



About the entropic structure of detailed balanced multi-species cross-diffusion equations [☆]

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Abstract

This paper links at the formal level the entropy structure of a multi-species cross-diffusion system of Shigesada–Kawasaki–Teramoto (SKT) type (cf. [1]) satisfying the detailed balance condition with the entropy structure of a reversible microscopic many-particle Markov process on a discretised space. The link is established by first performing a mean-field limit to a master equation over discretised space. Then the spatial discretisation limit is performed in a completely rigorous way. This by itself provides a novel strategy for proving global existence of weak solutions to a class of cross-diffusion systems.

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1. Introduction

We consider the population dynamics cross-diffusion system model coming out of the classical paper by Shigesada, Kawasaki and Teramoto [1] (SKT model) for $n \geq 2$ species without reaction term. For clarity, we suppose that the species live on the torus $\mathbb{T} = [0, 1)$ with periodic boundary conditions. Thus, the density $u_i := u_i(t, x)$ of species $i = 1, \dots, n$ evolves as

$$\partial_t u_i = \Delta \left(D_i u_i + \sum_{j=1}^n A_{ij} u_j u_i \right) \quad (1)$$

with diffusion constants $D_i \geq 0$, self-diffusion coefficients $A_{ii} > 0$ and cross-diffusion coefficients $A_{ij} \geq 0$ for $i, j = 1, \dots, n$.

For this system (1), Chen, Daus and Jüngel showed in [2] that

$$\mathcal{H}(u) := \int_{\mathbb{T}} \sum_{i=1}^n \pi_i [u_i \log(u_i(x)) - u_i(x) + 1] dx \quad (2)$$

with positive constants $\pi_i > 0$ for $i = 1, \dots, n$ is an entropy (Lyapunov) functional if the following condition holds

$$\pi_i A_{ij} = \pi_j A_{ji} \quad \text{for } i, j = 1, \dots, n, \quad (3)$$

which for $n \geq 3$ gives a constraint on the cross-diffusion coefficients A_{ij} . Under this condition (they called it *detailed balance condition*), the authors were then able to construct global weak solutions to (1) for an arbitrary number of population species with the help of the gradient estimates coming from the entropy production of the entropy (2).

The motivation of this work is to understand the origin of the entropy (2) under the condition (3). In particular, we wanted to link the condition (3) to the detailed balance equation of finite-state Markov chains, where the detailed balance equation has been identified as necessary and sufficient condition for the existence of a gradient flow structure with respect to the relative entropy [3–5].

In this work, we establish the formal link between the entropy structure of (1) and the entropy structure of a microscopic many-particle Markov process on a discrete space. The link is established in two steps. In the first step, we perform a formal mean-field limit keeping the spatial discretisation fixed. The resulting system is a quadratic master equation. In the second step, we then refine the spatial discretisation and arrive at the cross-diffusion system (1).

In this many-particle derivation, the condition (3) enters as a natural necessary condition for the construction of a reversible Markov process and the constants π_i can be interpreted as relative portions in the many-particle model.

In both limits, the entropy structure is preserved and, in particular, the master equation on the discretised space has the corresponding entropy structure. This allows us to perform the

spatial discretisation limit in a rigorous way, which is an interesting result by itself (which will be discussed after the statement of our main Theorem 8 in Section 3).

Note that the transfer of the entropy structure from a microscopic model towards a mesoscopic model has been extensively studied for equations belonging to other classes. The spatially homogeneous Boltzmann equation is for example a model in which many results have been proven (cf. [6]). It shares some features with the SKT model (quadraticity of course, but also diffusive properties when the angular cutoff of Grad is not performed).

For the second rigorous limit from the space discretised master equation to the SKT cross-diffusion system, similar discrete in space approximation schemes for the SKT model were studied in [7–9], but they are not necessarily entropy preserving. Very recently, an entropy preserving numerical scheme was proposed in [10], though not for the SKT model, but for a volume-filling type cross-diffusion system.

Other approaches have been proposed for obtaining cross-diffusion equations of SKT type out of microscopic models. First (stochastic) approaches from particle models to reaction–diffusion systems trace back to Oelschläger [11] in the late 1980s. Recently, Fontbona and Méléard [12] managed to prove the convergence from realistic individual-based models in a suitable limit towards non-local (convoluted w.r.t. space) SKT-type systems. Note that because of the lacking evidence of existence and uniqueness of strong solutions to the limiting model, it looks difficult to provide a rigorous proof of passage to the limit towards the full (i.e. nontriangular) local multi-species SKT system when one starts with a microscopic model (whether on a discrete set of positions or on a continuous set of positions, using a nonlocality which disappears in the limit). Note, however, that very recently, Moussa [21] managed to prove the convergence in the case of strictly triangular limiting local SKT model with bounded coefficients starting on a continuous set of positions with a nonlocality which disappears in the limit by using duality techniques (introduced for instance by Pierre and Schmitt in [13]).

2. Formal mean-field limit

For the microscopic derivation, we first consider a many-particle system on a fixed spatial discretisation. The spatial discretisation consists of M positions given by

$$\Omega_M = \{x_k : k = 0, \dots, M-1\} \quad \text{with} \quad x_k = \frac{k}{M} = kh, \quad (4)$$

which is understood in the periodic setting, and where we set $h = M^{-1}$.

Given the relative fractions π_1, \dots, π_n with $\pi_i > 0$ between the species, we consider the many-particle system with $\lfloor \pi_i N \rfloor$ particles of species $i = 1, \dots, n$, where $\lfloor \pi_i N \rfloor$ denotes the largest integer smaller than $\pi_i N$. The aim of this section is to obtain a suitable master equation when $N \rightarrow \infty$.

The microscopic configuration is given by

$$\underline{x} := (x_1^1, \dots, x_1^{\lfloor \pi_1 N \rfloor}, x_2^1, \dots, x_2^{\lfloor \pi_2 N \rfloor}, \dots, x_n^1, \dots, x_n^{\lfloor \pi_n N \rfloor}) \in \Omega_M^{\otimes (\lfloor \pi_1 N \rfloor + \dots + \lfloor \pi_n N \rfloor)} =: \Omega_M^N$$

and this configuration is set to evolve in time as a time-continuous Markov chain.

The distribution over the microscopic configurations at time t is given by a density $\mu_t^N \in \mathcal{P}(\Omega_M^N)$. In terms of statistical physics, this means that we consider an ensemble over the microscopic configurations.

We assume that the particles within a species are indistinguishable. The class of such measures is denoted by $\mathcal{P}_s(\Omega_M^N)$ and defined as follows:

Definition 1 (Indistinguishability). A measure $\mu \in \mathcal{P}(\Omega_M^N)$ is in $\mathcal{P}_s(\Omega_M^N)$ if and only if for all permutations $\sigma_1, \dots, \sigma_n$ of resp. $\{1, \dots, \lfloor \pi_1 N \rfloor\}, \dots, \{1, \dots, \lfloor \pi_n N \rfloor\}$ and configurations $\underline{x} \in \Omega_M^N$ it holds that

$$\begin{aligned} & \mu^N(x_1^{\sigma_1(1)}, \dots, x_1^{\sigma_1(\lfloor \pi_1 N \rfloor)}, x_2^{\sigma_2(1)}, \dots, x_2^{\sigma_2(\lfloor \pi_2 N \rfloor)}, \dots, x_n^{\sigma_n(1)}, \dots, x_n^{\sigma_n(\lfloor \pi_n N \rfloor)}) \\ &= \mu^N(x_1^1, \dots, x_1^{\lfloor \pi_1 N \rfloor}, x_2^1, \dots, x_2^{\lfloor \pi_2 N \rfloor}, \dots, x_n^1, \dots, x_n^{\lfloor \pi_n N \rfloor}). \end{aligned}$$

By the indistinguishability, the distribution of a typical particle is given by the marginal distribution. For this, we first introduce the following notation for projections.

Definition 2 (Projections). Let $p = (p_1, \dots, p_n)$ and N be such that $p_i \leq \lfloor \pi_i N \rfloor$ for $i = 1, \dots, n$. We define the projection

$$\mathbb{P}^{N;(p)} : \mathcal{P}(\Omega_M^N) \mapsto \mathcal{P}(\Omega_M^{\otimes(p_1+\dots+p_n)})$$

by

$$\begin{aligned} (\mathbb{P}^{N;(p)} \mu^N)(\underline{x}) := & \sum_{x_1^{p_1+1} \in \Omega_M} \cdots \sum_{x_1^{\lfloor \pi_1 N \rfloor} \in \Omega_M} \sum_{x_2^{p_2+1} \in \Omega_M} \cdots \sum_{x_2^{\lfloor \pi_2 N \rfloor} \in \Omega_M} \cdots \sum_{x_n^{p_n+1} \in \Omega_M} \cdots \sum_{x_n^{\lfloor \pi_n N \rfloor} \in \Omega_M} \\ & \mu^N(x_1^1, \dots, x_1^{\lfloor \pi_1 N \rfloor}, x_2^1, \dots, x_2^{\lfloor \pi_2 N \rfloor}, \dots, x_n^1, \dots, x_n^{\lfloor \pi_n N \rfloor}) \end{aligned}$$

for

$$\underline{x} := (x_1^1, \dots, x_1^{p_1}, x_2^1, \dots, x_2^{p_2}, \dots, x_n^1, \dots, x_n^{p_n}).$$

For $\mu^N \in \mathcal{P}(\Omega_M^N)$, we denote the marginal by

$$\mu^{N;(p)} = \mathbb{P}^{N;(p)} \mu^N \in \mathcal{P}(\Omega_M^{\otimes(p_1+\dots+p_n)}).$$

We then expect to recover the master equation from the first marginals

$$u_i := \mu^{N;(e_i)},$$

where $e_i = (0, \dots, 0, 1, 0, \dots, 0)$ denotes the unit vector with n components, where the 1 is at the i -th component.

The quadratic terms are expected to originate from a binary interaction in the particle model. The diffusion is the result of a random walk and the nonlinearity given in the SKT model (1) is expected to come out from jumps of particles interacting at the same position.

The entropy structure is expected to be linked to the reversibility of the Markov chain. We therefore introduce a binary interaction which happens in a reversible way. This can be realised by imposing the same jump for the interacting particles.

This leads us to consider the following class of particle models, describing the evolution of the microscopic configuration.

Definition 3 (*Reversible particle model*). Let D_i and D_{ij} be nonnegative constants such that $D_{ij} = D_{ji}$ for $i, j = 1, \dots, n$. For a fixed N , define the time-continuous Markov chain on Ω_M^N by the transitions

$$\left. \begin{aligned} \underline{x} &\rightarrow \underline{x} + \underline{e}_i^a + \underline{e}_j^b \\ \underline{x} &\rightarrow \underline{x} - \underline{e}_i^a - \underline{e}_j^b \end{aligned} \right\} \quad \text{with rate } \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N}$$

$$\left. \begin{aligned} \underline{x} &\rightarrow \underline{x} + \underline{e}_i^a \\ \underline{x} &\rightarrow \underline{x} - \underline{e}_i^a \end{aligned} \right\} \quad \text{with rate } D_i$$

for $i, j = 1, \dots, n$ and $a = 1, \dots, \lfloor \pi_i N \rfloor$, $b = 1, \dots, \lfloor \pi_j N \rfloor$, where \underline{e}_i^a is the vector with components of value zero at all places, except for the a th particle of species i , where the value is $h = 1/M$. The Markov chain is defined to have no other transitions.

Remark 1. The transition rates are well-defined if and only if $D_{ij} = D_{ji}$, which will lead to condition (3).

From the construction, we directly see the reversibility.

Lemma 2. *The Markov chain given in Definition 3 is reversible and the stationary distribution is the homogeneous distribution, where each $\underline{x} \in \Omega_M^N$ has the same probability $|\Omega_M^N|^{-1} = M^{-(\lfloor \pi_1 N \rfloor + \dots + \lfloor \pi_n N \rfloor)}$.*

Proof. This can be obtained by a direct computation. \square

We now suppose that the microscopic configuration evolves according to the Markov chain. Then the distribution μ^N solves the following linear ODE:

$$\begin{aligned} \frac{d}{dt} \mu^N(\underline{x}) &= \sum_{i=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} D_i \left[\mu^N(\underline{x} + \underline{e}_i^a) + \mu^N(\underline{x} - \underline{e}_i^a) - 2\mu^N(\underline{x}) \right] \\ &\quad + \frac{1}{2} \sum_{i=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} \sum_{j=1}^n \sum_{b=1}^{\lfloor \pi_j N \rfloor} \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \\ &\quad \times \left[\mu^N(\underline{x} + \underline{e}_i^a + \underline{e}_j^b) + \mu^N(\underline{x} - \underline{e}_i^a - \underline{e}_j^b) - 2\mu^N(\underline{x}) \right]. \end{aligned} \quad (5)$$

Here we used that $x_i^a = x_j^b$ holds after the pairwise interaction if and only if it holds before, so that we can factor it out (that is, $\delta_{x_i^a = x_j^b} = \delta_{(\underline{x} + \underline{e}_i^a)_i^a = (\underline{x} + \underline{e}_j^b)_j^b} = \delta_{(\underline{x} - \underline{e}_i^a)_i^a = (\underline{x} - \underline{e}_j^b)_j^b}$).

We further suppose that the particles are indistinguishable, which is propagated in time.

Lemma 3 (*Propagation of indistinguishability*). *Suppose that μ^N is the distribution for the Markov chain given in Definition 3. If $\mu^N \in \mathcal{P}_s(\Omega_M^N)$ initially holds, then it also holds at all later times.*

Proof. It follows directly from the definition of the transition rates, which respect the indistinguishability. \square

We now write explicitly the formula emphasizing the entropy structure of our reversible Markov process, we recall that due to [4], the time-reversible many-particle continuous time Markov chain is a gradient flow of the relative entropy with respect to its stationary distribution.

Lemma 4. *We assume that $D_i \geq 0$, and $D_{ij} = D_{ji} \geq 0$ for all $1 \leq i, j \leq n$. We also assume that μ^N is initially strictly positive. Then, the entropy functional defined by*

$$\tilde{\mathcal{H}}(\mu^N) := \sum_{\underline{x}} \mu^N(\underline{x}) \log \left(\frac{\mu^N(\underline{x})}{M^{\lfloor \pi_1 N \rfloor + \dots + \lfloor \pi_n N \rfloor}} \right) \quad (6)$$

is decreasing with respect to time, i.e.

$$\frac{d}{dt} \tilde{\mathcal{H}}(\mu^N) \leq 0 \quad \text{for all } t > 0$$

along the flow of (5).

Proof. Note first that the strict positivity of μ^N is maintained in the evolution of the process, so that the logarithm of μ^N is always well defined.

The proof works in a totally analogous way as the proof of (14), where the entropy decay is shown on the macroscopic level. For completeness, we sketch the proof also here, by using the following notation for any function $f : \Omega_M^N \rightarrow (0, \infty)$:

$$\begin{aligned} \Delta_{\underline{e}_i^a}(f(\underline{x})) &:= f(\underline{x} + \underline{e}_i^a) + f(\underline{x} - \underline{e}_i^a) - 2f(\underline{x}), \\ \Delta_{(\underline{e}_i^a + \underline{e}_j^b)}(f(\underline{x})) &:= f(\underline{x} + \underline{e}_i^a + \underline{e}_j^b) + f(\underline{x} - \underline{e}_i^a - \underline{e}_j^b) - 2f(\underline{x}), \\ \nabla_{\underline{e}_i^a}^+(f(\underline{x})) &:= f(\underline{x} + \underline{e}_i^a) - f(\underline{x}), \\ \nabla_{(\underline{e}_i^a + \underline{e}_j^b)}^+(f(\underline{x})) &:= f(\underline{x} + \underline{e}_i^a + \underline{e}_j^b) - f(\underline{x}). \end{aligned}$$

Here \underline{e}_i^a is the vector with components of value zero at all places, except for the a th particle of species i , where the value is $h = 1/M$. This coincides with the notation of a discrete Laplacian and discrete gradient up to positive scaling constants. We will introduce them more rigorously on the level of the master equation in Section 3. Thanks to the periodicity of the domain and to a discrete integration by parts (see detailed formulas at the beginning of Section 3), it holds that

$$\begin{aligned} \frac{d}{dt} \tilde{\mathcal{H}}(\mu^N) &= \sum_{\underline{x}} \left(\log \mu^N(\underline{x}) + 1 \right) \frac{d}{dt} \left(\mu^N(\underline{x}) \right) \\ &= \sum_{\underline{x}} \sum_{i=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} D_i \left(\log \mu^N(\underline{x}) + 1 \right) \Delta_{\underline{e}_i^a} \left(\mu^N(\underline{x}) \right) \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{2} \sum_{\underline{x}} \sum_{i,j=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} \sum_{b=1}^{\lfloor \pi_j N \rfloor} \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \left(\log \mu^N(\underline{x}) + 1 \right) \Delta_{(\underline{e}_i^a + \underline{e}_j^b)} \left(\mu^N(\underline{x}) \right) \\
 & = - \sum_{\underline{x}} \sum_{i=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} D_i \nabla_{(\underline{e}_i^a)}^+ \left(\log \mu^N(\underline{x}) \right) \cdot \nabla_{(\underline{e}_i^a)}^+ \left(\mu^N(\underline{x}) \right) \\
 & \quad - \frac{1}{2} \sum_{\underline{x}} \sum_{i,j=1}^n \sum_{a=1}^{\lfloor \pi_i N \rfloor} \sum_{b=1}^{\lfloor \pi_j N \rfloor} \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \nabla_{(\underline{e}_i^a + \underline{e}_j^b)}^+ \left(\log \mu^N(\underline{x}) \right) \\
 & \quad \times \nabla_{(\underline{e}_i^a + \underline{e}_j^b)}^+ \left(\mu^N(\underline{x}) \right) \\
 & \leq 0,
 \end{aligned}$$

thanks to the monotonicity of $x \mapsto \log x$. \square

The evolution of the marginals is given by the BBGKY hierarchy.

Lemma 5 (BBGKY hierarchy). *Suppose that $\mu^N \in \mathcal{P}_s(\Omega_M^N)$ is the density evolving according to (5). Then the marginals evolve as*

$$\frac{d}{dt} \mu^{N;(p)}(\underline{x}) = I + II + III,$$

where

$$\begin{aligned}
 I &= D_i \sum_{i=1}^n \sum_{a=1}^{p_i} [\mu^{N;(p)}(\underline{x} + \underline{e}_i^a) + \mu^{N;(p)}(\underline{x} - \underline{e}_i^a) - 2\mu^{N;(p)}(\underline{x})], \\
 II &= \frac{1}{2} \sum_{i=1}^n \sum_{a=1}^{p_i} \sum_{j=1}^n \sum_{b=1}^{p_j} \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \\
 & \quad \times [\mu^{N;(p)}(\underline{x} + \underline{e}_i^a + \underline{e}_j^b) + \mu^{N;(p)}(\underline{x} - \underline{e}_i^a - \underline{e}_j^b) - 2\mu^{N;(p)}(\underline{x})],
 \end{aligned}$$

with \underline{e}_i^a defined as the vector of size $p_1 + \dots + p_n$ with all coordinates with value 0, except the coordinate of index $p_1 + \dots + p_{i-1} + a$, which value is $1/M = h$. Finally,

$$\begin{aligned}
 III &= \sum_{i=1}^n \sum_{a=1}^{p_i} \sum_{j=1}^n \sum_{x_j^{p_j+1} \in \Omega_M} \delta_{x_i^a = x_j^{p_j+1}} D_{ij} \frac{\lfloor \pi_j N \rfloor - p_j}{N} \\
 & \quad \times \left[\mu^{N;(p+e_j)}((\underline{x} \# x_j^{p_j+1}) + \tilde{e}_i^a + \tilde{e}_j^{p_j+1}) + \mu^{N;(p+e_j)}((\underline{x} \# x_j^{p_j+1}) - \tilde{e}_i^a - \tilde{e}_j^{p_j+1}) \right. \\
 & \quad \left. - 2\mu^{N;(p+e_j)}((\underline{x} \# x_j^{p_j+1})) \right]
 \end{aligned}$$

with

$$(\underline{x} \# x_j^{p_j+1}) = (x_1^1, \dots, x_1^{p_1}, \dots, x_j^1, \dots, x_j^{p_j}, x_j^{p_j+1}, x_{j+1}^1, \dots, x_{j+1}^{p_{j+1}}, \dots, x_n^1, \dots, x_n^{p_n}),$$

i.e. \underline{x} with $x_j^{p_j+1}$ added between $x_j^{p_j}$ and x_{j+1}^1 , and where \tilde{e}_i^a is defined as the vector of size $p_1 + \dots + (p_j + 1) + \dots + p_n$ with all coordinates with value 0, except the coordinate of index $p_1 + \dots + p_j + 1$, which value is $1/M = h$.

The term I is the standard linear diffusion. The term II is the quadratic interaction between the considered particles, which should be negligible as $N \rightarrow \infty$. The term III is the interaction between the considered particles and the averaged particles, which leads to the quadratic term. The interaction between the averaged particles does not appear in the projection.

Proof. Take the projection $\mathbb{P}^{N;(p)}$. The terms I and II follow directly. The third term appears as

$$III = \sum_{i=1}^n \sum_{a=1}^{p_i} \sum_{j=1}^n \sum_{b=p_j+1}^{\lfloor \pi_j N \rfloor} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \mathbb{P}^{N;(p)} [\mu^N(\underline{x} + \underline{e}_i^a + \underline{e}_j^b) + \mu^N(\underline{x} - \underline{e}_i^a - \underline{e}_j^b) - 2\mu^N(\underline{x})],$$

where we ordered the pair (i, a) and (j, b) so that the factor $1/2$ is not appearing there. Thanks to the indistinguishability, this takes the claimed form. \square

Thus, as usually in the BBGKY hierarchy (tracing back to [14]), in order to compute the evolution of the one-particle marginals u_i , we need the knowledge of the two-particle marginals, whose evolution in turn requires the three-particle marginals.

In order to close an equation on u_i , we thus need an additional assumption. This assumption has been identified as chaos by Kac [15], in a mathematical setting following the famous Stoßzahlansatz by Boltzmann (first suggested by J. Clerk Maxwell in [16]). It states that in the limit $N \rightarrow \infty$, the different particles are becoming independent. In terms of the measure μ^N , it means that

$$\begin{aligned} & \mu^N(x_1^1, \dots, x_1^{\lfloor \pi_1 N \rfloor}, x_2^1, \dots, x_2^{\lfloor \pi_2 N \rfloor}, \dots, x_n^1, \dots, x_n^{\lfloor \pi_n N \rfloor}) \\ & \approx u_1(x_1^1) \cdots u_1(x_1^{\lfloor \pi_1 N \rfloor}) u_2(x_2^1) \cdots u_2(x_2^{\lfloor \pi_2 N \rfloor}) \cdots u_n(x_n^1) \cdots u_n(x_n^{\lfloor \pi_n N \rfloor}), \end{aligned} \quad (7)$$

as $N \rightarrow \infty$. The formal idea is that the interaction between two particles is scaled as N^{-1} so that the correlation between two particles should also be scaled as N^{-1} . Therefore, as $N \rightarrow \infty$, the particles become independent in the limit. In a way for a rigorous mathematical treatment, Kac suggested to initially assume the factorisation and then prove that this is preserved in time with an error going to zero as $N \rightarrow \infty$ (propagation of chaos).

Proposition 6. *Formally, as $N \rightarrow \infty$ we have under the Stoßzahlansatz that the marginals u_i evolve as*

$$\begin{aligned} \frac{d}{dt} u_i(x) &= D_i \left[u_i(x+h) + u_i(x-h) - 2u_i(x) \right] \\ &+ \sum_{j=1}^n D_{ij} \pi_j \left[u_j(x+h) u_i(x+h) + u_j(x-h) u_i(x-h) - 2u_j(x) u_i(x) \right]. \end{aligned} \quad (8)$$

Proof. This follows from Lemma 5, where in the term III , we see that $\frac{\lfloor \pi_i N \rfloor - p_i}{N} \rightarrow \pi_j$, and we reduce the two-marginal density as a product by (7). \square

This gives the desired quadratic master equation with the final rate $A_{ij} := D_{ij}\pi_j$. This is equivalent to the detailed balance equation (3), which follows from the symmetry $D_{ij} = D_{ji}$ in the following way:

$$\pi_i A_{ij} = \pi_i D_{ij} \pi_j = \pi_j D_{ji} \pi_i = \pi_j A_{ji} \quad \text{for all } 1 \leq i, j \leq n.$$

Thanks to the chaos assumption, we can relate the relative entropy of μ^N to the relative entropy of the u_i using the following proposition.

Proposition 7. *Assume*

$$\begin{aligned} & \mu^N(x_1^1, \dots, x_1^{\lfloor \pi_1 N \rfloor}, x_2^1, \dots, x_2^{\lfloor \pi_2 N \rfloor}, \dots, x_n^1, \dots, x_n^{\lfloor \pi_n N \rfloor}) \\ &= u_1(x_1^1) \cdots u_1(x_1^{\lfloor \pi_1 N \rfloor}) u_2(x_2^1) \cdots u_2(x_2^{\lfloor \pi_2 N \rfloor}) \cdots u_n(x_n^1) \cdots u_n(x_n^{\lfloor \pi_n N \rfloor}), \end{aligned}$$

then

$$\frac{1}{N} \tilde{\mathcal{H}}(\mu^N) = \sum_{\underline{x}} \mu^N(\underline{x}) \log \left(\frac{\mu^N(\underline{x})}{M^{\lfloor \pi_1 N \rfloor + \cdots + \lfloor \pi_n N \rfloor}} \right) = \frac{1}{N} \sum_{i=1}^n \sum_{\ell=0}^{M-1} \lfloor \pi_i N \rfloor u_i(x_\ell) \log \left(\frac{u_i(x_\ell)}{M} \right)$$

Proof. This follows from expanding the logarithm as product and using that the u_i are probability distributions. \square

When $N \rightarrow \infty$, this last quantity converges towards $\sum_{i=1}^n \pi_i \sum_{\ell=0}^{M-1} u_i(x_\ell) \log \left(\frac{u_i(x_\ell)}{M} \right)$. Because of Lemma 4 and Proposition 6, we expect that this quantity decreases along the flow of eq. (8). We shall indeed prove this in the next section, thus establishing the link between the entropy structure for eq. (8) (and its limit when the discretisation step h tends to 0) and the classical relative entropy of Markov chains.

3. Rigorous derivation to the cross-diffusion system

Starting from the Markov chain defined in Definition 3, we showed in the last section how performing the mean-field limit on the formal level leads to the spatial discretisation (8) of the SKT system (1). In fact, we expect this particular discretisation to preserve the entropy structure of the Markov chain. In this section we shall check this property and use it to pass rigorously to the limit when the discretisation step h tends to 0, thus recovering the existence of weak solutions for the SKT model.

For this, we recall the discretisation $\Omega_M = \{x_k = kh : k = 0, \dots, M-1\}$ with $h = M^{-1}$ from (4). Moreover, we introduce the discrete derivatives and discrete Laplacian by

$$\begin{aligned} (\nabla_h^+ f)(x) &:= \frac{f(x+h) - f(x)}{h}, & (\nabla_h^- f)(x) &:= \frac{f(x) - f(x-h)}{h}, \\ (\Delta_h f)(x) &:= [\nabla_h^- (\nabla_h^+ f)](x) = [\nabla_h^+ (\nabla_h^- f)](x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}. \end{aligned}$$

We now rewrite (8) together with its initial boundary conditions (and $A_{ij} := \pi_j D_{ij}$), after a suitable rescaling in time (such that ∂_t is replaced by $h^2 \partial_t$). This yields

$$\begin{cases} \partial_t u_i(t, x_k) = D_i [\Delta_h u_i(t, \cdot)](x_k) + \left[\Delta_h \left(u_i(t, \cdot) \sum_{j=1}^n A_{ij} u_j(t, \cdot) \right) \right](x_k), & k = 0, \dots, M-1, \\ u_i(0, x_k) = u_i^0(x_k) \geq 0, & k = 0, \dots, M-1, \quad i = 1, \dots, n, \\ u_i(t, x_0) = u_i(t, x_M), \quad u_i(t, x_{-1}) = u_i(t, x_{M-1}), & \forall t, \quad i = 1, \dots, n. \end{cases} \quad (9)$$

Given the values $(w(x_k))_{k=0, \dots, M-1}$ over Ω_M , let $\tilde{w} : \mathbb{T} \mapsto \mathbb{R}$ be the linear interpolant (P_1 discretisation), which can be defined by

$$\tilde{w}(x) := \sum_{k=0}^{M-1} w(x_k) T(x - x_k) + w(x_0) T(x - x_M), \quad (10)$$

where

$$T(x) = (1 - |x|/h) \mathbb{I}_{[|x| \leq h]}. \quad (11)$$

With this we can state our main theorem.

Theorem 8. *Let $D_i \geq 0$ and $A_{ij} \geq 0$ be coefficients satisfying*

- (i) $A_{ii} > 0$ (strict positivity of self-diffusion),
- (ii) $\pi_i A_{ij} = \pi_j A_{ji}$ for some constants $\pi_i > 0$ (detailed balance equation).

We also assume continuous positive initial data $u_i^0 := u_i^0(x) > 0$ on \mathbb{T} for all $1 \leq i \leq n$.

Then for all $M \in \mathbb{N}$, there exists a unique global solution $u_i := u_i(t, x_k) > 0$ of class C^∞ to the discrete system (9) with $h := 1/M$.

Denoting $[\tilde{u}_i]^M$ the interpolant obtained from $u_i(t, x_k)$ by formula (10), then there exists a subsequence such that the following holds: $[\tilde{u}_i]^M \rightarrow_{M \rightarrow \infty} u_i$ in $L^{4-\varepsilon}([0, T] \times \mathbb{T})$ for all $T > 0$ and $\varepsilon > 0$, where $u_i \in L^4([0, T] \times \mathbb{T}) \cap L^2([0, T], H^1(\mathbb{T}))$ is a weak solution to the SKT system $\partial_t u_i = \Delta(D_i u_i + \sum_{j=1}^n A_{ij} u_i u_j)$ (with initial data u_i^0 and periodic boundary conditions), in the following sense: For all $\varphi \in C_c^2([0, \infty) \times \mathbb{T})$ and for all $i = 1, \dots, n$,

$$\begin{aligned} & - \int_{\mathbb{T}} u_i(0, x) \varphi(0, x) dx - \int_0^\infty \int_{\mathbb{T}} u_i(t, x) \partial_t \varphi(t, x) dx dt \\ & = \int_0^\infty \int_{\mathbb{T}} \left[D_i u_i(t, x) + \sum_{j=1}^n A_{ij} u_i(t, x) u_j(t, x) \right] \Delta \varphi(t, x) dx dt. \end{aligned}$$

The existence of weak solutions to the SKT model has been known for a long time in the case of two equations, and it has been studied more recently in the case of more than two species,

under the detailed balance condition (cf. [17,2]). We do not go beyond the existing theory of existence in this paper. We, however, present an approximation procedure which is extremely simple (it consists only in discretizing w.r.t. the space variable) compared to most previous procedures (cf. for example [18,19]).

Though this approximation procedure is presented here only in the specific case of the quadratic SKT model without reaction terms under the assumption of detailed balance in dimension 1 and in the presence of self-diffusion, our feeling is that it can be easily extended to more general cases. First, one can introduce (not too quickly increasing) reaction terms. Second, one can go to higher space dimensions $d \geq 1$ keeping periodic boundary conditions. In a third step, by introducing a reasonable grid, one can expect that the same procedure works for any reasonably smooth domain with Neumann boundary conditions. Moreover, one can also think of non quadratic cases, provided that a good Lyapunov functional is known, or of the quadratic case without self-diffusion when the standard diffusion term or the reaction terms are sufficient to guarantee the equintegrability. It is less clear if duality arguments (cf. for example [20]) are compatible with this approximation (as they are when time discretisation is performed, cf. [21]): this issue will be investigated in future works.

The possibility of extending the formal results of the first part to more general systems (thus giving a microscopic background for an entropy structure which is known to exist at the macroscopic level) will also be studied further, especially in the direction of non quadratic systems, and systems presenting exclusion processes, see for instance [22–24].

We now begin the

Proof of Theorem 8. We first observe that there exists a unique global solution $t \in \mathbb{R}_+ \mapsto (u_1(t, x_k), \dots, u_n(t, x_k))$ with $u_i(t, x_k) \geq 0$ to the ODE system (9). We briefly sketch the proof of this result, which uses standard theorems for ODEs.

We denote by $T_1 > 0$ the maximal time of existence for the equation (obtained thanks to Cauchy–Lipschitz theorem), and by $T_2 \in]0, T_1[$ the maximal time for which $u_i(t, x_k) > 0$ for all i, k and $t \in [0, T_2[$. Note that $T_2 > 0$ because all initial data are assumed to be strictly positive.

On the interval $[0, T_2[$, we use the conservation of the total number of individuals (of each species)

$$\frac{d}{dt} \left(\sum_{k=0}^{M-1} u_i(t, x_k) \right) = 0,$$

for $i = 1, \dots, n$, and get that

$$\forall t \in]0, T_2[, \quad i = 1, \dots, n, \quad k = 0, \dots, M-1, \quad 0 \leq u_i(t, x_k) \leq C, \quad (12)$$

where $C := \sup_{i=1, \dots, n} \left[\sum_{k=0}^{M-1} u_i(0, x_k) \right]$.

Then, we observe that on the interval $[0, T_2[$,

$$\begin{aligned} h^2 \partial_t u_i(t, x_k) &= D_i [u_i(t, x_k + h) + u_i(t, x_k - h) - 2u_i(t, x_k)] \\ &\quad + \sum_{j=1}^n A_{ij} [(u_i u_j)(t, x_k + h) + (u_i u_j)(t, x_k - h) - 2(u_i u_j)(t, x_k)] \end{aligned}$$

$$\begin{aligned} &\geq -2D_i u_i(t, x_k) - 2 \sum_{j=1}^n A_{ij}(u_i u_j)(t, x_k) \\ &\geq -2(D_i + C \sum_{j=1}^n A_{ij}) u_i(t, x_k), \end{aligned}$$

and consequently

$$u_i(t, x_k) \geq u_i(0, x_k) \exp\left(-\frac{2}{h^2} \left[D_i + C \sum_{j=1}^n A_{ij}\right] T_2\right) > 0 \quad \text{for all } t \in [0, T_2].$$

Then $T_2 = T_1$, and finally thanks to estimate eq. (12), $T_1 = \infty$.

3.1. Discrete system

We start by studying the discrete system and establishing the main *a priori* estimates, which are uniform with respect to the spatial discretisation M . Those estimates are a direct consequence of the entropy structure of our models.

Lemma 9. *Under the same assumptions on the coefficients and initial data as in Theorem 8, the unique solution to the system (9) satisfies the following a priori estimates, for some constants $C_T > 0$ depending only on T , the initial data, and the coefficients π_i , A_{ij} and D_i :*

$$\sum_{i=1}^n \int_0^T h \sum_{k=0}^{M-1} |(\nabla_h^+ u_i)(t, x_k)|^2 dt \leq C_T, \quad (13)$$

and

$$\frac{d}{dt} \mathcal{H}^h(u(t, \cdot)) \leq 0, \quad \sup_{t \in [0, T]} \mathcal{H}^h(u(t, \cdot)) \leq C_T, \quad (14)$$

where

$$\mathcal{H}^h(u) := \sum_{i=1}^n h \sum_{k=0}^{M-1} \pi_i \left[u_i(x_k) \log(u_i(x_k)) - u_i(x_k) + 1 \right]. \quad (15)$$

Remark 10. The normalised entropy described at the end of Section 2 differs from \mathcal{H}^h in (15) only by terms which are constant with respect to time t (due to mass conservation), thus the entropy dissipation of those terms is 0.

For the proof, we rely on the following elementary properties for the discrete derivatives:

(i) Discrete integration by parts: For all 1-periodic functions $p, q : \mathbb{R} \rightarrow \mathbb{R}$,

$$\sum_{k=0}^{M-1} (\nabla_h^+ p)(x_k) q(x_k) = - \sum_{k=0}^{M-1} p(x_k) (\nabla_h^- q)(x_k); \quad (16)$$

(ii) Discrete product rule: For all functions $p, q : \mathbb{R} \rightarrow \mathbb{R}$,

$$(\nabla_h^+(pq))(x) = p(x+h) (\nabla_h^+ q)(x) + (\nabla_h^+ p)(x) q(x). \quad (17)$$

Proof. By using the abbreviation $\tilde{a}_{ij} := \pi_i A_{ij}$ (and therefore assuming that $\tilde{a}_{ij} = \tilde{a}_{ji}$ for all $i, j \in \{1, \dots, n\}$), we can compute

$$\begin{aligned} \frac{d}{dt} \mathcal{H}^h(u) &= \sum_{i=1}^n \sum_{k=0}^{M-1} h \pi_i \partial_t u_i(x_k) \log u_i(x_k) \\ &= \sum_{i=1}^n \sum_{k=0}^{M-1} h \pi_i \left(\Delta_h \left[D_i u_i + u_i \sum_{j=1}^n A_{i,j} u_j \right] \right)(x_k) \log u_i(x_k) \\ &= h \sum_{i=1}^n \sum_{k=0}^{M-1} D_i \pi_i \log u_i(x_k) (\Delta_h u_i)(x_k) + h \sum_{i,j=1}^n \sum_{k=0}^{M-1} \tilde{a}_{ij} \log u_i(x_k) (\Delta_h(u_i u_j))(x_k) \\ &= -h \sum_{i=1}^n \sum_{k=0}^{M-1} D_i \pi_i (\nabla_h^+(\log u_i))(x_k) (\nabla_h^+(u_i))(x_k) \\ &\quad - h \sum_{i,j=1}^n \sum_{k=0}^{M-1} \tilde{a}_{ij} (\nabla_h^+(\log u_i))(x_k) (\nabla_h^+(u_i u_j))(x_k) \\ &= -h \sum_{i=1}^n \sum_{k=0}^{M-1} D_i \pi_i (\nabla_h^+(\log u_i))(x_k) (\nabla_h^+(u_i))(x_k) \\ &\quad - \frac{h}{2} \sum_{i,j=1}^n \sum_{k=0}^{M-1} \tilde{a}_{ij} (\nabla_h^+(\log(u_i u_j)))(x_k) (\nabla_h^+(u_i u_j))(x_k) \\ &\leq -4h \sum_{i=1}^n \sum_{k=0}^{M-1} D_i \pi_i |\nabla_h^+(\sqrt{u_i})(x_k)|^2 - 2h \sum_{i,j=1}^n \sum_{k=0}^{M-1} \tilde{a}_{ij} |\nabla_h^+(\sqrt{u_i u_j})(x_k)|^2 \leq 0. \end{aligned}$$

We used above the elementary inequality $(x - y)(\log x - \log y) \geq 4(\sqrt{x} - \sqrt{y})^2$ for all $x > 0$, $y > 0$.

We end up the proof of estimate (14) by noticing that all terms above are nonpositive and by integrating between 0 and T . Estimate (13) is obtained by using only the self diffusion terms (that is, the ones corresponding to \tilde{a}_{ij} , for $i = j$) and also by integrating between 0 and T .

Next, we introduce for $1 \leq p < \infty$ the discrete norm for $(w(x_k))_{k=0,\dots,M-1}$ by defining

$$\|w\|_{h,p}^p := h \sum_{k=0}^{M-1} |w(x_k)|^p. \quad (18)$$

With the help of the following lemma, we can switch between the discrete norm and the norm of the continuous linear interpolant \tilde{w} of w defined in (10):

Lemma 11. For $1 \leq p < \infty$ and $w(x_k) \geq 0$, $k = 0, \dots, M-1$, it holds that

$$\|\tilde{w}\|_{L^p(\mathbb{T})}^p \leq \|w\|_{h,p}^p \leq \frac{p+1}{2} \|\tilde{w}\|_{L^p(\mathbb{T})}^p, \quad (19)$$

$$\|\nabla \tilde{w}\|_{L^p(\mathbb{T})}^p = \|\nabla_h^+ w\|_{h,p}^p, \quad (20)$$

where $\|w\|_{h,p}$ is the discrete norm defined in (18), and \tilde{w} is the linear interpolant defined in (10).

Remark 12. The factor $2/(p+1)$ is necessary, as can be seen from the case when $w(x_k) = 1$ for $k = 1$ and $w(x_k) = 0$ otherwise.

Proof. Note that the linear interpolant \tilde{w} can also be rewritten as

$$\tilde{w}(x) = \sum_{k=0}^{M-1} \left(\alpha_k(x) w(x_k) + (1 - \alpha_k(x)) w(x_{k+1}) \right) \mathbb{I}_{[x_k, x_{k+1})}(x), \quad (21)$$

where $w(x_M) := w(x_0)$ and

$$\alpha_k(x) = \frac{x_{k+1} - x}{h}.$$

For $x \in [x_k, x_{k+1})$ with $k = 0, \dots, M-1$, we know thanks to (21) that

$$\tilde{w}(x) = \alpha_k(x) w(x_k) + (1 - \alpha_k(x)) w(x_{k+1}).$$

Since $x \mapsto x^p$ is convex, we see that

$$|\tilde{w}(x)|^p \leq \alpha_k(x) |w(x_k)|^p + (1 - \alpha_k(x)) |w(x_{k+1})|^p,$$

so that integrating between x_k and x_{k+1} , we get

$$\int_{x_k}^{x_{k+1}} |\tilde{w}(x)|^p dx \leq \frac{h}{2} |w(x_k)|^p + \frac{h}{2} |w(x_{k+1})|^p,$$

which shows the first part of (19).

In the other direction, we find that

$$\begin{aligned} \int_{x_k}^{x_{k+1}} |\tilde{w}(x)|^p dx &= h \int_{\beta=0}^1 |\beta w(x_k) + (1-\beta)w(x_{k+1})|^p d\beta \\ &= \frac{h}{p+1} \frac{[w(x_{k+1})]^{p+1} - [w(x_k)]^{p+1}}{w(x_{k+1}) - w(x_k)} \\ &\geq \frac{h}{p+1} \left[[w(x_{k+1})]^p + [w(x_k)]^p \right], \end{aligned}$$

where we used the elementary inequality

$$\frac{A^{p+1} - B^{p+1}}{A - B} \geq A^p + B^p \quad \text{for all } A, B \geq 0. \quad (22)$$

This elementary inequality is easily proved (by considering A/B). This finishes the proof of (19).

For (20), we see that for $k = 0, \dots, M-1$,

$$\nabla \tilde{w}(x) = (\nabla_h^+ w)(x_k) \quad \text{for } x \in (x_k, x_{k+1}).$$

This implies

$$\begin{aligned} \|\nabla \tilde{w}\|_{L^p(\mathbb{T})}^p &= \int_{\mathbb{T}} |\nabla \tilde{w}(x)|^p dx = \sum_{k=0}^{M-1} \int_{x_k}^{x_{k+1}} |\nabla \tilde{w}(y)|^p dy \\ &= \sum_{k=0}^{M-1} h |(\nabla_h^+ w)(x_k)|^p = \|\nabla_h^+ w\|_{h,p}^p. \quad \square \end{aligned}$$

3.2. Uniform a priori estimates for the linear interpolant

From now on, when we interpolate functions which depend on t , we systematically write $\tilde{w}(t, x)$ instead of $\widetilde{w(t, \cdot)}(x)$. We also use the notation C_T for any constant depending on the time T , on the initial data and the parameters π , $A_{i,j}$ and D_i of the problem, but not on the discretisation parameter $h = 1/M$.

Combining Lemma 9 and Lemma 11, we obtain for \tilde{u}_i with $i = 1, \dots, n$ that

$$\sup_{t \in [0, T]} \int_{\mathbb{T}} \tilde{u}_i(t, x) dx \leq C_T, \quad (23)$$

$$\int_0^T \int_{\mathbb{T}} |\nabla \tilde{u}_i(t, x)|^2 dx dt \leq C_T. \quad (24)$$

Using the Gagliardo–Nirenberg inequality, this implies for $p \in [1, 4]$ that

$$\int_0^T \int_{\mathbb{T}} |\tilde{u}_i(t, x)|^p dx dt \leq C_T. \quad (25)$$

Note that in the estimate above, when the dimension $d = 1$ is replaced by a more general dimension d , the maximal value 4 of p is replaced by $2 + 2/d$.

Indeed, the Gagliardo–Nirenberg interpolation allows to estimate $\|\tilde{u}_i\|_{L^p(\mathbb{T})}$ by $\|\nabla \tilde{u}_i\|_{L^2(\mathbb{T})}^\theta \|\tilde{u}_i\|_{L^1(\mathbb{T})}^{1-\theta}$. Choosing $\theta p = 2$, means that $\theta = (2d(p-1))/((d+2)p) \in [0, 1]$ so that $p = 2 + 2/d$. With this choice, we find

$$\begin{aligned} \|\tilde{u}_i\|_{L^p([0,T], L^p(\mathbb{T}))}^p &= \int_0^T \|\tilde{u}_i\|_{L^p(\mathbb{T})}^p dt \\ &\leq C \int_0^T \|\nabla \tilde{u}_i\|_{L^2(\mathbb{T})}^{\theta p} \|\tilde{u}_i\|_{L^1(\mathbb{T})}^{(1-\theta)p} dt \\ &\leq C \|\tilde{u}_i\|_{L^\infty([0,T], L^1(\mathbb{T}))}^{(1-\theta)p} \int_0^T \|\nabla \tilde{u}_i\|_{L^2(\mathbb{T})}^{\theta p} dt \\ &\leq C \|\tilde{u}_i\|_{L^\infty([0,T], L^1(\mathbb{T}))}^{(1-\theta)p} \|\nabla \tilde{u}_i\|_{L^2([0,T] \times \mathbb{T})}^2. \end{aligned}$$

Using Lemma 11, we can relate the estimate back to the discrete system as

$$\int_0^T h \sum_{k=0}^{M-1} |u_i(t, x_k)|^p dt \leq C_T, \quad \text{for all } p \in [1, 4]. \quad (26)$$

We now show that for all $\phi \in W^{1,\infty}(\mathbb{T})$,

$$\int_0^T \left| \partial_t \int_{\mathbb{T}} \tilde{u}_i(t, x) \phi(x) dx \right| dt \leq C_T \|\phi\|_{W^{1,\infty}(\mathbb{T})}. \quad (27)$$

Indeed, performing a discrete integration by parts in x_k (cf. (16)) and performing the translation $x \mapsto x + h$ inside the integral over \mathbb{T} , we get that

$$\begin{aligned} &\partial_t \int_{\mathbb{T}} \tilde{u}_i(t, x) \phi(x) dx \\ &= \sum_{k=0}^{M-1} \left[\Delta_h \left(D_i u_i(t, \cdot) + u_i(t, \cdot) \sum_{j=1}^n A_{ij} u_j(t, \cdot) \right) \right] (x_k) \int_{\mathbb{T}} T(x - x_k) \phi(x) dx \end{aligned}$$

$$\begin{aligned}
&= - \sum_{k=0}^{M-1} \left[\nabla_h^+ \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) \int_{\mathbb{T}} [(\nabla_h^+ T)(x - \cdot)](x_k) \phi(x) dx \\
&= \sum_{k=0}^{M-1} \left[\nabla_h^+ \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) \int_{\mathbb{T}} \frac{T(x - x_k) - T(x - x_{k+1})}{h} \phi(x) dx \\
&= - \sum_{k=0}^{M-1} \left[\nabla_h^+ \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) \int_{\mathbb{T}} T(x - x_k) [\nabla_h^+ \phi](x) dx.
\end{aligned}$$

By the discrete product rule (17), this can be estimated as

$$\begin{aligned}
&\int_0^T \left| \partial_t \int_{\mathbb{T}} \tilde{u}_i(t, x) \phi(x) dx \right| dt \\
&\leq \int_0^T \sum_{k=0}^{M-1} \left| \left[\nabla_h^+ \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) \right| \int_{\mathbb{T}} T(x - x_k) |[\nabla_h^+ \phi](x)| dx dt \\
&\leq \|\nabla_h^+ \phi\|_{\infty} h \int_0^T \sum_{k=0}^{M-1} \left| \left[\nabla_h^+ \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) \right| dt \\
&\leq \|\nabla_h^+ \phi\|_{\infty} \int_0^T h \sum_{k=0}^{M-1} \sum_{j=1}^n A_{ij} |u_i(t, x_k + h)| |[\nabla_h^+ u_j(t, \cdot)](x_k)| dt \\
&\quad + \|\nabla_h^+ \phi\|_{\infty} \int_0^T h \sum_{k=0}^{M-1} \sum_{j=1}^n A_{ij} |u_j(t, x_k)| |[\nabla_h^+ u_i(t, \cdot)](x_k)| dt \\
&\quad + \|\nabla_h^+ \phi\|_{\infty} \int_0^T h \sum_{k=0}^{M-1} D_i |[\nabla_h^+ u_i(t, \cdot)](x_k)| dt \\
&\leq \|\nabla_h^+ \phi\|_{\infty} \sum_{j=1}^n A_{ij} \left(\int_0^T h \sum_{k=0}^{M-1} |u_i(t, x_k + h)|^2 dt \right)^{1/2} \left(\int_0^T h \sum_{k=0}^{M-1} |[\nabla_h^+ u_j(t, \cdot)](x_k)|^2 dt \right)^{1/2} \\
&\quad + \|\nabla_h^+ \phi\|_{\infty} \sum_{j=1}^n A_{ij} \left(\int_0^T h \sum_{k=0}^{M-1} |u_j(t, x_k)|^2 dt \right)^{1/2} \left(\int_0^T h \sum_{k=0}^{M-1} |[\nabla_h^+ u_i(t, \cdot)](x_k)|^2 dt \right)^{1/2} \\
&\quad + \|\nabla_h^+ \phi\|_{\infty} D_i \left(\int_0^T h \left(\sum_{k=0}^{M-1} 1 \right) dt \right)^{1/2} \left(\int_0^T h \sum_{k=0}^{M-1} |[\nabla_h^+ u_i(t, \cdot)](x_k)|^2 dt \right)^{1/2}
\end{aligned}$$

$$\leq C_T [n \max_{i,j} A_{ij} + \max_i D_i] \|\phi\|_{W^{1,\infty}(\mathbb{T})} \left[T^{1/2} + \max_j \left(\int_0^T h \sum_{k=0}^{M-1} |u_j(t, x_k)|^2 dt \right)^{1/2} \right] \\ \leq C_T,$$

where we used estimates (13) and (26).

3.3. Compactness

In order to stress the dependence w.r.t. the spatial discretisation, we denote by $[\tilde{u}_i]^M$ the interpolant associated to the discrete system on Ω_M .

The classical Aubin–Lions lemma shows with the estimates (24), (25) and (27) that there exists a subsequence such that

$$[\tilde{u}_i]^M \rightarrow_{M \rightarrow \infty} u_i \quad \text{strongly in } L^{4-\varepsilon}([0, T] \times \mathbb{T})$$

for some $u_i \in L^4([0, T] \times \mathbb{T}) \cap L^2([0, T], H^1(\mathbb{T}))$.

3.4. Passing to the limit

We now show that the limit is a solution in the weak formulation stated in Theorem 8.

We first find that the interpolation $[\tilde{u}_i]^M$ of the discrete solution on Ω_M satisfies for all test functions $\varphi := \varphi(t, x) \in C_c([0, +\infty) \times \mathbb{T})$ and $i = 1, \dots, N$ that

$$- \int_{\mathbb{T}} [\tilde{u}_i]^M(0, x) \varphi(0, x) dx - \int_0^\infty \int_{\mathbb{T}} [\tilde{u}_i]^M(t, x) \partial_t \varphi(t, x) dx dt \\ = D_i \int_0^\infty \int_{\mathbb{T}} [\tilde{u}_i]^M(t, x) \Delta_h \varphi(t, x) dx dt + \sum_{j=1}^n A_{ij} \int_0^\infty \int_{\mathbb{T}} [\widetilde{u_i u_j}]^M(t, x) \Delta_h \varphi(t, x) dx dt, \quad (28)$$

where $[\widetilde{u_i u_j}]^M$ is the interpolant (in the sense of (10)) of $u_i u_j$ from the values on Ω_M .

Indeed, differentiating the interpolant $[\tilde{u}]^M$ in time, we find from the ODE system (9) that

$$\partial_t [\tilde{u}_i]^M(t, x) = \sum_{k=0}^{M-1} \left[\Delta_h \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) T(x - x_k). \quad (29)$$

Multiplying with the compact test function φ and integrating shows that

$$- \int_{\mathbb{T}} [\tilde{u}_i]^M(0, x) \varphi(0, x) dx - \int_0^\infty \int_{\mathbb{T}} [\tilde{u}_i]^M \partial_t \varphi dx dt \\ = \int_0^\infty \int_{\mathbb{T}} \sum_{k=0}^{M-1} \left[\Delta_h \left(D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right) \right] (x_k) T(x - x_k) \varphi(t, x) dx dt$$

$$\begin{aligned}
 &= \int_0^\infty \int_{\mathbb{T}} \sum_{k=0}^{M-1} \left[D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right] (x_k) \Delta_h [T(x - \cdot)](x_k) \varphi(t, x) \, dx \, dt \\
 &= \int_0^\infty \sum_{k=0}^{M-1} \left[D_i u_i(t, \cdot) + \sum_{j=1}^n A_{ij} u_i(t, \cdot) u_j(t, \cdot) \right] (x_k) \int_{\mathbb{T}} T(x - x_k) (\Delta_h \varphi)(x) \, dx \, dt \\
 &= D_i \int_0^\infty \int_{\mathbb{T}} [\tilde{u}_i]^M(t, x) \Delta_h \varphi(t, x) \, dx \, dt + \sum_{j=1}^n A_{ij} \int_0^\infty \int_{\mathbb{T}} [\widetilde{u_i u_j}]^M(t, x) \Delta_h \varphi(t, x) \, dx \, dt,
 \end{aligned}$$

so that (28) holds.

Next, we use the following result explaining how the linear interpolation behaves on products:

Lemma 13. *Under the assumptions of Theorem 8, the following estimate holds:*

$$\int_0^T \int_{\mathbb{T}} \left| [\widetilde{u_i u_j}]^M(t, x) - [\tilde{u}_i]^M(t, x) [\tilde{u}_j]^M(t, x) \right| \, dx \, dt \leq C_T h.$$

Proof. For $x \in [x_k, x_{k+1})$ the representation formula (21) shows for $i = 1, \dots, n$ that

$$\begin{aligned}
 [\tilde{u}_i]^M(t, x) &= \alpha_k(x) u_i(t, x_k) + (1 - \alpha_k(x)) u_i(t, x_{k+1}), \\
 [\widetilde{u_i u_j}]^M(t, x) &= \alpha_k(x) [(u_i u_j)(t, x_k)] + (1 - \alpha_k(x)) [(u_i u_j)(t, x_{k+1})],
 \end{aligned}$$

where we recall that $\alpha_k(x) = (x_{k+1} - x)/h$. Then, for $x \in [x_k, x_{k+1})$:

$$\begin{aligned}
 &\left| [\widetilde{u_i u_j}]^M(t, x) - [\tilde{u}_i]^M(t, x) [\tilde{u}_j]^M(t, x) \right| \\
 &= \left| \alpha_k(x) [(u_i u_j)(t, x_k)] + (1 - \alpha_k(x)) [(u_i u_j)(t, x_{k+1})] \right. \\
 &\quad \left. - \left([\alpha_k(x) u_i(t, x_k) + (1 - \alpha_k(x)) u_i(t, x_{k+1})] [\alpha_k(x) u_j(t, x_k) + (1 - \alpha_k(x)) u_j(t, x_{k+1})] \right) \right| \\
 &\leq \alpha_k(x) (1 - \alpha_k(x)) \left(|u_i(t, x_k) + u_i(t, x_{k+1})| \right) |u_j(t, x_{k+1}) - u_j(t, x_k)|.
 \end{aligned}$$

Consequently, we get that

$$\begin{aligned}
 &\int_0^T \int_{\mathbb{T}} \left| [\widetilde{u_i u_j}]^M - [\tilde{u}_i]^M [\tilde{u}_j]^M \right| \, dx \, dt \\
 &\leq \int_0^T \left(\sum_{k=0}^{M-1} \int_{x_k}^{x_{k+1}} \alpha_k(x) (1 - \alpha_k(x)) \, dx (|u_i(t, x_k)| + |u_i(t, x_{k+1})|) |u_j(t, x_{k+1}) - u_j(t, x_k)| \right) \, dt
 \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{6} \int_0^T \sum_{k=0}^{M-1} h (|u_i(t, x_k)| + |u_i(t, x_{k+1})|) |u_j(t, x_{k+1}) - u_j(t, x_k)| dt \\
&\leq \frac{1}{3} \int_0^T \left(\sum_{k=0}^{M-1} h |u_i(t, x_k)|^2 \right)^{1/2} \left(\sum_{k=0}^{M-1} h |u_j(t, x_{k+1}) - u_j(t, x_k)|^2 \right)^{1/2} dt \\
&= \frac{1}{3} h \left(\int_0^T \sum_{k=0}^{M-1} h |u_i(t, x_k)|^2 dt \right)^{1/2} \left(\int_0^T \sum_{k=0}^{M-1} h |(\nabla_h^+ u_j(t, \cdot))(x_k)|^2 dt \right)^{1/2}.
\end{aligned}$$

This concludes the proof with the estimates (13) and (26). \square

Thanks to the lemma above, the weak formulation (28) of the discretised system implies that for all $\varphi := \varphi(t, x) \in C_c([0, T) \times \mathbb{T})$ and $i \in 1, \dots, n$,

$$\begin{aligned}
& - \int_{\mathbb{T}} [\tilde{u}_i]^M(0, \cdot) \varphi(0, \cdot) dx \\
& - \int_0^\infty \int_{\mathbb{T}} \left([\tilde{u}_i]^M \partial_t \varphi + \left[D_i [\tilde{u}_i]^M + \sum_{j=1}^n A_{ij} [\tilde{u}_i]^M [\tilde{u}_j]^M \right] \Delta_h \varphi \right) dx dt = \mathcal{O}(h).
\end{aligned} \tag{30}$$

We end up the proof of Theorem 8 by observing that the limit satisfies

$$- \int_{\mathbb{T}} u_i(0, \cdot) \varphi(0, \cdot) dx - \int_0^\infty \int_{\mathbb{T}} \left(u_i \partial_t \varphi + \left[D_i u_i + \sum_{j=1}^n A_{ij} u_i u_j \right] \Delta \varphi \right) dx dt = 0.$$

Indeed,

$$\begin{aligned}
& \left| - \int_{\mathbb{T}} u_i(0, \cdot) \varphi(0, \cdot) dx - \int_0^\infty \int_{\mathbb{T}} \left(u_i \partial_t \varphi + \left[D_i u_i + \sum_{j=1}^n A_{ij} u_i u_j \right] \Delta \varphi \right) dx dt \right| \\
& \leq \int_{\mathbb{T}} |u_i(0, \cdot) - [\tilde{u}_i]^M(0, \cdot)| |\varphi(0, \cdot)| dx + \int_0^\infty \int_{\mathbb{T}} |u_i - [\tilde{u}_i]^M| |\partial_t \varphi| dx dt \\
& + \sum_{j=1}^n A_{ij} \int_0^\infty \int_{\mathbb{T}} |[\tilde{u}_i]^M [\tilde{u}_j]^M - u_i u_j| |\Delta_h \varphi| dx dt + D_i \int_0^\infty \int_{\mathbb{T}} |[\tilde{u}_i]^M - u_i| |\Delta_h \varphi| dx dt \\
& + \int_0^\infty \int_{\mathbb{T}} |D_i u_i + \sum_{j=1}^n A_{ij} u_i u_j| |\Delta_h \varphi - \Delta \varphi| dx dt + \mathcal{O}(h).
\end{aligned}$$

The first integral tends to 0 because $u_i(0, \cdot)$ is continuous on \mathbb{T} . The second and fourth integrals converge to 0 because $[\tilde{u}_i]^M \rightarrow u_i$ strongly in L^1 , the third integral converges to 0 because $[\tilde{u}_i]^M \rightarrow u_i$ strongly in L^2 , and the last integral converges to 0 since φ is smooth. \square

This concludes the proof of Theorem 8.

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