

# A DISCRETE BOUNDEDNESS-BY-ENTROPY METHOD FOR FINITE-VOLUME APPROXIMATIONS OF CROSS-DIFFUSION SYSTEMS

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ABSTRACT. An implicit Euler finite-volume scheme for general cross-diffusion systems with volume-filling constraints is proposed and analyzed. The diffusion matrix may be nonsymmetric and not positive semidefinite, but the diffusion system is assumed to possess a formal gradient-flow structure that yields  $L^\infty$  bounds on the continuous level. Examples include the Maxwell–Stefan systems for gas mixtures, tumor-growth models, and systems for the fabrication of thin-film solar cells. The proposed numerical scheme preserves the structure of the continuous equations, namely the entropy dissipation inequality as well as the nonnegativity of the concentrations and the volume-filling constraints. The discrete entropy structure is a consequence of a new vector-valued discrete chain rule. The existence of discrete solutions, their positivity, and the convergence of the scheme is proved. The numerical scheme is implemented for a one-dimensional Maxwell–Stefan model and a two-dimensional thin-film solar cell system. It is illustrated that the convergence rate in space is of order two and the discrete relative entropy decays exponentially.

## 1. INTRODUCTION

Cross-diffusion is a phenomenon in multi-species systems, in which the gradient of the concentration of one species induces a flux of the other species. Examples include gas mixtures, ion transport through membranes, and tumor-growth models. Mathematically, cross-diffusion is described by quasilinear parabolic equations with a non-diagonal diffusion matrix. The analysis of such systems is challenging since the diffusion matrix is generally neither symmetric nor positive semidefinite, and standard tools like maximum principles and regularity theory generally do not apply. In recent years, it has been found that a class of cross-diffusion systems, which describe volume-filling effects in mixtures, possess global bounded weak solutions [9, 32]. The existence proof is based on the formal gradient-flow

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or entropy structure of the cross-diffusion equations, leading to the so-called boundedness-by-entropy method. In this paper, we develop a discrete version of this method for finite-volume approximations of cross-diffusion systems, preserving the structure of the continuous equations, namely nonnegativity, boundedness, mass control, and entropy dissipation, and converging to the continuous equations when the mesh parameters tend to zero.

**1.1. The boundedness-by-entropy method.** We consider the cross-diffusion system

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

where  $u = (u_1, \dots, u_n)$  is the vector of volume or mass fractions and  $\Omega \subset \mathbb{R}^2$  is a bounded domain. The volume or mass fraction of the solvent  $u_0$  is defined by  $u_0 = 1 - \sum_{i=1}^n u_i$  such that the identity  $\sum_{i=0}^n u_i = 1$  is fulfilled. These equations describe the evolution of fluid mixtures or multicomponent systems [33]. We prescribe no-flux boundary and initial conditions:

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

where  $\nu$  denotes the exterior unit normal vector to  $\partial\Omega$ . The diffusion matrix  $A(u) = (A_{ij}(u))$  is generally neither symmetric nor positive definite obstructing the use of standard techniques. This problem can be overcome when the system possesses a formal gradient-flow or entropy structure. In the following, we explain this structure.

First, we introduce the open simplex

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

and let a strictly convex function  $h \in C^2(D; [0, \infty))$  with  $h(u) = \sum_{i=0}^n h_i(u_i)$  be given. Note that  $u_0$  is a function of  $u = (u_1, \dots, u_n)$ , so  $h$  depends only on  $(u_1, \dots, u_n)$ . Furthermore, we set  $\mathcal{H}[u] = \int_{\Omega} h(u) dx$ . Choosing  $h'(u)$  as a test function in the weak formulation of (1), a formal computation gives

$$(3) \quad \frac{d\mathcal{H}}{dt} + \int_{\Omega} \nabla u : h''(u) A(u) \nabla u dx = 0, \quad 0 < t < T,$$

where  $h''(u)$  is the Hessian of  $h$ , and “:” is the Frobenius matrix product. If  $h''(u)A(u)$  is positive (semi-) definite, we call  $h$  an entropy density,  $\mathcal{H}$  an entropy, and (3) an entropy (dissipation) inequality. In many applications, there exist  $c_A > 0$  and  $0 < s \leq 1$  such that for  $z \in \mathbb{R}^n$  and  $u \in D$ ,

$$z^\top h''(u) A(u) z \geq c_A \sum_{i=1}^n u_i^{2(s-1)} z_i^2.$$

This means that  $h''(u)A(u)$  is positive definite but possibly involving a singularity at  $u_i = 0$ . We refer to [32] and Section 3 for some examples. In this situation, (3) provides an  $L^2(\Omega)$  estimate for  $\nabla u_i^s$ . Moreover, if  $h' : D \rightarrow \mathbb{R}^n$  is invertible, we conclude an  $L^\infty(\Omega)$

bound for  $u_i$ . Indeed, the strategy of the existence analysis is to solve (1) in the entropy variable  $w = h'(u)$  and to define the volume fractions a posteriori via  $u = (h')^{-1}(w)$ . Since  $(h')^{-1} : \mathbb{R}^n \rightarrow D$ , it holds that  $u(x, t) \in D$ , which gives the desired  $L^\infty(\Omega)$  bound. With these tools, the global existence of bounded weak solutions to (1)–(2) can be proved [32].

The existence result may be surprising in view of the fact that the diffusion matrix in (1) may be not positive (semi-) definite, but it can be understood by observing that the positive definiteness of  $h''(u)A(u)$  implies that equations (1) are parabolic in the sense of Petrovskii [33, Remark 4.3]. Another explanation is that equations (1) can be written equivalently as

$$(4) \quad \partial_t u_i(w) - \operatorname{div} \left( \sum_{j=1}^n B_{ij}(w) \nabla w \right) = 0, \quad i = 1, \dots, n,$$

where the so-called Onsager matrix  $B = (B_{ij})$ , defined by  $B(w) = A(u(w))h''(u(w))^{-1}$ , is positive (semi-) definite. The task is to “translate” this strategy to a finite-volume setting.

**1.2. Key ideas.** The derivation of the entropy inequality (3) is based on the chain rule  $h''(u)\nabla u = \nabla h'(u)$ . To formulate a discrete version, we assume that  $\Omega$  is the union of cells  $K$  and let  $\sigma = K|L$  be the edge between two neighboring cells  $K$  and  $L$  inside of  $\Omega$ . The discrete volume fraction  $u_i$  is constant on each cell, and we write  $u_{i,K}$  for its value. The value on the edge is denoted by  $u_{i,\sigma}$ .

When the entropy density equals the sum  $h(u) = \sum_{i=1}^n h_i(u_i)$ , the Hessian  $h''(u)$  is diagonal, and the discrete chain rule can be formulated componentwise as

$$(5) \quad h_i''(u_{i,\sigma})(u_{i,K} - u_{i,L}) = h_i'(u_{i,K}) - h_i'(u_{i,L}) \quad \text{for } \sigma = K|L.$$

If  $h_i''$  is strictly monotone, there exists a unique solution  $u_{i,\sigma}$  to (5) by the mean-value theorem. In the case of the Boltzmann entropy  $h_i(u_i) = u_i(\log u_i - 1) + 1$ , this leads to the logarithmic mean

$$(6) \quad u_{i,\sigma} = \frac{u_{i,K} - u_{i,L}}{\log u_{i,K} - \log u_{i,L}},$$

which has been used to develop entropy-conservative schemes for hyperbolic conservation laws [29] and entropy-dissipative schemes for drift-diffusion equations [5].

In the present case, we assume that  $h(u) = \sum_{i=0}^n h_i(u_i)$ . Unfortunately, the Hessian  $h''(u)$  is not diagonal, since  $\partial^2 h / (\partial u_i \partial u_j) = \delta_{ij} h_i''(u_i) + h_0''(u_0)$ . Then the vector-valued mean-value theorem does not allow us to determine  $u_{i,\sigma}$  like in (5). We overcome this issue by introducing two ideas.

Our *first idea* is to define  $u_{0,K} = 1 - \sum_{i=1}^n u_{i,K}$  on the cells but to define  $u_{0,\sigma}$  (as well as  $u_{i,\sigma}$  for  $i = 1, \dots, n$ ) from (5). Thus, in general,  $u_{0,\sigma} \neq 1 - \sum_{i=1}^n u_{i,\sigma}$ . We set  $u_K = (u_{1,K}, \dots, u_{n,K})$ ,  $u_\sigma = (u_{0,\sigma}, \dots, u_{n,\sigma})$ , and  $H_{ij}(u_\sigma) = \delta_{ij} h_i''(u_{i,\sigma}) + h_0''(u_{0,\sigma})$  for  $i, j = 1, \dots, n$ . The matrix  $H(u_\sigma) = (H_{ij}(u_\sigma))$  is similar to the Hessian  $h''$  with the exception that we use  $u_{0,\sigma}$  as the argument of  $h_0''$  and not  $1 - \sum_{i=1}^n u_{i,\sigma}$ . This means that  $H$  depends on all variables  $u_{0,\sigma}, \dots, u_{n,\sigma}$ , while  $h$  is a function of  $u_{1,K}, \dots, u_{n,K}$ . We prove in Lemma

4 that

$$(7) \quad \sum_{j=1}^n H_{ij}(u_\sigma)(u_{j,K} - u_{j,L}) = (h'(u_K) - h'(u_L))_i, \quad i = 1, \dots, n,$$

holds, which is the desired discrete chain rule.

Furthermore, we need the positive (semi-) definiteness of  $h''(u)A(u)$  at  $u_\sigma$ . Since we have replaced  $h''$  by the matrix  $H(u_\sigma)$ , which contains the new variable  $u_{0,\sigma}$ , we cannot evaluate  $A(u)$  at  $(u_{1,\sigma}, \dots, u_{n,\sigma})$ . Instead, our *second idea* is to interpret the diffusion matrix  $A$  as a function of  $u_\sigma = (u_{0,\sigma}, \dots, u_{n,\sigma})$ , called  $A_\sigma$ , and to impose the positive definiteness condition

$$(8) \quad z^\top H(u_\sigma)A_\sigma(u_\sigma)z \geq c_A \sum_{i=1}^n u_{i,\sigma}^{2(s-1)} z_i^2 \quad \text{for all } z \in \mathbb{R}^n.$$

**1.3. An illustrative example.** Let us explain the second idea on a simple example with the diffusion matrix

$$(9) \quad A = \begin{pmatrix} 1 - u_1 & -u_1 \\ -u_2 & 1 - u_2 \end{pmatrix} \quad \text{for } u = (u_1, u_2) \in D.$$

Equations (1) with this diffusion matrix can be formally derived in the diffusion limit from the Euler equations with friction forces [33, Example 4.3]. We present in Section 3 further examples. We choose the entropy density

$$h(u) = \sum_{i=0}^2 u_i (\log u_i - 1) + 3, \quad \text{where } u_0 = 1 - u_1 - u_2,$$

and compute

$$h''(u) = \begin{pmatrix} 1/u_1 + 1/u_0 & 1/u_0 \\ 1/u_0 & 1/u_2 + 1/u_0 \end{pmatrix}, \quad h''(u)A(u) = \begin{pmatrix} 1/u_1 & 0 \\ 0 & 1/u_2 \end{pmatrix}.$$

This shows that  $h''(u)A(u)$  is positive definite with  $z^\top h''(u)A(u)z = z_1^2/u_1 + z_2^2/u_2$  for all  $u \in D$  and  $z \in \mathbb{R}^2$ .

For the numerical approximation, we write the diffusion matrix as

$$\tilde{A}(u_0, u) = \frac{1}{a(u)} \begin{pmatrix} u_0 + u_2 & -u_1 \\ -u_2 & u_0 + u_1 \end{pmatrix}, \quad \text{where } a(u) = u_0 + u_1 + u_2.$$

Of course, this matrix and (9) coincide if the identity  $u_0 + u_1 + u_2 = 1$  holds. In the numerical scheme, we do not impose this condition on the edges. Instead, we define

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

and  $A_\sigma(u_\sigma) := \tilde{A}(u_\sigma)$ , where  $u_{i,\sigma}$  for  $i = 0, 1, 2$  is given by (6). Although  $u_{0,\sigma} + u_{1,\sigma} + u_{2,\sigma} \neq 1$  is not guaranteed, we find that

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

and (8) is satisfied for  $s = 1/2$ . Note the factor  $a(u_\sigma)$  in the definition of  $A_\sigma$  is crucial for this result and that  $u_{i,\sigma} > 0$  for all  $i$  cannot be guaranteed in general. However, we prove that  $0 < a(u_\sigma) \leq 1$  holds in the present case; see the paragraph after Theorem 1.

When  $1/a(u_\sigma) > 1$ , this factor may be interpreted as an artificial diffusion coefficient. Yet, even if in general  $a(u_\sigma) \neq 1$ , as  $a(u_\sigma)$  is the sum of the logarithmic mean between  $u_{i,K}$  and  $u_{i,L}$  of *each* species, we always observe in our numerical experiments (not shown here) that  $a(u_\sigma)$  is of order one. Moreover, the solution is very close to that one obtained from a finite-volume scheme with arithmetic mean (which preserves the volume-filling constraint) instead of the logarithmic mean. Thus, as expected, this factor does *not* lead to over-diffusive results. Let us notice that the situation may be different if, for instance,  $a(u_\sigma)$  was only given by  $u_{1,\sigma}$  or  $u_{2,\sigma}$  (or even  $u_{1,\sigma} + u_{2,\sigma}$ ). In this case, we can build initial data such that  $1/a(u_\sigma)$  is much larger than one at least for the first time steps, leading to over-diffusive solutions.

**1.4. State of the art.** First existence results for cross-diffusion systems were stated under restrictive conditions on the nonlinearities [40]. Amann [2] showed that weak solutions to strongly coupled parabolic systems exist globally if their  $W^{1,p}$  norm with  $p > d$  can be controlled. Alt and Luckhaus [1] proved global existence results for systems of the form (4) with uniformly positive definite Onsager matrices. Global *bounded* weak solutions were shown for a special cross-diffusion system with volume-filling effects by Burger et al. [9] and later for a general class of systems in [32], based on the underlying entropy structure. Such systems arise naturally in the modeling of gas mixtures and in multi-species population dynamics [33, 44].

Structure-preserving finite-volume-type schemes were first designed for hyperbolic conservation laws fulfilling entropy stability or entropy conservation [43]. The application to cross-diffusion systems is more recent. A convergence study of a finite-volume approximation for a nondegenerate cross-diffusion problem was carried out in [3], based on classical quadratic energy estimates. Finite-volume approximations that satisfy a discrete entropy inequality were suggested and analyzed in [10, 12, 13, 16, 37, 38], while finite-volume schemes for cross-diffusion systems preserving the volume-filling constraints were developed in [10, 12, 16, 28].

The preservation of the entropy structure is achieved by designing a discrete chain rule. In the literature, the elementary inequality  $(u - v)(\log u - \log v) \geq 4(\sqrt{u} - \sqrt{v})^2$  is used as a discrete version of the chain rule  $\nabla u \cdot \nabla \log u = 4|\nabla \sqrt{u}|^2$  [10, 24] and the logarithmic mean (6) as a discrete version of the chain rule  $u \nabla \log u = \nabla u$  [5, 13, 22]. The more general chain rule (5) was suggested in our previous work [38]. In all these examples, the discrete chain rule is defined componentwise.

In the discrete gradient method for differential equations, related discrete chain rules are formulated to achieve energy conservation or entropy dissipation; see the review [42]. Examples are given by the Gonzales scheme [25] and the mean-value discrete gradient [27]. The latter technique was extended to the average vector field method [14], which uses an average of the differential operator  $\operatorname{div}(B \nabla w)$  and is based on the vector-valued mean-value theorem. However, it seems to be difficult to extract gradient estimates from these discrete

gradients. Here, we consider for the first time (up to our knowledge) a vector-valued chain rule leading to gradient estimates.

Let us also mention related approaches for diffusion problems. For finite-difference schemes, entropy-stable and entropy-dissipative discretizations were developed in, e.g., [31, 39, 41], extending Tadmor's framework or using upwind approximations. When the equations possess a variational structure involving the variational derivative of the energy/entropy, discrete variational derivatives were defined in [21]. This approach was extended to fourth-order parabolic equations [8], but it seems not to cover cross-diffusion systems. Energy-dissipative schemes for scalar equations were developed also for higher-order time integrations; see, e.g., [26] for Runge–Kutta methods and [35] for one-leg multistep methods. Unfortunately, these techniques cannot be easily adapted to our setting. Interesting approaches are the discontinuous Galerkin time discretization of [18], whose use in finite-volume schemes has still to be explored, and the space-time Galerkin approach of [7], which needs a regularizing term.

The paper is organized as follows. The numerical scheme and our main results (existence of discrete solutions, positivity, and convergence of the scheme) are introduced in Section 2. We present some examples of cross-diffusion models that satisfy our main assumptions in Section 3. In Section 4, the existence of solutions is proved, while the convergence of the scheme is shown in Section 5. Finally, some numerical examples are presented in Section 6.

## 2. NUMERICAL SCHEME AND MAIN RESULTS

**2.1. Notation and definitions.** Let  $\Omega \subset \mathbb{R}^2$  be a bounded, polygonal domain. We consider only two-dimensional domains, but the generalization to higher space dimensions is straightforward. An admissible mesh of  $\Omega$  is given by (i) a family  $\mathcal{T}$  of open polygonal control volumes (or cells), (ii) a family  $\mathcal{E}$  of edges, and (iii) a family  $\mathcal{P}$  of points  $(x_K)_{K \in \mathcal{T}}$  associated to the control volumes and satisfying Definition 9.1 in [19]. This definition implies that the straight line  $\overline{x_K x_L}$  between two centers of neighboring cells is orthogonal to the edge  $\sigma = K|L$  between two cells. For instance, Voronoï meshes satisfy this condition [19, Example 9.2]. The size of the mesh is denoted by  $\Delta x = \max_{K \in \mathcal{T}} \text{diam}(K)$ . The family of edges  $\mathcal{E}$  is assumed to consist of interior edges  $\mathcal{E}_{\text{int}}$  satisfying  $\sigma \subset \Omega$  and boundary edges  $\sigma \in \mathcal{E}_{\text{ext}}$  satisfying  $\sigma \subset \partial\Omega$ . For given  $K \in \mathcal{T}$ ,  $\mathcal{E}_K$  is the set of edges of  $K$ , and it splits into  $\mathcal{E}_K = \mathcal{E}_{\text{int},K} \cup \mathcal{E}_{\text{ext},K}$ . For any  $\sigma \in \mathcal{E}$ , there exists at least one cell  $K \in \mathcal{T}$  such that  $\sigma \in \mathcal{E}_K$ .

We need the following definitions. For  $\sigma \in \mathcal{E}$ , we introduce the distance

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

where  $d$  is the Euclidean distance in  $\mathbb{R}^2$ , and the transmissibility coefficient

$$(10) \quad \tau_\sigma = \frac{m(\sigma)}{d_\sigma},$$

where  $m(\sigma)$  denotes the Lebesgue measure of  $\sigma$ . The mesh is assumed to satisfy the following regularity assumption: There exists  $\zeta > 0$  such that for all  $K \in \mathcal{T}$  and  $\sigma \in \mathcal{E}_K$ ,

$$(11) \quad d(x_K, \sigma) \geq \zeta d_\sigma.$$

Let  $T > 0$ ,  $N_T \in \mathbb{N}$  and introduce the time step size  $\Delta t = T/N_T$  as well as the time steps  $t_k = k\Delta t$  for  $k = 0, \dots, N_T$ . We denote by  $\mathcal{D}$  the admissible space-time discretization of  $\Omega_T = \Omega \times (0, T)$  composed of an admissible mesh  $\mathcal{T}$  and the values  $(\Delta t, N_T)$ .

Next, we introduce the functional spaces. The space of piecewise constant functions is defined by

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

where  $\mathbf{1}_K$  is the characteristic function on  $K$ . In order to define a norm on this space, we first introduce the notation

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

for  $K \in \mathcal{T}$ ,  $\sigma \in \mathcal{E}_K$  and the discrete operators

$$D_{K,\sigma} v := v_{K,\sigma} - v_K, \quad D_\sigma v := |D_{K,\sigma} v|.$$

The (squared)  $L^2$  norm, the discrete  $H^1$  seminorm, and the discrete  $H^1$  norm on  $V_{\mathcal{T}}$  are given by, respectively,

$$\begin{aligned} \|v\|_{0,2,\mathcal{T}}^2 &= \sum_{K \in \mathcal{T}} m(K) |v_K|^2, \\ |v|_{1,2,\mathcal{T}}^2 &= \sum_{\sigma \in \mathcal{E}} \tau_\sigma |D_\sigma v|^2, \\ \|v\|_{1,2,\mathcal{T}}^2 &= |v|_{1,2,\mathcal{T}}^2 + \|v\|_{0,2,\mathcal{T}}^2. \end{aligned}$$

We associate to these norms a dual norm with respect to the  $L^2$  inner product,

$$\|v\|_{-1,2,\mathcal{T}} = \sup \left\{ \int_{\Omega} v w dx : w \in V_{\mathcal{T}}, \|w\|_{1,2,\mathcal{T}} = 1 \right\}.$$

It holds that

$$\left| \int_{\Omega} v w dx \right| \leq \|v\|_{-1,2,\mathcal{T}} \|w\|_{1,2,\mathcal{T}} \quad \text{for } v, w \in V_{\mathcal{T}}.$$

Finally, we introduce the space  $V_{\mathcal{T},\Delta t}$  of piecewise constant functions with values in  $V_{\mathcal{T}}$ ,

$$V_{\mathcal{T},\Delta t} = \left\{ v : \bar{\Omega} \times [0, T] \rightarrow \mathbb{R} : \exists (v^k)_{k=1,\dots,N_T} \subset V_{\mathcal{T}}, v(x, t) = \sum_{k=1}^{N_T} v^k(x) \mathbf{1}_{(t_{k-1}, t_k]}(t) \right\},$$

equipped with the discrete  $L^2(0, T; H^1(\Omega))$  norm

$$\left( \sum_{k=1}^{N_T} \Delta t \|v^k\|_{1,2,\mathcal{T}}^2 \right)^{1/2} \quad \text{for all } v \in V_{\mathcal{T},\Delta t}.$$

**2.2. Numerical scheme.** We define the finite-volume scheme for the cross-diffusion model (1) and (2). We first approximate the initial functions by

$$(12) \quad u_{i,K}^0 = \frac{1}{m(K)} \int_K u_i^0(x) dx \quad \text{for } K \in \mathcal{T}, \quad i = 0, \dots, n.$$

Let  $u_K^{k-1} = (u_{1,K}^{k-1}, \dots, u_{n,K}^{k-1})$  and  $u_{0,K}^{k-1} = 1 - \sum_{i=1}^n u_{i,K}^{k-1}$  be given for  $K \in \mathcal{T}$ . Then the values  $u_{i,K}^k$  are determined by the implicit Euler finite-volume scheme

$$(13) \quad m(K) \frac{u_{i,K}^k - u_{i,K}^{k-1}}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{i,K,\sigma}^k = 0,$$

$$(14) \quad \mathcal{F}_{i,K,\sigma}^k = - \sum_{j=1}^n \tau_\sigma A_{ij,\sigma}(u_\sigma^k) D_{K,\sigma} u_j^k \quad \text{for } K \in \mathcal{T}, \quad \sigma \in \mathcal{E}_K,$$

and  $\tau_\sigma$  is defined by (10). The matrix  $A_\sigma = (A_{ij,\sigma})$  satisfies  $A_\sigma(u_0, u) = A(u)$  for all  $u \in D$  and  $u_0 = 1 - \sum_{i=1}^n u_i$ . By definition of the discrete operator  $D_{K,\sigma}$ , the discrete fluxes vanish on the boundary edges, guaranteeing the no-flux boundary conditions. Thus, we only need to define in (14) the mean vector  $u_\sigma^k = (u_{0,\sigma}^k, \dots, u_{n,\sigma}^k)$  for every  $\sigma = K|L \in \mathcal{E}_{\text{int}}$ :

$$(15) \quad u_{i,\sigma}^k = \begin{cases} \tilde{u}_{i,\sigma}^k & \text{if } u_{i,K}^k > 0, \quad u_{i,L}^k > 0, \quad \text{and } u_{i,K}^k \neq u_{i,L}^k, \\ u_{i,K}^k & \text{if } u_{i,K}^k = u_{i,L}^k > 0, \\ 0 & \text{else,} \end{cases}$$

where  $\tilde{u}_{i,K}^k \in (0, 1)$  is the unique solution to

$$(16) \quad h_i''(\tilde{u}_{i,\sigma}^k) D_{K,\sigma} u_i^k = D_{K,\sigma} h_i'(u_i^k) \quad \text{for } K \in \mathcal{T}, \quad \sigma \in \mathcal{E}_{\text{int},K}, \quad i = 0, \dots, n.$$

If  $h_i''$  is continuous and strictly monotone, the existence of a unique value  $\tilde{u}_{i,\sigma}^k$  follows from the mean-value theorem. Moreover, if  $u_{i,K}^k, u_{i,L}^k \geq 0$  we have for  $i = 0, \dots, n$ ,

$$0 \leq \min\{u_{i,K}^k, u_{i,L}^k\} \leq u_{i,\sigma}^k \leq \max\{u_{i,K}^k, u_{i,L}^k\} \leq 1.$$

**2.3. Main results.** Given the entropy density  $h(u) = \sum_{i=1}^n h_i(u_i) + h_0(u_0)$ , we define for  $u \in V_{\mathcal{T}}$  the discrete entropy

$$\mathcal{H}[u] = \sum_{K \in \mathcal{T}} m(K) h(u_K),$$

and replace the Hessian  $h''$  by the matrix

$$(17) \quad H_{ij}(u_\sigma) = \delta_{ij} h_i''(u_{i,\sigma}) + h_0''(u_{0,\sigma}), \quad u_\sigma \in (0, 1)^{n+1}, \quad i, j = 1, \dots, n,$$

where  $u_{i,\sigma}$  is defined by (15). Note that this matrix is symmetric and positive definite (if  $h_i$  is strictly convex).

We impose the following hypotheses:

**(H1)** Domain:  $\Omega \subset \mathbb{R}^2$  is a bounded polygonal domain and  $D = \{u = (u_1, \dots, u_n) \in (0, 1)^n : \sum_{i=1}^n u_i < 1\}$ .

**(H2)** Discretization:  $\mathcal{D}$  is an admissible discretization of  $\Omega_T = \Omega \times (0, T)$  satisfying (11).



- (H3) Initial data:  $u^0 = (u_1^0, \dots, u_n^0) \in L^1(\Omega; D)$  satisfies  $\int_{\Omega} h(u^0) dx < \infty$ . We set  $u_0^0 = 1 - \sum_{i=1}^n u_i^0$ .
- (H4) Entropy density:  $h(u) = \sum_{i=1}^n h_i(u_i) + h_0(u_0)$  for  $u \in D$  and  $u_0 = 1 - \sum_{i=1}^n u_i$ , where  $h \in C^0(\bar{D}; [0; \infty))$  is convex,  $h' : D \rightarrow \mathbb{R}$  is invertible,  $h_i \in C^2(0, 1)$ ,  $h_i''$  is strictly decreasing, and there exists  $c_h > 0$  such that  $h_i(x) \geq c_h(x - 1)$  for all  $0 \leq x \leq 1$ ,  $i = 1, \dots, n$ .
- (H5) Diffusion matrix:  $A \in C^{0,1}(\bar{D}; \mathbb{R}^{n \times n})$  and there exists a matrix  $A_{\sigma} \in C^{0,1}([0, 1] \times (0, 1)^n; \mathbb{R}^{n \times n})$  such that  $A(u) = A_{\sigma}(u_{\sigma})$  for all  $u \in D$  with  $u_i = u_{i,\sigma}$  for  $i = 1, \dots, n$  and  $u_{0,\sigma} = 1 - \sum_{i=1}^n u_i$ . We assume that  $\|A_{\sigma}(0, u)\| < \infty$ , where  $\|\cdot\|$  denotes some matrix norm, for all  $u = (u_1, \dots, u_n) \in (0, 1)^n$  satisfying  $\sum_{i=1}^n u_i \leq 1$ , and there exist numbers  $c_A > 0$ ,  $0 < s < 1$  such that for all  $z \in \mathbb{R}^n$  and for some  $u_{\sigma} \in (0, 1)^{n+1}$ ,

$$z^{\top} H(u_{\sigma}) A_{\sigma}(u_{\sigma}) z \geq c_A \sum_{i=1}^n u_{i,\sigma}^{2(s-1)} z_i^2.$$

These assumptions include all hypotheses needed in the boundedness-by-entropy method; see [32]. We also need additional conditions. First, the entropy density in Hypothesis (H4) has a particular structure including the Boltzmann entropy for volume-filling models. The strict monotonicity of  $h_i''$  is required to define properly the mean value  $\tilde{u}_{i,\sigma}^k$  in (15). Admissible examples are  $h_i(s) = s(\log s - 1) + 1$  and, more generally,  $h_i(s) = \int_a^s \log q(z) dz$  with  $a \in (0, 1)$ ,  $q \in C^2(0, 1) \cap C^0([0, 1])$  is strictly monotone,  $qq'' > (q')^2$ ,  $q(0) = 0$ , and  $q(0)/q'(0) = 0$ .

Second, the positive definiteness condition in Hypothesis (H5) is formulated for the matrix  $H(u_{\sigma})$ , which replaces the Hessian  $h''$ , and the modified diffusion matrix  $A_{\sigma}(u_{\sigma})$ . This modification is needed to take care of the fact that  $u_{0,\sigma}$  can generally not be identified with  $1 - \sum_{i=1}^n u_{i,\sigma}$ . If this identification is possible, the matrices  $h''A$  and  $HA_{\sigma}$  coincide. The Lipschitz continuity of  $A_{\sigma}$  is needed in the proof of the convergence of the scheme but not for the existence analysis. We prove below (see Theorem 1) that  $u_{i,\sigma}^k > 0$  holds for all  $i = 1, \dots, n$  but only  $u_{0,\sigma}^k \geq 0$ . Our analysis can be extended under suitable assumptions to the case  $s = 1$  and allowing for source terms in (1); see Remarks 6, 7, and 11.

The first main result is as follows.

**Theorem 1** (Existence of discrete solutions). *Let Hypotheses (H1)–(H5) hold. Then there exists a solution  $u_K^k = (u_{1,K}^k, \dots, u_{n,K}^k)$  to scheme (12)–(15) satisfying  $u_K^k \in D$  for  $K \in \mathcal{T}$  and  $0 < u_{i,\sigma}^k < 1$  for  $\sigma \in \mathcal{E}_{\text{int}}$ ,  $k \geq 1$ ,  $i = 1, \dots, n$ . Moreover, the following discrete entropy inequality holds:*

$$(18) \quad \mathcal{H}[u^k] + c_A \Delta t \sum_{i=1}^n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} u_{i,\sigma}^{2(s-1)} (D_{\sigma} u_i^k)^2 \leq \mathcal{H}[u^{k-1}].$$

The proof of Theorem 1 is based on a topological degree argument and the entropy estimate (18), which follows from the discrete chain rule (7). Generally, we cannot exclude that  $\sum_{i=0}^n u_{i,\sigma}^k > 1$ . However, when the entropy is given by the Boltzmann entropy  $h_i(u_i) = u_i(\log u_i - 1) + 1$ , it holds that  $\sum_{i=0}^n u_{i,\sigma}^k \leq 1$ , since the logarithmic mean is not larger than

the arithmetic mean, i.e.  $u_{i,\sigma}^k \leq (u_{i,K}^k + u_{i,L}^k)/2$  for  $\sigma = K|L$  and  $\sum_{i=0}^n u_{i,\sigma}^k \leq \sum_{i=0}^n (u_{i,K}^k + u_{i,L}^k)/2 = 1$ . This shows that the volume-filling constraints are fully satisfied.

For the convergence result, we need some notation. For  $K \in \mathcal{T}$  and  $\sigma \in \mathcal{E}_K$ , we define the cell  $T_{K,\sigma}$  of the dual mesh:

- If  $\sigma = K|L \in \mathcal{E}_{\text{int},K}$ , then  $T_{K,\sigma}$  is that cell (“diamond”) whose vertices are given by  $x_K, x_L$ , and the end points of the edge  $\sigma$ .
- If  $\sigma \in \mathcal{E}_{\text{ext},K}$ , then  $T_{K,\sigma}$  is that cell (“triangle”) whose vertices are given by  $x_K$  and the end points of the edge  $\sigma$ .

The cells  $T_{K,\sigma}$  define a partition of  $\Omega$ . It follows from the property that the straight line  $\overline{x_K x_L}$  between two neighboring centers of cells is orthogonal to the edge  $\sigma = K|L$  that

$$\mathfrak{m}(\sigma)d(x_K, x_L) = 2 \mathfrak{m}(T_{K,\sigma}) \quad \text{for } \sigma = K|L \in \mathcal{E}_{\text{int}}.$$

The approximate gradient of  $v \in V_{\mathcal{T},\Delta t}$  is defined by

$$\nabla^{\mathcal{D}} v(x, t) = \frac{\mathfrak{m}(\sigma)}{\mathfrak{m}(T_{K,\sigma})} (\mathbb{D}_{K,\sigma} v^k) \nu_{K,\sigma} \quad \text{for } x \in T_{K,\sigma}, \quad t \in (t_{k-1}, t_k],$$

where  $\nu_{K,\sigma}$  is the unit vector that is normal to  $\sigma$  and points outwards of  $K$ .

We introduce a family  $(\mathcal{D}_m)_{m \in \mathbb{N}}$  of admissible space-time discretizations of  $\Omega_T$  indexed by the size  $\eta_m = \max\{\Delta x_m, \Delta t_m\}$  of the mesh, satisfying  $\eta_m \rightarrow 0$  as  $m \rightarrow \infty$ . We denote by  $\mathcal{T}_m$  the corresponding meshes of  $\Omega$  and by  $\Delta t_m$  the corresponding time step sizes. Finally, we set  $\nabla^m := \nabla^{\mathcal{D}_m}$ .

**Theorem 2** (Convergence of the scheme). *Let the assumptions of Theorem 1 hold, let  $(\mathcal{D}_m)_{m \in \mathbb{N}}$  be a family of admissible meshes satisfying (11) uniformly in  $m \in \mathbb{N}$ . Let  $(u_m)_{m \in \mathbb{N}}$  be a family of finite-volume solutions to (12)–(15) constructed in Theorem 1. Then there exists a function  $u = (u_1, \dots, u_n) \in L^2(0, T; H^1(\Omega; \mathbb{R}^n))$  satisfying  $u(x, t) \in \overline{D}$  for a.e.  $(x, t) \in \Omega_T$  and for  $i = 1, \dots, n$ ,*

$$\begin{aligned} u_{i,m} &\rightarrow u_i \quad \text{strongly in } L^p(\Omega_T), \quad 1 \leq p < \infty, \\ \nabla^m u_{i,m} &\rightharpoonup \nabla u_i \quad \text{weakly in } L^2(\Omega_T) \quad \text{as } m \rightarrow \infty, \end{aligned}$$

up to a subsequence, and  $u$  is a weak solution to (1) and (2), i.e., for all  $\psi_i \in C_0^\infty(\Omega \times [0, T])$ , it holds that for all  $i = 1, \dots, n$ ,

$$(19) \quad \int_0^T \int_\Omega u_i \partial_t \psi_i dx dt + \int_\Omega u_i^0 \psi_i(0) dx = \int_0^T \int_\Omega \sum_{j=1}^n A_{ij}(u) \nabla u_j \cdot \nabla \psi_i dx dt.$$

The proof is based on uniform estimates deduced from the entropy inequality (18) and the compactness result from [23], giving a.e. convergence of a subsequence of  $(u_m)$ . We follow the strategy of [15] to show that the limit satisfies (1) in the weak sense (19).

### 3. EXAMPLES AND COUNTER-EXAMPLE

**3.1. Three-species Maxwell–Stefan equations.** The Maxwell–Stefan equations describe the evolution of the partial densities in a multicomponent fluid, with diffusion fluxes

originating from friction forces. The diffusion matrix of the Fock–Onsager formulation is defined for the three-species case by

$$A(u) = \frac{1}{\alpha(u)} \begin{pmatrix} d_2 + (d_0 - d_2)u_1 & (d_0 - d_1)u_1 \\ (d_0 - d_2)u_2 & d_1 + (d_0 - d_1)u_2 \end{pmatrix},$$

where  $\alpha(u) = d_1 d_2 (1 - u_1 - u_2) + d_0 d_1 u_1 + d_0 d_2 u_2$ ,

where  $u_1, u_2$  are the volume fractions of the components of the fluid mixture and  $d_i$  are some positive parameters [33]. The third constituent is given by  $u_0 = 1 - u_1 - u_2$ . We introduce the entropy density

$$(20) \quad h(u) = u_1(\log u_1 - 1) + u_2(\log u_2 - 1) + u_0(\log u_0 - 1) + 3, \quad u \in D.$$

Then the Hessian of  $h$  equals

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

Now, for the finite-volume scheme, let  $(u_{1,K}, \dots, u_{n,K}) \in D$  be given for every  $K \in \mathcal{T}$ , we define for all  $\sigma = K|L \in \mathcal{E}_{int}$  and  $i = 0, \dots, n$ ,

$$(21) \quad u_{i,\sigma} = \begin{cases} \frac{u_{i,K} - u_{i,L}}{\log(u_{i,K}) - \log(u_{i,L})} & \text{if } u_{i,K} > 0, u_{i,L} > 0, \text{ and } u_{i,K} \neq u_{i,L}, \\ u_{i,K} & \text{if } u_{i,K} = u_{i,L} > 0, \\ 0 & \text{else,} \end{cases}$$

and

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

$$A_\sigma(u_\sigma) = \frac{1}{\alpha_\sigma(u_\sigma)} \begin{pmatrix} d_2(u_{2,\sigma} + u_{0,\sigma}) + d_0 u_{1,\sigma} & (d_0 - d_1)u_{1,\sigma} \\ (d_0 - d_2)u_{2,\sigma} & d_1(u_{1,\sigma} + u_{0,\sigma}) + d_0 u_{2,\sigma} \end{pmatrix},$$

where  $\alpha_\sigma(u_\sigma) = d_1 d_2 u_{0,\sigma} + d_0 d_1 u_{1,\sigma} + d_0 d_2 u_{2,\sigma}$ .

Note that  $A_\sigma = A$  if  $u_{0,\sigma} = 1 - u_{1,\sigma} - u_{2,\sigma}$ . We compute for  $z = (z_1, z_2) \in \mathbb{R}^2$ ,

$$H(u_\sigma)A_\sigma(u_\sigma) = \frac{u_{0,\sigma} + u_{1,\sigma} + u_{2,\sigma}}{\alpha_\sigma(u_\sigma)} \begin{pmatrix} d_2/u_{1,\sigma} + d_0/u_{0,\sigma} & d_0/u_{0,\sigma} \\ d_0/u_{0,\sigma} & d_1/u_{2,\sigma} + 1/u_{0,\sigma} \end{pmatrix},$$

$$z^\top H(u_\sigma)A_\sigma(u_\sigma)z = \frac{u_{0,\sigma} + u_{1,\sigma} + u_{2,\sigma}}{\alpha_\sigma(u_\sigma)} \left( \frac{d_2}{u_{1,\sigma}} z_1^2 + \frac{d_1}{u_{2,\sigma}} z_2^2 + \frac{d_0}{u_{0,\sigma}} (z_1 + z_2)^2 \right)$$

$$\geq c \left( \frac{z_1^2}{u_{1,\sigma}} + \frac{z_2^2}{u_{2,\sigma}} \right),$$

where  $c = \max\{d_0 d_1, d_0 d_1, d_1 d_2\} > 0$ . This fulfills Hypothesis (H5) with  $s = 1/2$ . Moreover, Theorem 1 shows that  $u_{i,\sigma} > 0$  for  $i = 1, 2$ . Thus,  $\alpha_\sigma(u_\sigma)$  is positive and  $A_\sigma$  is well defined.

**3.2. A cross-diffusion system for thin-film solar cells.** The physical vapor deposition process for the fabrication of thin-film crystalline solar cells can be described by the following cross-diffusion equations:

$$(22) \quad \partial_t u_i = \operatorname{div} \left( \sum_{j=0}^n a_{ij} (u_j \nabla u_i - u_i \nabla u_j) \right), \quad i = 0, \dots, n,$$

where  $u_i$  are the volume fractions of the components of the thin film and  $a_{ij} > 0$  satisfies  $a_{ij} = a_{ji}$  for all  $i, j = 1, \dots, n$ . Since  $\sum_{i=0}^n u_i = 1$ , we can remove, as in [4], the equation for the species  $i = 0$ , leading to equations (1) with the diffusion matrix  $A(u) = (A_{ij}(u))$ , where

$$(23) \quad A_{ii}(u) = \sum_{k=1, k \neq i}^n (a_{ik} - a_{i0}) u_k + a_{i0}, \quad A_{ij}(u) = -(a_{ij} - a_{i0}) u_i \quad \text{for } j \neq i,$$

and  $i, j = 1, \dots, n$ . In this case, we consider the entropy density (20) and for  $(u_{1,K}, \dots, u_{n,K}) \in D$  given for every  $K \in \mathcal{T}$ , we define for all  $\sigma = K|L \in \mathcal{E}_{int}$  and  $i = 0, \dots, n$  the coefficient  $u_{i,\sigma}$  as in (21). Then we choose the following matrices:

$$(24) \quad H_{ii}(u_\sigma) = \frac{1}{u_{i,\sigma}} + \frac{1}{u_{0,\sigma}}, \quad H_{ij}(u_\sigma) = \frac{1}{u_{0,\sigma}} \quad \text{for } j \neq i,$$

$$(25) \quad A_{ii,\sigma}(u_\sigma) = \sum_{k=1, k \neq i}^n (a_{ik} - a_{i0}) u_{k,\sigma} + a_{i0}, \quad A_{ij,\sigma}(u_\sigma) = -(a_{ij} - a_{i0}) u_{i,\sigma} \quad \text{for } j \neq i.$$

We claim that Hypothesis (H5) holds with  $s = 1/2$ . The proof follows the strategy in [4, Section 3.1], but since generally  $\beta \neq 1$ , we need to modify slightly the arguments. To this end, we introduce the matrix  $P(u_\sigma)$  with elements  $P_{ij}(u_\sigma) = \delta_{ij} - u_{i,\sigma}$  for  $i, j = 1, \dots, n$ . A computation shows that

$$(H(u_\sigma)P(u_\sigma))_{ii} = \frac{1}{u_{i,\sigma}} + \frac{1-\beta}{u_{0,\sigma}}, \quad (H(u_\sigma)P(u_\sigma))_{ij} = \frac{1-\beta}{u_{0,\sigma}} \quad \text{for } i \neq j.$$

Recall that  $\beta \leq 1$ . Then  $H(u_\sigma)P(u_\sigma)$  is positive definite with

$$z^\top H(u_\sigma)P(u_\sigma)z = \sum_{i=1}^n \frac{z_i^2}{u_{i,\sigma}} + \frac{1-\beta}{u_{0,\sigma}} \sum_{i,j=1}^n (z_i + z_j)^2 \geq \sum_{i=1}^n \frac{z_i^2}{u_{i,\sigma}}$$

for any  $z \in \mathbb{R}^n$ . We also need the matrix  $\Lambda(u_\sigma)$  with elements  $\Lambda_{ij}(u_\sigma) = \delta_{ij}/u_{i,\sigma}$  and  $\alpha = \min_{i,j=1,\dots,n} a_{ij} > 0$ . The previous inequality gives

$$z^\top (H(u_\sigma)A_\sigma(u_\sigma) - \alpha\Lambda(u_\sigma))z \geq z^\top H(u_\sigma)(A_\sigma(u_\sigma) - \alpha P(u_\sigma))z.$$

Denoting by  $\tilde{A}_\sigma(u_\sigma)$  the matrix with coefficients  $a_{ij} - \alpha$  instead of  $a_{ij}$  and introducing the matrix  $D(u_\sigma)$  with elements  $D_{ij}(u_\sigma) = u_{i,\sigma}$  for  $i, j = 1, \dots, n$ , it follows that  $A_\sigma(u_\sigma) - \alpha P(u_\sigma) = \tilde{A}_\sigma(u_\sigma) + \alpha D(u_\sigma)$ . Therefore,

$$z^\top (H(u_\sigma)A_\sigma(u_\sigma) - \alpha\Lambda(u_\sigma))z \geq z^\top (H(u_\sigma)\tilde{A}_\sigma(u_\sigma) + \alpha H(u_\sigma)D(u_\sigma))z.$$

It remains to show that  $H(u_\sigma)\tilde{A}_\sigma(u_\sigma)$  and  $H(u_\sigma)D(u_\sigma)$  are positive semidefinite. All elements of  $H(u_\sigma)D(u_\sigma)$  are given by the same value  $\beta/u_{0,\sigma}$ , and so this matrix is positive semidefinite. Furthermore,  $H(u_\sigma)\tilde{A}_\sigma(u_\sigma)$  is positive semidefinite if and only if  $\tilde{A}_\sigma(u_\sigma)H(u_\sigma)^{-1}$  is positive semidefinite. (At this point, we use the symmetry of  $H(u_\sigma)$ .) Since the elements of the inverse  $H(u_\sigma)^{-1}$  are

$$H(u_\sigma)_{ii}^{-1} = \frac{1}{\beta}(\beta - u_{i,\sigma})u_{i,\sigma}, \quad H(u_\sigma)_{ij}^{-1} = -\frac{1}{\beta}u_{i,\sigma}u_{j,\sigma} \quad \text{for } i \neq j$$

and  $i, j = 1, \dots, n$ , we obtain

$$\begin{aligned} (\tilde{A}_\sigma(u_\sigma)H(u_\sigma)^{-1})_{ii} &= (a_{i0} - \alpha)\frac{u_{i,\sigma}}{\beta}(\beta - u_{i,\sigma}) + \frac{1}{\beta} \sum_{k=1, j \neq i}^n (a_{ij} - \alpha)u_{i,\sigma}u_{j,\sigma}, \\ (\tilde{A}_\sigma(u_\sigma)H(u_\sigma)^{-1})_{ij} &= -\frac{1}{\beta}(a_{ij} - \alpha)u_{i,\sigma}u_{j,\sigma} \quad \text{for } i \neq j. \end{aligned}$$

Consequently, using the symmetry of  $(a_{ij})$ ,

$$\begin{aligned} z^\top \tilde{A}_\sigma(u_\sigma)H(u_\sigma)^{-1}z &= \frac{1}{\beta} \sum_{i=1}^n (a_{i0} - \alpha)u_{i,\sigma}(\beta - u_{i,\sigma})z_i^2 + \frac{1}{\beta} \sum_{i=1}^n \sum_{j=1, j \neq i}^n (a_{ij} - \alpha)u_{i,\sigma}u_{j,\sigma}(z_i^2 - z_i z_j) \\ &= \frac{1}{\beta} \sum_{i=1}^n (a_{i0} - \alpha)u_{i,\sigma}(\beta - u_{i,\sigma})z_i^2 + \frac{1}{2\beta} \sum_{i \neq j} (a_{ij} - \alpha)u_{i,\sigma}u_{j,\sigma}(z_i^2 + z_j^2 - 2z_i z_j) \geq 0. \end{aligned}$$

We conclude that

$$z^\top (H(u_\sigma)A_\sigma(u_\sigma) - \alpha\Lambda(u_\sigma))z \geq 0.$$

Summarizing, the result reads as follows.

**Lemma 3.** *et  $u_\sigma \in (0, 1)^{n+1}$  be defined by (21) and  $H(u_\sigma)$  and  $A_\sigma(u_\sigma)$  by (24)–(25) and assume that  $a_{ij} = a_{ji}$  for all  $i, j = 1, \dots, n$  and  $\alpha = \min_{i,j=1,\dots,n} a_{ij} > 0$ . Then for any  $z \in \mathbb{R}^n$ ,*

$$z^\top H(u_\sigma)A_\sigma(u_\sigma)z \geq \alpha \sum_{i=1}^n \frac{z_i^2}{u_{i,\sigma}}.$$

Already in [13], a convergent two-point flux approximation finite-volume scheme for this model with a logarithmic mean was introduced, but with a different strategy. Indeed, the authors of [13] noticed that if all diffusion coefficients are equal, system (22) reduces to  $n + 1$  uncoupled heat equations, and they rewrite the equations as

$$\partial_t u_i - a^* \Delta u_i = \operatorname{div} \left( \sum_{j=0}^n (a_{ij} - a^*) (u_j \nabla u_i - u_i \nabla u_j) \right), \quad i = 0, \dots, n,$$

where  $a^* > 0$  is arbitrary. Then they designed their scheme for this equivalent system and proved its convergence, using similar techniques as in our paper. However, the numerical

results depend on the choice of  $a^*$ , and choosing  $a^* > 0$  too large overestimates the diffusion. In our approach, we avoid the artificial parameter  $a^*$  but still obtain full structure preservation of the scheme.

**3.3. Tumor-growth model.** The growth of an avascular tumor can be modeled in the framework of fluid dynamics and continuum mechanics by diffusion fluxes of the tumor cells, the extracellular matrix (ECM), and the interstitial fluid (water, nutrients). The diffusion matrix of the tumor-growth model of [30] is given by

$$A(u) = \begin{pmatrix} 2u_1(1-u_1) - \beta\theta u_1 u_2^2 & -2\beta u_1 u_2(1+\theta u_1) \\ -2u_1 u_2 + \beta\theta(1-u_2)u_2^2 & 2\beta u_2(1-u_2)(1+\theta u_1) \end{pmatrix},$$

where  $u_1$  is the volume fraction of the tumor cells and  $u_2$  is the volume fraction of the ECM. The volume fraction of the interstitial fluid is denoted by  $u_0$ , and it holds that  $u_0 + u_1 + u_2 = 1$ . The entropy density and the mobility coefficients are defined as in the previous examples, and we choose  $H(u_\sigma)$  as before. Furthermore, we define

$$A_\sigma(u_\sigma) = \frac{1}{a(u_\sigma)} \begin{pmatrix} 2u_{1,\sigma}(u_{0,\sigma} + u_{2,\sigma}) - \beta\theta u_{1,\sigma} u_{2,\sigma}^2 & -2\beta u_{1,\sigma} u_{2,\sigma}(1 + \theta u_{1,\sigma}) \\ -2u_{1,\sigma} u_{2,\sigma} + \beta\theta(u_{0,\sigma} + u_{1,\sigma})u_{2,\sigma}^2 & 2\beta u_{2,\sigma}(u_{0,\sigma} + u_{1,\sigma})(1 + \theta u_{1,\sigma}) \end{pmatrix},$$

where  $a(u_\sigma) = u_{0,\sigma} + u_{1,\sigma} + u_{2,\sigma}$  is a correction factor. The corresponding cross-diffusion system has an entropy structure under the condition  $\theta < 4/\sqrt{\beta}$  [36]. We compute

$$z^\top H(u_\sigma) A_\sigma(u_\sigma) z = 2z_1^2 + \beta\theta u_{2,\sigma} z_1 z_2 + 2\beta(1 + \theta u_{1,\sigma}) z_2^2 \geq \delta(z_1^2 + z_2^2),$$

where  $\delta > 0$  depends on  $\beta$  and  $\theta$ . This does not fulfill Hypothesis (H5) since  $s = 1$ . Moreover, we cannot deduce that  $a(u_\sigma) > 0$  from Theorem 1. For instance, if  $\sigma = K|L$  and  $u_{1,K} = u_{2,L} = 0$ ,  $u_{1,L} = u_{2,K} = 1$ , we obtain  $u_{0,K} = u_{0,L} = 0$  and  $u_{i,\sigma} = 0$  for all  $i = 0, 1, 2$ . In fact, we observe in our numerical simulations that  $a(u_\sigma)$  may vanish. This can be prevented by adding an artificial diffusion term of the form  $\delta \Delta u_i$  with  $\delta > 0$  for  $i = 1, 2$ . Then Hypothesis (H5) is satisfied with  $s = 1/2$ . However, such terms regularize the solutions in such a way that the ‘‘spikes’’ observed in [36, Figure 1] are smoothed out. Thus, the accurate numerical simulation in the case  $s = 1$  is still an open problem.

#### 4. PROOF OF THEOREM 1

We first prove a discrete version of the chain rule  $h''(u)\nabla u = \nabla h'(u)$ .

**Lemma 4** (Discrete chain rule). *Let  $H_{ij}(u_\sigma)$  be defined by (17), where  $u \in D$  and  $u_\sigma$  is given by (15). Then for all  $\sigma \in \mathcal{E}_{\text{int},K}$ , it holds that*

$$H(u_\sigma) D_{K,\sigma} u^k = D_{K,\sigma} h'(u^k).$$

*Proof.* Let  $\sigma = K|L \in \mathcal{E}_{\text{int},K}$  and  $i \in \{1, \dots, n\}$ . By definition (15), we find that

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

using  $\sum_{j=1}^n u_{i,K} = 1 - u_{0,K}$  in the last step. Since  $u \in D$ , we have either  $u_{i,\sigma} = \tilde{u}_{i,\sigma}$  or  $u_{i,\sigma} = u_{i,K} = u_{i,L}$ . Therefore,

$$\begin{aligned} \sum_{j=1}^n H_{ij}(u_\sigma^k) D_{K,\sigma} u_j^k &= h'_i(u_{i,L}) - h'_i(u_{i,K}) - (h'_0(u_{0,L}) - h'_0(u_{i,K})) \\ &= D_{K,\sigma} h'_i(u^k) - D_{K,\sigma} h'_0(u^k) = D_{K,\sigma} (\partial h / \partial u_i)(u^k). \end{aligned}$$

The result also holds when  $\sigma \in \mathcal{E}_{\text{ext},K}$ , since then  $D_{K,\sigma} u_j^k = 0$ . This finishes the proof.  $\square$

The existence proof is similar to [38, Section 2] and we repeat only the main arguments. The proof of the positivity statements, however, is new.

*Step 1: Fixed-point problem.* We proceed by induction over  $k \in \mathbb{N} \cup \{0\}$ . If  $k = 0$ , we have  $u_K^0 \in D$  for  $K \in \mathcal{T}$  by Hypothesis (H3). Let  $u^{k-1}$  be given such that  $u_K^{k-1} \in D$  for  $K \in \mathcal{T}$ . We construct  $u^k$  from a fixed-point argument. For this, let  $R > 0$ ,  $\varepsilon > 0$  and set

$$Z_R = \{w = (w_1, \dots, w_n) \in V_{\mathcal{T}}^n : \|w_i\|_{1,2,\mathcal{T}} < R \text{ for } i = 1, \dots, n\}.$$

We define the mapping  $F_\varepsilon : Z_R \rightarrow \mathbb{R}^{n\theta}$ ,  $F_\varepsilon(w) = w^\varepsilon$ , where  $\theta = \#\mathcal{T}$  and  $w^\varepsilon = (w_1^\varepsilon, \dots, w_n^\varepsilon)$  solves the linear system

$$(26) \quad \varepsilon \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} w_i^\varepsilon - \varepsilon m(K) w_{i,K}^\varepsilon = \frac{m(K)}{\Delta t} (u_{i,K} - u_{i,K}^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{i,K,\sigma},$$

for  $K \in \mathcal{T}$ ,  $i = 1, \dots, n$ , where  $\mathcal{F}_{i,K,\sigma}$  is defined in (14) and  $u_K = (h')^{-1}(w_K) \in D$ . The regularization in  $\varepsilon$  is needed, since the diffusion matrix is only positive semidefinite in the variable  $w^\varepsilon$ . The existence of a unique solution  $w^\varepsilon$  to (26) is a consequence of the proof of [19, Lemma 9.2]. The continuity of  $F_\varepsilon$  is shown as in [38, Section 4] by exploiting the fact that  $w \in Z_R$  is bounded and so does  $u = (h')^{-1}(w)$ , yielding the estimate  $\varepsilon \|w_i^\varepsilon\|_{1,2,\mathcal{T}} \leq C(R)$  for some constant  $C(R) > 0$ .

We claim that  $F_\varepsilon$  admits a fixed point. To this end, we use a topological degree argument [17, Chap. 1] and prove that the Brouwer topological degree satisfies  $\deg(I - F_\varepsilon, Z_R, 0) = 1$ . It is sufficient to verify that any solution  $(w^\varepsilon, \rho) \in \overline{Z}_R \times [0, 1]$  to the fixed-point equation  $w^\varepsilon = \rho F_\varepsilon(w)$  satisfies  $(w^\varepsilon, \rho) \notin \partial Z_R \times [0, 1]$  for sufficiently large values of  $R > 0$ . Let  $(w^\varepsilon, \rho)$  be a fixed point and  $\rho \neq 0$  (the case  $\rho = 0$  is clear). Then  $w^\varepsilon$  solves

$$(27) \quad \varepsilon \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} w_i^\varepsilon - \varepsilon m(K) w_{i,K}^\varepsilon = \rho \left( \frac{m(K)}{\Delta t} (u_{i,K}^\varepsilon - u_{i,K}^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{i,K,\sigma}^\varepsilon \right),$$

for all  $K \in \mathcal{T}$  and  $i = 1, \dots, n$ , where  $u_K^\varepsilon = (h')^{-1}(w_K^\varepsilon)$  and  $\mathcal{F}_{i,K,\sigma}^\varepsilon$  is defined as in (14) with  $u$  replaced by  $u^\varepsilon$ . Because of  $u_{i,K}^\varepsilon \in D$  we have  $u_{i,K}^\varepsilon > 0$  for  $K \in \mathcal{T}$  and  $i = 0, \dots, n$ .

*Step 2: Discrete entropy inequality.* The key step of the proof is the following lemma.

**Lemma 5** (Discrete entropy inequality). *Let the assumptions of Theorem 1 hold, let  $0 < \rho \leq 1$ ,  $\varepsilon > 0$ , and let  $u^\varepsilon$  be a solution to (27). Then  $u_{i,\sigma}^\varepsilon > 0$  for all  $\sigma \in \mathcal{E}$ ,  $i = 0, \dots, n$*

and

$$(28) \quad \rho\mathcal{H}[u^\varepsilon] + \rho c_A \Delta t \sum_{i=1}^n \sum_{\sigma \in \mathcal{E}} \tau_\sigma (u_{i,\sigma}^\varepsilon)^{2(s-1)} (D_\sigma u_i^\varepsilon)^2 + \varepsilon \Delta t \sum_{i=1}^n \|w_i^\varepsilon\|_{1,2,\mathcal{T}}^2 \leq \rho\mathcal{H}[u^{k-1}].$$

*Proof.* First, we prove that  $u_{i,\sigma}^\varepsilon > 0$  for all  $\sigma \in \mathcal{E}$  and  $i = 0, \dots, n$ . Indeed, if  $\sigma \in \mathcal{E}_{\text{ext},K}$ , we have  $u_{i,K}^\varepsilon = u_{i,K,\sigma}^\varepsilon > 0$  and hence  $u_{i,\sigma}^\varepsilon = u_{i,K}^\varepsilon > 0$ . Thus, let  $\sigma = K|L \in \mathcal{E}_{\text{int},K}$ . Again, if  $u_{i,K}^\varepsilon = u_{i,L}^\varepsilon > 0$ , it follows that  $u_{i,\sigma}^\varepsilon > 0$ . Otherwise,  $u_{i,\sigma}^\varepsilon$  is the unique solution to

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

and we deduce from the strict monotonicity that  $u_{i,\sigma}^\varepsilon \geq \min\{u_{i,K}^\varepsilon, u_{i,L}^\varepsilon\} > 0$ .

Next, multiplying (27) by  $\Delta t w_{i,K}^\varepsilon$ , summing over  $i = 1, \dots, n$  and  $K \in \mathcal{T}$ , and applying discrete integration by parts, we find that

$$\begin{aligned} 0 &= \rho \sum_{i=1}^n \sum_{K \in \mathcal{T}} m(K) (u_{i,K}^\varepsilon - u_{i,K}^{k-1}) w_{i,K}^\varepsilon - \rho \Delta t \sum_{i=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \mathcal{F}_{i,K,\sigma}^\varepsilon D_{K,\sigma} w_i^\varepsilon \\ &\quad + \varepsilon \Delta t \sum_{i=1}^n \|w_i^\varepsilon\|_{1,2,\mathcal{T}}^2 = I_1 + I_2 + I_3. \end{aligned}$$

We know from Hypothesis (H4) that  $h$  is convex such that, because of  $w_K^\varepsilon = h'(u_K^\varepsilon)$ ,

$$I_1 \geq \rho \sum_{K \in \mathcal{T}} m(K) (h(u_K^\varepsilon) - h(u_K^{k-1})) = \rho (\mathcal{H}[u^\varepsilon] - \mathcal{H}[u^{k-1}]).$$

Furthermore, by Lemma 4, the symmetry of  $(H_{ij})$ , and Hypothesis (H5),

$$\begin{aligned} I_2 &= \rho \Delta t \sum_{i,j=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma A_{ij}(u_\sigma^\varepsilon) D_{K,\sigma} u_j^\varepsilon D_{K,\sigma} (h'(u^\varepsilon))_i \\ &= \rho \Delta t \sum_{i,j=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma (H(u_\sigma^\varepsilon) D_{K,\sigma} u^\varepsilon)_i A_{ij}(u_\sigma^\varepsilon) D_{K,\sigma} u_j^\varepsilon \\ &= \rho \Delta t \sum_{i,j,\ell=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma D_{K,\sigma}(u_\ell^\varepsilon) H_{\ell i}(u_\sigma^\varepsilon) A_{ij}(u_\sigma^\varepsilon) D_{K,\sigma} u_j^\varepsilon \\ &= \rho \Delta t \sum_{j,\ell=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma D_{K,\sigma} u_\ell^\varepsilon (H(u_\sigma^\varepsilon) A(u_\sigma^\varepsilon))_{\ell j} D_{K,\sigma} u_j^\varepsilon \\ &\geq \rho c_A \Delta t \sum_{j=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma (u_{j,\sigma}^\varepsilon)^{2(s-1)} (D_{K,\sigma} u_j^\varepsilon)^2. \end{aligned}$$



Putting these estimates together, we conclude the proof.  $\square$

We continue with the topological degree argument. Choosing

$$R = \frac{1}{\sqrt{\varepsilon\Delta t}} \mathcal{H}[u^{k-1}]^{1/2} + 1,$$

the previous lemma leads to

$$\varepsilon\Delta t \sum_{i=1}^n \|w_i^\varepsilon\|_{1,2,\mathcal{T}}^2 \leq \rho \mathcal{H}[u^{k-1}] \leq \varepsilon\Delta t (R-1)^2,$$

which gives  $\sum_{i=1}^n \|w_i^\varepsilon\|_{1,2,\mathcal{T}}^2 < R^2$ . We conclude that  $w^\varepsilon \notin \partial Z_R$  and  $\deg(I - F_\varepsilon, Z_R, 0) = 1$ . Thus,  $F_\varepsilon$  admits at least one fixed point.

*Step 3: Limit  $\varepsilon \rightarrow 0$ .* By construction of  $u^\varepsilon$ , we have  $u_K^\varepsilon = (h')^{-1}(w_K^\varepsilon) \in D$  for  $K \in \mathcal{T}$ . Thus,  $\|u_i^\varepsilon\|_{0,\infty,\mathcal{T}} := \max_{K \in \mathcal{T}} |u_{i,K}^\varepsilon| \leq 1$  for  $i = 0, \dots, n$ , and there exists a subsequence (not relabeled) such that  $u_{i,K}^\varepsilon \rightarrow u_{i,K}^k \in [0, 1]$  as  $\varepsilon \rightarrow 0$  for  $K \in \mathcal{T}$ ,  $i = 1, \dots, n$  and satisfying  $u_K^k = (u_{1,K}^k, \dots, u_{n,K}^k) \in \overline{D}$ . Moreover, there exists a subsequence such that  $u_{i,\sigma}^\varepsilon \rightarrow u_{i,\sigma}^k \in [0, 1]$  as  $\varepsilon \rightarrow 0$  for  $\sigma \in \mathcal{E}_{\text{int}}$  and  $i = 0, \dots, n$ , and  $u_{0,\sigma}^k$  is given by (15). In view of the bound for  $\sqrt{\varepsilon}w_i^\varepsilon$ , we have, again for a subsequence,  $\varepsilon w_{i,K}^\varepsilon \rightarrow 0$ .

We show that the total mass  $\int_\Omega u_i^k dx$  is positive for  $i = 1, \dots, n$ . For this, we write  $w_{i,K}^{\varepsilon,k} := w_{i,K}^\varepsilon$ , sum over  $K \in \mathcal{T}$  in (27), and use the local balance equations  $\mathcal{F}_{i,K,\sigma}^\varepsilon + \mathcal{F}_{i,L,\sigma}^\varepsilon = 0$  and  $\tau_\sigma D_{K,\sigma} w^\varepsilon + \tau_\sigma D_{L,\sigma} w^\varepsilon = 0$  for all  $\sigma = K|L \in \mathcal{E}_{\text{int}}$  to deduce that, by induction,

$$\begin{aligned} \sum_{K \in \mathcal{T}} m(K) u_{i,K}^\varepsilon &= \sum_{K \in \mathcal{T}} m(K) u_{i,K}^{k-1} - \varepsilon\Delta t \sum_{K \in \mathcal{T}} m(K) w_{i,K}^{\varepsilon,k} \\ &= \sum_{K \in \mathcal{T}} m(K) u_{i,K}^0 - \varepsilon\Delta t \sum_{j=1}^k \sum_{K \in \mathcal{T}} m(K) w_{i,K}^{\varepsilon,k}, \end{aligned}$$

for  $i = 1, \dots, n$ . The limit  $\varepsilon \rightarrow 0$  yields

$$(29) \quad \sum_{K \in \mathcal{T}} m(K) u_{i,K}^k = \sum_{K \in \mathcal{T}} m(K) u_{i,K}^0 = \int_\Omega u_i^0(x) dx > 0 \quad \text{for } i = 1, \dots, n,$$

where the positivity in the last step follows from Hypothesis (H3).

Next, we show that  $0 < u_{i,\sigma}^k < 1$  for all  $\sigma \in \mathcal{E}_{\text{int}}$  and  $i = 1, \dots, n$ . In view of definition (15) of  $u_{i,\sigma}^k$  and  $\sum_{i=1}^n u_{i,K}^k \leq 1$ , it is sufficient to show that  $u_{i,K}^k > 0$  for all  $K \in \mathcal{T}$  and  $i = 1, \dots, n$ . Let  $i \in \{1, \dots, n\}$  be fixed. Assume by contradiction that  $u_{i,K}^k = 0$  for some  $K \in \mathcal{T}$ . Then  $u_{i,\sigma}^k = 0$  for  $\sigma = K|L \in \mathcal{E}_{\text{int}}$ . The entropy inequality gives

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

and in the limit  $\varepsilon \rightarrow 0$

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

Thus,  $u_{i,\sigma}^k = 0$  implies that  $u_{i,L}^k = 0$  (here we need  $s < 1$ ). Next, let  $L'$  be a neighboring cell of  $L$ . By the previous argument, it follows that also  $u_{i,L'}^k = 0$ . Repeating this argument

for all cells in  $\mathcal{T}$ , we find that  $u_{i,K}^k = 0$  for all  $K \in \mathcal{T}$ . Consequently,  $\sum_{K \in \mathcal{T}} m(K) u_{i,K}^k = 0$ , which contradicts (29). This shows in particular that  $u_{0,K}^k = 1 - \sum_{i=1}^n u_{i,K}^k < 1$  and hence  $u_K^k \in D$  for all  $K \in \mathcal{T}$ . Moreover, we deduce from the definition of  $u_{i,\sigma}^k$  that  $0 < u_{i,\sigma}^k < 1$  holds for all  $\sigma = K|L \in \mathcal{E}_{\text{int}}$  and  $i = 1, \dots, n$ .

Note that  $u_{0,\sigma}^k = 0$  may be possible, which explains the condition  $\|A_\sigma(u_\sigma)\| < \infty$  in Hypothesis (H5) whenever  $u_{0,\sigma} = 0$ . Thus, together with the continuity of  $A_{ij,\sigma}$  on  $[0, 1] \times (0, 1)^n$  and the bounds on  $u_{i,\sigma}^k$  for  $i = 1, \dots, n$ , we can pass to the limit  $\varepsilon \rightarrow 0$  in (27) and (28) to finish the proof of Theorem 1.

**Remark 6** (Case  $s = 1$ ). The existence of discrete solutions to scheme (12)–(15) and the validity of the entropy inequality can be extended to the case  $s = 1$  if  $\|A_\sigma(0)\| < \infty$ . This is possible since the singular term  $(u_{i,\sigma}^k)^{2(s-1)}$  disappears when  $s = 1$  and the proof simplifies. However, we cannot ensure in general that  $u_{i,\sigma}^k > 0$  holds for  $\sigma \in \mathcal{E}_{\text{int}}$ ,  $k \geq 1$ ,  $i = 1, \dots, n$ . For the existence of discrete solutions, the condition  $\|A_\sigma(0)\| < \infty$  is crucial. The example in Section 3.3 shows that the modified matrix  $A_\sigma$  may contain the factor  $a(u_\sigma) = \sum_{i=1}^n c_i u_{i,\sigma}$  for some  $c_i > 0$ , necessary to prove the positive (semi-) definiteness of  $HA_\sigma$ . In this situation,  $\|A_\sigma(0)\|$  is not a number, and the existence of a discrete solution cannot be guaranteed.  $\square$

**Remark 7** (Source terms). Our analysis still holds when we include source terms of the type  $f_i(u)$  on the right-hand side of (1). We need to assume that  $f_i \in C^0(\bar{D})$  and that there exist constants  $C_f > 0$ ,  $c_f \geq 0$  such that for all  $u \in D$ ,

$$(30) \quad \sum_{i=1}^n f_i(u)(h'_i(u_i) + h'_0(u_0)) \leq C_f(1 + h(u)) \quad \text{and} \quad f_i(u) \geq -c_f u_i \quad \text{for } i = 1, \dots, n.$$

If we assume, in addition to Hypotheses (H1)–(H5), the condition  $\Delta t < 1/C_f$  on the time step size, then the statement of Theorem 1 holds with the modified entropy inequality

$$(1 - C_f \Delta t) \mathcal{H}[u^k] + c_A \Delta t \sum_{i=1}^n \sum_{\sigma \in \mathcal{E}} \tau_\sigma u_{i,\sigma}^{2(s-1)} (D_\sigma u_i^k)^2 \leq \mathcal{H}[u^{k-1}] + C_f \Delta t m(\Omega).$$

This inequality is a direct consequence of the first assumption in (30); see, e.g., the proof of [38, Theorem 1]. The second assumption in (30) allows us to adapt the proof of the positivity of the total mass in Step 3, giving after an induction

$$\sum_{K \in \mathcal{T}} m(K) u_{i,K}^k \geq \frac{\int_\Omega u_i^0(x) dx}{(1 + c_f \Delta t)^k} > 0.$$

The remaining proof is unchanged.  $\square$

## 5. PROOF OF THEOREM 2

We prove first some estimates uniform in  $\Delta x$  and  $\Delta t$  and then deduce the compactness properties.

5.1. **A priori estimates.** We introduce the discrete time derivative of a function  $v \in V_{\mathcal{T}, \Delta t}$ :

$$\partial_t^{\Delta t} v(x, t) = \partial_t^{\Delta t} v^k(x) = \frac{1}{\Delta t} (v^k(x) - v^{k-1}(x)), \quad (x, t) \in \bar{\Omega} \times (t_{k-1}, t_k], \quad k = 1, \dots, N_T.$$

**Lemma 8** (Uniform estimates). *Let the assumptions of Theorem 1 hold. Then there exists a constant  $C > 0$  independent of  $\Delta x$  and  $\Delta t$  such that for all  $i = 1, \dots, n$ ,*

$$\max_{k=1, \dots, N_T} \|u_i^k\|_{0,1,\mathcal{T}} + \sum_{k=1}^{N_T} \Delta t \|u_i^k\|_{1,2,\mathcal{T}}^2 + \sum_{k=1}^{N_T} \Delta t \|\partial_t^{\Delta t} u_i^k\|_{-1,2,\mathcal{T}}^2 \leq C.$$

*Proof.* We sum (18) over  $k = 1, \dots, j$  (with  $j \leq N_T$ ) and  $i = 1, \dots, n$ , and use the facts that  $0 < u_{i,\sigma}^k \leq 1$  and  $s < 1$  to obtain

$$\mathcal{H}[u^j] + c_A \sum_{k=1}^j \Delta t \sum_{i=1}^n \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma u_i^k)^2 \leq \mathcal{H}[u^0].$$

Since the entropy dominates the  $L^1$  norm thanks to (H4), the previous inequality implies that

$$\max_{k=1, \dots, j} \sum_{i=1}^n \|u_i^k\|_{0,1,\mathcal{T}} + \sum_{k=1}^j \Delta t \sum_{i=1}^n |u_i^k|_{1,2,\mathcal{T}}^2 \leq \mathcal{H}[u^0] + c_h \text{m}(\Omega).$$

The discrete Poincaré–Wirtinger inequality [6, Theorem 3.6] gives the existence of a constant  $C$  only depending on  $u^0$  and  $\Omega$  such that  $\sum_{k=1}^j \Delta t \|u_i^k\|_{0,2,\mathcal{T}}^2 \leq C$ .

For the estimate of the discrete time derivative, we choose  $\phi \in V_{\mathcal{T}}$  with  $\|\phi\|_{1,2,\mathcal{T}} = 1$  and multiply scheme (13) by  $\phi_K$ , sum over  $K \in \mathcal{T}$ ,  $k = 1, \dots, N_T$ , and apply discrete integration by parts:

$$\sum_{K \in \mathcal{T}} \text{m}(K) \frac{u_{i,K}^k - u_{i,K}^{k-1}}{\Delta t} \phi_K = - \sum_{j=1}^n \sum_{\substack{\sigma \in \mathcal{E}_{\text{int}} \\ \sigma = K|L}} \tau_\sigma A_{ij}(u_\sigma^k) D_{K,\sigma} u_j^k D_{K,\sigma} \phi =: J_1.$$

The boundedness of  $u_{i,\sigma}^k$  and the Cauchy-Schwarz inequality imply that

$$|J_1| \leq \sum_{j=1}^n \max_{\Omega} |A_{ij}(u_\sigma^k)| |u_j^k|_{1,2,\mathcal{T}} |\phi|_{1,2,\mathcal{T}} \leq C \sum_{j=1}^n \|u_j^k\|_{1,2,\mathcal{T}} \|\phi\|_{1,2,\mathcal{T}}.$$

We infer that

$$\sum_{k=1}^{N_T} \Delta t \left\| \frac{u_i^k - u_i^{k-1}}{\Delta t} \right\|_{-1,2,\mathcal{T}}^2 = \sup_{\|\phi\|_{1,2,\mathcal{T}}=1} \sum_{k=1}^{N_T} \Delta t \left| \sum_{K \in \mathcal{T}} \text{m}(K) \frac{u_i^k - u_i^{k-1}}{\Delta t} \phi_K \right|^2 \leq C.$$

This finishes the proof.  $\square$

**5.2. Compactness properties.** Let  $(\mathcal{D}_m)_{m \in \mathbb{N}}$  be a sequence of admissible meshes of  $\Omega_T$  satisfying the mesh regularity (11) uniformly in  $m \in \mathbb{N}$ . We claim that the estimates from Lemma 8 imply the strong convergence of a subsequence of  $(u_{i,m})$ .

**Proposition 9** (Strong convergence). *Let the assumptions of Theorem 2 hold and let  $(u_m)_{m \in \mathbb{N}}$  be a sequence of discrete solutions to (12)–(15) constructed in Theorem 1. Then there exists a subsequence of  $(u_m)$ , which is not relabeled, and  $u = (u_1, \dots, u_n) \in L^\infty(\Omega_T)$  such that for any  $i = 1, \dots, n$ ,*

$$u_{i,m} \rightarrow u_i \quad \text{strongly in } L^p(\Omega_T) \text{ as } m \rightarrow \infty, \quad 1 \leq p < \infty.$$

*Proof.* The result follows from the discrete Aubin–Lions lemma of [23, Theorem 3.4] if the following two properties are satisfied:

- (i) For any sequence  $(v_m)_{m \in \mathbb{N}} \subset V_{\mathcal{T}_m}$  such that there exists  $C > 0$  with  $\|v_m\|_{1,2,\mathcal{T}_m} \leq C$  for all  $m \in \mathbb{N}$ , there exists  $v \in L^2(\Omega)$  satisfying, up to a subsequence,  $v_m \rightarrow v$  strongly in  $L^2(\Omega)$ .
- (ii) If  $v_m \rightarrow v$  strongly in  $L^2(\Omega)$  and  $\|v_m\|_{-1,2,\mathcal{T}_m} \rightarrow 0$  as  $m \rightarrow \infty$ , then  $v = 0$ .

Property (i) follows from [20, Lemma 5.6], while property (ii) can be replaced by the condition that  $\|\cdot\|_{1,2,\mathcal{T}_m}$  and  $\|\cdot\|_{-1,2,\mathcal{T}_m}$  are dual norms with respect to the  $L^2(\Omega)$  norm, thanks to [23, Remark 6], which is the case here. Then [23, Theorem 3.4] implies that there exists a subsequence (not relabeled) such that  $u_{i,m} \rightarrow u_i$  strongly in  $L^2(0, T; L^2(\Omega))$  as  $m \rightarrow \infty$ . We deduce from the  $L^\infty$  bound for  $(u_{i,m})$  that  $u_{i,m} \rightarrow u_i$  strongly in  $L^p(\Omega_T)$  for any  $1 \leq p < \infty$ .  $\square$

**Lemma 10** (Convergence of the gradient). *Under the assumptions of Proposition 9, there exists a subsequence of  $(u_m)_{m \in \mathbb{N}}$  such that for  $i = 1, \dots, n$ ,*

$$\nabla^m u_{i,m} \rightharpoonup \nabla u_i \quad \text{weakly in } L^2(\Omega_T) \text{ as } m \rightarrow \infty,$$

where  $\nabla^m$  is defined in Section 2.

*Proof.* Lemma 8 implies that  $(\nabla^m u_{i,m})$  is bounded in  $L^2(\Omega_T)$ . Thus, for a subsequence,  $\nabla^m u_{i,m} \rightharpoonup v_i$  weakly in  $\Omega_T$  as  $m \rightarrow \infty$ . It is shown in [15, Lemma 4.4] that  $v_i = \nabla u_i$ .  $\square$

**5.3. Convergence of the scheme.** We show that the limit  $u$  from Proposition 9 is a weak solution to (1)–(2). Let  $i \in \{1, \dots, n\}$  be fixed, let  $\psi_i \in C_0^\infty(\Omega \times [0, T])$  be given, and let  $\eta_m := \max\{\Delta x, \Delta t_m\}$  be sufficiently small such that  $\text{supp}(\psi_i) \subset \{x \in \Omega : d(x, \partial\Omega) > \eta_m\} \times [0, T]$ . Furthermore, let  $\psi_{i,K}^k := \psi_i(x_K, t_k)$ . We multiply scheme (13) by  $\Delta t_m \psi_{i,K}^{k-1}$  and sum over  $K \in \mathcal{T}_m$  and  $k = 1, \dots, N_T$ . Then  $F_1^m + F_2^m = 0$ , where

$$\begin{aligned} F_1^m &= \sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}_m} m(K) (u_{i,K}^k - u_{i,K}^{k-1}) \psi_{i,K}^{k-1}, \\ F_2^m &= - \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma A_{\sigma,ij} (u_\sigma^k) D_{K,\sigma} u_j^k \psi_{i,K}^{k-1}. \end{aligned}$$

Furthermore, we introduce

$$F_{10}^m = - \int_0^T \int_{\Omega} u_{i,m} \partial_t \psi_i dx dt - \int_{\Omega} u_{i,m}(x,0) \psi_i(x,0) dx,$$

$$F_{20}^m = \sum_{j=1}^n \int_0^T \int_{\Omega} A_{ij}(u_m) \nabla^m u_{j,m} \cdot \nabla \psi_i dx dt.$$

It follows from the convergence results from the previous subsection, the continuity of  $A_{ij}$ , and the assumption on the initial data that, as  $m \rightarrow \infty$ ,

$$F_{10}^m + F_{20}^m \rightarrow - \int_0^T \int_{\Omega} u_i \partial_t \psi_i dx dt - \int_{\Omega} u_i^0(x) \psi_i(x,0) dx + \sum_{j=1}^n \int_0^T \int_{\Omega} A_{ij}(u) \nabla u_j \cdot \nabla \psi_i dx dt.$$

We prove that  $F_{j0}^m - F_j^m \rightarrow 0$  as  $m \rightarrow \infty$  for  $j = 1, 2$ , since this shows that  $F_{10}^m + F_{20}^m \rightarrow 0$ , finishing the proof.

We start with the first difference  $F_{10}^m - F_1^m$ . It is shown in [15, Theorem 5.2], using the  $L^\infty(\Omega_T)$  bound for  $u_{i,m}$  and the regularity of  $\phi$ , that  $F_{10}^m - F_1^m \rightarrow 0$ . It remains to verify that  $|F_{20}^m - F_2^m| \rightarrow 0$ . To this end, we apply discrete integration by parts and write  $F_2^m = F_{21}^m + F_{22}^m$ , where

$$F_{21}^m = \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma A_{ij}(u_K^k) \mathbb{D}_{K,\sigma} u_j^k \mathbb{D}_{K,\sigma} \psi_i^{k-1},$$

$$F_{22}^m = \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma (A_{\sigma,ij}(u_\sigma^k) - A_{\sigma,ij}(u_{0,K}^k, u_K^k)) \mathbb{D}_{K,\sigma} u_j^k \mathbb{D}_{K,\sigma} \psi_i^{k-1}.$$

Here, we used the equality  $A_\sigma(u_{0,K}^k, u_K^k) = A(u_K^k)$  since  $u_K^k \in D$  and  $u_{0,K}^k = 1 - \sum_{i=1}^n u_{i,K}^k$  for all  $K \in \mathcal{T}$ , coming from Hypothesis (H5). The definition of the discrete gradient  $\nabla^m$  in Section 2.3 gives

$$|F_{20}^m - F_{21}^m| \leq \sum_{j=1}^n \sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} m(\sigma) |A_{ij}(u_K^k)| |\mathbb{D}_{K,\sigma} u_j^k|$$

$$\times \left| \int_{t_{k-1}}^{t_k} \left( \frac{\mathbb{D}_{K,\sigma} \psi_i^{k-1}}{d_\sigma} - \frac{1}{m(T_{K,\sigma})} \int_{T_{K,\sigma}} \nabla \psi_i \cdot \nu_{K,\sigma} dx \right) dt \right|.$$

It is shown in the proof of [15, Theorem 5.1] that there exists a constant  $C_0 > 0$  such that

$$\left| \int_{t_{k-1}}^{t_k} \left( \frac{\mathbb{D}_{K,\sigma} \psi_i^{k-1}}{d_\sigma} - \frac{1}{m(T_{K,\sigma})} \int_{T_{K,\sigma}} \nabla \psi_i \cdot \nu_{K,\sigma} dx \right) dt \right| \leq C_0 \Delta t_m \eta_m.$$

Hence, by the uniform  $L^\infty$  bound for  $u^k$  and the Cauchy–Schwarz inequality,

$$|F_{20}^m - F_{21}^m| \leq C_0 \eta_m \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} m(\sigma) |A_{ij}(u_K^k)| |\mathbb{D}_{K,\sigma} u_j^k|$$

$$\leq C\eta_m \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \|u_j^k\|_{1,2,\mathcal{T}_m} \left( \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} m(\sigma) d_\sigma \right)^{1/2}.$$

We deduce from the mesh regularity (11) and the assumption  $\Omega \subset \mathbb{R}^2$  that

$$\sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} m(\sigma) d_\sigma \leq \frac{1}{\zeta} \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} m(\sigma) d(x_K, \sigma) \leq \frac{2}{\zeta} \sum_{K \in \mathcal{T}_m} m(K) = \frac{2}{\zeta} m(\Omega).$$

Hence, we have

$$|F_{20}^m - F_{21}^m| \leq C\eta_m \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \|u_j^k\|_{1,2,\mathcal{T}_m} \leq C\eta_m \rightarrow 0.$$

For the estimate of  $F_{22}^m$ , we need the Lipschitz continuity of  $A_{\sigma,ij}$ , the upper bound  $u_{\ell,\sigma}^k \leq (u_{\ell,K}^k + u_{\ell,L}^k)/2$  for  $\sigma \in \mathcal{E}_{\text{int}}$  and  $\ell = 0, \dots, n$ , the equality  $u_{0,K}^k = 1 - \sum_{\ell=1}^n u_{\ell,K}^k$  for all  $K \in \mathcal{T}$ , and the Cauchy–Schwarz inequality:

$$\begin{aligned} |F_{22}^m| &\leq C\eta_m \|\psi_i\|_{C^1(\bar{\Omega}_T)} G_m, \quad \text{where} \\ G_m &= \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma |A_{\sigma,ij}(u_\sigma^k) - A_{\sigma,ij}(u_{0,K}^k, u_K^k)| D_\sigma u_j^k \\ &\leq C \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma \left( \sum_{\ell=0}^n |u_{\ell,\sigma}^k - u_{\ell,K}^k| \right) D_\sigma u_j^k \\ &\leq \frac{C}{2} \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma \left( \sum_{\ell=0}^n |u_{\ell,L}^k - u_{\ell,K}^k| \right) D_\sigma u_j^k \\ &\leq C \sum_{\ell,j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}_m} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \tau_\sigma D_\sigma u_\ell^k D_\sigma u_j^k \\ &\leq C \left( \sum_{\ell=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma u_\ell^k)^2 \right)^{1/2} \left( \sum_{j=1}^n \sum_{k=1}^{N_T} \Delta t_m \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma u_j^k)^2 \right)^{1/2}. \end{aligned}$$

By Lemma 8, the right-hand side is bounded uniformly in  $m$ . Thus,  $|F_{22}^m| \leq C\eta_m \rightarrow 0$  and  $|F_{20}^m - F_2^m| \leq |F_{20}^m - F_{21}^m| + |F_{22}^m| \rightarrow 0$  as  $m \rightarrow \infty$ . This finishes the proof.

**Remark 11.** Let us mention some possible extensions of Theorem 2. We can easily adapt the proof to the case  $s = 1$  if we assume in addition to (H5) that  $\|A_\sigma(0)\| < \infty$  holds. Moreover, we can include source terms  $f_i \in C^0(\bar{D})$  for  $i = 1, \dots, n$  such that the conditions (30) and  $\Delta t_m < 1/C_f$  for  $m \in \mathbb{N}$  are fulfilled. Then, following the proof in [38, Theorem 2], we can show that Theorem 2 still holds.  $\square$

## 6. NUMERICAL EXAMPLES

We present in this section some numerical experiments in one and two space dimensions.

**6.1. Implementation of the scheme.** The finite-volume scheme (12)–(15) is implemented in MATLAB. Since the numerical scheme is implicit in time, we have to solve a nonlinear system of equations at each time step. In the one-dimensional case, we use Newton’s method. Starting from  $u^{k-1} = (u_1^{k-1}, u_2^{k-1})$ , we apply a Newton method with precision  $\varepsilon = 10^{-10}$  to approximate the solution to the scheme at time step  $k$ . In the two-dimensional case, we use a Newton method complemented by an adaptive time-stepping strategy to approximate the solution of the scheme at time  $t_k$ . More precisely, starting again from  $u^{k-1} = (u_1^{k-1}, u_2^{k-1})$ , we launch a Newton method. If the method does not converge with precision  $\varepsilon = 10^{-10}$  after at most 50 steps, we multiply the time step by a factor 0.2 and restart the Newton method. At the beginning of each time step, we increase the value of the previous time step size by multiplying it by 1.1. Moreover, we impose the condition  $10^{-8} \leq \Delta t_k \leq 10^{-2}$  with an initial time step size set to  $10^{-5}$ .

**6.2. Test case 1: Rate of convergence in space.** In this section, we illustrate the order of convergence in space for the Maxwell–Stefan model presented in Section 3.1 in one space dimension with  $\Omega = (0, 1)$ . We consider a similar test case as in [34, Section 6.2] but with a discontinuous initial datum  $u_1^0$ . We choose the coefficients  $d_0 = 1/0.168$ ,  $d_1 = 1/0.68$ , and  $d_2 = 1/0.883$  and impose the initial datum

$$u_1^0(x) = 0.8 \cdot \mathbf{1}_{(0,0.5)}(x), \quad u_2^0(x) = 0.2.$$

Since exact solutions to the Maxwell-Stefan model are not explicitly known, we compute a reference solution on a uniform mesh composed of 5120 cells and with time step size  $\Delta t = (1/5120)^2$ . We use this rather small value of  $\Delta t$ , because the Euler discretization in time exhibits a first-order convergence rate, while we expect, as observed for instance in [13], a second-order convergence rate in space for scheme (12)–(15), due to the logarithmic mean used to approximate the mobility coefficients in the numerical fluxes. We compute approximate solutions on uniform meshes made of 40, 80, 160, 320, 640, and 1280 cells, respectively. In Figure 1, we present the sum of the  $L^1(\Omega)$  norms of the differences between the approximate solution  $u_i$  and the average of the reference solution  $u_{i,\text{ref}}$  at the final time  $T = 10^{-2}$ . As expected, we observe a second-order convergence rate in space as in [34].

**6.3. Test case 2: Long-time behavior.** Following [13, Section 5.3], we study the long-time behavior of the scheme for the cross-diffusion system for thin-film solar cells, introduced in Section 3.2, with reactions terms. More precisely, for  $\Omega = (0, 1)^2$  and the final time  $T = 15$ , we consider the system

$$(31) \quad \partial_t u_1 - \operatorname{div} (A_{11}(u) \nabla u_1 + A_{12}(u) \nabla u_2) = r_1(u),$$

$$(32) \quad \partial_t u_2 - \operatorname{div} (A_{21}(u) \nabla u_1 + A_{22}(u) \nabla u_2) = -2r_1(u),$$

where

$$r_1(u) = (u_2^+)^2 - 1000u_1^+(1 - u_1 - u_2)^+,$$

and the coefficients of the diffusion matrix  $A(u)$  are given by (23). We choose, similar to [13],  $a_{10} = 1$ ,  $a_{20} = 0.1$ ,  $a_{12} = 0$ , and  $a_{21} = 0$ . Observe that these coefficients do not satisfy

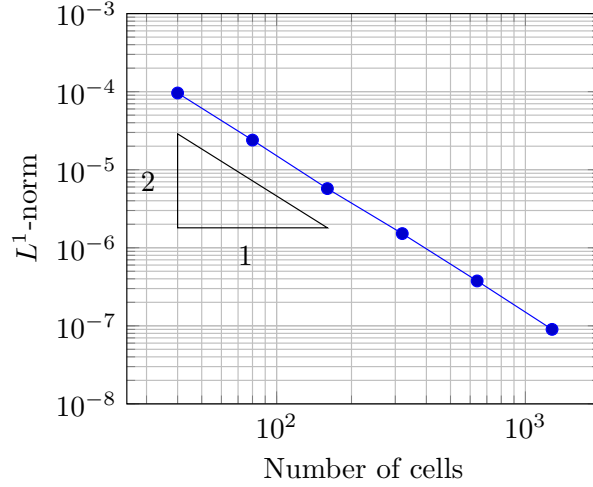


FIGURE 1. Test case 1:  $L^1$  norm of the error in space at final time  $T = 10^{-2}$ .

the assumptions of Lemma 3. Finally, we impose the initial datum

$$u_1^0(x, y) = \frac{9}{44} \frac{\mathbf{1}_{(0,0.5)^2}(x, y)}{0.5^2}, \quad u_2^0(x, y) = \frac{2}{11} \frac{\mathbf{1}_{(0.5,1)^2}(x, y)}{0.5^2}.$$

The steady state of this system is given by

$$u_1^\infty = \frac{9}{44} - \alpha, \quad u_2^\infty = \frac{2}{11} + 2\alpha,$$

where  $\alpha = (-5\sqrt{206530} + 4504)/10956$  is the unique root of the polynomial of degree two given by  $r_1(u^\infty)$  which ensures the nonnegativity of the steady state  $u^\infty = (u_1^\infty, u_2^\infty)$ , see [13, Section 5.3] for more details.

Let us notice that the source terms in (31)–(32) do not satisfy the assumptions (30) of Remark 7. Indeed, in this case, we consider the (discrete) relative Boltzmann entropy

$$(33) \quad \mathcal{H}[u|u^\infty] = \sum_{i=0}^2 \sum_{K \in \mathcal{T}} m(K) \left( u_{i,K} \log \frac{u_{i,K}}{u_i^\infty} + u_i^\infty - u_{i,K} \right),$$

with  $u_0^\infty = 1 - u_1^\infty - u_2^\infty$ . Now, since by construction of  $u^\infty$  we have  $\log(u_1^\infty u_0^\infty) - 2 \log(u_2^\infty) = \log(1000)$ , we conclude that

$$r_1(u)(h'_1(u_1) + h'_0(u_0)) - 2r_1(u)(h'_2(u_2) + h'_0(u_0)) = r_1(u) (\log(1000u_1u_0) - \log(u_2^2)) \leq 0.$$

In particular, under the assumptions of Lemma 3 and adapting the proof of Theorem 1, the following discrete entropy inequality holds:

$$\mathcal{H}[u^k|u^\infty] + \alpha \Delta t \sum_{i=1}^n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma (D_\sigma(u_i^k)^{1/2})^2 \leq \mathcal{H}[u^{k-1}|u^\infty],$$



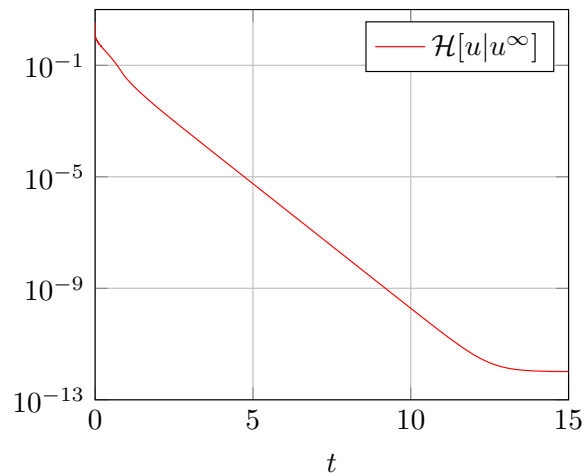


FIGURE 2. Test case 2: Discrete relative entropy versus time.

with  $\alpha = \min_{i,j=1,\dots,2} a_{ij}$ . Then, arguing as in [11], there exist constants  $\kappa > 0$  (depending on  $u^0$ ) and  $\lambda > 0$  (depending on  $\alpha$ ,  $u^0$ , and  $\zeta$ ) such that

$$\sum_{i=1}^n \|u_i^k - u_i^\infty\|_{0,1,\mathcal{T}}^2 \leq \kappa \mathcal{H}[u^0|u^\infty] e^{-\lambda t_k} \quad \text{for all } k \geq 1.$$

Figure 2 illustrates, in semilogarithmic scale and for a mesh of  $\Omega$  made of 3584 triangles (see [38, Fig. 2 left]), the temporal evolution of the discrete relative entropy (33). As in [13], we observe an exponential decay towards the steady state, although the assumptions of Lemma 3 are not fulfilled.

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