Mathematical modeling of complex systems
Part 3. Hydrodynamics

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Joint work with S. Motsch ;
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Summary

1. Introduction
2. From particle to Mean-Field model
3. From Mean-Field to Hydrodynamics
4. Properties of the hydro model
5. Conclusion

1. Introduction

Complex system

- System with interacting agents without leaders
  - emergence of large scale space-time structures
  - produced by local interactions only

Local interactions

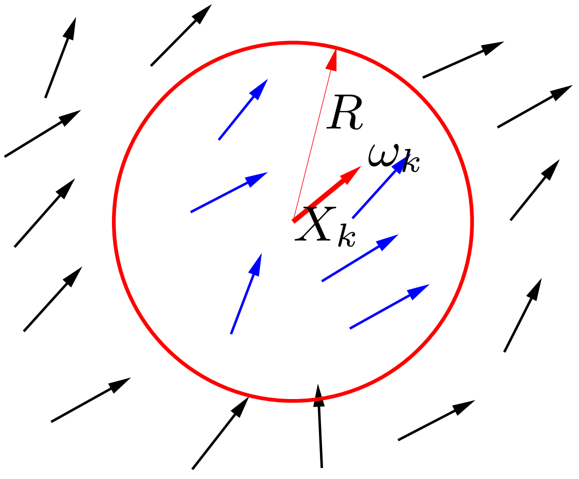
- Local interactions are complex & difficult to access from experiments
- Classical micro-macro approach is bottom-up
- Complex systems require top-down approach
  - use macro model to probe the data and extract the relevant information
- Important to link micro interactions to macro model
- Justification of macroscopic limits difficult
  - $\exists$ correlations: chaos assumption may not be true

Hydrodynamic limit of the Vicsek model

- Leave justification of chaos assumption aside
- Three steps
  - time-continuous particle (IBM) model
  - Mean-field kinetic limit
  - Hydrodynamic limit
- Difficulty
  - dimension of invariants $<$ dimension of equilibria
  - New concept of 'Generalized Collisions Invariants'
  - 1st derivation of non-conservative model from kinetics

2. From particles to mean-field model

Vicsek model [Vicsek et al, PRL 95]



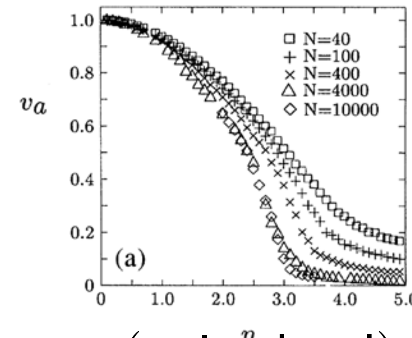
- Time-discrete model:
  - $t^n = n\Delta t$
  - k-th individual
  - X_k^n: position at t^n
  - ω_k^n: velocity with $|\omega_k^n| = 1$

- $$X_k^{n+1} = X_k^n + \omega_k^n \, \Delta t$$
  $$\omega_k^{n+1} = \bar{\omega}_k^n + \text{ noise (uniform in small angle interval)}$$
  $$\bar{\omega}_k^n = \frac{J_k^n}{|J_k^n|}, \quad J_k^n = \sum_{j,\, |X_j^n - X_k^n| \leq R} \omega_j^n$$

- Alignment to neighbours' mean velocity plus noise

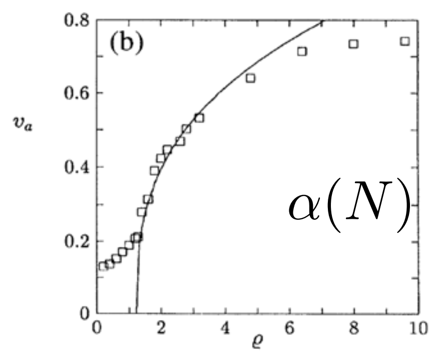
Phase transition to aligned state

➠ As noise decreases
[Vicsek et al, PRL 95]

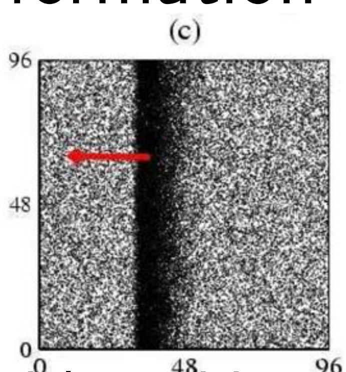


α(noise level)

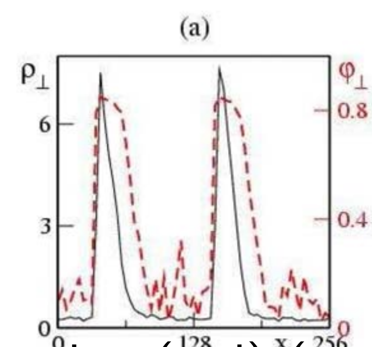
➠ As density increases
[Vicsek et al, PRL 95]



➠ Band formation [Chaté et al]



Particle positions



ρ (black) and α (red) (cross section)

Time continuous Vicsek algorithm

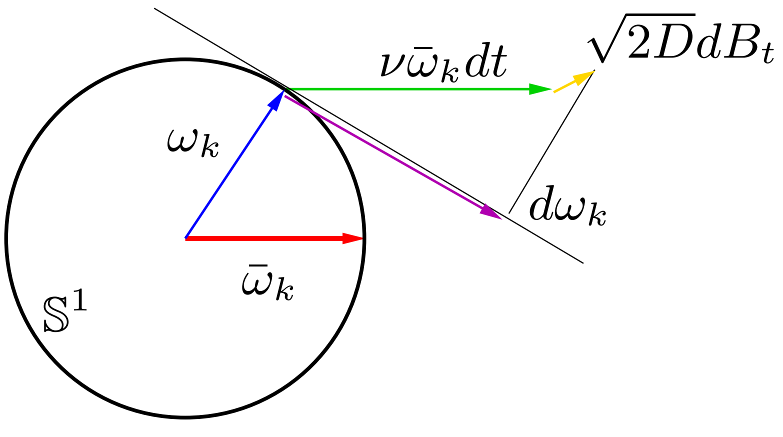
- Time continuous dynamics:

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

$$d\omega_k(t) = (\mathrm{Id} - \omega_k \otimes \omega_k)(\nu \bar{\omega}_k dt + \sqrt{2D} dB_t)$$

$$\bar{\omega}_k = \frac{J_k}{|J_k|}, \quad J_k = \sum_{j, |X_j - X_k| \le R} \omega_j$$

- Recover original Vicsek by:
  - Time discretization Δt
  - Gaussian noise $\to$ uniform
  - $\nu \Delta t = 1$



Mean-field model

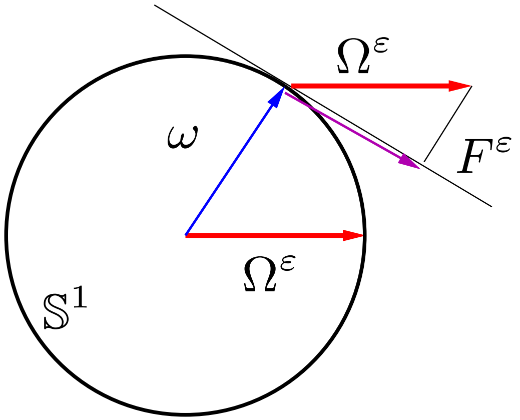
- $f(x, \omega, t) =$ 1-particle proba distr.
  - satisfies a Fokker-Planck equation
  - Scaling to macro variables $\tilde{x} = \varepsilon x$, $\tilde{t} = \varepsilon t$, $\varepsilon \ll 1$
  - local interaction: $\tilde{R} = \varepsilon R$

- Fokker-Planck eq. in scaled variables

$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon) + \nabla_\omega \cdot (F^\varepsilon f^\varepsilon) = D\Delta_\omega f^\varepsilon$$

$$F^\varepsilon = (\mathrm{Id} - \omega \otimes \omega)\Omega^\varepsilon$$

$$\Omega^\varepsilon = \frac{j^\varepsilon}{|j^\varepsilon|}, \quad j^\varepsilon = \int_{|v|=1} v f^\varepsilon(x, v, t)\, dv$$



  - Ω^ε is the direction of the local flux

3. From Mean-Field to Hydrodynamics

Collision operator

- Model can be written

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

  - with collision operator

$$Q(f) = -\nabla_\omega \cdot (F_f\, f) + D\Delta_\omega f$$

$$F_f = (\mathrm{Id} - \omega \otimes \omega)\Omega_f$$

$$\Omega_f = \frac{j_f}{|j_f|}, \quad j_f = \int_{|v|=1} v f(x,v,t)\, dv$$

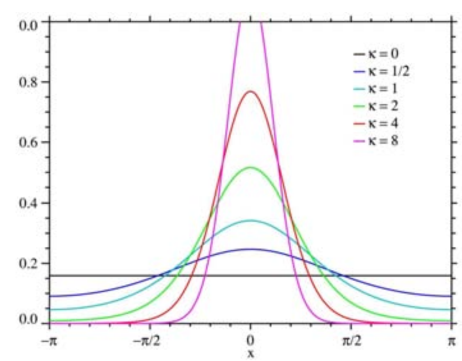
- Problem: find the limit $\varepsilon \to 0$

- Equilibrium manifold: $\mathcal{E} = \{f \,|\, Q(f) = 0\}$

- Rewrite

$$Q(f) = \nabla_\omega \cdot [-F_f \, f + D\nabla_\omega f]$$

  - Introduce the solution of $[\ldots] = 0$
  - $\forall \Omega \in \mathbb{S}^1$, $\exists$ a unique normalized solution $f = M_\Omega$ such that $\Omega_f = \Omega$



- Von-Mises distribution:

$$M_\Omega(\omega) = Z^{-1} \exp \beta(\omega \cdot \Omega), \qquad \int M_\Omega(\omega)\, d\omega = 1, \quad \beta = D^{-1}$$

- $Q(f)$ can be written

$$Q(f) = D\,\nabla_\omega \cdot \left[M_{\Omega_f} \nabla_\omega \left(\frac{f}{M_{\Omega_f}} \right) \right]$$

- Entropy inequality

$$H(f) = \int Q(f) \frac{f}{M_{\Omega_f}}\, d\omega = -D \int M_{\Omega_f} \left| \nabla_\omega \left(\frac{f}{M_{\Omega_f}} \right) \right|^2 \leq 0$$

- $\mathcal{E} = \{ \rho M_\Omega(\omega)$ for arbitrary $\rho \in \mathbb{R}_+$ and $\Omega \in \mathbb{S}^2$ $\}$ (or $\mathbb{S}^1$ in dim 2)
  - dim $\mathcal{E} = \begin{cases} 3 & \text{in dimension } 3 \\ 2 & \text{in dimension } 2 \end{cases}$

2nd step: Collision invariants (conserved quantity)

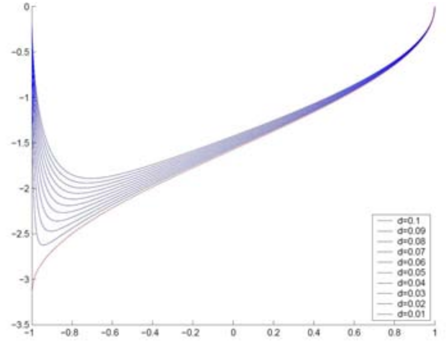
- Function $\psi(\omega)$ such that $\int Q(f)\psi \, d\omega = 0, \quad \forall f$
  - Form a vector space $\mathcal{C}$
  - Multiply eq. by ψ: ε^{-1} term disappears
  - Find a conservation law
  - Limit fully determined if dim $\mathcal{C} =$ dim $\mathcal{E}$
- Here dim $\mathcal{C} = 1$ because $\mathcal{C} =$ Span$\{1\}$
  - conservation of mass
  - dim $\mathcal{E} = 3 >$ dim $\mathcal{C} = 1$ (in dimension 3)
  - Is the limit problem ill-posed ?

Generalized collision invariants

- Given Ω, find ψ_Ω a GCI, such that

$$\int Q(f)\psi_\Omega \, d\omega = 0, \quad \forall f \text{ such that } \Omega_f = \Omega$$

- Given Ω, the GCI form a 3-dim vector space spanned by 1 and $\vec{\psi}_\Omega(\omega)$



- $\vec{\psi}_\Omega(\omega) = \frac{\Omega\times\omega}{|\Omega\times\omega|} g(\Omega\cdot\omega)$
  $g(\mu)$ sol. of elliptic eq:

$$-(1-\mu^2)\partial_\mu(e^{\mu/D}(1-\mu^2)\partial_\mu g) + e^{\mu/D} g = -(1-\mu^2)^{3/2} e^{\mu/D}$$

- Multiply FP eq by $\vec{\psi}_{\Omega_{f^\varepsilon}}$
  - $O(\varepsilon^{-1})$ terms disappear
  - Let $\varepsilon \to 0$: $\quad f^\varepsilon \to \rho M_\Omega$ and $\vec{\psi}_{\Omega_{f^\varepsilon}} \to \vec{\psi}_\Omega$
  - Gives:

$$\int \left(\partial_t(\rho M_\Omega) + \omega \cdot \nabla_x(\rho M_\Omega)\right) \vec{\psi}_\Omega \, d\omega = 0$$

- Not a conservation equation because of dependence of $\vec{\psi}_\Omega$ upon Ω

Macro version of Vicsek model

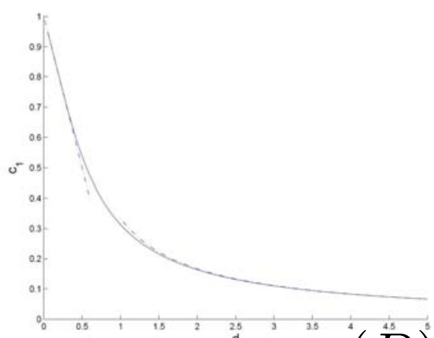
➠ density $\rho(x,t)$; flux director $\Omega(x,t)$:

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

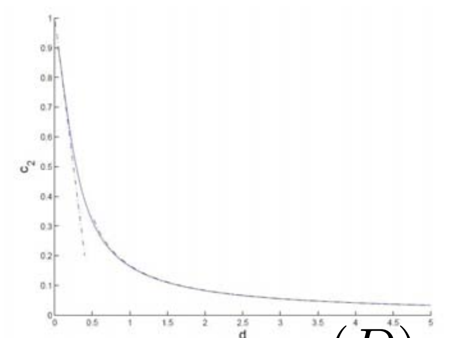
$$\rho \, (\partial_t \Omega + c_2 (\Omega \cdot \nabla) \Omega) + D \, (\mathrm{Id} - \Omega \otimes \Omega) \nabla_x \rho = 0$$

$$|\Omega| = 1$$

➠ c_1, c_2: constants (moments of M_Ω and g), $c_2 < c_1$



$c_1(D)$



$c_2(D)$

4. Properties of the hydrodynamic model

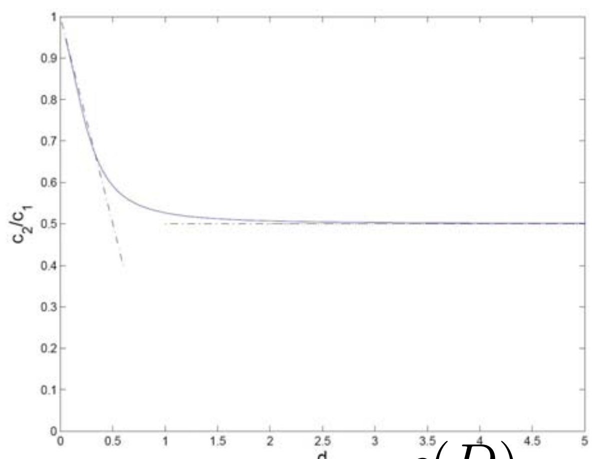
- By time rescaling: $c = c_2/c_1 < 1, \quad d = D/c_1$

Density $\rho(x,t)$, flux director $\Omega(x,t)$:

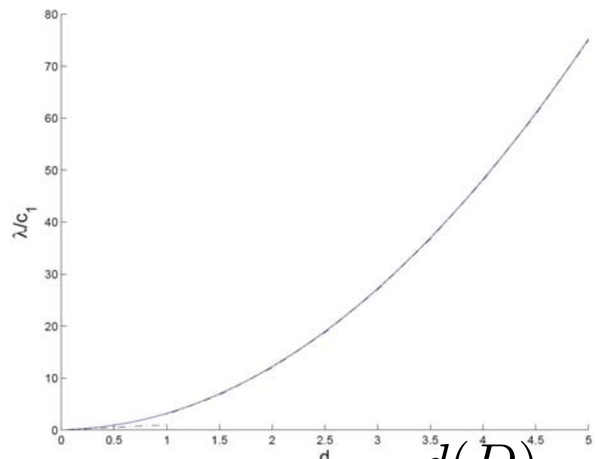
$$\partial_t \rho + \nabla_x \cdot (\rho \Omega) = 0$$

$$\rho \, (\partial_t \Omega + c(\Omega \cdot \nabla)\Omega) + d \, (\mathsf{Id} - \Omega \otimes \Omega) \nabla_x \rho = 0$$

$$|\Omega| = 1$$



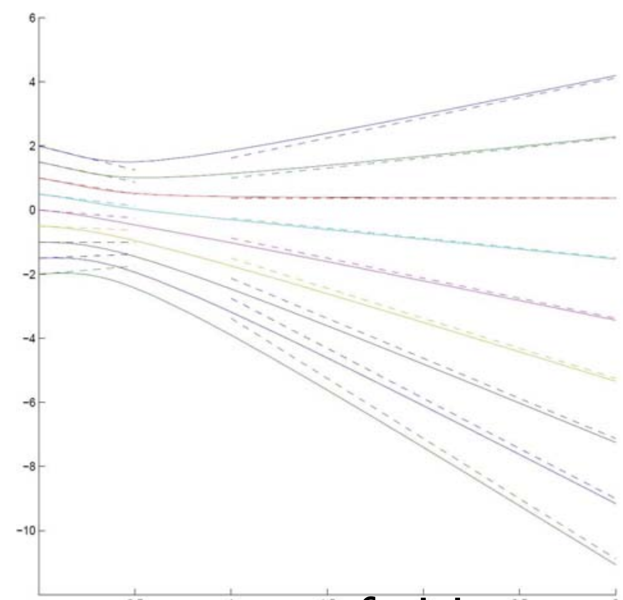
$c(D)$



$d(D)$

- Hyperbolic model with geometric constraint
  - Non-conservative terms arise from the constraint
  - Hydro & relaxation limits do not commute
- Velocity information travels slower than mass flow
  - like traffic
  - reinforced by forward vision

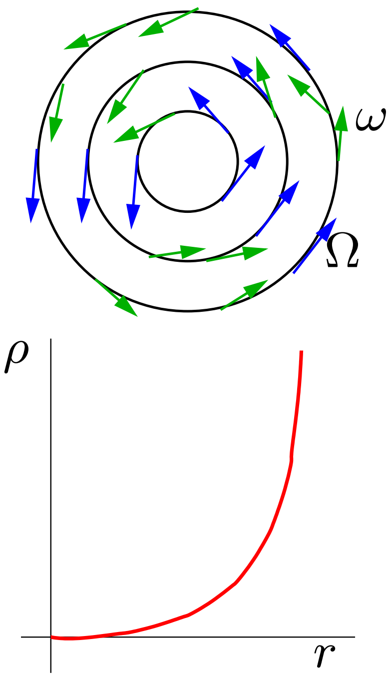
    [Frouvelle]



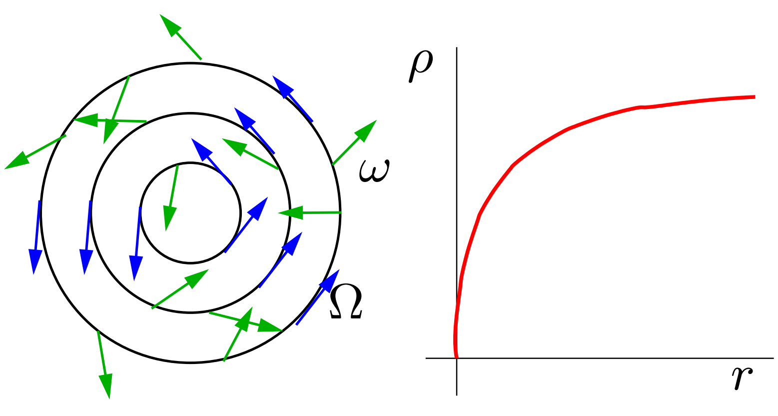
$c(D)$ for various apertures of vision cone

Mills are stationary solutions

- Mills: $\rho(r) = \rho_0 \, (r \, / \, r_0)^{c/d}$, $\Omega = x^\perp / r$
- Shape depends on noise level
  - small noise: $\rho(r)$ convex: sharp edged mills
  - large noise: $\rho(r)$ concave: fuzzy edges



small noise

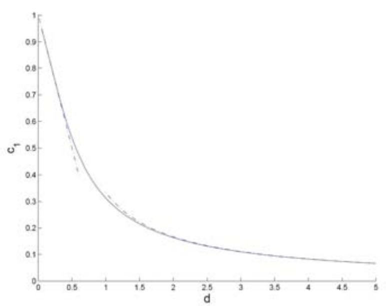


large noise

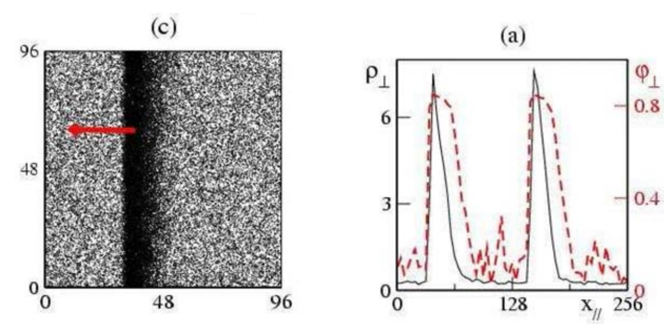
- Stability of mills ?

Order parameter

- $c_1 = |j_{M_\Omega}| =$ order parameter
  - $c_1 \sim 1$: aligned
  - $c_1 \sim 0$: random
- Vicsek: c_1 not uniform in space
- Hydro model: c_1 uniform (fixed by D)
  - Cure: make $D(\rho)$ (fluctuations ?) see [Frouvelle]



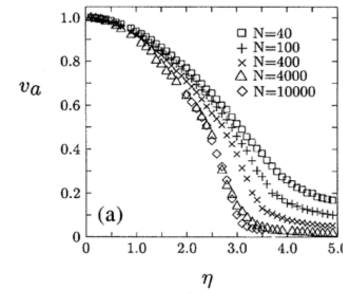
$c_1(D)$



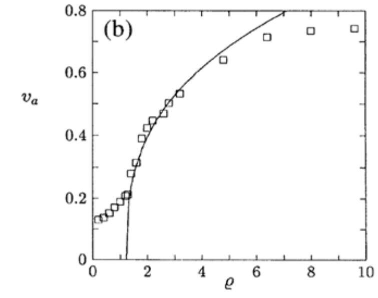
after [Chaté et al]: particle simulations
show band formation ; ρ & c_1 (cross section)

Phase transitions

- Vicsek model has phase transitions

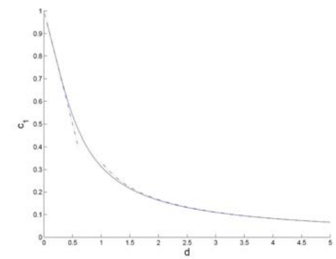


$c_1(D)$



$c_1(\rho)$

- Hydro model has **no** phase transitions



$c_1(D)$

- Different regimes
  - Vicsek: interaction radius is $O(1)$ (instead of $O(\varepsilon)$)
  - number of particle not large: Mean-Field and Hydro limits not valid

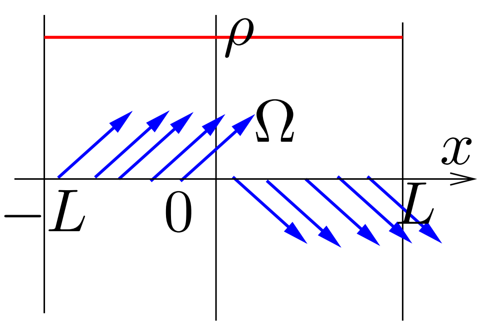
- Difficulty: geometric constraint $|\Omega| = 1$
  - No theoretical framework
  - Chen-Levermore-Liu theory does not apply
  - Shock speed undefined, no entropy, . . .
- Model $=$ relaxation limit of conservative model

$$\partial_t(\rho\Omega) + c\nabla \cdot (\rho\Omega \otimes \Omega) + d\,\nabla_x \rho = -\epsilon^{-1}\rho(1 - |\Omega|^2)\Omega$$

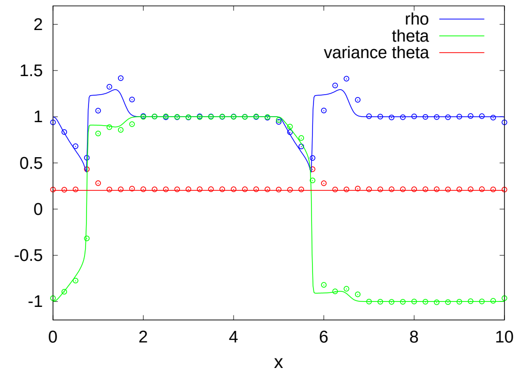
- Numerical methods [Motsch & Navoret]: compare
  - Standard methods
  - Method based on a splitting of the relaxation model

Vicsek vs Hydro

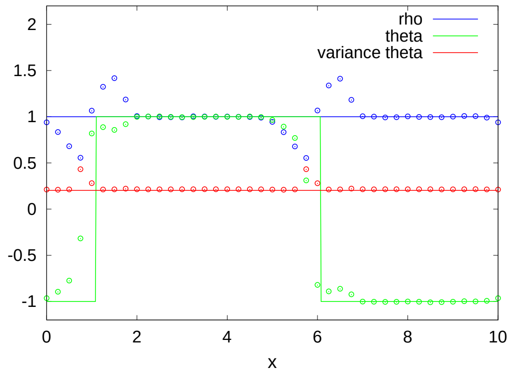
Initial conditions



Relaxation-based



Standard



- Initial contact discontinuity $\theta \longrightarrow -\theta$ at $x = 0$
- Vicsek (dots) and Hydro (solid line)
- $\rho(x)$ (blue), $\theta(x)$ green, $c_1(x)$ red $\Omega = (\cos\theta, \sin\theta)$
- Excellent agreement with relaxation-based meth.
- Wrong results with standard meth.

Vicsek vs Hydro (cont)

- Initial contact discontinuity resolved by complex wave pattern
  - not reproduced by standard methods
  - Confirms the need for a theory of these systems

5. Conclusion

Hydrodynamics of Vicsek particles

- Hydrodynamics of Vicsek model
  - derived under appropriate scaling hypotheses
- Non-standard features have been outlined
  - lack of collision invariants
- A new concept has been proposed
  - Generalized Collision Invariant
- 1st derivation of non-conservative model from kinetic theory
  - [D. Motsch, M3AS, Vol. 18, (2008)]

About the Hydrodynamic model

- Excellent agreement with Vicsek particle model
  - provided relaxation formulation is used
- Geometrical constraint
  - requires theoretical investigations
- Improvements required:
  - non-constant order parameter
  - possibility of phase transition
  - more general alignement dynamics
- Further refinements
  - work in progress by A. Frouvelle