# Mean-field-type limits of interacting particle systems for multiple species

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1. Introduction
2. First particle system
3. Second particle system

# Motivation

Aim: rigorous derivation of cross-diffusion systems ($i = 1, \ldots, n$)

$$\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j\right), \quad u_i(0) = u_{i,0} \quad \text{in } \mathbb{R}^d$$

Applications: population dynamics, ion transport in cells, fluids, etc.

Single-species particle system:

$$dX^k = -\frac{1}{N}\sum_{j=1, j\neq k}^N \nabla B(X^k - X^j)dt + \sqrt{2\sigma}dW^k(t), \quad k = 1, \ldots, N$$

with $X^k(t)$ stochastic processes ("random position"), $W^k(t)$ independent Wiener processes, $B$ interaction potential (Lipschitz)

Heuristic argument for limit $N \to \infty$:

$$\frac{1}{N}\sum_{j\neq k}\nabla B(x - X^j) \sim \mathrm{E}(\nabla B) = \int_{\mathbb{R}^d}\nabla B(x-y)u(y)dy = \nabla B * u$$

- Limit eq. for probability density: $\partial_t u = \operatorname{div}(u(\nabla B * u)) + \sigma\Delta u$
- Localization limit $B \to \delta_0$: $\partial_t u = \sigma\Delta u + \operatorname{div}(u\nabla u)$

# Overview

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# First particle system

Stochastic processes $X_i^k(t)$ solve SDE

$$dX_i^k = -\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N \nabla B_{ij}^\eta(X_i^k - X_j^\ell)dt + \sqrt{2\sigma_i}dW_i^k(t), \quad X_i^k(0) = \xi_i^k$$

- Species index $i = 1, \ldots, n$, particle index $k = 1, \ldots, N$
- $W_i^k$ independent Wiener processes, $\sigma_i > 0$, $\xi_i^1, \ldots, \xi_i^N$ iid with common density $u_{i,0}$
- Interaction potential: $B_{ij}^\eta(x) = \eta^{-d}B_{ij}(x/|\eta|)$, $\int_{\mathbb{R}^d} B_{ij}dx = a_{ij} \Rightarrow$

$$\|B_{ij}^\eta\|_{L^1(\mathbb{R}^d)} = \|B_{ij}\|_{L^1(\mathbb{R}^d)}, \quad B_{ij}^\eta \to a_{ij}\delta_0 \quad \text{in } \mathcal{D}'$$

- Expect: $N \to \infty$ leads to "nonlocal" SDE, $\eta \to 0$ leads to local SDE with probability density satisfying PDE (by Itô's lemma)

# Mean-field-type limit in first particle system

Idea: consider intermediate particle system

- "Microscopic" particle system: $(i = 1, \ldots, n,\ k = 1, \ldots, N)$

$$dX_i^k = -\sum_{j=1}^n \frac{1}{N} \sum_{\ell=1}^N \nabla B_{ij}^\eta (X_i^k - X_j^\ell) dt + \sqrt{2\sigma_i} dW_i^k(t), \quad X_i^k(0) = \xi_i^k$$

- "$N \to \infty$" $\Rightarrow$ intermediate particle system: $u_{\eta,j}$ solves nonlocal PDE

$$d\overline{X}_i^k = -\sum_{j=1}^n (\nabla B_{ij}^\eta * u_{\eta,j})(\overline{X}_i^k(t), t) dt + \sqrt{2\sigma_i} dW_i^k(t), \quad \overline{X}_i^k(0) = \xi_i^k$$

- $\eta \to 0 \Rightarrow$ "macroscopic" particle system:

$$d\widehat{X}_i^k = -\sum_{j=1}^n a_{ij} \nabla u_j (\widehat{X}_i^k(t), t) dt + \sqrt{2\sigma_i} dW_i^k(t), \quad \widehat{X}_i^k(0) = \xi_i^k$$

- Density function $u_i = \mathrm{Law}(\widehat{X}_i^k)$ associated to $\widehat{X}_i^k$ solves

$$\partial_t u_i = \sigma_i \Delta u_i + \operatorname{div}\left( u_i \sum_{j=1}^n a_{ij} \nabla u_j \right)$$

# Mean-field-type limit in first particle system

$$dX_i^k = -\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N \nabla B_{ij}^\eta(X_i^k - X_j^\ell)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

$$d\overline{X}_i^k = -\sum_{j=1}^n (\nabla B_{ij}^\eta * u_{\eta,j})(\overline{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

$$d\widehat{X}_i^k = -\sum_{j=1}^n a_{ij}\nabla u_j(\widehat{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

**Theorem (L. Chen-Daus-A.J. 2019)**

*Let $N \in \mathbb{N}$, $\delta \in (0,1)$ "small", $\eta^{-2d-4} \le \delta \log N$. Then*

$$\sup_{k=1,\ldots,N} \mathbb{E}\bigg(\sum_{i=1}^n \sup_{0<s<T}\big|X_i^k(s) - \widehat{X}_i^k(s)\big|\bigg) \le C(T)\eta.$$

Idea of proof: exploit Lipschitz continuity of $B_{ij}$ and estimate

$$\mathrm{E}\Big(\sup_{0<s<T}\big|X_i^k - \widehat{X}_i^k\big|\Big) \le \mathrm{E}\Big(\sup_{0<s<T}\big|X_i^k - \overline{X}_i^k\big|\Big) + \mathrm{E}\Big(\sup_{0<s<T}\big|\overline{X}_i^k - \widehat{X}_i^k\big|\Big)$$

# Mean-field-type limit in first particle system

$$dX_i^k = -\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N \nabla B_{ij}^\eta(X_i^k - X_j^\ell)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

$$d\overline{X}_i^k = -\sum_{j=1}^n (\nabla B_{ij}^\eta * u_{\eta,j})(\overline{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

$$d\widehat{X}_i^k = -\sum_{j=1}^n a_{ij}\nabla u_j(\widehat{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t)$$

**Theorem (L. Chen-Daus-A.J. 2019)**

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Idea of proof: exploit Lipschitz continuity of $B_{ij}$ and estimate

$$\mathrm{E}\Big(\sup_{0<s<T}\left|X_i^k - \widehat{X}_i^k\right|\Big) \le C(T)N^{-1/2+C\delta} + C(T)\eta \le C(T)\eta$$

# First limit system: entropy structure

$$\partial_t u_i = \sigma_i \Delta u_i + \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j, \quad i = 1, \ldots, n$$

Entropy structure: let $\exists\, \pi_i > 0$: $\pi_i a_{ij} = \pi_j a_{ji}$, $A = (\pi_i a_{ij})$ pos. def.

- Shannon-type entropy density: $h_1(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$

$$\frac{d}{dt} \int_{\mathbb{R}^d} h_1(u) dx + 4 \int_{\mathbb{R}^d} \sum_{i=1}^n \pi_i \sigma_i |\nabla \sqrt{u_i}|^2 dx + \lambda_A \int_{\mathbb{R}^d} \sum_{i=1}^n |\nabla u_i|^2 dx \le 0$$

- Rao-type entropy density: $h_2(u) = \frac{1}{2} \sum_{i,j=1}^n \pi_i a_{ij} u_i u_j$

$$\frac{d}{dt} \int_{\mathbb{R}^d} h_2(u) dx + \lambda_{A\sigma} \int_{\mathbb{R}^d} \sum_{i=1}^n |\nabla u_i|^2 dx + \int_{\mathbb{R}^d} \sum_{i=1}^n \pi_i u_i |\nabla p_i(u)|^2 dx \le 0$$

- Numerical analysis: A.J.-Zurek 2020
- Mathematical analysis: A.J.-Portisch-Zurek 2021

# Overview

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# Second particle system

Let $X_i^k(t)$ be stochastic processes for $i = 1, \ldots, n$, $k = 1, \ldots, N$

$$dX_i^k = -\nabla U_i(X_i^k)dt + \sqrt{2\sigma_i + 2F_N^\eta(X)}\,dW_i^k(t), \quad X_i^k(0) = \xi_i^k$$

$$F_N^\eta(X) = \sum_{j=1}^n \frac{1}{N} \sum_{\ell=1}^N B_{ij}^\eta(X_i^k - X_j^\ell)$$

- $W_i^k$ independent Wiener processes, $\sigma_i > 0$, $\xi_i^1, \ldots, \xi_i^N$ iid with common density $u_{i,0}$, $U_i$ environmental potential
- Interaction potential: $B_{ij}^\eta(x) = \eta^{-d} B_{ij}(x/|\eta|)$, $\int_{\mathbb{R}^d} B_{ij}dx = a_{ij} \Rightarrow$

$$\|B_{ij}^\eta\|_{L^1(\mathbb{R}^d)} = \|B_{ij}\|_{L^1(\mathbb{R}^d)}, \quad B_{ij}^\eta \to a_{ij}\delta_0 \quad \text{in } \mathcal{D}'$$

- Compared to first system: interacting diffusion coefficients
- Expectation:

$$F_N^\eta(X) \sim \sum_{j=1}^n \mathrm{E}(B_{ij}) = \sum_{j=1}^n B_{ij} * u_j \sim \sum_{j=1}^n a_{ij}u_j \ \Rightarrow \ \Delta\Big(u_i \sum_{j=1}^n a_{ij}u_j\Big)$$

# Mean-field-type limit in second particle system

Idea: consider intermediate particle system

- "Microscopic" particle system: $(i = 1, \ldots, n,\ k = 1, \ldots, N)$

$$dX_i^k = -\nabla U_i(X_i^k)dt + \Big(2\sigma_i + 2\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N B_{ij}^\eta(X_i^k - X_j^\ell)\Big)^{1/2} dW_i^k(t)$$

- $N \to \infty$ leads to intermediate particle system:

$$d\overline{X}_i^k = -\nabla U_i(\overline{X}_i^k)dt + \Big(2\sigma_i + 2\sum_{j=1}^n B_{ij}^\eta * u_{\eta,j}(\overline{X}_i^k(t), t)\Big)^{1/2} dW_i^k(t)$$

- $\eta \to 0$ leads to "macroscopic" particle system:

$$d\widehat{X}_i^k = -\nabla U_i(\widehat{X}_i^k)dt + \Big(2\sigma_i + 2\sum_{j=1}^n a_{ij} u_j(\widehat{X}_i^k(t), t)\Big)^{1/2} dW_i^k(t)$$

- Density function $u_i = \mathrm{Law}(\widehat{X}_i^k)$ associated to $\widehat{X}_i^k$ solves

$$\partial_t u_i = \operatorname{div}(u_i \nabla U_i) + \Delta\Big(u_i\Big(\sigma_i + \sum_{j=1}^n a_{ij} u_j\Big)\Big)$$

# Mean-field-type limit in second particle system

$$dX_i^k = -\nabla U_i(X_i^k)dt + \left(2\sigma_i + 2\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N B_{ij}^\eta(X_i^k - X_j^\ell)\right)^{1/2} dW_i^k(t),$$

$$d\widehat{X}_i^k = -\nabla U_i(\widehat{X}_i^k)dt + \left(2\sigma_i + 2\sum_{j=1}^n a_{ij}u_j(\widehat{X}_i^k(t),t)\right)^{1/2} dW_i^k(t)$$

**Theorem (L. Chen-Daus-Holzinger-A.J. 2020)**

*Let $U_i(x) = -\frac{1}{2}|x|^2$, $N \in \mathbb{N}$, $\delta \in (0,1)$ "small", $\eta^{-2d-3} \le \delta \log N$. Then*

$$\sup_{k=1,\ldots,N} \mathbb{E}\left(\sum_{i=1}^n \sup_{0<s<T} \left|X_i^k(s) - \widehat{X}_i^k(s)\right|\right) \le C(T)\eta.$$

Idea of proof: similarly as for first particle system, but estimates more delicate since $U_i$, $\nabla U_i \notin L^2(\mathbb{R}^d)$

# Generalization

$$dX_i^k = -\nabla U_i(X_i^k)dt + \left(2\sigma_i + 2\sum_{j=1}^n f_\eta\left(\frac{1}{N}\sum_{\ell=1}^N B_{ij}^\eta(X_i^k - X_j^\ell)\right)\right)^{1/2} dW_i^k(t)$$

- Function $f_\eta \in C^{0,1}(\mathbb{R})$ satisfies $f_\eta \to f \in C^{0,1}_{\mathrm{loc}}(\mathbb{R})$
- Mean-field-type limit:

$$\partial_t u_i = \operatorname{div}(u_i \nabla U_i) + \Delta\left(u_i\left(\sigma_i + \sum_{j=1}^n f(a_{ij}u_j)\right)\right)$$

By-product: porous-medium equation ($n = 1$)

- Mean-field limit in

$$dX^k = \left(2\sigma + 2f_\eta\left(\frac{1}{N}\sum_{\ell=1}^N B_{ij}^\eta(X^k - X^\ell)\right)\right)^{1/2} dW^k$$

gives $\partial_t u = \sigma\Delta u + \Delta(uf(u))$

- Other derivation by Figalli-Philipowski 2008 from

$$dX^k = -\left[\nabla B^\eta * (B^\eta * u_\eta)^{m-1}\right]dt + \sqrt{2\sigma}dW^k, \ u_\eta(t) = \mathrm{Law}(X^k(t))$$

gives $\partial_t u = \sigma\Delta u + \frac{m-1}{m}\Delta(u^m)$, $m > 1$

# Second limit system

$$\partial_t u_i = \operatorname{div}(u_i \nabla U_i) + \Delta(u_i p_i(u)), \quad p_i(u) = \sigma_i + \sum_{j=1}^n a_{ij} u_j$$

- Suggested by Shigesada, Kawasaki, Teramoto in 1979
- Mathematical analysis: L. Chen-A.J. 2004 ($n = 2$), Dreher 2008 ($n = 2$, $\mathbb{R}^d$), X. Chen-Daus-A.J. 2018 ($n \geq 2$)

Entropy structure: let $\exists \pi_i > 0 : \pi_i a_{ij} = \pi_j a_{ji}$
Shannon-type entropy density: $h_1(u) = \sum_{i=1}^n \pi_i u_i (\log u_i - 1)$

$$\frac{d}{dt} \int_{\mathbb{R}^d} h_1(u) dx + 4 \int_{\mathbb{R}^d} \sum_{i=1}^n \pi_i \sigma_i |\nabla \sqrt{u_i}|^2 dx + 2 \int_{\mathbb{R}^d} \sum_{i=1}^n \pi_i a_{ii} |\nabla u_i|^2 dx \leq 0$$

Comparison with first mean-field system:

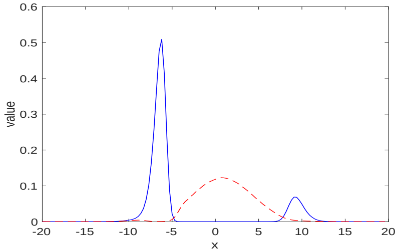
- Additional diffusion in second model weakens segregation effect
- First model possesses two entropies

# Numerical comparison of "microscopic" particle systems

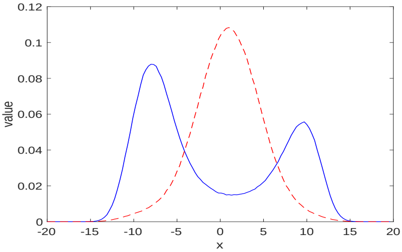
$$dX_i^k = -\sum_{j=1}^{n} \frac{1}{N} \sum_{\ell=1}^{N} \nabla B_{ij}^{\eta}(X_i^k - X_j^{\ell})dt + \sqrt{2\sigma_i}dW_i(t)$$

$$dY_i^k = -\nabla U_i(Y_i^k)dt + \left(2\sigma_i + 2\sum_{j=1}^{n} \frac{1}{N} \sum_{\ell=1}^{N} B_{ij}^{\eta}(Y_i^k - Y_j^{\ell})\right)^{1/2} dW_i^k(t)$$

- Euler-Maruyama discretization, Gaussian initial data, parallelized
- $B_{ij}(x) = e^{-1/(1-x^2)} 1_{\{|x| \leq 1\}}$, $U_i = 0$, 5000 particles, 500 simulations
- Parameter: $\sigma_1 = 1$, $\sigma_2 = 2$, $a_{11} = 0$, $a_{12} = 355$, $a_{21} = 25$, $a_{22} = 0$




First particle system: strong segregation




Second particle system (SKT)

# Summary and open questions

## Summary:

- Derivation of $\partial_t u_i = \sigma_i \Delta u_i + \operatorname{div}(u_i \sum_j a_{ij} \nabla u_j)$ from

$$dX_i^k = -\sum_{j=1}^{n} \frac{1}{N} \sum_{\ell=1}^{N} \nabla B_{ij}^{\eta}(X_i^k - X_j^{\ell})dt + \sqrt{2\sigma_i}dW_i^k(t)$$

- Derivation of $\partial_t u_i = \sigma_i \Delta u_i + \Delta(u_i \sum_j a_{ij} u_j) + \operatorname{div}(u_i \nabla U_i)$ from

$$dX_i^k = -\nabla U_i(X_i^k)dt + \left(2\sigma_i + 2\sum_{j=1}^{n} \frac{1}{N} \sum_{\ell=1}^{N} B_{ij}^{\eta}(X_i^k - X_j^{\ell})\right)^{1/2} dW_i^k(t)$$

## Perspectives and open questions:

- Random-batch method for particle systems, cf. Shi Jin (cooperation with E. Daus, M. Fellner)
- Fluctuations: include first-order correction $\to$ stochastic PDE (cooperation with L. Chen, E. Daus, A. Holzinger)
- Can we justify $\partial_t u_i = \sigma_i \Delta u_i + \Delta(u_i p_i(u)) + \sqrt{2\sigma(u)} dW_i$?