure, we detail the hypotheses. We set $\mathcal{D} := (0,\infty)^n$.

(H1) Domain: $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) is a bounded polygonal domain.

(H2) Discretization: $(\mathcal{T}, \mathcal{E}, \mathcal{P})$ and $(\Delta t, N)$ is a space-time discretization of $\Omega \times (0,T)$ composed of an admissible mesh $\mathcal{T}$ and the values $\Delta t > 0$, $N \in \mathbb{N}$.

(H3) Initial data: $u^0 = (u_1^0, \ldots, u_n^0) \in L^1(\Omega; \overline{\mathcal{D}})$ satisfies $\int_\Omega h(u^0)\mathrm{d}x < \infty$.

(H4) Entropy density: $h(u) = \sum_{i=1}^n h_i(u_i)$, where $h_i \in C^2(0,\infty) \cap C^0([0,\infty))$ is nonnegative and convex, $h_i' : (0,\infty) \to \mathbb{R}$ is invertible, h_i'' is strictly monotone, and there exists $c_h > 0$ such that $h_i(s) \ge c_h(s-1)$ for $s \ge 0$, $i = 1, \ldots, n$.

(H5) Diffusion matrix: $A \in C^0(\overline{\mathcal{D}}; \mathbb{R}^{n\times n})$, and there exist $c_A > 0$, $s \ge 1/2$ such that

$$z^T h''(u) A(u) z \ge c_A \sum_{i=1}^n u_i^{2s-2} z_i^2 \quad \text{for all } z \in \mathbb{R}^n,\ u \in \mathcal{D}.$$

(H6) Source terms: $r = (r_1, \ldots, r_n) \in C^0(\overline{\mathcal{D}}; \mathbb{R}^n)$, and there exists $C_r > 0$ such that for all $u \in \overline{\mathcal{D}}$,

$$r(u) \cdot h'(u) \le C_r(1 + h(u)).$$

Assuming that a solution to scheme (4.15)–(4.16) exists, the discrete entropy

$$\mathcal{H}_d(u^k) = \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) h_i(u_{i,K}^k), \quad k \ge 0,$$

fulfills a discrete entropy inequality, showing that the scheme preserves the entropy structure.

Theorem 4.10 (Discrete entropy inequality)**.** *Let Hypotheses (H1)–(H6) hold and let $u^k = (u_1^k, \ldots, u_n^k) \in V_{\Delta x}^n$ be a solution to (4.15)–(4.18) satisfying $u_{i,K}^k > 0$ for $K \in \mathcal{T}$, $k \ge 1$, and $i = 1, \ldots, n$. Then, for any $k \ge 1$,*

$$(1 - C_r\Delta t)\mathcal{H}_d(u^k) + c_A\Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (u_{i,\sigma}^k)^{2s-2} (\mathrm{D}_{K,\sigma} u_i^k)^2 \le \mathcal{H}_d(u^{k-1}) + C_r\Delta t \mathrm{m}(\Omega). \tag{4.19}$$

In particular, if $C_r = 0$, the discrete entropy $k \mapsto \mathcal{H}_d(u^k)$ is nonincreasing.

Proof. Let $w_{i,K}^k := h'(u_{i,K}^k)$ for $i = 1, \ldots, n$ be the entropy variables. We multiply scheme (4.15) by $w_{i,K}^k$ and sum over $i = 1, \ldots, n$ and $K \in \mathcal{T}$. Then $I_1 + I_2 + I_3 = 0$, where

$$I_1 = \frac{1}{\Delta t} \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_{i,K}^k - u_{i,K}^{k-1}) w_{i,K}^k,$$

$$I_2 = \sum_{i=1}^n \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k w_{i,K}^k,$$

$$I_3 = -\sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) r_i(u_K^k) w_{i,K}^k.$$

The convexity of $z \mapsto h_i(z)$ for $z > 0$ implies that $(z-y)h_i'(z) \ge h_i(z) - h_i(y)$ for all $y, z > 0$. Hence, the first term becomes

$$I_1 \ge \frac{1}{\Delta t}\sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(h_i(u_{i,K}^k) - h_i(u_{i,K}^{k-1})\big) = \frac{1}{\Delta t}\big(\mathcal{H}_d(u^k) - \mathcal{H}_d(u^{k-1})\big).$$

We rewrite the second term by using discrete integration by parts and the chain rule (4.18):

$$\begin{aligned} I_2 &= -\sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} F_{i,K,\sigma}^k \mathrm{D}_{K,\sigma} w_{i,K}^k \\ &= \sum_{i,j=1}^n \sum_{\sigma=K|L\in\mathcal{E}_{\rm int}} \tau_\sigma A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_j^k \mathrm{D}_{K,\sigma}h_i'(u_i^k) \\ &= \sum_{i,j=1}^n \sum_{\sigma=K|L\in\mathcal{E}_{\rm int}} \tau_\sigma h_i''(u_{i,\sigma}^k) A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_i^k \mathrm{D}_{K,\sigma}u_j^k. \end{aligned}$$

This expression is bounded from below by Hypothesis (H5):

$$I_2 \ge c_A \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (u_{i,\sigma}^k)^{2s-2} (\mathrm{D}_{K,\sigma}u_i^k)^2.$$

Finally, we deduce from Hypothesis (H6) that

$$I_3 \ge -C_r \sum_{K\in\mathcal{T}} \mathrm{m}(K)(1 + h(u_K^k)) = -C_r\Delta t(\mathrm{m}(\Omega) + \mathcal{H}_d(u^k)).$$

These estimates yield

$$\mathcal{H}_d(u^k) + c_A\Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (u_{i,\sigma}^k)^{2s-2} (\mathrm{D}_{K,\sigma}u_i^k)^2 \le C_r\Delta t(\mathrm{m}(\Omega) + \mathcal{H}_d(u^k)),$$

finishing the proof. □

The nonnegativity of solutions is a by-product of the existence analysis which is based on the formulation in terms of entropy variables.

Theorem 4.11 (Existence of discrete solutions)**.** *Let Hypotheses (H1)–(H6) hold and let* $\Delta t < 1/C_r$*. Then there exists a solution* $u^k = (u_1^k, \ldots, u_n^k) \in V_{\Delta x}^n$ *to scheme* (4.15)–(4.18) *satisfying*

$$u_{i,K}^k \ge 0 \quad \textit{for all } K \in \mathcal{T},\ k \ge 1,\ i = 1, \ldots, n.$$

If $s \ge 1$*,* u^k *satisfies the discrete entropy inequality* (4.19)*.*

The proof of this result is based on Schaefer's fixed-point theorem.

Theorem 4.12 (Schaefer)**.** *Let X be a finite-dimensional vector space and $S : X \to X$ be a continuous mapping. We assume that the set*

$$Y := \{v \in X : \exists \theta \in [0,1],\ v = \theta S(v)\}$$

is bounded. Then S has a fixed point.

The idea of the theorem is a homotopy argument: Setting $Y_\theta = \{v \in X : v = \theta S(v)\}$, we have $Y = \cup_{\theta\in[0,1]} Y_\theta$. The idea is to "deform" the nonempty set $Y_0 = \{0\}$ to Y_1 by means of the sets Y_θ. The theorem states that if we have a bound on any fixed point of the mapping θS for $\theta \in [0,1]$, then Y_1 is nonempty, and there exists a fixed point of S. In nonlinear PDEs, the bounds are a consequence of a priori estimates. In this sense, supposing that a solution to the nonlinear PDE exists, the a priori estimates show that a solution indeed exists. Theorem 4.12 is a consequence of Brouwer's fixed-point theorem. It is also valid in infinite-dimensional spaces if S is compact. We refer to [6, Sec. 9.2.2] for a proof.

Proof of Theorem 4.11. We proceed by induction. If $k = 0$, we have $u_{i,K}^k \geq 0$ for all $K \in \mathcal{T}$, $i = 1, \ldots, n$ by Hypothesis (H3). Assume that there exists a solution u^{k-1} to scheme (4.15)–(4.16) satisfying $u_{i,K}^{k-1} \geq 0$ for $K \in \mathcal{T}$, $i = 1, \ldots, n$. For the construction of u^k, we use a fixed-point argument.

▶ *Step 1: Construction of the fixed-point operator.* Let $\varepsilon > 0$ and define the operator $S : V_{\Delta x}^n \to V_{\Delta x}^n$, $S(v) = w$, where $w \in V_{\Delta x}^n$ is the unique solution to

$$\varepsilon \mathrm{m}(K) w_{i,K} = -\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}(v) - u_{i,K}^{k-1}) - \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}(v) + \mathrm{m}(K) r_i(u_K(v)), \tag{4.20}$$

Here, we interpret the densities as functions of v, i.e.

$$u_{i,K}(v) := (h_i')^{-1}(v_{i,K}), \quad F_{i,K,\sigma}(v) := -\sum_{j=1}^n \tau_\sigma A_{ij}(u_\sigma(v)) \mathrm{D}_{K,\sigma} u_j(v), \tag{4.21}$$

and $u_\sigma(v)$ is determined by (4.17) with $(u_{i,K}^k, u_{i,K,\sigma}^k)$ replaced by $(u_{i,K}(v), u_{i,K,\sigma}(v))$. The finite-dimensional space $V_{\Delta x}$ is endowed with the norm

$$\|w_i\|_{0,2,\mathcal{T}} = \left(\sum_{K\in\mathcal{K}} \mathrm{m}(K) w_{i,K}^2\right)^{1/2}.$$

Since $V_{\Delta x}$ is finite-dimensional, in fact all norms are equivalent. The regularization on the left-hand side of (4.20) is needed to prove the existence of solutions in the entropy variable formulation (to obtain a bound in terms of w_i) and to conclude that $u_{i,K}(v) = (h_i')^{-1}(v_{i,K})$ is positive (which follows from the fact that $(h_i')^{-1}$ maps $\mathbb{R}^n$ to $(0,\infty)^n$).

▶ *Step 2: Continuity of S.* Let $i \in \{1, \ldots, n\}$ be fixed. We show first an a priori estimate. For this, we multiply (4.20) by $w_{i,K}$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$\varepsilon \|w_i\|_{0,2,\mathcal{T}}^2 = -\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}(v) - u_{i,K}^{k-1}) w_{i,K} + \sum_{\sigma=K|L\in\mathcal{E}_{\mathrm{int}}} F_{i,K,\sigma}(v) \mathrm{D}_{K,\sigma} w_i \tag{4.22}$$

$$+\sum_{K\in\mathcal{T}}\mathrm{m}(K)r_i(u_K(v))w_{i,K} =: J_1+J_2+J_3.$$

It follows from the Cauchy–Schwarz inequality and definition (4.21) of $F_{i,K,\sigma}(v)$ that

$$\begin{aligned}
J_1 &\le \frac{1}{\Delta t}\|u_i(v)-u_i^{k-1}\|_{0,2,\mathcal{T}}\|w_i\|_{0,2,\mathcal{T}},\\
J_2 &= \bigg(\sum_{j=1}^n\sum_{\sigma\in\mathcal{E}}\tau_\sigma A_{ij}(u_\sigma(v))(\mathrm{D}_{K,\sigma}u_j(v))^2\bigg)^{1/2}\bigg(\sum_{\sigma\in\mathcal{E}}\tau_\sigma(\mathrm{D}_{K,\sigma}w_i)^2\bigg)^{1/2},\\
J_3 &\le \|r_i(u(v))\|_{0,2,\mathcal{T}}\|w_i\|_{0,2,\mathcal{T}}.
\end{aligned}$$

We infer from (4.22) that

$$\varepsilon\|w_i\|_{0,2,\mathcal{T}}^2 \le C\Big(1+\max_{i=1,\ldots,n}\|v_i\|_{0,2,\mathcal{T}}\Big)\|w_i\|_{0,2,\mathcal{T}},$$

since $u_i(v)$ depends only on v and all norms are equivalent on $V_{\Delta x}$. Here, $C>0$ is some constant being independent of v and w. This shows that

$$\|w_i\|_{0,2,\mathcal{T}} \le C\varepsilon^{-1}\Big(1+\max_{i=1,\ldots,n}\|v_i\|_{0,2,\mathcal{T}}\Big). \tag{4.23}$$

Next, we turn to the continuity of S. Let $(v^m)_{m\in\mathbb{N}}\subset V_{\Delta x}^n$ be such that $v^m\to v$ as $m\to\infty$. Then $(v^m)_m$ is bounded. Estimate (4.23) implies that also $(w^m)_m$, defined by $w^m:=S(v^m)$, is bounded. By the theorem of Bolzano–Weierstraß, there exists a subsequence of (w^m), which is not relabeled, such that $w^m\to w$ as $m\to\infty$. Passing to the limit $m\to\infty$ in scheme (4.20) and taking into account the continuity of the nonlinear functions, we conclude that w_i is a solution to (4.20) and $w=S(v)$. Because of the uniqueness of the limit function, the whole sequence converges. This proves that S is continuous.

▶ *Step 3: Existence of a fixed point.* Let $\theta\in[0,1]$ and let $w=\theta S(w)$, i.e., w_i solves

$$\varepsilon\mathrm{m}(K)w_{i,K} = -\theta\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}(w)-u_{i,K}^{k-1}) - \theta\sum_{\sigma\in\mathcal{E}_K}F_{i,K,\sigma}(w) + \theta\mathrm{m}(K)r_i(u_K(w)).$$

We have to show that w is uniformly bounded. By Hypothesis (H4), we can define $u_i(w):=(h_i')^{-1}(w_i)>0$. The proof of Theorem 4.10 shows the following discrete entropy inequality:

$$\begin{aligned}
&(1-C_r\Delta t)\mathcal{H}(u^k)+\varepsilon\Delta t\sum_{i=1}^n\|w_i\|_{0,2,\mathcal{T}}^2\\
&\quad+\theta c_A\Delta t\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}}\tau_\sigma(u_{i,\sigma}^k)^{2s-2}(\mathrm{D}_{K,\sigma}u_i^k)^2 \le \theta\mathcal{H}(u^{k-1})+\theta C_r\Delta t\mathrm{m}(\Omega),
\end{aligned} \tag{4.24}$$

which differs from the inequality in Theorem 4.10 by the additional norm for w_i and the factor $\theta\in[0,1]$. Set

$$R^2 := \frac{1}{\varepsilon\Delta t}\big(\mathcal{H}(u^{k-1})+C_r\Delta t\mathrm{m}(\Omega)\big).$$

Then $\|w_i\|_{0,2,\mathcal{T}}^2 \le \theta R^2 \le R^2$. Since the value R is universal (it does not depend on w or θ), this shows that the set $\{w : w = \theta S(w) \text{ for some } \theta \in [0,1]\}$ is bounded. By Schaefer's fixed-point theorem, there exists a solution $w^\varepsilon := w$ to (4.20) with $v = w$.

▶ *Step 4: Limit $\varepsilon \to 0$ and nonnegativity.* We define $u_i^\varepsilon := (h_i')'(w_i^\varepsilon)$. By Hypothesis (H4), this function is positive. We pass to the limit $\varepsilon \to 0$ in the variable u_i^ε and not w_i^ε, since we do not have an ε-independent estimate for w_i^ε. To derive such a bound for u_i^ε, we use the condition $h_i(u_{i,K}^\varepsilon) \ge c_h(u_{i,K}^\varepsilon - 1)$ from Hypothesis (H4). This is the only place where we use this property. We infer from (4.24) for $\theta = 1$ that, for any $K \in \mathcal{T}$,

$$c_h \mathrm{m}(K)(u_{i,K}^\varepsilon - 1) \le \mathrm{m}(K) h_i(u_{i,K}^\varepsilon) \le \mathcal{H}_d(u^\varepsilon) \le \frac{\mathcal{H}_d(u^{k-1}) + C_r \Delta t \mathrm{m}(\Omega)}{1 - C_r \Delta t}.$$

Hence, $(u_{i,K}^\varepsilon)$ is bounded uniformly in ε, and there exists a subsequence (not relabeled) such that $u_{i,K}^\varepsilon \to u_{i,K}^k$ as $\varepsilon \to 0$. We deduce from inequality (4.24) with $\theta = 1$ that

$$\varepsilon \|w_i^\varepsilon\|_{0,2,\mathcal{T}}^2 \le (\Delta t)^{-1}\big(\mathcal{H}_d(u^{k-1}) + C_r \Delta t \mathrm{m}(\Omega)\big),$$

which implies a bound for $\sqrt{\varepsilon} w_{i,K}^\varepsilon$. Consequently, $\varepsilon w_{i,K}^\varepsilon \to 0$ as $\varepsilon \to 0$. Therefore, we can pass to the limit $\varepsilon \to 0$ in scheme (4.20) with $v = w$ to deduce the existence of a solution u^k to (4.15)–(4.16). As $u_{i,K}^\varepsilon$ is positive, its limit function $u_{i,K}^k$ is nonnegative. Finally, assuming that $s \ge 1$, we can pass to the limit $\varepsilon \to 0$ in the approximate discrete entropy inequality (4.24) with $\theta = 1$, showing that u^k satisfies the discrete entropy inequality (4.19). □

In the case $s < 1$, the limit $\varepsilon \to 0$ in the regularized discrete entropy inequality (4.24) with $\theta = 1$ is nontrivial since the expression $(u_{i,\sigma}(w^\varepsilon))^{2s-2}$ diverges if $u_{i,\sigma}(w^\varepsilon) \to 0$. Under rather weak additional assumptions, we are able to prove that the limit $u_{i,\sigma}^k$ is positive, which removes the singularity and makes possible the limit $\varepsilon \to 0$ in the discrete entropy inequality also for $s < 1$.

Proposition 4.13. *Let Hypothesis (H6) with $s < 1$ hold, $\int_\Omega u_i^0 \mathrm{d}x > 0$, and let $r_i(u) \ge -c_r u_i$ for $u \in [0,\infty)^n$, $i = 1,\ldots,n$. Furthermore, let $u^k \in V_{\Delta x}^n$ be the solution to scheme (4.15)–(4.16) constructed in Theorem 4.11. Then*

$$u_{i,K}^k > 0 \quad \text{for all } K \in \mathcal{T},\ k \in \mathbb{N},\ i = 1,\ldots,n,$$

and u^k satisfies the discrete entropy inequality (4.19) for any $s \ge 1/2$.

Proof. The proof is taken from [14, Sec. 4]. First, we show that the total mass $\int_\Omega u_i^k \mathrm{d}x$ is positive, thanks to the assumption $r_i(u) \ge -c_r u_i$. To this end, we sum (4.20) with $v = w^k$ over $K \in \mathcal{T}$, set $u_{i,K}^\varepsilon := u_{i,K}(w^\varepsilon)$, and use the local balance equations $F_{i,K,\sigma}(w^k) + F_{i,L,\sigma}(w^k) = 0$ to deduce that, by induction,

$$\begin{aligned}\sum_{K\in\mathcal{T}} \mathrm{m}(K) u_{i,K}^\varepsilon &= \sum_{K\in\mathcal{T}} \mathrm{m}(K) u_{i,K}^{k-1} - \varepsilon\Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K) w_{i,K}^k + \Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K) r_i(u_K^\varepsilon) \\ &\ge \sum_{K\in\mathcal{T}} \mathrm{m}(K) u_{i,K}^\varepsilon - \varepsilon\Delta t \sum_{j=1}^k \sum_{K\in\mathcal{T}} \mathrm{m}(K) w_{i,K}^j - c_r \Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K) u_{i,K}^\varepsilon.\end{aligned}$$

Denoting by $u_{i,K}^k$ the limit function of $u_{i,K}^\varepsilon$ as $\varepsilon\to 0$, this limit yields

$$\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^k \ge \sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^0 - c_r\Delta t\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^k.$$

We infer that

$$\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^k \ge \frac{\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^{k-1}}{1+c_r\Delta t} \ge \frac{\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^0}{(1+c_r\Delta t)^k} > 0. \tag{4.25}$$

With this bound at hand, we proceed to the proof of the positivity of $u_{i,K}^k$. Let $i\in\{1,\ldots,n\}$ and $k\in\mathbb{N}$ be fixed. Assume by contradiction that there exists $K\in\mathcal{T}$ such that $u_{i,K}^k=0$. The approximate discrete entropy inequality (4.24) shows that

$$(u_{i,\sigma}^\varepsilon)^{2(s-1)}(\mathrm{D}_{K,\sigma}u_i^\varepsilon)^2 \le C(\Delta t,u^{k-1}),$$

and hence,

$$(u_{i,L}^\varepsilon - u_{i,K}^\varepsilon)^2 \le C(\Delta t,u^{k-1})(u_{i,\sigma}^\varepsilon)^{2-2s}.$$

This becomes in the limit $\varepsilon\to 0$ (because of $s<1$):

$$(u_{i,L}^k)^2 = (u_{i,L}^k - u_{i,K}^k)^2 \le C(\Delta t,u^{k-1})(u_{i,\sigma}^k)^{2-2s}.$$

Now, $u_{i,K}^k=0$ implies that $u_{i,\sigma}^k=0$ and consequently $u_{i,L}^k=0$. Let L' be a neighboring control volume of L. By the same argument as before, it follows that also $u_{i,L'}^k=0$. Repeating this argument for all control volumes in the finite set $\mathcal{T}$, we infer that $u_{i,K}^k=0$ for all $K\in\mathcal{T}$. Then the total mass vanishes, $\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}^k=0$, which contradicts (4.25). We conclude that $u_{i,K}^k>0$ for all $K\in\mathcal{T}$. □

4.2.2. Examples. We present some examples for which the model assumptions (H4)–(H6) are fulfilled.

► *Shigesada–Kawaski–Teramoto system.* We consider equations (4.13)–(4.14) with the diffusion coefficients

$$A_{ij}(u) = \delta_{ij}\biggl(a_{i0}+\sum_{k=1}^n a_{ik}u_k\biggr)a_{ij}u_i, \quad i,j=1,\ldots,n,$$

and the Lotka–Volterra source terms

$$r_i(u) = u_i\biggl(b_{i0}-\sum_{j=1}^n b_{ij}u_j\biggr), \quad i=1,\ldots,n,$$

where the parameters satisfy $a_{ii}>0$, $b_{ii}>0$ for $i=1,\ldots,n$ and $a_{ij}\ge 0$, $b_{ij}\ge 0$ for $i\ne j$. For $n=2$, we recover the Shigesada–Kawasaki–Teramoto population system without environmental potential, introduced in Section 2.1.1.

To verify Hypotheses (H4)–(H6), we choose the entropy density

$$h_B(u)=\sum_{i=1}^n h_i(u_i), \quad \text{where } h_i(u_i)=\pi_i\bigl(u_i(\log u_i-1)+1\bigr), \quad u\in[0,\infty)^n,$$

and the numbers $\pi_i > 0$ satisfy the detailed-balance condition $\pi_i a_{ij} = \pi_j a_{ji}$ for $i \neq j$. Then the mean $\widetilde{u}_{i,\sigma}^k$ in (4.17) specializes to the logarithmic mean

$$\widetilde{u}_{i,\sigma}^k = \frac{1}{\pi_i} \frac{u_{i,K,\sigma}^k - u_{i,K}^k}{\log u_{i,K,\sigma}^k - \log u_{i,K}^k} \quad \text{for } K \in \mathcal{K},\ \sigma \in \mathcal{E}_K. \tag{4.26}$$

Since $h_i'(u_i) = \pi_i \log u_i$ is invertible as a function from $(0,\infty)$ to $\mathbb{R}$, Hypothesis (H4) is satisfied. A computation shows that (see Lemma 2.1)

$$z^T h_B''(u) A(u) z \geq \sum_{i=1}^n \pi_i \left(\frac{4a_{i0}}{u_i} + 2a_{ii} \right) z_i^2 \quad \text{for } z \in \mathbb{R}^n$$

holds, so Hypothesis (H5) is fulfilled with $s = 1$ (and $s = 1/2$ if $a_{i0} > 0$). It remains to check Hypothesis (H6) for the source terms.

With the elementary inequalities $z \log z + \mathrm{e}^{-1} \geq 0$ and $z \leq z(\log z - 1) + \mathrm{e}$, we find that

$$\begin{aligned}
\sum_{i=1}^n r_i(u) h_i'(u_i) &= \sum_{i=1}^n \pi_i \left(u_i \log u_i + \frac{1}{\mathrm{e}} \right) \left(b_{i0} - \sum_{j=1}^n b_{ij} u_j \right) - \frac{1}{\mathrm{e}} \sum_{i=1}^n \pi_i \left(b_{i0} - \sum_{j=1}^n b_{ij} u_j \right) \\
&\leq \sum_{i=1}^n \pi_i b_{i0} \left(u_i \log u_i + \frac{1}{\mathrm{e}} \right) + \frac{1}{\mathrm{e}} \sum_{j=1}^n \left(\sum_{i=1}^n \pi_i b_{ij} \right) u_j \\
&\leq \sum_{i=1}^n \pi_i b_{i0} \left(u_i (\log u_i - 1) + u_i + \frac{1}{\mathrm{e}} \right) + \sum_{j=1}^n \left(\sum_{i=1}^n \pi_i b_{ij} \right) \big(u_j (\log u_j - 1) + \mathrm{e} \big) \\
&\leq C_r (1 + h(u))
\end{aligned}$$

for some $C_r > 0$ only depending on the coefficients π_i and b_{ij}.

We conclude from Theorem 4.11 that there exists a finite-volume solution to scheme (4.15)–(4.16), which is nonnegative componentwise and which satisfies the discrete entropy inequality (4.19) if $s = 1$ and $a_{i0} = 0$. Moreover, if $a_{i0} > 0$, we have $s = 1/2$, and restricting the Lotka–Volterra terms to the case $b_{ij} = 0$ for all $i \neq j$, we have $r_i(u) \geq -b_{ii} u_i$. Then Proposition 4.13 shows that the discrete solution is positive componentwise and that the discrete entropy inequality holds.

▶ *Busenberg–Travis model.* The generalized Busenberg–Travis model from Section 2.1.2 has the diffusion matrix $A_{ij}(u) = u_i a_{ij}$ for $i, j = 1, \ldots, n$. With the Boltzmann entropy density of the previous subsection, we have

$$z^T h_B''(u) A(u) z = \sum_{i,j=1}^n \pi_i a_{ij} z_i z_j \geq \alpha |z|^2 \quad \text{for } z \in \mathbb{R}^n,$$

if the matrix $(\pi_i a_{ij})$ is symmetric positive definite with smallest eigenvalue $\alpha > 0$. Thus, Hypothesis (H5) is satisfied with $s = 1$, and according to Theorem 4.11, scheme (4.15)–(4.16) possesses a discrete solution with nonnegative components and satisyfing the discrete entropy inequality (4.19).

The Busenberg–Travis system has another entropy density, namely the Rao entropy density

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

introduced in Section 2.1.2. One may ask whether scheme (4.15)–(4.16) satisfies a discrete Rao entropy inequality, which is an equality at the continuous level:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega h_R(u)\mathrm{d}x + \sum_{i=1}^n \int_\Omega \pi_i u_i |\nabla p_i(u)|^2 \mathrm{d}x = 0, \quad \text{where } p_i(u) = \sum_{j=1}^n a_{ij}u_j.$$

This is indeed the case. To see this, we rewrite scheme (4.15)–(4.16) as

$$\frac{\mathrm{m}(K)}{\Delta}(u_{i,K}^k - u_{i,K}^{k-1}) + \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k = 0, \quad i = 1,\ldots,n, \tag{4.27}$$

$$F_{i,K,\sigma}^k = -\tau_\sigma u_{i,\sigma}^k \mathrm{D}_{K,\sigma} p_i(u^k), \tag{4.28}$$

for $K\in\mathcal{T}$, $\sigma\in\mathcal{E}_K$, $k\ge 1$, where $u_{i,\sigma}^k$ is defined in (4.17) and (4.26). This expression coincides with the general definition (4.16). We claim that the numerical flux (4.28) preserves the nonnegativity of the densities and the entropy inequality. We define the discrete Rao entropy by

$$\mathcal{H}_R(u^k) = \sum_{K\in\mathcal{T}} \mathrm{m}(K) h_R(u_K^k). \tag{4.29}$$

Lemma 4.14. *Let $u^k\in V_{\Delta x}^n$ be a solution to (4.27)–(4.28) and let $(\pi_i a_{ij})_{ij}$ be positive semidefinite. Then $u_{i,K}^k\ge 0$ for all $K\in\mathcal{T}$, $k\in\mathbb{N}$, $i=1,\ldots,n$, and*

$$\mathcal{H}_R(u^k) + \Delta t\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}} \tau_\sigma u_{i,\sigma}^k (\mathrm{D}_{K,\sigma}p_i(u^k))^2 \le \mathcal{H}_R(u^{k-1}), \quad k\ge 1.$$

For this lemma, it is sufficient to assume the positive semidefiniteness of $(\pi_i a_{ij})$. However, we should assume that at least $a_{ii}>0$, since $\mathcal{H}_R(u^k)\ge\sum_{i=1}^n\sum_{K\in\mathcal{T}}\mathrm{m}(K)a_{ii}(u_{i,K}^k)^2$ then implies an $L^2(\Omega)$ bound for u_i^k. Positive definiteness of $(\pi_i a_{ij})$ is needed to prove the convergence of the scheme.

Proof. Similarly as in the proof of Lemma 4.8, we assume by induction that $u_{i,K}^{k-1}\ge 0$ for all $K\in\mathcal{T}$ for some $k\ge 1$ and some fixed $i\in\{1,\ldots,n\}$. We multiply (4.27) by $(u_{i,K}^k)^- = \min\{0,u_{i,K}^k\}$, sum over $K\in\mathcal{T}$, and use discrete integration by parts:

$$\begin{aligned}\sum_{K\in\mathcal{T}}\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}^k - u_{i,K}^{k-1})(u_{i,K}^k)^- &= \sum_{\sigma=K|L\in\mathcal{E}_{\mathrm{int}}} F_{i,K,\sigma}^k\big((u_{i,L}^k)^- - (u_{i,K}^k)^-\big)\\ &= -\sum_{\sigma=K|L\in\mathcal{E}_{\mathrm{int}}}\tau_\sigma u_{i,\sigma}^k\big(p_i(u_L^k)-p_i(u_K^k)\big)\big((u_{i,L}^k)^- - (u_{i,K}^k)^-\big).\end{aligned} \tag{4.30}$$

If both $u_{i,L}^k \geq 0$ and $u_{i,K}^k \geq 0$, then the right-hand side vanishes. If $u_{i,L}^k < 0$ or $u_{i,K}^k < 0$, we have $u_{i,\sigma}^k = 0$ by definition. (Observe that the definition $u_{i,\sigma}^k = \min\{u_{i,K}^k, u_{i,L}^k\}$ would lead to the same result.) Thus, the right-hand side of (4.30) vanishes in either case, and we conclude that

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}[(u_{i,K}^k)^-]^2 = 0.$$

This shows that $u_{i,K}^k \geq 0$ for any $K \in \mathcal{T}$.

Next, we multiply scheme (4.27) by $\pi_i p_i(u_K^k)$, sum over $K \in \mathcal{T}$ and $i = 1, \ldots, n$, and use discrete integration by parts:

$$\begin{aligned}\sum_{i=1}^n \sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}\pi_i(u_{i,K}^k - u_{i,K}^{k-1})p_i(u_K^k) &= \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \pi_i F_{i,K,\sigma}^k \mathrm{D}_{K,\sigma} p_i(u^k) \\ &= -\sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma \pi_i u_{i,\sigma}^k (\mathrm{D}_{K,\sigma} p_i(u^k))^2.\end{aligned}$$

Inserting the definition of $p_i(u_K^k)$ and using the assumption $\pi_j a_{ji} = \pi_i a_{ij}$, we calculate the left-hand side:

$$\begin{aligned}\sum_{i=1}^n \pi_i(u_{i,K}^k - u_{i,K}^{k-1})p_i(u_K^k) &= \sum_{i,j=1}^n \pi_i a_{ij}(u_{i,K}^k - u_{i,K}^{k-1})u_{j,K}^k \\ &= \frac{1}{2}\sum_{i,j=1}^n \pi_i a_{ij}(u_{i,K}^k - u_{i,K}^{k-1})u_{j,K}^k + \frac{1}{2}\sum_{i,j=1}^n \pi_j a_{ji}(u_{j,K}^k - u_{j,K}^{k-1})u_{i,K}^k \\ &= \frac{1}{2}\sum_{i,j=1}^n \pi_i a_{ij}\big((u_{i,K}^k - u_{i,K}^{k-1})u_{j,K}^k + (u_{j,K}^k - u_{j,K}^{k-1})u_{i,K}^k\big) \\ &= \frac{1}{2}\sum_{i,j=1}^n \pi_i a_{ij}\big(u_{i,K}^k u_{j,K}^k - u_{i,K}^{k-1}u_{j,K}^{k-1}\big) + \frac{1}{2}\sum_{i,j=1}^n \pi_i a_{ij}(u_{i,K}^k - u_{i,K}^{k-1})(u_{j,K}^k - u_{j,K}^{k-1}) \\ &\geq \mathcal{H}_R(u^k) - \mathcal{H}_R(u^{k-1}),\end{aligned}$$

since the last sum is nonnegative due to the positive semidefiniteness of the matrix $(\pi_i a_{ij})$. This shows that

$$\mathcal{H}_R(u^k) - \mathcal{H}_R(u^{k-1}) \leq -\sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma \pi_i u_{i,\sigma}^k (\mathrm{D}_{K,\sigma} p_i(u^k))^2,$$

concluding the proof. □

4.3. Finite volumes for volume-filling systems

In the previous section, the entropy density was assumed to be given by the sum of the entropy densities of the various species. Then its Hessian is diagonal, which allowed us to define the discrete chain rule

$$h_i''(\widetilde{u}_{i,\sigma})(u_{i,L} - u_{i,K}) = h_i'(u_{i,L}) - h_i'(u_{i,K}) \quad \text{for } \sigma = K|L \tag{4.31}$$

component by component by using the standard mean-value theorem. This idea cannot be used if the entropy density contains mixed terms, like in volume-filling models. Indeed, consider a fluid mixture of n components with mass fractions $u_1,\ldots,u_n$ dissolved in a solvent with mass fraction u_0. We assume that the sum of all components including the solvent adds up to one, $\sum_{i=0}^n u_i=1$, which means that the fluid is saturated. Thus, we are looking for values in the simplex

$$\mathcal{D}:=\left\{u=(u_1,\ldots,u_n)\in(0,1)^n:\sum_{i=1}^n u_i<1\right\}. \tag{4.32}$$

In many applications, like the Maxwell–Stefan model introduced in Section 2.2, the entropy density is given by the sum

$$h(u)=\sum_{i=0}^n h_i(u_i)=\sum_{i=1}^n h_i(u_i)+h\biggl(1-\sum_{i=1}^n u_i\biggr),\quad u\in\mathcal{D},$$

and we interpret $h(u)$ as a function of $u=(u_1,\ldots,u_n)$, since the solvent fraction can be computed from all the other mass fractions. In this situation, the Hessian of $h(u)$ is not diagonal, $\partial^2 h/(\partial u_i\partial u_j)=\delta_{ij}h_i''(u_i)+h_0''(u_0)$. Then the mean-value theorem does not allow us to formulate a discrete chain rule.

Following [14], we overcome this issue by introducing two ideas. First, we define the solvent fraction $u_{0,K}=1-\sum_{i=1}^n u_{i,K}$ on the control volumes, but we define $u_{0,\sigma}$ as well as $u_{1,\sigma},\ldots,u_{n,\sigma}$ independently from the discrete chain rule (4.31). Then we cannot expect that the values on the edges sum up to one, i.e., generally $u_{0,\sigma}\neq 1-\sum_{i=1}^n u_{i,\sigma}$; see the discussion in Remark 4.18 below. Then, setting

$$u_K=(u_{1,K},\ldots,u_{n,K})\in\mathcal{D}\subset\mathbb{R}^n,\quad u_\sigma=(u_{0,\sigma},\ldots,u_{n,\sigma})\in\mathbb{R}^{n+1},$$

we introduce the modified Hessian

$$H_{ij}(u_\sigma):=\delta_{ij}h_i''(u_{i,\sigma})+h_0''(u_{0,\sigma}),\quad i,j=1,\ldots,n, \tag{4.33}$$

where $u_{i,\sigma}$ for $i=0,\ldots,n$ is defined as in (4.17), i.e.

$$u_{i,\sigma}^k=\begin{cases}\widetilde{u}_{i,\sigma}^k & \text{if } u_{i,K}^k>0,\ u_{i,K,\sigma}^k>0,\text{ and } u_{i,K}^k\neq u_{i,K,\sigma}^k,\\ u_{i,K}^k & \text{if } u_{i,K}^k=u_{i,K,\sigma}^k>0,\\ 0 & \text{else,}\end{cases} \tag{4.34}$$

and $\widetilde{u}_{i,\sigma}$ is determined from the discrete chain rule (4.31). The matrix $H(u_\sigma)=(H_{ij}(u_\sigma))_{ij}\in\mathbb{R}^{n\times n}$ differs from the Hessian h'' by the fact that we use $u_{0,\sigma}$ as the argument of h_0'' and not $1-\sum_{i=1}^n u_{i,\sigma}$. Thus, H depends on the $n+1$ variables $u_{0,\sigma},\ldots,u_{n,\sigma}$, while h'' is a function of the n variables $u_{1,K},\ldots,u_{n,K}$. Relaxing the identity $u_{0,\sigma}=1-\sum_{i=1}^n u_{i,\sigma}$ provides us with some flexibility to prove a vector-valued discrete chain rule; see Proposition 4.15 below.

The second idea is to interpret also the diffusion matrix A, which is defined for the n variables $u_1,\ldots,u_n$, as a function of the $n+1$ variables $u_\sigma=(u_{0,\sigma},\ldots,u_{n,\sigma})$, called A_σ. If $u_{0,\sigma}=1-\sum_{i=1}^n u_{i,\sigma}$, then both matrices coincide, $A_\sigma(u_\sigma)=A(u_{1,\sigma},\ldots,u_{n,\sigma})$. Generally, we have $u_{0,\sigma}\neq 1-\sum_{i=1}^n u_{i,\sigma}$ and so, both matrices may not coincide. Although we reformulate A by A_σ by using the relation $u_{0,\sigma}=1-\sum_{i=1}^n u_{i,\sigma}$, we do not use it anymore in the numerical scheme. In some sense, this relation is encoded in the definition of A_σ. The mathematical reason

for this choice is that we need the positive (semi-) definiteness of $h''(u)A(u)$ at u_σ. Since we have replaced $h''(u)$ by the matrix $H(u_\sigma)$, by consistency, we need to switch to the variable u_σ also in the matrix A, leading to $A_\sigma(u_\sigma)$. We suppose that $H(u_\sigma)A_\sigma(u_\sigma)$ is positive definite in the sense of Hypothesis (H5); see Section 4.2.1.

Let us discuss both ideas in more detail.

▶ *Discrete chain rule.* We show that the scalar chain rule (4.31) indeed leads to a vector-valued chain rule.

Proposition 4.15 (Discrete chain rule)**.** *Let $u \in V_{\Delta x}^n$ be such that $u(x) \in \mathcal{D}$ for $x \in \Omega$, let u_σ be defined by* (4.31) *and* (4.34)*, and let H_{ij} be given by* (4.33)*. Then*

$$H(u_\sigma)\mathrm{D}_{K,\sigma}u = \mathrm{D}_{K,\sigma}h'(u) \quad \text{for } K \in \mathcal{T},\ \sigma \in \mathcal{E}_K.$$

Proof. We fix $i \in \{1,\dots,n\}$, $\sigma = K|L \in \mathcal{E}_{\mathrm{int},K}$, and let $u(x) \in \mathcal{D}$. It follows from definition (4.33) of $H_{ij}(u_\sigma)$ and $\sum_{j=1}^n u_{j,K} = 1 - u_{0,K}$ that

$$\begin{aligned}\sum_{j=1}^n H_{ij}(u_\sigma)\mathrm{D}_{K,\sigma}u_j &= h_i''(u_{i,\sigma})(u_{i,L}-u_{i,K}) + h_0''(u_{0,\sigma})\sum_{j=1}^n (u_{j,L}-u_{j,k}) \\ &= h_i''(u_{i,\sigma})(u_{i,L}-u_{i,K}) - h_0''(u_{0,\sigma})(u_{0,L}-u_{0,K}).\end{aligned}$$

The choice $u(x) \in \mathcal{D}$ implies that the components of u do not vanish, so either $u_{i,\sigma} = \widetilde{u}_{i,\sigma}$ or $u_{i,\sigma} = u_{i,K} = u_{i,L}$, by definition (4.34). Then the scalar discrete chain rule (4.31) gives

$$\begin{aligned}\sum_{j=1}^n H_{ij}(u_\sigma)\mathrm{D}_{K,\sigma}u_j &= (h_i'(u_{i,L}) - h_i'(u_{i,K})) - (h_0'(u_{0,L}) - h_0'(u_{0,K})) \\ &= \mathrm{D}_{K,\sigma}h_i'(u) - \mathrm{D}_{K,\sigma}h_0'(u) = \mathrm{D}_{K,\sigma}\left(\frac{\partial h}{\partial u_i}(u)\right).\end{aligned}$$

The result also holds when $\sigma \in \mathcal{E}_{\mathrm{ext},K}$, since then $\mathrm{D}_{K,\sigma}u_j = 0$. This ends the proof. □

The proof that the discrete solution has values in $\mathcal{D}$ relies on the entropy structure and is proved in a similar way as in the previous subsection in the proof of the existence of discrete solutions; see Theorem 4.11.

▶ *Definition of A_σ.* As an illustrative example, we consider the Maxwell–Stefan equations from Section 2.2:

$$\begin{aligned}A(u) &= \frac{1}{a(u)}\begin{pmatrix} d_{02}+(d_{12}-d_{02})u_1 & (d_{12}-d_{01})u_1 \\ (d_{12}-d_{02})u_2 & d_{01}+(d_{12}-d_{01})u_2\end{pmatrix}, \\ &\text{where } a(u) = d_{01}d_{02}(1-u_1-u_2) + d_{01}d_{12}u_1 + d_{02}d_{12}u_2,\end{aligned}$$

and d_{01}, d_{02} ,$d_{12} > 0$, $u = (u_1,u_2)$. The entropy density equals $h(u) = \sum_{i=0}^2 u_i(\log u_i - 1)$ with the Hessian

$$h''(u) = \begin{pmatrix} 1/u_1 + 1/u_0 & 1/u_0 \\ 1/u_0 & 1/u_2 + 1/u_0\end{pmatrix},$$

recalling that $u_0 = 1 - u_1 - u_2$. The discrete Hessian reads as

$$H(u_\sigma) = \begin{pmatrix} 1/u_{1,\sigma} + 1/u_{0,\sigma} & 1/u_{0,\sigma} \\ 1/u_{0,\sigma} & 1/u_{2,\sigma} + 1/u_{0,\sigma} \end{pmatrix}.$$

To formulate the matrix A_σ, we replace $d_{02}(1-u_1)$ by $d_{02}(u_0+u_2)$ and $d_{01}(1-u_2)$ by $d_{01}(u_0+u_1)$ such that

$$A_\sigma(u_\sigma) = \frac{1}{a_\sigma(u_\sigma)} \begin{pmatrix} d_{02}(u_{0,\sigma}+u_{2,\sigma}) + d_{12}u_{1,\sigma} & (d_{12}-d_{01})u_{1,\sigma} \\ (d_{12}-d_{02})u_{2,\sigma} & d_{01}(u_{0,\sigma}+u_{1,\sigma}) + d_{12}u_{2,\sigma} \end{pmatrix}, \tag{4.35}$$

where $a_\sigma(u_\sigma) = d_{01}d_{02}u_{0,\sigma} + d_{01}d_{12}u_{1,\sigma} + d_{02}d_{12}u_{2,\sigma}$.

Notice that $A = A_\sigma$ if $u_{0,\sigma} = 1 - u_{1,\sigma} - u_{2,\sigma}$. We set $I_\sigma := u_{0,\sigma} + u_{1,\sigma} + u_{2,\sigma} \neq 1$. A computation shows that

$$z^T H(u_\sigma) A_\sigma(u_\sigma) z = \frac{I_\sigma}{a_\sigma(u_\sigma)} \left(\frac{d_2}{u_{1,\sigma}} z_1^2 + \frac{d_1}{u_{2,\sigma}} z_2^2 + \frac{d_0}{u_{0,\sigma}} (z_1+z_2)^2 \right) \geq c \left(\frac{z_1^2}{u_{1,\sigma}} + \frac{z_2^2}{u_{2,\sigma}} \right),$$

where $c := \min\{d_{01}, d_{02}\} / \max\{d_{01}d_{02}, d_{01}d_{12}, d_{02}d_{12}\}$, since

$$\frac{I_\sigma}{a_\sigma(u_\sigma)} = \frac{u_{0,\sigma}+u_{1,\sigma}+u_{2,\sigma}}{d_{01}d_{02}u_{0,\sigma} + d_{01}d_{12}u_{1,\sigma} + d_{02}d_{12}u_{2,\sigma}} \geq \frac{1}{\max\{d_{01}d_{02}, d_{01}d_{12}, d_{02}d_{12}\}}.$$

We infer that the matrix $H(u_\sigma)A_\sigma(u_\sigma)$ satisfies Hypothesis (H5) with $s = 1/2$. We show below that $u_{i,\sigma} > 0$ for $i = 1, 2$ so that $a_\sigma(u_\sigma)$ is positive and A_σ is well defined.

There is no clear recipe how to construct the matrix A_σ. The idea is to replace some expressions to introduce $u_{0,\sigma}$ instead of $u_{i,\sigma}$ in such a way that $H(u_\sigma)A_\sigma(u_\sigma)$ satisfies the positive definiteness condition of Hypothesis (H5) from Section 4.2.1.

We summarize the finite-volume scheme:

$$\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}^k - u_{i,K}^{k-1}) + \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k = \mathrm{m}(K) r_i(u_K^k), \quad i = 1, \ldots, n, \tag{4.36}$$

$$F_{i,K,\sigma}^k = -\sum_{j=1}^n \tau_\sigma A_{\sigma,ij}(u_\sigma^k) \mathrm{D}_{K,\sigma} u_j^k \quad \text{for } K \in \mathcal{T},\ \sigma \in \mathcal{E}_K, \tag{4.37}$$

the mean values $u_{i,\sigma}^k$ are determined from (4.34), and $\widetilde{u}_{i,\sigma}^k \in (0,1)$ is the unique solution to

$$h_i''(\widetilde{u}_{i,\sigma}^k) \mathrm{D}_{K,\sigma} u_i^k = \mathrm{D}_{K,\sigma} h_i'(u_i^k) \quad \text{for } K \in \mathcal{T},\ \sigma \in \mathcal{E}_{\mathrm{int},K},\ i = 0, \ldots, n. \tag{4.38}$$

We show now some properties of this scheme. We introduce the discrete entropy

$$\mathcal{H}_d(u^k) = \sum_{i=0}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) h_i(u_{i,K}^k), \quad k \geq 0.$$

Theorem 4.16 (Discrete entropy inequality)**.** *Let Hypotheses (H1)–(H6) from Section 4.2.1 hold with sums over $i = 0, \ldots, n$ and let $u^k = (u_1^k, \ldots, u_n^k) \in V_{\Delta x}^n$ be a solution to (4.36)–(4.38) satisfying $u_{i,K}^k > 0$ for $K \in \mathcal{T}$, $k \geq 0$, and $i = 0, \ldots, n$. Then, for any $k \geq 1$,*

$$(1 - C_r\Delta t)\mathcal{H}_d(u^k) + c_A \Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (u_{i,\sigma}^k)^{2s-2} (\mathrm{D}_{K,\sigma} u_i^k)^2 \leq \mathcal{H}_d(u^{k-1}) + C_r \Delta t \mathrm{m}(\Omega).$$

PROOF. The proof is similar to that one of Theorem 4.10. Therefore, we highlight only the different parts of the proof. First, we prove that $u_{i,\sigma}^k > 0$ for $\sigma \in \mathcal{E}$, $i = 0, \ldots, n$. If $\sigma \in \mathcal{E}_{\mathrm{ext},K}$, we have $u_{i,K}^k = u_{i,K,\sigma}^k > 0$ and, by definition (4.34), $u_{i,\sigma}^k = u_{i,K}^k > 0$. If $\sigma = K|L \in \mathcal{E}_{\mathrm{int},K}$, we have either $u_{i,K}^k = u_{i,L}^k > 0$ and then $u_{i,\sigma}^k > 0$, or $u_{i,\sigma}^k$ is the unique solution to

$$h_i''(u_{i,\sigma}^k) = \frac{h_i'(u_{i,L}^k) - h_i'(u_{i,K}^k)}{u_{i,L}^k - u_{i,K}^k} > 0.$$

We already know that $u_{i,\sigma}^k \ge \min\{u_{i,K}^k, u_{i,L}^k\} > 0$.

Next, define the entropy variable $w^k := h'(u^k)$. Then $w_{i,K}^k = h_i'(u_{i,K}^k) + h_0'(u_{0,K}^k)$ for $i = 1, \ldots, n$. We multiply scheme (4.36) by $w_{i,K}^k$, sum over $K \in \mathcal{T}$ and $i = 1, \ldots, n$, and use discrete integration by parts in the sum with the numerical flux. Then $I_1 + I_2 + I_3 = 0$, where

$$\begin{aligned}
I_1 &= \frac{1}{\Delta t}\sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_{i,K}^k - u_{i,K}^{k-1})w_{i,K}^k, \\
I_2 &= -\sum_{i=1}^n \sum_{\sigma=K|L\in\mathcal{E}_{\mathrm{int}}} F_{i,K,\sigma}^k \mathrm{D}_{K,\sigma} w_i^k, \\
I_3 &= \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) r_i(u_K^k) w_{i,K}^k.
\end{aligned}$$

The convexity of h, due to Hypothesis (H4), implies that

$$\begin{aligned}
I_1 &= \frac{1}{\Delta t}\sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_K^k - u_K^{k-1})\cdot h'(u_K^k) \\
&\ge \frac{1}{\Delta t}\sum_{K\in\mathcal{T}} \mathrm{m}(K)(h(u_K^k) - h(u_K^{k-1})) = \frac{1}{\Delta t}\big(\mathcal{H}_d(u^k) - \mathcal{H}_d(u^{k-1})\big).
\end{aligned}$$

The discrete chain rule in Proposition 4.15 and the symmetry of $H(u_\sigma)$ show that

$$\begin{aligned}
I_2 &= \sum_{i,j=1}^n \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}}\\ \sigma=K|L}} \tau_\sigma A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_j^k \mathrm{D}_{K,\sigma}(h'(u^k))_i \\
&= \sum_{i,j=1}^n \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}}\\ \sigma=K|L}} \tau_\sigma \big(H(u^k)\mathrm{D}_{K,\sigma}u^k\big)_i A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_j^k \\
&= \sum_{i,j=1}^n \sum_{\ell=1}^n \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}}\\ \sigma=K|L}} \tau_\sigma \mathrm{D}_{K,\sigma}u_\ell^k H_{\ell i}(u_\sigma^k) A_{ij}(u_\sigma^k)\mathrm{D}_{K,\sigma}u_j^k \\
&= \sum_{i,j=1}^n \sum_{\ell=1}^n \sum_{\substack{\sigma\in\mathcal{E}_{\mathrm{int}}\\ \sigma=K|L}} \tau_\sigma \mathrm{D}_{K,\sigma}u_\ell^k \big(H(u_\sigma^k)A(u_\sigma^k)\big)_{\ell j}\mathrm{D}_{K,\sigma}u_j^k
\end{aligned}$$

$$\ge c_A \sum_{j=1}^n \sum_{\substack{\sigma\in\mathcal{E}_{\rm int}\\ \sigma=K|L}} \tau_\sigma (u_{j,\sigma}^k)^{2s-2} (\mathrm{D}_{K,\sigma} u_j^k)^2.$$

We deduce from Hypothesis (H6) that

$$\begin{aligned} I_3 &= \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) r_i(u_K^k)\big(h_i'(u_{i,K}^k) + h_0'(u_{0,K}^k)\big) \\ &\le C_r \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K)(1+h(u_K^k)) = C_r(\mathcal{H}_d(u^k) + \mathrm{m}(\Omega)). \end{aligned}$$

Inserting these estimates into $I_1 + I_2 + I_3 = 0$ and proceeding as in the proof of Theorem 4.10 concludes the proof. □

As in the previous section, the bound $u_{i,K}^k \in \mathcal{D}$ is a consequence of the formulation in entropy variables. We call this approach the *discrete boundedness-by-entropy method*. For the existence analysis, we need an additional hypothesis:

(H7) There exists a matrix A_σ which is Lipschitz continuous on $[0,1]\times(0,1)^n$ such that $A(u) = A_\sigma(u_\sigma)$ for all $u\in\mathcal{D}$ with $u_i = u_{i,\sigma}$ for $i=1,\ldots,n$ and $u_{0,\sigma} = 1 - \sum_{i=1}^n u_i$, as well as $\|A_\sigma(0,u)\| < \infty$ for all $u\in(0,1)^n$ satisfying $\sum_{i=1}^n u_i \le 1$, where $\|\cdot\|$ is an arbitrary matrix norm,

Theorem 4.17 (Existence of discrete solutions)**.** *Let Hypotheses (H1)–(H7) hold with the exceptions that the sums are from $i=0,\ldots,n$ and that $s<1$. Furthermore, let $\Delta t < 1/C_r$. Then there exists a solution $u^k = (u_1^k,\ldots,u_n^k) \in V_{\Delta x}^n$ to scheme (4.36)–(4.38) satisfying*

$$u_K^k \in \mathcal{D} \quad \text{for } K\in\mathcal{T}, \quad 0 < u_{i,\sigma}^k < 1 \quad \text{for } \sigma\in\mathcal{E}_{\rm int}$$

and for all $k\ge 1$ and $i=1,\ldots,n$. Moreover, u^k satisfies the discrete entropy inequality in Theorem (4.16).

Proof. The proof is very similar to that one of Theorem 4.11. We still need to verify that $0 < u_{i,\sigma}^k < 1$ for $\sigma\in\mathcal{E}_{\rm int}$, $i=1,\ldots,n$. In view of definition (4.34) and $\sum_{i=0}^n u_{i,K}^k \le 1$, it is sufficient to show that $u_{i,K}^k > 0$ for all $K\in\mathcal{T}$, $i=1,\ldots,n$. This property was shown in the proof of Proposition 4.13 under the condition that $r_i(u) \ge -c_r u_i$ for some $c_r > 0$. Here, we exploit the boundedness of $\mathcal{D}$ to infer that $|r_i|$ is bounded on $\overline{\mathcal{D}}$, and the lower bound is satisfied. Since $u_{0,\sigma}^k = 0$ is possible, we need the condition $\|A_\sigma(u_\sigma)\| < \infty$ in Hypothesis (H7) whenever $u_{0,\sigma}^k = 0$. From this point on, the proof follows the lines of the proof of Theorem 4.11. □

Remark 4.18 (Upper bound)**.** Theorem 4.17 states in particular that the solution satisfies for $K\in\mathcal{T}$ and $\sigma\in\mathcal{E}_{\rm int}$,

$$0 < u_{i,K}^k < 1, \quad 0 < u_{i,\sigma}^k < 1 \quad \text{for } i=1,\ldots,n, \quad \sum_{i=1}^n u_{i,K}^k < 1,$$

but we cannot exclude that $\sum_{i=0}^n u_{i,\sigma}^k > 1$. When the entropy is given by the Boltzmann-type entropy density $h(u) = \sum_{i=0}^n u_i(\log u_i - 1)$, we deduce from the fact that the logarithmic mean is not larger than the arithmetic mean that

$$\sum_{i=0}^n u_{i,\sigma}^k \le \frac{1}{2}\sum_{i=0}^n (u_{i,K}^k + u_{i,L}^k) = 1 \quad \text{for } \sigma \in \mathcal{E}_{\rm int},\ k \ge 0,$$

In this situation, we obtain $u_\sigma^k \in \overline{\mathcal{D}}$. □

Remark 4.19 (Case $s = 1$)**.** The condition $\|A_\sigma(0, u_\sigma)\| < \infty$ is crucial. Indeed, the matrix A_σ in example (4.35) contains the factor $1/a_\sigma(u_\sigma)$ that is infinite if $u_\sigma = 0$. Since we do not require that $\sum_{i=0}^n u_{i,\sigma}^k = 1$, this may happen. Then the quantity $\|A_\sigma(u_\sigma)\|$ is not a number, and the existence of a discrete solution cannot be guaranteed. □

References for Chapter 4

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