Aggregation versus Diffusion in Mathematical Biology

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Lecture 4: Kinetic Models

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Outline

1. IBM’s or Particle models

2. Kinetic Models and measure solutions
   - Ideas of the Proof

3. Qualitative Properties
   - Cucker-Smale model
   - Variations

4. Conclusions
Types of interaction

Swarming = Aggregation of agents of similar size and body type generally moving in a coordinated way.

Highly developed social organization: insects (locusts, ants, bees ...), fishes, birds, micro-organisms (myxo-bacteria, ...) and artificial robots for unmanned vehicle operation.

Interaction regions between individuals$^a$

$^a$Barbaro, Birnir et al. (2008).

- Repulsion Region: $R_k$.
- Attraction Region: $A_k$.
- Orientation Region: $O_k$. 
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Model with an asymptotic velocity

D’Orsogna, Bertozzi et al. model (PRL 2006):

\[
\begin{align*}
\frac{dx_i}{dt} &= v_i, \\
\frac{dv_i}{dt} &= (\alpha - \beta |v_i|^2)v_i - \sum_{j \neq i} \nabla U(|x_i - x_j|). 
\end{align*}
\]

Model assumptions:

- Self-propulsion and friction terms determine an asymptotic speed of \(\sqrt{\alpha/\beta}\).
- Attraction/Repulsion modeled by an effective pairwise potential \(U(x)\).

\[U(r) = -C_A e^{-r/\ell_A} + C_R e^{-r/\ell_R}.\]
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Velocity consensus model

Cucker-Smale Model (IEEE Automatic Control 2007):

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\begin{aligned}
\frac{dx_i}{dt} &= v_i, \\
\frac{dv_i}{dt} &= \sum_{j=1}^{N} a_{ij} (v_j - v_i),
\end{aligned}
\]

with the communication rate, \( \gamma \geq 0 \):

\[
a_{ij} = a(|x_i - x_j|) = \frac{1}{(1 + |x_i - x_j|^2)^\gamma}.
\]

Unconditional flocking: \( \gamma \leq 1/2 \); Ha-Tadmor, Ha-Liu, Carrillo-Fornasier-Toscani-Rosado.

Conditional flocking: \( \gamma > 1/2 \).
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Mesoscopic models

Model with asymptotic velocity + Attraction/Repulsion:

\[ \frac{\partial f}{\partial t} + v \cdot \nabla_x f + \text{div}_v [ (\alpha - \beta |v|^2) vf ] - \text{div}_v [ (\nabla_x U \ast \rho) f ] = 0. \]

Velocity consensus Model:

\[ \frac{\partial f}{\partial t} + v \cdot \nabla_x f = \nabla_v \cdot \left[ \left( \int_{\mathbb{R}^{2d}} \frac{v - w}{(1 + |x - y|^2)^{\gamma}} f(y, w, t) \, dy \, dw \right) f(x, v, t) \right] \]

:= \xi(f)(x,v,t)

Orientation, Attraction and Repulsion:

\[ \frac{\partial f}{\partial t} + v \cdot \nabla_x f - \text{div}_v [ (\nabla_x U \ast \rho) f ] = \nabla_v \cdot [ \xi'(f)(x, v, t) f(x, v, t) ] . \]
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Well-posedness in probability measures\(^1\)

Existence, uniqueness and stability

Take a potential \( U \in C^2_b(\mathbb{R}^d) \), and \( f_0 \) a measure on \( \mathbb{R}^d \times \mathbb{R}^d \) with compact support. There exists a solution \( f \in C([0, +\infty); \mathcal{P}_1(\mathbb{R}^d)) \) in the sense of solving the equation through the characteristics: \( f_t := P^t \# f_0 \) with \( P^t \) the flow map associated to the equation.

Moreover, the solutions remains compactly supported for all time with a possibly growing in time support.

Moreover, given any two solutions \( f \) and \( g \) with initial data \( f_0 \) and \( g_0 \), there is an increasing function depending on the size of the support of the solutions and the parameters, such that

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W_1(f_t, g_t) \leq \alpha(t) W_1(f_0, g_0)
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Convergence of the particle method

- **Empirical measures**: if $x_i, v_i : [0, T) \rightarrow \mathbb{R}^d$, for $i = 1, \ldots, N$, is a solution to the ODE system,

$$\begin{align*}
\frac{dx_i}{dt} &= v_i, \\
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\end{align*}$$

then the $f : [0, T) \rightarrow \mathcal{P}_1(\mathbb{R}^d)$ given by

$$f_N(t) := \sum_{i=1}^{N} m_i \delta_{(x_i(t), v_i(t))}$$

is the solution corresponding to initial atomic measures.

- Convergence of approximations of measures by particles due to the stability at any given time $T$ as an alternative derivation of the kinetic models.
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Mean-Field Limit

Convergence of approximations of measures by particles due to the stability at any given time $T$ as an alternative derivation of the kinetic models.

Just take as many particles as needed in order to have

$$W_1(f_t, f^N_t) \leq \alpha(t) \ W_1(f_0, f^N_0) \to 0 \quad \text{as } N \to \infty$$

by sampling the initial data in a suitable way.

The sequences of particle solutions becomes a Cauchy sequence with the distance $W_1$ converging to the solution of the kinetic equation.
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   - Ideas of the Proof

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Proof of the Theorem

Conditions on $E$:

1. $E$ is continuous on $[0, T] \times \mathbb{R}^d$,

2. For some $C > 0$,

   $|E(t, x)| \leq C_E(1 + |x|), \quad \text{for all } t, x \in [0, T] \times \mathbb{R}^d,$

3. $E$ is locally Lipschitz with respect to $x$, i.e., for any compact set $K \subseteq \mathbb{R}^d$ there is some $L_K > 0$ such that

   $|E(t, x) - E(t, y)| \leq L_K|x - y|, \quad t \in [0, T], \quad x, y \in K.$
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Proof of the Theorem

\[
\partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f + \text{div}_v((\alpha - \beta |v|^2)vf) = 0,
\]

which is a linear first-order equation. The associated characteristic system of ODE’s is

\[
\frac{d}{dt} X = V,
\]

\[
\frac{d}{dt} V = E(t, X) + V(\alpha - \beta |V|^2).
\]

Flow Map:

Given \((X_0, V_0) \in \mathbb{R}^d \times \mathbb{R}^d\) there exists a unique solution \((X, V)\) to the ODE system in \(C^1([0, T]; \mathbb{R}^d \times \mathbb{R}^d)\) satisfying \(X(0) = X_0\) and \(V(0) = V_0\). In addition, there exists a constant \(C\) which depends only on \(T, |X_0|, |V_0|, \alpha, \beta\) and the constant \(C_E\), such that

\[
|(X(t), V(t))| \leq |(X_0, V_0)| e^{Ct} \quad \text{for all } t \in [0, T].
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\]
We can thus consider the flow at time $t \in [0, T)$ of ODE’s equations

$$\mathcal{T}_E^t : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d.$$ 

Again by basic results in ode’s, the map $(t, x, v) \mapsto \mathcal{T}_E^t (x, v) = (X, V)$ with $(X, V)$ the solution at time $t$ to the ODE system with initial data $(x, v)$, is jointly continuous in $(t, x, v)$.

For a measure $f_0 \in \mathcal{P}_1(\mathbb{R}^d \times \mathbb{R}^d)$, the function

$$f : [0, T) \to \mathcal{P}_1(\mathbb{R}^d \times \mathbb{R}^d), \quad t \mapsto f_t := \mathcal{T}_E^t f_0$$

is the unique measure solution to the linear PDE.
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Proof of the Theorem

Estimates on characteristics:

- Taking characteristics with initial data inside a fixed ball then there exists $R > 0$ depending on $T$, in which the whole trajectories are inside a possibly larger ball of radius $R$ for all times $t \in [0, T]$.

- For some constant $C$ which depends only on $\alpha, \beta, R$ and $\text{Lip}_R(E^i)$, for all $P_0$ in $B_R$

$$\left| \mathcal{T}_{E^1}^t(P_0) - \mathcal{T}_{E^2}^t(P_0) \right| \leq \frac{e^{Ct} - 1}{C} \sup_{s \in [0,T]} \left\| E^1_s - E^2_s \right\|_{L^\infty(B_R)}.$$  

- For some constant $C$ as before

$$\left| \mathcal{T}_E^t(P_1) - \mathcal{T}_E^t(P_2) \right| \leq |P_1 - P_2| e^{C \int_0^t (\text{Lip}_R(E_s) + 1) \, ds}, \quad t \in [0, T].$$
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  $$\left| \mathcal{T}^t_{E_1}(P^0) - \mathcal{T}^t_{E_2}(P^0) \right| \leq \frac{e^{Ct} - 1}{C} \sup_{s \in [0,T)} \| E^1_s - E^2_s \|_{L^\infty(B_R)}.$$

- For some constant $C$ as before

  $$\left| \mathcal{T}^t_E(P_1) - \mathcal{T}^t_E(P_2) \right| \leq |P_1 - P_2| e^{C \int_0^t (\text{Lip}_R(E_s) + 1) \, ds}, \quad t \in [0, T].$$
Proof of the Theorem

Error on transported measures through different flows:

Let $P_1, P_2 : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be two Borel measurable functions. Also, take $f \in \mathcal{P}_1(\mathbb{R}^d)$. Then,

$$W_1(T_1\#f, T_2\#f) \leq \|T_1 - T_2\|_{L^\infty(\text{supp} f)}.$$  

Continuity in time for solutions of the linear transport:

$$W_1(T^s E\#f, T^t E\#f) \leq C|t - s|, \quad \text{for any } t, s \in [0, T].$$

Error on transported measures through different initial data:

Take a locally Lipschitz map $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $f, g \in \mathcal{P}_1(\mathbb{R}^d)$, both with compact support contained in the ball $B_R$. Then,

$$W_1(T\#f, T\#g) \leq L W_1(f, g),$$  

where $L$ is the Lipschitz constant of $T$ on the ball $B_R$. 
Proof of the Theorem

Error on transported measures through different flows:

Let $P_1, P_2 : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be two Borel measurable functions. Also, take $f \in \mathcal{P}_1(\mathbb{R}^d)$. Then,

$$W_1(\mathcal{T}_1 \# f, \mathcal{T}_2 \# f) \leq \|\mathcal{T}_1 - \mathcal{T}_2\|_{L^\infty(\text{supp} f)}.$$ 

Continuity in time for solutions of the linear transport:

$$W_1(\mathcal{T}^s_E \# f, \mathcal{T}^t_E \# f) \leq C |t - s|, \quad \text{for any } t, s \in [0, T].$$

Error on transported measures through different initial data:

Take a locally Lipschitz map $\mathcal{T} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $f, g \in \mathcal{P}_1(\mathbb{R}^d)$, both with compact support contained in the ball $B_R$. Then,

$$W_1(\mathcal{T} \# f, \mathcal{T} \# g) \leq L W_1(f, g),$$

where $L$ is the Lipschitz constant of $\mathcal{T}$ on the ball $B_R$. 
Proof of the Theorem

\[ W_1(f_t, g_t) = W_1(\mathcal{T}_f^t \# f_0, \mathcal{T}_g^t \# g_0) \]
\[ \leq W_1(P_f^t \# f_0, P_g^t \# f_0) + W_1(P_g^t \# f_0, P_g^t \# g_0) \]
\[ \leq \| P_f^t - P_g^t \|_{L^\infty(\text{supp} f_0)} + L_t W_1(f_0, g_0) \]
\[ \leq C_2 \int_0^t e^{C_2(t-s)} \| E[f_s] - E[g_s] \|_{L^\infty(B_R)} \, ds + L_t W_1(f_0, g_0) \]
\[ \leq C_3 \text{Lip}_{2R}(\nabla U) \int_0^t e^{C_4(t-s)} W_1(f_s, g_s) \, ds + e^{C_1t} W_1(f_0, g_0). \]
Proof of the Theorem

\[ W_1(f_t, g_t) = W_1(\mathcal{T}_f^t \# f_0, \mathcal{T}_g^t \# g_0) \]
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\[ \leq C_3 \text{Lip}_2 R (\nabla U) \int_0^t e^{C_4(t-s)} W_1(f_s, g_s) \, ds + e^{C_1 t} W_1(f_0, g_0). \]
Outline

1 IBM’s or Particle models

2 Kinetic Models and measure solutions
   - Ideas of the Proof

3 Qualitative Properties
   - Cucker-Smale model
   - Variations

4 Conclusions
Asymptotic Flocking

Let us consider the $N_p$-particle system:

\[
\begin{align*}
\frac{dx_i}{dt} &= v_i, \quad x_i(0) = x_i^0 \\
\frac{dv_i}{dt} &= \sum_{j=1}^{N_p} m_j a(|x_i - x_j|) (v_j - v_i), \quad v_i(0) = v_i^0,
\end{align*}
\]

Due to translation invariance, w.l.o.g. the mean velocity is zero and thus the center of mass is preserved along the evolution, i.e.,

\[
\sum_{i=1}^{N_p} m_i v_i(t) = 0 \quad \text{and} \quad \sum_{i=1}^{N_p} m_i x_i(t) = x_c
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for all $t \geq 0$ and $x_c \in \mathbb{R}^d$. 
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\]

for all $t \geq 0$ and $x_c \in \mathbb{R}^d$. 
Asymptotic Flocking

Find a bound independent of the number of particles for the time it takes for all the particles to travel at the mean velocity.
Unconditional Non-universal Flocking Result for Particles

The unique measure-valued solution for the CS kinetic model with $\gamma \leq 1/2$, with a finite number of particles given by

$$\tilde{\mu}(t) = \sum_{i=1}^{N_p} m_i \delta(x - x_i(t)) \delta(v - v_i(t)),$$

satisfies that

$$\lim_{t \to \infty} W_1 (\tilde{\mu}(t), \tilde{\mu}^\infty) = 0$$

with

$$\tilde{\mu}^\infty = \sum_{i=1}^{N_p} m_i \delta(x - x_i^\infty - mt) \delta(v - m)$$

with $m$ the initial mean velocity of the particles.
Asymptotic Flocking

Unconditional Non-universal Flocking Result for general measures

Given $\mu_0 \in \mathcal{M}(\mathbb{R}^{2d})$ compactly supported, then the unique measure-valued solution to the CS kinetic model with $\gamma \leq 1/2$, satisfies the following bounds on their supports:

$$\text{supp } \mu(t) \subset B(x_c(0) + mt, R^x(t)) \times B(m, R^y(t))$$

for all $t \geq 0$, with $R^x(t) \leq \bar{R}$ and $R^y(t) \leq R_0 e^{-\lambda t}$ with $\bar{R}$ depending only on the initial support radius.
Asymptotic Flocking

Let us fix any $R_0^x > 0$ and $R_0^v > 0$, such that all the initial velocities lie inside the ball $B(0, R_0^v)$ and all positions inside $B(x_c, R_0^x)$.

Let us define the function $R^v(t)$ to be

$$R^v(t) := \max \{|v_i(t)|, \ i = 1, \ldots, N_p\}.$$
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Let us define the function $R^v(t)$ to be

$$R^v(t) := \max \{|v_i(t)|, \ i = 1, \ldots, N_p\}.$$
Choosing the label $i$ to be the one achieving the maximum, we get

$$\frac{d}{dt} R^v(t)^2 = \frac{d}{dt} |v_i|^2 = -2 \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] \, a(|x_i - x_j|).$$

Because of the choice of the label $i$, we have that $(v_i - v_j) \cdot v_i \geq 0$ for all $j \neq i$ that together with $a \geq 0$ imply $R^v(t) \leq R^v_0$ for all $t \geq 0$. 

\[ (v_i - v_j) \cdot v_i \geq 0 \]
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Because of the choice of the label $i$, we have that $(v_i - v_j) \cdot v_i \geq 0$ for all $j \neq i$ that together with $a \geq 0$ imply $R^v(t) \leq R_0^v$ for all $t \geq 0$. 
Asymptotic Flocking

Coming back to the equation for the positions,

$$|x_i(t) - x_i^0| \leq R_v^0 t \quad \text{for all } t \geq 0 \text{ and all } i = 1, \ldots, N_p.$$ 

$$a(|x_i - x_j|) \geq \frac{1}{[1 + 4R_0^2(1 + t)^2]^{\gamma}} \quad \text{for all } t \geq 0 \text{ and all } i, j = 1, \ldots, N_p,$$

with $R_0 = \min(R_0^x, R_0^v)$.

Coming back to the equation for the maximal velocity

$$\frac{d}{dt} R_v(t)^2 = -2 \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] \ a(|x_i - x_j|)$$

$$\leq -2 \frac{2}{[1 + 4R_0^2(1 + t)^2]^{\gamma}} \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i]$$

$$= -\frac{2}{[1 + 4R_0^2(1 + t)^2]^{\gamma}} R_v(t)^2 : = -f(t) R_v(t)^2,$$
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Coming back to the equation for the positions,

$$|x_i(t) - x_i^0| \leq R_0^v t \quad \text{for all } t \geq 0 \text{ and all } i = 1, \ldots, N_p.$$ 

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$$\frac{d}{dt} R^v(t)^2 = -2 \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] \ a(|x_i - x_j|)$$

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Asymptotic Flocking

Gronwall’s lemma:

\[ R^v(t) \leq R_0^v \exp \left\{ -\frac{1}{2} \int_0^t f(s) \, ds \right\}. \]

For \( \gamma \leq 1/2 \), the function \( f(t) \) is not integrable at \( \infty \) and therefore

\[ \lim_{t \to \infty} \int_0^t f(s) \, ds = +\infty \]

and \( R^v(t) \to 0 \) as \( t \to \infty \) giving the convergence to a single point, its mean velocity, of the support for the velocity.

Again for the position variables, we get

\[
\begin{cases}
\int_0^t |v_i(s)| \, ds \leq C_1 \int_0^t (1 + s)^{-1-\epsilon} \, ds & \gamma < 1/2 \\
\int_0^t |v_i(s)| \, ds \leq C \int_0^t \frac{1}{1 + s} \, ds = C \log(1 + t) & \gamma = 1/2.
\end{cases}
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Gronwall’s lemma:

\[ R^v(t) \leq R^v_0 \exp \left\{ -\frac{1}{2} \int_0^t f(s) \, ds \right\}. \]

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\int_0^t |v_i(s)| \, ds \leq C \int_0^t \frac{1}{1 + s} \, ds = \text{Clog}(1 + t) & \text{if } \gamma = 1/2,
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\end{cases}
\]
Asymptotic Flocking

There exists $R_i^x > 0$ such that

$$|x_i(t) - x_i^0| \leq R_i^x$$

Now, $a(|x_i(t) - x_j(t)|) \geq a(2\bar{R}^x)$,

$$\frac{d}{dt} R^v(t)^2 = -2 \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] a(|x_i - x_j|)$$

$$\leq -2a(2\bar{R}^x) \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] = -2a(2\bar{R}^x)R^v(t)^2$$

from which we finally deduce the exponential decay to zero of $R^v(t)$. 
Asymptotic Flocking

There exists $R_1^x > 0$ such that

$$|x_i(t) - x_0^i| \leq R_1^x$$

Now, $a(|x_i(t) - x_j(t)|) \geq a(2\bar{R}^x)$,

$$\frac{d}{dt} R^v(t)^2 = -2 \sum_{j \neq i} m_j [(v_i - v_j) \cdot v_i] a(|x_i - x_j|)$$

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Outline

1. IBM’s or Particle models
2. Kinetic Models and measure solutions
   - Ideas of the Proof
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4. Conclusions
Cucker-Smale with local influence regions:

\[
\begin{align*}
\frac{dx_i}{dt} &= v_i, \\
\frac{dv_i}{dt} &= \sum_{j \in \Sigma_i(t)} a(|x_i - x_j|)(v_j - v_i),
\end{align*}
\]

where \( \Sigma_i(t) \subset \{1, \ldots, N\} \) is the set of dependence, given by

\[
\Sigma_i(t) := \left\{ 1 \leq \ell \leq N : \frac{(x_\ell - x_i) \cdot v_i}{|x_\ell - x_i||v_i|} \geq \alpha \right\}.
\]

Cone of Vision:
Leadership, Geometrical Constraints, and Cone of Influence

Cucker-Smale with local influence regions:

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\left\{ \begin{array}{l}
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Cone of Vision:
Roosting Forces

Adding a roosting area to the model:

\[
\begin{cases}
\frac{dx_i}{dt} = v_i, \\
\frac{dv_i}{dt} = (\alpha - \beta |v_i|^2)v_i - \sum_{j \neq i} \nabla U(|x_i - x_j|) - v_i \perp \nabla x_i \left[ \phi(x_i) \cdot v_i \perp \right].
\end{cases}
\]

with the roosting potential \( \phi \) given by \( \phi(x) := \frac{b}{4} \left( \frac{|x|}{R_{Roost}} \right)^4. \)

Roosting effect: milling flocks \( N = 400, R_{roost} = 20. \)
Adding Noise

Self-Propelling/Friction/Interaction with Noise Particle Model:

\[
\begin{align*}
\dot{x}_i &= v_i, \\
\dot{v}_i &= \left[ (\alpha - \beta |v_i|^2) v_i - \nabla x_i \sum_{j \neq i} U(|x_i - x_j|) \right] dt + \sqrt{2\sigma} d\Gamma_i(t),
\end{align*}
\]

where \( \Gamma_i(t) \) are \( N \) independent copies of standard Wiener processes with values in \( \mathbb{R}^d \) and \( \sigma > 0 \) is the noise strength. The Cucker–Smale Particle Model with Noise:

\[
\begin{align*}
\dot{x}_i &= v_i dt, \\
\dot{v}_i &= \sum_{j=1}^{N} a(|x_j - x_i|)(v_j - v_i) dt + \sqrt{2\sigma} \sum_{j=1}^{m} a(|x_j - x_i|) d\Gamma_i(t).
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Mean-field: Growing at infinity Lipschitz constants treated by moment bounds.
Adding Noise

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Mean-field: Growing at infinity Lipschitz constants treated by moment bounds.
Simple modelling of the three main mechanisms leads to complicated patterns. More information from particular species should be included to make more realistic models (Helmelrijk & collaborators, ...)

Millings can be understood as kinetic measure solutions concentrated on certain velocities. Geometric constraints: velocities on a sphere. Stability of these patterns?

Mean field limit for less singular potentials than Newtonian and less smooth than locally Lipschitz potentials allowing for more "generic" initial data.

Phase transition from ordered to disordered state driven by noise: (Liu-Frouvelle, 2011) (Barbaro-Cañizo-C.-Degond, work in preparation).

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- Simple modelling of the three main mechanisms leads to complicated patterns. More information from particular species should be included to make more realistic models (Helmelrijk & collaborators, ...)

- Millings can be understood as kinetic measure solutions concentrated on certain velocities. Geometric constraints: velocities on a sphere. Stability of these patterns?

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