# Deterministic particle approximation for nonlocal transport equations

Emanuela Radici

École polytechnique fédérale de Lausanne

*Dynamics and Discretization: PDEs, Sampling, and Optimization*

*Simons Institute for the Theory of Computing*

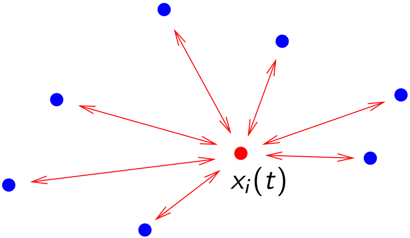
$29^{th}$ *October* 2021

EPFL

# Plan of the talk

- Nonlocal transport equations with linear and nonlinear mobility
- Deterministic particle approximation for nonlinear mobility
- Deterministic particle approximation for linear mobility
- Application to opinion dynamics

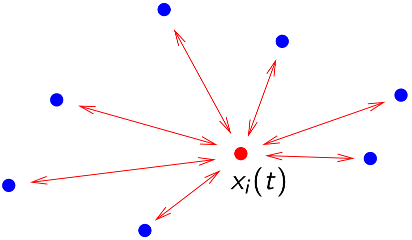
$N$ particles located at positions $x_1(t), \dots, x_N(t)$




energetical setting:

- nonlocal interaction potential $W$ depending on the relative distance of the particles
- no inertia (negligible in many socio-biological phenomena)

$N$ particles located at positions $x_1(t), \dots, x_N(t)$




energetical setting:

- nonlocal interaction potential $W$ depending on the relative distance of the particles
- no inertia (negligible in many socio-biological phenomena)

$$\boxed{\dot{x}_i(t) = -\frac{1}{N} \sum_{j \neq i} \nabla W(x_i(t) - x_j(t))}$$

$$\updownarrow$$

$$\boxed{\partial_t \rho = \nabla \cdot (\rho \nabla W * \rho)}$$

$$\dot{x}_i = -\frac{1}{N}\sum_{j\neq i} \nabla W(x_i - x_j)$$

$$\Updownarrow$$

$$\partial_t \rho = \nabla \cdot (\rho \nabla W * \rho)$$

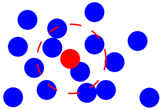
(non exaustive) Literature

[Bertozzi, Carrillo, Laurent, Rosado, Brandman]
*$L^p$ theory*

[Ambrosio, Gigli, Savaré]
*optimal transport with smooth potentials*

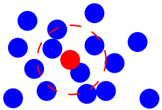
[Carrillo, Choi, Di Francesco, Figalli, Hauray, Laurent, Slepčev]
*optimal transport with midly-singular potentials*

# Linear vs Nonlinear mobility

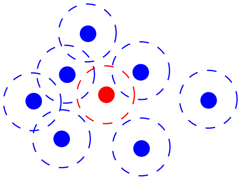


If the potential $W$ is attractive then the particles tend to concentrate (the density $\rho$ can blow up)

# Linear vs Nonlinear mobility



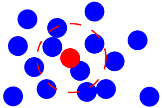
If the potential $W$ is attractive then the particles tend to concentrate (the density $\rho$ can blow up)



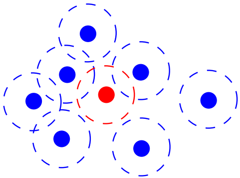
one way to prevent the overcrowding effect is to let the mobility depend also on a velocity term that decreases where the concentration is higher

$v : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ s.t. $v' \leq 0$, $spt\, v = [0, R]$
(ex. $v(\rho) = (1 - \rho)_+$)

# Linear vs Nonlinear mobility



If the potential $W$ is attractive then the particles tend to concentrate (the density $\rho$ can blow up)



one way to prevent the overcrowding effect is to let the mobility depend also on a velocity term that decreases where the concentration is higher

$v : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ s.t. $v' \leq 0$, $spt\, v = [0, R]$ (ex. $v(\rho) = (1-\rho)_+$)

$$\boxed{\partial_t \rho = \nabla \cdot (\rho v(\rho) \nabla W * \rho)}$$

# state of the art in the scalar case

$$\begin{cases} \partial_t \rho = \partial_x(\rho v(\rho) W' * \rho) & [0, T] \times \mathbb{R} \\ \rho(0, \cdot) = \rho_0 & \rho_0 \in BV \cap \mathcal{P}_{cmpt} \cap L^\infty(\mathbb{R}) \end{cases}$$

We call $\rho_i := \frac{1}{N(x_{i+1} - x_i)}$ the local reconstruction of the macroscopic density

**Theorem (Di Francesco, Fagioli, R. 2019)**

*Let $W \in W^{3,\infty}_{loc}(\mathbb{R})$ be even and attractive, i.e. $W'(x)x \geq 0$, then the many particle limit of the system*

$$\dot{x}_i = -N^{-1} v(\rho_{i-1}) \sum_{j<i} W'(x_i - x_j) - N^{-1} v(\rho_i) \sum_{j>i} W'(x_i - x_j)$$

*is the unique entropy solution of the Cauchy problem.*

Outlines of the proof:

- *Discrete Maximum Principle* $\rho_i \leq \|\rho_0\|_{L^\infty}$

Outlines of the proof:

- *Discrete Maximum Principle* $\rho_i \leq \|\rho_0\|_{L^\infty}$
- *Density approximations*

$$\rho^N(t,x) := \sum_{i=0}^{N-1} \rho_i(t)\, \mathbf{1}_{[x_i(t),x_{i+1}(t))}(x)$$

Outlines of the proof:

- *Discrete Maximum Principle* $\rho_i \leq \|\rho_0\|_{L^\infty}$
- *Density approximations*

$$\rho^N(t,x) := \sum_{i=0}^{N-1} \rho_i(t)\, \mathbf{1}_{[x_i(t),x_{i+1}(t))}(x)$$

- *strong $L^1$ compactness* follows from
  - *BV estimates* $\int_0^T \big(|supp\,\rho^N(t,\cdot)| + TV[\rho^N(t,\cdot)]\big)\,dt < \infty$
  - *continuity in time* $W_1(\rho^N(t,\cdot), \rho^N(s,\cdot)) \leq C(TV[\rho_0])|t-s|$

Outlines of the proof:

- *Discrete Maximum Principle* $\rho_i \leq \|\rho_0\|_{L^\infty}$
- *Density approximations*

$$\rho^N(t,x) := \sum_{i=0}^{N-1} \rho_i(t)\, \mathbf{1}_{[x_i(t), x_{i+1}(t))}(x)$$

- *strong $L^1$ compactness* follows from
  - *BV estimates* $\int_0^T \left(|supp\, \rho^N(t,\cdot)| + TV[\rho^N(t,\cdot)]\right) dt < \infty$
  - *continuity in time* $W_1(\rho^N(t,\cdot), \rho^N(s,\cdot)) \leq C(TV[\rho_0])|t-s|$
- *Kruzkov entropy inequality* holds for $\rho^N$ up to an error vanishing in the many particle limit

Outlines of the proof:

- *Discrete Maximum Principle* $\rho_i \leq \|\rho_0\|_{L^\infty}$
- *Density approximations*

$$\rho^N(t,x) := \sum_{i=0}^{N-1} \rho_i(t)\, \mathbf{1}_{[x_i(t),x_{i+1}(t))}(x)$$

- *strong $L^1$ compactness* follows from
  - *BV estimates* $\int_0^T \left(|supp\, \rho^N(t,\cdot)| + TV[\rho^N(t,\cdot)]\right) dt < \infty$
  - *continuity in time* $W_1(\rho^N(t,\cdot), \rho^N(s,\cdot)) \leq C(TV[\rho_0])|t-s|$
- *Kruzkov entropy inequality* holds for $\rho^N$ up to an error vanishing in the many particle limit
- uniqueness follows by a stability result of Karlsen and Risebro

# state of the art in the scalar case

$$\begin{cases} \partial_t \rho = \partial_x(\rho v(\rho) W' * \rho) + \partial_{xx}\phi(\rho) & [0,T]\times[0,\ell] \\ \rho(0,\cdot) = \rho_0 & \rho_0 \in BV \cap L^\infty \cap \mathcal{P}([0,\ell]), \gg 0 \\ v(\rho)\partial_x(a(\rho) + W * \rho) = 0 & [0,T]\times(\{0\}\cup\{\ell\}) \end{cases}$$

through the relation $\phi(\rho) = \int_0^\rho \xi v(\xi) a'(\xi) d\xi$,

**Theorem** (Fagioli, R. 2018)

*Let $W \in W^{3,\infty}_{loc}(\mathbb{R})$ be even and attractive, and $\phi \in Lip([0,\infty))$, s.t. $\phi(0) = 0$ and $\phi' \geq 0$, then the many particle limit of the system $\dot{x}_N = \dot{x}_0 = 0$ and $\dot{x}_i = \dot{x}_i^d + \dot{x}_i^{nL}$, where*

$$\dot{x}_i^d = N(\phi(\rho_{i-1}) - \phi(\rho_i))$$

$$\dot{x}_i^{nL} = -N^{-1} v(\rho_i) \sum_{j>i} W'(x_i - x_j) - N^{-1} v(\rho_{i-1}) \sum_{j<i} W'(x_i - x_j),$$

*is the unique entropy solution of the Cauchy problem.*

# state of the art in the scalar case

$$\begin{cases} \partial_t \rho = \partial_x(\rho v(\rho) V(x)) & [0,T]\times\mathbb{R} \\ \rho(0,\cdot) = \rho_0 & \rho_0 \in BV \cap \mathcal{P}_{cmpt} \cap L^\infty(\mathbb{R}) \end{cases}$$

**Theorem** (Di Francesco, Stivaletta 2020)

*Let $V \in W^{2,\infty}(\mathbb{R})$ be*

*positive* $\longrightarrow \quad \dot{x}_i = v(\rho_i)V(x_i)$

*negative* $\longrightarrow \quad \dot{x}_i = v(\rho_{i-1})V(x_i)$

*repulsive* $\longrightarrow \quad \dot{x}_i = V(x_i)v(\rho_{i-1})\mathbf{1}_{\leq 0}(x_i) + V(x_i)v(\rho_i)\mathbf{1}_{>0}(x_i)$

*attractive* $\longrightarrow \quad \dot{x}_i = V(x_i)v(\rho_i)\mathbf{1}_{\leq 0}(x_i) + V(x_i)v(\rho_{i-1})\mathbf{1}_{>0}(x_i)$

*Then the many particle limit of the corresponding system is the unique entropy solution of the Cauchy problem.*

# state of the art in the scalar case

$$\begin{cases} \partial_t \rho = \partial_x(\rho v(\rho)(W' * \rho - V'(x)) & [0,T] \times \mathbb{R} \\ \rho(0,\cdot) = \rho_0 & \rho_0 \in BV \cap \mathcal{P}_{cmpt} \cap L^\infty(\mathbb{R}) \end{cases}$$

**Theorem** (Fagioli, Tse 2021)

*Let $V \in C^2(\mathbb{R})$ with $V'$ having linear growth and $W$ be a radially symmetric interaction potential satisfying one of the following*

- $W \in C^1(\mathbb{R})$ *and* $W' \in W^{2,\infty}(\mathbb{R})$ *with linear growth,*
- $W(x) = \pm|x|$,

*then the many particle limits of the system*

$$\dot{x}_i(t) = v(\rho_i)U_i^+ + v(\rho_{i-1})U_i^-, \quad U_i = -N^{-1}\sum_{j\neq i} W'(x_i - x_j) - V'(x_i)$$

*correspond to the unique entropy solution of the Cauchy problem.*

# state of the art in the scalar case

$$\begin{cases} \partial_t \rho = \partial_x(\rho v(\rho)(W' * \rho - V(t,x)) & [0,T] \times \mathbb{R} \\ \rho(0,\cdot) = \rho_0 & \rho_0 \in BV \cap \mathcal{P}_{cmpt} \cap L^\infty(\mathbb{R}) \end{cases}$$

**Theorem** (R., Stra 2021)

*Let* $W \in L^1([0,T], W^{1,\infty}_{loc}(\mathbb{R}) \cap W^{3,\infty}_{loc}(\mathbb{R}_{\lessgtr 0}))$ *and* $V \in L^1([0,T], W^{2,\infty}_{loc}(\mathbb{R}))$, *then the many particle limits of the systems*

$$\dot{x}_i(t) = -v_i N^{-1} \sum_{j \neq i} W'\big(t, x_i - x_j\big) + v_i V(t, x_i) \ = v_i \hat{U}_i(t)$$

$$\dot{x}_i(t) = -v_i \sum_{j=0}^{N} (\rho_{j+1} - \rho_j) W(t, x_i - x_j) + v_i V(t, x_i) = v_i \bar{U}_i(t)$$

*where* $v_i = v(\rho_i)$ *if* $U_i \geq 0$ *and* $v_i = v(\rho_{i-1})$ *if* $U_i \leq 0$, *correspond to the unique entropy solution of the Cauchy problem.*

# Numerics

Pure aggregative regime

$$v(\rho) = (1-\rho)_+, \quad W = \mathcal{N}(0,1), \quad \rho_0(x) = 0.2\,\mathbf{1}_{[-0.5,0]}(x) + 0.6\,\mathbf{1}_{[0.5,1]}(x)$$

# Numerics

Non uniqueness of weak solutions

$$v(\rho) = (1-\rho)_+, \quad W = \mathcal{N}(0,1), \quad \rho_0(x) = \mathbf{1}_{[-0.5,0]}(x) + \mathbf{1}_{[0.5,1]}(x)$$

# Numerics

Aggregative and diffusive regime

$$v(\rho) = (1-\rho)_+, \quad W = \mathcal{N}(0,1), \quad \rho_0(x) = \frac{3}{4}(1-x^2)\mathbf{1}_{[-1,1]}(x)$$

$$a(\rho) = \frac{1}{20}\rho^2\mathbf{1}_{[0,\frac{2}{5})}(\rho) + \frac{1}{125}\mathbf{1}_{[\frac{2}{5},\frac{3}{5})}(\rho) + \left[\frac{1}{125} + \frac{1}{20}\left(\rho - \frac{3}{5}\right)^2\right]\mathbf{1}_{[\frac{3}{5},\infty)}(\rho)$$

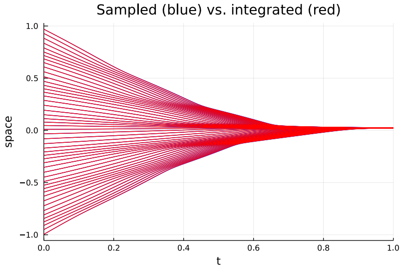
New particle scheme

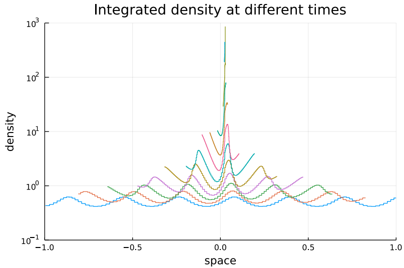
$v(\rho) = (1-\rho)_+, \quad W(x) = -5\ln(|x|+1), \quad V(t,x) = -(x - sin(3t))^3,$
$\rho_0(x) = \mathbf{1}_{[-1,-0.5]}(x) + \mathbf{1}_{[0,0.5]}(x), \quad N = 80$ vs $N = 240$

New particle scheme

$v(\rho) = (1-\rho)_+, \quad W(x) = -5\ln(|x|+1), \quad V(t,x) = -(x - sin(3t))^3,$
$\rho_0(x) = \mathbf{1}_{[-1,-0.5]}(x) + \mathbf{1}_{[0,0.5]}(x),$ sampled vs integrated

# Numerics

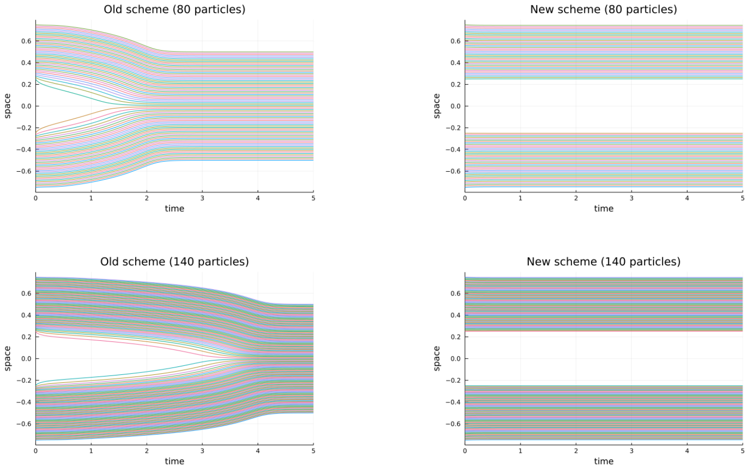



$$v(\rho) = \frac{1}{1+\rho}, \quad W(x) = 5\ln(|x|+1), \quad V(t,x) = 0,$$

$$\rho_0(x) \approx \frac{1}{2} + \text{oscillations}, \quad \text{non vanishing } v$$

# Comparison old scheme vs new scheme




$$v(\rho) = (1-\rho)_+, \quad W(x) = 5\ln(|x|+1), \quad \rho_0(x) = \mathbf{1}_{[-0.75,-0.25]}(x) + \mathbf{1}_{[0.25,0.75]}(x)$$

# diffusion in unbounded domains

$$\begin{cases} \partial_t \rho = \partial_x(\rho W' * \rho) + \partial_{xx}\phi(\rho) & [0, T] \times \mathbb{R} \\ \rho(0, \cdot) = \rho_0 & \rho_0 \in L^\infty \cap \mathcal{P}_1(\mathbb{R}), \end{cases}$$

**Theorem** (Daneri, R., Runa 2021)

*Let $W \in W^{2,\infty} \cap W^{1,1}(\mathbb{R}_{\lessgtr 0}) \cap C(\mathbb{R})$ be even, $\phi \in C^1(\mathbb{R})$ is a diffusion of the form $\phi(\rho) = \rho U'(\rho) - U(\rho)$ for $U \geq 0$ with suitable growth conditions (including the class $\phi(\rho) = \rho^m$, $m \geq 1$), and $\rho_0$ be an initial datum with finite energy. Then the many particle limits of the systems*

$$\dot{x}_i^L = -N^{-1} \sum_{j \neq i} W'(x_i - x_j) + N(\phi(\rho_{i-1}) - \phi(\rho_i))$$

*of the approximated problem on the torus $\mathbb{T}_L$ converge to the unique bounded weak solution of the Cauchy problem in $L^1([0, T] \times \mathbb{R})$.*

# Linear mobility case

Outlines of the proof:

- *Gradient flow* of

$$\mathcal{E}_L(\nu) = \frac{1}{2} \int_{\mathbb{T}_L \times \mathbb{T}_L} W(x-y) d\nu d\nu + \int_{\mathbb{T}_L} U(\nu)$$

# Linear mobility case

Outlines of the proof:

- *Gradient flow* of

$$\mathcal{E}_L(\nu) = \frac{1}{2}\int_{\mathbb{T}_L \times \mathbb{T}_L} W(x-y)d\nu d\nu + \int_{\mathbb{T}_L} U(\nu)$$

- *Energy estimates* along the density approximations

$$\frac{d\mathcal{E}_L(\rho_N^L(t))}{dt} \leq C(W', W'')\frac{L}{\sqrt{N}}$$

# Linear mobility case

Outlines of the proof:

- *Gradient flow* of

$$\mathcal{E}_L(\nu) = \frac{1}{2}\int_{\mathbb{T}_L \times \mathbb{T}_L} W(x-y)d\nu d\nu + \int_{\mathbb{T}_L} U(\nu)$$

- *Energy estimates* along the density approximations

$$\frac{d\mathcal{E}_L(\rho_N^L(t))}{dt} \leq C(W', W'')\frac{L}{\sqrt{N}}$$

- *Discrete Maximum Principle* for $\phi(\rho_N^L)$ and $\rho_N^L$

# Linear mobility case

Outlines of the proof:

- *Gradient flow* of

$$\mathcal{E}_L(\nu) = \frac{1}{2}\int_{\mathbb{T}_L\times\mathbb{T}_L} W(x-y)d\nu d\nu + \int_{\mathbb{T}_L} U(\nu)$$

- *Energy estimates* along the density approximations

$$\frac{d\mathcal{E}_L(\rho_N^L(t))}{dt} \leq C(W', W'')\frac{L}{\sqrt{N}}$$

- *Discrete Maximum Principle* for $\phi(\rho_N^L)$ and $\rho_N^L$
- $L^1$ *compactness* on $[0, T]\times\mathbb{T}_L$ and also on $[0, T]\times\mathbb{R}$

# Opinion Dynamics

A further application of the deterministic particle approach concerns the theory of *opinion dynamics*

$$\partial_t \rho = \partial_x \left( \frac{\lambda}{2} D^2(x) \partial_x \phi(\rho) + \rho \mathrm{P}[\rho] \right) \qquad x \in [-1, 1],\ t \in [0, T]$$

where

$$\mathrm{P}[\rho](x, t) = \int_{-1}^{1} P(x, y)(x - y)\rho(t, y) dy$$

- $0 \leq P \leq 1$ models the local relevance of the compromise.
  Standard choices are $P(x_1, x_2) = 1$ or $P(x_1, x_2) = (1 - x_1^2)^{1+\alpha}$ with $\alpha > 0$
- $D$ models the diffusion of the single opinion.
  Standard choice is $D(x) = (1 - x^2)^{\alpha/2}$ with $\alpha > 0$
- $\phi$ is some standard diffusion function, for example of porous medium type
- $\lambda$ is some positive constant that is obtained in deducing this PDE as limit of the Bolzmann equation

The corresponding particle scheme is

$$\dot{x}_i = \frac{\lambda}{2} N D^2(x_i)(\phi(R_{i-1}) - \phi(R_i)) + \frac{1}{N}\sum_{j=0}^{N} P(x_i, x_j)(x_i - x_j) \qquad i = 1\dots, N-1$$

with the boundary conditions $\dot{x}_0 = \dot{x}_N = 0$. If we assume that

- $P$ is such that $0 \leq P(\cdot) \leq 1$ and $P'$ is Lipschitz in the first component
- $D = (1 - x^2)^{\alpha/2}$ for some $\alpha \geq 1$
- $\phi : [0, \infty) \to \infty$ is Lipschitz, non-decreasing and $\phi(0) = 0$

**Theorem** (Fagioli,R. 2020)

*If the initial datum $\rho_0$ is far from vacuum, we can prove that the sequence $\rho^N$ is well defined and it $L^1$-converges to some density $\rho$ satisfying*

$$\int_0^T \int_{-1}^1 \rho\partial_t\varphi + \phi(\rho)\partial_x(D^2(x)\partial_x\varphi) - \rho\mathrm{P}[\rho]\partial_x\varphi \, dx \, dt = 0$$

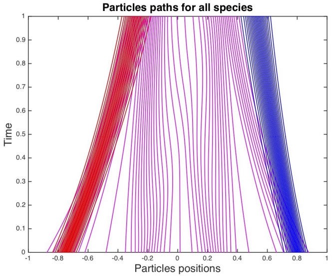
*for every $\varphi \in \mathcal{C}_c^\infty((0, T) \times (-1, 1))$ with $\partial_x\varphi(\pm 1) = 0$.*

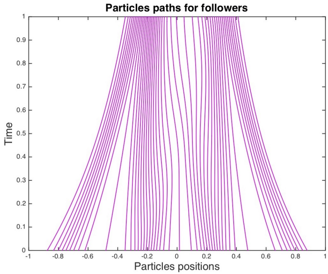
One can generalize this approach to study the opinion dynamics of a society which is composed by a populations of followers $f$, a red party $r$, a blue party $b$. Then the corresponding system is

$$\begin{cases} \partial_t f = \partial_x \left( \frac{\lambda_f}{2} D^2 \partial_x \phi_f(f) + f(\mathrm{P}_{f,f}[f] + \mathrm{P}_{f,r}[r] + \mathrm{P}_{f,b}[b]) \right) \\ \partial_t r = \partial_x \left( \frac{\lambda_r}{2} D^2 \partial_x \phi_r(r) + r(\mathrm{P}_{r,r}[r] + \mathrm{P}_{r,b}[b]) \right) \\ \partial_t b = \partial_x \left( \frac{\lambda_b}{2} D^2 \partial_x \phi_b(b) + b(\mathrm{P}_{b,b}[b] + \mathrm{P}_{b,r}[r]) \right) \end{cases}$$

masses: $m_b = 0.5, \; m_r = 0.4, \; m_f = 1$

Parameters: $\lambda_i = 0.05, \; \phi_f = \phi_r = \phi_b = \frac{u^2}{2}, \; P_{f,f} = P_{r,r} = P_{b,b} = 1,$
$P_{r,b} = P_{b,r} = \frac{1}{2}(1 - x_{r/b}^2), \quad P_{f,r} = P_{f,b} = \frac{1}{10}(1 - x_f^2)$



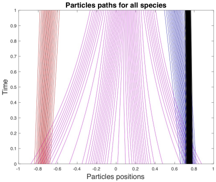



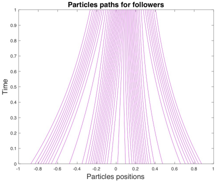
We can add even the dependece of an eventual population $g$ of fake followers owned by one of the parties (trolls). Then the corresponding system is

$$\begin{cases} \partial_t f = \partial_x \left( \frac{\lambda_f}{2} D^2 \partial_x \phi_f(f) + f(\mathrm{P}_{f,f}[f] + \mathrm{P}_{f,f}[g] + \mathrm{P}_{f,r}[r] + \mathrm{P}_{f,b}[b]) \right) \\ \partial_t r = \partial_x \left( \frac{\lambda_r}{2} D^2 \partial_x \phi_r(r) + r(\mathrm{P}_{r,r}[r] + \mathrm{P}_{r,b}[b]) \right) \\ \partial_t b = \partial_x \left( \frac{\lambda_b}{2} D^2 \partial_x \phi_b(b) + b(\mathrm{P}_{b,b}[b] + +\mathrm{P}_{b,r}[r]) \right) \\ \partial_t g = \partial_x \left( g \mathrm{P}_{g,b}[b] \right) \end{cases}$$

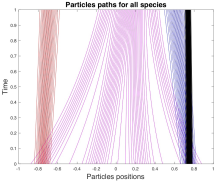
$$P_{g,b} = 1 - (x_g - x_b)^2$$

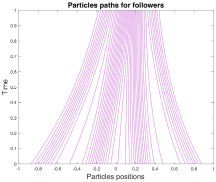
$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.1$



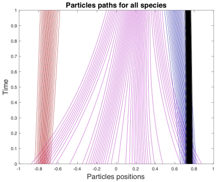



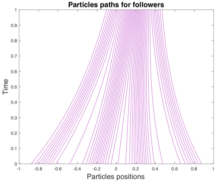

$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.2$




$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.3$

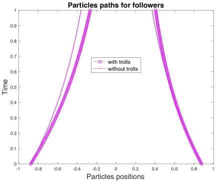


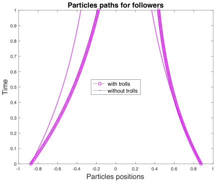



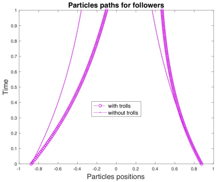
$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.1$

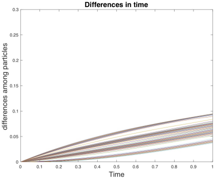
$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.2$

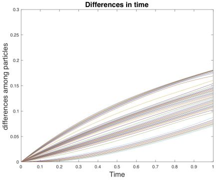
$m_f = 1, m_r = 0.4,$
$m_b = 0.2, m_g = 0.3$

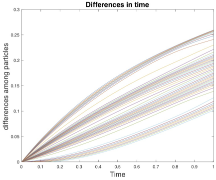


# Related open problems

1. diffusion & nonlinear mobility in unbounded domains with no box constraint
2. Lennard-Jones type potentials
3. Deterministic particle approach for 1D systems with nonlinear mobility
4. Deterministic particle approach on networks and higher dimension

# Related open problems

1. diffusion & nonlinear mobility in unbounded domains with no box constraint
2. Lennard-Jones type potentials
3. Deterministic particle approach for 1D systems with nonlinear mobility
4. Deterministic particle approach on networks and higher dimension

Thank you for your attention