### Some aspects of cross diffusion equations

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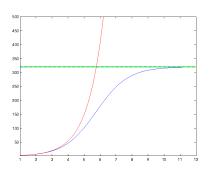
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#### Growth models for populations



#### Logistic model (Verhulst, 1838)

$$u'(t) = r_0 \left(1 - \frac{u(t)}{K}\right) u(t), \qquad u(t) = \frac{u(0) K}{u(0) + (K - u(0)) \exp(-r_0 t)}.$$

#### Growth models for populations

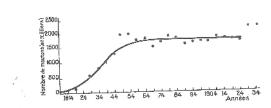
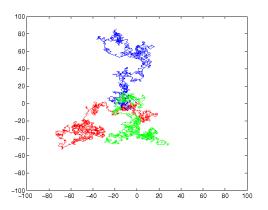
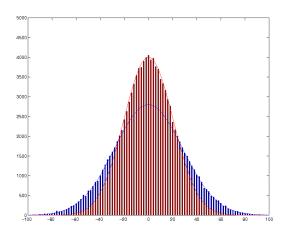


Fig. 62.—Le développement du mouton après son introduction en Tasmanie.

An example of observed data and of logistic "fit"



**Random walk**: We assume isotropy, and consider a scale of time and space which is large (w.r.t. the motion of one individual).



**Corresponding law**: convergence towards a Gaussian law with variance proportional to time.

Random walk  $S_p = \sum_{i=1}^p X_i$ , with  $X_i = \Delta x$  and  $X_i = -\Delta x$  each of probability 1/2, and independent.

Law of 
$$S_p$$
:  $P(S_p = q \Delta x) = 2^{-p} C_p^{\frac{q+p}{2}}$  (when  $|q| \leq p$  et  $q \equiv p[2]$ ).

We consider  $N(p\Delta t, x) := P(S_p \in [x - \Delta x, x + \Delta x])$ . Then for  $t = p \Delta t$ :

$$N(t, q \Delta x) = 2^{-p} C_p^{\frac{q+p}{2}}.$$

One uses the following asymptotic expansion:

#### Lemma:

$$2^{-p} C_p^{rac{q+p}{2}} \sim rac{2}{\sqrt{2\pi \, p}} \, e^{-rac{q^2}{2p}}$$

when  $p \to +\infty$ ,  $q^3 = o(p^2)$ .



When  $\Delta t \rightarrow 0$  and  $\Delta t^2 << \Delta x^3$ ,

$$N(t,x) \sim 2 \Delta x \sqrt{\frac{\Delta t}{\Delta x^2}} \frac{e^{-\{\frac{\Delta t}{\Delta x^2}\}\frac{x^2}{2t}}}{\sqrt{2\pi t}},$$

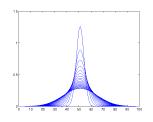
in such a way that  $rac{\Delta t}{\Delta x^2} 
ightarrow rac{1}{2D}$  and  $\Delta t 
ightarrow 0$ ,

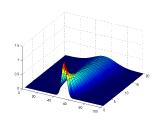
$$\frac{N(t,x)}{2\Delta x} \to u(t,x) = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}.$$

This last quantity is the elementary solution of the heat equation in dimension 1 with a diffusion coefficient D:

$$\frac{\partial u}{\partial t}(t,x) = D \frac{\partial^2 u}{\partial x^2}(t,x), \qquad u(0,x) = \delta_0(x).$$







**Diffusion (Fourier, 1822)**: Heat (diffusion) equation and its fundamental solution:

$$\frac{\partial u}{\partial t}(t,x) = D \frac{\partial^2 u}{\partial x^2}(t,x), \qquad u(0,x) = \delta_0(x).$$

$$u(t,x) = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}.$$



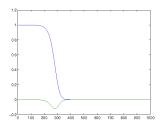
#### Traveling waves

Invasion model (Fisher; Kolmogoroff-Petrovsky-Piscounoff, 1937)

$$\frac{\partial u}{\partial t}(t,x) = D \frac{\partial^2 u}{\partial x^2}(t,x) + r_0 \left(1 - \frac{u(t,x)}{K}\right) u(t,x).$$

Obtained when both diffusion and logistic effects are considered.

#### Traveling waves



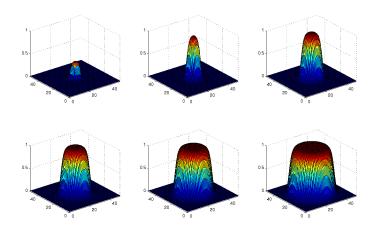
**In dimension 1**: One looks for u(t,x) = N(x-ct) solution of the PDE:

$$-c N'(z)-D N''(z)=r_0 \left(1-\frac{N(z)}{K}\right) N(z); \qquad N(-\infty)=K; \ N(\infty)=0.$$

**Theorem** (Kolmogoroff-Petrovsky-Piscounoff, 1937): Solutions to this heteroclinic junction problem in ODEs exist when  $c \ge c_0 = \sqrt{2 \, r_0 \, D}$ , critical speed of invasion associated to a population.

Those solutions are stable (in a setting to be made precise...) for the PDE if and only if  $c = c_0$ .

### 2D Traveling waves of invasion



#### Meaning of maps related to a biological invasion

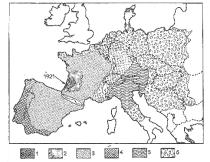


Fig. 63. - Progression du doryphore en Europe après son arrivée en 1921.



#### Competition models

#### Lotka, Volterra, 1925

Unknowns:  $u := u(t) \ge 0$ ,  $v := v(t) \ge 0$ , for  $t \ge 0$ .

Equations:

$$u'(t) = (r_1 - S_{11} u(t) - S_{12} v(t)) u(t),$$

$$v'(t) = (r_2 - S_{21} u(t) - S_{22} v(t)) v(t).$$

 $S_{ii} > 0$ : intraspecific competition

 $S_{ij} \geq 0$ ,  $i \neq j$ : interspecific competition

#### Competition models

Depending on the parameters  $r_i$ ,  $S_{ij}$ , and considering only nonnegative solutions, one has either (up to exchanging  $n_1$  and  $n_2$ ):

- **Strong competition**: The only stable equilibrium for the system of ODEs is  $(u, v) = (n_{10}, 0)$  with  $n_{10} > 0$ ; competitive exclusion.
- **Weak competition**: The only stable equilibrium for the system of ODEs is  $(u, v) = (n_{10}, n_{20})$  with  $n_{10} > 0$ ,  $n_{20} > 0$ ; coexistence.

#### Competition/Diffusion model

Unknowns: 
$$u_1 := u_1(t, x) \ge 0$$
,  $u_2 := u_2(t, x) \ge 0$ , for  $t \ge 0$ ,  $x \in \Omega$ .

Equations:

$$\partial_t u_1 - D_1 \Delta_x u_1 = (r_1 - S_{11} u_1 - S_{12} u_2) u_1,$$

$$\partial_t u_2 - D_2 \Delta_x u_2 = (r_2 - S_{21} u_1 - S_{22} u_2) u_2.$$

**No Turing instability** for such models: all steady homogeneous solutions which are stable for the ODEs are also stable for the PDEs; **No segregation of species appears** 

## A typical cross diffusion system: Shigesada-Kawasaki-Teramoto (SKT) model (1979)

Equations for the densities of population of two competing species:

$$\partial_t u_1 - \Delta_x \left( u_1 \left[ D_1 + A_{12} u_2 \right] \right) = (r_1 - S_{11} u_1 - S_{12} u_2) u_1,$$
  
 $\partial_t u_2 - \Delta_x \left( u_2 \left[ D_2 + A_{21} u_1 \right] \right) = (r_2 - S_{21} u_1 - S_{22} u_2) u_2.$ 

Neumann boundary condition (for  $t \ge 0$ ,  $x \in \partial\Omega$ )

$$\nabla_{\mathbf{x}} u_1(t,\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0, \quad \nabla_{\mathbf{x}} u_2(t,\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0.$$

Assumption:  $D_i > 0$ ,  $A_{12}$ ,  $A_{21} > 0$ ,  $r_i > 0$ ,  $S_{ij} > 0$ .

#### Modeling issue

Why 
$$\Delta_x(u_1 u_2) = \nabla_x \cdot (u_2 \nabla_x u_1) + \nabla_x \cdot (u_1 \nabla_x u_2)$$
 rather than  $\nabla_x \cdot (u_2 \nabla_x u_1)$ , or  $\Delta_x(u_1 u_2) = \nabla_x \cdot (u_2 \nabla_x u_1) + \beta \nabla_x \cdot (u_1 \nabla_x u_2)$ , avec  $\beta \neq 1$ ?

Answer (proposed by Iida, Izuhara, Mimura, Ninomiya, in the "triangular" case  $A_{21} = 0$ )

Possible interprétation based on a "microscopic" behavior: The species  $u_1$  exists in two states: quiet  $(u_{1A})$  and stressed  $(u_{1B})$ . The individuals of this species switch between the two states with a time scale  $\varepsilon$  and probability rates which depend on the concentration  $u_2$  of the other species.

#### Equations of the "microscopic" model

$$\partial_t u_{1A} - D_1 \Delta_x u_{1A} = (r_1 - S_{11} (u_{1A} + u_{1B}) - S_{12} u_2) u_{1A} + \frac{1}{\varepsilon} ((1 - u_2) u_{1B} - u_2 u_{1A}),$$

$$\partial_t u_{1B} - (D_1 + A_{12}) \Delta_x u_{1B} = (r_1 - S_{11} (u_{1A} + u_{1B}) - S_{12} u_2) u_{1B}$$
$$-\frac{1}{\varepsilon} ((1 - u_2) u_{1B} - u_2 u_{1A}),$$

$$\partial_t u_2 - D_2 \Delta_x u_2 = (r_2 - S_{21} (u_{1A} + u_{1B}) - S_{22} u_2) u_2.$$



#### Formal asymptotics when the time scales tends to 0

Assuming that 
$$u_{1A}^{\varepsilon} \to u_{1A}$$
,  $u_{1B}^{\varepsilon} \to u_{1B}$ ,  $u_{2}^{\varepsilon} \to u_{2}$ , 
$$(1-u_{2})\,u_{1B} = u_{2}\,u_{1A}, \qquad u_{1B} = u_{2}\,(u_{1A}+u_{1B}),$$
 and  $(u_{1A}+u_{1B},u_{2})$  satisfy 
$$\partial_{t}(u_{1A}+u_{1B}) - \Delta_{x} \left(D_{1}\,u_{1A}+(D_{1}+A_{12})\,u_{1B})\right)$$
 
$$= (r_{1}-S_{11}\,(u_{1A}+u_{1B})-S_{12}\,u_{2})\,(u_{1A}+u_{1B}),$$
 
$$\partial_{t}u_{2}-D_{2}\,\Delta_{x}u_{2} = (r_{2}-S_{21}\,(u_{1A}+u_{1B})-S_{22}\,u_{2})\,u_{2}.$$

Rigorous proof: Cf. LD-Trescases.

## Formal asymptotics when the time scales tends to 0 (II)

The SKT model (with  $A_{21} = 0$ ) is recovered by defining  $u_1 = u_{1A} + u_{1B}$ ,

$$\partial_t u_1 - \Delta_x \bigg( (D_1 + A_{12} u_2) u_1 \bigg) = (r_1 - S_{11} u_1 - S_{12} u_2) u_1.$$

The equation for  $u_2$  is conserved:

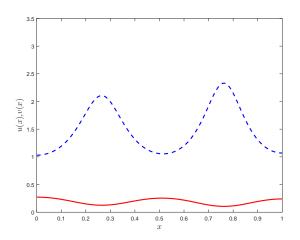
$$\partial_t u_2 - D_2 \Delta_x u_2 = (r_2 - S_{21} u_1 - S_{22} u_2) u_2.$$

#### Turing instability for the SKT model

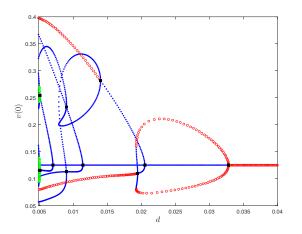
Existence of inhomogeneous steady states for the SKT model, interpreted as describing segregation situations

- At the numerical level: computation of those inhomogeneous steady states, and of associated bifurcation diagrams lida, Izuhara, Mimura, Ninomiya.
- At the rigorous level: justification of the numerical simulations thanks to computer-assisted proofs Breden, Castelli, Lessard, Vanicat.

## Segregation state



#### Bifurcation Diagram



Here, d is one of the parameters of the SKT model. The solutions in red are stable, the ones in blue and green unstable.

#### Results of existence for the non-triangular SKT system

Amann: Existence of local (in time) solutions

Kim; Masuda, Mimura; Shim: Existence of solutions for various types of coefficients in dimension 1

Li, Zhao: Existence of solutions when  $D_1 = D_2$ 

Chen, Jüngel, 2004: Existence of (weak) solutions thanks to the use of the functional

$$J(u_1, u_2) = A_{21} \int_{\Omega} (u_1 \ln u_1 - u_1 + 1) + A_{12} \int_{\Omega} (u_2 \ln u_2 - u_2 + 1)$$

#### Computation of the evolution of the functional J

$$\frac{d}{dt}J(u_1,u_2) + A_{21}D_1\int \frac{|\nabla_x u_1|^2}{u_1} + A_{12}D_2\int \frac{|\nabla_x u_2|^2}{u_2} + A_{12}A_{21}\int u_1u_2\left|\frac{\nabla_x u_1}{u_1} + \frac{\nabla_x u_2}{u_2}\right|^2 \le C(r_i, S_{ij}, A_{ij}).$$

After integration in time, for any T > 0,

$$\int_0^T \int_{\Omega} \left( \left| \nabla_x \sqrt{u_1} \right|^2 + \left| \nabla_x \sqrt{u_2} \right|^2 \right) < \infty.$$

If 
$$r_i = 0$$
,  $S_{ij} = 0$ ,

$$C=0; \qquad \frac{d}{dt}J(u_1,u_2)\leq 0.$$



#### Extensions for more general equations

**Theorem** (LD, Lepoutre, Moussa, Trescases) We assume that  $D_i > 0$ ,  $r_i \ge 0$ ,  $A_{ij} \ge 0$ , and  $S_{ij} > 0$ . We take  $0 < \beta_{ji} < 1$ , and  $\alpha_{12}, \alpha_{21} > 0$  such that

$$\alpha_{12} \, \alpha_{21} < 1.$$

Then there exists a weak solution to the system

$$\begin{split} \partial_t u_1 - \Delta_x \bigg[ \big( D_1 + A_{12} \, u_2^{\alpha_{12}} \big) \, u_1 \bigg] &= u_1 \, \bigg( r_1 - S_{11} \, u_1^{\beta_{11}} - S_{12} \, u_2^{\beta_{12}} \bigg), \\ \partial_t u_2 - \Delta_x \bigg[ \big( D_2 + A_{21} \, u_1^{\alpha_{21}} \big) \, u_2 \bigg] &= u_2 \, \bigg( r_2 - S_{21} \, u_1^{\beta_{21}} - S_{22} \, u_2^{\beta_{22}} \bigg), \end{split}$$

with Neumann boundary conditions, and suitable (nonnegative for all components) initial data.



#### Main a priori estimate used in the proof

Entropy (Lyapounov) estimate (case  $\alpha_{12} < 1$ ,  $\alpha_{21} < 1$ ),

$$egin{aligned} J^*(u_1,u_2)(T) + 4 \sum_{i 
eq j} A_{ij} D_j \int_0^T \int_\Omega \left| 
abla_x \sqrt{u_j^{lpha_{ij}}} 
ight|^2 \ &+ 4 \, A_{12} A_{21} \, \int_0^T \int_\Omega \left| 
abla_x \sqrt{u_2^{lpha_{12}} u_1^{lpha_{21}}} 
ight|^2 \leq \, J^*(u_{10},u_{20}) + C(T), \end{aligned}$$

where

$$J^*(u_1, u_2) := \sum_{i \neq j} \frac{A_{ij} \alpha_{ij}}{1 - \alpha_{ij}} \int_{\Omega} \left[ \left( u_j - \frac{u_j^{\alpha_{ij}}}{\alpha_{ij}} \right) - \left( 1 - \frac{1}{\alpha_{ij}} \right) \right].$$

#### The entropic structure

#### General equation

$$\partial_t U - \Delta_{\times}[A(U)] = R(U),$$

with 
$$A, R : \mathbb{R}^I \to \mathbb{R}^I$$
, and  $U := U(t, x) : \mathbb{R}_+ \times \Omega (\Omega \subset \mathbb{R}^N) \to (\mathbb{R}_+)^I$ .

For any  $\Phi: (\mathbb{R}_+)^l \to \mathbb{R}_+$ , if R = 0, and  $\langle \ , \ \rangle$  is the Euclidian scalar product on  $\mathbb{R}^l$ ,

$$\begin{split} \frac{d}{dt} \int_{\Omega} \Phi(U) &= \int_{\Omega} \langle \nabla \Phi(U), \Delta_{x}[A(U)] \rangle \\ &= -\sum_{j=1}^{N} \int_{\Omega} \langle \partial_{x_{j}} U, D^{2} \Phi(U) D(A)(U) \partial_{x_{j}} U \rangle \leq 0 \end{split}$$

when  $\Phi$  is an entropy, that is when  $(D^2\Phi(U)D(A)(U))^{sym} \geq 0$ .



#### The entropic structure (II)

**Proposition** (LD, Lepoutre, Moussa, Trescases): Consider  $a_1, a_2 : \mathbb{R}_+^* \to \mathbb{R}_+$  two  $C^1$  functions, and

$$A(x_1,x_2) := (x_1 a_1(x_2), x_2 a_2(x_1)).$$

We assume that  $a_1, a_2$  are increasing and  $Det D(A) \ge 0$ , that is

$$\forall x_1, x_2 > 0,$$
  $a_1(x_2) a_2(x_1) \ge x_1 x_2 a_1'(x_2) a_2'(x_1).$ 

Then taking

$$\Phi(X) := \phi_1(x_1) + \phi_2(x_2),$$

where  $\phi_i$  is a nonnegative second primitive of  $z \mapsto a'_j(z)/z$   $(i \neq j)$ , we get an entropy.



#### The entropic structure (III)

**Proof**: We compute, for  $X = (x_1, x_2)$ ,

$$D(A)(X) = \begin{pmatrix} a_1(x_2) & x_1 a_1'(x_2) \\ x_2 a_2'(x_1) & a_2(x_1) \end{pmatrix}, \quad D^2(\Phi)(X) = \begin{pmatrix} \frac{a_2'(x_1)}{x_1} & 0 \\ 0 & \frac{a_1'(x_2)}{x_2} \end{pmatrix},$$

so that

$$M(X) := D^{2}(\Phi)(X) D(A)(X) = \begin{pmatrix} a'_{2}(x_{1})a_{1}(x_{2})/x_{1} & a'_{2}(x_{1})a'_{1}(x_{2}) \\ a'_{1}(x_{2})a'_{2}(x_{1}) & a'_{1}(x_{2})a_{2}(x_{1})/x_{2} \end{pmatrix}$$

is obviously symmetric. Since the functions  $a_i$  are increasing, all the coefficients of M(X) are nonnegative, so that  $\operatorname{Tr} M(X) \geq 0$ ; we also see that

$$\operatorname{Det} M(X) = \operatorname{Det} D^2(\Phi)(X) \operatorname{Det} D(A)(X) \geq 0.$$



## Example of a system of 3 equations for which an entropy exists (and existence holds)

System:

$$\begin{split} \partial_t u_1 - \Delta_x [u_1 \left( D_1 + u_2^s + u_3^s \right)] &= 0, \\ \partial_t u_2 - \Delta_x [u_2 \left( D_2 + u_1^s + u_3^s \right)] &= 0, \\ \partial_t u_3 - \Delta_x [u_3 \left( D_3 + u_1^s + u_2^s \right)] &= 0, \end{split}$$

for  $0 < s < 1/\sqrt{3}$  and  $D_1, D_2, D_3 > 0$ .

Entropy still of the form

$$\int_{\Omega} \left( \phi_1(u_1) + \phi_2(u_2) + \phi_3(u_3) \right) dx.$$

# Example of a system for which an entropy is known, but is not "additive" (and existence is not known)

System:

$$\partial_t u - \Delta_x [u v^2] = 0,$$
  
$$\partial_t v - d \Delta_x [v u^2] = 0.$$

#### Entropy structure:

$$\frac{d}{dt}\int_{\Omega}u^2\,v^2\,dx = -\int_{\Omega}\left(u^2\,v^4\left|\frac{\nabla_{\times}u}{u} + 2\,\frac{\nabla_{\times}v}{v}\right|^2 + d\,u^4\,v^2\left|2\,\frac{\nabla_{\times}u}{u} + \frac{\nabla_{\times}v}{v}\right|^2\right)dx.$$

## A method for building systems with entropies: Fast reaction limit of reaction-diffusion systems

Reaction-(nonlinear) diffusion system with fast reaction limit:

$$\begin{split} \partial_t u - \Delta_x(u^2) &= \frac{1}{\varepsilon} (v w - u), \\ \partial_t v - \Delta_x(v^2) &= -\frac{1}{\varepsilon} (v w - u), \\ \partial_t w - \Delta_x(w^2) &= -\frac{1}{\varepsilon} (v w - u). \end{split}$$

Entropy:

$$E = \int \left[ (u \ln u - u + 1) + (v \ln v - v + 1) + (w \ln w - w + 1) \right] dx.$$

#### Fast reaction limit of reaction-diffusion systems (II)

Formal limit: u = v w, and

$$\partial_t (v w + v) - \Delta_x (v^2 w^2 + v^2) = 0,$$
  
 $\partial_t (v w + w) - \Delta_x (v^2 w^2 + w^2) = 0.$ 

Entropy:

$$E = \int \left[ (v w \ln(v w) - v w + 1) + (v \ln v - v + 1) + (w \ln w - w + 1) \right] dx.$$

Rigorous passage to the limit: Bothe, Rolland

# Fast reaction limit of reaction-diffusion systems (III: structural stability)

Reaction-cross diffusion system with fast reaction limit:

$$\partial_t u - \Delta_x (u^2 + \eta u p(u, v)) = \frac{1}{\varepsilon} (v w - u),$$
  

$$\partial_t v - \Delta_x (v^2 + \eta v q(u, v)) = -\frac{1}{\varepsilon} (v w - u),$$
  

$$\partial_t w - \Delta_x (w^2) = -\frac{1}{\varepsilon} (v w - u).$$

Assumption:  $p \ge 0$ ,  $\partial_1 p \ge 0$ ,  $q \ge 0$ ,  $\partial_2 q \ge 0$ ,

$$\eta\left(||\partial_2 p||_{\infty} + ||\partial_1 q||_{\infty}\right) \leq 4.$$

Entropy:

$$E = \int \left[ (u \ln u - u + 1) + (v \ln v - v + 1) + (w \ln w - w + 1) \right] dx.$$

#### Fast reaction limit of reaction-diffusion systems (IV)

Formal limit: u = v w, and

$$\partial_t(v w + v) - \Delta_x(v^2 w^2 + v^2 + \eta v w p(v w, v) + \eta v q(v w, v)) = 0,$$
  
$$\partial_t(v w + w) - \Delta_x(v^2 w^2 + w^2 + \eta v w p(v w, v)) = 0.$$

Entropy:

$$E = \int \left[ (v w \ln(v w) - v w + 1) + (v \ln v - v + 1) + (w \ln w - w + 1) \right] dx.$$

Rigorous passage to the limit: Daus, LD, Jüngel

#### SKT system for an arbitrary number of species

System:

$$\partial_t u_i = \Delta_{\mathsf{x}} \left( \left[ D_i + \sum_{j=1}^n A_{ij} u_j \right] u_i \right)$$

Chen, Daus, Jüngel showed that

$$J(u_1,..,u_n) := \sum_{i=1}^n \int \pi_i \left[ u_i \ln(u_i) - u_i + 1 \right]$$

with positive constants  $\pi_i > 0$  for i = 1, ..., n, is an entropy if the following condition holds

$$\forall i,j \qquad \pi_i A_{ij} = \pi_j A_{ji}.$$

The system is then said to be **detailed balanced**.



#### SKT system for an arbitrary number of species (II)

We consider a dicretized space domain:  $\Omega_M = \{0, \frac{1}{M}, \frac{2}{M}, ..., 1\}$ , and nonnegative constants  $\pi_i, D_i, D_{ij}$  such that  $\sum_{i=1}^n \pi_i = 1$  and  $D_{ij} = D_{ji}$  for i, j = 1, ..., n.

We consider n species of particles located on  $\Omega_M$ . There are  $[\pi_i N]$  particles of species i.

We define the time-continuous Markov chain on  $\Theta_{M,N}:=\Omega_M^{[\pi_1N]+\cdots+[\pi_nN]}$  by the transitions

$$egin{aligned} x 
ightharpoonup x + e_i^a + e_j^b \ x 
ightharpoonup x - e_i^a - e_j^b \ \end{pmatrix} \qquad ext{with rate } \delta_{(i,a) 
eq (j,b)} \delta_{x_i^a = x_j^b} rac{D_{ij}}{N} \ & \times 
ightharpoonup x + e_i^a \ & \times 
ightharpoonup x - e_i^a \ \end{pmatrix} \qquad ext{with rate } D_i \ & \qquad ex$$

for i, j = 1, ..., n and  $a = 1, ..., [\pi_i N]$ ,  $b = 1, ..., [\pi_j N]$ , where  $e_i^a$  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.

## SKT system for an arbitrary number of species (III)

Associated master equation:

$$\frac{d}{dt}\mu^{N}(t,x) = \sum_{i=1}^{n} \sum_{a=1}^{[\pi_{i}N]} D_{i} \Big[ \mu^{N}(t,x+e_{i}^{a}) + \mu^{N}(t,x-e_{i}^{a}) - 2\mu^{N}(t,x) \Big] 
+ \frac{1}{2} \sum_{i=1}^{n} \sum_{a=1}^{[\pi_{i}N]} \sum_{j=1}^{n} \sum_{b=1}^{[\pi_{j}N]} \delta_{(i,a)\neq(j,b)} \delta_{x_{i}^{a}=x_{j}^{b}} \frac{D_{ij}}{N} \Big[ \mu^{N}(t,x+e_{i}^{a}+e_{j}^{b}) 
+ \mu^{N}(t,x-e_{i}^{a}-e_{j}^{b}) - 2\mu^{N}(t,x) \Big].$$

### SKT system for an arbitrary number of species (IV)

The functional defined by

$$\tilde{\mathcal{H}}(\mu^{N})(t) := \sum_{x} \mu^{N}(t, x) \ln \left( \frac{\mu^{N}(t, x)}{M^{[\pi_{1}N] + \dots + [\pi_{n}N]}} \right)$$

is decreasing with respect to time, i.e.

$$\frac{d}{dt}\tilde{\mathcal{H}}(\mu^N) \leq 0$$

along the flow of the master equation.

#### SKT system for an arbitrary number of species (V)

When  $N \to \infty$ , under the assumption (of indinstinguishability and) chaos propagation:

$$\begin{split} & \mu^{N}(t, x_{1}^{1}, \dots, x_{1}^{[\pi_{1}N]}, \dots, x_{n}^{1}, \dots, x_{n}^{[\pi_{n}N]}) \\ & \approx \textit{u}_{1}(t, x_{1}^{1}) \cdots \textit{u}_{1}(t, x_{1}^{[\pi_{1}N]}) \cdots \cdots \textit{u}_{n}(t, x_{n}^{1}) \cdots \textit{u}_{n}(t, x_{n}^{[\pi_{n}N]}), \end{split}$$

one can show that

$$\frac{d}{dt}u_i(t,x)=D_i\Big[u_i(t,x+h)+u_i(t,x-h)-2u_i(t,x)\Big]$$

$$+\sum_{j=1}^{n}D_{ij}\pi_{j}\Big[u_{j}(t,x+h)u_{i}(t,x+h)+u_{j}(t,x-h)u_{i}(t,x-h)-2u_{j}(t,x)u_{i}(t,x)\Big].$$

#### SKT system for an arbitrary number of species (VI)

When  $N \to \infty$ , under the assumption (of indinstinguishability and) chaos propagation,

$$\frac{1}{N}\tilde{\mathcal{H}}(\mu^{N}) = \sum_{x} \mu^{N}(x) \ln \left( \frac{\mu^{N}(x)}{M^{([\pi_{1}N] + \dots + [\pi_{n}N])}} \right)$$

$$\approx \frac{1}{N} \sum_{i=1}^{n} \sum_{\ell=0}^{M-1} [\pi_{i}N] u_{i}(x_{\ell}) \ln \left( \frac{u_{i}(x_{\ell})}{M} \right)$$

$$\to \sum_{i=1}^{n} \pi_{i} \sum_{\ell=0}^{M-1} u_{i}(x_{\ell}) \ln \left( \frac{u_{i}(x_{\ell})}{M} \right).$$

#### SKT system for an arbitrary number of species (VII)

When  $h=1/M\to 0$ , defining  $A_{ij}:=\pi_j\,D_{ij}$ , and rescaling in time (in such a way that  $\partial_t$  is replaced by  $h^2\,\partial_t$ ), one recovers the original SKT system for an arbitrary number of species:

$$\partial_t u_i = \Delta_{\mathsf{x}} \left( \left[ D_i + \sum_{j=1}^n A_{ij} u_j \right] u_i \right),$$

and its Lyapunov functional:

$$J(u_1,..,u_n) := \sum_{i=1}^n \int \pi_i \left[ u_i \ln(u_i) - u_i + 1 \right].$$

The condition  $\forall i, j \ D_{ij} = D_{ji}$  becomes the detailed balance condition:

$$\forall i, j \qquad \pi_i A_{ii} = \pi_i A_{ii}.$$