Quantitative particle approximation of nonlinear Fokker-Planck equations with singular kernels

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joint work with C. Olivera (Campinas) and A. Richard (CentraleSupélec) to appear in Ann Sc Norm Super Pisa'21+

Conference BSDE and Mean Field Systems
27 June 2022

Overview

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Nonlinear Fokker-Planck equation with singular interaction

- We study on $[0,T) \times \mathbb{R}^d$

$$\begin{cases} \partial_t u(t,x) = \Delta u(t,x) - \nabla \cdot \big(u(t,x)\ K *_x u(t,x)\big), \\ u(0,x) = u_0(x), \end{cases} \tag{NLFP}$$

  with K **locally integrable** and singular at 0.

- Our main interest : stochastic particle approximation of (NLFP).
- Why?
  - Macroscopic to microscopic description (and back!);
  - Numerical schemes...

Classical approach: mean-field interactions

- (NLFP) is seen as the FP equation for the non-linear process

$$\begin{cases} dX_t = K * u_t(X_t)dt + \sqrt{2}dW_t, \\ \mathcal{L}(X_t) = u_t. \end{cases} \qquad \text{(NLSDE)}$$

- Particle system in mean-field interaction :

$$dX_t^{i,N} = \frac{1}{N}\sum_{j=1}^{N} K(X_t^{i,N} - X_t^{j,N}) + \sqrt{2}dW_t^{i,N} \qquad \text{(PS)}$$

and its empirical measure $\mu^N_{\cdot} = \frac{1}{N}\sum_{i=1}^{N} \delta_{X^{i,N}_{\cdot}}$.
- Propagation of chaos : convergence in law of μ^N in $\mathcal{P}(\mathcal{C})$ towards the law of X.
- Issues: **K singular** $\to$ wellposedness of (PS), (NLSDE) and the propagation of chaos?
- Probabilistic approach to **singular** interactions:
  - Boltzmann, Burgers, Navier-Stokes, Keller-Segel equations, ...
  - studied by Bossy, Calderoni, Cattiaux, Fournier, Hauray, Jabin, Jourdain, Méléard, Mischler, Osada, Pulvirenti, Talay, ...

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Another viewpoint: moderate interaction

Motivated by singular attractive kernels for which either:

- existence of (PS) is unknown ;
- or existence ok, but convergence unknown.

Moderately interacting particles :

$$dX_t^{i,N} = F\Big(V^N * (K * \mu_t^N)(X_t^{i,N})\Big)dt + \sqrt{2}dW_t^{i,N},$$

where:

- $V^N(x) = N^{d\alpha}V(N^\alpha x), \alpha > 0$ and V a regular density;
- F a smooth cut-off.
- Some references : [Oelschläger'85], [Méléard & Roelly'87], [Jourdain & Méléard'98]

$\rightarrow$ A **semigroup approach** was recently developed by Flandoli, Olivera and their collaborators to get uniform (non-quantitative) convergence of $V^N * \mu^N$ towards a mild solution to:

FKPP, 2d Navier-Stokes equations, PDE-ODE system related to aggregation phenomena.

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Our main objectives

What assumptions on K and what suitable functional framework for (NLFP) so the following holds?

- Convergence of $\{\mu_t^N = \frac{1}{N}\sum_{i=1}^N \delta_{X_t^{i,N}},\, t \in [0,T]\}$ to the solution (NLFP) when $N \to \infty$:
  - which range of α?
  - what is the rate of convergence ?
- Well-posedness of (NLSDE).
- Propagation of chaos towards (NLSDE) (without the cut-off and the mollifier)

Which kernels?

A typical example in dimension $d \geq 2$ is the family of **Riesz kernels**:

$$K_s(x) = \pm \nabla \mathcal{V}_s(x)$$

where

$$\mathcal{V}_s(x) := \begin{cases} |x|^{-s} & \text{if } s \in (0, d-1) \\ -\log|x| & \text{if } s = 0 \end{cases}, \quad x \in \mathbb{R}^d.$$

Examples:

- Coulomb interactions: K_s, with $s = d-2$ ($d \geq 3$);
- 2d Navier-Stokes equation (vorticity): $K(x) = \frac{x^\perp}{|x|^2}$;
- Parabolic-elliptic Keller-Segel model: $K(x) = -\chi \frac{x}{|x|^d}$ (*attractive*...);
- Some attractive-repulsive kernels.

Overview

Assumptions on K and α

(H_K):

(i) $K \in L^{\boldsymbol{p}}(\mathcal{B}_1)$, for some $\boldsymbol{p} \in [1, +\infty]$;

(ii) $K \in L^{\boldsymbol{q}}(\mathcal{B}_1^c)$, for some $\boldsymbol{q} \in [1, +\infty]$;

(iii) There exists $\boldsymbol{r} \geq \max(\boldsymbol{p}', \boldsymbol{q}')$ and $\boldsymbol{\zeta} \in (0, 1]$ such that:

$$\mathcal{N}_{\boldsymbol{\zeta}}(K * f) \lesssim \|f\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}, \quad \forall f \in L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d).$$

($\mathcal{N}_\zeta$ the Hölder seminorm of parameter $\boldsymbol{\zeta}$.)

(H_α): α and $\boldsymbol{r}$ satisfy

$$0 < \alpha < \frac{1}{d + 2d(\frac{1}{2} - \frac{1}{\boldsymbol{r}}) \vee 0}.$$

- Notice here that for $f \in L^1 \cap L^r(\mathbb{R}^d)$ one has

$$\|K * f\|_{L^\infty(\mathbb{R}^d)} \leq C_{K,d} \|f\|_{L^1 \cap L^r(\mathbb{R}^d)}.$$

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Convergence of the mollified empirical measure

Assume (always today) that $u_0 \geq 0$ and $\int_{\mathbb{R}^d} u_0 = 1$.

Proposition

Let K satisfying (H_K)(i)-(ii), $u_0 \in L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)$ with $\boldsymbol{r} \geq \max(\boldsymbol{p}', \boldsymbol{q}')$. There exists $T > 0$ and a unique $u : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ s.t.

$$u \in \mathcal{C}([0,T]; L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d))$$

and

$$u_t = e^{t\Delta} u_0 - \int_0^t \nabla \cdot (e^{(t-s)\Delta}(u_s \, K * u_s)) \, ds, \quad 0 \leq t \leq T.$$

Denote by T_{max} the maximal existence time.

Convergence of the mollified empirical measure

Theorem ([O.-R.-T. Ann Sc Norm Super Pisa'21+])

Let $T < T_{max}$ and assume (H_K) and (H_α). Under suitable conditions on the initial conditions, we have for $\{u_t^N = V^N * \mu_t^N,\ t \in [0,T]\}_{N\in\mathbb{N}}$ *:*
$\forall \varepsilon > 0$ *and* $\forall m \geq 1$,

$$\Big\| \|u^N - u\|_{T, L^1\cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \Big\|_{L^m(\Omega)} \lesssim \Big\| \|u_0^N - u_0\|_{L^1\cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \Big\|_{L^m(\Omega)} + N^{-\varrho+\varepsilon},$$

where

$$\varrho = \min\left(\alpha\boldsymbol{\zeta}, \frac{1}{2}\left(1 - \alpha(d + d(1-\frac{2}{\boldsymbol{r}}) \vee 0)\right)\right).$$

Without the cutoff F in the drift of the particles, we get:

Corollary

For any $\varepsilon \in (0, \varrho)$, *any* $\eta > 0$ *and any* $m \geq 1$,

$$\mathbb{P}\left(\|u_t^N - u_t\|_{T, L^1 \cap L^r(\mathbb{R}^d)} \geq \eta\right) \lesssim \frac{1}{\eta^m}\Big(\big\| \|u_0^N - u_0\|_{L^1 \cap L^r(\mathbb{R}^d)} \big\|_{L^m(\Omega)} + N^{-\varrho+\varepsilon}\Big)^m .$$

Some consequences and remarks

- Same rate for the genuine empirical measure of (PS)

$$\left\| \sup_{t\in[0,T]} \|\mu_t^N - u_t\|_0 \right\|_{L^m(\Omega)} \leq C\, N^{-\varrho+\varepsilon},$$

  where $\|\cdot\|_0$ denotes the Kantorovich-Rubinstein metric

- The rate in the previous results holds almost surely.
- Cannot expect here a $N^{-\frac{1}{2}}$ rate of convergence because of the short range interactions : "best possible" $N^{-\alpha}$.

Applications

- **Coulomb-type kernels** (like Biot-Savart in $d=2$, Riesz with $s=d-2$),
  - convergence happens for $\alpha < \frac{1}{2(d-1)}$ $\quad (d=2 \Rightarrow \alpha = (\frac{1}{2})^{-})$;
  - best possible rate is $\varrho = \left(\frac{1}{2(d+1)}\right)^{-}$ (obtained for $\alpha = \left(\frac{1}{2(d+1)}\right)^{+}$, $\boldsymbol{r} = +\infty$, $\boldsymbol{\zeta} = 1$).

- **Keller-Segel parabolic elliptic** ($d=2:$ global solution $\chi < 8\pi$, blow up in finite time otherwise).
  - we get the above rate for any value of χ;
  - the result holds even if the PDE explodes in finite time ($\chi > 8\pi$).

- **The Riesz kernels with** $s > d-2$ do not satisfy (H_K)(iii). However, by imposing more regularity on the initial conditions and smaller values of α, we get a rate of convergence for singular Riesz kernels with $s \in (d-2, d-1)$.

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Sketch of proof

- Derive the SPDE satisfied by the mollified empirical measure u^N in its mild form

$$u_t^N(x) = e^{t\Delta}u_0^N(x) - \int_0^t \nabla \cdot e^{(t-s)\Delta}\langle \mu_s^N, V^N(x-\cdot)F\big(K * u_s^N(\cdot)\big)\rangle \, ds \\ -\frac{1}{N}\sum_{i=1}^N \int_0^t e^{(t-s)\Delta}\nabla V^N(x - X_s^{i,N}) \cdot dW_s^i, \quad x \in \mathbb{R}^d$$

applying Itô's formula to $G_{t,V^N}(s, x-\cdot) := e^{(t-s)\Delta}V^N(x-\cdot)$ on each particle between 0 and t for x and t fixed. (sum up, $\frac{1}{N}$, rearrange..)

- For $q \geq 1$ establish that

$$\sup_{N\in\mathbb{N}^*} \mathbb{E}\left[\sup_{t\in[0,T]} \left\|u_t^N\right\|_{L^r(\mathbb{R}^d)}^q\right] < \infty.$$

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Decompose $\|u_t^N - u_t\|_{L^1 \cap L^r}$ into several terms (u is the unique sln of the mild equation with cut-off):

$$
\begin{aligned}
u_t^N(x) - u_t(x) = e^{t\Delta}(u_0^N - u_0)(x) + E_t(x) - M_t^N(x) \\
+ \int_0^t \nabla \cdot e^{(t-s)\Delta} \Big(u_s F(K * u_s) - u_s^N F(K * u_s^N) \Big)(x) \, ds,
\end{aligned}
$$

where we have set

$$
E_t(x) := \int_0^t \nabla \cdot e^{(t-s)\Delta} \langle \mu_s^N, V^N(x - \cdot) \Big(F\big(K * u_s^N(x)\big) - F\big(K * u_s^N(\cdot)\big) \Big) \rangle \, ds,
$$

$$
M_t^N(x) := \frac{1}{N} \sum_{i=1}^N \int_0^t e^{(t-s)\Delta} \nabla V^N(x - X_s^{i,N}) \cdot dW_s^i. \tag{1}
$$

Pivoting in the last term and using that

$$\|K * f\|_{L^\infty(\mathbb{R}^d)} \leq C_{K,d} \|f\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}$$

$$\|u_t^N - u_t\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \leq \|u_0^N - u_0\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} + C \int_0^t \frac{1}{\sqrt{t-s}} \|u_s^N - u_s\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} ds$$
$$+ \|E_t\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} + \|M_t^N\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}.$$

Using the Grönwall lemma for convolution integrals, we obtain

$$\begin{aligned} \|u^N - u\|_{t, L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \leq C\Big(& \|u_0^N - u_0\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \\ & + \|E\|_{t, L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} + \|M^N\|_{t, L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}\Big). \end{aligned} \tag{2}$$

It remains to control the moments of $\|E\|_{t, L^q(\mathbb{R}^d)}$ and $\|M\|_{t, L^q(\mathbb{R}^d)}$ for $q \in \{1, \boldsymbol{r}\}$. This is where the two expression in the definition of the speed ρ appear.

Observe that (positivity of F, heat kernel)

$$\|E_t\|_{L^q(\mathbb{R}^d)} \leq C \int_0^t \frac{1}{(t-s)^{\frac{1}{2}}} \Big(\int_{\mathbb{R}^d} \langle \mu_s^N, V^N(x-\cdot) \Big| F\big(K * u_s^N(\cdot)\big) - F\big(K * u_s^N(x)\big) \Big| \rangle^q \, dx \Big)^{\frac{1}{q}} \, ds.$$

F Lipschitz and the $\boldsymbol{\zeta}$-Hölder continuity of $K * u^N$ give

$$\|E_t\|_{L^q(\mathbb{R}^d)} \leq C \int_0^t \frac{\|u_s^N\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}}{(t-s)^{\frac{1}{2}}} \left(\int_{\mathbb{R}^d} \langle \mu_s^N, V^N(x-\cdot) \, |\cdot - x|^{\boldsymbol{\zeta}} \rangle^q \, dx \right)^{\frac{1}{q}} \, ds.$$

Since V is compactly supported (wlog, assume $supp(V) \subset B_1$), we have that $V^N(x-y) \, |y-x|^{\boldsymbol{\zeta}} \leq N^{-\alpha\boldsymbol{\zeta}} V^N(x-y)$. Thus

$$\begin{aligned} \|E_t\|_{L^q(\mathbb{R}^d)} &\leq \frac{C}{N^{\alpha\boldsymbol{\zeta}}} \int_0^t \frac{1}{(t-s)^{\frac{1}{2}}} \|u_s^N\|_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \|u_s^N\|_{L^q(\mathbb{R}^d)} \, ds \\ &\leq \frac{C}{N^{\alpha\boldsymbol{\zeta}}} \int_0^t \frac{1}{(t-s)^{\frac{1}{2}}} \|u_s^N\|^2_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \, ds, \end{aligned}$$

Apply Hölder's inequality with $p = \frac{3}{2}$ to obtain

$$\|E_t\|_{L^q(\mathbb{R}^d)} \leq \frac{C}{N^{\alpha\boldsymbol{\zeta}}} \left(\int_0^t (t-s)^{-\frac{3}{4}}\, ds \right)^{\frac{2}{3}} \left(\int_0^t \|u_s^N\|^6_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)}\, ds \right)^{\frac{1}{3}}.$$

Finally, we have from Jensen's inequality that for $m \geq 3$,

$$\left\| \|E\|_{t, L^q(\mathbb{R}^d)} \right\|_{L^m(\Omega)} \leq \frac{C}{N^{\alpha\boldsymbol{\zeta}}} \left(\int_0^t \mathbb{E}\left[\|u_s^N\|^{2m}_{L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)} \right] ds \right)^{\frac{1}{m}}$$

and the bound uniform bounds on u^N permits to conclude that

$$\left\| \|E\|_{t, L^q(\mathbb{R}^d)} \right\|_{L^m(\Omega)} \leq \frac{C}{N^{\alpha\boldsymbol{\zeta}}}. \tag{3}$$

This inequality immediately extends to $1 \leq m < 3$.

Sketch of proof

Main issue: control the moments of

$$\sup_{t\leq T}\|\frac{1}{N}\sum_{i=1}^{N}\int_0^t e^{(t-s)\triangle}\nabla V^N(X_s^i-\cdot)dW_s^i\|_{L^1\cap L^r(\mathbb{R}^d)}.$$

- Not a martingale, fix the time in the heat operator and it becomes one;
- to control the $L^1\cap L^r(\mathbb{R}^d)$ norm, use stochastic integration techniques in infinite-dimensional spaces [van Neerven et al.'07];
- use Garsia-Rodemich-Rumsey's lemma to put the $\sup$ inside.

Note that this is where the limitation on α (H_α) arises.

Overview

Definition

Assume (H_K)(i)-(ii), $u_0 \in L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d)$ with $\boldsymbol{r} \geq \max(\boldsymbol{p}', \boldsymbol{q}')$ and consider the canonical space $\mathcal{C}([0,T];\mathbb{R}^d)$ equipped with its canonical filtration. We say that $\mathbb{Q} \in \mathcal{P}(\mathcal{C}([0,T];\mathbb{R}^d))$ solves the nonlinear martingale problem associated to (NLSDE) if:

(i) $\mathbb{Q}_0 = u_0$;

(ii) For any $t \in (0,T]$, $\mathbb{Q}_t$ has density q_t and $q \in \mathcal{C}([0,T]; L^1 \cap L^{\boldsymbol{r}}(\mathbb{R}^d))$;

(iii) For any $f \in \mathcal{C}_c^2(\mathbb{R}^d)$, the process $(M_t)_{t\in[0,T]}$ defined as

$$M_t := f(w_t) - f(w_0) - \int_0^t \Big[\Delta f(w_s) + \nabla f(w_s) \cdot (K * q_s(w_s))\Big] ds$$

is a $\mathbb{Q}$-martingale, where $(w_t)_{t\in[0,T]}$ denotes the canonical process.

The nonlinear process

Proposition

Let $T < T_{max}$. Then the martingale problem related to (NLSDE) *is well-posed.*

$\Rightarrow$ the McKean-Vlasov equation (NLSDE) admits a unique weak solution $\widetilde{X}$. Combined with the convergence theorem, it comes:

$$\left\| \max_{i\in\{1,\dots,N\}} \sup_{t\in[0,T]} |X_t^{i,N} - \widetilde{X}_t^i| \right\|_{L^m(\Omega)} \leq C\, N^{-\varrho+\varepsilon}, \quad \forall N \in \mathbb{N}^*.$$

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Propagation of chaos

Theorem

Same hypotheses as in previous Theorem + Assume that $\{X_0^i,\ i \in \mathbb{N}\}$ *are identically distributed and that* $\langle u_0^N, \varphi\rangle \xrightarrow{\mathbb{P}} \langle u_0, \varphi\rangle$, $\forall \varphi \in \mathcal{C}_b(\mathbb{R}^d)$. *Then*

$$\mu_.^N \xrightarrow{(d)} \mathbb{Q},$$

where $\mathbb{Q}$ *is the law of the solution of* (NLSDE).

Example: $2d$ Keller-Segel parabolic-elliptic equation. We obtain local existence and uniqueness of (NLSDE) for all values of χ and the propagation of chaos towards it.

Propagation of chaos

Theorem

Same hypotheses as in previous Theorem + Assume that $\{X_0^i,\ i \in \mathbb{N}\}$ *are identically distributed and that* $\langle u_0^N, \varphi\rangle \xrightarrow{\mathbb{P}} \langle u_0, \varphi\rangle$, $\forall \varphi \in \mathcal{C}_b(\mathbb{R}^d)$*. Then*

$$\mu_{\cdot}^N \xrightarrow{(d)} \mathbb{Q},$$

where $\mathbb{Q}$ *is the law of the solution of* (NLSDE)*.*

Example: $2d$ Keller-Segel parabolic-elliptic equation. We obtain local existence and uniqueness of (NLSDE) for all values of χ and the propagation of chaos towards it.

Sketch of proof

Usual strategy:

(1) Consider the nonlinear MP with cutoff;
(2) Prove the tightness of the family $\Pi^N := \mathcal{L}(\mu^N)$ in the space $\mathcal{P}(\mathcal{P}(\mathcal{C}([0,T];\mathbb{R}^d)))$;
(3) Prove that any limit point Π^∞ of Π^N is $\delta_{\mathbb{Q}}$.
(4) Lift the cutoff.

(3) is the most technical part:

- work in fact on

$$\mathcal{H} := \mathcal{P}(\mathcal{C}([0,T];\mathbb{R}^d)) \times \mathcal{C}([0,T];L^1 \cap L^r(\mathbb{R}^d))$$

  with $\widetilde{\Pi}^N = \mathcal{L}(\mu^N, u^N)$ (as in [Méléard & Roelly'87]).
- introduce a quadratic functional Γ on $\mathcal{H}$, which depends on the form of the martingale problem.
- use the convergence of $\widetilde{\Pi}^N$ to $\widetilde{\Pi}^\infty$ to prove that $\Gamma = 0$ $\widetilde{\Pi}^\infty$-a.e. This is where μ^N and the particle system appear.
- deduce that the first coordinate of $\widetilde{\Pi}^\infty$ solves the nonlinear MP (with cutoff).

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Overview

Recent progress

- In a recent work [Guo & Luo '21] extend our method to particles with common noise:

$$dX_t^{i,N} = V^\varepsilon * (K * \mu_t^N)(X_t^{i,N})dt + \sqrt{2\nu}\sum_k \sigma_k^N(X_t^{i,N})dW_t^k,$$

and quantify its convergence (in a two step procedure) to

$$\partial_t u(t,x) = \nu\Delta u(t,x) - \nabla\cdot\big(u(t,x)\ K *_x u(t,x)\big)$$

for a class of kernels such as repulsive Riesz kernels for $s \in [0, d-2]$.

- Rate of convergence for the IPS without cutoff, working on the torus:

$$\limsup_{N\to+\infty} N^{\varrho-\varepsilon} \sup_{t\in[0,T]} \|u_t^N - u_t\|_{L^p(\mathbb{T}^d)} \leq X\ a.s.$$

- Extension to Burgers.

Some next steps

- Numerical applications : use our result to quantify the convergence of a scheme coming from the moderately interacting particles.

- Treat non-Markovian particle systems : e.g. the parabolic-parabolic Keller-Segel model.
- Improve the constraint on α by changing the functional space.

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