

The Scharfetter-Gummel scheme for the aggregation-diffusion equation and vanishing diffusion limit

Anastasiia Hraivoronska (Université Claude Bernard - Lyon 1)

joint work with **André Schlichting** and **Oliver Tse**
Preprint arXiv:2306.02226

Gradient flows face-to-face 3, Lyon, 14 September 2023

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla (\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega \quad (\text{ADE})$$

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega \quad (\text{ADE})$$

- ▶ Population dynamics $\Lambda(x) = w(|x|)$. Attractive forces $w'(r) > 0$, repulsive forces $w'(r) < 0$.

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega \quad (\text{ADE})$$

- ▶ Population dynamics $\Lambda(x) = w(|x|)$. Attractive forces $w'(r) > 0$, repulsive forces $w'(r) < 0$.
- ▶ The Morse potential

$$\Lambda(x) = C_r e^{-|x|/\ell_r} - C_a e^{-|x|/\ell_a}$$

with $C_r \geq C_a > 0$ and $\ell_a > \ell_r$.

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega$$

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega$$

- ▶ bounded convex domain $\Omega \subset \mathbb{R}^d$;

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega$$

- ▶ bounded convex domain $\Omega \subset \mathbb{R}^d$;
- ▶ a diffusion coefficient $\varepsilon > 0$;

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega$$

- ▶ bounded convex domain $\Omega \subset \mathbb{R}^d$;
- ▶ a diffusion coefficient $\varepsilon > 0$;
- ▶ an interaction potential $\Lambda \in \operatorname{Lip}(\mathbb{R}^d) \cap C^1(\mathbb{R}^d \setminus \{0\})$ (pointy).
- ▶ no-flux boundary condition

$$\varepsilon \partial_\nu \rho + \rho \partial_\nu(\Lambda * \rho) = 0 \quad \text{on } \partial\Omega,$$

ν denotes the outer normal vector on $\partial\Omega$.

Aggregation-diffusion equation

$$\partial_t \rho = \varepsilon \Delta \rho + \operatorname{div}(\rho \nabla(\Lambda * \rho)) \quad \text{in } (0, T) \times \Omega$$

- ▶ bounded convex domain $\Omega \subset \mathbb{R}^d$;
- ▶ a diffusion coefficient $\varepsilon > 0$;
- ▶ an interaction potential $\Lambda \in \operatorname{Lip}(\mathbb{R}^d) \cap C^1(\mathbb{R}^d \setminus \{0\})$ (pointy).
- ▶ no-flux boundary condition

$$\varepsilon \partial_\nu \rho + \rho \partial_\nu(\Lambda * \rho) = 0 \quad \text{on } \partial\Omega,$$

ν denotes the outer normal vector on $\partial\Omega$.

Gradient flow in $(\mathcal{P}(\Omega), W_2)$ with respect to the driving energy:

$$\mathcal{E}_\varepsilon(\rho) = \varepsilon \int_{\Omega} \log \frac{d\rho}{d\mathcal{L}^d}(x) \rho(dx) + \frac{1}{2} \int_{\Omega} \int_{\Omega} \Lambda(x-y) \rho(dx) \rho(dy)$$

Zoo of numerical schemes

- ▶ Based on the JKO scheme

$$\rho_k^\tau = \arg \min_{\rho \in \mathcal{P}(\Omega)} \left\{ \mathcal{E}_\varepsilon(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_{k-1}^\tau) \right\}$$

purely continuous [Benamou-Brenier '00]; semi-discrete

[Benamou-Carlier-Merigot-Oudet '16], [Kitagawa-Mérogot-Thibert '19]; purely

discrete [Cuturi '13]; other [Carrillo-Ranetbauer-'16]

Zoo of numerical schemes

- ▶ Based on the JKO scheme

$$\rho_k^\tau = \arg \min_{\rho \in \mathcal{P}(\Omega)} \left\{ \mathcal{E}_\varepsilon(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_{k-1}^\tau) \right\}$$

purely continuous [Benamou-Brenier '00]; semi-discrete

[Benamou-Carlier-Merigot-Oudet '16], [Kitagawa-Mérogot-Thibert '19]; purely discrete [Cuturi '13]; other [Carrillo-Ranetbauer-'16]

- ▶ Discretize the equation directly

[Bailo-Carrillo-Murakawa-Schmidtchen '20], [Zhang-Hu '21], [Schlichting-Seis '22]

Zoo of numerical schemes

- ▶ Based on the JKO scheme

$$\rho_k^\tau = \arg \min_{\rho \in \mathcal{P}(\Omega)} \left\{ \mathcal{E}_\varepsilon(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_{k-1}^\tau) \right\}$$

purely continuous [Benamou-Brenier '00]; semi-discrete

[Benamou-Carlier-Merigot-Oudet '16], [Kitagawa-Mérogot-Thibert '19]; purely

discrete [Cuturi '13]; other [Carrillo-Ranetbauer-'16]

- ▶ Discretize the equation directly

[Bailo-Carrillo-Murakawa-Schmidtchen '20], [Zhang-Hu '21], [Schlichting-Seis '22]

- ▶ Deterministic particle approximations:

$$\rho^N = \sum_{i=1}^N m_i \delta_{x_i(t)}$$

[Carrillo-Craig-Patacchini '19]

Zoo of numerical schemes

- ▶ Based on the JKO scheme

$$\rho_k^\tau = \arg \min_{\rho \in \mathcal{P}(\Omega)} \left\{ \mathcal{E}_\varepsilon(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_{k-1}^\tau) \right\}$$

purely continuous [Benamou-Brenier '00]; semi-discrete

[Benamou-Carlier-Merigot-Oudet '16], [Kitagawa-Mérogot-Thibert '19]; purely

discrete [Cuturi '13]; other [Carrillo-Ranetbauer-'16]

- ▶ Discretize the equation directly

[Bailo-Carrillo-Murakawa-Schmidtchen '20], [Zhang-Hu '21], [Schlichting-Seis '22]

- ▶ Deterministic particle approximations:

$$\rho^N = \sum_{i=1}^N m_i \delta_{x_i(t)}$$

[Carrillo-Craig-Patacchini '19]

Structure-preserving properties

1. Preserving positivity of solutions. If $\rho_0 \geq 0$, then $\rho_t \geq 0$ for all $t > 0$.

Structure-preserving properties

1. Preserving positivity of solutions. If $\rho_0 \geq 0$, then $\rho_t \geq 0$ for all $t > 0$.
2. Conservation of mass

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \rho(\mathrm{d}x) &= \int_{\Omega} \operatorname{div}(\varepsilon \nabla \rho + \rho(\nabla \Lambda * \rho)) \mathrm{d}x \\ &= \int_{\partial\Omega} (\varepsilon \nabla \rho + \rho(\nabla \Lambda * \rho)) \cdot \nu \mathrm{d}x = 0. \end{aligned}$$

Structure-preserving properties

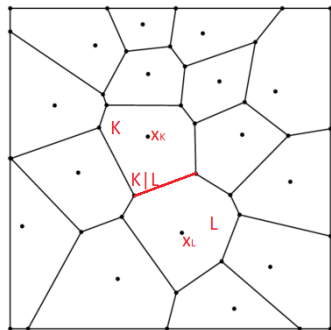
1. Preserving positivity of solutions. If $\rho_0 \geq 0$, then $\rho_t \geq 0$ for all $t > 0$.
2. Conservation of mass

$$\begin{aligned}\frac{d}{dt} \int_{\Omega} \rho(\mathrm{d}x) &= \int_{\Omega} \operatorname{div}(\varepsilon \nabla \rho + \rho(\nabla \Lambda * \rho)) \mathrm{d}x \\ &= \int_{\partial \Omega} (\varepsilon \nabla \rho + \rho(\nabla \Lambda * \rho)) \cdot \nu \mathrm{d}x = 0.\end{aligned}$$

3. Dissipation of the driving energy

$$\frac{d}{dt} \mathcal{E}(\rho_t) = \int_{\Omega} \mathcal{E}'(x) \partial_t \rho(x) \mathrm{d}x = - \int_{\Omega} |\nabla \mathcal{E}'(x)|^2 \rho_t(\mathrm{d}x) \leq 0.$$

The idea of finite-volume schemes

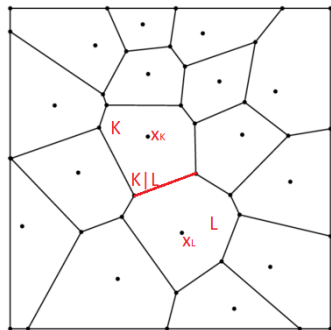


$$\partial_t \rho + \operatorname{div} j = 0 \quad \text{on } (0, T) \times \Omega$$

Tessellation $(\mathcal{T}^h, \Sigma^h)$

$$h = \max_{K \in \mathcal{T}^h} \operatorname{diam}(K)$$

The idea of finite-volume schemes



$$\partial_t \rho + \operatorname{div} j = 0 \quad \text{on } (0, T) \times \Omega$$

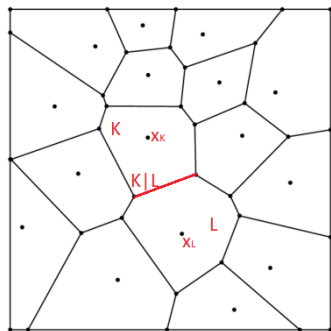
Integrating over the control volumes $K \in \mathcal{T}^h$:

$$\int_K \partial_t \rho + \int_K \operatorname{div} j = 0.$$

Tessellation $(\mathcal{T}^h, \Sigma^h)$

$$h = \max_{K \in \mathcal{T}^h} \operatorname{diam}(K)$$

The idea of finite-volume schemes



$$\partial_t \rho + \operatorname{div} j = 0 \quad \text{on } (0, T) \times \Omega$$

Integrating over the control volumes $K \in \mathcal{T}^h$:

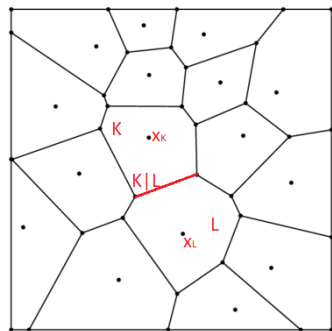
$$\int_K \partial_t \rho + \int_K \operatorname{div} j = 0.$$

$$\partial_t \rho_K^h + \int_{\partial K} j \cdot n \, d\mathcal{H}^{d-1} = 0$$

Tessellation $(\mathcal{T}^h, \Sigma^h)$

$$h = \max_{K \in \mathcal{T}^h} \operatorname{diam}(K)$$

The idea of finite-volume schemes



Tessellation $(\mathcal{T}^h, \Sigma^h)$

$$h = \max_{K \in \mathcal{T}^h} \text{diam}(K)$$

$$\partial_t \rho + \text{div } j = 0 \quad \text{on } (0, T) \times \Omega$$

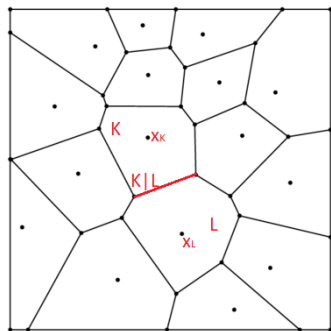
Integrating over the control volumes $K \in \mathcal{T}^h$:

$$\int_K \partial_t \rho + \int_K \text{div } j = 0.$$

$$\partial_t \rho_K^h + \int_{\partial K} j \cdot n \, d\mathcal{H}^{d-1} = 0$$

$$\partial_t \rho_K^h + \sum_{L \sim K} \int_{(K|L)} j \cdot n_{KL} \, d\mathcal{H}^{d-1} = 0$$

The idea of finite-volume schemes



Tessellation $(\mathcal{T}^h, \Sigma^h)$

$$h = \max_{K \in \mathcal{T}^h} \text{diam}(K)$$

$$\partial_t \rho + \text{div } j = 0 \quad \text{on } (0, T) \times \Omega$$

Integrating over the control volumes $K \in \mathcal{T}^h$:

$$\int_K \partial_t \rho + \int_K \text{div } j = 0.$$

$$\partial_t \rho_K^h + \int_{\partial K} j \cdot n \, d\mathcal{H}^{d-1} = 0$$

$$\partial_t \rho_K^h + \sum_{L \sim K} \int_{(K|L)} j \cdot n_{KL} \, d\mathcal{H}^{d-1} = 0$$

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0$$

The Scharfetter-Gummel flux

$$\partial_t \rho + \operatorname{div} j = 0$$

$$j = \varepsilon \nabla \rho + \rho \nabla (\Lambda * \rho)$$

Finite-volume approximation:

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

The Scharfetter-Gummel flux

$$\partial_t \rho + \operatorname{div} j = 0$$

$$j = \varepsilon \nabla \rho + \rho \nabla (\Lambda * \rho)$$

Finite-volume approximation:

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

The idea of the Scharfetter-Gummel is **solving a cell problem**.

$$u \in C^2([x_K, x_L])$$

$$\begin{cases} -\partial_x (\varepsilon \partial_x u + u q_{K|L}^h) = 0 & \text{on } [x_K, x_L] \\ u(x_K) = \rho_K^h / |K|, \quad u(x_L) = \rho_L^h / |L| \end{cases} \quad (\text{Cell-Pr})$$

Define $\mathcal{J}_{K|L}^\rho := \varepsilon \partial_x u + u q_{K|L}^h$.

Scharfetter-Gummel flux

The solution of (Cell-Pr) is

$$\mathcal{J}_{K|L}^\rho = \varepsilon \tau_{K|L} \left(\beta(q_{K|L}/\varepsilon) u_K^h - \beta(-q_{K|L}/\varepsilon) u_L^h \right),$$

where

- ▶ u^h is the density $u_K^h := \frac{\rho^K}{|K|}$ for all $K \in \mathcal{T}^h$;
- ▶ the transmission coefficient $\tau_{K|L} := \frac{|(K|L)|}{|x_L - x_K|}$ for all $(K, L) \in \Sigma^h$;
- ▶ β is the Bernoulli function $\beta(s) = \frac{s}{e^s - 1}$
- ▶ $q_{K|L}$ is a discrete approximation for $\nabla(\Lambda * \rho)$:

$$q_{K|L} = \sum_{M \in \mathcal{T}^h} (\Lambda(x_M - x_L) - \Lambda(x_M - x_K)) \rho_M^h$$

Properties of the Scharfetter-Gummel flux

1. If $\Lambda \equiv 0$, then

$$\mathcal{J}_{K|L}^\rho = \varepsilon \tau_{K|L} (u_K^h - u_L^h).$$

2. In the vanishing diffusion limit $\varepsilon \rightarrow 0$, the flux converges to the upwind scheme:

$$\mathcal{J}_{K|L}^\rho = \tau_{K|L} (q_{K|L}^+ u_K^h - q_{K|L}^- u_L^h)$$

Properties of the Scharfetter-Gummel flux

1. If $\Lambda \equiv 0$, then

$$\mathcal{J}_{K|L}^\rho = \varepsilon \tau_{K|L} (u_K^h - u_L^h).$$

2. In the vanishing diffusion limit $\varepsilon \rightarrow 0$, the flux converges to the upwind scheme:

$$\mathcal{J}_{K|L}^\rho = \tau_{K|L} (q_{K|L}^+ u_K^h - q_{K|L}^- u_L^h)$$

3. [Schlichting-Seis '22] The Scharfetter-Gummel scheme is:
 - + Positivity preserving;
 - + Mass conservative;
 - + Energy-dissipative;
 - ? Does it have a gradient structure?

Convergence and asymptotic limits

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0$$

$$\mathcal{J}_{K|L}^\rho = \varepsilon \tau_{K|L} (\beta(q_{K|L}/\varepsilon) u_K^h - \beta(-q_{K|L}/\varepsilon) u_L^h)$$

$$\partial_t \rho = \operatorname{div}(\varepsilon \nabla \rho + \rho \nabla(\Lambda * \rho))$$

Scharfetter–Gummel scheme $\xrightarrow{h \rightarrow 0}$ **Aggregation-diffusion equation**

$\downarrow \varepsilon \rightarrow 0$

Upwind scheme $\xrightarrow{h \rightarrow 0}$

$\downarrow \varepsilon \rightarrow 0$

Aggregation equation

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0$$

$$\mathcal{J}_{K|L}^\rho = \tau_{K|L} (q_{K|L}^+ u_K^h - q_{K|L}^- u_L^h)$$

$$\partial_t \rho = \operatorname{div}(\rho \nabla(\Lambda * \rho))$$

A definition of GF solutions via energy-dissipation balance

$$\mathcal{I}(\rho, j) := \int_0^T \{ \mathcal{R}(\rho_t, j_t) + \mathcal{R}^*(\rho_t, -\nabla \mathcal{E}'(\rho_t)) \} dt + \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0).$$

Definition

A measure-flux pair (ρ, j) is called a gradient flow solution if

$$\partial_t \rho + \operatorname{div} j = 0 \quad \text{and} \quad \mathcal{I}(\rho, j) = 0.$$

A definition of GF solutions via energy-dissipation balance

$$\mathcal{I}(\rho, j) := \int_0^T \{ \mathcal{R}(\rho_t, j_t) + \mathcal{R}^*(\rho_t, -\nabla \mathcal{E}'(\rho_t)) \} dt + \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0).$$

Definition

A measure-flux pair (ρ, j) is called a gradient flow solution if

$$\partial_t \rho + \operatorname{div} j = 0 \quad \text{and} \quad \mathcal{I}(\rho, j) = 0.$$

W_2 -gradient structure:

$$\mathcal{R}(\rho, j) = \frac{1}{2} \int_{\Omega} \left| \frac{dj}{d\rho} \right|^2 d\rho$$

$$\mathcal{D}(\rho) := \mathcal{R}^*(\rho, -\nabla \mathcal{E}'(\rho)) = \frac{1}{2} \int_{\Omega} |\nabla \mathcal{E}'(\rho)|^2 d\rho$$

Gradient structure for the S-G scheme

Remember the finite-volume approximation (the discrete continuity equation):

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

Gradient structure for the S-G scheme

Remember the finite-volume approximation (the discrete continuity equation):

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

We need to choose a driving energy \mathcal{E}_h and a dissipation potential \mathcal{R}_h such that

$$\mathcal{J}_{K|L}^\rho = D_2 \mathcal{R}_h^*(\rho^h, -\bar{\nabla} \mathcal{E}'_h(\rho^h)). \quad (\text{KRh})$$

Gradient structure for the S-G scheme

Remember the finite-volume approximation (the discrete continuity equation):

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

We need to choose a driving energy \mathcal{E}_h and a dissipation potential \mathcal{R}_h such that

$$\mathcal{J}_{K|L}^\rho = D_2 \mathcal{R}_h^*(\rho^h, -\bar{\nabla} \mathcal{E}'_h(\rho^h)). \quad (\text{KRh})$$

$$\mathcal{E}_h(\rho^h) = \varepsilon \sum_{K \in \mathcal{T}^h} \log(u_K^h) \rho_K^h + \frac{1}{2} \sum_{(K,L) \in \mathcal{T}^h \times \mathcal{T}^h} \Lambda_{KL}^h \rho_K^h \rho_L^h, \quad u_K^h := \frac{\rho_K^h}{|K|}$$

Gradient structure for the S-G scheme

Remember the finite-volume approximation (the discrete continuity equation):

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0, \quad K \in \mathcal{T}^h.$$

We need to choose a driving energy \mathcal{E}_h and a dissipation potential \mathcal{R}_h such that

$$\mathcal{J}_{K|L}^\rho = D_2 \mathcal{R}_h^*(\rho^h, -\bar{\nabla} \mathcal{E}_h'(\rho^h)). \quad (\text{KRh})$$

$$\mathcal{E}_h(\rho^h) = \varepsilon \sum_{K \in \mathcal{T}^h} \log(u_K^h) \rho_K^h + \frac{1}{2} \sum_{(K,L) \in \mathcal{T}^h \times \mathcal{T}^h} \Lambda_{KL}^h \rho_K^h \rho_L^h, \quad u_K^h := \frac{\rho_K^h}{|K|}$$

$$\mathcal{R}_h^*(\rho^h, \xi^h) = 2 \sum_{(K,L) \in \Sigma^h} \tau_{K|L} \alpha_\varepsilon^* \left(u_K^h, u_L^h, \frac{\xi_{KL}^h}{2} \right)$$

The convergence result with diffusion

Let $\{(\mathcal{T}^h, \Sigma^h)\}_{h>0}$ satisfy the inner ball and orthogonality assumptions. Assume that $(\rho^h, j^h)_{h>0}$ are discrete gradient flow solutions of the Scharfetter-Gummel scheme with $\sup_{h>0} \mathcal{E}_h(\rho_0^h) < \infty$.

Then there exists a subsequence of $\{(\hat{\rho}^h, \hat{j}^h)\}_{h>0}$ and a pair (ρ, j) such that

1. (ρ, j) satisfies (CE)
 - ▶ $d\hat{\rho}_t^h / d\mathcal{L}^d \rightarrow u_t$ in $L^1(\Omega)$ for every $t \in [0, T]$;
 - ▶ $\int \hat{j}_t^h dt \rightharpoonup^* \int j_t dt$ weakly-*
2. The following estimate holds:

$$\liminf_{h \rightarrow 0} \mathcal{I}_h(\rho^h, j^h) \geq \mathcal{I}(\rho, j).$$

3. The limit pair (ρ, j) is a minimizer of the Otto energy-dissipation functional $\mathcal{I}(\rho, j)$ and, consequently, is the gradient flow solution of

$$\partial_t \rho = \operatorname{div}(\varepsilon \nabla \rho + \rho \nabla(\Lambda * \rho)).$$

Γ -convergence of the Fisher information

Recall the energy-dissipation functional:

$$\mathcal{I}(\rho, j) := \int_0^T \{ \mathcal{R}(\rho_t, j_t) + \mathcal{R}^*(\rho_t, -\nabla \mathcal{E}'(\rho_t)) \} dt + \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0).$$

The Fisher information is defined as

$$\mathcal{D}(\rho) := \mathcal{R}^*(\rho, -\nabla \mathcal{E}'(\rho))$$

$$\mathcal{D}_\epsilon(\rho) = 2\epsilon^2 \int |\nabla \sqrt{u}|^2 dx + \epsilon \int \nabla u \cdot \nabla (\Lambda * \rho) dx + \frac{1}{2} \int |\nabla (\Lambda * \rho)|^2 d\rho$$

Γ -convergence of the Fisher information

Recall the energy-dissipation functional:

$$\mathcal{I}(\rho, j) := \int_0^T \{ \mathcal{R}(\rho_t, j_t) + \mathcal{R}^*(\rho_t, -\nabla \mathcal{E}'(\rho_t)) \} dt + \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0).$$

The Fisher information is defined as

$$\mathcal{D}(\rho) := \mathcal{R}^*(\rho, -\nabla \mathcal{E}'(\rho))$$

$$\mathcal{D}_\epsilon(\rho) = 2\epsilon^2 \int |\nabla \sqrt{u}|^2 dx + \epsilon \int \nabla u \cdot \nabla (\Lambda * \rho) dx + \frac{1}{2} \int |\nabla (\Lambda * \rho)|^2 d\rho$$

The discrete Fisher information:

$$\mathcal{D}_{\epsilon, h}(\rho^h) = \sum_{(K, L) \in \Sigma^h} \left[\beta_\epsilon(u_K^h, u_L^h) + \frac{\epsilon}{2} (u_L^h - u_K^h) q_{K|L}^h \tau_{K|L}^h + |q_{K|L}^h|^2 h_\epsilon(u_K^h, u_L^h, q_{K|L}^h) \right] \tau_{K|L}^h$$

$$\text{Goal: } \Gamma\text{-}\lim_{h \rightarrow 0} \mathcal{D}_{\epsilon, h} = \mathcal{D}_\epsilon$$

Γ -convergence of the Fisher information

$$\begin{aligned}\mathcal{F}_h(\varphi^h, Q_x) &= \frac{1}{2} \sum_{(K,L) \in \Sigma^h|_{Q_x}} (\varphi_L^h - \varphi_K^h)^2 \tau_{K|L}^h \\ &= \frac{1}{2} \sum_{(K,L) \in \Sigma^h|_{Q_x}} (\xi \cdot x_L - \xi \cdot x_K)^2 \tau_{K|L}^h \\ &= \frac{1}{2} \left\langle \xi, \sum_{(K,L) \in \Sigma^h|_{Q_x}} \tau_{K|L}^h (x_L - x_K) \otimes (x_L - x_K) \xi \right\rangle \\ &= \left\langle \xi, \frac{1}{|Q_x|} \int_{Q_x} \mathbb{T}^h(x) dx \xi \right\rangle\end{aligned}$$

$$\mathbb{T}^h(x) := \frac{1}{2} \sum_{K \in \mathcal{T}^h} \mathbb{I}_K(x) \sum_{L \sim K} \tau_{K|L} (x_L - x_K) \otimes (x_L - x_K)$$

What about the tensor?

$$\mathbb{T}^h(x) := \frac{1}{2} \sum_{K \in \mathcal{T}^h} \mathbb{I}_K(x) \sum_{L \sim K} \tau_{K|L}(x_L - x_K) \otimes (x_L - x_K)$$

For an admissible tessellation $\mathbb{T}^h \rightharpoonup^* \mathbb{T}$ in weakly-* in $\sigma(L^\infty, L^1)$.

What about the tensor?

$$\mathbb{T}^h(x) := \frac{1}{2} \sum_{K \in \mathcal{T}^h} \mathbb{I}_K(x) \sum_{L \sim K} \tau_{K|L}(x_L - x_K) \otimes (x_L - x_K)$$

For an admissible tessellation $\mathbb{T}^h \rightharpoonup^* \mathbb{T}$ in weakly-* in $\sigma(L^\infty, L^1)$.

Proposition HST '23

Let a family of tessellations $\{(\mathcal{T}^h, \Sigma^h)\}_{h>0}$ satisfy the orthogonality assumption $x_L - x_K \perp (K|L)$, then the family of tensors $\{\mathbb{T}^h\}_{h>0}$ is such that $\mathbb{T}^h \rightharpoonup^* \text{Id}$ weakly-* in $\sigma(L^\infty, L^1)$.

Convergence and asymptotic limits

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0$$

$$\mathcal{J}_{K|L}^\rho = \varepsilon \tau_{K|L} (\beta(q_{K|L}/\varepsilon) u_K^h - \beta(-q_{K|L}/\varepsilon) u_L^h)$$

$$\partial_t \rho = \operatorname{div}(\varepsilon \nabla \rho + \rho \nabla(\Lambda * \rho))$$

Scharfetter–Gummel scheme $\xrightarrow{h \rightarrow 0}$ Aggregation-diffusion equation

$\downarrow_{\varepsilon \rightarrow 0}$

Upwind scheme $\xrightarrow{h \rightarrow 0}$

$\downarrow_{\varepsilon \rightarrow 0}$

Aggregation equation

$$\partial_t \rho_K^h + \sum_{L \sim K} \mathcal{J}_{K|L}^\rho = 0$$

$$\mathcal{J}_{K|L}^\rho = \tau_{K|L} (q_{K|L}^+ u_K^h - q_{K|L}^- u_L^h)$$

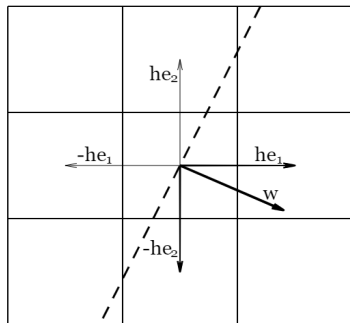
$$\partial_t \rho = \operatorname{div}(\rho \nabla(\Lambda * \rho))$$

[Lagoutière-Santambrogio-Tran Tien '23]

Tensor for the upwind scheme

$$\mathbb{T}_\varphi^h(x) := \frac{1}{2} \sum_{K \in \mathcal{T}^h} \mathbb{I}_K(x) \sum_{L \sim K} \tau_{K|L}(x_L - x_K) \otimes (x_L - x_K) v_K^\varphi$$

$$v_K^\varphi = \mathbb{I}_{\{M \in \mathcal{T}^h: \nabla \varphi(x_K) \cdot (x_M - x_K) > 0\}} + \frac{1}{2} \mathbb{I}_{\{M \in \mathcal{T}^h: \nabla \varphi(x_K) \cdot (x_M - x_K) = 0\}}$$



Upwind-to-aggregation limit

Let $\{(\mathcal{T}^h, \Sigma^h)\}_{h>0}$ be **Cartesian grids** and $\Lambda \in C^1$. Assume that $(\rho^h, j^h)_{h>0}$ are discrete gradient flow solutions of **the upwind scheme**. Then there exists a subsequence of $\{(\hat{\rho}^h, \hat{j}^h)\}_{h>0}$ and a pair (ρ, j) such that

1. (ρ, j) satisfies (CE)
 - ▶ $\hat{\rho}_t^h \rightharpoonup^* \rho_t$ **weakly-*** in $\mathcal{P}(\Omega)$ for every $t \in [0, T]$;
 - ▶ $\int \hat{j}_t^h dt \rightharpoonup^* \int j_t dt$ weakly-*
2. The following estimate holds:

$$\liminf_{h \rightarrow 0} \mathcal{I}_h(\rho^h, j^h) \geq \mathcal{I}(\rho, j).$$

3. The limit pair (ρ, j) is a minimizer of the Otto energy-dissipation functional $\mathcal{I}(\rho, j)$ and, consequently, is the gradient flow solution of

$$\partial_t \rho = \operatorname{div}(\rho \nabla(\Lambda * \rho)).$$

Outlook and open problems

1. More singular potentials.
2. Generalization for non-linear mobility or non-linear diffusion.
3. Improve the discrete-to-continuum limit from the upwind scheme to the aggregation equation.
4. Rates of convergence.

Outlook and open problems

1. More singular potentials.
2. Generalization for non-linear mobility or non-linear diffusion.
3. Improve the discrete-to-continuum limit from the upwind scheme to the aggregation equation.
4. Rates of convergence.

Thank you for your attention!

Hraivoronska, A., Schlichting, A., Tse, O. (2023). Variational convergence of the Scharfetter-Gummel scheme to the aggregation-diffusion equation and vanishing diffusion limit. arXiv preprint arXiv:2306.02226.

'Cosh' dissipation potential:

$$\mathcal{R}_h^*(\rho^h, \bar{\nabla}\varphi^h) = \sum_{(K,L) \in \Sigma^h} \Psi^*((\bar{\nabla}\varphi^h)(K,L)) \sqrt{u_K^h u_L^h} \vartheta_{KL}^h$$

with $\Psi^*(s) = 4(\cosh(s/2) - 1)$.

Discrete-to-continuum EDP convergence:

$$\partial_t \rho_K^h = \sum_{L \sim K} (\rho_K^h \kappa_{KL}^h - \rho_L^h \kappa_{LK}^h)$$

$$\partial_t \rho^h + \overline{\text{div}} j^h = 0$$

$$\mathcal{I}_h(\rho^h, j^h) = 0$$

$\xrightarrow{h \rightarrow 0}$

$$\partial_t \rho = \Delta \rho + \nabla(\rho \nabla V)$$

$$\partial_t \rho + \text{div } j = 0$$

$$\mathcal{I}(\rho, j) = 0$$

Gradient structure for the S-G scheme

Lemma [H.-Schlichting-Tse '23]

The Scharfetter-Gummel flux \mathcal{J}^ρ satisfies

$$\mathcal{J}_{K|L}^\rho = D_2 \mathcal{R}_h^*(\rho^h, -\bar{\nabla} \mathcal{E}'_h(\rho^h))$$

with the 'cosh' dual dissipation potential \mathcal{R}_h^* with the weights

$$\vartheta_{KL} = \frac{\tau_{K|L}}{\exp(-\Lambda_K^h/\varepsilon)} \frac{2 q_{K|L}/\varepsilon}{\exp(\Lambda_L^h/\varepsilon) - \exp(\Lambda_K^h/\varepsilon)},$$

where $q_{K|L} = \sum_{M \in \mathcal{T}^h} (\Lambda_{ML}^h - \Lambda_{MK}^h) \rho_M^h$ and $\Lambda_K^h = \sum_{M \in \mathcal{T}^h} \Lambda_{MK}^h \rho_M^h$.

The de-tilting trick

ED functional

$$\mathcal{I}_h(\rho^h, j^h) = \int_0^T \{ \mathcal{R}_h(\rho_t^h, j_t^h) + \mathcal{R}_h^*(\rho_t^h, -\bar{\nabla} \mathcal{E}'_h(\rho_t^h)) \} dt + \mathcal{E}_h(\rho_T) - \mathcal{E}_h(\rho_0)$$

Along the solution:

$$\xi_{KL}^h = -\bar{\nabla} \mathcal{E}'_h(\rho^h)(K, L) = -\varepsilon \log \frac{u_L^h}{u_K^h} + q_{K|L}^h$$

$$q_{K|L}^h = \varepsilon \log \frac{u_K^h}{u_L^h} - \xi_{KL}^h = \varepsilon \left(\log \left(u_K^h e^{-\xi_{KL}^h/2\varepsilon} \right) - \log \left(u_L^h e^{\xi_{KL}^h/2\varepsilon} \right) \right)$$

New way to write the flux:

$$\mathcal{J}_{K|L}^{h,\rho} = \varepsilon \sinh \left(\frac{\xi_{KL}^h}{2\varepsilon} \right) \Lambda_H \left(u_K^h e^{-\frac{\xi_{KL}^h}{2\varepsilon}}, u_L^h e^{\frac{\xi_{KL}^h}{2\varepsilon}} \right) |K| \stackrel{!}{=} D_2 \mathcal{R}_{\varepsilon,h}^*(\rho^h, \xi^h)(K, L)$$

De-tilted structure

De-tilted dual dissipation potential

$$\mathcal{R}_h^*(\rho^h, \xi^h) = 2 \sum_{(K,L) \in \Sigma^h} \tau_{K|L} \alpha_\varepsilon^* \left(u_K^h, u_L^h, \frac{\xi_{KL}^h}{2} \right),$$

where

$$\alpha_\varepsilon^*(a, b, \xi) = \varepsilon \int_0^\xi \sinh \left(\frac{x}{\varepsilon} \right) \Lambda_H(ae^{-x/\varepsilon}, be^{x/\varepsilon}) dx$$

with the *harmonic-logarithmic mean*

$$\Lambda_H(s, t) = \frac{1}{\Lambda(1/s, 1/t)} \quad \text{with} \quad \Lambda(s, t) = \frac{s - t}{\log s - \log t}. \quad (1)$$

Discrete-to-continuous convergence

1. Compactness. There exists a subsequence such that $(\rho^h, j^h) \rightarrow (\rho, j)$ and $\partial_t \rho + \nabla \cdot j = 0$.
2. The limit ED functional:

$$\left. \begin{array}{l} \liminf \mathcal{R}_h(\rho^h, j^h) \geq \mathcal{R}(\rho, j) \\ \liminf \mathcal{D}_h(\rho^h) \geq \mathcal{D}(\rho) \\ \liminf \mathcal{E}_h(\rho^h) \geq \mathcal{E}(\rho) \end{array} \right\} \implies \liminf_{h \rightarrow 0} \mathcal{I}_h(\rho^h, j^h) \geq \mathcal{I}(\rho, j)$$

3. Prove that \mathcal{I} is proper ED functional (chain rule):

$$0 = \liminf_{h \rightarrow 0} \mathcal{I}_h(\rho^h, j^h) \geq \mathcal{I}(\rho, j) \stackrel{?}{\geq} 0.$$

4. Recover the limit equation.