Mathematical modeling of self-organized dynamics: from microscopic to macroscopic description

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G. Theraulaz, J. Gautrais (CRCA, Toulouse)

UC Davis, Applied Math PDE Seminar

Outline

Motivation

- Individuals have only local interactions
- There is no leader inside the group ($\Rightarrow$ *self-organization*)
- The global organization of the group is at a much larger scale than the individual size

How can we connect individual and global dynamics ?

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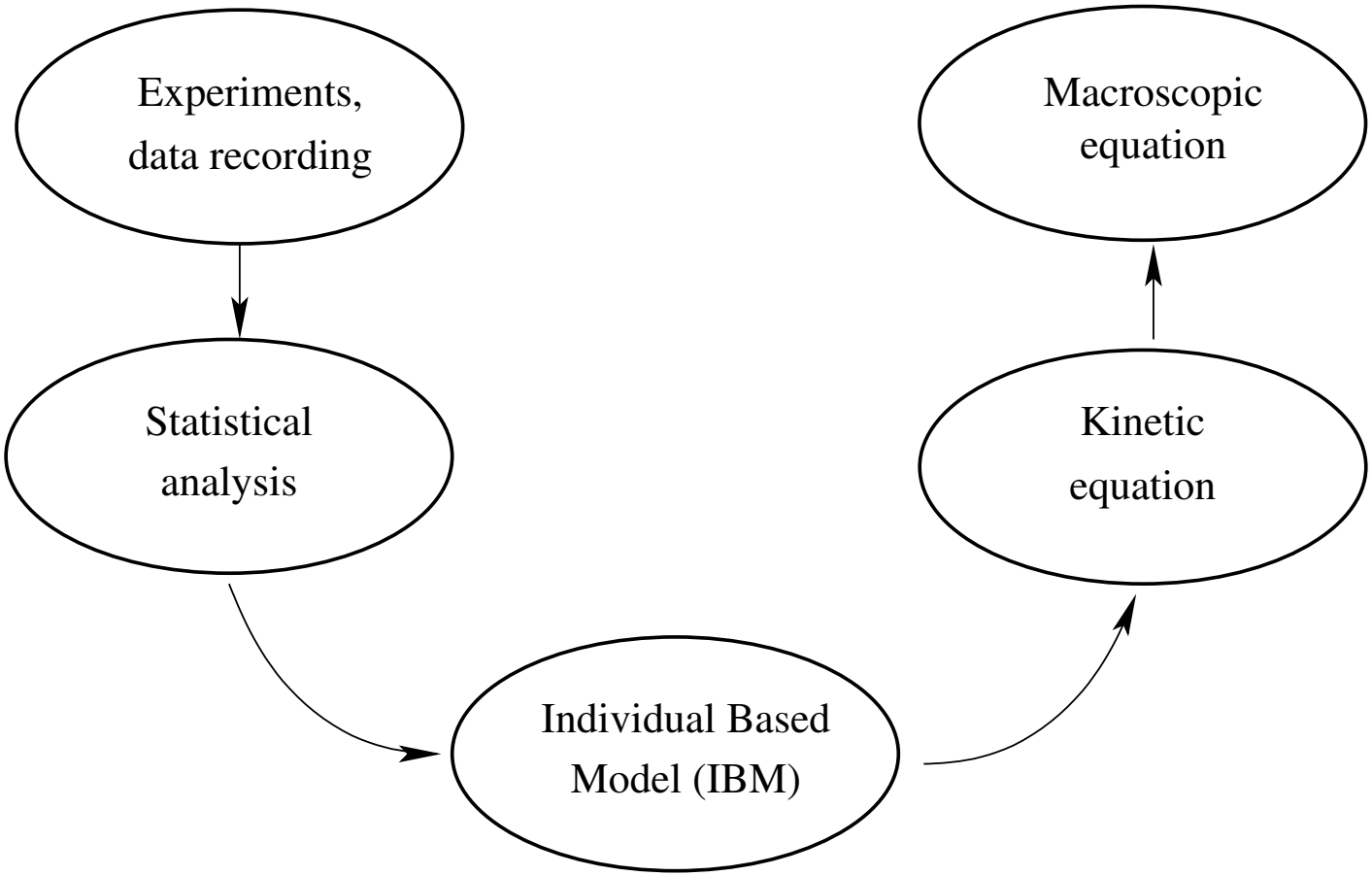
Methodology



Identify the rules
for individual behavior

Capture the global
behavior of the system

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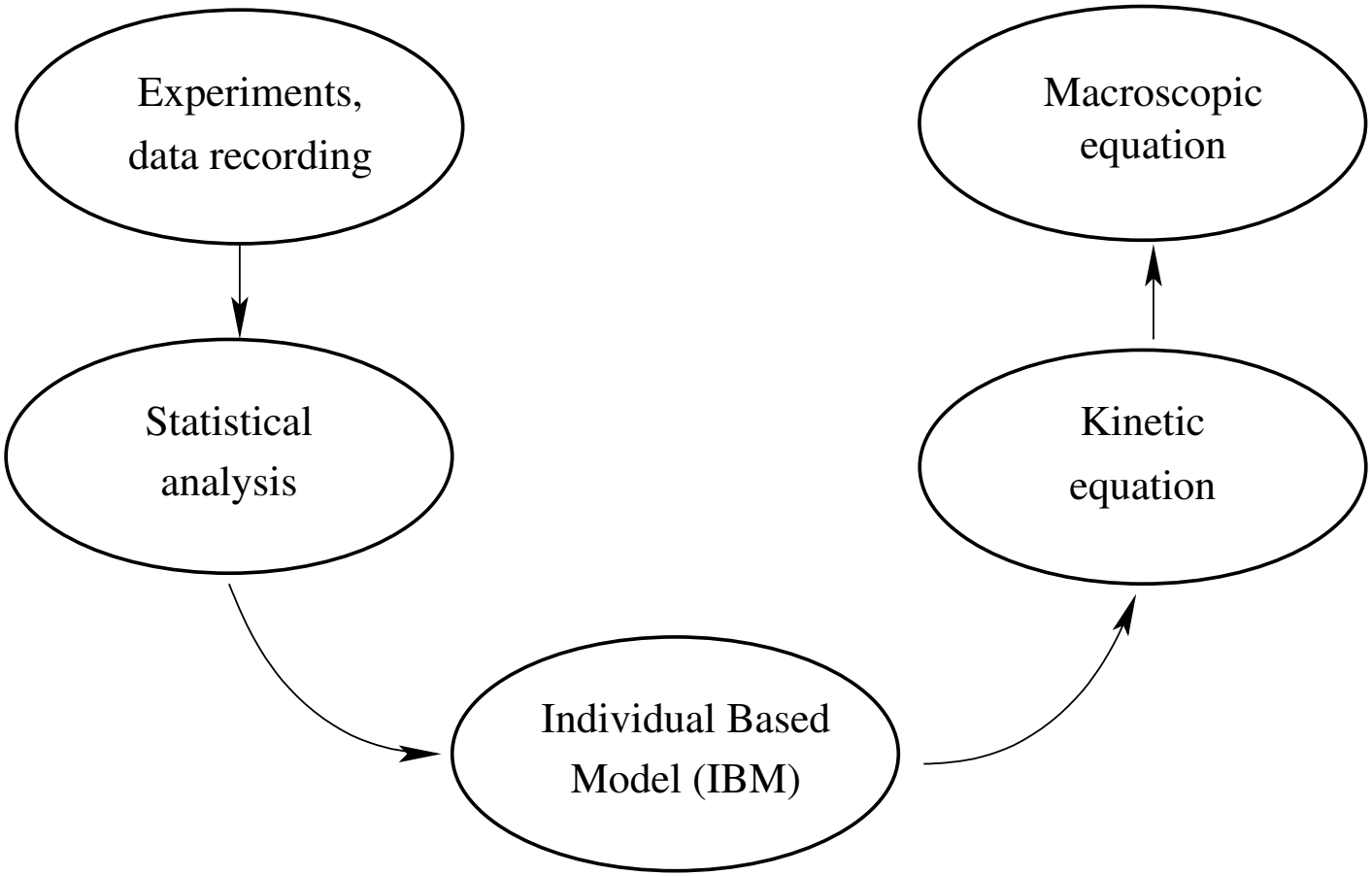

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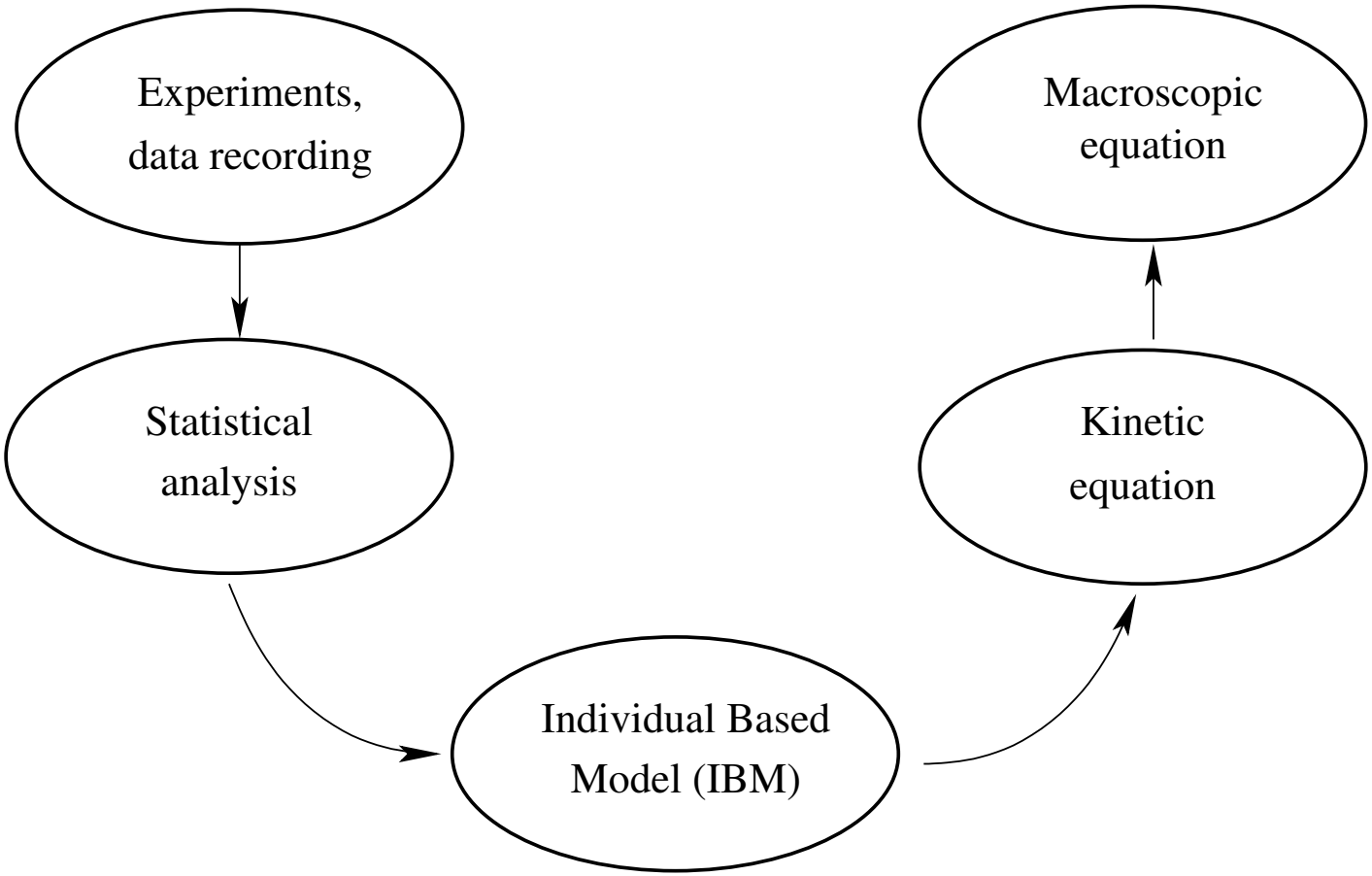

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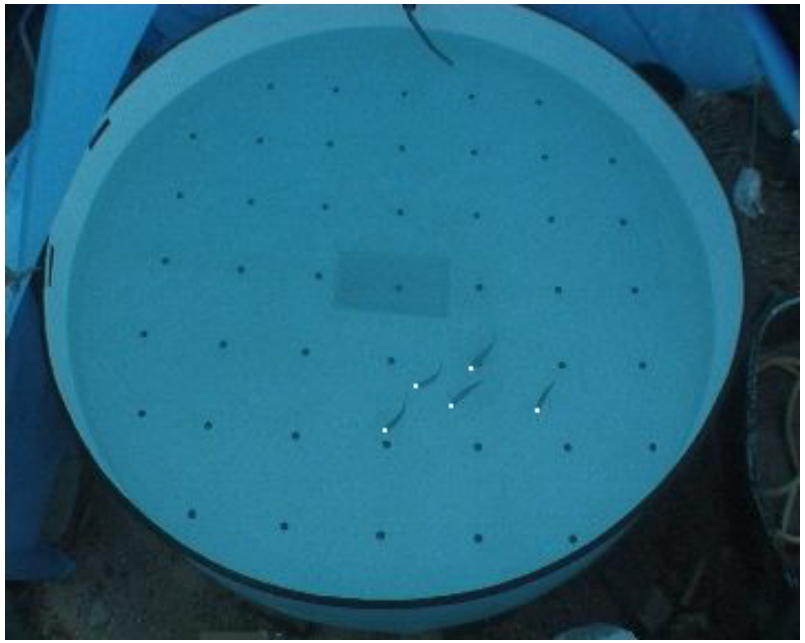
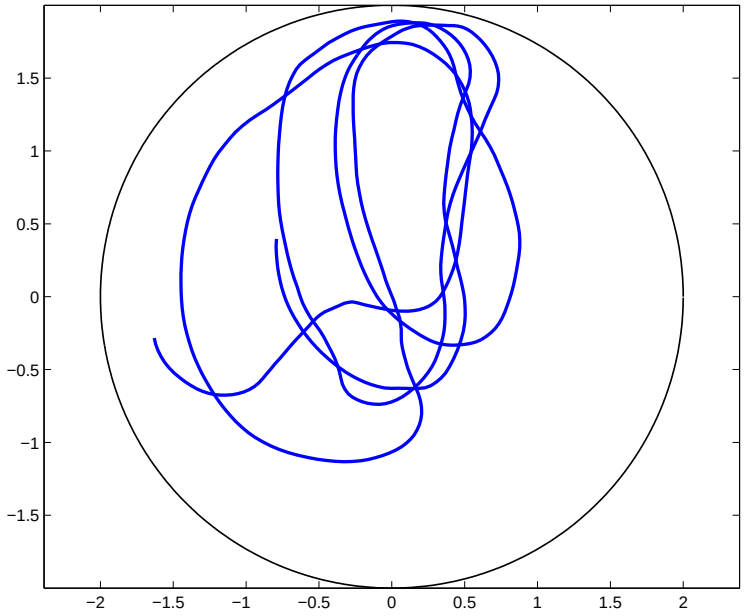
Experiments for fish



- The diameter of the basin is 4 meters
- Species studied: Kuhlia mugil (20-25 cm)

Video , data recorded

An example of trajectory :



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- The trajectory is smooth, the fish seems to turn constantly

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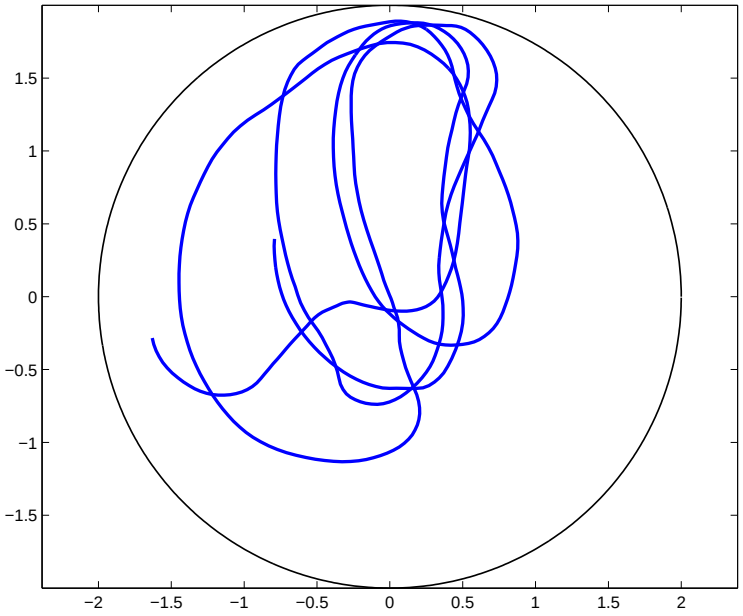

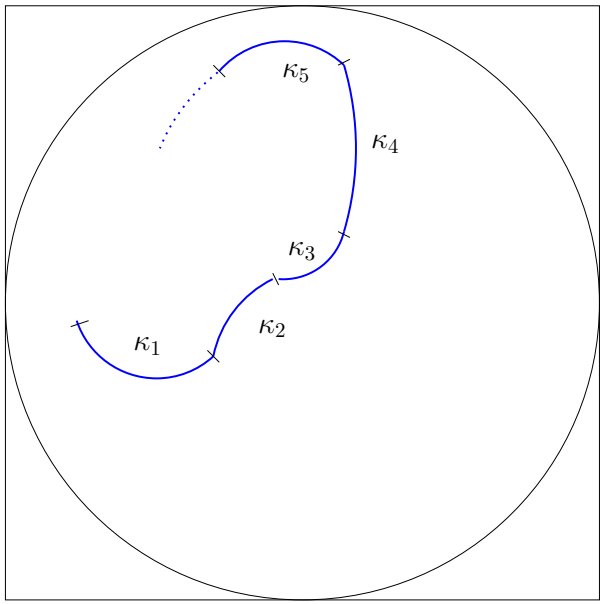

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PTW model

The model proposed is the following:

$$\begin{aligned} \frac{d\vec{x}}{dt} &= c\vec{\tau}(\theta) \\ \frac{d\theta}{dt} &= c\kappa \\ d\kappa &= -a\kappa\, dt + b\, dB_t \end{aligned}$$

where c is the speed, a the inverse of a relaxation time, b the intensity of diffusion.

We call this model "Persistent Turning Walker" (PTW)[1].

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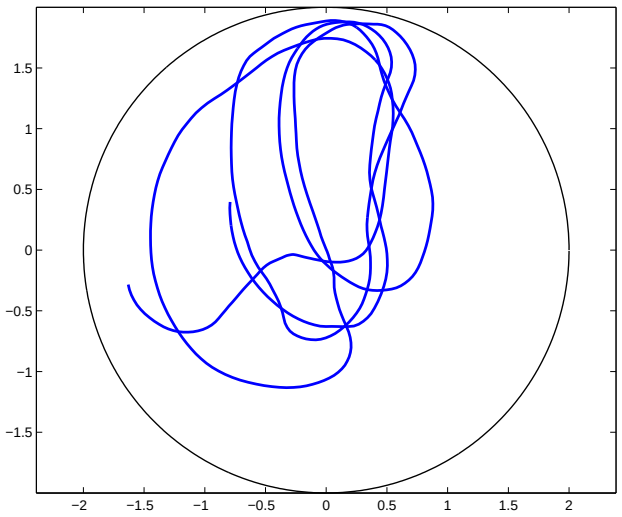
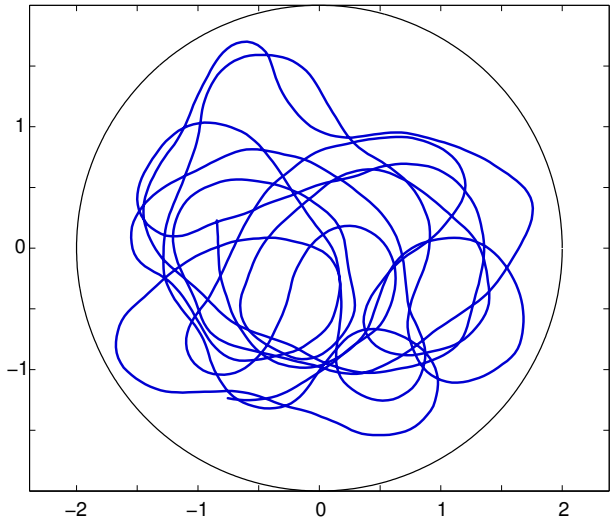
Comparison Data and Model



Experiment



Simulation (PTW model)

Derivation of a diffusion equation

To analyze the large scale dynamics of the PTW model, it is more convenient to manipulate the density distribution of particles $\mathbf{f}(\mathbf{t}, \mathbf{x}, \theta, \kappa)$.

PTW model

$$\begin{aligned} \frac{d\vec{x}}{dt} &= \vec{\tau}(\theta) \\ \frac{d\theta}{dt} &= \kappa \\ d\kappa &= -\kappa\, dt + \sqrt{2}\alpha\, dB_t \end{aligned}$$

(in scaled variables)

Kinetic equation

$$\partial_t f + \vec{\tau} \cdot \nabla_{\vec{x}} f$$

with

$$Lf = -\kappa \partial_\theta f + \partial_\kappa(\kappa f) + \alpha^2 \partial_{\kappa^2} f$$

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$$\partial_t f + \vec{\tau}\cdot\nabla_{\vec{x}} f + \kappa\partial_\theta f - \partial_\kappa(\kappa f) = \alpha^2 \partial_{\kappa^2} f$$

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$$Lf = -\kappa\partial_\theta f + \partial_\kappa(\kappa f) + \alpha^2\partial_{\kappa^2} f$$

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Derivation of a macroscopic model

- Step 1. *Diffusive scaling*: $t' = \varepsilon^2 t,\ x' = \varepsilon x$.
  In these *macroscopic* variables, f^ε satisfies:

$$\varepsilon \partial_t f^\varepsilon + \vec{\tau} \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} L(f^\varepsilon). \tag{1}$$

- Step 2. *Hilbert expansion*: $f^\varepsilon = f^0 + \varepsilon f^1 + \ldots$

$$\partial_t f^0 = \frac{1}{\varepsilon^2} L(f^1) + \frac{1}{\varepsilon} L(f^2) + \ldots$$

  with M a Gaussian with zero mean and unit variance.

- Step 3. *Integrate* in (θ, κ):

$$\int_{\theta,\kappa} \left(\varepsilon \partial_t f^\varepsilon + \vec{\tau} \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} L(f^\varepsilon) \right) d\theta d\kappa.$$

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$$Lf^0 = 0 \quad \Rightarrow \quad f^0 = \rho^0(x) \frac{\mathcal{N}(\kappa)}{2\pi} \quad (\textit{equilibrium})$$

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Diffusion equation

Thm.[2] The distribution f^ε solution of (1) satisfies:

$$f^\varepsilon \overset{\varepsilon \to 0}{\rightharpoonup} \rho^0 \frac{\mathcal{N}(\kappa)}{2\pi},$$

with:

$$\partial_t \rho^0 + \nabla_{\vec{x}} \cdot J^0 = 0,$$
$$J^0 = -D \nabla_{\vec{x}} \rho^0,$$

where $D = \int_0^\infty \exp^{-\alpha^2(-1+s+e^{-s})}\, ds$.

Probabilistic point of view.

$$= x_0 + \int_0 \cos(\theta_s)\, ds$$

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Probabilistic point of view.

$$x(t) = x_0 + \int_0^t \cos(\theta_s)\, ds \quad \overset{\varepsilon \to 0}{\longrightarrow} \quad 0 \quad + \quad D\, \widetilde{B}_{t'}$$

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$$x^\varepsilon(t') = \varepsilon x_0 + \varepsilon \int_0^{t'/\varepsilon^2} \cos(\theta_s)\, ds \overset{\varepsilon \to 0}{\longrightarrow} 0 + D\, \widetilde{B}_{t'}$$

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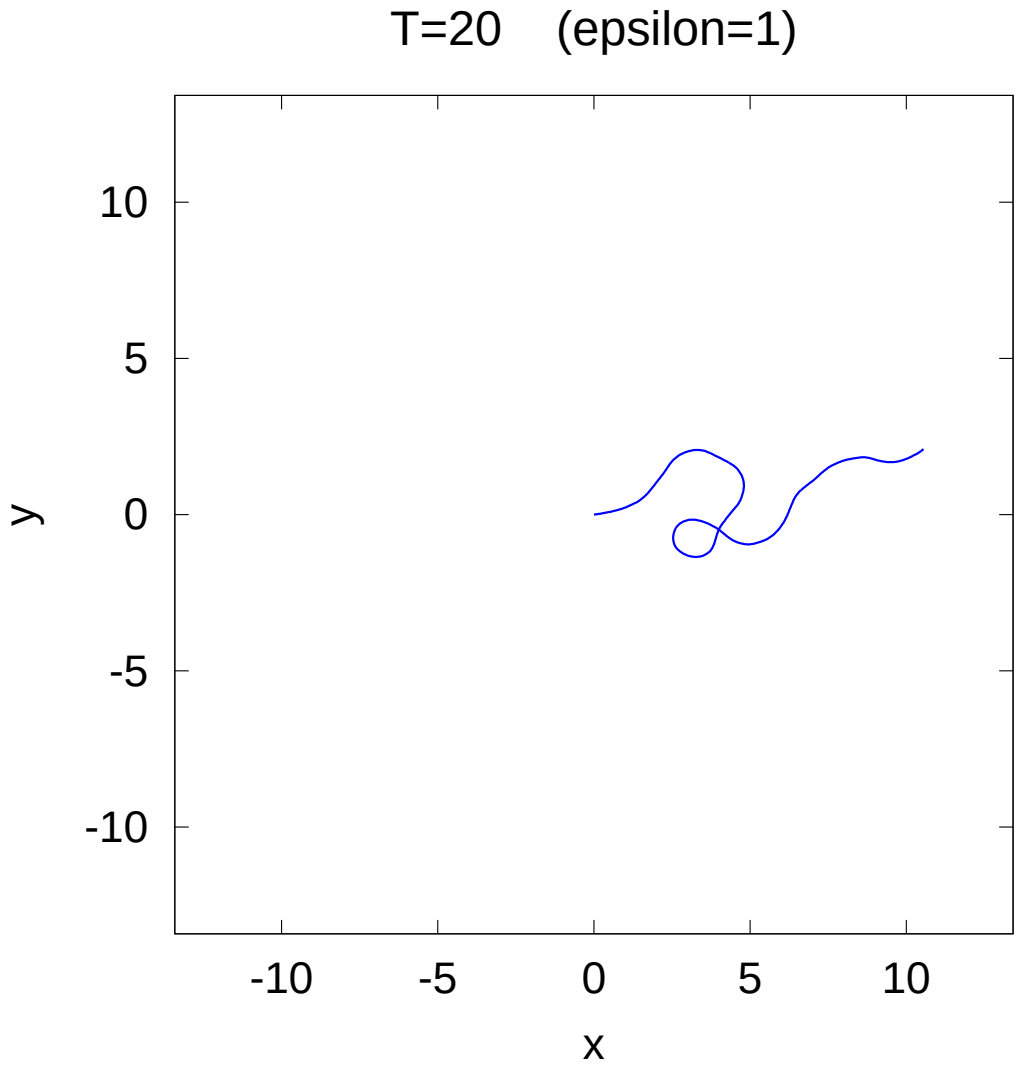
Illustration: one trajectory $\vec{x}(t)$



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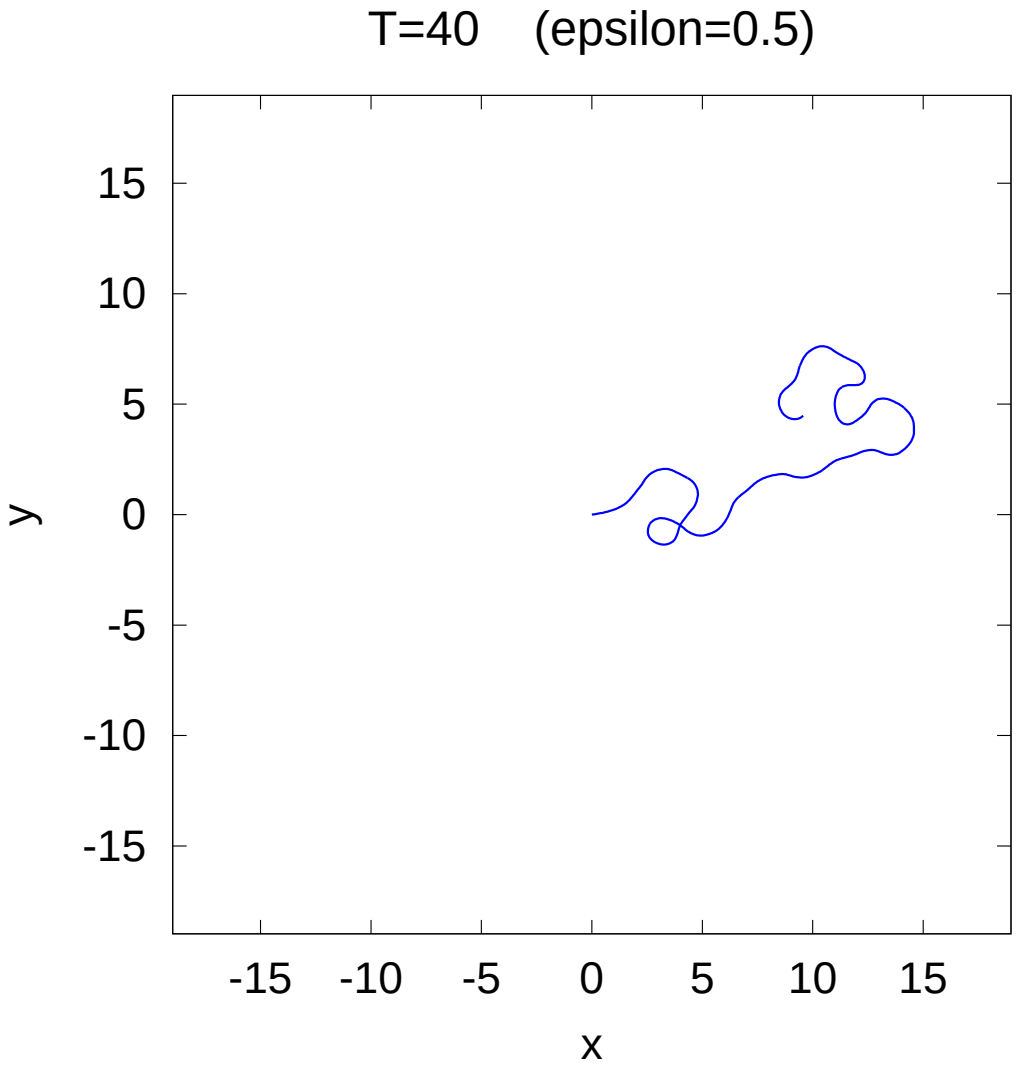

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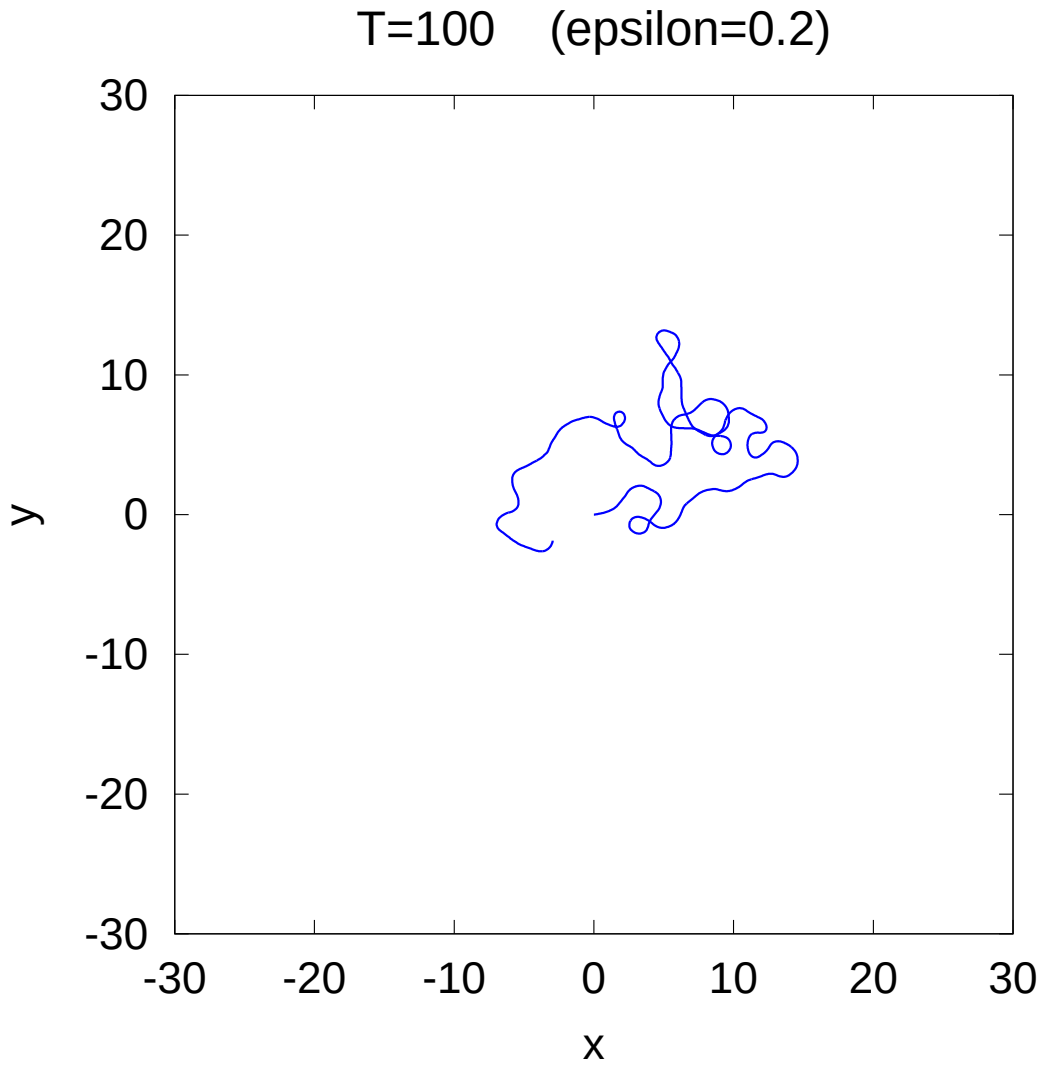

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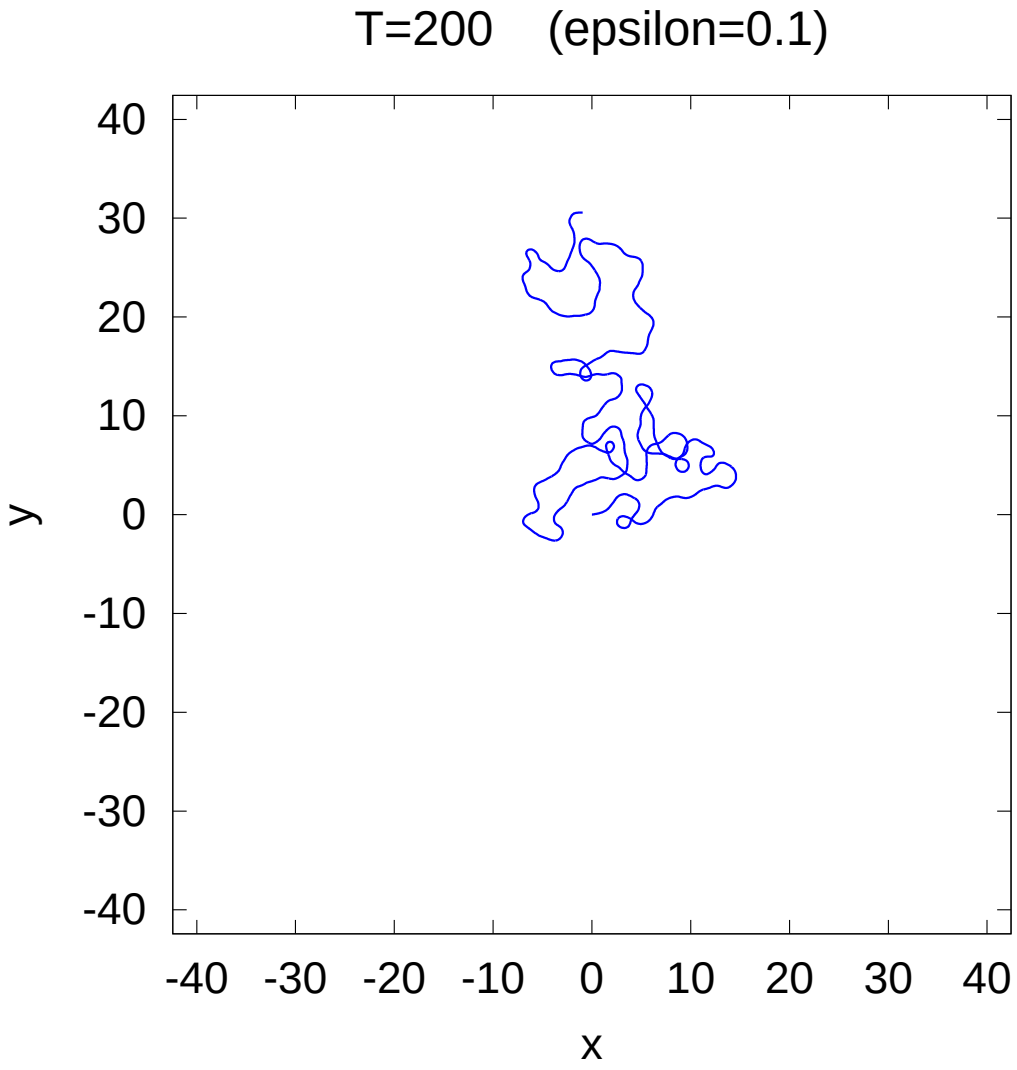

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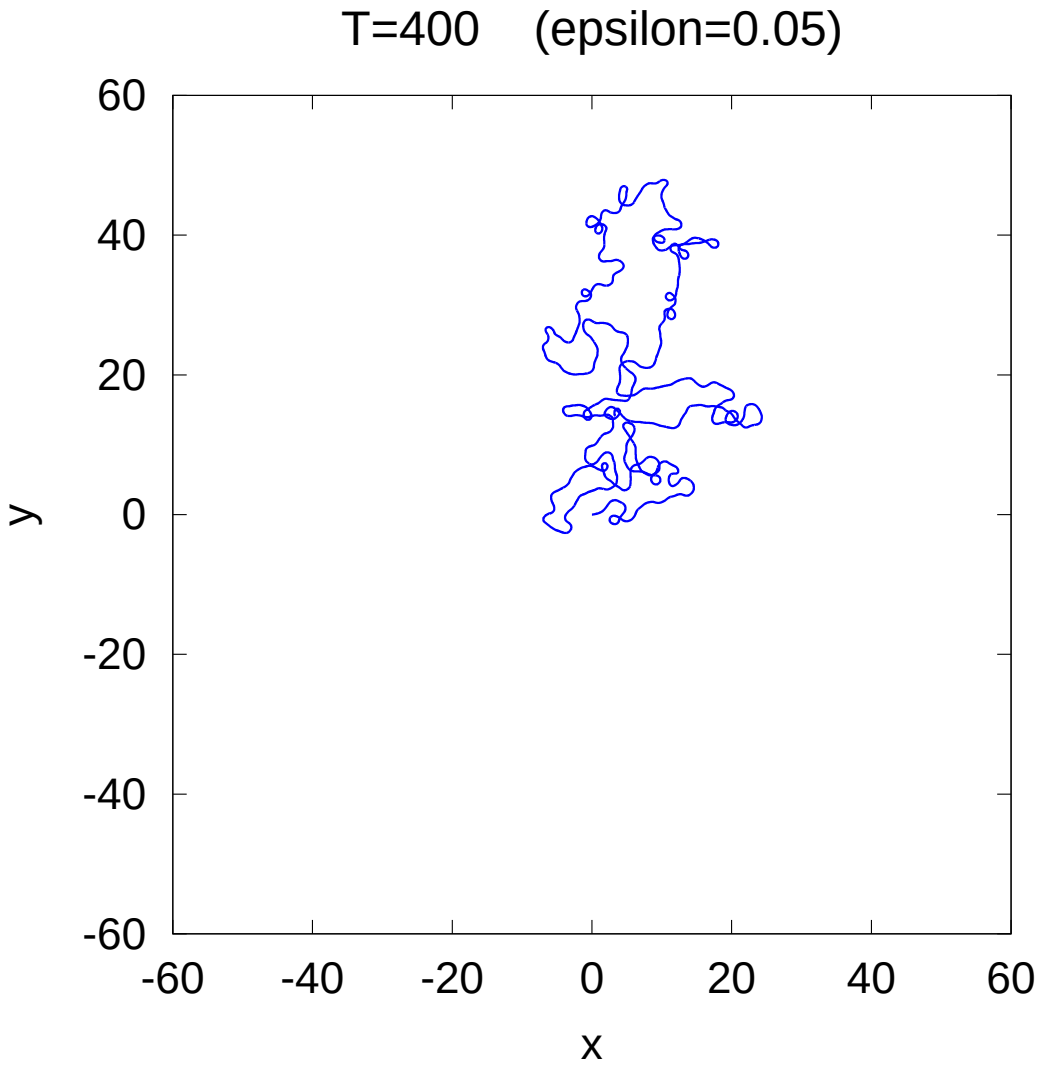

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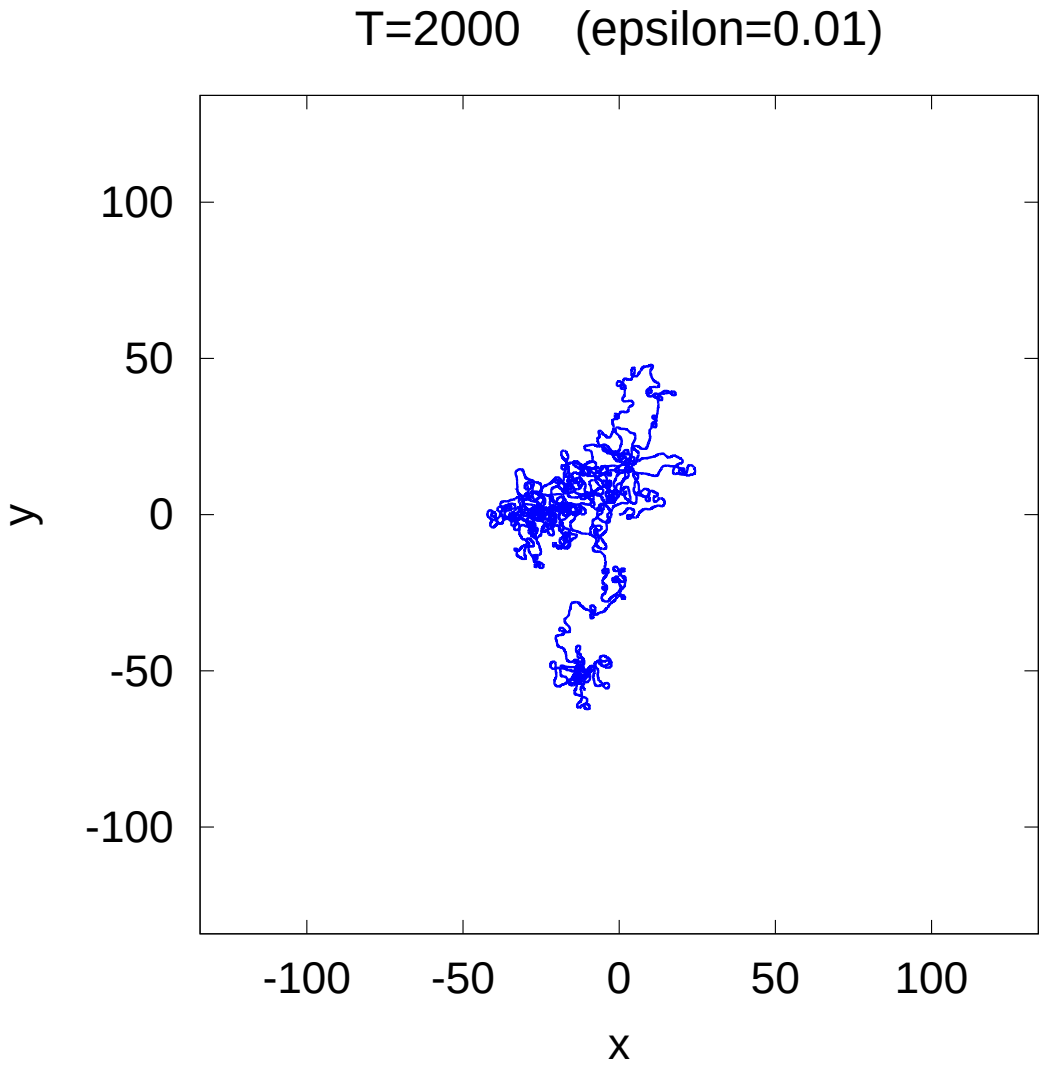

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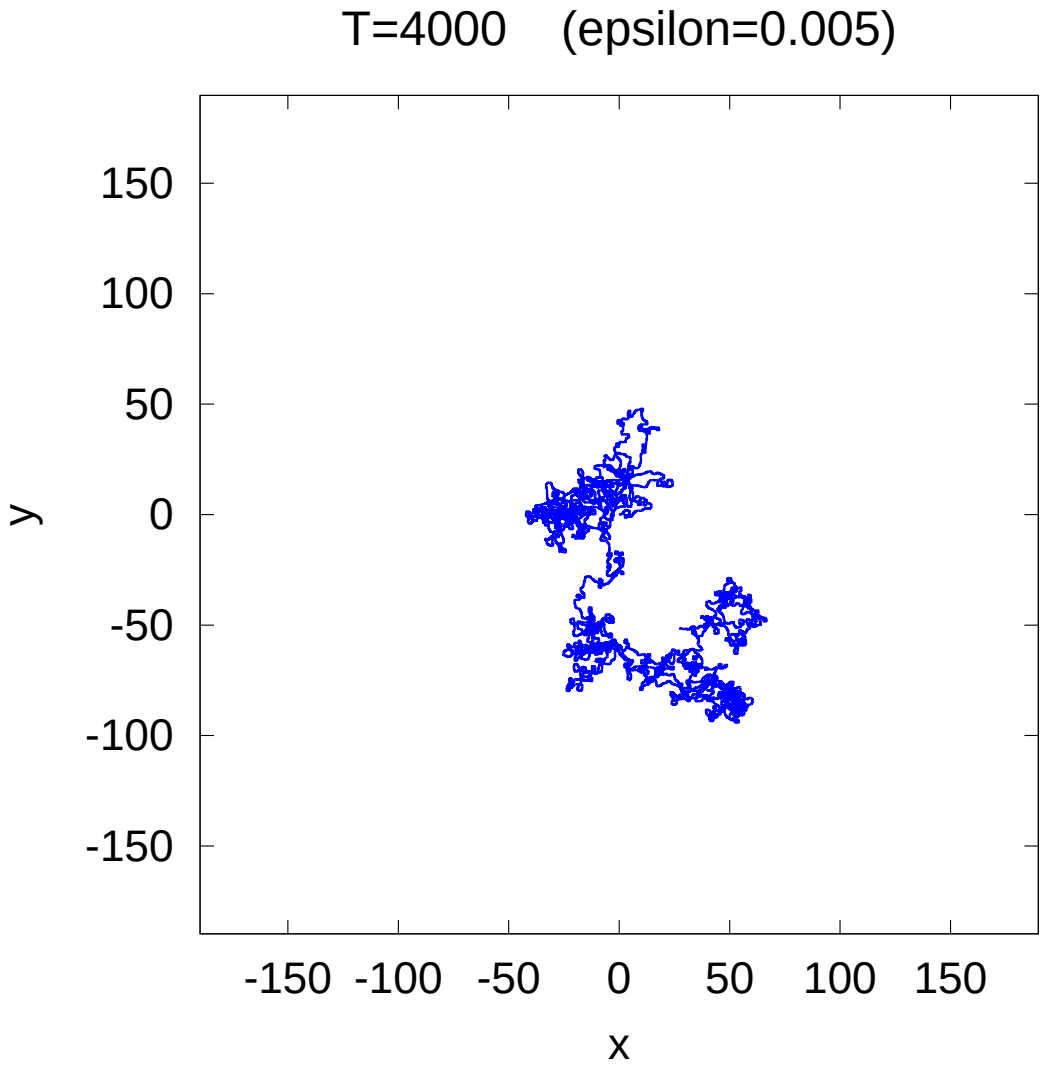
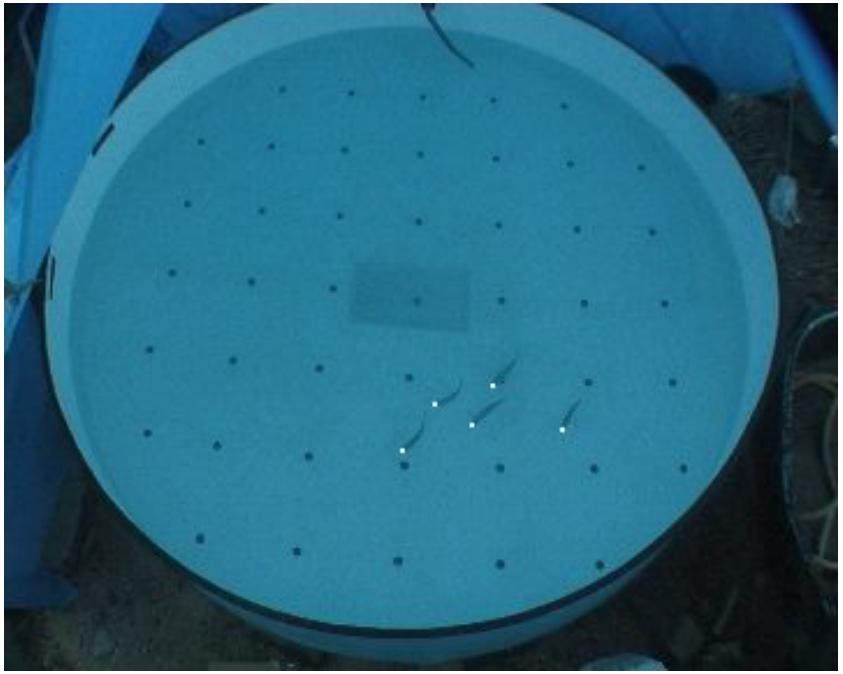


Fish in interaction

- In group, fish are usually aligned
- To measure this effect, we observe the velocity of the neighbors in the frame of reference of one fish :



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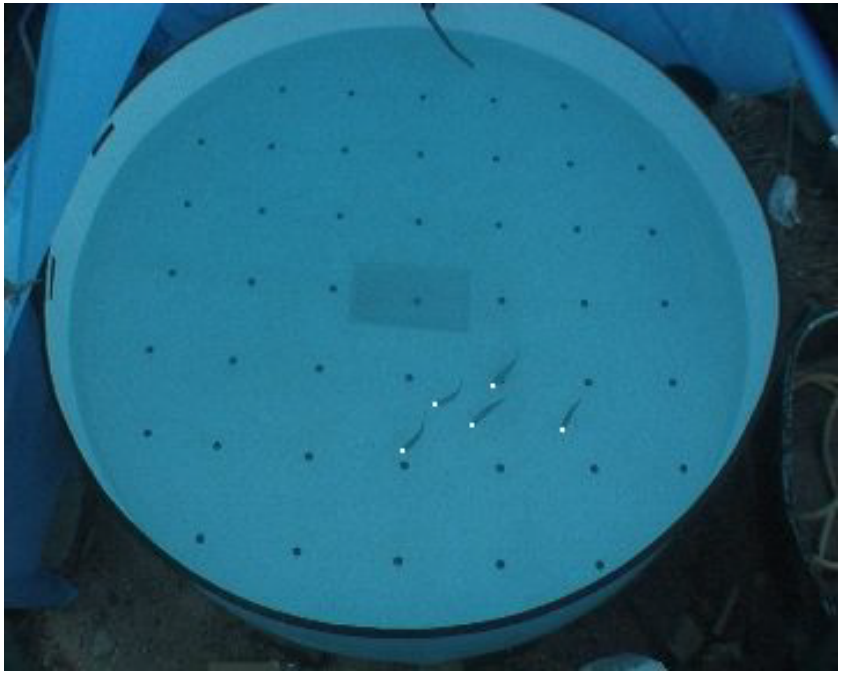

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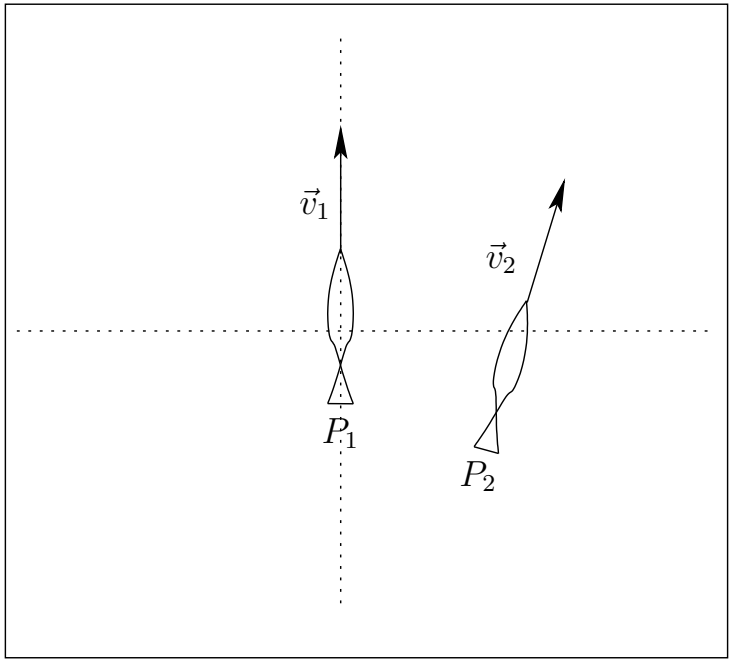

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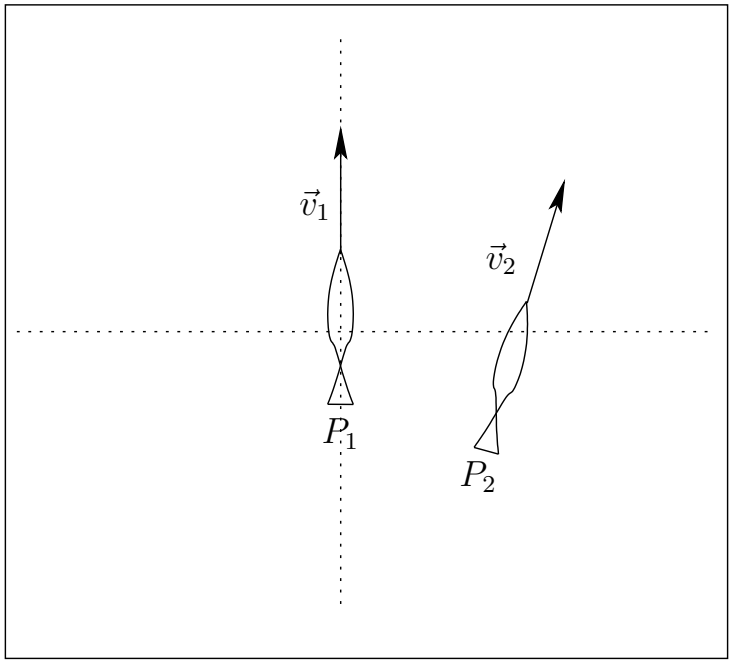

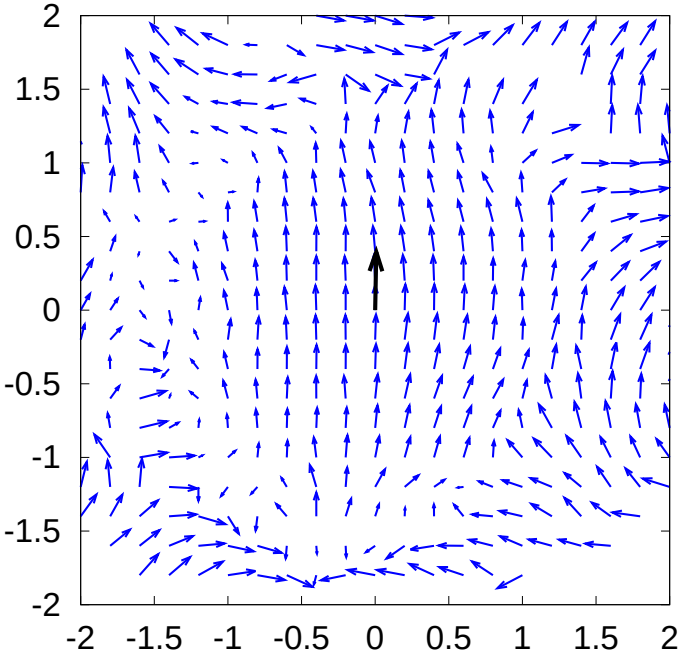

Experimental data

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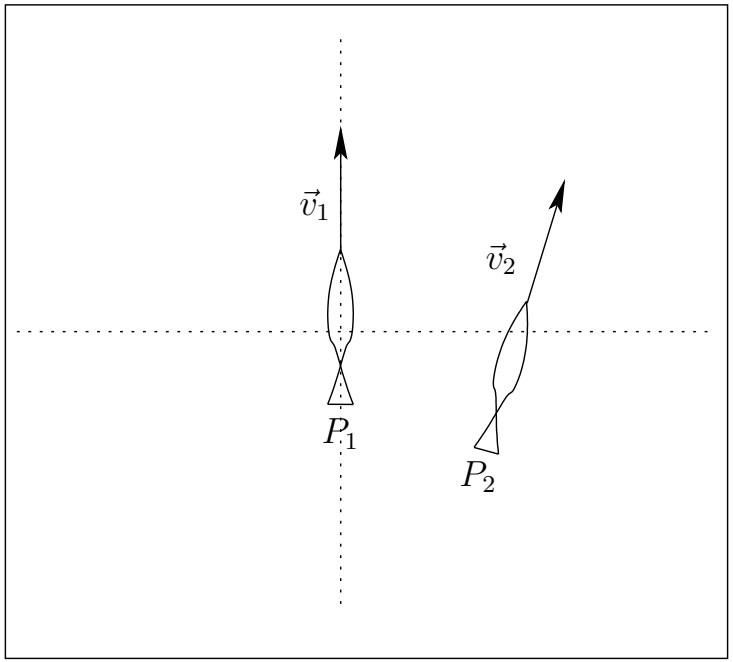
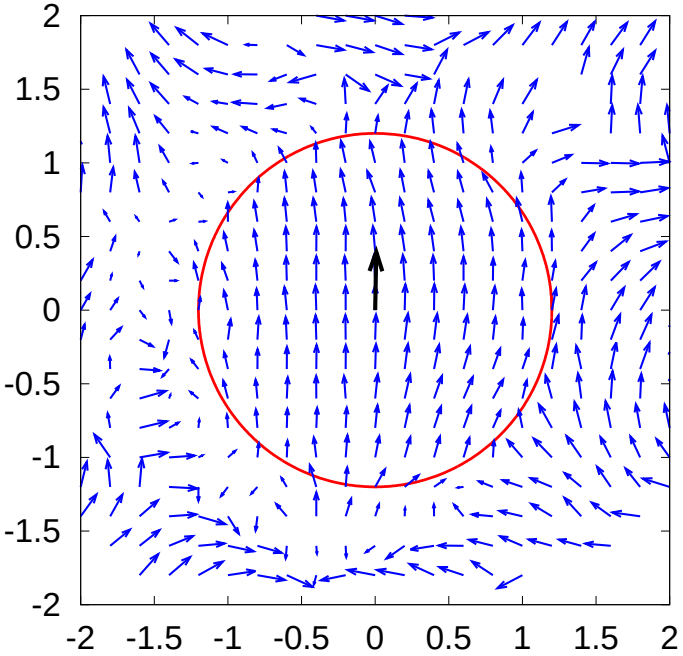
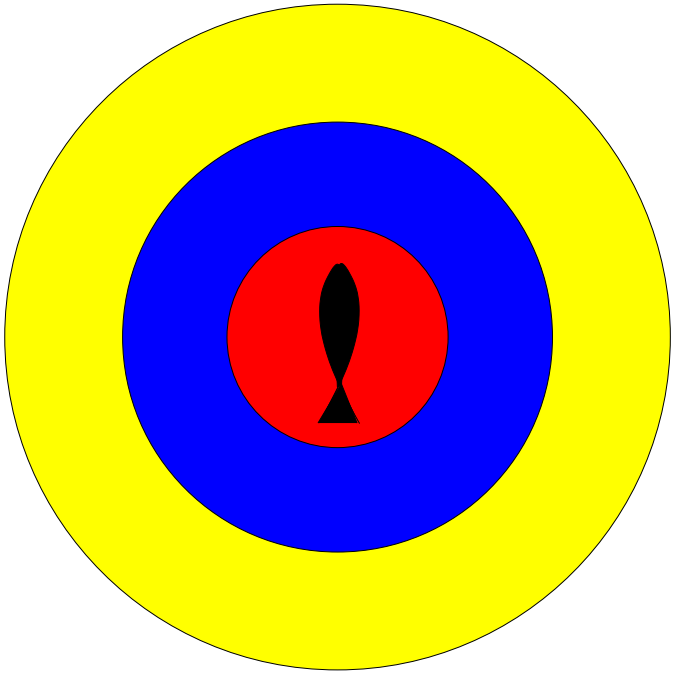




Experimental data

Fish in interaction

Classical model with 3 zones



: attraction

: alignment

: repulsive

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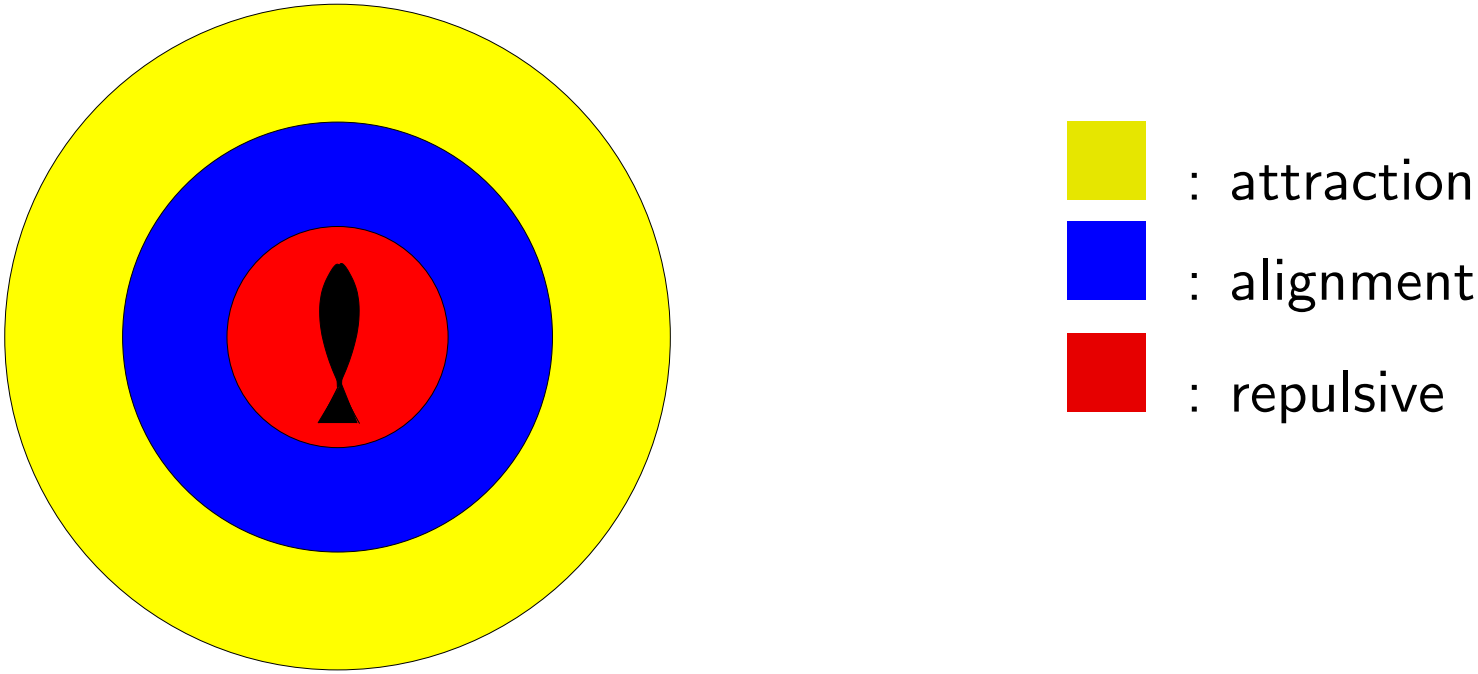

Ref.: Aoki (1982), Reynolds (1986),
Huth-Wissel (1992), Couzin et al. (2002),...

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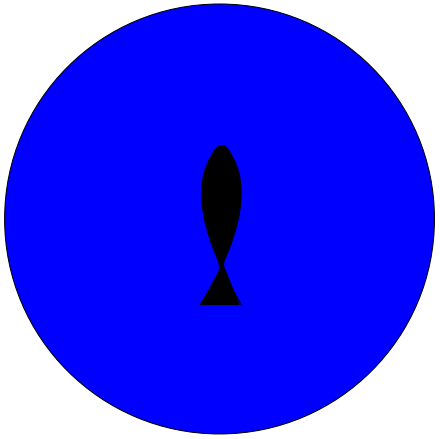


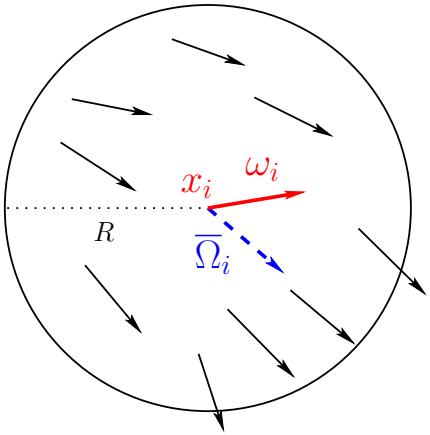
: alignment

Ref.: Vicsek (1995), Gregoire-Chaté (2004), Cucker-Smale (2007), Ha-Tadmor (2008),...

Outline

Vicsek model ('95)

Discrete dynamics:



$$\begin{aligned} x_i^{n+1} &= x_i^n + \Delta t\, \omega_i^n \\ \omega_i^{n+1} &= \overline{\Omega}_i^n + \epsilon \end{aligned} \qquad (2)$$

with $\overline{\Omega}_i^n = \dfrac{\sum_{|x_j - x_i| < R}\ \omega_j^n}{\left|\sum_{|x_j - x_i| < R}\ \omega_j^n\right|}$, ϵ noise.

Continuous dynamics:

$$\begin{aligned} \frac{dx_i}{dt} &= \omega_i \\ d\omega_i &= (\mathrm{Id} - \omega_i \otimes \omega_i)(\nu\, \overline{\Omega}_i\, dt + \sqrt{2D}\, dB_t) \end{aligned} \qquad (3)$$

Remark. eq. (3) + "$\nu \Delta t = 1$" $\Rightarrow$ eq. (2)

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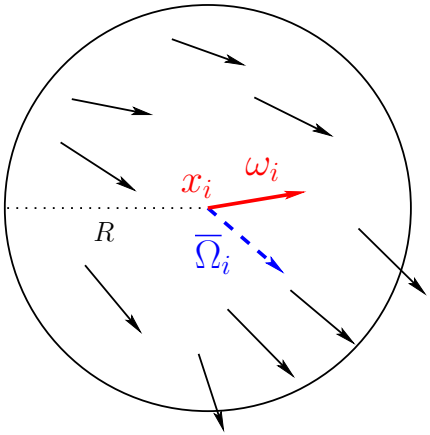

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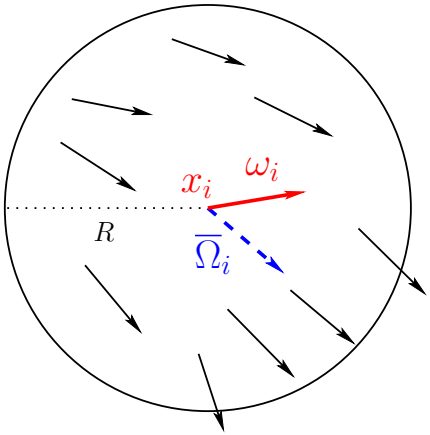

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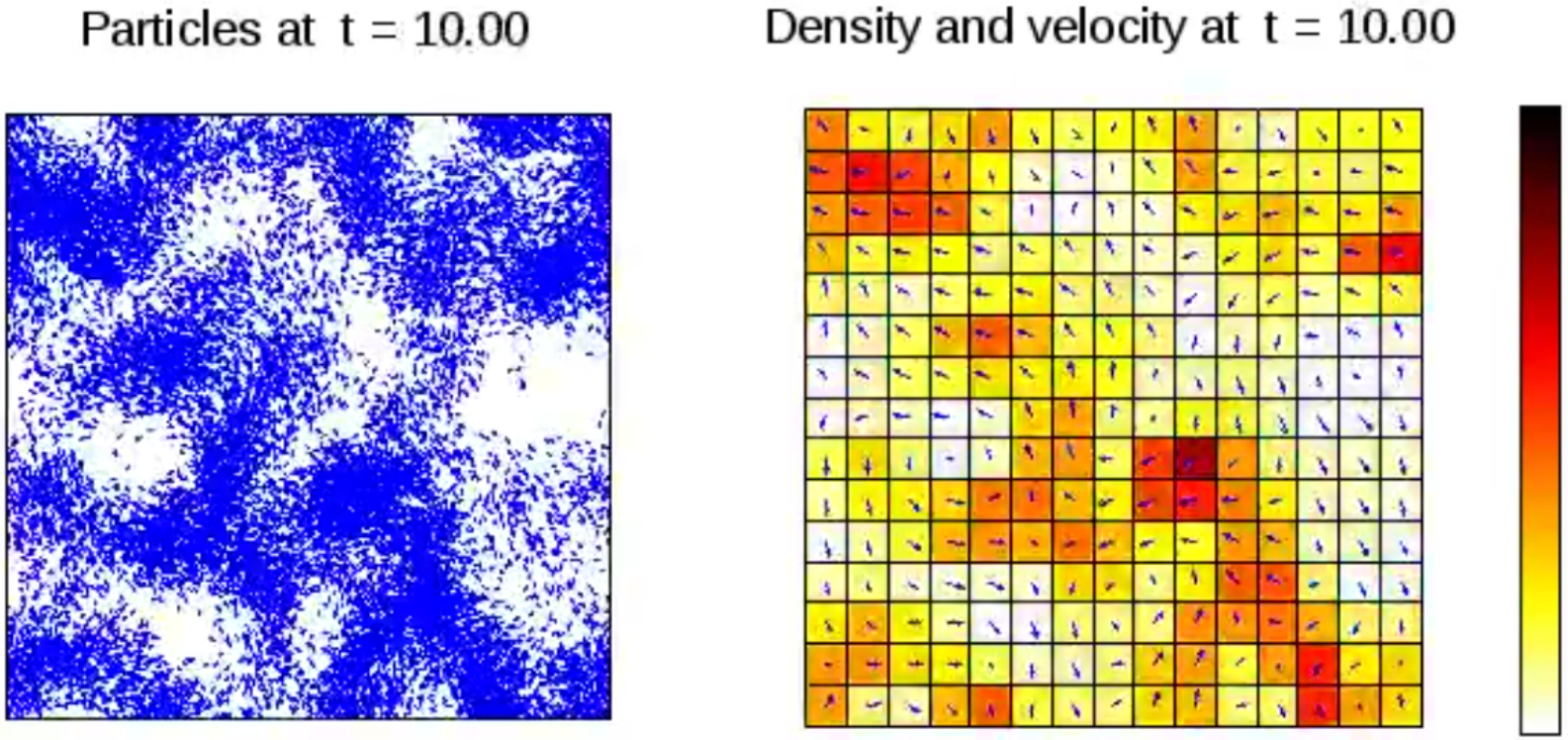
Particles at t = 10.00
Density and velocity at t = 10.00

Kinetic equation

Under the *hypothesis of propagation of chaos*[3], the density of particles $f(t,x,\omega)$ satisfies:

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

with :

$$F(x,\omega) = (\mathrm{Id} - \omega \otimes \omega)\, \nu \overline{\Omega}(x) \quad , \quad \overline{\Omega}(x) = \frac{J(x)}{|J(x)|}$$

$$J(x) = \int_{|y-x|<R,\, \omega^* \in \mathbb{S}^1} \omega^*\, f(y,\omega^*)\, dy\, d\omega^*$$

- The alignment is expressed by the operator $\nabla_\omega \cdot F f$,
- The randomness is expressed by $D \Delta_\omega f$.

[3] **Sznitman**, Saint-Flour (89)

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Kinetic equation

Finally, f satisfies:

$$\partial_t f + \omega \cdot \nabla_x f = Q(f) \tag{4}$$

with: $Q(f) = -\nabla_\omega \cdot (Ff) + D\Delta_\omega f$.

- The *equilibrium* of $Q(f)$ (i.e. $Qf = 0$) are the Von Mises distributions:

$$\mathcal{M}_\Omega(\omega) = C \exp\left(\frac{\omega \cdot \Omega}{T}\right)$$

  where $T = D/\nu$ and Ω is an arbitrary direction.
- The *total momentum* is **not** preserved by the operator:

$$\int_\omega Q(f)\omega \, d\omega \neq 0.$$

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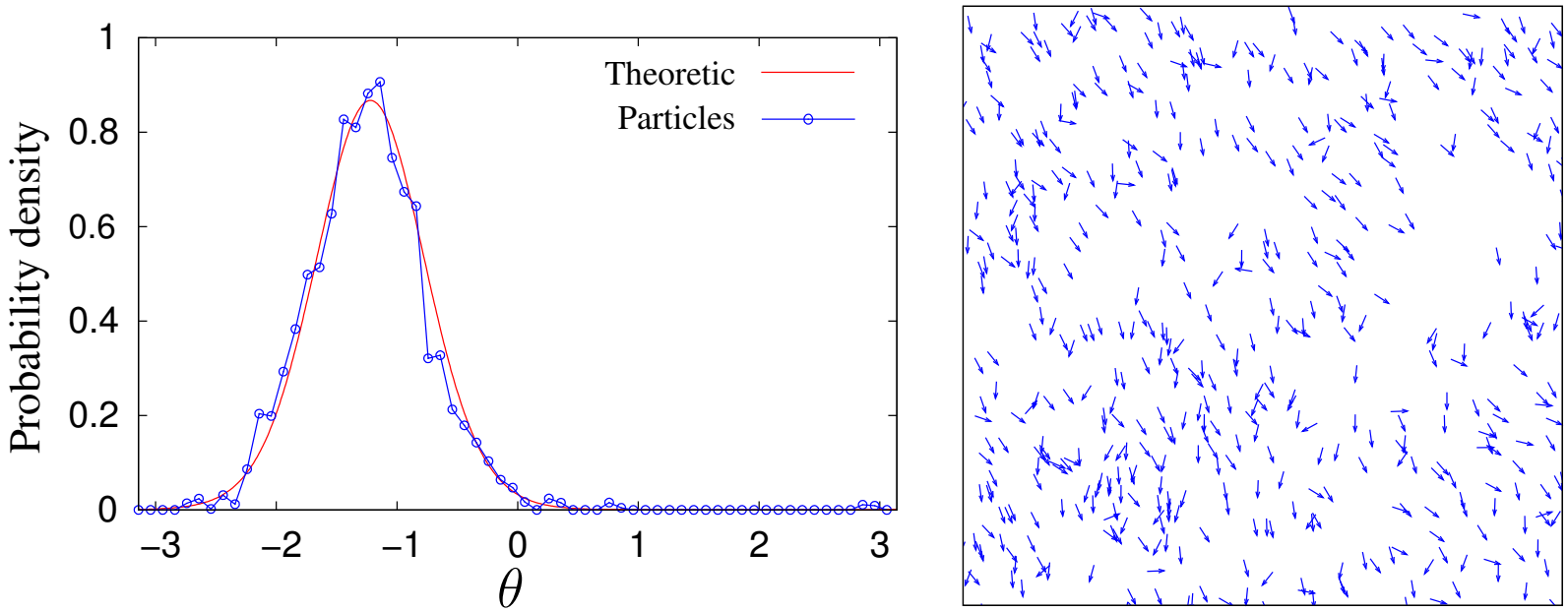

Figure: *Local* distribution of velocity f (**Left**) for a simulation in a *small* domain (**Right**).

Derivation of a hyperbolic system

- Step 1. *Hydrodynamic scaling*: $t' = \varepsilon t,\ x' = \varepsilon x$.
  In these macroscopic variables, f^ε satisfies:

$$\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon). \tag{5}$$

- Step 2. Hilbert expansion: $f^\varepsilon = f^0 + \varepsilon f^1 + \ldots$

  $\Rightarrow$ Equation for the equilibrium

- Step 3. Integrate (5) against the *collisional invariants*

$$\int_\omega [\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)]\, \psi\, d\omega$$

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<u>Problem</u>: Only **one** quantity is preserved by Q.

Momentum is **not** *preserved by the dynamics*

Def. ψ is a if for every f

$$\int_\omega Q(f)\psi \, d\omega = 0 \quad \Rightarrow \quad \int_\omega f \, Q^*_{\Omega_f}(\psi) \, d\omega = 0$$

Then, we can integrate the kinetic equation:

$$\int_\omega [\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)] \begin{pmatrix} 1 \\ \varphi_{\Omega^\varepsilon}(\omega) \end{pmatrix} d\omega$$

Derivation of a hyperbolic system

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Def. ψ is a collisional invariant if for every f satisfying $\int_\omega \omega f \, d\omega \, // \, \Omega$

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Hyperbolic system

Thm.[4] The distribution f^ε solution of (5) satisfies:

$$f^\varepsilon \overset{\varepsilon \to 0}{\rightharpoonup} \rho\, \mathcal{M}_\Omega(\omega)$$

Hyperbolic system

$$\begin{aligned}
&\partial_t \rho + c_1 \nabla_x \cdot (\rho \Omega) = 0, \\
&\rho(\partial_t \Omega + c_2 (\Omega \cdot \nabla_x)\Omega) + \lambda\,(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0, \\
&|\Omega| = 1
\end{aligned}$$

where c_1, c_2 and λ depend on $T = D/\nu$.

Remarks:

- the system obtained is hyperbolic...
- ...but non-conservative (due to the constraint $|\Omega| = 1$)
- ρ and Ω have different convection speeds ($c_1 \neq c_2$).

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- The model is non-conservative...
- ...and has a geometric constraint

$\Rightarrow$ *No available theory to deal with this system.*

Numerical simulation

We want to numerically solve the macroscopic Vicsek (**MV**) model:

$$\begin{aligned}
&\partial_t \rho + c_1 \nabla_x \cdot (\rho \Omega) = 0, \\
&\rho(\partial_t \Omega + c_2 (\Omega \cdot \nabla_x)\Omega) + \lambda\,(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0, \\
&|\Omega| = 1
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Splitting method

The main idea of this method is to replace the geometric constraint ($|\Omega| = 1$) by a relaxation operator:

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

In the limit $\eta \to 0$, we recover the original MV model.

To solve numerically this system, we proceed in two steps (*splitting*):

- Step 1: we solve the relaxation part (hyperbolic part)
- Step 2: we solve the relaxation part (ODE part)

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To solve numerically this system, we proceed in two steps (*splitting*):

- Step 1: we solve the transport equation (without the constraint)
- Step 2: we project the solution on the constraint

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- Second, we solve the relaxation part :

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Other numerical methods

In one direction, the system is written:

$$\begin{aligned} \partial_t \rho + c_1 \partial_x (\rho \cos\theta) &= 0 \\ \partial_t \theta + c_2 \cos\theta \, \partial_x \theta - \lambda \frac{\sin\theta}{\rho} \partial_x \rho &= 0. \end{aligned} \tag{6}$$

Multiplying (6) by $1/\sin\theta$ and integrating in θ, we find a *conservative formulation* of the MV model.

Solving the conservative formulation gives another method
$\Rightarrow$ **Conservative method**

Remark. Other methods can be developed using the "non-conservative" form of the MV model (e.g. *upwind scheme*).

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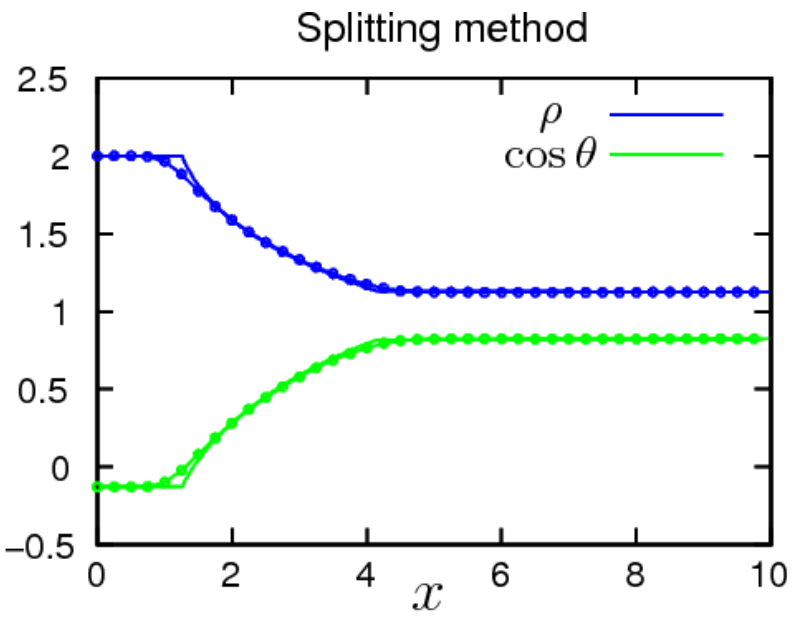
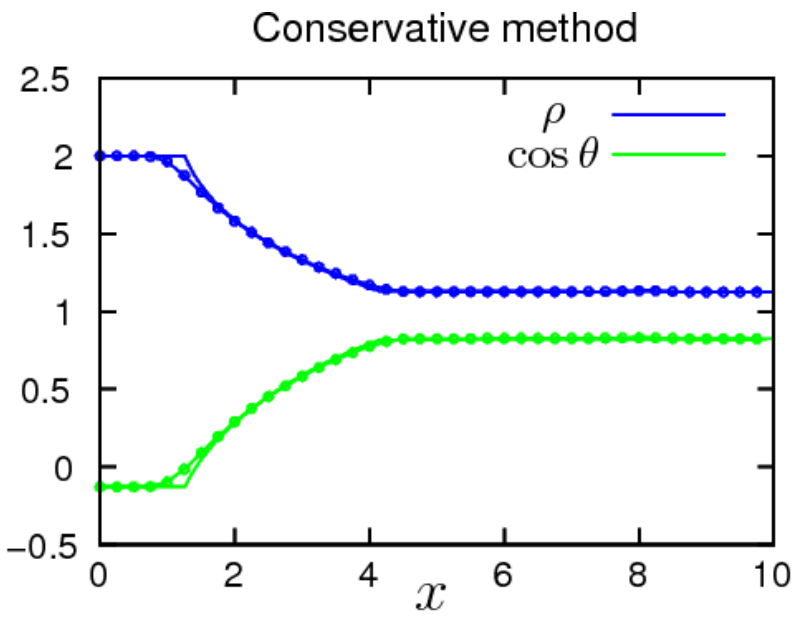
Simulations 1

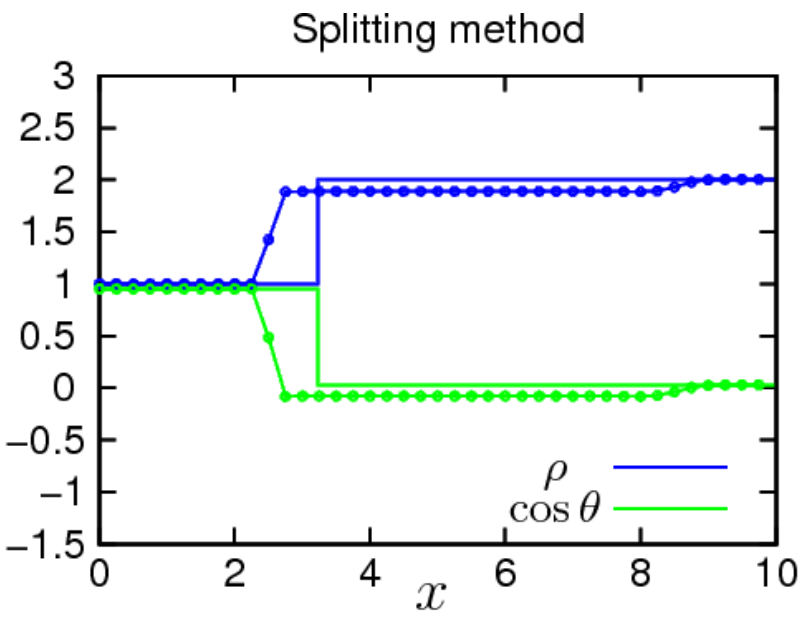
The numerical schemes agree with each other on *rarefaction waves* (smooth solutions)

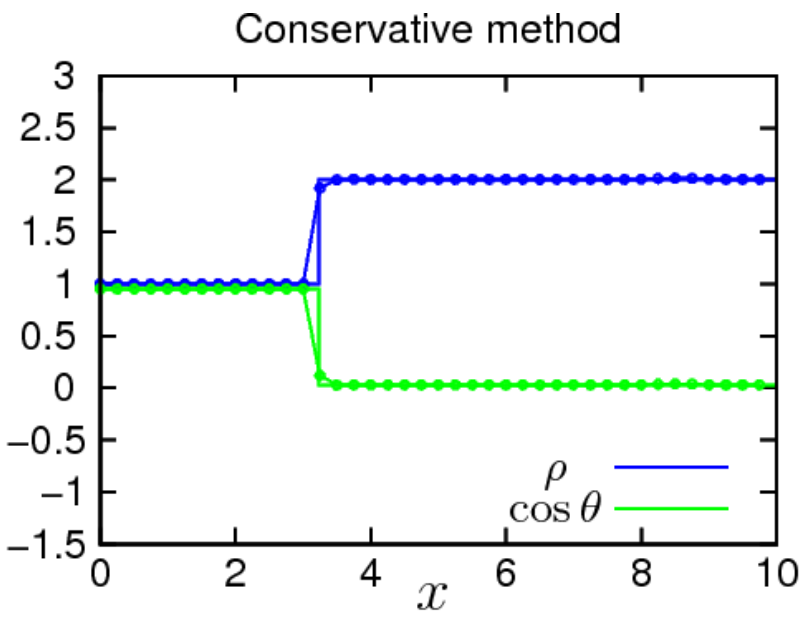




Simulations 2

However, the numerical schemes disagree when the solution is a *shock wave* (**non-smooth** solutions)





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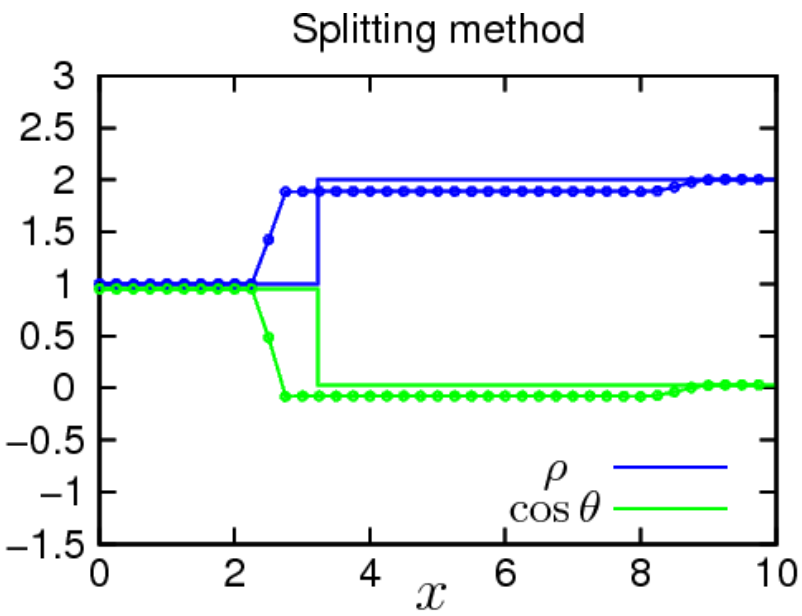

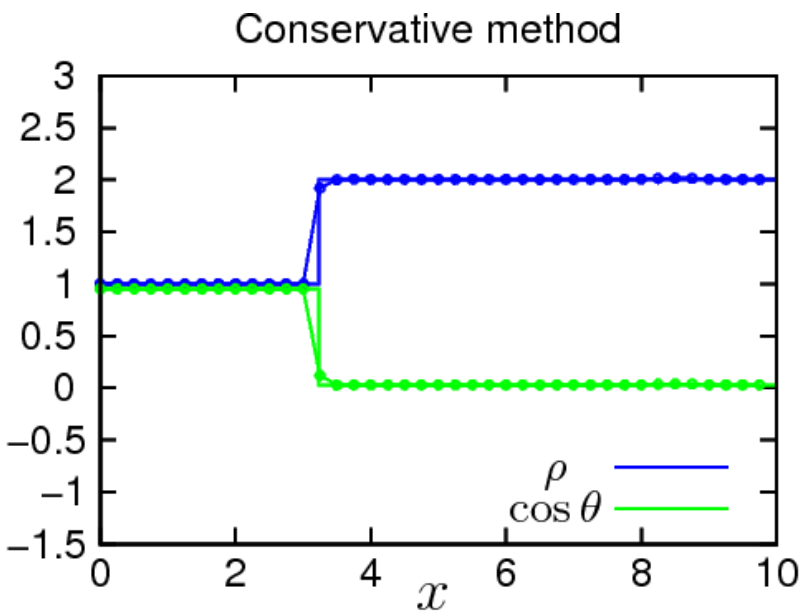

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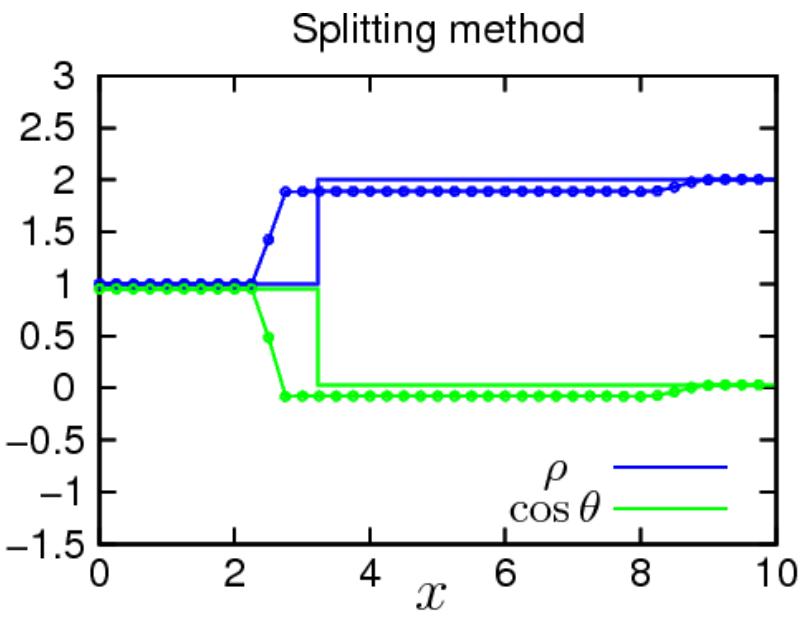

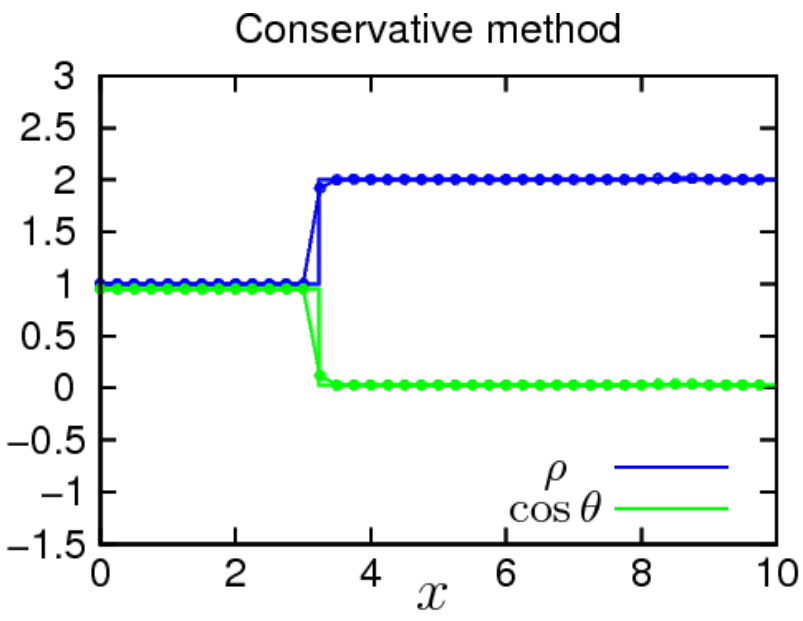

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Particle simulations

Since there is **no** theoretical solution to test our numerical simulations, we use the microscopic Vicsek model as a *benchmark*:

$$\frac{dx_k^\varepsilon}{dt} = \omega_k^\varepsilon,$$

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We use Riemann problem as initial condition.

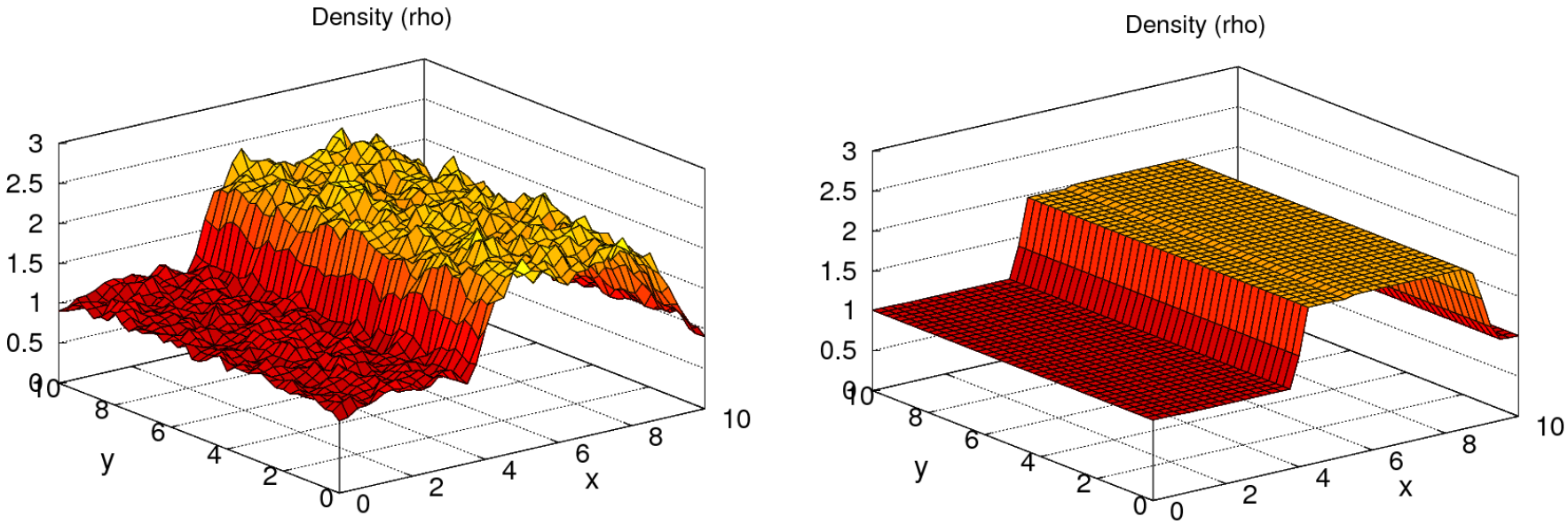

Figure: Density ρ: Micro (left) and Macro (right)

We take a cross section of the distribution in the x-direction:

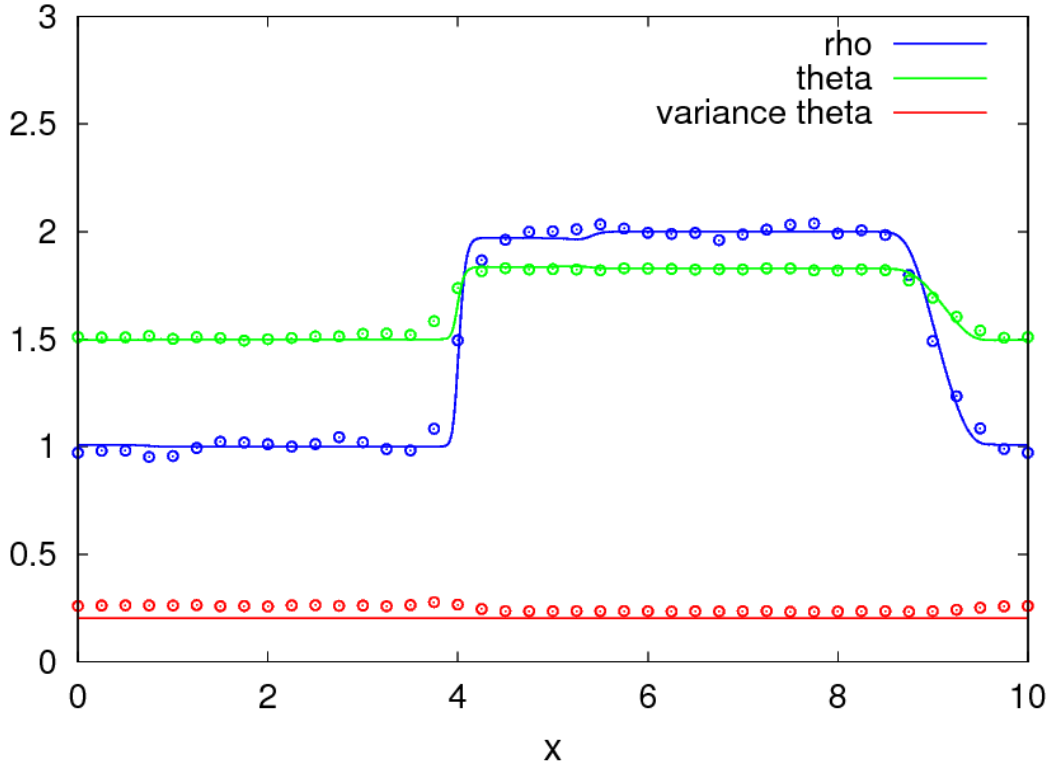

Figure: macro. equation (line) and micro. equation (dot) at time $t = 2$.

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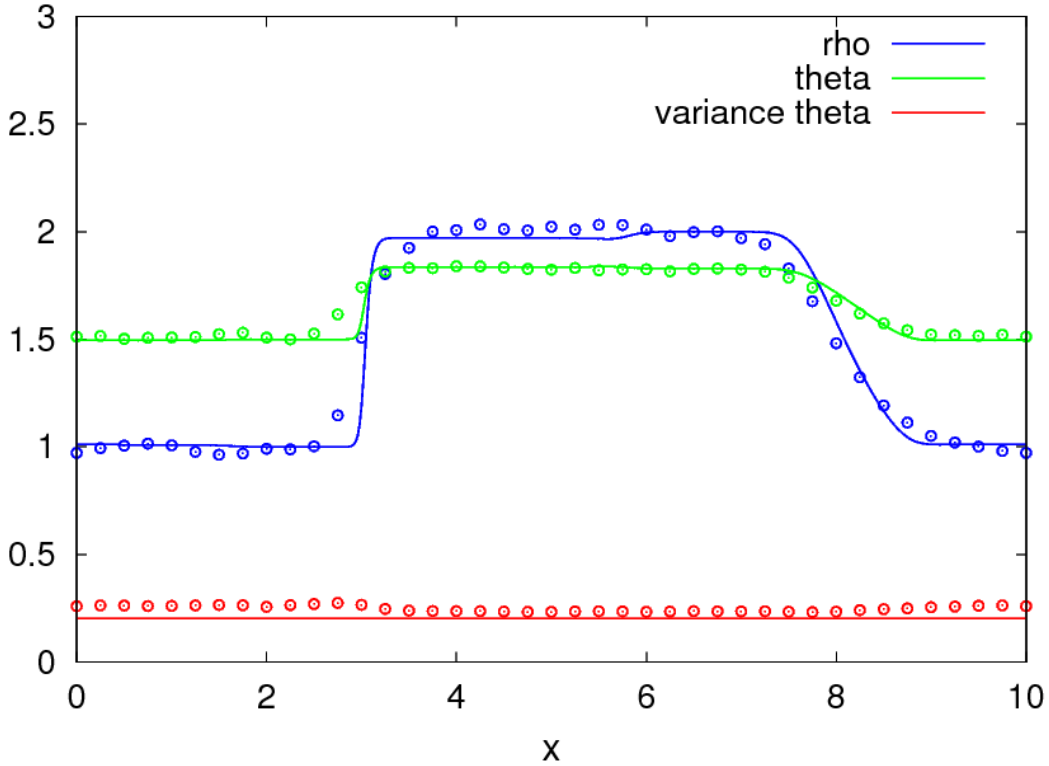
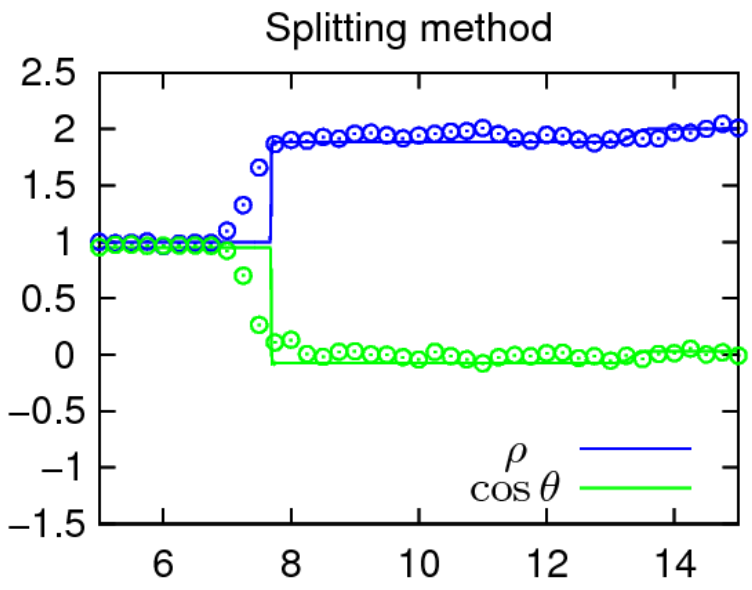
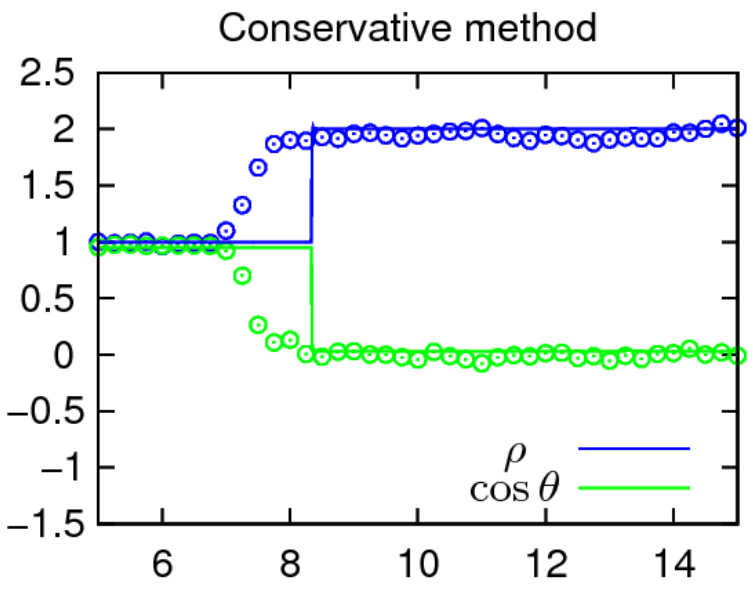


Figure: macro. equation (line) and micro. equation (dot) at time $t = 4$.

Micro vs macro

We compare the solutions of the MV model with the particles for the shock-wave solution:





The splitting method has the "correct speed".

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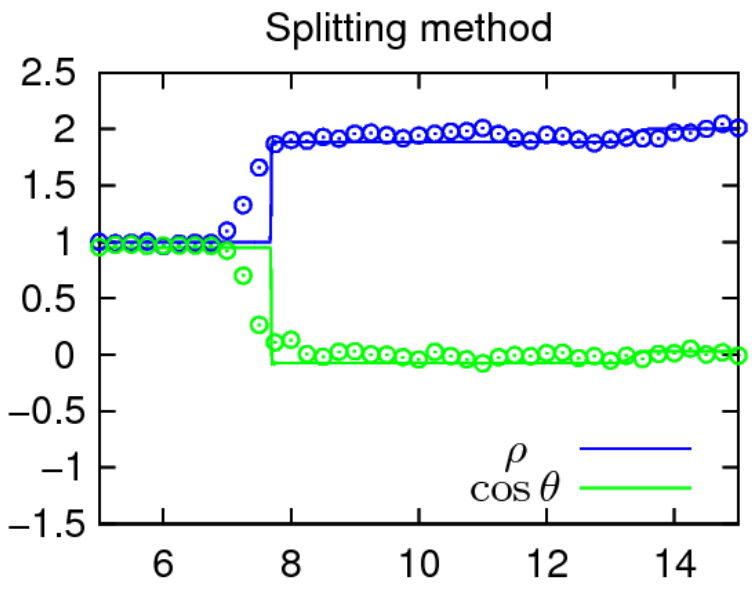

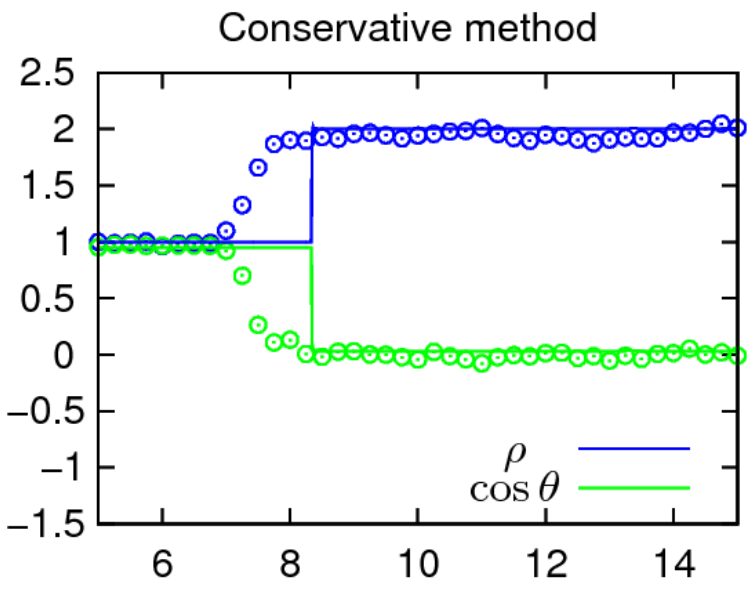

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Contact discontinuity

For an initial condition given as a *contact discontinuity*, a weak solution is given by a traveling wave.
We observe numerically another type of solution[5]:

[5] **M., Navoret**, SIAM Multiscale Modeling & Simulation (2011)

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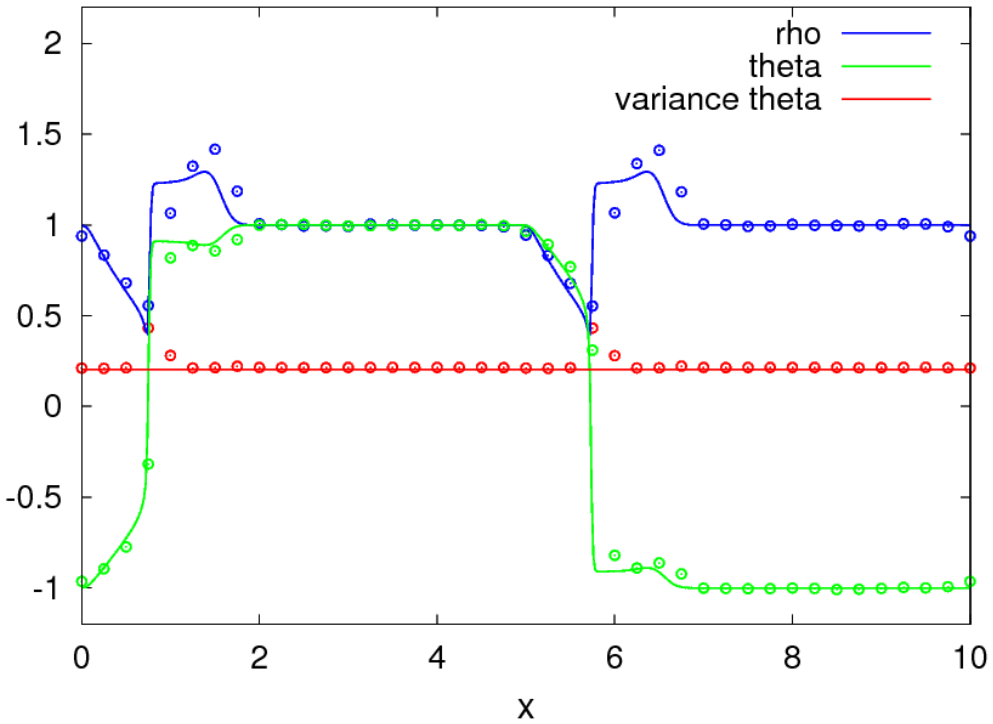

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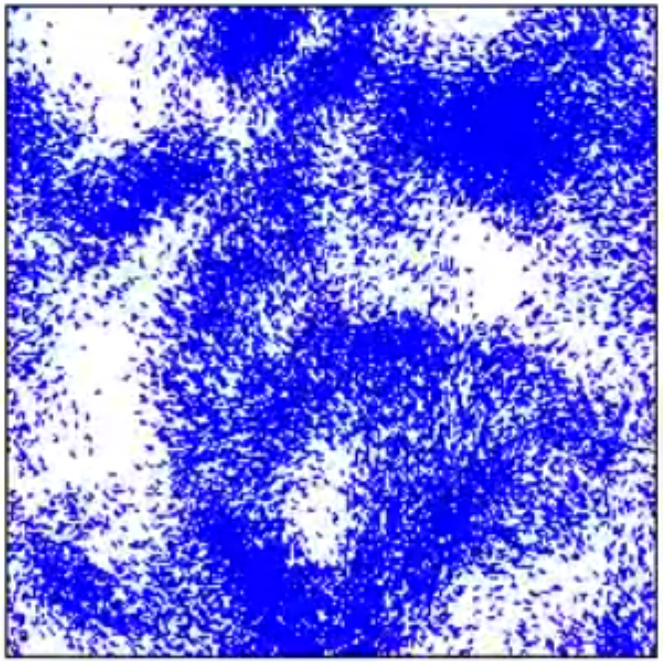
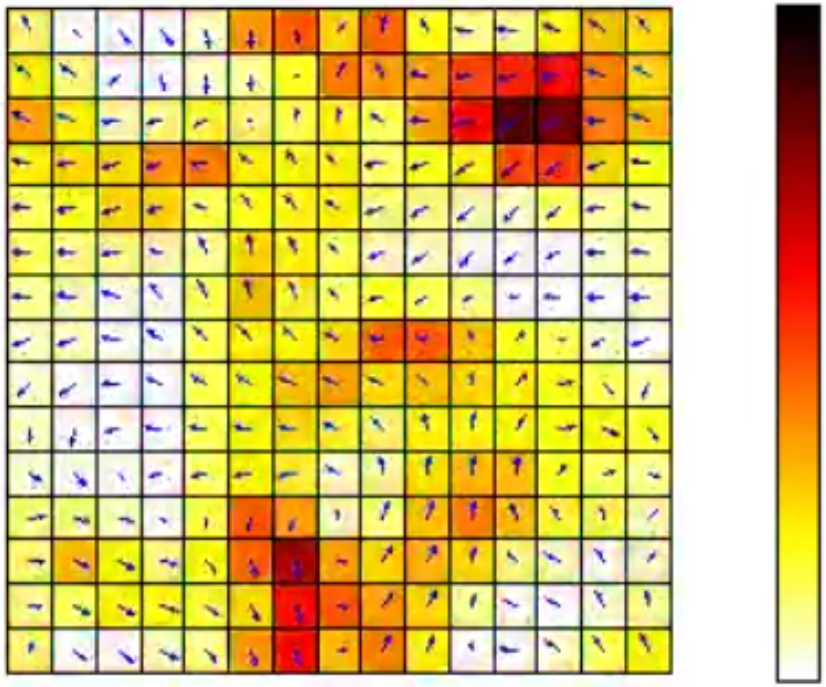
General case

How about *non-standard* initial condition?





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