Variational convergence of the Scharfetter-Gummel scheme

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joint work with **André Schlichting** and **Oliver Tse**

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Outline

Aggregation-diffusion equation and Otto gradient structure

Scharfetter-Gummel scheme and generalized gradient structure

Discrete-to-continuum convergence

Models with non-local interaction

Given $\rho_0 = \rho_{in} \in \mathcal{P}(\Omega)$,

$$\partial_t \rho = \varepsilon \Delta \rho + \mathrm{div}\big(\rho \nabla (W * \rho)\big) \qquad \text{in } (0, T) \times \Omega \qquad \text{(ADE)}$$

Mogilner-Edelstein–Keshet '98, Morale-Capasso-Oelschläger '05, Topaza-Bertozzib-Lewisc '06, Carrillo-DiFrancesco-Figalli-Laurent-Slepčev '11, Carrillo-Craig-Yao '19

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

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

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

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  with $C_r \geq C_a > 0$ and $\ell_a > \ell_r$.
- Chemotaxis: aggregation of bacteria through chemical signals. Patlak-Keller-Segel system in $\mathbb{R}^2$ with

$$W(x) = -\frac{1}{2\pi} \log |x|$$

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Aggregation-diffusion equation

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

- curve of probability measures $t \mapsto \rho_t \in \mathcal{P}(\Omega)$ with given $\rho = \rho_{in} \in \mathcal{P}(\Omega)$;
- bounded convex domain $\Omega \subset \mathbb{R}^d$;
- a diffusion coefficient $\varepsilon > 0$;
- an interaction potential $W \in \operatorname{Lip}(\mathbb{R}^d) \cap C^1(\mathbb{R}^d \setminus \{0\})$ (pointy).
- no-flux boundary condition

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

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

Otto gradient structure

$$\partial_t \rho = \operatorname{div}\big(\varepsilon \nabla \rho + \rho \nabla (W * \rho)\big) \qquad \text{in } (0,T) \times \Omega$$

has the gradient structure in $(\mathcal{P}(\Omega), W_2)$ with respect to the driving energy:

$$\mathcal{E}(\rho) = \varepsilon \int_\Omega \log \frac{\mathrm{d}\rho}{\mathrm{d}\mathcal{L}^d}\, \mathrm{d}\rho + \frac{1}{2} \iint_{\Omega \times \Omega} W(x-y)\rho(\mathrm{d}x)\rho(\mathrm{d}y)$$

Jordan-Kinderlehrer-Otto '98, Otto '01, Ambrosio-Gigli-Savaré '08

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$$\mathcal{E}'(\rho) = \varepsilon \log \frac{\mathrm{d}\rho}{\mathrm{d}\mathcal{L}^d} + (W * \rho)$$

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The aggregation-diffusion equation in the "gradient-flow" form

$$\partial_t \rho + \mathrm{div} j = 0 \tag{CE}$$

$$j = \rho \nabla \mathcal{E}'(\rho) \tag{KR}$$

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Energy-dissipation balance

Rewrite the equation as the continuity equation and the kinetic relation

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Formulate (KR) by using the dual dissipation potential

$$\mathcal{R}^*(\rho, \nabla\varphi) := \frac{1}{2}\int_\Omega |\nabla\varphi|^2 \, \mathrm{d}\rho$$

$$j = D_2 \mathcal{R}^*\big(\rho, -\nabla\mathcal{E}'(\rho)\big)$$

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A variational characterization of (KR) via Legendre-Fenchel duality:

$$\mathcal{R}(\rho, j) + \mathcal{R}^*\big(\rho, -\nabla\mathcal{E}'(\rho)\big) = \big\langle j, -\nabla\mathcal{E}'(\rho)\big\rangle$$

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Energy-dissipation principle:

$$\int_0^T \big\{\mathcal{R}(\rho_t, j_t) + \mathcal{R}^*\big(\rho_t, -\nabla\mathcal{E}'(\rho_t)\big)\big\}\, \mathrm{d}t + \mathcal{E}(\rho_T) = \mathcal{E}(\rho).$$

A definition of (continuous) gradient flow solutions

The energy-dissipation functional

$$\mathcal{I}(\rho, j) := \int_0^T \left\{\mathcal{R}(\rho_t, j_t) + \mathcal{D}(\rho_t)\right\} \mathrm{d}t + \mathcal{E}(\rho_T) - \mathcal{E}(\rho),$$

with the Fisher information

$$\begin{aligned}\mathcal{D}(\rho) &= \mathcal{R}^*(\rho, -\nabla\mathcal{E}'(\rho)) \\ &= 2\varepsilon^2 \int |\nabla\sqrt{\rho}|^2 + \varepsilon \int \nabla\rho \cdot \nabla(W * \rho) + \frac{1}{2}\int |\nabla(W * \rho)|^2 \rho.\end{aligned}$$

Note that $\mathcal{I}(\rho, j) \geq 0$ for **any** (ρ, j) satisfying (CE).

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Definition

A measure-flux pair (ρ, j) is called an Otto gradient flow solution if it satisfies the continuity equation

$$\partial_t \rho + \operatorname{div} j = 0 \qquad \text{(CE)}$$

and it is the minimizer of the *energy-dissipation functional* $\mathcal{I}(\rho, j)$.

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The Scharfetter-Gummel flux

$$\partial_t \rho + \operatorname{div} j = 0$$
$$j = \varepsilon \nabla \rho + \rho \nabla (W * \rho)$$

Finite-volume approximation (semi-discrete):

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

Scharfetter-Gummel '69, Farrell-Gartland Jr. '91, Eymard-Fuhrmann-Gärtner '06, Bessemoulin-Chatard '12, Schlichting-Seis '22

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

The idea of the Scharfetter-Gummel is **solving a cell problem.** Given $q_{K|L} \sim \nabla(W * \rho)$, find $u \in C^2([x_K, x_L])$:

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

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

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Scharfetter-Gummel flux

The solution of (Cell-Pr) is

$$\mathcal{J}^{\rho}_{K|L} = \varepsilon\tau^h_{K|L}\left(B(q_{K|L}/\varepsilon)u^h_K - B(-q_{K|L}/\varepsilon)u^h_L\right),$$

where

- u^h is the density $u^h_K := \dfrac{\rho^K}{|K|}$ for all $K \in \mathcal{T}^h$;
- the transmission coefficient $\tau^h_{K|L} := \dfrac{|(K|L)|}{|x_L - x_K|}$ for all $(K, L) \in \Sigma^h$;
- B is the Bernoulli function $B(s) = \dfrac{s}{e^s - 1}$
- $q_{K|L}$ is a discrete approximation for $\nabla(W * \rho)$:

$$q_{K|L} = \sum_{M\in\mathcal{T}^h}\big(W(x_M - x_L) - W(x_M - x_K)\big)\rho^h_M$$

Properties of the Scharfetter-Gummel flux

- If $W \equiv 0$, then

$$\mathcal{J}^{\rho}_{K|L} = \varepsilon \tau^{h}_{K|L}(u^{h}_{K} - u^{h}_{L}).$$

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$$\mathcal{J}^{\rho}_{K|L} = \varepsilon \tau^{h}_{K|L}(u^{h}_{K} - u^{h}_{L}).$$

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

$$\mathcal{J}^{\rho}_{K|L} = \tau^{h}_{K|L}\big(q^{+}_{K|L} u^{h}_{K} - q^{-}_{K|L} u^{h}_{L}\big)$$

Convergence and asymptotic limits

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

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

$$\partial_t \rho = \mathrm{div}\big(\varepsilon \nabla \rho + \rho \nabla (W * \rho)\big)$$

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

$\big\downarrow \epsilon\to 0$ $\qquad\qquad$ $\big\downarrow \epsilon\to 0$

Upwind scheme $\xrightarrow{h\to 0}$ **Aggregation equation**

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

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

$$\partial_t \rho = \mathrm{div}\big(\rho \nabla (W * \rho)\big)$$

Generalized gradient structure for the S-G scheme

$$\partial_t \rho_K^h + \sum_{L\sim K} j_{K|L}^h = 0, \qquad K \in \mathcal{T}^h \qquad \text{(CEh)}$$

$$j_{K|L}^h = D_2 R_h^*(\rho^h, -\overline{\nabla} E_h'(\rho^h)) \qquad \text{(KRh)}$$

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(KRh) is equivalent to $\mathcal{I}_h(\rho^h, j^h) = 0$ with the ED functional

$$\mathcal{I}_h(\rho^h, j^h) = \int_0^T \left\{ R_h(\rho_t^h, j_t^h) + R_h^*\big(\rho_t^h, -\overline{\nabla} E_h'(\rho_t^h)\big) \right\} \mathrm{d}t + E_h(\rho_T) - E_h(\rho)$$

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The de-tilted dual dissipation potential

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

$$\text{with} \quad \alpha_\varepsilon^*(a,b,\xi) = \varepsilon \int^\xi \sinh\left(\frac{x}{\varepsilon}\right) \Lambda_H\left(ae^{-x/\varepsilon}, be^{x/\varepsilon}\right) \mathrm{d}x$$

with the *harmonic-logarithmic mean*

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

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$$\partial_t \rho_K^h + \sum_{L\sim K} j_{K|L}^h = 0, \qquad K \in \mathcal{T}^h \tag{CEh}$$

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The driving energy:

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

The discrete Fisher information

Decomposition

$\alpha_\varepsilon^*(a, b, -\varepsilon \log \sqrt{b/a} + q/2) = \beta_\varepsilon(a, b) + \frac{\varepsilon}{2}(b - a)q + |q|^2 \chi_\varepsilon(a, b, q)$,

with $\beta_\varepsilon(a, b) := \alpha_\varepsilon^*(a, b, -\varepsilon \log \sqrt{b/a})$ leads to

$$D_h(\rho^h) = R_h^*(\rho^h, -\overline{\nabla} E_h'(\rho^h)) = D_h^0(\rho^h) + D_h^1(\rho^h) + D_h^2(\rho^h)$$

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with $\beta_\varepsilon(a, b) := \alpha^*_\varepsilon(a, b, -\varepsilon \log \sqrt{b/a})$ leads to

$$D_h(\rho^h) = R^*_h(\rho^h, -\overline{\nabla} E'_h(\rho^h)) = D^0_h(\rho^h) + D^1_h(\rho^h) + D^2_h(\rho^h)$$

$$D^0_h(\rho^h) = \sum_{(K,L)\in\Sigma^h} \beta_\varepsilon(u^h_K, u^h_L)\, \tau^h_{K|L},$$

$$\frac{\varepsilon^2}{8} \frac{(a-b)^2}{\frac{a+b}{2}} \leq \beta_\varepsilon(a, b) \leq \frac{\varepsilon^2}{2} |\sqrt{b} - \sqrt{a}|^2, \qquad a, b \geq 0$$

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$\alpha_\varepsilon^*(a,b,-\varepsilon\log\sqrt{b/a}+q/2)=\beta_\varepsilon(a,b)+\frac{\varepsilon}{2}(b-a)q+|q|^2\chi_\varepsilon(a,b,q)$,

with $\beta_\varepsilon(a,b):=\alpha_\varepsilon^*(a,b,-\varepsilon\log\sqrt{b/a})$ leads to

$$D_h(\rho^h)=R_h^*(\rho^h,-\overline{\nabla}E_h'(\rho^h))=D_h^0(\rho^h)+D_h^1(\rho^h)+D_h^2(\rho^h)$$

$$D_h^0(\rho^h)=\sum_{(K,L)\in\Sigma^h}\beta_\varepsilon(u_K^h,u_L^h)\,\tau_{K|L}^h,$$

$$\frac{\varepsilon^2}{8}\frac{(a-b)^2}{\frac{a+b}{2}}\le\beta_\varepsilon(a,b)\le\frac{\varepsilon^2}{2}|\sqrt{b}-\sqrt{a}|^2,\qquad a,b\ge 0$$

$$D_h^1(\rho^h)=\frac{\varepsilon}{2}\sum_{(K,L)\in\Sigma^h}(u_L^h-u_K^h)\,q_{K|L}^h\tau_{K|L}^h,$$

$$D_h^2(\rho^h)=\frac{1}{2}\sum_{(K,L)\in\Sigma^h}|q_{K|L}^h|^2\,\chi_\varepsilon(u_K^h,u_L^h,q_{K|L}^h)\,\tau_{K|L}^h.$$

Gradient flow solutions of the Scharfetter-Gummel scheme

Energy-dissipation functional

$$\mathcal{I}_h(\rho^h, j^h) = \int_0^T \left\{ R_h(\rho^h_t, j^h_t) + D_h\big(\rho^h_t\big) \right\} \mathrm{d}t + E_h(\rho_T) - E_h(\rho).$$

Definition

A measure-flux pair (ρ^h, j^h) is called a generalized (E_h, R_h, R_h^*) gradient flow solution if it satisfies the continuity equation

$$\partial_t \rho^h + \overline{\mathrm{div}}\, j^h = 0 \qquad \text{(CEh)}$$

and it is the minimizer of the energy-dissipation functional $\mathcal{I}(\rho^h, j^h)$.

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2. The limit ED functional:

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

Sandier-Serfati('04), Mielke('16)

Discrete-to-continuous convergence

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

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

4. Recover the limit equation.

Forkert-Maas-Portinale '22, H.-Tse '23, H.-Schlichting-Tse '24

The convergence result with the fixed diffusion coefficient

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 $\sup_{h>0} E_h(\rho^h) < \infty$.

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

1. (ρ, j) satisfies (CE)
   - $\mathrm{d}\hat{\rho}^h_t / \mathrm{d}\mathcal{L}^d \to u_t$ in $L^1(\Omega)$ for every $t \in [0, T]$;
   - $\int_\cdot \hat{\jmath}^h_t \,\mathrm{d}t \rightharpoonup^* \int_\cdot j_t \,\mathrm{d}t$ weakly-$*$.
2. The following estimate holds:

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

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

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

Upwind-to-aggregation convergence

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

1. (ρ, j) satisfies (CE)
   - $\hat{\rho}^h_t \rightharpoonup^* \rho_t$ **weakly-$*$ in** $\mathcal{P}(\Omega)$ for every $t \in [0, T]$;
   - $\int_\cdot \hat{\jmath}^h_t \, \mathrm{d}t \rightharpoonup^* \int_\cdot j_t \, \mathrm{d}t$ weakly-$*$.
2. The following estimate holds:

$$\liminf_{h \to 0} \mathcal{I}_{h,\varepsilon=0}(\rho^h, j^h) \geq \mathcal{I}(\rho, j).$$

3. The limit pair (ρ, j) is a minimizer of the Otto energy-dissipation functional $\mathcal{I}_{\varepsilon=0}(\rho, j)$ and, consequently, is the gradient flow solution of

$$\partial_t \rho = \operatorname{div}\left(\rho \nabla (W * \rho)\right).$$

Continuity equation and reconstruction

Goal: Given (ρ^h, j^h) such that $\partial_t \rho^h + \overline{\text{div}} j^h = 0$ on $\mathcal{T}^h$,
find $(\hat{\rho}^h, \hat{\jmath}^h)$ satisfying $\partial_t \hat{\rho}^h + \text{div} \hat{\jmath}^h = 0$ on Ω and $(\hat{\rho}^h, \hat{\jmath}^h) \to (\rho, j)$.

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$$\hat\rho^h := \hat u^h \mathcal{L}^d, \quad \hat u^h := \sum_{K \in \mathcal{T}^h} u_K^h 1_K, \qquad \hat\jmath^h := \sum_{(K,L) \in \Sigma^h} j_{K|L}^h \sigma_{K|L}^h.$$

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Relation between gradients (a small OT trick):

$$\begin{aligned}
\overline{\nabla} \varphi^h(K, L) &= \varphi^h(L) - \varphi^h(K) \\
&= \int_{\mathbb{R}^d} \varphi(y) \frac{1_L(y)}{|L|} \, \mathrm{d}y - \int_{\mathbb{R}^d} \varphi(x) \frac{1_K(x)}{|K|} \, \mathrm{d}x \\
&= \int_{\mathbb{R}^d} (\varphi(T_{KL} x) - \varphi(x)) \frac{1_K(x)}{|K|} \, \mathrm{d}x \\
&= \int_{\mathbb{R}^d} \int^1 \nabla \varphi(x + \tau^h (T_{KL} x - x)) \cdot (T_{KL} x - x) \frac{1_K(x)}{|K|} \, \mathrm{d}\tau^h \, \mathrm{d}x \\
&= \int_{\mathbb{R}^d} \nabla \varphi(x) \cdot \sigma_{KL}(\mathrm{d}x).
\end{aligned}$$

Compactness for flux

Lemma

There exists a Borel family $(j_t)_{t\in[0,T]} \subset \mathcal{M}(\Omega;\mathbb{R}^d)$ such that (up to subsequence)

$$J^h = \int_\cdot \hat{\jmath}_t^h \,\mathrm{d}t \rightharpoonup^* \int_\cdot j_t \,\mathrm{d}t \quad \text{weakly-}* \text{ in } \mathcal{M}([0,T]\times\Omega;\mathbb{R}^d).$$

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$$R_h(\rho^h_t, j^h_t) = \sup_{\xi^h} \Big\{ \sum_{(K,L)\in\Sigma^h} \xi^h_{K|L} j^h_{K|L}(t) - R^*_h(\rho^h_t,\xi^h) \Big\}$$
$$\geq \lambda|\hat{\jmath}^h_t|(\Omega) - R^*_h\big(\rho^h_t, \lambda\,\mathrm{sign}(j^h_{K|L})|\sigma^h_{K|L}|(\Omega)\big) \geq \lambda|\hat{\jmath}^h_t|(\Omega) - R^*_h\big(\rho^h_t,\lambda h\big)$$

$$\sup_{h>0}\int_0^T \widetilde{\Psi}\left(|\hat{\jmath}^h_t|(\Omega)\right)\,\mathrm{d}t \leq \sup_{h>0}\int_0^T R_h(\rho^h_t, j^h_t)\,\mathrm{d}t \leq \sup_{h>0} E_h(\rho^h) < \infty$$

$$\sup_{h>0}|J^h|([0,T]\times\Omega) \leq 2d\Big(\sup_{h>0}\int_0^T R_h(\rho^h_t,j^h_t)\,\mathrm{d}t + CT\Big) < \infty$$

Strong L^1 compactness for densities pointwise in time

For $\hat{u}^h := \sum_{K \in \mathcal{T}^h} u_K^h 1_K$, we have

$$D\hat{u}^h = \frac{1}{2} \sum_{(K,L) \in \Sigma^h} (u_K^h - u_L^h) n_{K|L} \mathcal{H}^{d-1}|_{(K|L)}.$$

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$$\begin{aligned}
|D\hat{u}^h|(\Omega) &\leq \frac{1}{2} \sum_{(K,L) \in \Sigma^h} |u_K^h - u_L^h||(K|L)| \leq \frac{1}{2} \sum_{(K,L) \in \Sigma^h} |u_K^h - u_L^h| h \tau_{K|L}^h \\
&\leq \left(\sum_{(K,L) \in \Sigma^h} \frac{\left|u_L^h - u_K^h\right|^2}{u_L^h + u_K^h} \tau_{K|L}^h \right)^{1/2} \left(\sum_{(K,L) \in \Sigma^h} (u_K^h + u_L^h)\, h^2 \tau_{K|L}^h \right)^{1/2} \\
&\leq C \sqrt{D_h^0(\rho^h)}.
\end{aligned}$$

Strong L^1 compactness for the curve of densities

Lemma

There exists $u \in L^1((0,T); L^1(\Omega))$ and a (not relabelled) subsequence such that

$$\hat{u}_t^h \to u_t \quad \text{in } L^1(\Omega) \text{ for } t \in (0,T).$$

[Rossi-Savaré '03]: compactness in measure = tightness + weak integral equicontinuity

$$\sup_{h>0} \int_0^T \|\hat{u}_t^h\|_{BV}^2 \, \mathrm{d}t \le C\left(T + \sup_{h>0} \int_0^T D_h(\rho_t^h) \, \mathrm{d}t\right) \le C\left(T + \sup_{h>0} E_h(\rho^h)\right)$$

$$\lim_{\tau^h \to 0} \sup_{h>0} \int^{T-\tau^h} d_{BL}(\hat{\rho}_{t+\tau^h}^h, \hat{\rho}_t^h) \, \mathrm{d}t = 0$$

Compactness in $\mathcal{M}((0,T), L^1(\Omega))$ + uniform integrability = Compactness in $L^1((0,T), L^1(\Omega))$

Liminf for the dissipation potential

Goal: Prove that $\liminf_{h\to 0} R_h(\rho^h, j^h) \geq \mathcal{R}(\rho, j)$

By duality:

$$\liminf_{h\to 0} R_h(\rho^h, j^h) \geq \mathcal{R}(\rho, j) \iff \limsup_{h\to 0} R_h^*(\rho^h, \overline{\nabla}\varphi^h) \leq \mathcal{R}^*(\rho, \nabla\varphi)$$

Use $\varphi \in C^2$, $\varphi_K^h = \varphi(x_K)$, and the Taylor expansion.

Γ-convergence of the Fisher information

Theorem

The Γ-limit of D_h w.r.t. L^2-topology is

$$\mathcal{D}(\rho) = \begin{cases} 2\varepsilon^2 \int |\nabla \sqrt{u}|^2 + \varepsilon \int \nabla u \cdot \nabla (W * \rho) + \frac{1}{2} \int |\nabla (W * \rho)|^2 \, \mathrm{d}\rho \\ +\infty \qquad \text{if } \sqrt{u} \notin H^1 \end{cases}$$

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Discrete Fisher information:

$$D_h(\rho^h) = \sum_{(K,L) \in \Sigma^h} \beta_\varepsilon(u_K^h, u_L^h)\, \tau_{K|L}^h + D_h^1(\rho^h) + D_h^2(\rho^h)$$

$$\frac{\varepsilon^2}{4} \frac{(a-b)^2}{a+b} \le \beta_\varepsilon(a,b) \le \frac{\varepsilon^2}{2} |\sqrt{b} - \sqrt{a}|^2, \qquad a, b \ge 0$$

Localization technique of Γ-convergence for D_h^0. Continuous convergence for D_h^1 and D_h^2.

Localization technique

1. Define a *localized* version $D_h(\cdot, A)$ depending on the domain of integration $A \subset \Omega$.
2. Show $\mathcal{D}(\cdot, A) = \Gamma\text{-}\lim D_h(\cdot, A)$.
3. Prove that $\mathcal{D}(\sqrt{u}, A)$ has an integral representation by showing:
   3.1 growth conditions;
   3.2 inner regularity;
   3.3 subadditivity;
   3.4 locality.
4. Identify the limit:

$$D(\sqrt{u}, \Omega) = \begin{cases} \displaystyle\int_\Omega |\nabla \sqrt{u}|^2 \, \mathrm{d}\mathcal{L}^d & \text{if } \sqrt{u} \in H^1(\Omega), \\ +\infty & \text{otherwise.} \end{cases}$$

The convergence result with the fixed diffusion coefficient

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 $\sup_{h>0} E_h(\rho^h) < \infty$.

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

1. (ρ, j) satisfies (CE)
   - $\mathrm{d}\hat{\rho}^h_t / \mathrm{d}\mathcal{L}^d \to u_t$ in $L^1(\Omega)$ for every $t \in [0, T]$;
   - $\int_\cdot \hat{\jmath}^h_t \,\mathrm{d}t \rightharpoonup^* \int_\cdot j_t \,\mathrm{d}t$ weakly-$*$.
2. The following estimate holds:

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

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

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

Γ-convergence for general discrete quadratic functionals

For a discrete diffusion equation

$$D_h(\rho^h) = \sum_{(K,L)\in\Sigma^h} \left|\sqrt{u_L^h} - \sqrt{u_K^h}\right|^2 \tau_{K|L}^h$$

Using the localization technique of Γ-convergence, we prove that

$$\Gamma\text{-}\lim_{h\to 0} D_h(\rho^h) = \int |\nabla\sqrt{u}|^2 \,\mathrm{d}\mathcal{L}^d.$$

The Γ-convergence holds for more general functionals with relaxed orthogonality and more general weights θ^h

$$\tilde{D}_h(\rho^h) = \sum_{(K,L)\in\Sigma^h} \left|\sqrt{u_L^h} - \sqrt{u_K^h}\right|^2 \theta_{K|L}^h$$

$$\Gamma\text{-}\lim_{h\to 0} \tilde{D}_h(\rho^h) = \int \langle \nabla\sqrt{u}, \mathbb{T}(x)\nabla\sqrt{u}\rangle \,\mathrm{d}x$$

Consequence: The discrete diffusion equation with edge activities θ^h converges to $\partial_t\rho = \mathrm{div}\big(\mathbb{T}(\nabla\rho)\big)$

Diffusion tensor

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

- Limit diffusion tensor: $\mathbb{T}^h \rightharpoonup^* \mathbb{T}$

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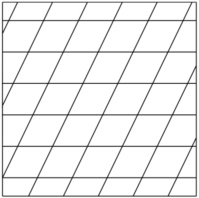
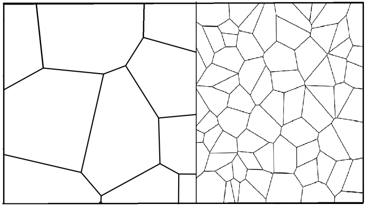
- If the tessellation satisfies the orthogonality assumption and $\theta^h_{K|L} = \tau^h_{K|L}$, then $\mathbb{T} = \mathrm{Id}$.
- Other examples:





$$\mathbb{T} = \begin{pmatrix} 1+\alpha^4 & \alpha^2(1-\alpha^2) \\ \alpha^2(1-\alpha^2) & (1-\alpha^2)^2 \end{pmatrix}$$

$$\alpha = \cos\gamma$$

$$\mathbb{T}(x) = \mathbb{T}_1 1_{\text{left part}}(x) + \mathbb{T}_2 1_{\text{right part}}(x)$$

Outlook and open problems

We obtained a discrete-to-continuum convergence result for the semi-discrete Scharfetter-Gummel scheme for the aggregation-diffusion equation.

Possible improvements:

1. Include more singular potentials.
2. Generalization for non-linear mobility or non-linear diffusion.
3. Rates of convergence.