Collective dynamics in life sciences

Lecture 2: the Vicsek model

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Summary

1. The Vicsek model

Individual-Based (aka particle) model

self-propelled $\Rightarrow$ all particles have same constant velocity a

align with their neighbours up to a certain noise

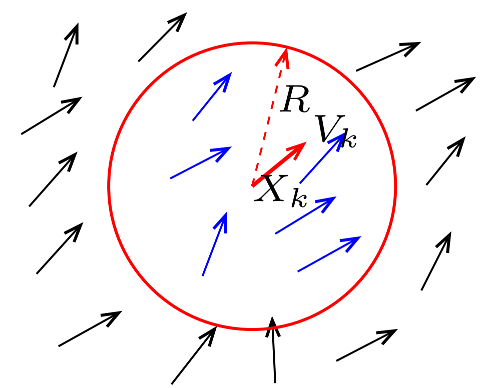
Time-discrete model

k-th particle position X_k^n, velocity direction V_k^n, at $t^n = n\Delta t$

$$X_k^{n+1} = X_k^n + aV_k^n \Delta t, \quad |V_k^n| = 1$$

$$\mathcal{J}_k^n = \sum_{j,\,|X_j^n - X_k^n| \le R} V_j^n, \quad \bar{V}_k^n = \frac{\mathcal{J}_k^n}{|\mathcal{J}_k^n|}$$

$$\arg(V_k^{n+1}) = \arg(\bar{V}_k^n + \tau_k^n)$$



τ_k^n drawn uniformly in $[-\tau, \tau]$; $R =$ interaction range

$\mathcal{J}_k^n =$ local particle flux in interaction disk

$\bar{V}_k^n =$ neighbors' average direction

2. Mean-Field model

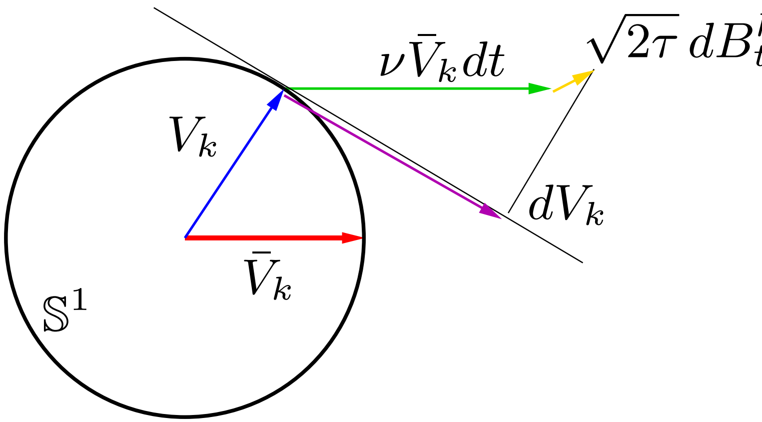
Passage to time continuous dynamics:

requires introduction of new parameter: interaction frequency ν

$$\dot{X}_k(t) = aV_k(t)$$

$$dV_k(t) = P_{V_k^\perp} \circ (\nu \bar{V}_k dt + \sqrt{2\tau}\, dB_t^k), \quad P_{V_k^\perp} = \mathrm{Id} - V_k \otimes V_k$$

$$\mathcal{J}_k = \sum_{j,\, |X_j - X_k| \leq R} V_j, \quad \bar{V}_k = \frac{\mathcal{J}_k}{|\mathcal{J}_k|}$$



Recover original Vicsek by:

Time discretization Δt s.t. $\nu \Delta t = 1$

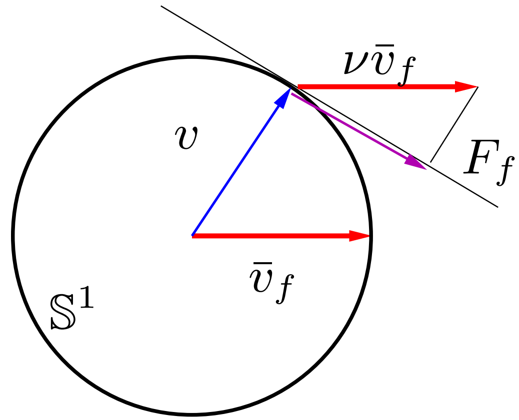
Gaussian noise $\to$ uniform

Dimension $n = 2$; here $(X_k, V_k) \in \mathbb{R}^n \times \mathbb{R}^n$, $n \geq 2$

Mean-field model

$f(x, v, t) =$ particle probability density

satisfies a Fokker-Planck equation



$$\partial_t f + a v \cdot \nabla_x f + \nabla_v \cdot (F_f f) = \tau \Delta_v f$$

$$F_f(x, v, t) = P_{v^\perp}(\nu \bar{v}_f(x, t)), \quad P_{v^\perp} = \mathrm{Id} - v \otimes v$$

$$\bar{v}_f(x, t) = \frac{\mathcal{J}_f(x, t)}{|\mathcal{J}_f(x, t)|}, \quad \mathcal{J}_f(x, t) = \int_{|y-x|<R} \int_{\mathbb{S}^{n-1}} f(y, w, t)\, w \, dw \, dy$$

$\mathcal{J}_f(x, t) =$ particle flux in a neighborhood of x

$\bar{v}_f(x, t) =$ direction of this flux

$F_f(x, v, t)) =$ projection of the flux direction on $v^\perp$

$(x, v) \in \mathbb{R}^n \times \mathbb{S}^{n-1}$; $\nabla_v \cdot$, ∇_v: div and grad on $\mathbb{S}^{n-1}$

Δ_v Laplace-Beltrami operator on the sphere

Passage to dimensionless units

Highlights important physical scales & small parameters

Choose time scale t_0, space scale $x_0 = at_0$

Set f scale $f_0 = 1/x_0^n$, F scale $F_0 = 1/t_0$

Introduce dimensionless parameters $\bar{\nu} = \nu t_0$, $\bar{\tau} = \tau t_0$, $\bar{R} = \frac{R}{x_0}$

Change variables $x = x_0 x'$, $t = t_0 t'$, $f = f_0 f'$, $F = F_0 F'$

Get the scaled Fokker-Planck system (omitting the primes):

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (F_f f) = \bar{\tau} \Delta_v f$$

$$F_f(x,v,t) = P_{v^\perp}(\bar{\nu} \bar{v}_f(x,t)), \quad P_{v^\perp} = \mathrm{Id} - v \otimes v$$

$$\bar{v}_f(x,t) = \frac{\mathcal{J}_f(x,t)}{|\mathcal{J}_f(x,t)|}, \quad \mathcal{J}_f(x,t) = \int_{|y-x|<\bar{R}} \int_{\mathbb{S}^{n-1}} f(y,w,t)\, w \, dw \, dy$$

Macroscoping scaling

Choice of t_0 such that $\bar{\tau} = \frac{1}{\varepsilon}$, $\varepsilon \ll 1$

Macroscopic scale:

there are many velocity diffusion events within one time unit

Assumption 1: $k := \frac{\bar{\nu}}{\bar{\tau}} = \mathcal{O}(1)$

Social interaction and diffusion act at the same scale

Implies $\bar{\nu}^{-1} = \mathcal{O}(\varepsilon)$, i.e. mean-free path is microscopic

Assumption 2: $\bar{R} = \varepsilon$

Interaction range is microscopic

and of the same order as mean-free path $\bar{\nu}^{-1}$

Possible variant: $\bar{R} = \mathcal{O}(\sqrt{\varepsilon})$: interaction range still small

but large compared to mean-free path. To be investigated later

With Assumption 2 ($\bar{R} = \mathcal{O}(\varepsilon)$)

Interaction is local at leading order: by Taylor expansion:

$$\mathcal{J}_f = J_f + \mathcal{O}(\varepsilon^2), \quad J_f(x,t) = \int_{\mathbb{S}^{n-1}} f(x,w,t)\, w\, dw$$

$J_f(x,t)$ = local particle flux. From now on, neglect $\mathcal{O}(\varepsilon^2)$ term

Fokker-Planck eq. in scaled variables

$$\varepsilon(\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon) + \nabla_v \cdot (F^\varepsilon f^\varepsilon) = \Delta_v f^\varepsilon$$

$$F^\varepsilon(x,v,t) = k P_{v^\perp} u_{f^\varepsilon}(x,t)$$

$$u_{f^\varepsilon}(x,t) = \frac{J_{f^\varepsilon}}{|J_{f^\varepsilon}|}, \quad J_{f^\varepsilon}(x,t) = \int_{\mathbb{S}^{n-1}} f^\varepsilon(x,w,t)\, w\, dw$$

Hydrodynamic model is obtained in the limit $\varepsilon \to 0$

3. Self-Organized Hydrodynamics (SOH)

Model can be written

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)$$

with collision operator

$$Q(f) = -\nabla_v \cdot (F_f \, f) + \Delta_v f$$

$$F_f = k P_{v^\perp} u_f$$

$$u_f = \frac{J_f}{|J_f|}, \quad J_f = \int_{\mathbb{S}^{n-1}} f(x,w,t) \, w \, dw$$

When $\varepsilon \to 0$, $f^\varepsilon \to f$ (formally) such that $Q(f) = 0$

$\Rightarrow$ importance of the solutions of $Q(f) = 0$ (equilibria)

Q acts on v-variable only ((x,t) are just parameters)

Force F_f can be written: $F_f(v) = k\,\nabla_v(u_f \cdot v)$

Note u_f independent of v ((x,t) are fixed)

Rewrite:

$$\begin{aligned} Q(f)(v) &= \nabla_v \cdot \big[- f\, k \nabla_v (u_f \cdot v) + \nabla_v f \big] \\ &= \nabla_v \cdot \big[f\, \nabla_v(-k\, u_f \cdot v + \ln f) \big] \end{aligned}$$

Let $u \in \mathbb{S}^{n-1}$ be given: Solutions of $\nabla_v(-k\, u \cdot v + \ln f) = 0$ are proportional to :

$$f(v) = M_{ku}(v) := \frac{e^{k u \cdot v}}{\int_{\mathbb{S}^{n-1}} e^{k u \cdot v} dv}$$

von Mises-Fisher (VMF) distribution

Again:

$$M_{ku}(v) := \frac{e^{ku\cdot v}}{\int_{\mathbb{S}^{n-1}} e^{ku\cdot v} dv}$$

$k > 0$: concentration parameter; $u \in \mathbb{S}^{n-1}$: orientation

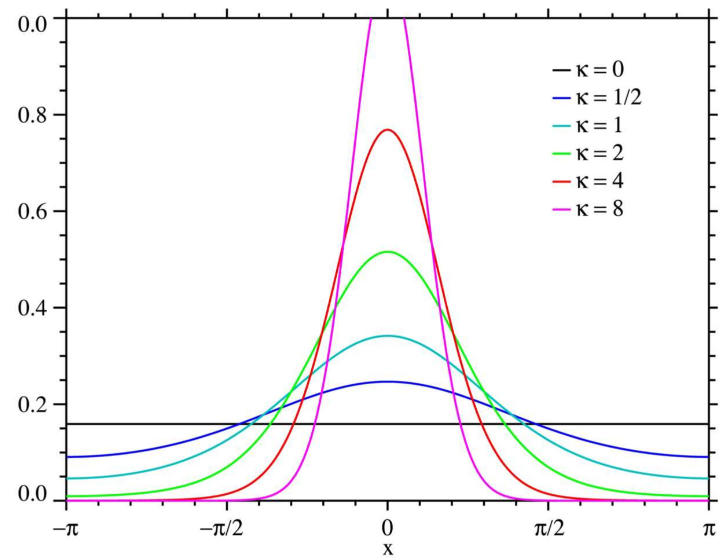
Order parameter: $c_1(k) = \int_{\mathbb{S}^{n-1}} M_{ku}(v)\ u \cdot v\, dv$

$k \overset{\nearrow}{\to} c_1(k)$, $0 \leq c_1(k) \leq 1$

Flux: $\int_{\mathbb{S}^{n-1}} M_{ku}(v)\, v\, dv = c_1(k) u$

Here:

concentration parameter k
and order parameter $c_1(k)$
are constant



Equilibria

Definition: equilibrium manifold $\mathcal{E} = \{f(v) \,|\, Q(f) = 0\}$

Theorem: $\mathcal{E} = \{ \rho M_{ku}$ for arbitrary $\rho \in \mathbb{R}_+$ and $u \in \mathbb{S}^{n-1}\}$

Note: dim mediumblue $\mathcal{E} = n$

Proof: follows from entropy inequality:

$$H(f) = \int Q(f) \frac{f}{M_{ku_f}} \, dv = - \int M_{ku_f} \Big| \nabla_v \big(\frac{f}{M_{ku_f}} \big) \Big|^2 \leq 0$$

follows from $Q(f) = \nabla_v \cdot \big[M_{ku_f} \nabla_v \big(\frac{f}{M_{ku_f}} \big) \big]$

Then, $Q(f) = 0$ implies $H(f) = 0$ and $\frac{f}{M_{ku_f}} =$ Constant

and f is of the form ρM_{ku}

Reciprocally, if $f = \rho M_{ku}$, then, $u_f = u$ and $Q(f) = 0$

Use of equilibria

$f^\varepsilon \to f$ as $\varepsilon \to 0$ with $v \to f(x,v,t) \in \mathcal{E}$ for all (x,t)

Implies that $f(x,v,t) = \rho(x,t) M_{ku(x,t)}$

Need to specify the dependence of ρ and u on (x,t)

Requires n equations since $(\rho, u) \in \mathbb{R}_+ \times \mathbb{S}^{n-1}$ are determined by n independent real quantities

f satisfies

$\partial_t f + v \cdot \nabla_x f = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} Q(f^\varepsilon)$

Problem: $\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} Q(f^\varepsilon)$ is not known

Trick:

Collision invariant

is a function $\psi(v)$ such that $\int Q(f)\psi \, dv = 0, \quad \forall f$

Form a linear vector space $\mathcal{C}$

Multiply eq. by ψ: ε^{-1} term disappears

Find a conservation law:

$$\partial_t \Big(\int_{\mathbb{S}^{n-1}} f(x,v,t)\, \psi(v)\, dv \Big) + \nabla_x \cdot \Big(\int_{\mathbb{S}^{n-1}} f(x,v,t)\, \psi(v)\, v\, dv \Big) = 0$$

Have used that ∂_t or ∇_x and $\int \ldots dv$ can be interchanged

Limit fully determined if dim $\mathcal{C}$ = dim $\mathcal{E} = n$

$\mathcal{C}$ = Span$\{1\}$. Interaction preserves mass but no other quantity

Due to self-propulsion, no momentum conservation

dim $\mathcal{C} = 1 <$ dim $\mathcal{E} = n$. Is the limit problem ill-posed ?

Use of CI: mass conservation eq.

Proof that $\psi(v) = 1$ is a CI ?

Obvious. $Q(f) = \nabla_v \cdot [\ldots]$ is a divergence

By Stokes theorem on the sphere, $\int Q(f)\, dv = 0$

Use of the CI $\psi(v) = 1$: Get the conservation law

$$\partial_t \Big(\int_{\mathbb{S}^{n-1}} f(x,v,t)\, dv \Big) + \nabla_x \cdot \Big(\int_{\mathbb{S}^{n-1}} f(x,v,t)\, v\, dv \Big) = 0$$

With $f = \rho M_{ku}$ we have

$$\int f(x,v,t)\, dv = \rho(x,t), \quad \int f(x,v,t)\, v\, dv = \rho c_1 u$$

We end up with the mass conservation eq.

$$\partial_t \rho + c_1 \nabla_x \cdot (\rho u) = 0$$

Given $u \in \mathbb{S}^{n-1}$, Define $\mathcal{Q}_u(f) = \nabla_v \cdot \left[M_{ku} \nabla_v \left(\frac{f}{M_{ku}} \right) \right]$

Note $f \to \mathcal{Q}_u(f)$ is linear and $Q(f) = \mathcal{Q}_{u_f}(f)$

A function $\psi_u(v)$ is a GCI associated to u, iff

$$\int \mathcal{Q}_u(f) \psi_u \, dv = 0, \quad \forall f \text{ such that } u_f \parallel u$$

The set of GCI $\mathcal{G}_u$ is a linear vector space

Theorem: Given $u \in \mathbb{S}^{n-1}$, $\mathcal{G}_u$ is the n-dim vector space :

$\mathcal{G}_u = \{ v \mapsto C + h(u \cdot v) \, \beta \cdot v,$ with arbitrary $C \in \mathbb{R}$ and $\beta \in \mathbb{R}^n$ with $\beta \cdot u = 0 \}$.

Introduce $\cos\theta = u \cdot v$ and $h(\cos\theta) = g(\theta) / \sin\theta$

g is the unique solution in V of problem $Lg = \sin\theta$ with

$$Lg(\theta) = - \sin^{2-n}\theta \; e^{-k \, \cos\theta} \left(\sin^{n-2}\theta \; e^{k \, \cos\theta} \; g'(\theta) \right)' + (n-2) \sin^{-2}\theta \, g(\theta)$$

$$V = \{ g \mid (n-2) (\sin\theta)^{\frac{n}{2}-2} g \in L^2(0,\pi), \; (\sin\theta)^{\frac{n}{2}-1} g \in H_0^1(0,\pi) \}$$

Use of GCI: velocity equation

Use GCI $h(u\cdot v)\beta\cdot v$ for $\beta\in\mathbb{R}^n$ with $\beta\cdot u=0$

Equivalently, use the vector valued function $\vec\psi_u(v)=h(u\cdot v)P_{u^\perp}v$

Multiply FP eq by GCI $\vec\psi_{u_{f^\varepsilon}}$: $O(\varepsilon^{-1})$ terms disappear

$$\int Q(f)\,\vec\psi_{u_f}\,dv=\int \mathcal{Q}_{u_f}(f)\vec\psi_{u_f}\,dv=0 \quad \text{by property of GCI}$$

Gives:
$$\int(\partial_t f^\varepsilon+v\cdot\nabla_x f^\varepsilon)\,\vec\psi_{u_{f^\varepsilon}}\,dv=0$$

As $\varepsilon\to 0$: $f^\varepsilon\to\rho M_{ku}$ and $\vec\psi_{u_{f^\varepsilon}}\to\vec\psi_u$ Leads to:

$$\int\big(\partial_t(\rho M_{ku})+v\cdot\nabla_x(\rho M_{ku})\big)\,\vec\psi_u\,dv=0$$

Not a conservation equation

because of dependence of $\vec\psi_u$ upon (x,t) through u

∂_t or ∇_x and $\int\ldots dv$ cannot be interchanged

Velocity equation (II)

Velocity equation takes the form:

$$\rho\big(\partial_t u + c_2 (u \cdot \nabla_x) u\big) + P_{u^\perp} \nabla_x \rho = 0$$

Computations are straightforward but tedious

Coefficient c_2 depends on GCI

$$c_2 = \frac{\int_0^\pi \cos\theta \, h(\cos\theta) \, e^{k \cos\theta} \, \sin^n \theta \, d\theta}{\int_0^\pi h(\cos\theta) \, e^{k \cos\theta} \, \sin^n \theta \, d\theta}$$

Resulting system: SOH

Self-Organized Hydrodynamics (SOH)

System for the density $\rho(x,t)$ and velocity direction $u(x,t)$:

$$\partial_t \rho + c_1 \nabla_x (\rho u) = 0$$

$$\rho \left(\partial_t u + c_2 (u \cdot \nabla_x) u \right) + P_{u^\perp} \nabla_x \rho = 0$$

$$|u| = 1$$

Rigorous limit $\varepsilon \to 0$

[N Jiang, L Xiong, T-F Zhang, arXiv:1508.04640]

4. Properties of the SOH model and extensions

Properties

$$\partial_t \rho + c_1 \nabla_x \cdot (\rho u) = 0$$

$$\rho \left(\partial_t u + c_2 (u \cdot \nabla_x) u \right) + P_{u^\perp} \nabla_x \rho = 0, \quad |u| = 1$$

Similar to Compressible Euler eqs. of gas dynamics

System of hyperbolic eqs.

But major differences:

Geometric constraint $|u| = 1$

Preserved in time if satisfied by the initial condition

thanks to the projection operator $P_{u^\perp}$

But system not in conservative form

i.e. spatial derivatives not in divergence form

$c_2 \neq c_1$: loss of Galilean invariance

Vision anisotropy (or blind zone) reinforces this effect

[Frouvelle, M3AS 2012]

Existence of solutions

Local existence of smooth solutions

[PD Liu Motsch Panferov, MAA 20 (2013) 089]

in 2D and in 3D under the condition:

$\exists$ a direction ω and $|u_0 \times \omega| \geq C > 0$ at $t = 0$

Both rely on symmetrization and energy estimates

Non-smooth solutions

Non-conservative model, no entropy

Shock relations unknown

SOH is relaxation limit $\zeta \to 0$ of:

$$\partial_t(\rho u) + c_2 \nabla_x \cdot (\rho u \otimes u) + \nabla_x \rho = -\frac{1}{\zeta} \rho (1 - |u|^2) u$$

But limit system not conservative:

Relaxation theory not applicable

Shock-wave solutions

Selection principle: physically valid solutions =

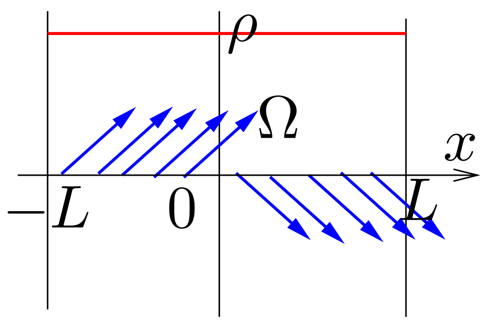
consistent approximations of the Vicsek particle system

Numerical observation [S Motsch, L Navoret, MMS 9 (2011) 1253]

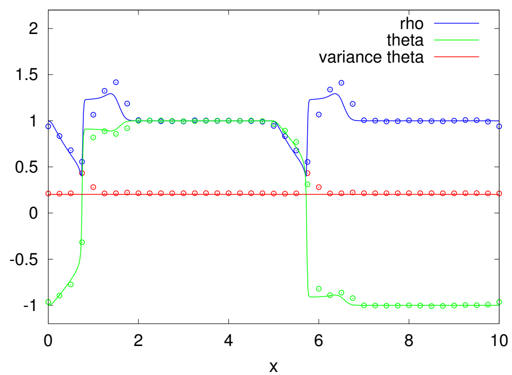
Relaxation based scheme → valid solutions

Standard shock capturing methods → not valid

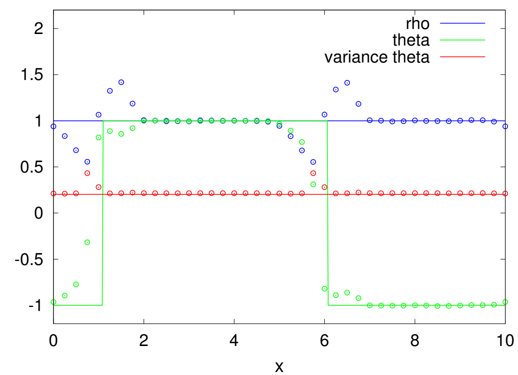
Initial conditions



Relaxation-based



Standard



Vicsek (dots), SOH (solid line), ρ (blue), θ (green), c_1 (red)

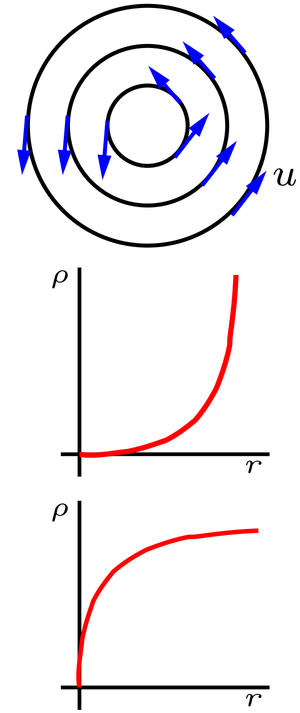
Mills: $\rho(r) = \rho_0 \, (r \, / \, r_0)^{c/d}, \quad u = x^\perp / r$

are stationary solutions. Stability ?

Shape depends on noise level

small noise: $\rho(r)$ convex: sharp edged mills

large noise: $\rho(r)$ concave: fuzzy edges



Previous models of active fluids

use average velocity (i.e. $c_1 u$)

[Toner, Tu & Ramaswamy, Annals of Physics 2005]

except e.g. [Baskaran & Marchetti, PRL 2008]

who use 'polarization vector' ρu

Ext. 1: large interaction range (i)

So far: scaling of interaction range $\bar{R}$ is such that $\bar{R} = \varepsilon$

$\bar{R}$ is microscopic and of the same order as the mean-free path $\bar{\nu}^{-1}$

Different possibility is $\bar{R} = \sqrt{\varepsilon}$

$\bar{R}$ is still microscopic

i.e. infinitesimally small at the macroscopic scale

but much larger than the mean-free path $\bar{\nu}^{-1}$

Interaction force must be Taylor expanded at the next order

$$F_f = k P_{v^\perp} \Big(u_f + \varepsilon \frac{H}{|J_f|} P_{u_f^\perp} \Delta_x J_f \Big) + \mathcal{O}(\varepsilon^2)$$

H is a constant which only depends on the dimension

Ext. 1: large interaction range (ii)

The $\mathcal{O}(\varepsilon)$ term comes into the FP eq

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + \frac{kH}{|J_{f^\varepsilon}|} \nabla_v \cdot \left(P_{v^\perp} P_{u^\perp_{f^\varepsilon}} \Delta_x J_{f^\varepsilon} \, f^\varepsilon \right) = \frac{1}{\varepsilon} Q(f^\varepsilon)$$

Its contribution in the SOH model needs to be evaluated

The resulting model is:

$$\partial_t \rho + c_1 \nabla_x \cdot (\rho u) = 0$$

$$\rho \left(\partial_t u + c_2 (u \cdot \nabla_x) u \right) + P_{u^\perp} \nabla_x \rho = c_3 P_{u^\perp} \Delta_x (\rho u), \quad |u| = 1$$

Viscous version of the SOH model

Similar to the compressible Navier-Stokes system

Scaling retains non-local effects via velocity diffusion

Local existence of smooth solutions in 2D. No result in 3D.

$c_3 = kH((n-1) + c_2) > 0$

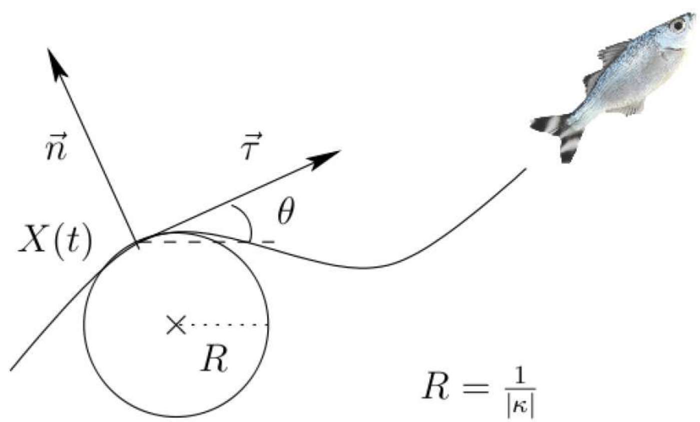
Ext 2: curvature control

Agents control curvature instead of direction

like driver with steering wheel

and try to align with neighbors

Persistent Turner [Gautrais et al, J. Math. Biol. 2009]



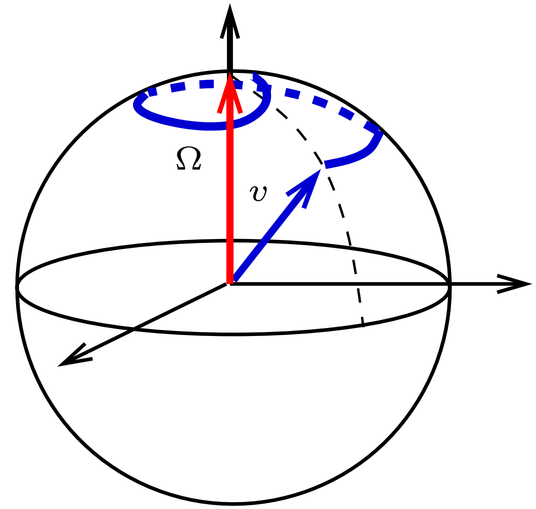
Macro model is SOH

Add precession (dimension $= 3$)

$$\varepsilon(\partial_t f + v \cdot \nabla_x f) = -\nabla_v \cdot (F_f f) + \Delta_v f$$

$$F_f = k P_{v^\perp} \bar{v}_f + \alpha \bar{v}_f \times v$$

$$\bar{v}_f = u_f + \varepsilon \frac{H}{|J_f|} P_{u_f^\perp} \Delta_x J_f, \quad u_f = \frac{J_f}{|J_f|}$$



The limit model is SOH with precession

$$\partial_t \rho + c_1 \nabla_x (\rho u) = 0$$

$$\rho\{\partial_t u + c_2 \cos\delta \, (u \cdot \nabla_x) u + c_2 \sin\delta \, u \times ((u \cdot \nabla_x) u)\} + P_{u^\perp} \nabla_x \rho +$$
$$+ kH \, \{-(2 + c_2 \cos\delta) P_{u^\perp} \Delta_x (\rho u) + (c_2 \sin\delta - \alpha) u \times \Delta_x (\rho u)\} = 0$$

δ related to precession speed α

The Landau-Lifschitz-Gilbert equation

Special case: no self-propulsion and $\rho = 1$. Gives:

$$\partial_t u + kH\big\{(2d + c_2 \cos\delta)\,(u \times (u \times \Delta_x u)) + (c_2 \sin\delta - \alpha)\,(u \times \Delta_x u)\big\} = 0$$

Landau-Lifschitz-Gilbert equation

First (to our knowledge) microscopic derivation of LLG eq.

5. Conclusion

Summary & Perspectives

Macroscopic models of collective dynamics

- require new concepts to face new challenges
- lack of conservation properties, phase transitions, . . .

The Self-Organized Hydrodynamic (SOH) model

- is the paradigmatic fluid model for collective dynamics
- Its mathematical analysis is widely open
- It has potential to model a vast category of self-organization phenomena