Mathematical models of self-organization

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Summary

1. Introduction

Emergence

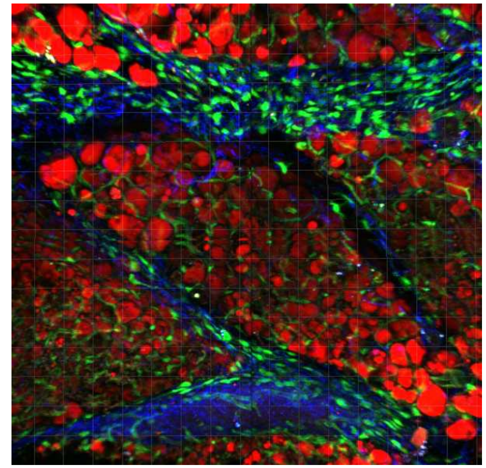
Emergence is the phenomenon by which:

interacting many-particle (or agent) systems

exhibit large-scale self-organized structures

not explicitly encoded in the agents' interaction rules

Typical emergent phenomena are



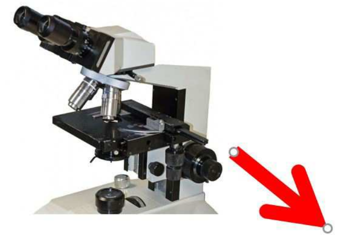
- pattern formation
  - ex: a biological tissue
- coordination
  - ex: a bird flock
- self-organization
  - ex: pedestrian lanes

Emergence is a key process

of life and social systems by which

they self-organize into functional systems

Questions



Understand link between:

individual behavior (micro model: ODE or SDE)

& large-scale structure (macro model: PDE)

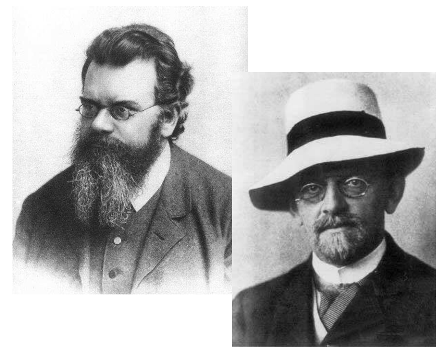
Requires rigorous passage "micro $\to$ macro"

Why macro models ?

Computational time

Analysis: stability, bifurcations, . . .

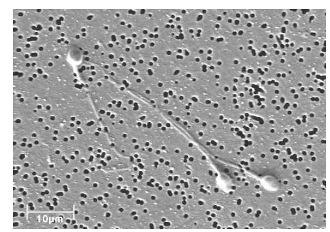
Data (images) inform on the macro scale



What is special about emergent systems ?

"micro $\to$ macro" Boltzmann, Hilbert, . . .

Lions (94), Villani (10), Hairer (14), Figalli (18) . . .



Unusual features

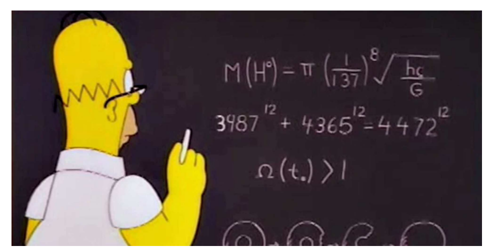
Lack of propagation of chaos

Lack of conservations: particles are "active"

Coexistence of $\neq$ phases

Complex underlying geometrical structures

$\Rightarrow$ revisit classical concepts



2. Directional coordination: the Vicsek model

Directional coordination: the Vicsek model

2.1 Presentation

Tamàs Vicsek (Budapest)

Individual-Based (i.e. particle) model

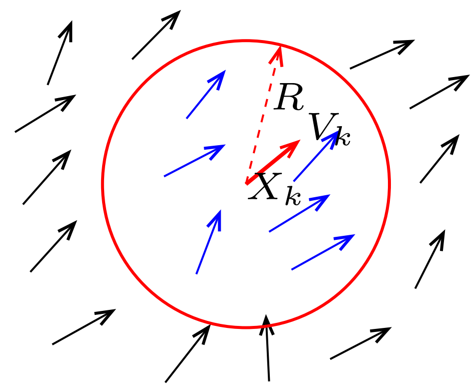
- self-propelled $\Rightarrow$ all particles have same constant speed $= 1$
- align with their neighbors up to some noise
- Particle q: position $X_q(t) \in \mathbb{R}^n$, velocity direction $V_q(t) \in \mathbb{S}^{n-1}$

$$\dot{X}_q(t) = V_q(t)$$

$$dV_q(t) = P_{V_q^\perp} \circ (k U_q dt + \sqrt{2}\, dB_t^q)$$

$$U_q = \frac{J_q}{|J_q|}, \quad J_q = \sum_{j,\, |X_j - X_q| \leq R} V_j$$

- $R =$ interaction range
- $k = k(|J_q|) =$ alignment frequency
- $J_q =$ local particle flux in interaction disk
- $U_q =$ neighbors' average direction
- $P_{V_q^\perp} = \mathrm{Id} - V_q \otimes V_q =$ orth. proj. on $V_q^\perp$
- $\circ =$ Stratonovitch: guarantees $|V_q(t)| = 1$, $\forall t$



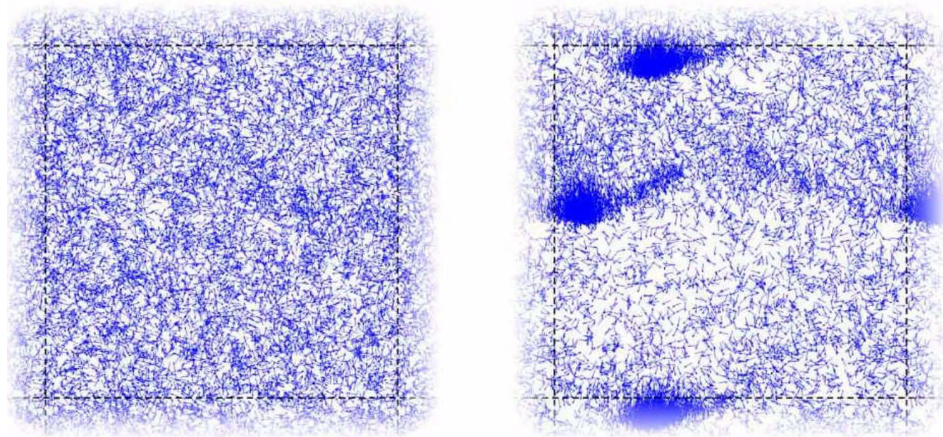
"Minimal model" for collective dynamics

Phase transition in Vicsek model

Phase transition

symmetry breaking

disordered $\to$ aligned

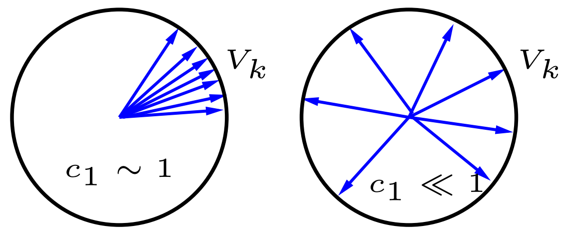


small k large k

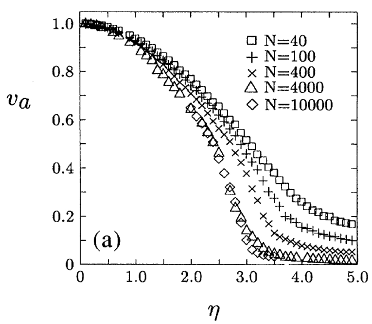
Simulations by A. Frouvelle

Order parameter measures alignment

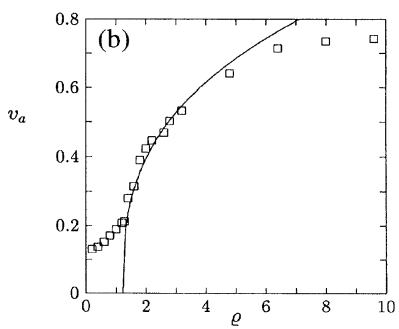
$$c_1 = \left| N^{-1} \sum_q V_q \right|, \quad 0 \le c_1 \le 1$$



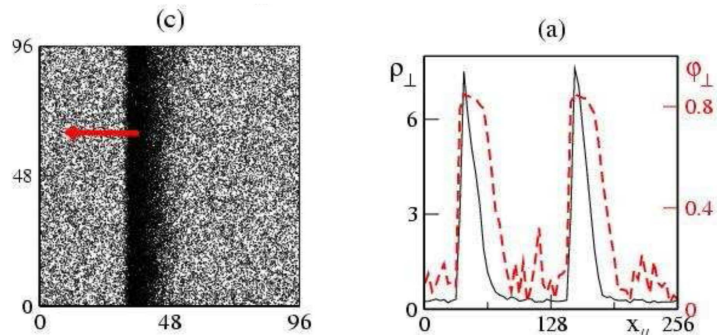
c_1 vs $1/k$



c_1 vs density



band formation



after [Chaté et al, PRE 2008]

Mean-field model

$f(x,v,t) =$ particle probability density with $(x,v) \in \mathbb{R}^n \times \mathbb{S}^{n-1}$

satisfies a Fokker-Planck equation

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

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

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

$J_f(x,t) =$ particle flux in a neighborhood of x

$u_f(x,t) =$ direction of this flux

$k u_f(x,t) =$ alignment force (with $k = k(|J_f|)$)

$F_f(x,v,t)) =$ projection of alignment force on $\{v\}^\perp$

$P_{v^\perp} = \mathrm{Id} - v \otimes v =$ projection on $\{v\}^\perp$

$\nabla_v \cdot$, ∇_v: div and grad on $\mathbb{S}^{n-1}$; $\Delta_v =$ Laplace-Beltrami on $\mathbb{S}^{n-1}$

From particle to mean-field

Requires number of particles $N \to \infty$

Define empirical measure:

$$f^N(x,v,t) = N^{-1} \sum_{q=1}^N \delta_{(X_q(t),V_q(t))}(x,v)$$

$f^N \to f$ where f satisfies Fokker-Planck

Formal derivation in [D., Motsch: M3AS 18 (2008) 1193]

Rigorous convergence proof:

Classical: particle models with smooth interaction e.g. [Spohn]

Difficulty here is handling constraint $|v| = 1$

Done for $k(|J_f|) = |J_f|$ in [Bolley Canizo Carrillo: AML 25 (2012) 339]

Open for $k(|J_f|) = 1$ (difficulty: controling singularity at $J_f = 0$)

Existence and uniqueness of solutions to Fokker-Planck

[Gamba, Kang: ARMA 222 (2016) 317]

Other collective dynamics models do not normalize velocities

e.g. Cucker-Smale, Motsch-Tadmor $\to$ huge literature

Directional coordination: the Vicsek model

2.2 Space-homogeneous case: phase transitions

[A. Frouvelle, Jian-Guo Liu, SIMA 44 (2012) 791]
[PD., A. Frouvelle, Jian-Guo Liu, JNLS 23 (2013), 427]
[PD., A. Frouvelle, Jian-Guo Liu, ARMA 216 (2015) 63-115]

Amic Frouvelle (Dauphine)

Jian-Guo Liu (Duke)

Forget the space-variable: $\nabla_x \equiv 0$: $f(v,t)$, $v \in \mathbb{S}^{n-1}$

$\partial_t f = -\nabla_v \cdot (F_f f) + \Delta_v f := Q(f) =$ collision operator

$$F_f = k(|J_f|)\, P_{v^\perp} u_f, \quad u_f = \frac{J_f}{|J_f|}, \quad J_f = \int_{\mathbb{S}^{n-1}} f(v',t)\, v'\, dv'$$

Set: $\rho(t) = \int f(v,t)\, dv$. Then $\partial_t \rho = 0$. So, $\rho(t) = \rho =$ Constant

Global existence results

for $k(|J_f|)/|J_f|$ smooth: [Frouvelle Liu: SIMA 44 (2012) 791]

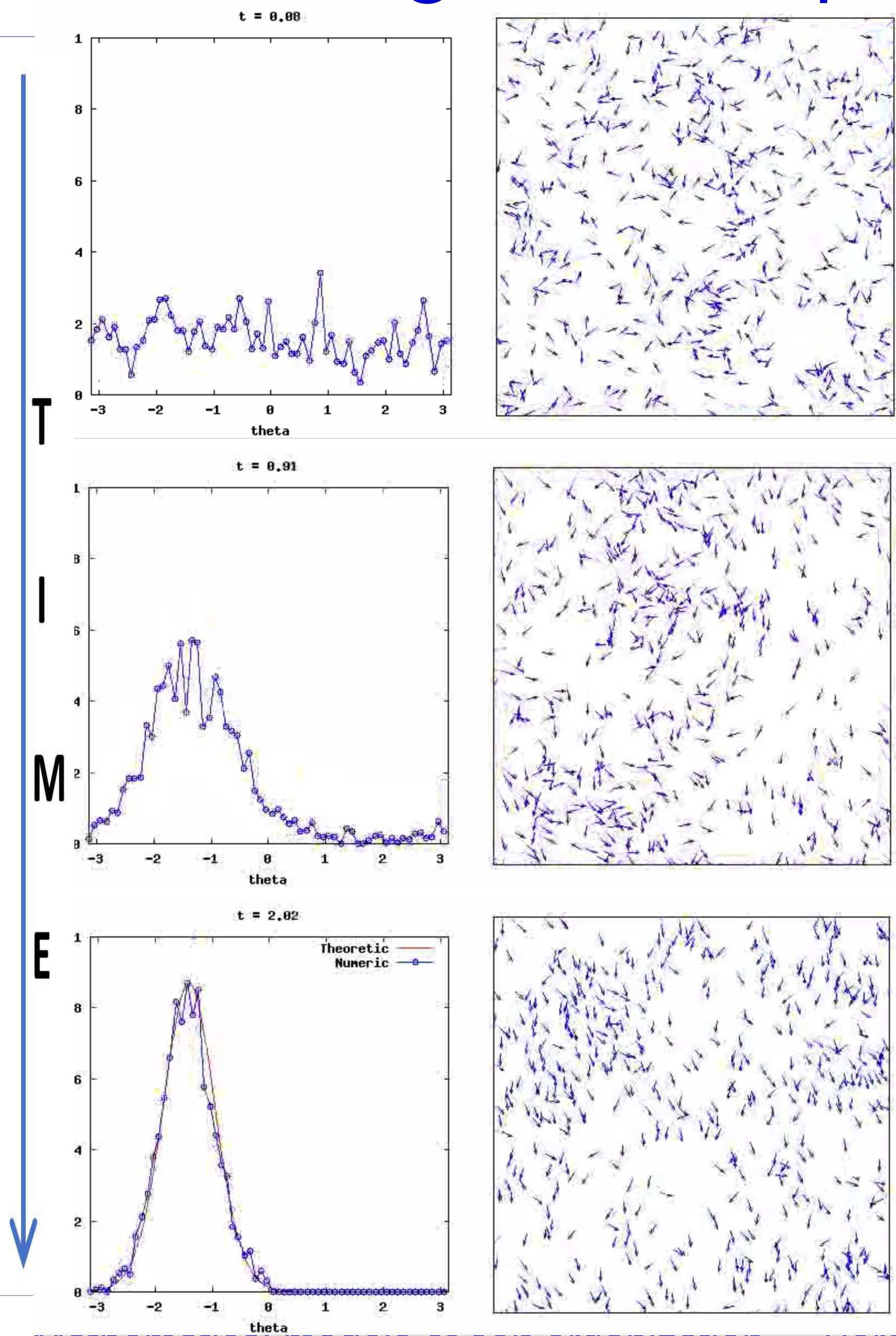
& [D. Frouvelle Liu: JNLS 23 (2013) 427 & ARMA 216 (2015) 63]

for $k(|J_f|) = 1$: [Figalli Kang Morales: ARMA 227 (2018) 869]

Equilibria: solutions of $Q(f) = 0$

Simulation of convergence to equilibrium

Histogram of velocity directions in $(-\pi, \pi)$



positions and velocity vectors of particles in periodic box

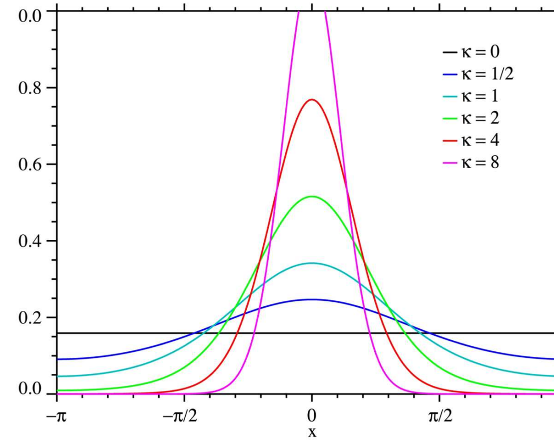
Simulation by S. Motsch

Equilibria are VMF distributions

(VMF = Von Mises-Fisher) given by

$$f(v) = \rho \, M_{\kappa u}(v), \qquad M_{\kappa u}(v) = \frac{e^{\kappa \, u \cdot v}}{\int e^{\kappa \, u \cdot v} \, dv}$$

where orientation $u \in \mathbb{S}^{n-1}$ is arbitrary
and concentration parameter $\kappa = k(|J_f|)$



Order parameter: $c_1(\kappa) = \int M_{\kappa u}(v) \, u \cdot v \, dv \in [0,1]$, $c_1(\kappa) \nearrow$

Compatibility equation: $|J_f| = \rho c_1(\kappa) = \rho c_1(k(|J_f|))$

introducing $j(\kappa) =$ inverse function of $k(|J_f|)$, can be recast in

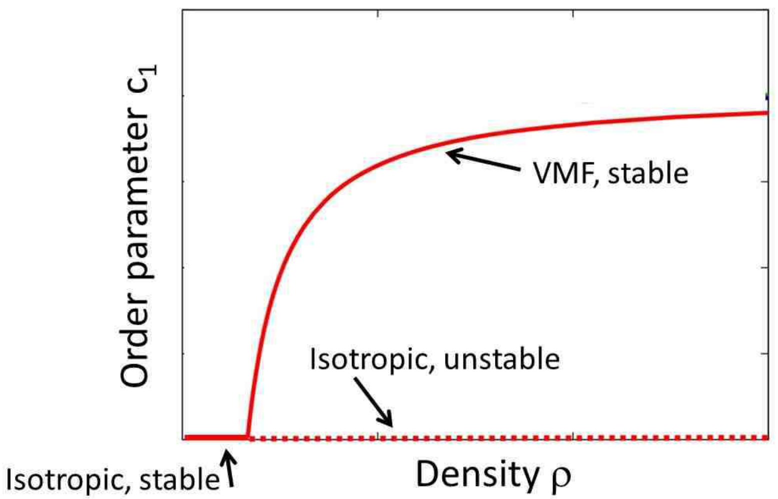
$$\kappa = 0 \quad \text{or} \quad \rho = \frac{j(\kappa)}{c_1(\kappa)}$$

Number of roots and local monotony of $\frac{j(\kappa)}{c_1(\kappa)}$ determine
number of equilibria and their stability

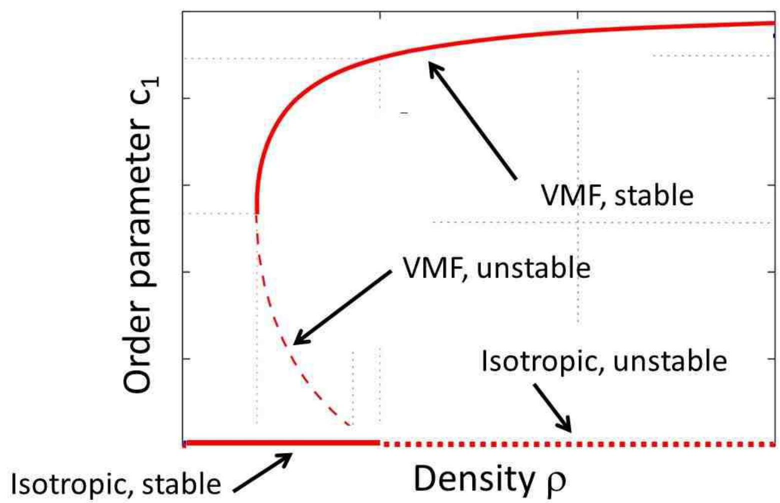
Examples

Ex. 1: $k(|J|) = \frac{|J|}{1+|J|}$: continuous phase transition

Ex. 2: $k(|J|) = |J| + |J|^2$: discontinuous phase transition



Ex. 1



Ex.2

Free energy: $\mathcal{F}(f) = \int f \, \ln f \, dv - \Phi(|J_f|)$ with $\Phi' = k$

Free energy dissipation: $\frac{d}{dt}\mathcal{F}(f) = -\mathcal{D}(f) \leq 0$

$$\mathcal{D}(f) = \tau(|J_f|) \int f \left| \nabla_v f - k(|J_f|)(v \cdot u_f) \right|^2 dv$$

f is an equilibrium iff $\mathcal{D}(f) = 0$

Free energy decays with time towards an equilibrium

Unstable VMF are local max or saddle-points of $\mathcal{F}$

Stable VMF are local min of $\mathcal{F}$

$\mathcal{F}$ estimates L^2-distance to local equilibrium:

$$\|f(t) - \rho M_{\kappa u_f(t)}\|^2_{L^2} \sim \mathcal{F}(f(t)) - \mathcal{F}(\rho M_{\kappa u_f(t)}) \searrow$$

Convergence to equilibrium with explicit rate

relies on entropy-entropy dissipation estimates: cf Villani, ...

$\mathcal{D}(f) \geq 2\lambda_\kappa(\mathcal{F}(f) - \mathcal{F}(M_{\kappa u})) +$ "small"

Directional coordination: the Vicsek model

2.3 Space-inhomogeneous case: macroscopic limit

[PD, S. Motsch: M3AS 18 Suppl. (2008) 1193]
[PD., A. Frouvelle, Jian-Guo Liu, JNLS 23 (2013), 427]
[PD., A. Frouvelle, Jian-Guo Liu, ARMA 216 (2015) 63-115]

Sebastien Motsch (Arizona State)

Space-inhomogeneous model

Restore x-dependence:

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (F_f f) = \Delta_v f, \quad F_f(x,v,t) = P_{v^\perp}(k u_f(x,t)),$$

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

Macroscopic scaling: change variables to $x' = \varepsilon x$, $t' = \varepsilon t$

(x', t') = macroscopic space and time variables

Scaled model (dropping primes): $\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)$

where $Q(f)$ collision operator studied above

limit $\varepsilon \to 0$ leads to macroscopic model

When $\varepsilon \to 0$, $f^\varepsilon \to f$ s. t. $Q(f) = 0 \Rightarrow f$ is an equilibrium

Hypothesis: k = Constant $\Rightarrow$ only equilibria are VMF ρM_{ku}

$\exists$ unique VMF equilibrium ; $\nexists$ isotropic equilibrium

No phase transition

When $\varepsilon \to 0$ $f^\varepsilon(x,v,t) \to \rho(x,t) M_{ku(x,t)}(v)$

space non-homogeneous $\Rightarrow$ $\rho(x,t)$ and $u(x,t)$ are not constant

ρ and u determined by macroscopic equations

Resulting system is Self-Organized Hydrodynamics (SOH)

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

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

$$|u| = 1$$

Classically: use collision invariants: $\psi(v) \mid \int Q(f) \psi \, dv = 0, \; \forall f$

Requires dimension { CI } $=$ number of equations

Here dimension { CI } $= 1 <$ number of equations $(= n)$

Generalized collision invariants (GCI) overcome the problem

first proposed in [PD, S. Motsch: M3AS 18 Suppl. (2008) 1193]

GCI ψ satisfies CI property with smaller class of f

Finding ψ involves inverting the "adjoint" of Q

c_2 is found as a moment of GCI ψ; $c_1 =$ order parameter

Remarks

SOH is similar to Compressible Euler eqs. of gas dynamics

- Continuity eq. for ρ
- Material derivative of u balanced by pressure force $-\nabla_x \rho$

But with major differences:

- geometric constraint $|u| = 1$ (ensured by projection operator $P_{u^\perp}$)
- $c_2 \neq c_1$: loss of Galilean invariance

Hyperbolic system

- but not in conservative form: shock solutions not well-defined

Local existence of smooth solutions in 2D and 3D

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

- Existence / uniqueness of non-smooth solutions open
- Rigorous limit $\varepsilon \to 0$ proved:

[N Jiang, L Xiong, T-F Zhang, SIMA 48 (2016) 3383]

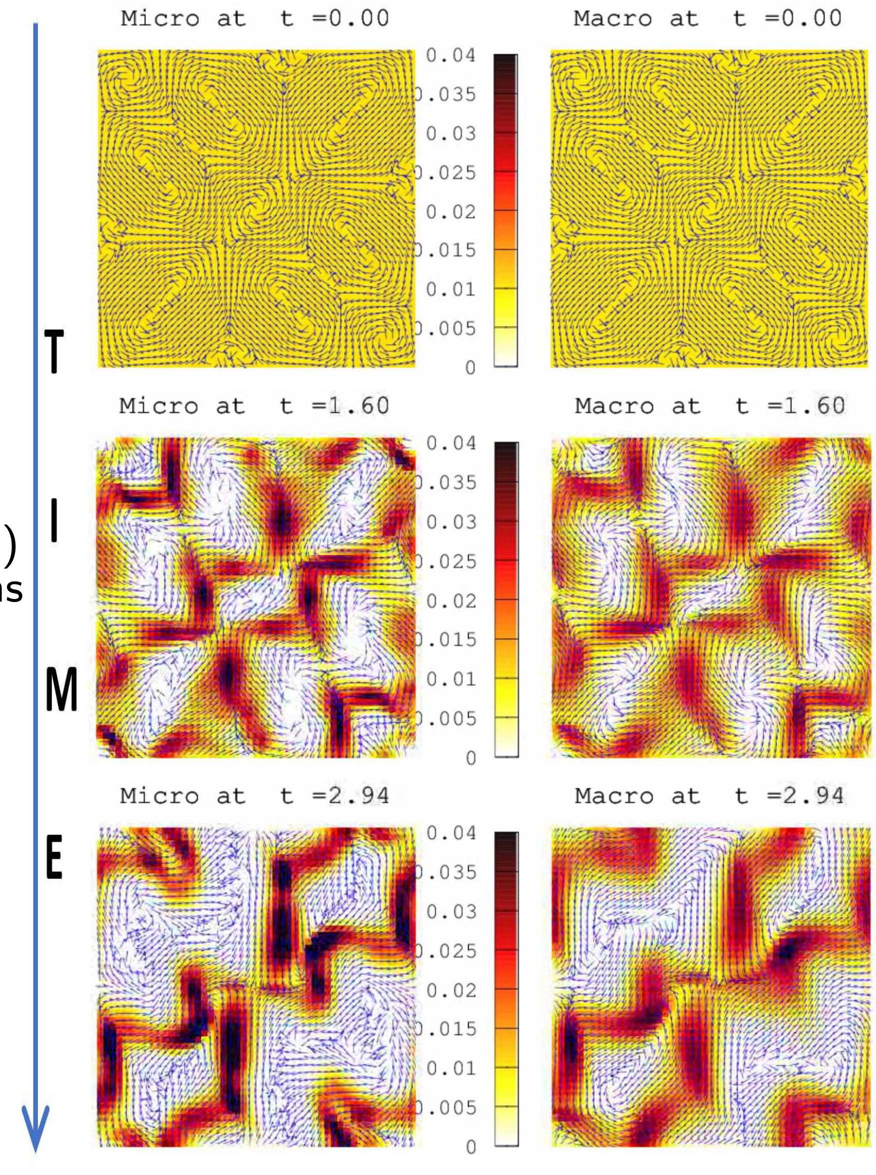
Differences (but also similarities) with the Toner-Tu model

[J Toner, Y Tu, PRL 75 (1995) 4326]

- built on symmetry considerations

Micro (Vicsek)

Density (color code)
& velocity directions



Macro (SOH)

Density (color code)
& velocity directions

Simulation by
G. Dimarco,
TBN. Mac,
N. Wang

3. Body attitude coordination

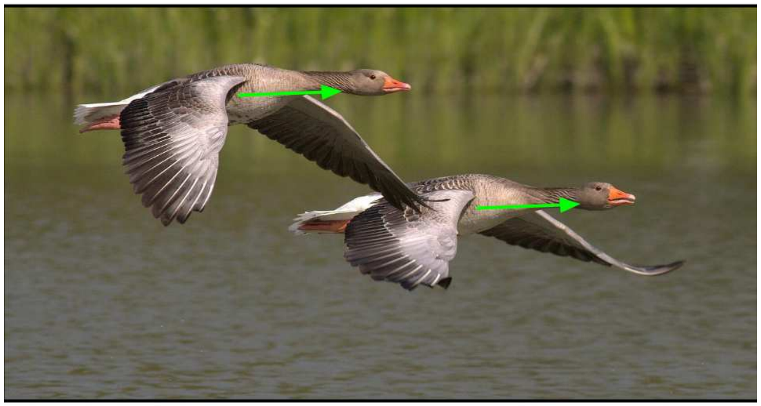
[PD, A. Frouvelle, S. Merino-Aceituno, M3AS 27 (2017) 1005]
[PD, A. Frouvelle, S. Merino-Aceituno, A. Trescases, MMS 16 (2018) 28]

Arianne Trescases (Toulouse) & Sara Merino-Aceituno (Sussex & Vienna)

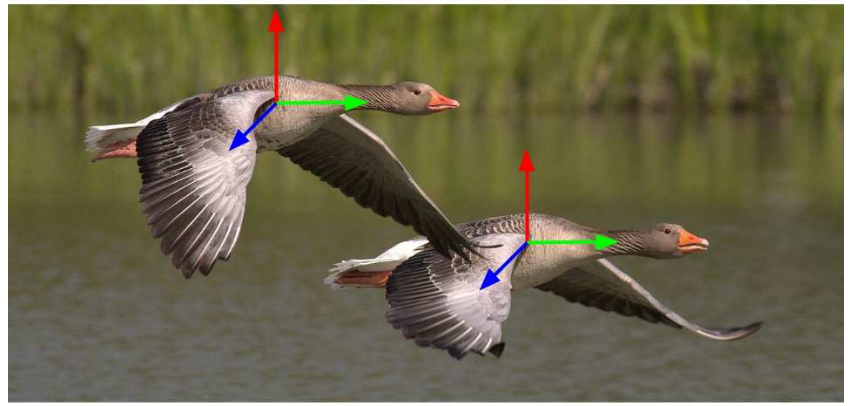
A new alignment dynamics

Self-propelled agents which align with their neighbors

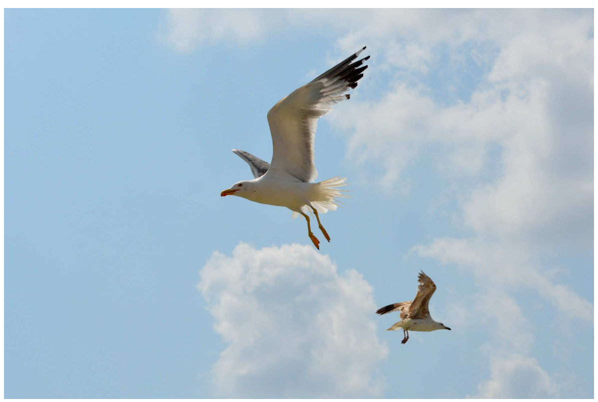
- Vicsek model: Alignment of their directions of motion
- New model: Alignment of their full body attitude

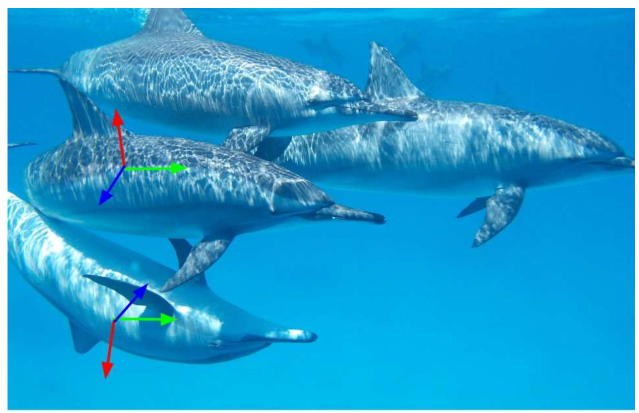


Vicsek model



Body attitude alignment

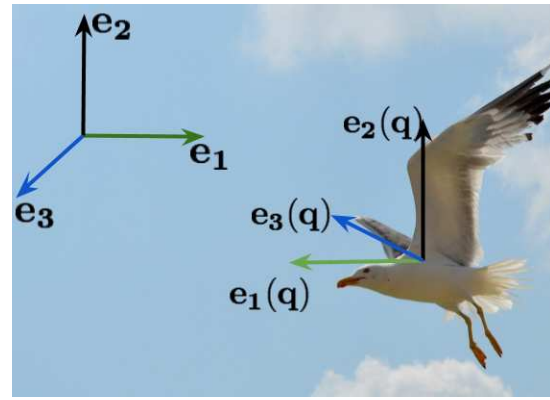




$X_q(t) \in \mathbb{R}^n$: position of the q-th subject at time t. $\quad q \in \{1, \ldots, N\}$

$A_q(t) \in \mathsf{SO}(n)$: rotation mapping reference frame $(e_1, \ldots, e_n)$ to subject's body frame

$A_q(t)e_1 \in \mathbb{S}^{n-1}$: propulsion direction



$$\dot{X}_q(t) = A_q(t)e_1$$

$$dA_q(t) = P_{T_{A_q(t)}\mathsf{SO}(n)} \circ (k\bar{A}_q dt + \sqrt{2}\, dB_t^q),$$

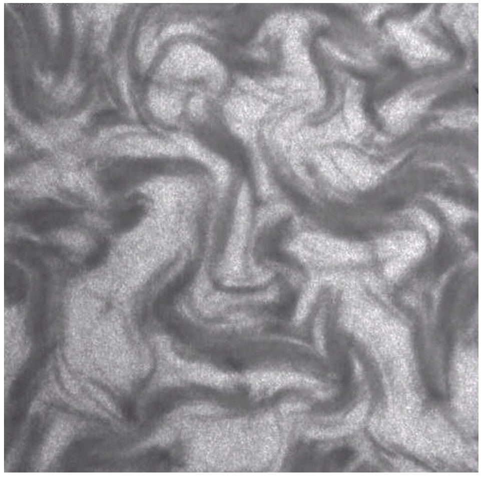
$$\bar{A}_q = \mathsf{PD}(M_q(t)), \quad M_q(t) = \sum_{j,\, |X_j - X_q| \leq R} A_j(t)$$

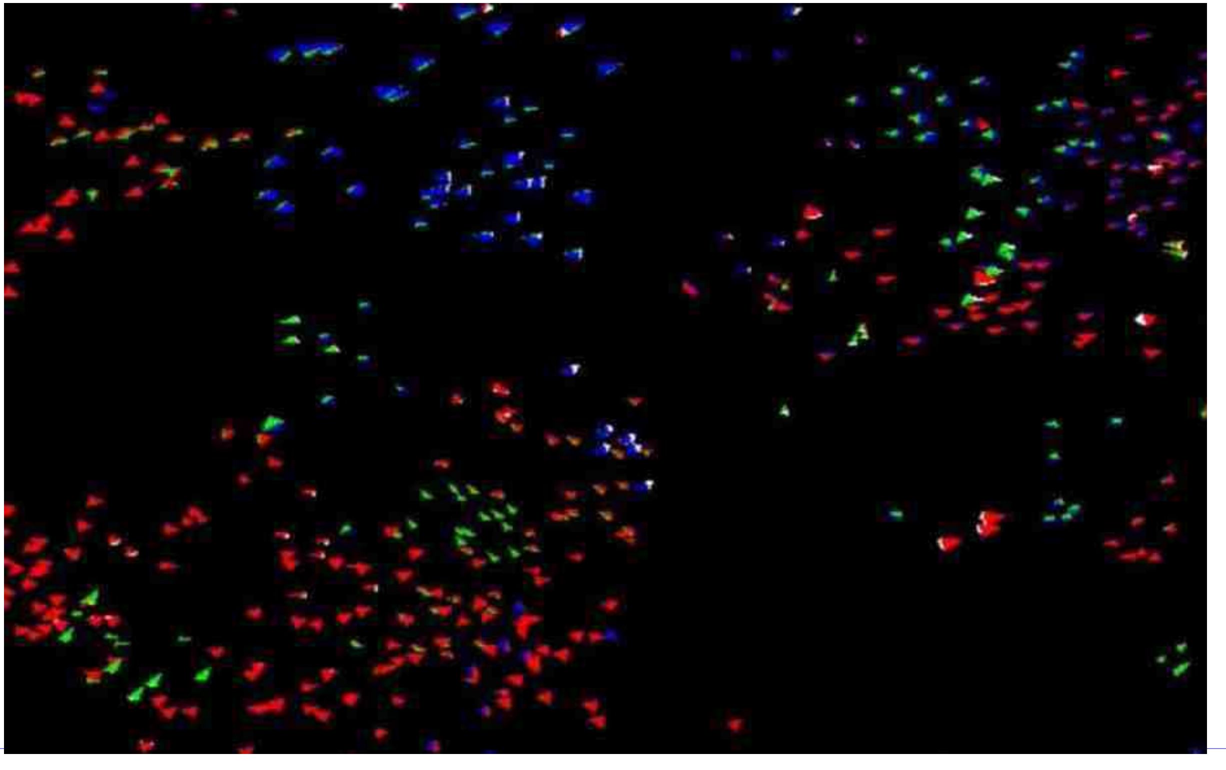
M_q arithmetic mean of neighbors' A matrices

$\bar{A}_q = \mathsf{PD}(M_q) \Leftrightarrow \exists S_q$ symmetric s.t. $M_q = \bar{A}_q S_q$ (polar decomp.)

$P_{T_{A_q(t)}\mathsf{SO}(n)}$ projection on the tangent $T_{A_q(t)}\mathsf{SO}(n)$, maintains $A_q(t) \in \mathsf{SO}(n)$

Sperm observed through microscope





positions and body attitudes of particles in periodic cube

Simulation by M. Biskupiak

Understand the differences between Vicsek and body alignment

do gradients of body frames genuinely influence motion ?

$\rightarrow$ use macroscopic model to shed light on this question

Main steps of derivation of macroscopic model:

(i) take $N \to \infty$ and obtain mean-field model

(ii) rescale mean-field model by ε (micro to macro scales ratio)

(iii) take $\varepsilon \to 0$ and obtain macro model

Step (iii): $f^\varepsilon = f^\varepsilon(x, A, t)$ with $x \in \mathbb{R}^n$, $A \in \mathrm{SO}(n)$ solves

$$\partial_t f^\varepsilon + (Ae_1) \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon); \quad Q(f) = -\nabla_A \cdot (F_f f) + \Delta_A f$$

$$F_f = k\, P_{T_A} B_f, \quad B_f = \mathrm{PD}(M_f), \quad M_f = \int_{\mathrm{SO(n)}} f(x, A', t)\, A'\, dA'$$

Equilibria are VMF-like: $Q(f) = 0 \Leftrightarrow \exists \rho > 0,\ B \in \mathrm{SO}(n)$ s.t.

$$f(A) = \rho\, M_{kB}(A), \quad M_{kB}(A) = \frac{e^{k\, B \cdot A}}{\int e^{k\, B \cdot A}\, dA}$$

ρ: density; B: mean body-frame. Depend on (x, t). Satisfy macro Eqs.

Self-Organized Hydrodynamics for Body orientation (SOHB)

provide Eqs for density $\rho > 0$ and mean body-frame $B \in \mathrm{SO}(3)$

$$\partial_t \rho + \nabla \cdot (c_1 \, \rho B_1) = 0$$

$$\partial_t B + c_2 (B_1 \cdot \nabla) B + \big[c_3 B \times \nabla \log \rho + c_4 (B_1 \times \mathrm{curl} B + (\mathrm{div} B) B_1) \big]_\times B = 0.$$

with $B_1 = B e_1$ mean propagation direction

$\forall w \in \mathbb{R}^3$, $[w]_\times$ is the matrix of $x \mapsto w \times x$.

Define matrix $\mathcal{D}(B)$ by $(w \cdot \nabla) B = [\mathcal{D}(B) w]_\times B$, $\forall w \in \mathbb{R}^3$

$\mathrm{div} B = \mathrm{Tr}\{\mathcal{D}(B)\}$; $\mathrm{curl} B$ is s.t. $[\mathrm{curl} B]_\times = \mathcal{D}(B) - \mathcal{D}(B)^T$

Derivation uses generalized collision invariants

$c_2, \ldots, c_4$ are moments of GCI. $c_1 =$ "order parameter"

use of special parametrization of $\mathrm{SO}(3) \sim$ quaternions

Remarks: formal derivation still unknown in dimension ≥ 4

derivation in 3D is formal; mathematical theory is empty

available: phase transitions in simpler model (w. A. Diez)

using quaternions, model $\equiv$ polymer model in 4D

SOHB in frame representation

Define local frame $B = [B_1, B_2, B_3]$ Then, SOHB is written

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho B_1) = 0$$

$$\rho \big(\partial_t B_1 + c_2 (B_1 \cdot \nabla_x) B_1\big) + P_{B_1^\perp} \big(c_3 \nabla_x \rho - c_4 \rho \, \mathsf{curl} B\big) = 0$$

$$\rho \big(\partial_t B_2 + c_2 (B_1 \cdot \nabla_x) B_2\big) - \big[B_2 \cdot \big(c_3 \nabla_x \rho - c_4 \rho \, \mathsf{curl} B\big)\big] B_1 + c_4 \rho \, (\mathsf{div} B) B_3 = 0$$

$$\rho \big(\partial_t B_3 + c_2 (B_1 \cdot \nabla_x) B_3\big) - \big[B_3 \cdot \big(c_3 \nabla_x \rho - c_4 \rho \, \mathsf{curl} B\big)\big] B_1 - c_4 \rho \, (\mathsf{div} B) B_2 = 0$$

with

$$\mathsf{curl} B = (B_1 \cdot \nabla_x) B_1 + (B_2 \cdot \nabla_x) B_2 + (B_3 \cdot \nabla_x) B_3$$

$$\mathsf{div} B = \big[(B_1 \cdot \nabla_x) B_2\big] \cdot B_3 + \big[(B_2 \cdot \nabla_x) B_3\big] \cdot B_1 + \big[(B_3 \cdot \nabla_x) B_1\big] \cdot B_2$$

If $c_4 = 0$, reduces to Vicsek-SOH model for ρ and $u = B_1$:

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

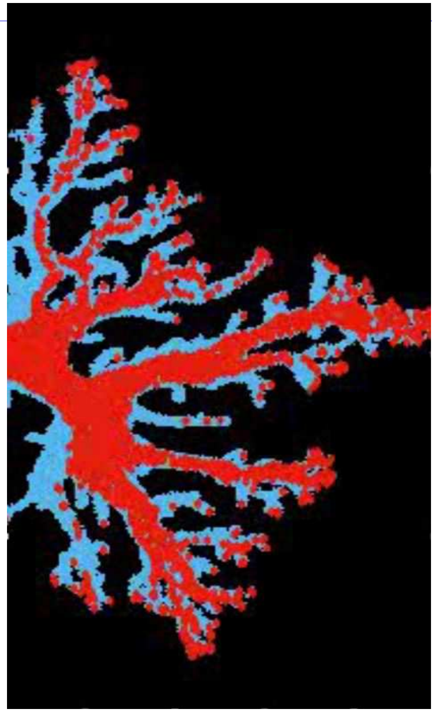
$$\rho \big(\partial_t u + c_2 (u \cdot \nabla_x) u\big) + P_{u^\perp} (c_3 \nabla_x \rho) = 0$$

But $c_4 \neq 0$ in general

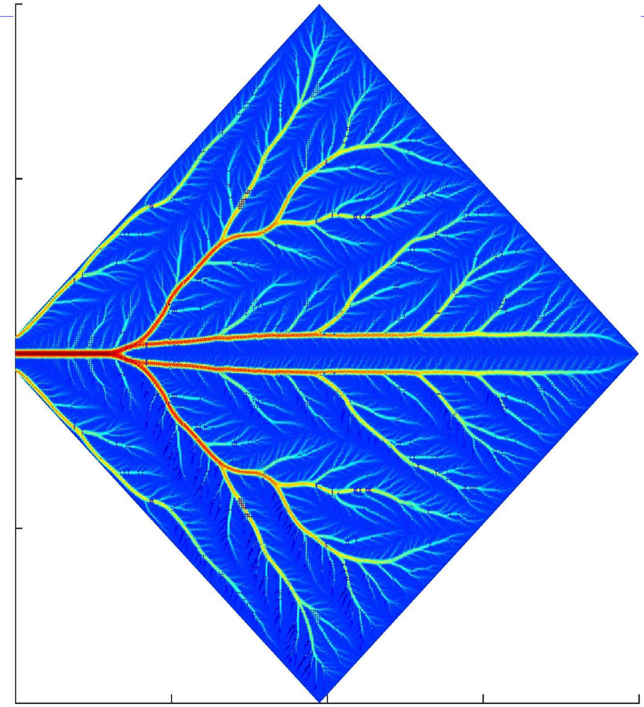
gradients of body frames genuinely influence motion

4. Reflection: network formation models

Models of network formation



Micro[1]



Macro[2]

Main difference: in order to produce the network structure:

- macro (right) requires the presence of a nonlinear decay term
- micro (left) does not require

[1] [arxiv 1812.09992] with P. Aceves-Sanchez, B. Aymard (Nice), D. Peurichard (INRIA Paris), L. Casteilla & A. Lorsignol (Stromalab, Toulouse), P. Kennel & F. Plouraboué (Fluid Mech. Toulouse)

[2] [Hu & Cai, PRL 111 (2013) 138701], [Haskovec, Markowich, Perthame, Schlottbom, NLA 138 (2016) 127]

Macro models seem less prone to pattern formation

than micro models

and require additional mechanisms

Are macroscopic models too deterministic ?

May require additional stochastic terms, leading to SPDE

How to rigorously derive such terms ?

Why is ability to pattern formation lost at coarse-graining ?

Breakdown of propagation of chaos at large time scales ?

Suggestion that this may be the case in

[E. Carlen, PD, B. Wennberg, M3AS 23 (2013) 1339]

5. Conclusion

Summary / Perspectives

Emergence = development of large-scale structures
by agents interacting locally without leader

Modelling emergence presents new challenges:
- lack of conservations due to agents' active character
- possible breakdown of propagation of chaos

Emergence = phase transition from disorder to patterns
analyzed through bifurcation theory

Agents may carry inner geometrical structures
which influence the large-scale structures

New models constructed by combining various
inner geometrical structures and interactions

Needed to describe living and social systems complexity
and are source of new fascinating mathematical questions