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

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UC Davis, Applied Math PDE Seminar
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Motivation

- Individuals have only local interactions
- There is no leader inside the group (⇒ 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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How can we connect individual and global dynamics?
Methodology

- Experiments, data recording
- Statistical analysis
- Individual Based Model (IBM)
- Identify the rules for individual behavior

- Kinetic equation
- Macroscopic equation
- Capture the global behavior of the system
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Outline

1 PTW model
   - Experiments and model
   - Derivation of a diffusion equation

2 Vicsek model
   - The model
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3 Numerical schemes
   - Splitting method
   - Particle simulations
   - Micro vs macro
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:

- The norm of the velocity is constant
- The trajectory is smooth, the fish seems to turn constantly
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The model proposed is the following:

\[
\begin{align*}
    \frac{d\bar{x}}{dt} &= c\bar{\tau}(\theta) \\
    \frac{d\theta}{dt} &= c\kappa \\
    d\kappa &= -a\kappa\,dt + b\,dB_t
\end{align*}
\]

where \( c \) is the speed, \( a \) the inverse of a relaxation time, and \( b \) the intensity of diffusion.

We call this model “Persistent Turning Walker” (PTW)\(^1\).

\(^1\text{Gautrais et al., J. Math. Biol. (2009)}\)
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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 $f(t, x, \theta, \kappa)$.

**PTW model**

\[
\begin{align*}
\frac{d\bar{x}}{dt} &= \bar{\tau}(\theta) \\
\frac{d\theta}{dt} &= \kappa \\
\frac{d\kappa}{dt} &= -\kappa \, dt + \sqrt{2\alpha} \, dB_t
\end{align*}
\]

(in scaled variables)

**Kinetic equation**

\[
\partial_t f + \bar{\tau} \cdot \nabla_{\bar{x}} f
\]

with

\[
Lf = -\kappa \partial_\theta f + \partial_\kappa (\kappa f) + \alpha^2 \partial_{\kappa^2} f
\]
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**PTW model**

$$\frac{d \bar{x}}{dt} = \bar{\tau}(\theta)$$

$$\frac{d \theta}{dt} = \kappa$$

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\frac{d\theta}{dt} &= \kappa \\
d\kappa &= -\kappa dt + \sqrt{2\alpha} dB_t
\end{align*}
\]

*(in scaled variables)*

**Kinetic equation**

\[
\partial_t f + \vec{\tau} \cdot \nabla_x f + \kappa \partial_\theta f - \partial_\kappa (\kappa f) = \alpha^2 \partial_{\kappa^2} f
\]

with

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\]
Derivation of a macroscopic model

- **Step 1. Diffusive scaling**: \( t' = \varepsilon^2 t, \ x' = \varepsilon x \).

  In these ***macroscopic*** variables, \( f^\varepsilon \) satisfies:

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

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

  \( L f^0 = 0 \) \( \Rightarrow \) \( f^0 = \rho^0(x) e^{\frac{\theta^2}{2\sigma^2}} \) (equilibrium)

  with \( N^\theta \) a Gaussian with zero mean and variance \( \sigma^2 \).

- **Step 3. Integrate in (\( \theta, \kappa \))**: 

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

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  \]
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- **Step 3.** *Integrate in \((\theta, \kappa)\):*

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  \]
The distribution $f^\varepsilon$ solution of (1) satisfies:

$$f^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \rho^0 \frac{\mathcal{N}(\kappa)}{2\pi},$$

with:

$$\partial_t \rho^0 + \nabla \cdot J^0 = 0,$$

$$J^0 = -D \nabla \rho^0,$$

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

Probabilistic point of view.

$$= x_0 + \int_0^\infty \cos(\theta_s) ds \xrightarrow{\varepsilon \rightarrow 0} 0 + D \beta.$$
**Diffusion equation**

**Thm.**\(^2\) The distribution \(f^\varepsilon\) solution of (1) satisfies:

\[
f^\varepsilon \xrightarrow{\varepsilon \to 0} \rho^0 \frac{\mathcal{N}(\kappa)}{2\pi},
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\[
J^0 = -D \nabla \bar{x} \rho^0,
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where \(D = \int_{0}^{\infty} \exp(-\alpha^2(-1+s+e^{-s})) \, ds\).

**Probabilistic point of view.**

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\]

\(^2\)Degond, M., J. Stat. Phys. ,

\(\square\)
**Thm.** The distribution $f^\epsilon$ solution of (1) satisfies:

$$f^\epsilon \xrightarrow{\epsilon \to 0} \rho^0 \frac{\mathcal{N}(\kappa)}{2\pi},$$

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**Thm.**² The distribution $f^\varepsilon$ solution of (1) satisfies:

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with:

$$\partial_t \rho^0 + \nabla \vec{x} \cdot J^0 = 0,$$

$$J^0 = -\mathcal{D} \nabla \vec{x} \rho^0,$$

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

**Probabilistic** point of view.

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

**Thm.**\(^2\) The distribution \(f^\varepsilon\) solution of (1) satisfies:

\[
\lim_{\varepsilon \to 0} f^\varepsilon \rightarrow \rho^0 \frac{\mathcal{N}(\kappa)}{2\pi},
\]

with:

\[
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\text{Diffusion equation} \\
\partial_t \rho^0 + \nabla \cdot J^0 &= 0, \\
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\end{align*}
\]

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

**Probabilistic** point of view.

\[
\begin{align*}
\chi^\varepsilon(t') &= \varepsilon x_0 + \varepsilon \int_0^{t'/\varepsilon^2} \cos(\theta_s) \, ds \\
&\xrightarrow{\varepsilon \to 0} 0 + D \tilde{B}_{t'}.
\end{align*}
\]

Diffusion equation

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

$T=20$ (epsilon=1)
Illustration: one trajectory $\vec{x}(t)$

![Graph](attachment:image.png)
Illustration: one trajectory $\vec{x}(t)$
Illustration: one trajectory $\vec{x}(t)$

$T=200$ (epsilon=0.1)
Illustration: one trajectory $\vec{x}(t)$
Illustration: one trajectory $\vec{x}(t)$
Illustration: one trajectory $\vec{x}(t)$
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:
Fish in interaction

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\[ \vec{v}_1 \]
\[ \vec{v}_2 \]

\[ P_1 \]
\[ P_2 \]
Fish in interaction

- In group, fish are usually aligned
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\[ \vec{v}_1 \quad \vec{v}_2 \]

**Experimental data**
Fish in interaction

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\[
\vec{v}_1 \quad \vec{v}_2
\]

Experimental data
Fish in interaction

Classical model with 3 zones

- attraction
- alignment
- repulsive
Fish in interaction

Classical model with 3 zones

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

Classical model with 3 zones

Outline

1. PTW model
   - Experiments and model
   - Derivation of a diffusion equation

2. Vicsek model
   - The model
   - Derivation of a hyperbolic system

3. Numerical schemes
   - Splitting method
   - Particle simulations
   - Micro vs macro
**Vicsek model ('95)**

**Discrete dynamics:**

\[
\begin{align*}
    x_i^{n+1} &= x_i^n + \Delta t \omega_i^n \\
    \omega_i^{n+1} &= \overline{\Omega}_i^n + \epsilon
\end{align*}
\]  

with \( \overline{\Omega}_i^n = \frac{\sum |x_j - x_i| < R \omega_j^n}{\sum |x_j - x_i| < R \omega_j^n} \), \( \epsilon \) noise.

**Continuous dynamics:**

\[
\begin{align*}
    \frac{dx_i}{dt} &= \omega_i \\
    d\omega_i &= (\text{Id} - \omega_i \otimes \omega_i)(\nu \overline{\Omega}_i dt + \sqrt{2D} dB_t)
\end{align*}
\]  

Remark. eq. (3) + “\( \nu \Delta t = 1 \)” \( \Rightarrow \) eq. (2)
Vicsek model ('95)

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\[ x_{i}^{n+1} = x_{i}^{n} + \Delta t \omega_{i}^{n} \]

\[ \omega_{i}^{n+1} = \Omega_{i}^{n} + \epsilon \]

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Continuous dynamics:

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Remark. eq. (3) + “\( \nu \Delta t = 1 \)” \( \Rightarrow \) eq. (2)
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:

\[
\partial_t f + \omega \cdot \nabla_x f + \nabla_\omega \cdot (Ff) = D \Delta_\omega f,
\]

with:

\[
F(x, \omega) = (\text{Id} - \omega \otimes \omega) \nu \Omega(x), \quad \Omega(x) = \frac{J(x)}{|J(x)|}
\]

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

- The alignment is expressed by the operator \(\nabla_\omega \cdot Ff\),
- The randomness is expressed by \(D \Delta_\omega f\).

\(^3\)Sznitman, Saint-Flour (89)
Kinetic equation

Under the hypothesis of propagation of chaos\(^3\), the density of particles \(f(t,x,\omega)\) satisfies:

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\]

with:

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F(x,\omega) = (\text{Id} - \omega \otimes \omega) \nu \bar{\Omega}(x), \quad \bar{\Omega}(x) = \frac{J(x)}{|J(x)|}
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## Kinetic equation

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- The **alignment** is expressed by the operator \( \nabla_\omega \cdot Ff \),
- The **randomness** is expressed by \( D\Delta_\omega f \).

\(^3\text{Sznitman}, \text{Saint-Flour (89)}\)
Kinetic equation

Finally, $f$ satisfies:

\begin{equation}
\partial_t f + \omega \cdot \nabla_x f = Q(f)
\end{equation}

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:

\[ M_\Omega(\omega) = C \exp \left( \frac{\omega \cdot \Omega}{T} \right) \]

where $T = D/\nu$ and $\Omega$ is an arbitrary direction.

- The total momentum is not preserved by the operator:

\[ \int_\omega Q(f)\omega \, d\omega \neq 0. \]
Finally, $f$ satisfies:

$$\partial_t f + \omega \cdot \nabla_x f = Q(f)$$

with:

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

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

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Kinetic equation

Finally, $f$ satisfies:

\[
\partial_t f + \omega \cdot \nabla_x f = Q(f)
\]  \hspace{2cm} (4)

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- 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)
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- The *total momentum* is **not** preserved by the operator:
  \[
  \int_\omega Q(f)\omega \, d\omega \neq 0.
  \]
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, \( f^{\varepsilon} \) satisfies:

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

- **Step 2.** Hilbert expansion: \( f^{\varepsilon} = f^0 + \varepsilon f^1 + ... \)
  
  \( \Rightarrow f^0 \) is an equilibrium: \( f^0(x, \omega) = \rho^0(x) M_{\omega}(\rho^0(\omega)) \)

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

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

  with \( \psi \) such that \( \int_{\omega} Q(f) \psi \; d\omega = 0 \).
Derivation of a hyperbolic system

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

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Problem: Only one quantity is preserved by $Q$.

*Momentum is not preserved by the dynamics*

*Def.* $\psi$ is a if for every $f$ satisfying $\int_\Omega f \psi d\omega / / 0$

$\int_\omega Q(f)\psi d\omega = 0 \Rightarrow \int_\omega f Q^*_\Omega(\psi) d\omega = 0 \Rightarrow \psi = \{\varphi_{\Omega^c}^\prime(\omega)\}$

with $\varphi_{\Omega}$ a solution of: $Q^*(\varphi_{\Omega}) = \omega \times \Omega$.

Then, we can integrate the kinetic equation:

$\int_\omega \left[ \partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon) \right] \left( \frac{1}{\varphi_{\Omega^c}(\omega)} \right) d\omega$
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Hyperbolic system

**Thm.** The distribution \( f^\varepsilon \) solution of (5) satisfies:

\[
f^\varepsilon \xrightarrow{\varepsilon \to 0} \rho \mathcal{M}_\Omega (\omega)
\]

where \( \rho \) and \( \Omega \) have different convection speeds \( (c_1 \neq c_2) \).

**Remarks:**
- the system obtained is hyperbolic...
- ...but non-conservative (due to the constraint \( |\Omega| = 1 \))


where \( c_1, c_2 \) and \( \lambda \) depend on \( T = D/\nu \).
Thm.\textsuperscript{4} The distribution $f^{\varepsilon}$ solution of (5) satisfies:

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\begin{align*}
\partial_t \rho &+ c_1 \nabla_x \cdot (\rho \Omega) = 0, \\
\rho (\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega) &+ \lambda (\text{Id} - \Omega \otimes \Omega) \nabla_x \rho = 0, \\
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\cite{Degond2008}
Applications

- Combine PTW and Vicsek model


- Extend the method for attraction-alignment-repulsion model


Perspectives

- Study numerically the kinetic equation
  
  joint work with I. Gamba, J. Haack

- Corroborate the macroscopic model with experimental data
  
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Outline

1. PTW model
   - Experiments and model
   - Derivation of a diffusion equation

2. Vicsek model
   - The model
   - Derivation of a hyperbolic system

3. Numerical schemes
   - Splitting method
   - Particle simulations
   - Micro vs macro
Numerical simulation

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

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\begin{align*}
\partial_t \rho + c_1 \nabla_x \cdot (\rho \Omega) &= 0, \\
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Two difficulties:

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

\[\Rightarrow \text{No available theory to deal with this system.}\]
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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):

- First, we solve the conservative part (left-hand-side).
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To solve numerically this system, we proceed in two steps (splitting):

- First, we solve the conservative part (left-hand-side)...
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Other numerical methods

In one direction, the system is written:

\[ \partial_t \rho + c_1 \partial_x (\rho \cos \theta) = 0 \]
\[ \partial_t \theta + c_2 \cos \theta \partial_x \theta - \lambda \frac{\sin \theta}{\rho} \partial_x \rho = 0. \]  \(\text{(6)}\)

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

Solving the conservative formulation gives another method

\[ \Rightarrow \text{Conservative method} \]

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

Question: What is the correct solution? Do we have it?

⇒ Go back to the microscopic model...
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Question: What is the correct solution? Do we have it?

⇒ Go back to the microscopic model...
Particle simulations

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

\[
\frac{dx_k^e}{dt} = \omega_k^e, \\
\frac{d\omega_k^e}{dt} = \frac{1}{\varepsilon} (I - \omega_k^e \otimes \omega_k^e) (\nu \bar{\Omega}_k^e \, dt + \sqrt{2D} \, dB_t),
\]

with

\[
\bar{\Omega}_k^e = \frac{J_k^e}{|J_k^e|}, \quad J_k^e = \sum_{j, |x_j^e - x_k^e| \leq \varepsilon R} \omega_j^e.
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\]
We use Riemann problem as initial condition.

Figure: Density $\rho$: Micro (left) and Macro (right)
We take a cross section of the distribution in the $x$-direction:

![Graph showing macro. equation (line) and micro. equation (dot) at time $t = 2$.](image)

**Figure:** macro. equation (line) and micro. equation (dot) at time $t = 2$. 
We take a cross section of the distribution in the $x$-direction:

![Graph showing 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”.

\[ \rho \cos \theta \]
We compare the solutions of the MV model with the particles for the shock-wave solution:

The splitting method has the “correct speed”.
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)
Contact discontinuity

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General case

How about *non-standard* initial condition?
General case

How about *non-standard* initial condition?

Micro at $t = 40.00$

Macro at $t = 40.00$