# Kinetic and Hydrodynamic modelling of Active Particle Systems

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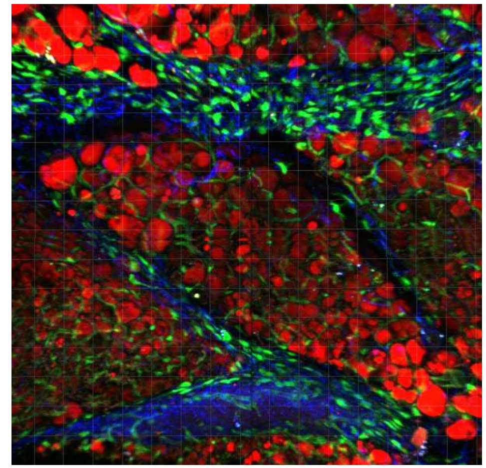
# Summary

1. Introduction
2. Directional coordination: the Vicsek model
3. Space-homogeneous case: phase transitions
4. Space-inhomogeneous case: macroscopic limit
5. Conclusion

# 1. Introduction

self-organization (aka 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)

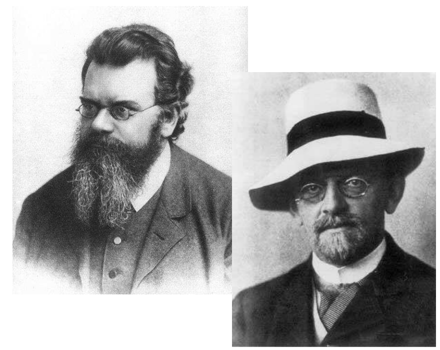
Requires rigorous passage "micro → macro"

Why macro models ?

Computational time

Analysis: stability, bifurcations, . . .

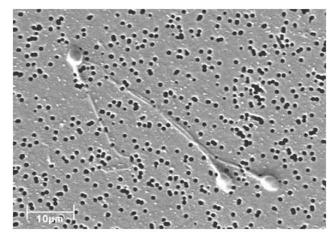
Data (images) inform on the macro scale



What is special about emergent systems ?

"micro → macro" Boltzmann, Hilbert, . . .

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



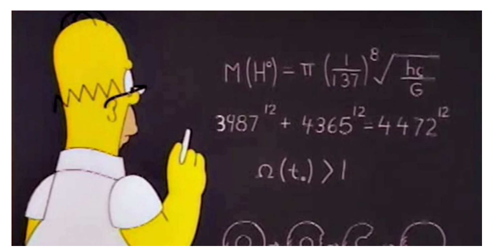
Unusual features

Lack of propagation of chaos

Lack of conservations: particles are "active"

Coexistence of ≠ phases

Complex underlying geometrical structures




⇒ revisit classical concepts

# 2. Directional coordination: the Vicsek model

Tamàs Vicsek (Budapest)

Individual-Based (i.e. particle) model

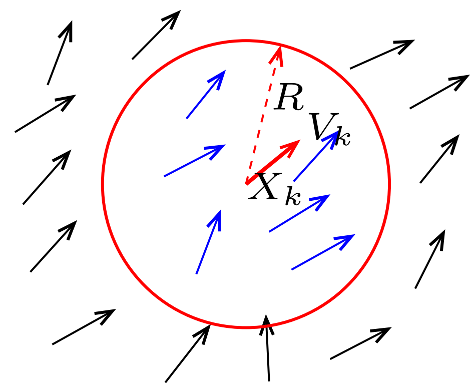
- self-propelled $\Rightarrow$ all particles have same constant speed $= 1$
- align with their neighbors up to some noise
- Particle $q$: position $X_q(t) \in \mathbb{R}^n$, velocity direction $V_q(t) \in \mathbb{S}^{n-1}$

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

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

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

- $R =$ 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 $|V_q(t)| = 1$, $\forall t$



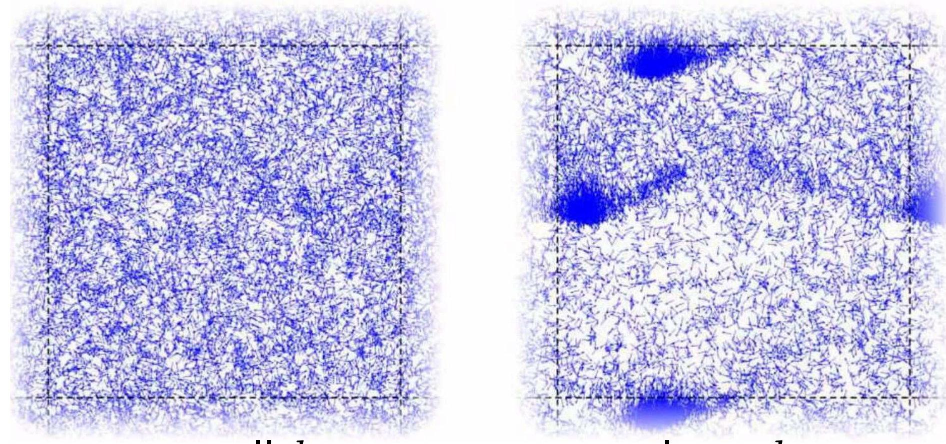

"Minimal model" for collective dynamics

# Phase transition in Vicsek model

## Phase transition

symmetry breaking

disordered $\to$ aligned

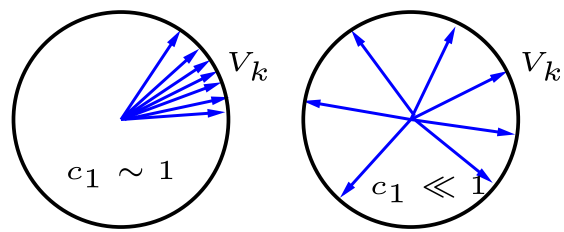


small $k$ large $k$

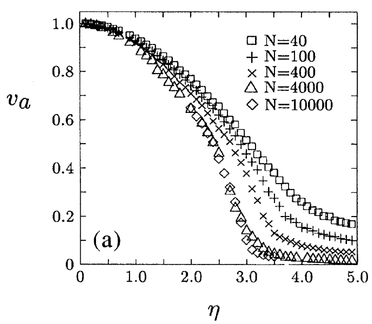
Simulations by A. Frouvelle

## Order parameter measures alignment

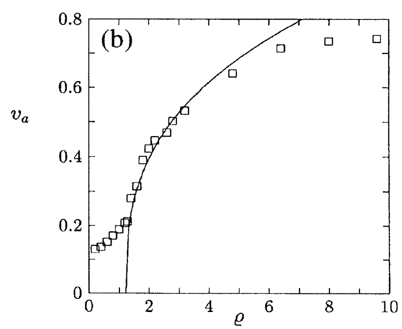
$$c_1 = \left| N^{-1} \sum_q V_q \right|, \quad 0 \le c_1 \le 1$$



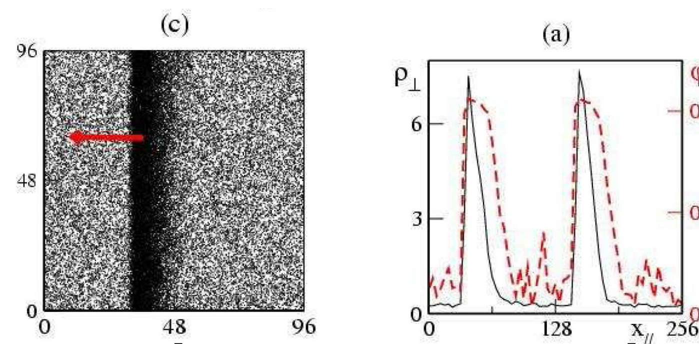

$c_1$ vs $1/k$




$c_1$ vs density

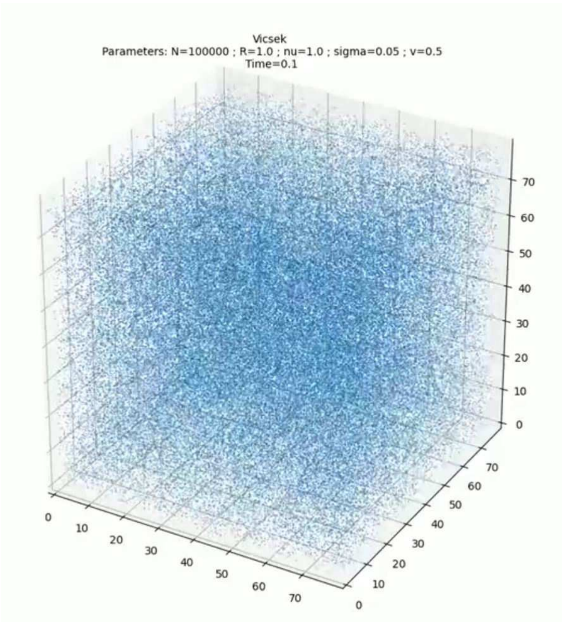



band formation

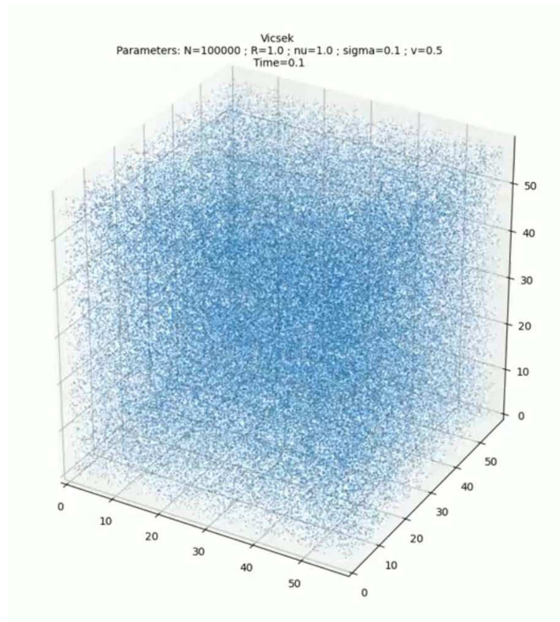



after [Chaté et al, PRE 2008]

# Some 3D simulations by Antoine Diez




bands from disorder




bands from flock

# 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 $\{v\}^\perp$
$\nabla_v \cdot$, $\nabla_v$: 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 2008)]

## 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 (2012)]

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

## Existence and uniqueness of solutions to Fokker-Planck

[Gamba, Kang (2016); Figalli, Kang, Morales (2018); Briant, Merino (2020)]

Other collective dynamics models do not normalize velocities

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

# 3. Space-homogeneous case: phase transitions

initiated with

## Amic Frouvelle and Jian-Guo Liu

Frouvelle Liu (SIMA 2012), D. Frouvelle Liu (JNLS 2013 & ARMA 2015)
Barbaro D. (DCDS B 2014), Barbaro Cañizo Carrillo D. (MMS 2016)
D. Diez Frouvelle Merino (JNLS 2020), Frouvelle (arxiv 2020)

Amic

Jian-Guo

# Spatially homogeneous case

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

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

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

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 2012),
D. Frouvelle Liu (JNLS 2013 & ARMA 2015]

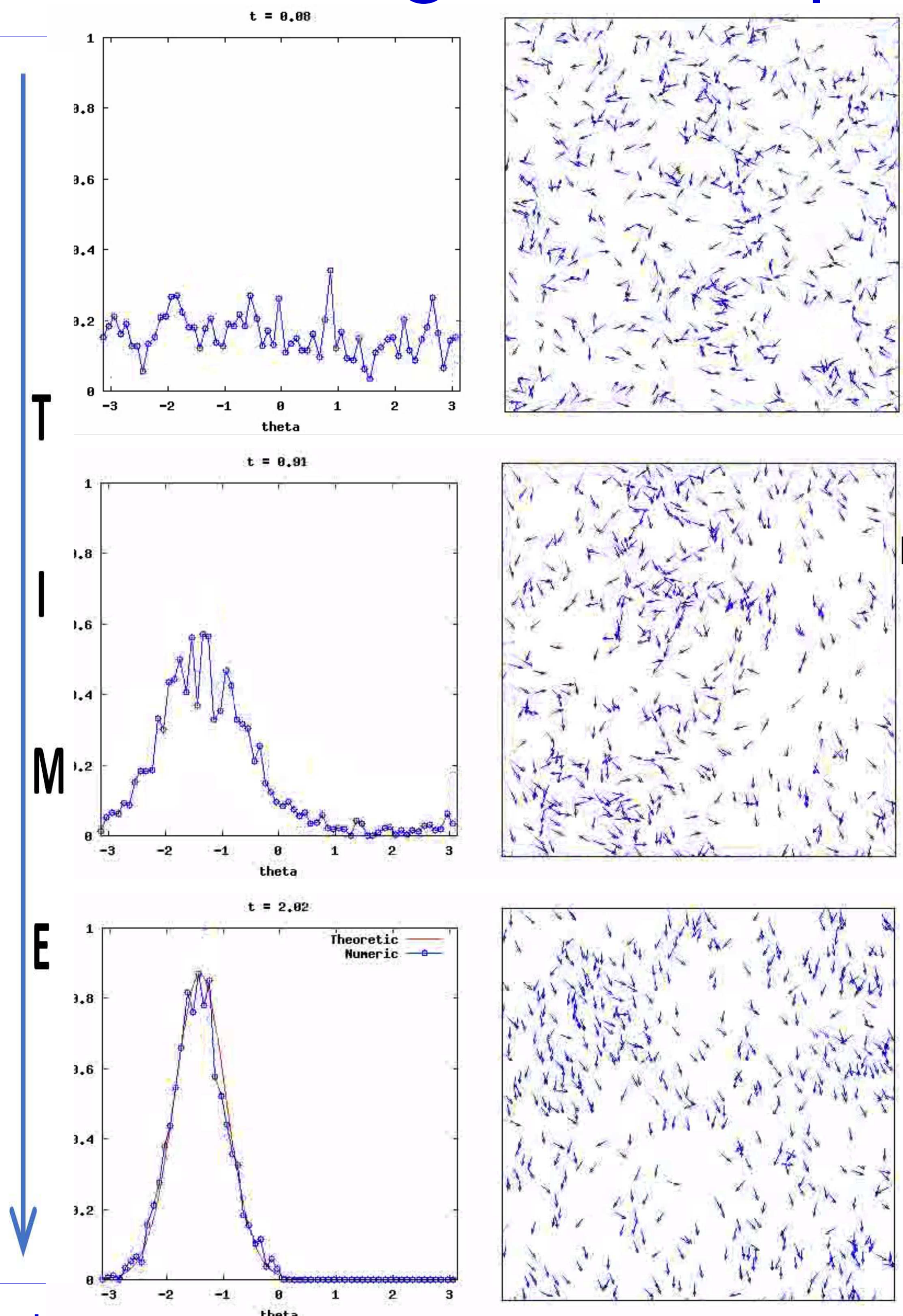
for $k(|J_f|) = 1$: [Figalli Kang Morales (ARMA 2018)]

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

# Simulation of convergence to equilibrium

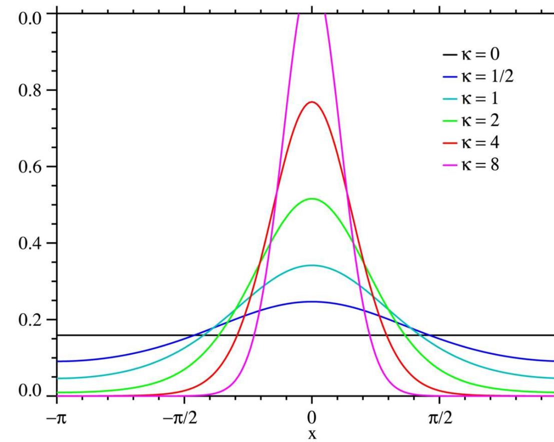


Histogram of velocity directions in $(-\pi, \pi)$




positions and velocity vectors of particles in periodic box

Simulation by S. Motsch




(VMF = Von Mises-Fisher) given by

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

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

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

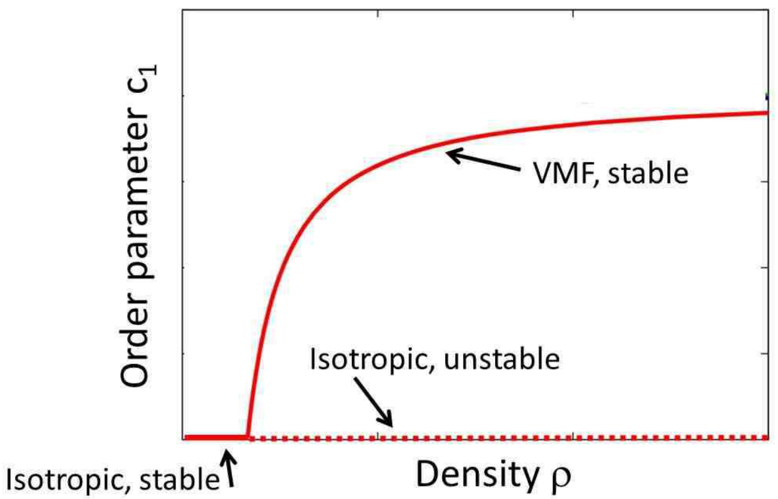
Number of roots and local monotony of $\frac{j(\kappa)}{c_1(\kappa)}$ determine

number of equilibria and their stability

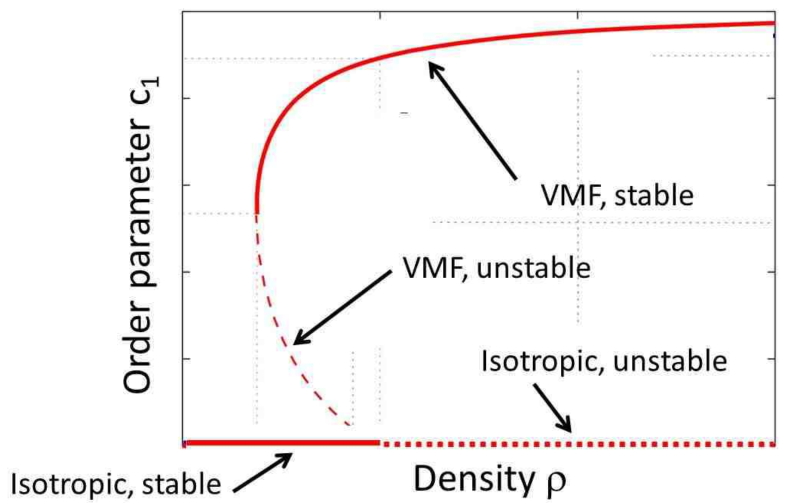
# Examples

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, ...

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

# 4. Space-inhomogeneous case: macroscopic limit

initiated with

## Sebastien Motsch

D. Motsch (M3AS 2008), D. Liu Motsch Panferov (MAA 2013)
D. Dimarco Mac Wang (CMS 2015)
Aceves-Sanchez Bostan Carrillo D. (MBE 2019)

Sebastien Motsch

Giacomo Dimarco

Pedro Aceves-Sanchez

# 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 $\rho M_{ku}$

$\exists$ 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 inhomogeneous $\Rightarrow$ $\rho(x,t)$ and $u(x,t)$ are not constant

$\rho$ and $u$ determined by macroscopic equations

Resulting system is Self-Organized Hydrodynamics (SOH)

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

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

$$|u| = 1$$

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

Requires dimension { CI } = number of equations

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

Generalized collision invariants (GCI) overcome the problem

first proposed in [D Motsch (M3AS 2008)]

GCI $\psi$ satisfies CI property with smaller class of $f$

Finding $\psi$ involves inverting the "adjoint" of $Q$

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

# Remarks

SOH is similar to Compressible Euler eqs. of gas dynamics
- Continuity eq. for $\rho$
- 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
- [D. Liu Motsch Panferov (MAA 2013)]
- Existence / uniqueness of non-smooth solutions open
- Rigorous limit $\varepsilon \to 0$ proved: [Jiang Xiong Zhang (SIMA 2016)]

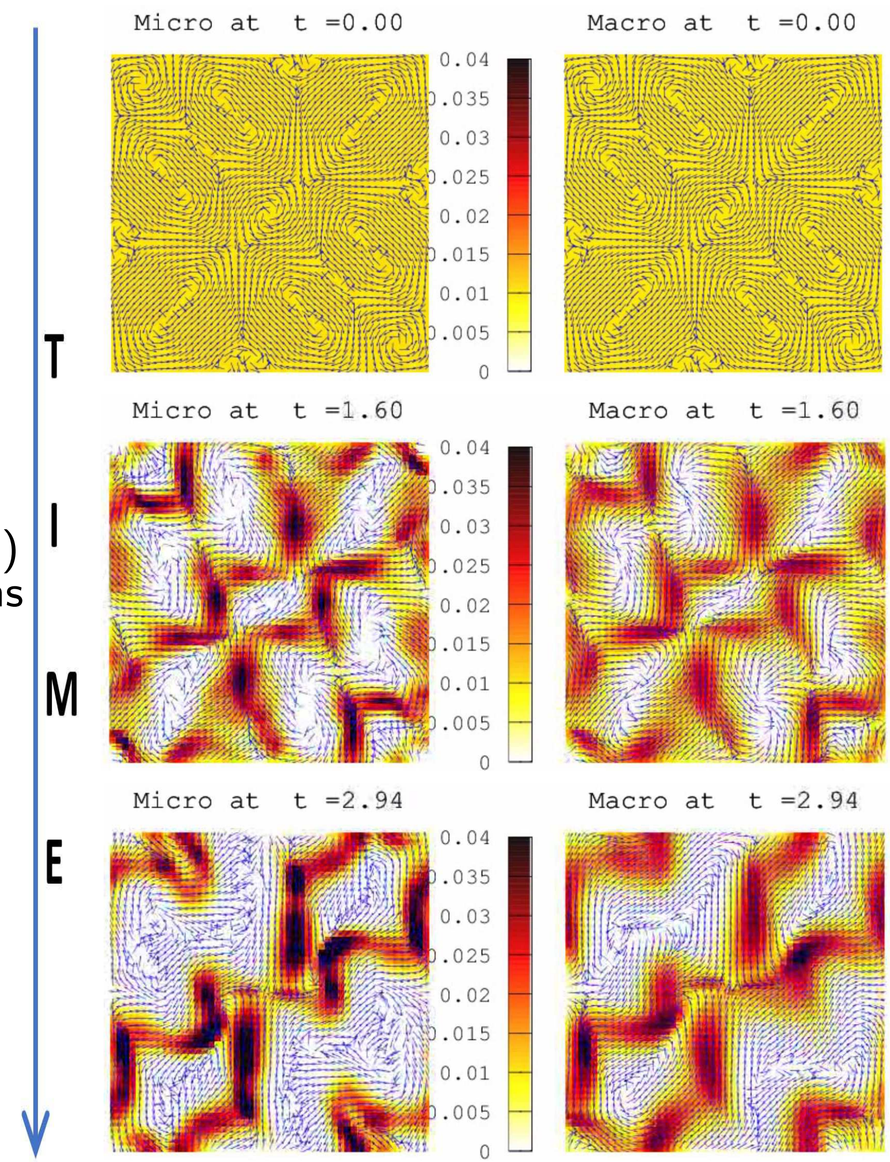
Differences (but also similarities) with the Toner-Tu model
- [Toner Tu (PRL 1995)] built on symmetry considerations

Numerical simulations [Motsch Navoret (MMS 2011),
Gamba Haack Motsch (JCP 2015), Dimarco Motsch (M3AS 2016)]

# Comparison between micro and macro

Micro (Vicsek)

Density (color code)
& velocity directions




Macro (SOH)

Density (color code)
& velocity directions

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

# 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

Needed to describe living and social systems complexity

and are source of new fascinating mathematical questions