Aggregation-Diffusion equations: stationary states, gradient flows, radial symmetry and metastability

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Interactions between PDE and Probability

Outline

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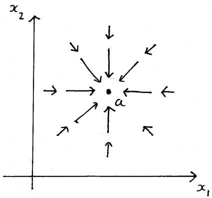
Aggregation for particles - Continuum Model

One particle attracted/repelled by a fixed location $x = a$

$$\dot{X} = -\nabla U(X - a) \qquad U(x) = U(-x), U(0) = 0\,, U \in C^1(\mathbb{R}^d/\{0\}, \mathbb{R})$$

Multiple particles attracted/repelled by one another

$$\dot{X}_i = -\sum_{j \neq i} m_j \, \nabla U(X_i - X_j)$$



$\rho(t, x)$ = density of particle at time t

$$v(x) = -\int_{\mathbb{R}^d} \nabla U(x - y) \, \rho(y) dy$$

So $\boxed{v = -\nabla U * \rho}$:

$$\begin{cases} \rho_t + \operatorname{div}(\rho v) = 0 \\ v = -\nabla U * \rho \end{cases}$$

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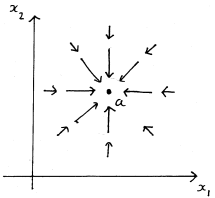

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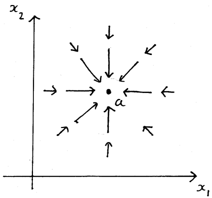

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Aggregation-Diffusion Equation

$$\begin{cases} \rho_t + \operatorname{div}(\rho v) = 0 \\ v = -\nabla U * \rho - \nabla P(\rho) \end{cases}$$

$\rho(t,x)$: density
$v(t,x)$: velocity field
$x \in \mathbb{R}^d$, $t > 0$

$U : \mathbb{R}^d \to \mathbb{R}$
"interaction potential"

$-\nabla U : \mathbb{R}^d \to \mathbb{R}^d$
"attracting/repelling field"

For which interaction repulsive/attractive potentials do we get convergence towards some nontrivial steady states?

How can we characterize these stationary states and what are their qualitative and stability properties?

If repulsion is modelled by diffusion, when does a balance between attraction and diffusion happen?

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Formal Gradient Flow

Basic Properties

1. **Conservation of the center of mass.**
2. **Liapunov Functional:** Gradient flow of

$$\mathcal{F}[\rho] = \frac{1}{2}\iint U(x-y)\,\rho(x)\,\rho(y)\,dxdy + \int_{\mathbb{R}^d} \Phi(\rho(x))\,dx$$

with respect to the Wasserstein distance W_2.
(C., McCann, Villani; RMI 2003, ARMA 2006).

The macroscopic equation can be rewritten as

$$\frac{\partial \rho}{\partial t}(t,x) = \mathrm{div}\left(\rho(t,x)\nabla\left[\frac{\delta\mathcal{F}}{\delta\rho}(t,x)\right]\right)$$

with $\frac{\delta\mathcal{F}}{\delta\rho} = U * \rho + \Phi'(\rho)$, $P'(\rho) = \rho\Phi'(\rho)$, and entropy dissipation:

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Free Energy Minimization: Stable Steady States

Minimization Problem

We want to find local minimizers of the total interaction energy

$$\mathcal{F}[\rho] := \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} U(x-y)\rho(x)\rho(y)\,dxdy + \int_{\mathbb{R}^d} \Phi(\rho(x))\,dx\,.$$

What is the right topology to talk about measures/densities being close?

When does a balance between attraction and repulsion (modelled either by nonlocality or diffusion) happen?

Recurrent Question in many fields:

- Statistical Mechanics & Crystallization: Typically very singular potentials at zero: Lennard-Jones.
- Semiconductors - Astrophysics - Chemotaxis: Macroscopic model obtained from Vlasov Equation under certain limits. Newtonian Potential.
- Economic Applications: Mean Field Games, Cournot-Nash Equilibria.
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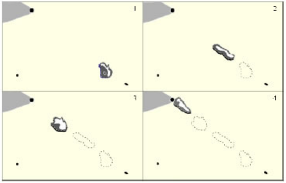
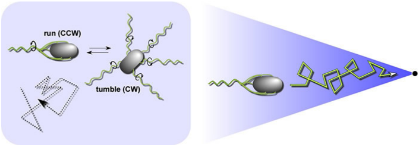
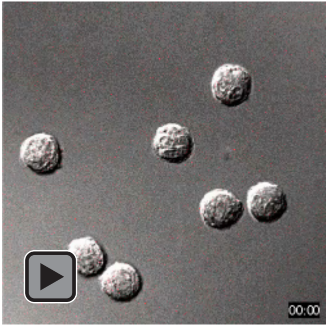
Cell/Bacteria Movement by Chemotaxis



$$\begin{cases} \dfrac{\partial n}{\partial t} = \Delta\Phi(n) - \chi\nabla\cdot(n\nabla c) & x \in \mathbb{R}^2\,,\ t > 0\,, \\ \dfrac{\partial c}{\partial t} - \Delta c = n - \alpha c & x \in \mathbb{R}^2\,,\ t > 0\,, \\ n(0,x) = n_0 \geq 0 & x \in \mathbb{R}^2\,. \end{cases}$$

Patlak (1953), Keller-Segel (1971), Nanjundiah (1973).





Movement and aggregation due to chemical signalling. Wikinut

J. Saragosti etal, PLoS Comput. Biol. 2010.

S. Volpe etal, PLoS One 2012.

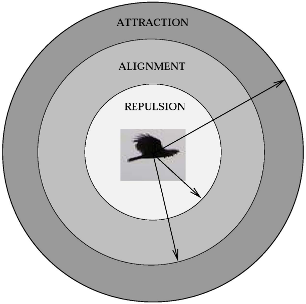
Individual Based Models (Particle models)

Swarming = Aggregation of agents of similar size and body type generally moving in a coordinated way.
Highly developed social organization: insects (locusts, ants, bees ...), fish, birds, micro-organisms,... and artificial robots for unmanned vehicle operation.

Interaction regions between individuals[a]

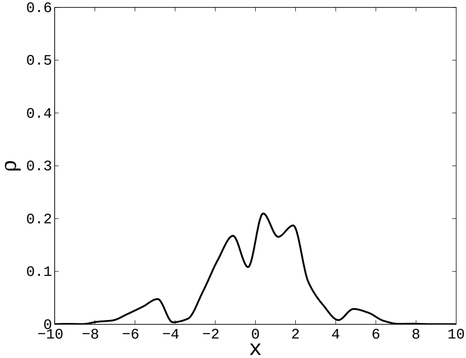
[a] Aoki, Helmerijk et al., Barbaro, Birnir et al.

- Repulsion Region: R_k.
- Attraction Region: A_k.
- Orientation Region: O_k.



Example: Aggregation with degenerate diffusion in 1D [1]

$$\rho_t = (\rho(\nu\rho^{m-1})_x)_x + (\rho(U * \rho)_x)_x \qquad \text{with } U(x) = -G(x) = -\frac{1}{2\pi}e^{-|x|^2/2}.$$



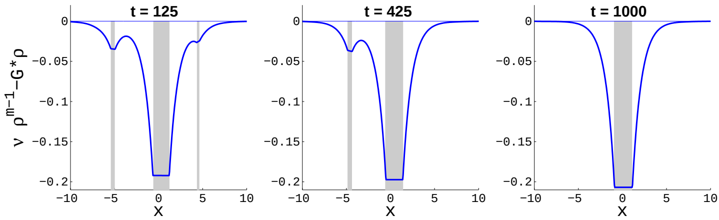
[1] J. A. Carrillo, A. Chertock, Y. Huang, CICP 2015

Example: Aggregation with degenerate diffusion in 1D

During the metastable stage, the solution to

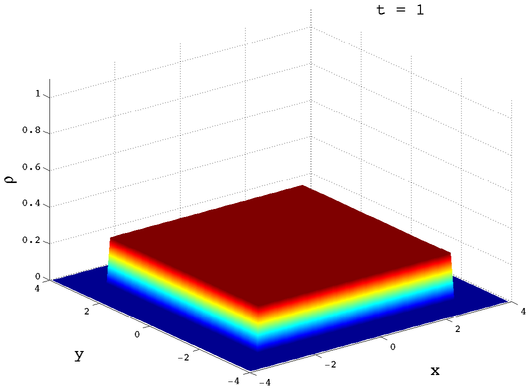
$$\rho_t = (\rho(\nu\rho^{m-1})_x)_x - (\rho(G * \rho)_x)_x$$

is almost steady on the support, or $\xi = \nu\nu\rho^{m-1} - G * \rho$ is close to a constant.



Example: Aggregation with degenerate diffusion in 2D

$$\rho_t = \nu \Delta \rho^m - \nabla \cdot (\rho \nabla G * \rho).$$



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Different Regimes

Homogeneous Aggregation-Diffusion

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\rho \nabla (\rho^{m-1} + U * \rho) \right)$$

Here, $U(\mathbf{x}) = |\mathbf{x}|^a / a$ with $-d < a$, $|\mathbf{x}|^0 / 0 = \log(x)$ by convention.

By scaling considerations, one can find 3 different regimes:

- Diffusion-dominated regime: $m > (d-a)/d$. Here, the intuition is that solutions exist globally in time and the aggregation effect only shows in the long-time behavior where we numerically observe nontrivial compactly supported stationary states (Sugiyama 2006, C.-Calvez 2006).
- Aggregation-dominated regime: $m < (d-a)/d$. Blow-up and diffusive behavior coexist for all values of the mass depending on the initial concentration (Sugiyama 2006, Chen-Liu-Wang 2014).
- Fair-Competition regime: $m = (d-a)/d$. Here the mass of the system is the critical quantity. There is a critical mass, separating the diffusive behavior from the blow-up behavior (Blanchet-C.-Laurençot).

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Diffusion-Dominated Regime in $\mathbb{R}^2$

Classical Keller-Segel with nonlinear diffusion $m > 1$

$$\frac{\partial \rho}{\partial t} = \Delta \rho^m + \frac{1}{2\pi} \nabla \cdot (\rho (\nabla \log |x| * \rho)) \quad \text{in } \mathbb{R}^2$$

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What are the long time asymptotics?

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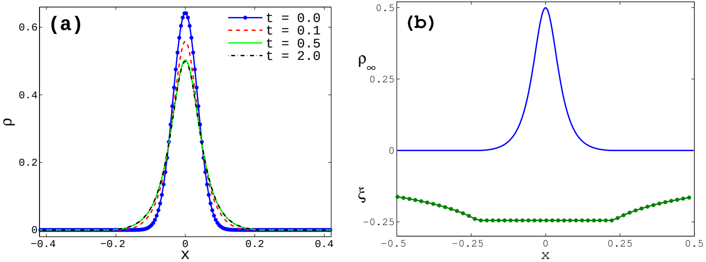

Figure: **(a)** The evolution of the solution with $m = 1.6$, $a = -0.5$ and total mass $M = 0.57$. **(b)** The steady state ρ_∞ and the corresponding $\xi = \rho_\infty^{m-1} + W * \rho_\infty$.

Outline

Minimization of the free energy functional

Free energy functional

$$\mathsf{G}[\rho] := \frac{1}{m-1}\int_{\mathbb{R}^2} \rho^m \, dx + \frac{1}{4\pi}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \log|x-y| \, \rho(x)\rho(y) \, dx \, dy \, .$$

Our goal is to minimize the functional $\mathsf{G}[\rho]$ defined on

$$\mathcal{Y}_M := \left\{ \rho \in L^1_+(\mathbb{R}^2) \cap L^m(\mathbb{R}^2) \,:\, \|\rho\|_1 = M, \int_{\mathbb{R}^2} x\rho(x)\,dx = 0 \right\}$$

Let $\rho^{\#}$ be the *spherical decreasing rearrangement of* ρ and define the class of radial densities as

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Existence & Uniqueness of radial global minimizer

[a] For any positive mass M, there exists a unique global radial minimizer $\rho_\infty \in \mathcal{Y}_M^{rad}$ of the free energy functional G in $\mathcal{Y}_M$.

[a] J. A. Carrillo, D. Castorina, B. Volzone, SIAM J. Math. Anal., 2015

Minimization of the free energy functional

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Uniqueness & Symmetry

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There is a unique radial global minimizer of the free energy functional G in $\mathcal{Y}_M$.

Idea: Mass comparison in radial coordinates.

Symmetry

Let $\rho \in \mathcal{Y}_M$ be any nonnegative compactly supported stationary state. Then ρ is radially symmetric upto translations.

Idea: non-standard Moving Plane type argument for the potential.

Open Problems at this point: Stationary Solutions & Long Time asymptotics

- We did not know how to disregard the existence of non compactly supported steady solutions. This is common to all diffusion-dominated problems.
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Outline

Conditions on Stationary Solutions and Potentials

General Aggregation-Diffusion Equation in the diffusion-dominated regime:

$$\frac{\partial \rho}{\partial t} = \Delta \rho^m + \nabla \cdot (\rho(\nabla U * \rho)) \text{ in } \mathbb{R}^d, \qquad m > 2 - \frac{2}{d}$$

Here, U satisfies the following four assumptions:

(K1) U is attracting, i.e., $U(x) \in C^1(\mathbb{R}^d \setminus \{0\})$ is radially symmetric $U(x) = \omega(r)$ and $\omega'(r) > 0$ for all $r > 0$ with $\omega(1) = 0$.

(K2) U is no more singular than the Newtonian kernel in $\mathbb{R}^d$ at the origin, i.e., there exists some $C_w > 0$ such that $\omega'(r) \leq C_w r^{1-d}$ for $r \leq 1$.

(K3) There exists some $C_w > 0$ such that $\omega'(r) \leq C_w$ for all $r > 1$.

(K4) Either $\omega(r)$ is bounded for $r \geq 1$ or there exists $C_w > 0$ such that for all $a, b \geq 0$:

$$\omega_+(a+b) \leq C_w(1 + \omega(1+a) + \omega(1+b)).$$

This includes the Newtonian potentials in any dimension.

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Symmetry result

Stationary States

Given $\rho_s \in L^1_+(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ we call it a stationary state if $\rho_s^m \in H^1_{loc}(\mathbb{R}^d)$, $\nabla\psi_s := \nabla U * \rho_s \in L^1_{loc}(\mathbb{R}^d)$, and it satisfies

$$\nabla \rho_s^m = -\rho_s \nabla \psi_s \text{ in } \mathbb{R}^d$$

in the sense of distributions in $\mathbb{R}^d$.

One can show under the assumptions on the potential U that any stationary solution ρ_s in the sense above satisfies

$$\frac{m}{m-1}\rho_s^{m-1} + U * \rho_s = C_i$$

in each connected component of $\{\rho_s > 0\}$. (C_i can differ in different components).

Radial Symmetry of Stationary States

[a] Let ρ_s be a stationary solution in the above sense. Then ρ_s must be radially decreasing up to a translation.

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Sketch of the proof

A crucial tool is again the gradient flow structure given by the free energy functional

$$\mathcal{E}[\rho] := \frac{1}{m-1} \int_{\mathbb{R}^d} \rho^m \, dx + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U(x-y)\, \rho(x)\rho(y)\, dx\, dy\,.$$

1. Assume there exists a stationary solution ρ_s that is NOT radially decreasing after any translation.
2. Then there exists a $(d-1)$-dimension hyperplane $H \subset \mathbb{R}^d$, such that H splits the mass of ρ_s into half and half, but ρ_s is not symmetric decreasing about H. WLOG set $H = \{x_1 = 0\}$.
3. We will construct a family of function ρ^ϵ that are perturbations around ρ_s, such that
$$\mathcal{E}[\rho^\epsilon] - \mathcal{E}[\rho_s] < -c\epsilon \quad \text{for all sufficiently small } \epsilon > 0,$$
where $c > 0$ depending on ρ_s and $\mathcal{K}$.
4. ρ^ϵ is constructed as the continuous Steiner symmetrization of ρ_s about H.

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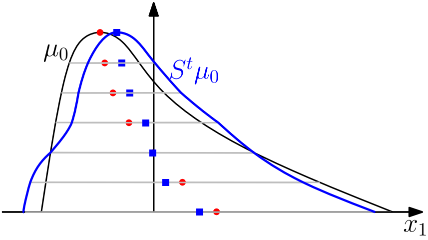
Properties of continuous Steiner symmetrization



ρ^ϵ satisfies the following:

- $\|\rho^\epsilon\|_m = \|\rho_s\|_m$.
- Since U is increasing in $|x|$ and ρ_s is not symmetric decreasing about H, one can show that $\int \rho^\epsilon(\rho^\epsilon * U)dx < \int \rho_s(\rho_s * U)dx$.
- It requires some messy work to prove

$$\int \rho^\epsilon(\rho^\epsilon * U)dx - \int \rho_s(\rho_s * U)dx < -c\epsilon$$

for some $c > 0$ (independent of ϵ) for all sufficiently small $\epsilon > 0$, but it can be quantitatively done.

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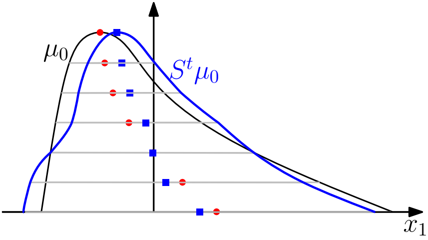

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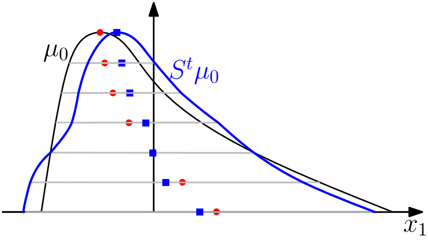

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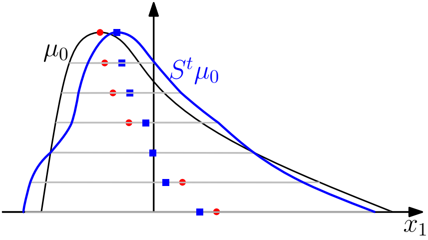

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Working towards a contradiction - Consequences

- With some extra work, one can modify ρ^ϵ into μ^ϵ, such that for all sufficiently small $\epsilon > 0$, in addition to

$$\mathcal{E}[\mu^\epsilon] - \mathcal{E}[\rho_s] < -c\epsilon \quad \text{for all sufficiently small } \epsilon > 0,$$

we also have:

$$|\mu^\epsilon(x) - \rho_s(x)| \le C\epsilon|\rho_s(x)| \quad \text{for all sufficiently small } \epsilon > 0.$$

- Combining the above pointwise estimate with the assumption that ρ_s is stationary, we have $|\mathcal{E}[\mu^\epsilon] - \mathcal{E}[\rho_s]| < C\epsilon^2$, contradicting the first inequality if $\epsilon > 0$ is sufficiently small. So there cannot be such a ρ_s!
- Uniqueness of stationary solutions upto translations and mass normalization is reduced to uniqueness of radially decreasing stationary solutions.

Characterization of Stationary States for Newtonian potential

Let ρ_s be a stationary solution in the above sense for Newtonian potentials. Then ρ_s must be radially decreasing up to a translation and given by the unique global minimizer ρ_∞ of the free energy functional upto translations (Lieb-Yau 1987, Kim-Yao 2012, C.-Castorina-Volzone 2015, C.-Sugiyama in preparation).

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Characterization of Stationary States for Newtonian potential

Let ρ_s be a stationary solution in the above sense for Newtonian potentials. Then ρ_s must be radially decreasing up to a translation and given by the unique global minimizer ρ_∞ of the free energy functional upto translations (Lieb-Yau 1987, Kim-Yao 2012, C.-Castorina-Volzone 2015, C.-Sugiyama in preparation).

Outline

Convergence for large time in 2D: Sketch of the proof

- Assume $\rho_0 \in L^1_+(\mathbb{R}^2, (1+|x|^2)dx) \cap L^\infty(\mathbb{R}^2)$.
- $\mathcal{E}[\rho(t,\cdot)] \le \mathcal{E}[\rho_0]$ implies $\iint \rho(t,x)\rho(t,y)\log|x-y|dxdy$ is uniformly bounded in time, which implies $\int \rho(t,x)\log(1+|x|)dx$ is uniformly bounded in time.
- By looking at the time evolution of the second moment $\int \rho(t,x)|x|^2dx$:

$$M_2[\rho(t,\cdot)] - M_2[\rho(0,\cdot)] = 4\int_0^t \int_{\mathbb{R}^2} \rho^m(t,x)\,dx\,dt - \frac{tM^2}{2\pi}$$

  we can show it is uniformly bounded for all time.

  This argument works for 2D only! It uses radially decreasing rearrangement comparison and the fact that the attractive contribution on the second moment only depends on the total mass in 2D.
- For any $t_n \to \infty$, the weak lower semicontinuity of the entropy dissipation, similar to Bian-Liu '13, gives that $\|\rho(t_{n_k},\cdot) - \rho_\infty\|_{L^1} \to 0$ for some $\tilde{\rho}$ along a subsequence $t_{n_k} \to \infty$, where $\tilde{\rho}$ is some stationary solution.
- Since the center of mass of $\rho(t,\cdot)$ is preserved, for any subsequence, $\tilde{\rho}$ must be the unique stationary solution with the same center of mass as ρ_0 given by ρ_∞ upto translations.

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Theorem (Large time asymptotics for the diffusion dominated Keller-Segel model in $\mathbb{R}^2$)

[a] *For any* $\rho_0 \in L^1_+(\mathbb{R}^2, (1+|x|^2)dx) \cap L^\infty(\mathbb{R}^2)$, *we have*

$$\lim_{t\to\infty} \|\rho(\cdot,t) - \rho_s\|_{L^q} = 0 \text{ for any } 1 \le q < \infty,$$

where ρ_s *is the (unique) stationary solution with the same mass and same center of mass as* ρ_0 *whose profile is given by the global minimizer of the free energy* ρ_∞.

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Conclusions

- Different regimes identified for aggregation-diffusion with homegenous pressure and kernels.
- Diffusion-Dominated regimes lead to Stationary States of each given mass.
- All stationary solutions of aggregation-diffusion problems under reasonable conditions on the potential and on the regularity are radially decreasing functions upto translations.
- Long time asymptotics is fine for the 2D classical degenerate Keller-Segel model. New confinement result.
- Long time asymptotics are still an open problem for the degenerate Keller-Segel model with $N \geq 3$ since confinement is challenging.
- References:

1. C.-Castorina-Volzone (SIMA 2015).
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