Aggregation of bacteria by chemotaxis: mathematical and numerical analysis

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Introduction

We are interested in the aggregation equation

$$\partial_t \rho + \mathrm{div}(a(\nabla_x W * \rho)\rho) = 0, \qquad \rho(t=0) = \rho^0,$$

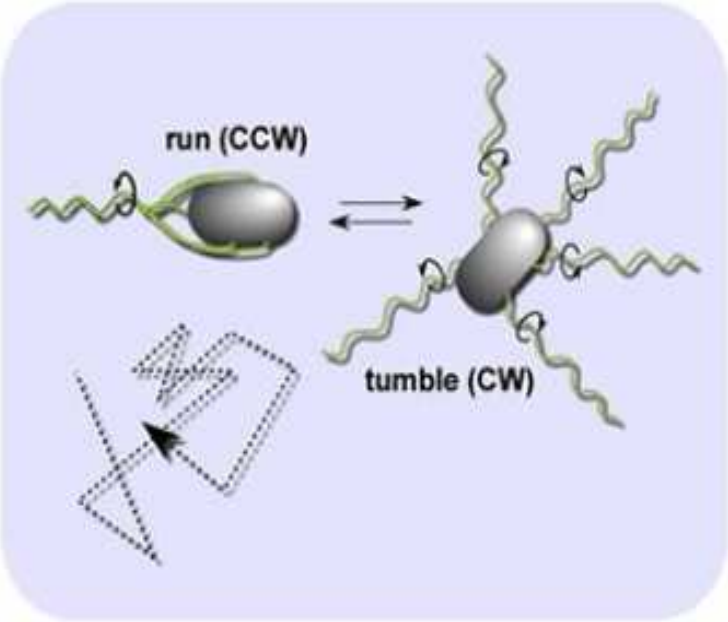
where

- $\rho \geq 0$ is the density of individuals ;
- $W : \mathbb{R}^d \to \mathbb{R}$ is an interaction potential describing the interaction between individuals (which is generally assumed to be *pointy*) ;
- $a : \mathbb{R}^d \to \mathbb{R}^d$ is a function (which is generally assumed to be *linear*).

Applications :

- bacterial motion by chemotaxis (Keller-Segel without diffusion),
- collective motion of individuals,
- pedestrians motions, ...

Motivation : bacterial chemotaxis



Bacteria like *Escherichia Coli* have several flagella allowing them to move. We can distinguish two phases :

- *run phases* : straight swim in a given direction.
- *tumble phases* : reorientation of cells in a direction depending on the chemoattractant concentration.

The resulting movement is due to the alternance of these two phases. Bacteria are able to find favorable location with high concentration of chemoattractant : they modulate the duration of their run phases (the frequency of tumbling is higher when bacteria go in unfavorable direction than when they go in favorable direction).

Kinetic model

We focus at a mesoscopic level of description, and consider the distribution function $f(t,x,v)$ at time t, position $x \in \mathbb{R}^d$ and velocity $v \in V$, V bounded domain of $\mathbb{R}^d$. Then the density $\rho(t,x) = \int_V f(t,x,v)\,dv$
The dynamics of f is given by the following kinetic model :

$$\underbrace{\partial_t f + v \cdot \nabla_x f}_{\text{run phase}} = \underbrace{\int_V (\phi(v' \cdot \nabla_x S) f(v') - \phi(v \cdot \nabla_x S) f(v))\,dv'}_{\text{tumble phase}},$$

where the chemoattractant, whose concentration is denoted S, is released by bacteria

$$(\partial_t S) - \underbrace{D_S \Delta S}_{\text{diffusion}} = \underbrace{\beta\rho}_{\text{birth}} - \underbrace{\alpha S}_{\text{death}}.$$

Kinetic model

Finally the kinetic model[1] we are considering reads :

$$\partial_t f + v \cdot \nabla_x f = \int_V (\phi(v' \cdot \nabla_x S) f(v') - \phi(v \cdot \nabla_x S) f(v))\, dv',$$

$$(\partial_t S) - D_S \Delta S + \alpha S = \beta \rho,$$

with $\rho := \int_V f(v)\, dv,$.

The function ϕ gives the rate of changing direction. We take $0 < \phi \leq 1$ and ϕ is nonincreasing which corresponds to positive chemotaxis.

1. Y. Dolak, C. Schmeiser, J. Math. Biol. 2005

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Assuming that the motion is mainly driven by tumbling,

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} \int_V (\phi(v' \cdot \nabla_x S) f(v') - \phi(v \cdot \nabla_x S) f(v))\, dv',$$

1. Y. Dolak, C. Schmeiser, J. Math. Biol. 2005

Formal hydrodynamic limit in 1D

For the sake of simplicity and clarity, we will consider the problem in 1D.

$$\partial_t f + v\partial_x f = \frac{1}{\varepsilon}\int_V (\phi(v'\partial_x S)f(v') - \phi(v\partial_x S)f(v))\,dv'.$$

- Conservation

$$\partial_t \rho + \operatorname{div} J = 0, \qquad J = \int_V v f(v)\,dv.$$

- Equilibrium. The elements in the kernel of the tumbling operator are such that

$$\int_V \phi(v'\partial_x S)f(v')\,dv' = |V|\phi(v\partial_x S)f(v).$$

Then, $f(v) = \frac{A}{|V|\phi(v\partial_x S)}$. Integrating,

$$\rho = \int_V f(v)\,dv = A\frac{1}{|V|}\int_V \frac{dv}{\phi(v\partial_x S)}.$$

Thus, the elements in the kernel are given by $\boxed{f(v) = \rho\Phi(v\partial_x S)}$.

Formal hydrodynamic limit in 1D

Finally, we have[2] that when $\varepsilon \to 0$, system

$$\partial_t f + v \cdot \partial_x f = \frac{1}{\varepsilon} \int_V (\phi(v' \partial_x S) f(v') - \phi(v \partial_x S) f(v))\, dv',$$
$$-\partial_{xx} S + S = \rho,$$

converges to

$$\partial_t \rho + \mathrm{div}(a(\partial_x S)\rho) = 0, \qquad -\partial_{xx} S + S = \rho.$$

This is the aggregation equation.

2. F. James, N. V., NoDEA 2013

Blow up for aggregation equation

We focus on the **aggregation equation**,

$$\partial_t \rho + \mathrm{div}(a(\nabla_x W * \rho)\rho) = 0.$$

Recall that in the case of chemotaxis the chemoattractant concentration is given by $S = W * \rho$.
We have the following result[3] :

- if W is smooth, existence of global solution, no blow up.
- if W has a singularity, blow up in finite time of weak solutions.
  Blow up : for all $p > 1$ we have that $\|\rho(t)\|_{L^p} \to +\infty$ in finite time.

3. (see Bertozzi et al., Carrillo et al., Laurent, Velasquez, ...)

Weak measure solutions for aggregation equation

$$\partial_t \rho + \mathrm{div}(a(\nabla_x W * \rho)\rho) = 0.$$

The L^1-norm is conserved, then we can work in the framework of measures solution.
Even in one dimension, a difficulty is that when $\rho \in \mathcal{M}_b(\mathbb{R})$, the quantity $a(\partial_x W * \rho)$ may have discontinuities. Thus the product $\rho a(\partial_x W * \rho)$ is not well-defined.

Ref : See Poupaud [MAA 02] (see also Dolbeault & Schmeiser [DCDS 09]), Nieto-Poupaud-Soler [ARMA 01] for a definition of the product when a is linear.

Ref : See Carrillo et al.[4] for such a problem in the framework of Gradient flows in the case $a = Id$.

4. Carrillo, DiFrancesco, Figalli, Laurent, Slepčev, Duke Math. J. 2010

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Aggregation equation as a transport equation

$$\partial_t \rho + \mathrm{div}(a(\nabla_x W * \rho)\rho) = 0, \qquad \rho(t=0) = \rho^0.$$

We consider the aggregation equation as a **conservative transport equation** with velocity $a(\nabla_x W * \rho)$ which may have discontinuities.

Objectives

- Existence and uniqueness of a weak measure solution, and its equivalence with the gradient flow solution.
- Design numerical schemes allowing to simulate the dynamics of the density after blow-up time.

Conservative transport equation

For the conservative transport equation

$$\partial_t u + \mathrm{div}(bu) = 0, \qquad u(t=0,x) = u^0.$$

If b is Lipschitz continuous, we can define the characteristics

$$X'(t,x) = b(t, X(t,x)), \qquad X(0,x) = x.$$

Then, the solution is given by the pushforward $u = X_\# u^0$. i.e. for all ϕ continuous, $\int \phi(x) u(dx) = \int \phi(X(t,x)) u^0(dx)$.

We notice that the definition $u = X_\# u^0$ is available also if u^0 is only a measure.

Conservative transport equation with discontinous coefficients

When b is not Lipschitz continous, one cannot guarantee the uniqueness of the flow X. But we have :

Filippov's flow

When b is one-sided Lipschitz, i.e. $\forall\, t > 0, x, y \in \mathbb{R}^d$,

$$\langle b(t,x) - b(t,y), x - y\rangle \leq \alpha(t)\|x-y\|^2, \quad \text{for } \alpha \in L^1(0,T).$$

Then there exists an unique Filippov's flow X.

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Idea : Assuming that we get two characteristics X and Y.

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|X(t)-Y(t)\|^2 &= \langle X'(t) - Y'(t), X(t) - Y(t)\rangle \\ &= \langle b(t,X(t)) - b(t,Y(t)), X(t) - Y(t)\rangle \\ &\leq \alpha(t)\|X(t)-Y(t)\|^2.\end{aligned}$$

With a Gronwall Lemma, $\|X(t) - Y(t)\| \leq e^{\int_0^t \alpha(s)ds}\|X(0) - Y(0)\|$.

Conservative transport equation with discontinous coefficients

Some remarks :

- In one dimension, the OSL condition is equivalent to $\partial_x b \leq \alpha$ in the sense of distributions.
- In higher dimension, the OSL condition is equivalent to

$$\frac{\nabla b + \nabla b^\top}{2} \leq \alpha(t)\mathrm{Id},$$

  in the sense of matrix distributions.
- **Examples :** For the Cauchy problem

$$y' = \sqrt{y}, \qquad y(0) = 0;$$

  we have two solutions $y(t) = \frac{1}{4}t^2$ and $y(t) = 0$.
  On the contrary, the Cauchy problem

$$y' = -\sqrt{y}, \qquad y(0) = 0;$$

  admits an unique solution $y = 0$.

Conservative transport equation with discontinous coefficients

Based on this Filippov's flow, we recall the results of [Poupaud-Rascle '97, Bouchut-James '98].

Poupaud-Rascle's solutions

Let $b \in L^1_{loc}([0,+\infty), L^\infty(\mathbb{R}^d))^d$ satisfying the OSL condition.
Then, for any $u^0 \in \mathcal{M}_b(\mathbb{R}^d)$, there exists a unique measure solution u in $C([0,+\infty); \mathcal{M}_b(\mathbb{R}^d))$ to the conservative transport equation with initial datum u^0 such that $u(t) = X(t)_\# u^0$, where X is the unique Filippov flow.

Remarks

- In one dimension, these solutions are equivalent to the duality solutions defined by Bouchut & James.
- A stability estimate for the Filippov flow has been recently obtained by Bianchini & Gloyer [CPDE '10] : if the velocity fields $b_n \rightharpoonup b$ weakly in L^1_{loc}, then the associated Filippov flows $X_n \to X$ locally in $C(\mathbb{R}^+ \times \mathbb{R}^d)$.

Aggregation equation as a transport equation

We come back to the aggregation equation in $\mathbb{R}^d$, $d \geq 1$, with $a = Id$,

$$\begin{aligned} &\partial_t \rho + \mathrm{div}_x \left((\nabla_x W * \rho)\rho \right) = 0, \qquad t > 0, \quad x \in \mathbb{R}^d, \\ &\rho(t=0) = \rho^0. \end{aligned}$$

We assume that the interaction potential $W : \mathbb{R}^d \to \mathbb{R}$ verifies

- $W \in C^1(\mathbb{R}^d \setminus \{0\})$, Lipschitz continuous, $W(x) = W(-x)$ and $W(0) = 0$.
- W is λ-concave for some $\lambda \geq 0$, i.e. $W(x) + \frac{\lambda}{2}|x|^2$ is concave :

$$\forall\, x, y \neq 0, \qquad \langle \nabla W(x) - \nabla W(y), x - y \rangle \leq \lambda |x - y|^2.$$

This set of potentials includes the class of so-called *pointy* potentials, for which ∇W is discontinuous in 0.
Examples : $W(x) = -\kappa|x|$ (Newtonian), $W(x) = e^{-\kappa|x|} - 1$ (Morse).

Stability of the flux

Since ∇W may be discontinuous in 0, we define

$$\widehat{\nabla W} = \begin{cases} \nabla W(x), & \text{for } x \neq 0; \\ 0, & \text{for } x = 0. \end{cases}$$

Lemma

If we have a regularization $W_n \to W$ such that $W_n \in C^1(\mathbb{R}^d)$, is odd, λ-concave and such that $\sup_{x \in \mathbb{R}^d \setminus B(0,\frac{1}{n})} |\nabla W_n(x) - \nabla W(x)| \leq \frac{1}{n}$.
If $\rho_n \rightharpoonup \rho$ weakly as measures.
Then, we have the weak convergence

$$(\nabla W_n * \rho_n)\rho_n \rightharpoonup (\widehat{\nabla W} * \rho)\rho.$$

OSL estimate

Then, we define

$$\widehat{a}_\rho(t,x) = \widehat{\nabla W} * \rho(t,x) = \int_{\mathbb{R}^d} \widehat{\nabla W}(x-z)\rho(t,dz).$$

We have

$$\begin{aligned}\langle \widehat{a}_\rho(t,x) - \widehat{a}_\rho(t,y), x-y\rangle &= \int_{\mathbb{R}^d} \langle \widehat{\nabla W}(x-z) - \widehat{\nabla W}(y-z), x-y\rangle \rho(dz) \\ &\leq \lambda |\rho|(\mathbb{R}^d)\|x-y\|^2,\end{aligned}$$

where we have used the λ-concavity of W in the last inequality.

Filippov characteristics

The macroscopic velocity $\widehat{a}_\rho$ is one-sided Lipschitz. Then, we can associate a Fillipov characteristics.

Existence and uniqueness result

For $\rho \in C([0,T], \mathcal{P}_2(\mathbb{R}^d))$ [5], we can define a Filippov characteristics $\widehat{X}$ associated to $\widehat{a}_\rho$. Then we have a push-forward measure $\widehat{\rho} = \widehat{X}_\# \rho^0$. But *a priori* we do not have that $\widehat{\rho}$ is the same as ρ.

However, we can prove

Theorem ($d \geq 1$)

Under above assumptions on W, ρ^0 given in $\mathcal{P}_2(\mathbb{R}^d)$, There exists a unique Filippov's flow X such that the pushforward measure $\rho := X_\# \rho^0$ satisfies in $\mathcal{D}'(\mathbb{R}^d)$

$$\partial_t \rho + \mathrm{div}_x \left(\widehat{a}_\rho \rho\right) = 0, \qquad \widehat{a}_\rho(t,x) = \widehat{\nabla W} * \rho.$$

By uniqueness, this solution is equivalent to the gradient flow solution.

5. $\mathcal{P}_2(\mathbb{R}^d)$ is the set of probability measures μ with finite second order moment $\int_{\mathbb{R}^d} |x|^2 \mu(dx) < +\infty$.

Existence and uniqueness result

- Existence relies on an approximation by Dirac measures and stability result ;
- Uniqueness relies on a contraction estimate in Wasserstein distance :

Contraction estimate

Under above assumptions on W, ρ^0 and $\widetilde{\rho}^0 \in \mathcal{P}_2(\mathbb{R}^d)$ Then the corresponding solutions $\rho = X_\# \rho^0$ and $\widetilde{\rho} = \widetilde{X}_\# \widetilde{\rho}^0$ verify

$$d_W(\rho(t), \widetilde{\rho}(t)) \leq e^{2\lambda t} d_W(\rho^0, \widetilde{\rho}^0).$$

Idea for the contraction estimate

Compute

$$\begin{aligned}
&\frac{d}{dt}\iint |X(t,x_1)-\widetilde{X}(t,x_2)|^2\gamma(dx_1,dx_2)\\
&\quad = 2\iint \langle a(t,X(t,x_1))-\widetilde{a}(t,\widetilde{X}(t,x_2)),X(t,x_1)-\widetilde{X}(t,x_2)\rangle\gamma(dx_1,dx_2)\\
&\quad = 2\iiiint \langle \nabla W(X(x_1)-X(y_1))-\nabla W(\widetilde{X}(x_2)-\widetilde{X}(y_2))),\\
&\qquad\qquad (X(x_1)-\widetilde{X}(x_2))\rangle\,\gamma(dx_1,dx_2)\gamma(dy_1,dy_2)
\end{aligned}$$

we may use the symmetry of W (exchanging the role of x and y) to obtain

$$\begin{aligned}
&= \iiiint \langle \nabla W(X(x_1)-X(y_1))-\nabla W(\widetilde{X}(x_2)-\widetilde{X}(y_2))),\\
&\qquad\qquad (X(x_1)-X(y_1)-\widetilde{X}(x_2)+\widetilde{X}(y_2))\rangle\,\gamma(dx_1,dx_2)\gamma(dy_1,dy_2)\\
&\le \lambda\iiiint |X(x_1)-X(y_1)-\widetilde{X}(x_2)+\widetilde{X}(y_2)|^2\,\gamma(dx_1,dx_2)\gamma(dy_1,dy_2),
\end{aligned}$$

where we use the λ-convexity of W. We conclude by a Gronwall argument (and by choosing γ as an optimal map with marginal ρ^0 and $\widetilde{\rho}^0$).

Plan

Numerical simulations for the aggregation equation

For the simplicity of the presentation, we consider the one dimensional case. But the approach can be easily extended to any dimension on a Cartesian mesh.

$$\partial_t \rho + \partial_x \big(\widehat{a}\rho\big) = 0, \quad \widehat{a} = \widehat{\partial_x W} * \rho.$$

Considering a Cartesian mesh of nodes $x_i = i\Delta x$, and time step Δt, $t^n = n\Delta t$, we introduce the conservative scheme :

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x}(J_{i+1/2}^n - J_{i-1/2}^n)$$
$$J_{i+1/2}^n = (a_i^n)^+ \rho_i^n - (a_{i+1}^n)^- \rho_{i+1}^n,$$

where $(a)^+ = \max\{0, a\}$ and $(a)^- = -\min\{0, a\}$.
The macroscopic velocity is discretized by

$$a_i^n = \sum_{k\in\mathbb{Z}} \rho_k^n \widehat{\partial_x W}(x_i - x_k).$$

Numerical simulations

Defining the reconstruction $\rho_\Delta^n = \sum_{i\in\mathbb{Z}} \rho_i^n \delta_{x_i}$, we may prove the weak convergence of $(\rho_\Delta^n)_n$ towards the weak measure solution of the aggregation equation *(under CFL condition)*. It allows to recover the dynamics after blow up :

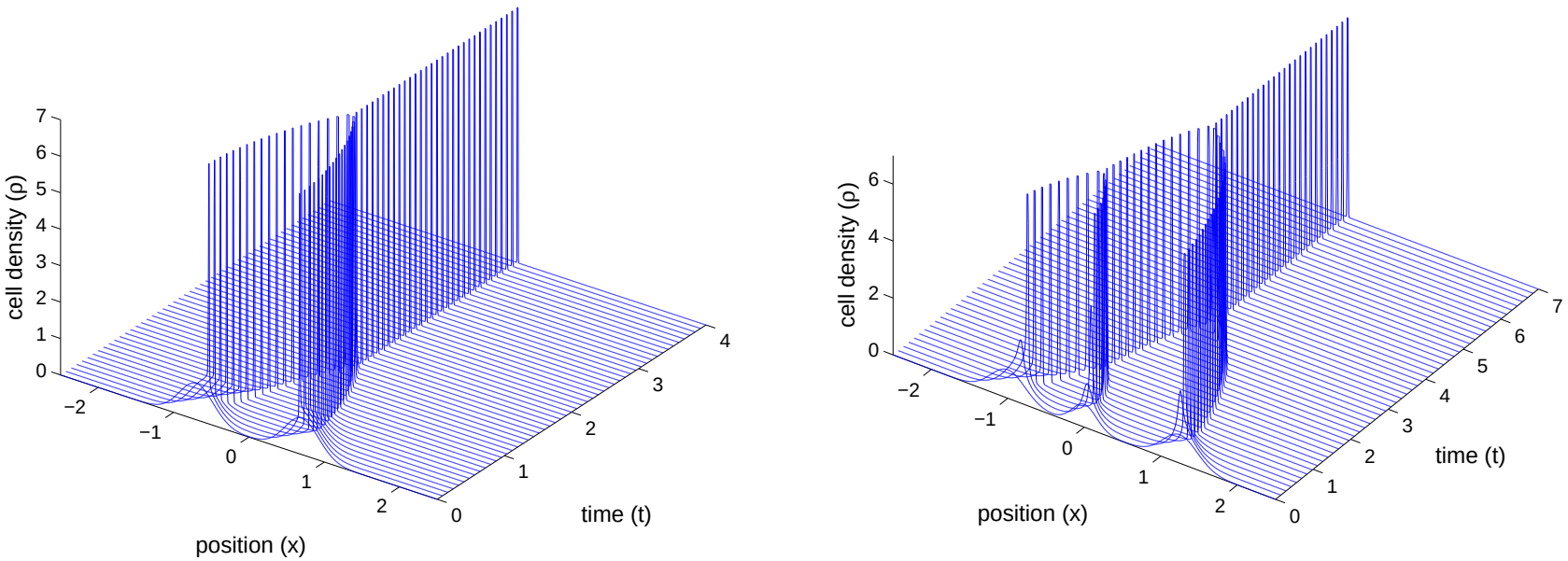

FIGURE: Dynamics of the density ρ for a Morse potential $W = e^{-5|x|} - 1$.

Remark on the scheme

We emphasize that the above scheme

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x}(J_{i+1/2}^n - J_{i-1/2}^n),$$
$$J_{i+1/2}^n = (a_i^n)^+ \rho_i^n - (a_{i+1}^n)^- \rho_{i+1}^n,$$

is different from the standard finite volume scheme where

$$J_{i+1/2}^n = (a_{i+1/2}^n)^+ \rho_i^n - (a_{i+1/2}^n)^- \rho_{i+1}^n.$$

A geometrical interpretation of the scheme is the following (under CFL condition) :

- The Delta mass ρ_i^n located at x_i moves with velocity a_i^n to the position $x_i + a_i^n \Delta t$;
- Then we make a linear interpolation of the mass between x_i and x_{i+1} if $a_i^n \geq 0$, or between x_{i-1} and x_i if $a_i^n \leq 0$.

Remark on the scheme

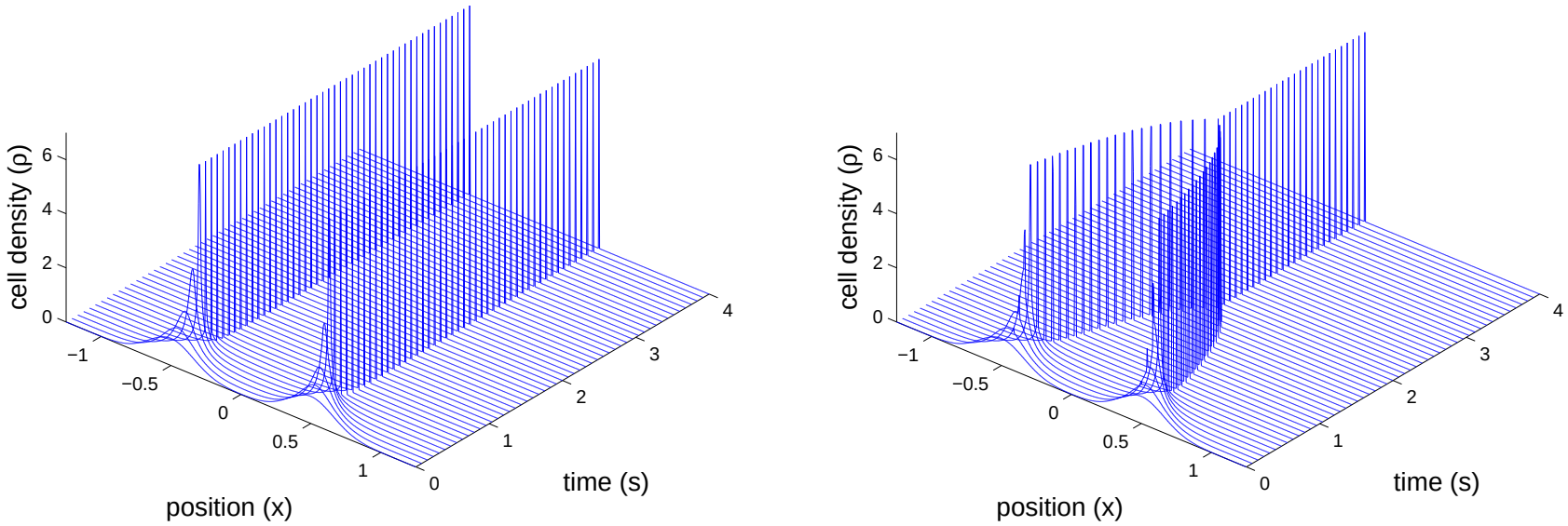

FIGURE: Numerical results for the one dimensional aggregation equation with an initial data given by the sum of two Gaussian functions. Left : Numerical results obtained with the standard finite volume upwind scheme. Right : Numerical results with the adapted upwind scheme.

Numerical simulations for two species

In order to illustrate the richness of the dynamics after blow up, we consider the case of two species in interaction. The model reads

$$\partial_t \rho_1 + \chi_1 \partial_x (\partial_x S \rho_1) = 0, \qquad \partial_t \rho_2 + \chi_2 \partial_x (\partial_x S \rho_2) = 0,$$
$$-\partial_{xx} S + S = \rho_1 + \rho_2.$$

Numerical simulations illustrate a complex dynamics with synchronisation or non-synchronisation of the dynamics of Dirac deltas.
Examples with $\chi_1 = 10$, $\chi_2 = 1$ for different initial data :

- synchronising dynamics
- non-synchronising dynamics
- non-synchronising dynamics
- more complex dynamics

Numerical simulations in higher dimension

In higher dimension, we use the same scheme and obtain similar results :

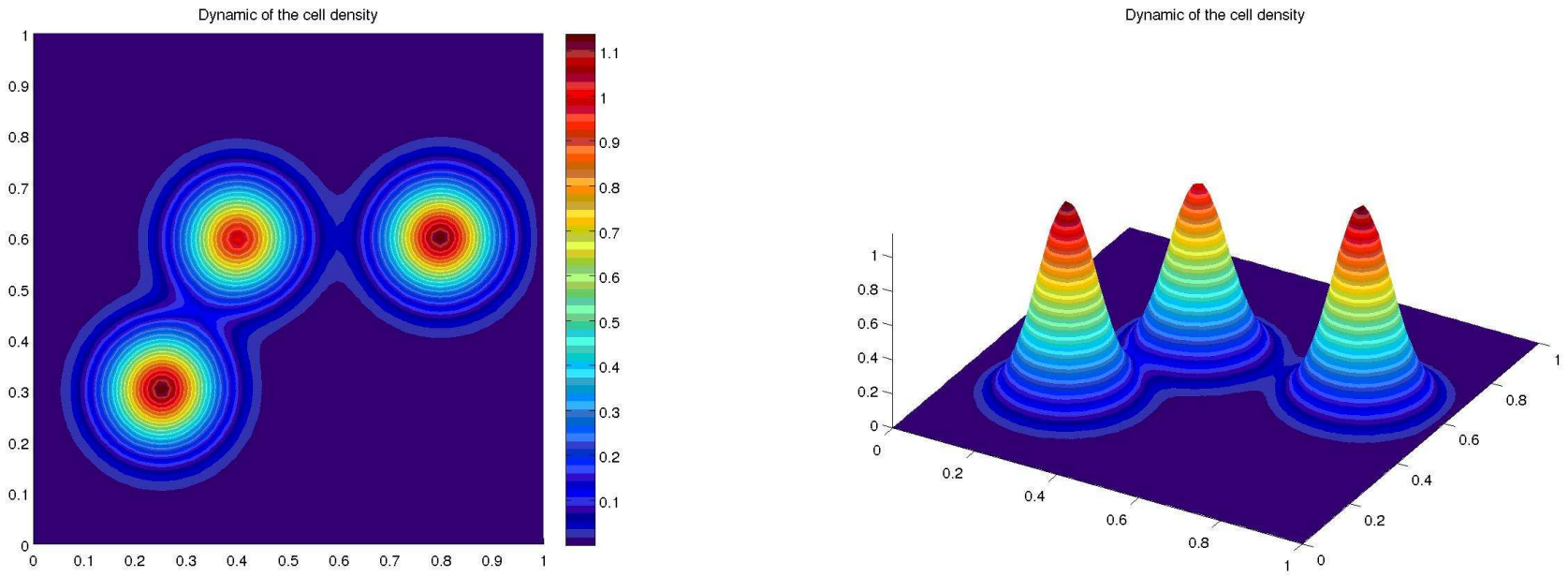

FIGURE: Dynamics of the density of bacteria ρ.

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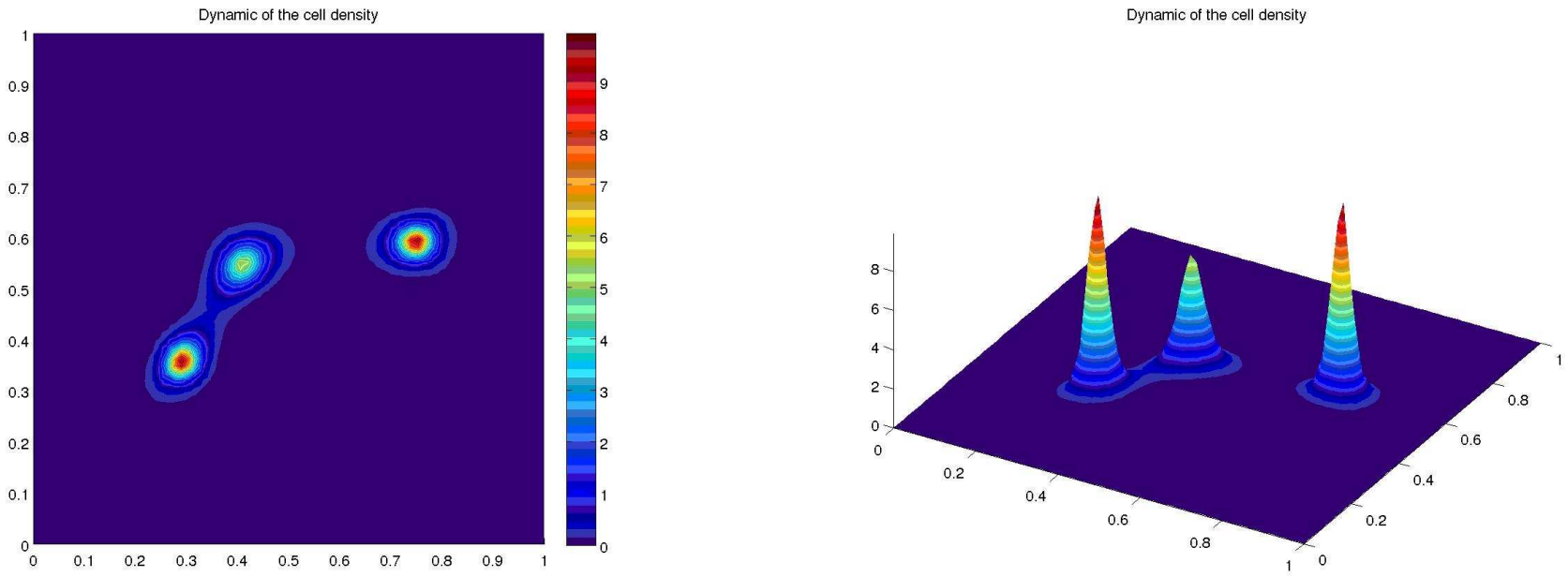

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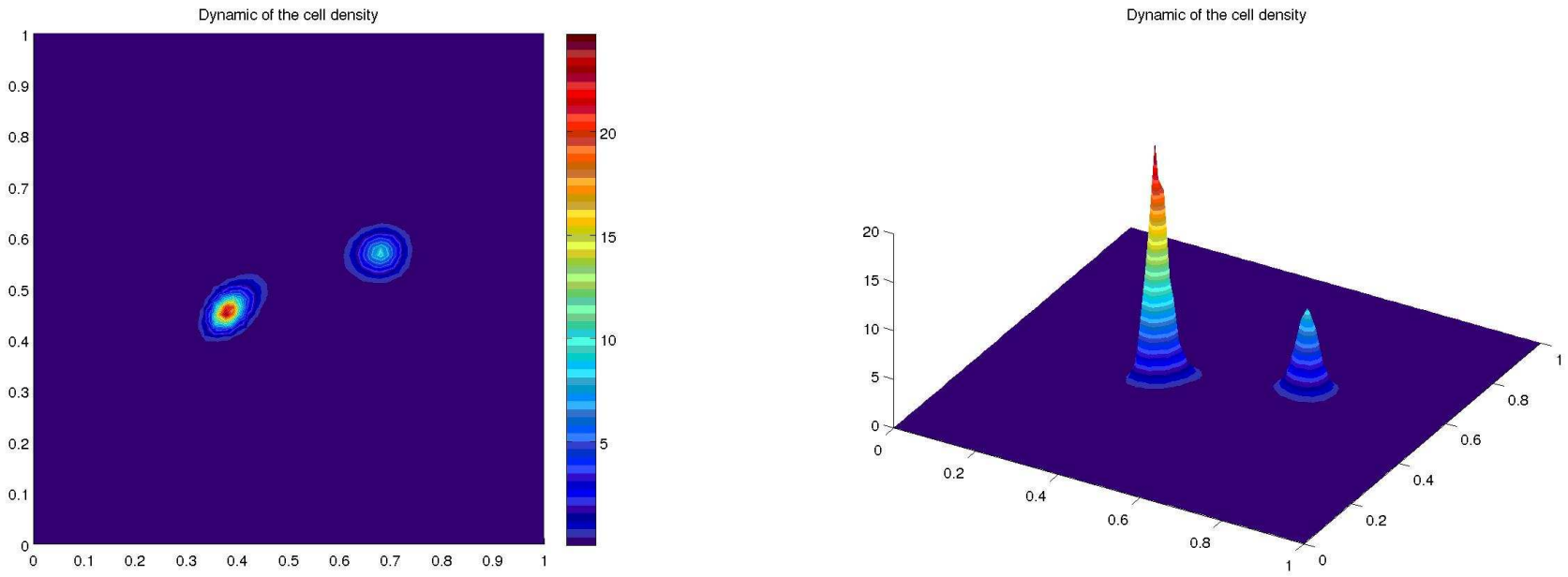

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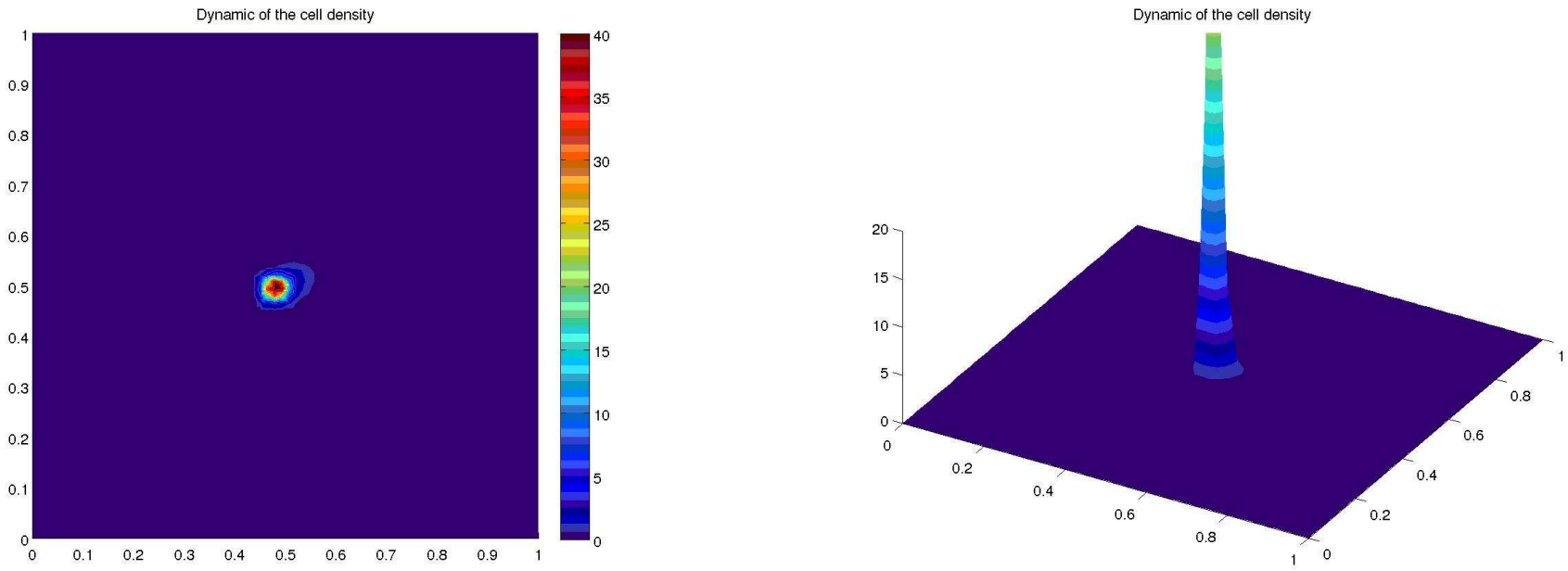

FIGURE: Dynamics of the density of bacteria ρ.

Convergence analysis

Order of convergence ($d \geq 1$)

Under the above assumptions on W. Let $\rho^0 \in \mathcal{P}_2(\mathbb{R}^d)$. Let $\rho = X_\# \rho^0$ be the unique measure solution to the aggregation equation with initial data ρ^{ini}. Let us define the reconstruction

$$\rho_\Delta^n = \sum_{J \in \mathbb{Z}^d} \rho_J^n \delta_{x_J},$$

where the approximation sequence (ρ_J^n) is computed thanks to the above upwind scheme. Then, under the CFL condition $w_\infty \frac{\Delta t}{\Delta x} \leq 1$, there exists a nonnegative constant C such that for all $n \in \mathbb{N}^*$,

$$d_W(\rho(t^n), \rho_{\Delta x}^n) \leq C\, e^{|\lambda|(1+\Delta t)t^n} \sqrt{t^n \Delta x}.$$

Remark : This order $1/2$ is optimal.

Convergence analysis

Idea of the proof

Define a random characteristics X_Δ such that $\rho_\Delta^n = X_\Delta(t_n)_\# \mathbb{P}_{\rho^0}$. Then we use the property of the Wasserstein distance

$$\begin{aligned} d_W(\rho(t^n), \rho_\Delta^n) &= d_W(X(t^n)_\# \mathbb{P}_{\rho^0}, X_\Delta(t^n)_\# \mathbb{P}_{\rho^0}) \\ &\leq \|X(t^n) - X_\Delta(t^n)\|_{L^2(\mathbb{P}_{\rho^0})} \\ &= \mathbb{E}\big(|X(t^n) - X_\Delta(t^n)|^2\big)^{1/2}, \end{aligned}$$

where $\mathbb{E}$ is the expectation.

Probabilistic interpretation

We rewrite the scheme as (in one dimension to simplify the scripture)

$$\rho_i^{n+1} = \rho_i^n \left[1 - \frac{\Delta t}{\Delta x}|a_i^n|\right] + \rho_{i+1}^n \frac{\Delta t}{\Delta x}(a_{i+1}^n)^- + \rho_{i-1}^n \frac{\Delta t}{\Delta x}(a_{i-1}^n)^+.$$

Probabilistic interpretation : The mass ρ_i^n located in x_i

- stays in x_i with probability $P_{i,i}^n = 1 - \frac{\Delta t}{\Delta x}|a_i^n|$;
- moves to x_{i-1} with probability $P_{i,i-1}^n = \frac{\Delta t}{\Delta x}(a_i^n)^-$;
- moves to x_{i+1} with probability $P_{i,i+1}^n = \frac{\Delta t}{\Delta x_i}(a_i^n)^+$.

We notice that $P_{ii} + P_{ii+1} + P_{ii-1} = 1$. The scheme rewrites

$$\rho_i^{n+1} = \rho_i^n P_{i,i}^n + \rho_{i+1}^n P_{i+1,i}^n + \rho_{i-1}^n P_{i-1,i}^n.$$

Then we may define a Markov chain by introducing the process $(K^n)_{n\in\mathbb{N}}$: K^n is the nth site occupied by the random process.

Probabilistic interpretation

We define the random characteristics by

$$\forall\, n \in \mathbb{N},\ \forall\, \omega \in \Omega = \mathbb{Z}^{\mathbb{N}}, \qquad X_\Delta^n(\omega) = x_{K^n(\omega)}.$$

Fundamental properties

(i) For all $i \in \mathbb{Z}$, we have,

$$\mathbb{E}^n(X_\Delta^{n+1} - X_\Delta^n) = \Delta t \int_{\mathbb{R}} \widehat{\nabla W}(X^n - y)\, \rho_{\Delta x}^n(dy).$$

(ii) We have $\rho_{\Delta x}^n = X_{\Delta\#}^n \mathbb{P}_{\rho_{\Delta x}^0}$.

Idea of the proof

(i) We compute the conditional expectation given the trajectory of the Markov chain up until time t^n :

$$\mathbb{E}^n(X_\Delta^{n+1} - X_\Delta^n) = \left(\Delta x (a_{K^n}^n)^+ \frac{\Delta t}{\Delta x} - \Delta x (a_{K^n}^n)^- \frac{\Delta t}{\Delta x}\right) = \Delta t a_{K^n}^n.$$

Probabilistic interpretation

(ii) For any $\mu \in \mathcal{P}(\mathbb{Z})$, we have, for all $n \in \mathbb{N}$,

$$X_\Delta^{n+1}{}_\# \mathbb{P}_\mu = \sum_{L \in \mathbb{Z}} \delta_{x_L} \mathbb{P}_\mu \big(K^{n+1} = L\big) = \sum_{L \in \mathbb{Z}} \sum_{J \in \mathbb{Z}} \delta_{x_L} \mathbb{P}_\mu \big(K^n = J\big) P^n_{J,L}.$$

Therefore,

$$X_\Delta^{n+1}{}_\# \mathbb{P}_\mu = \sum_{L \in \mathbb{Z}} \delta_{x_L} \Big(\mathbb{P}_\mu \big(K^n = L\big) P^n_{L,L} + \mathbb{P}_\mu \big(K^n = L-1\big) P^n_{L-1,L} + \mathbb{P}_\mu \big(K^n = L+1\big) P^n_{L+1,L} \Big).$$

Choosing $\mu = \rho^0_{\Delta x}$, the result follows from a straightforward induction, since we have

$$\rho_L^{n+1} = \rho_L^n P^n_{L,L} + \rho^n_{L+1} P^n_{L+1,L} + \rho^n_{L-1} P^n_{L-1,L}.$$

Proof of the convergence order

Idea of the proof

Recalling the previous estimate

$$d_W(\rho(t^n), \rho_\Delta^n) \leq \mathbb{E}\big(|X(t^n) - X_\Delta(t^n)|^2\big)^{1/2},$$

we are left to estimate the right hand side. We have

$$X(t^{n+1}, x) = X(t^n, x) + \int_{t^n}^{t^{n+1}} \widehat{a}_\rho(s, X(s,x))\, ds$$

$$X_\Delta(t^{n+1}, \omega) = X_\Delta(t^n, \omega) + \Delta t a_{K^n}^n(\omega) + h^n(\omega),$$

where we have $|h^n(\omega)| \leq \Delta x$ (due to CFL condition) and $\mathbb{E}^n(h^n) = 0$ (due to the fundamental properties).

$$\begin{aligned}|X(t^{n+1}) - X_\Delta(t^{n+1})|^2 &= |X(t^n) - X_\Delta(t^n)|^2 \\ &+ 2\int_{t^n}^{t^{n+1}} \langle \widehat{a}_\rho(s, X(s,x)) - a_{K^n}^n(\omega), X(t^n) - X_\Delta(t^n)\rangle\, ds \\ &+ \langle X(t^n) - X_\Delta(t^n), h^n(\omega)\rangle + O(\Delta t \Delta x).\end{aligned}$$

Proof of the convergence order

- *second term.* Using the fact that $\widehat{a}_\rho$ is bounded, we have for $s \in (t^n, t^{n+1})$, $|X(t^n) - X(s)| = O(\Delta t)$. Then, we may use the OSL estimate (after some computations) to prove that

$$\int_{t^n}^{t^{n+1}} \langle \widehat{a}_\rho(s,x) - a^n_{K^n}(\omega), X(t^n) - X_\Delta(t^n) \rangle \, ds \\ \leq \lambda \Delta t |X(t^n) - X_\Delta(t^n)|^2 + O(\Delta t \Delta x).$$

- *third term.* Taking the expected value knowing the position at time t^n, we have

$$\mathbb{E}^n(\langle X(t^n) - X_\Delta(t^n), h^n(\omega) \rangle) = \langle X(t^n) - X_\Delta(t^n), \mathbb{E}(h^n(\omega)) \rangle = 0.$$

We obtain

$$\mathbb{E}(|X(t^{n+1}) - X_\Delta(t^{n+1})|^2) \leq (1 + \lambda \Delta t) \mathbb{E}(|X(t^n) - X_\Delta(t^n)|^2) + O(\Delta t \Delta x).$$

The conclusion follows by a Gronwall lemma.

Conclusion and perspectives

We have presented an analysis of measures valued solutions for the aggregation equation with pointy potentials and provide a scheme allowing to recover the dynamics after blow-up.
This system can be obtained thanks to a hydrodynamical limit from a kinetic model. Numerical simulations of such kinetic models have interesting challenging issues. In particular, non-conservative products should be handle with care (work in collaboration with Laurent Gosse [CNR Roma]).

Several aspects are still under progress :

- Hydrodynamical limit in higher dimension.
- Model with internal variable describing the methylation level.
- Adding the nonlinear function a.

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Thanks you for your attention !