# Particle algorithm for McKean SDE: a short review on numerical analysis

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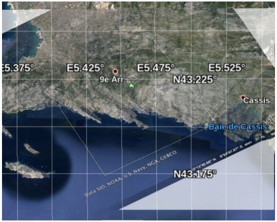
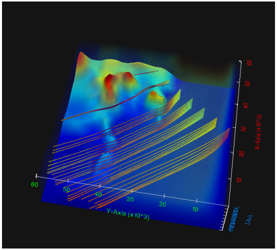
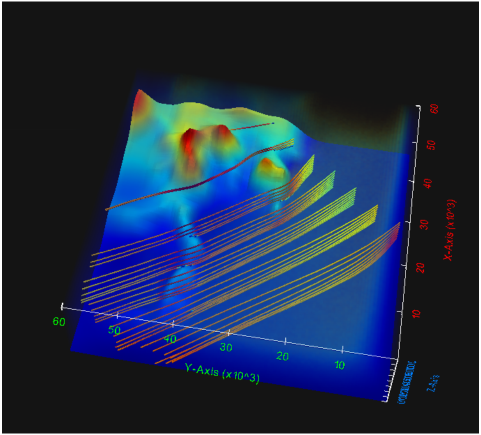
# Let's start with an example of simulation with particles






Stochastic Lagrangian model for wind simulation, forced with a WRF simulation, in the Marseille navigation basin (60 km $\times$ 60 km $\times$ 2 km. $150 \times 150 \times 200$ computation cells, with 96 particles in each cell ($432 \times 10^6$ particles). Time step is 10 seconds, with screen-out each 600 seconds.

*Simulation realized in collaboration with Yann Amice (Metigate) - 2016*

# Outline

► **Stochastic particle methods for McKean SDEs**

Method and introduction to the numerical analysis, for smooth coefficients

▷ **When the interaction kernels are non smooth functions**

Motivated by applications

Atmospheric boundary layer simulation

Wind farm simulation

▷ **Numerical analysis and numerical experiments**
for Stochastic Lagrangian models (toy version)

A PDE of conservation form

$$\begin{cases} \dfrac{\partial \rho_t}{\partial t} = \frac{1}{2}\sigma^2 \dfrac{\partial^2 \rho_t}{\partial x^2} - \dfrac{\partial}{\partial x}\left(B(t,x)\rho_t\right) \text{ in } \mathbb{R}, \\ \rho_{t=0} = \rho_0. \end{cases} \tag{1}$$

$B(t,x)$, bounded measurable

(1) is a Fokker-Planck Equation.
Set $(\mu, f) = \int_{\mathbb{R}} f(x)\mu(dx)$.

$\rho$ is a weak solution of (1), if for any test function $f \in C_b^2(\mathbb{R})$.

$$(\rho_t, f) = (\rho_0, f) + \int_0^t (\rho_s, \frac{1}{2}\sigma^2 f'' + B(s,\cdot)f')ds. \tag{2}$$

When $\rho_0$ is a probability measure, (1) (or (2)) describes the dynamics of the time-marginals of a stochastic process.

# Associated martingale problem

Let $(X_t)_{t\geq 0}$ the canonical process on $(C([0,+\infty),\mathbb{R}),\mathcal{B}(C([0,+\infty),\mathbb{R})))$.

For a probability $P$ on $(C([0,+\infty),\mathbb{R}),\mathcal{B}(C([0,+\infty),\mathbb{R})))$, we set $P_t = P \circ X_t^{-1}$.

**Definition - Martingale Problem**

$P$ on $(C([0,+\infty),\mathbb{R}),\mathcal{B}(C([0,+\infty),\mathbb{R})))$ is a solution of the martingale problem associated to $\mathcal{L} = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} + B(t,x)\frac{\partial}{\partial x}$ if

i) $P_0 = \rho_0$,

ii) $\forall f \in C_b^2(\mathbb{R})$, the process
$f(X_t) - f(X_0) - \int_0^t \left[\frac{1}{2}\sigma^2 f''(X_s) + B(s,X_s)f'(X_s)\right] ds$ is a $P$-martingale.

Existence and uniqueness for $X$ solution of

$$X_t = X_0 + \int_0^t B(s, X_s)ds + \sigma W_t.$$

For any test function $f$

$$\mathbb{E}f(X_t) = \mathbb{E}f(X_0) + \int_0^t \mathbb{E}\left[\frac{1}{2}\sigma^2 f''(X_s) + B(s, X_s)f'(X_s)\right] ds. \tag{3}$$

By setting $\rho_t = P \circ X_t^{-1}$ the $t$-time-marginal of $P$,
$\mathbb{E}f(X_t) = \int_{\mathbb{R}} f(x)\rho_t(dx) = (\rho_t, f)$ and (3) rewrites (2) :

$$(\rho_t, f) = (\rho_0, f) + \int_0^t (\rho_s, \frac{1}{2}\sigma^2 f'' + B(s, \cdot)f')ds.$$

# Numerical approximation, particle method

Main idea : approximate the measure $\rho_t$ by the empirical measure of a set of $N$ independent trials of the r.v. $X_t$.

Introducing $N$ particles of independent dynamics

$$X_t^i = X_0^i + \int_0^t B(s, X_s^i)ds + \sigma W_t^i, \quad i = 1, \ldots, N,$$

where $((X_0^i)_{i=1,\ldots,N})$ are i.i.d with law $\rho_0$, independent of the family of independent Brownian motions $((W_t^i), i = 1, \ldots, N)$.

$$\overline{U}_t^N = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_t^i}.$$

Do we have the convergence of the empirical measure $\overline{U}_t^N$ toward $\rho_t$ ?

- The parabolic problem has a smooth solution

$$\forall t > 0, \;\; \rho_t(dx) = \rho_t(x)dx.$$

Introduce a smoothing empirical measure by a *cut–off* function

$$\overline{U}_t^{N,\varepsilon}(x) = \left(\phi_\varepsilon * \overline{U}_t^N\right)(x) = \frac{1}{N}\sum_{i=1}^{N} \phi_\varepsilon(x - X_t^i)$$

where $\phi_\varepsilon(x) = \frac{1}{\varepsilon}\phi(\frac{x}{\varepsilon})$ and $\phi : \mathbb{R} \to \mathbb{R}$ smooth and such that $\int_{\mathbb{R}} \phi(x)dx = 1$.

At a given time $t$, we want the rate of convergence of the error :

$$\sup_{x\in\mathbb{R}} \mathbb{E}\left|\rho_t(x) - \overline{U}_t^{N,\varepsilon}(x)\right|.$$

Set $\rho_t^\varepsilon(x) = (\rho_t * \phi_\varepsilon)(x)$.

If $\phi$ is a $\theta$-order cut–off ( $\int_{\mathbb{R}} x^q \phi(x) dx = 0, \forall q \leq \theta - 1, \int_{\mathbb{R}} |x|^\theta |\phi(x)| dx < \infty$) and if $\rho_t$ is smooth enough

$$\|\rho_t^\varepsilon(x) - \rho_t(x)\|_{L^\infty(\mathbb{R})} \leq C\varepsilon^\theta \left\| \frac{\partial^\theta \rho_t}{\partial x^\theta} \right\|_{L^\infty(\mathbb{R})}$$

and

$$\sup_{x\in\mathbb{R}} \mathbb{E} \left| \rho(t,x) - \overline{U}_t^{N,\varepsilon}(x) \right| \leq C\varepsilon^\theta + \sup_{x\in\mathbb{R}} \mathbb{E} \left| \rho_t^\varepsilon(x) - \overline{U}_t^{N,\varepsilon}(x) \right|$$

with

$$\rho_t^\varepsilon(x) = \int_{\mathbb{R}} \phi_\varepsilon(x-y)\rho_t(y)dy = \mathbb{E}\phi_\varepsilon(x - X_t)$$

$$\overline{U}_t^{N,\varepsilon}(x) = \frac{1}{N} \sum_{i=1}^{N} \phi_\varepsilon(x - X_t^i).$$

The convergence is ensured by the strong law of large numbers.

More precisely,

$$\mathbb{E}\left|\overline{U}_t^{N,\varepsilon}(x) - \rho_t^\varepsilon(x)\right| = \mathbb{E}\left|\frac{1}{N}\sum_{i=1}^N \left[\phi_\varepsilon(x - X_t^i) - \mathbb{E}\phi_\varepsilon(x - X_t)\right]\right|$$

$$\leq \frac{1}{\sqrt{N}}\sqrt{\mathbb{E}\left(\phi_\varepsilon(x - X_t) - \mathbb{E}\phi_\varepsilon(x - X_t)\right)^2}$$

$$\leq \frac{1}{\sqrt{N}}\sqrt{\mathbb{E}\left(\phi_\varepsilon(x - X_t)\right)^2}$$

$$\leq \frac{1}{\sqrt{N}}\frac{1}{\sqrt{\varepsilon}}\|\phi\|_{L^\infty(\mathbb{R})}^{\frac{1}{2}}\sqrt{\mathbb{E}\phi_\varepsilon(x - X_t)}$$

$$= \frac{1}{\sqrt{N}}\frac{1}{\sqrt{\varepsilon}}\|\phi\|_{L^\infty(\mathbb{R})}^{\frac{1}{2}}\sqrt{\mathbb{E}\rho_t(Y^\varepsilon - x)}$$

$$\leq \frac{1}{\sqrt{\varepsilon N}}\|\phi\|_{L^\infty(\mathbb{R})}^{\frac{1}{2}}\|\rho_t\|_{L^\infty(\mathbb{R})}^{\frac{1}{2}}.$$

$$\overline{X}^i_{(k+1)\Delta t} = \overline{X}^i_{k\Delta t} + \Delta t B(k\Delta t, \overline{X}^i_{k\Delta t}) + \sigma(W^i_{(k+1)\Delta t} - W^i_{k\Delta t}).$$

$$\begin{aligned}
\mathbb{E}\left|\overline{U}^{N,\varepsilon}_{k\Delta t}(x) - \overline{U}^{N,\varepsilon,\Delta t}_{k\Delta t}(x)\right| &\leq \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left|\phi_\varepsilon(x - X^i_{k\Delta t}) - \phi_\varepsilon(x - \overline{X}^i_{k\Delta t})\right| \\
&\leq \sup_{x\in\mathbb{R}}\left|\phi'_\varepsilon(x)\right|\mathbb{E}\left|X^1_{k\Delta t} - \overline{X}^1_{t\Delta t}\right| \\
&\leq C\frac{\Delta t}{\varepsilon^2} \text{ (could by reduced to } C\frac{\Delta t}{\varepsilon}\text{).}
\end{aligned}$$

**Lemma**

$$\sup_{x\in\mathbb{R}}\mathbb{E}\left|u(t,x) - \overline{U}^{N,\varepsilon,\Delta t}_t(x)\right| + \mathbb{E}\left\|u(t,x) - \overline{U}^{N,\varepsilon,\Delta t}_t(x)\right\|_{L^1(\mathbb{R})}$$
$$\leq C_1\varepsilon^\theta + \frac{C_2}{\sqrt{\varepsilon N}} + C_3\frac{\Delta t}{\varepsilon}.$$

$$\left\{\begin{array}{l}\dfrac{\partial \rho_t}{\partial t} = \dfrac{1}{2}\displaystyle\sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j}\left(a_{ij}[x,\rho_t]\rho_t\right) - \sum_{i=1}^{d}\frac{\partial}{\partial x_i}\left(b_i[x,\rho_t]\rho_t\right)\\ \rho_0 \text{ a given probability measure on } \mathbb{R}^d.\end{array}\right. \tag{4}$$

where, for a probability measure $u$

$$b[x,u] = \int_{\mathbb{R}^d} b(x,y)u(dy); \text{ for } b(x,y)\ \mathbb{R}^d\text{-valued},$$

$$a[x,u] = \sigma[x,u]^t\sigma[x,u],$$

$$\sigma[x,u] = \int_{\mathbb{R}^d} \sigma(x,y)u(dy); \sigma(x,y)\ (d\times k) \text{ matrix-valued.}$$

Distribution equation : for any test function $f \in C_b^2(\mathbb{R}^d)$,

$$(\rho_t, f) = (\rho_0, f) + \int_0^t \left(\rho_s, \frac{1}{2}\sum_{i,j=1}^{d} a_{ij}[x,\rho_s]\frac{\partial^2 f}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i[x,\rho_s]\frac{\partial f}{\partial x_i}\right) ds \tag{5}$$

**Theorem [Méléard 95]**

for $b$ and $\sigma$ Lipschitz on $\mathbb{R}^{2d}$, for $\rho_0$ admitting a second order moment, there is existence and trajectorial uniqueness (given $X_0 \in L^2(\Omega)$ and $(W_t)$) and in law of the solution to the SDE

$$X_t = X_0 + \int_0^t \sigma[X_s, \rho_s] dW_s + \int_0^t b[X_s, \rho_s] ds,$$

where $\rho_s$ is the law of $X_s$.

(Proof from Sznitman 89, with $\sigma = 1$, and bounded $b$ ).
$\mathcal{P}_2 = \{$probability $P$ on $C([0,T], \mathbb{R}^d)$ such that $\mathbb{E}_P(\sup_{t\in[0,T]} |X_t^2|) < \infty\}$, endowed with the Wasserstein metric.

$$\Phi : \mathcal{P}_2 \ni m \mapsto \text{Law}(X_t^m, t \in [0,T]) \in \mathcal{P}_2$$
$$X_t^m = X_0 + \int_0^t \sigma[X_s^m, m_s] dW_s + \int_0^t b[X_s^m, m_s] ds.$$

admits a fix point in $\mathcal{P}_2$.

Idea : replace $\rho_t = \text{Law}(X_t)$ by the empirical measure $\mu^N = \frac{1}{N}\sum_{i=1}^{N} \delta_{X^{i,N}}$.

$$X_t^{i,N} = X_0^i + \int_0^t \sigma[X_s^{i,N}, \mu_s^N] dW_s^i + \int_0^t b[X_s^{i,N}, \mu_s^N] ds, \; i = 1, \ldots, N. \tag{6}$$

where $((X_0^i)_{i=1,\ldots,N})$ are i.i.d with law $\rho_0$, independent of the family of independent Brownian motions $((W_t^i), i = 1, \ldots, N)$.

(6) is well-posed when $b(x,y)$ $\sigma(x,y)$ are Lipschitz.

What convergence of $\mu_t^N$ toward $\rho_t$ ?

Let $E$ be a separable metric space and $\nu$ a probability measure on $E$. A sequence of symmetric probabilities $\nu^N$ on $E^N$ is $\nu$-chaotic if for any $\phi_1, \ldots, \phi_k \in C_b(E; \mathbb{R})$, $k \geq 1$,

$$\lim_{N \to \infty} \left\langle \nu^N, \phi_1 \otimes \ldots \otimes \phi_k \otimes 1 \ldots \otimes 1 \right\rangle = \prod_{l=1}^{k} \langle \nu, \phi_l \rangle.$$

Application : Let $(X^{1,N}, \ldots, X^{N,N})$, the set of $N$ particles satisfying (6), valued in $(C([0,T]; \mathbb{R}^d))^N$, with law $P^N$.

**Theorem (Méléard 95)**

If the initial of $(X_0^{1,N}, \ldots, X_0^{N,N})$ is $\rho_0$-chaotic, the chaos propagates and $P^N$ is $P$-chaotic where $P$ is the unique law of the McKean SDE.

The tow following assertions are equivalent : (Tanaka 82)

- $P^N$ is $P$-chaotic
- $\mu^N$ converges weakly toward the (deterministic) measure $P$

**Theorem (Méléard 95)**

$$\sup_N \mathbb{E}\left(\sup_{0\le t\le T} |X_t^{i,N}|^2\right) + \sup_N \mathbb{E}\left(\sup_{0\le t\le T} |X_t^{i}|^2\right) < \infty$$

$$\sup_N N\mathbb{E}\left(\sup_{0\le t\le T} |X_t^{i,N} - X_t^{i}|^2\right) < \infty,$$

where

$$X_t^i = X_0^i + \int_0^t \sigma[X_s^i, \rho_s] dW_s^i + \int_0^t b[X_s^i, \rho_s] ds$$

with $\rho_t = P \circ X_t^{-1}$.

## Numerical approximation

$$X_t = X_0 + \int_0^t \sigma[X_s, \rho_s]dW_s + \int_0^t b[X_s, \rho_s]ds, \text{ with } \rho_s = \text{Law}(X_s).$$

Spatial discretisation :

$$X_t^{i,N} \quad = \quad X_0^i + \int_0^t \sigma[X_s^{i,N}, \mu_s^N]dW_s^i + \int_)^t b[X_s^{i,N}, \mu_s^N]ds, i \leq N.$$

Time-Discretisation : $\Delta t > 0$, such that $T = K\Delta t$ for $K \in \mathbb{N}$,

$$\begin{cases} \bar{X}_{(k+1)\Delta t}^{i,N} = \bar{X}_{k\Delta t}^{i,N} + (\frac{1}{N}\sum_{j=1}^{N}\sigma(\overline{X}_{k\Delta t}^{i,N}, \overline{X}_{k\Delta t}^{j,N}))(W_{(k+1)\Delta t}^i - W_{k\Delta t}^i) \\ \qquad\qquad + \Delta t(\frac{1}{N}\sum_{j=1}^{N} b(\bar{X}_{k\Delta t}^{i,N}, \bar{X}_{k\Delta t}^{j,N})), \\ \bar{X}_{t=0}^{i,N} = X_0^i. \end{cases}$$

$$\overline{U}_{k\Delta t}^{N,\varepsilon,\Delta t}(x) = \frac{1}{N}\sum_{i=1}^{N}\phi_\varepsilon(x - \bar{X}_{k\Delta t}^{i,N}), \text{ pour un cut-off donné } \phi.$$

**Theorem (Bossy & Talay 97)**

Dimension $d = 1$.
Assume that $\rho_0(\cdot) \in C_K^2(\mathbb{R})$, $b(\cdot,\cdot) \in C_b^{2,2}(\mathbb{R}^2)$ and $s(\cdot,\cdot) \in C_b^3(\mathbb{R}^2)$.
Assume the strong ellipticity of the differential operator $\mathcal{L}$.
Then $\rho_t(\cdot) \in W^{2,1}(\mathbb{R})$ for all $t \in [0,T]$.
For a 2-order cut-off $\phi(x)$, $\forall\, k \leq K$,

$$\mathbb{E}\|\overline{U}_{k\Delta t}^{N,\varepsilon,\Delta t} - \rho_{k\Delta t}\|_{L^1(\mathbb{R})} \leq C_{b,\sigma,T,\rho_0}\left(\frac{1}{\varepsilon\sqrt{N}} + \varepsilon^2 + \frac{\sqrt{\Delta t}}{\varepsilon}\right).$$

$H(x) := \mathbb{1}_{\{x\geq 0\}}$, Heaviside function

$$\mathbb{E}\|(H * \rho_{k\Delta t})(x) - \frac{1}{N}\sum_{i=1}^{N} H(x - \overline{X}_{k\Delta t}^{i,N})\|_{L^1(\mathbb{R})} \leq C_{b,\sigma,T,\rho_0}\left(\frac{1}{\sqrt{N}} + \sqrt{\Delta t}\right).$$

**Theorem (Antonelli & Kohatsu-Higa 02)**

$d = 1$.
$b(\cdot,\cdot)$ and $s(\cdot,\cdot)$ $C^\infty(\mathbb{R}^2)$, with bounded derivatives.
A non degenerescency condition for $\mathcal{L}$ (needed by the use of Malliavin calculus framework).
$\phi(x)$ is the Gaussian density on $\mathbb{R}$.
$\varepsilon^2 = \Delta t$.

$$\mathbb{E}\|\overline{U}_{k\Delta t}^{N,\varepsilon,\Delta t} - \rho_{k\Delta t}\|_{L^1(\mathbb{R})} \leq C_{b,\sigma,T,\rho_0}\left(\frac{1}{\sqrt{\Delta t N}} + \Delta t + \frac{1}{\sqrt{N}}\right).$$

$H(x) := \mathbb{1}_{x\geq 0}$, Heaviside function,

$$\mathbb{E}\|(H * \rho_{k\Delta t})(x) - \frac{1}{N}\sum_{i=1}^{N} H(x - \overline{X}_{k\Delta t}^{i,N})\|_{L^1(\mathbb{R})} \leq C_{b,\sigma,T,\rho_0}\left(\frac{1}{\sqrt{N}} + \Delta t\right).$$

# Outline

- ▷ **Stochastic particle methods for McKean SDEs**

  Method and introduction to the numerical analysis, for smooth coefficients

- ► **and when the interaction kernels are non smooth functions**

  Motivated by applications
  - Atmospheric boundary layer simulation
  - Wind farm simulation

- ▷ **Numerical analysis and numerical experiments**
  for Stochastic Lagrangian models (toy version)

# Fluid particle model for turbulent flow : Convergence analysis ?

► Lagrangian McKean SDEs for fluid turbulent subscale models [Pope 95, 03; Durbin Speziale 94, Dreeben Pope 98, Waclawczyk Pozorski Minier 04, Bossy et al. 16]

$$\begin{cases} X_t = X_0 + \int_0^t U_s ds \\ (U_t, \Theta_t) = (U_0, \Theta_0) + \int_0^t \mathbb{E}_{\mathbb{P}} \left[ \ell(U_s, \Theta_s) \,|\, X_s \right] ds + \int_0^t \mathbb{E}_{\mathbb{P}} \left[ \gamma(U_s, \Theta_s) \,|\, X_s \right] dW_s, \end{cases}$$

Ingredient of the problem :

- Singular interaction (mean field) kernel in the diffusion term.
- degenerate diffusion coefficient

## Simplified the fluid particle model
## Goal : analyze the rate of convergence

$$\begin{cases} X_t = \Big[X_0 + \int_0^t U_s\,ds\Big] \mod \mathbf{1} \\ U_t = U_0 + \int_0^t B[X_s;\rho_s]\,ds + W_t, \quad \rho_t = \mathcal{L}(X_t,U_t), \quad \text{for all } t \le T \end{cases}$$

$$\mathbb{T} \times L^1(\mathbb{T}\times\mathbb{R}^d) \ni (x,\gamma) \mapsto B[x;\gamma] = \frac{\int_{\mathbb{R}^d} b(v)\gamma(x,v)\,dv}{\int_{\mathbb{R}^d}\gamma(x,v)dv} \mathbb{1}_{\{\int_{\mathbb{R}^d}\gamma(x,v)dv>0\}}$$

$$(t,x) \mapsto B[x;\rho(t)] = \mathbb{E}[b(U_t)\big|X_t = x]$$

The smoothed process $(X^\epsilon, U^\epsilon, \epsilon > 0)$ converges in law to $(X,U)$, by substituting the conditional expectation $B[x;\rho_t]$ with the kernel regression estimate

$$B_\epsilon[x;\rho] := \frac{\int_{\mathbb{T}\times\mathbb{R}^d} b(v)K_\epsilon(x-y)\,\rho(dy,dv)}{\int_{\mathbb{T}\times\mathbb{R}^d} K_\epsilon(x-y)\,\rho(dy,dv)},$$

where $K_\epsilon(x) := \frac{1}{\epsilon^d}K(\frac{x}{\epsilon})$ and $K$ is a kernel function.

$$\begin{cases} X_t^\epsilon = \Big[X_0 + \int_0^t U_s^\epsilon\,ds\Big] \mod \mathbf{1} \\ U_t^\epsilon = U_0 + \int_0^t B_\epsilon[X_s^\epsilon,\rho_s^\epsilon]\,ds + W_t, \quad \rho_t^\epsilon = \mathcal{L}(X_t^\epsilon,U_t^\epsilon), \quad \text{for all } t \le T. \end{cases}$$

# Numerical analysis of a non degenerate toy model (d=1)

$$Y_t = Y_0 + \int_0^t b[Y_s;\rho_s]ds + \sigma w_t, \quad \rho_t = \mathcal{L}(Y_t).$$

Assume $b$ symmetric $b(x,y) = b(x-y)$. $b[x,\rho_t] = \mathbb{E}b(x - Y_t)$.

Introduce $N$ particles:

Let $(w^i, i = 1,\dots,N)$ $N$-Brownian motion, independent of the i.i.d. $(Y_0^i, i = 1,\dots,N)$ with law $\rho_0$. We consider

$$Y_t^{i,N} = Y_0^i + \int_0^t \frac{1}{N}\sum_{j=1}^N b(Y_s^{i,N} - Y_s^{j,N})ds + \sigma w_t^i, \qquad \mu_t^N = \frac{1}{N}\sum_{i=1}^N \delta_{Y_t^{i,N}}.$$

## Lemma

Assume that there exists $r \geq 2$ such that $b(\cdot)$ is in $C_b^{r+1}(\mathbb{R})$, and $\rho_0 \in W^{r,\infty}(\mathbb{R}) \cap W^{r,1}(\mathbb{R})$.

Then $\rho_t \in W^{r,\infty}$, and for all test function $\phi \in C_c^3(\mathbb{R})$, there exists a positive constant $C$ such that

$$\sup_{t\in[0,T]} \mathbb{E}\left|\langle \phi, \mu_t^N - \rho_t\rangle\right| \leq \frac{C}{\sqrt{N}}.$$

where the constant $C$ is of the form $\beta\exp(\alpha\|b'\|_\infty t)$.

# Control of the drift error term

$$\forall t \in [0,T], \quad \mathcal{E}_{\text{drift}}(t) := \mathbb{E}\Big| b[Y_t^{1,N}, \rho_t] - \frac{1}{N}\sum_{j=1}^{N} b(Y_t^{1,N} - Y_t^{j,N})\Big|.$$

Notice that, with $Y_t^i = Y_0^i + \int_0^t b[Y_s^i; \rho_s]ds + \sigma w_t^i$,

$$\mathbb{E}|Y_t^1 - Y_t^{1,N}| = \mathbb{E}\Big| \int_0^t \left( b[Y_s^1, \rho_s] - \frac{1}{N}\sum_{j=1}^{N} b(Y_s^{1,N} - Y_s^{j,N}) \right) ds \Big|$$

Since $b$ is Lipschitz with constant $L = \|b'\|_\infty$, $x \mapsto b[x, \rho_t]$ is Lipschitz, and applying Gronwall Lemma

$$\mathbb{E}|Y_t^1 - Y_t^{1,N}| \le \int_0^t L\mathbb{E}|Y_s^1 - Y_s^{1,N}|ds + \int_0^t \mathcal{E}_{\text{drift}}(s)ds \le \int_0^t \exp(L(t-s))\mathcal{E}_{\text{drift}}(s)ds.$$

$$\mathcal{E}_{\text{drift}}(t) \le 3L\mathbb{E}|Y_t^{1,N} - Y_t^1| + \mathbb{E}\Big| b[Y_t^1, \rho_t] - \frac{1}{N}\sum_{j=1}^{N} b(Y_t^1 - Y_t^j)\Big|$$

$$\le \int_0^t 3L\exp(L(t-s))\mathcal{E}_{\text{drift}}(s)ds + \mathbb{E}\Big[\Big|\mathbb{E}b(x - Y_t) - \frac{1}{N}\sum_{j=1}^{N} b(x - Y_t^j)\Big|_{x=Y_t^1}\Big].$$

The $(Y^j, j \neq 1)$ being i.i.d. $\mathbb{E}\left[\Big|\mathbb{E}b(x - Y_t) - \frac{1}{N}\sum_{j=1}^{N} b(x - Y_t^j)\Big|^2_{x=Y_t^1}\right] \le \frac{C}{N}$.

Thus

$$\mathcal{E}_{\text{drift}}(t) \le \int_0^t 3L\exp(L(t-s))\mathcal{E}_{\text{drift}}(s)ds + \frac{C}{\sqrt{N}} \le \exp(4Lt)\frac{C\exp(-Lt)}{\sqrt{N}} \le \exp(3Lt)\frac{C}{\sqrt{N}}.$$

$$Y_t = Y_0 + \int_0^t \frac{1}{2}\rho_s(Y_s)ds + w_t, \quad \rho_t = \mathcal{L}(Y_t).$$

McKean 1967, Calderoni &Pulvirenti 1983, Sznitman & Varadhan 1986, Sznitman 1986.

$$Y_t^{i,N} = Y_0^i + \int_0^t K_\epsilon[Y_s^{i,N}; \mu_s^N]ds + \sigma w_t^i, \quad \mu_t^N = \sum_{i=1}^N \delta_{Y_t^{i,N}}$$

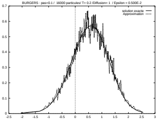
with $K_\epsilon[x;\gamma] := \int_{\mathbb{R}} K_\epsilon(x-y)\gamma(dy)$ with $K_\epsilon(z) = \frac{1}{\epsilon}K(\frac{z}{\epsilon})$ and $K$ positive function of mass equal to 1.

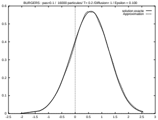
When $\rho_0 \in W^{2,1}(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$ then $\rho_t \in W^{2,1}(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$ for all finite $t > 0$ and

$$\|\rho_t - \rho_t^\epsilon\|_{L^1(\mathbb{R})} \leq C\epsilon^2,$$

where $Y_t^\epsilon = Y_0 + \int_0^t \frac{1}{2}K_\epsilon[Y_s^\epsilon; \rho_s^\epsilon]ds + w_t, \quad \rho_t^\epsilon = \mathcal{L}(Y_t^\epsilon)$.

From the previous lemma: $\sup_{t\in[0,T]} \mathbb{E}\left|\langle \phi, \mu^{N,\epsilon} - \rho_t\rangle\right| \leq C\left(\epsilon^2 + \frac{\exp(C/\epsilon)}{\sqrt{N}}\right).$




Numerical experiments are more optimistic :
($\rho_0(dx) = \mathbb{1}_{[0,1]}$ with $N = 16000$, $T = 0.2$, $\sigma = 1$, $\epsilon = 0.5 10^{-2}$ left, $\epsilon = 0.1$ right)

# A symptomatic case

$$Y_t = Y_0 + \int_0^t \frac{1}{2}\rho_s(Y_s)ds + w_t, \quad \rho_t = \mathcal{L}(Y_t).$$

McKean 1967, Calderoni &Pulvirenti 1983, Sznitman & Varadhan 1986, Sznitman 1986. When

$\rho_0 \in W^{2,1}(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$ then $\rho_t \in W^{2,1}(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$ for all finite $t > 0$ and

$$\|\rho_t - \rho_t^\epsilon\|_{L^1(\mathbb{R})} \leq C\epsilon^2,$$

Define

$$Y_t^{i,N} = Y_0^i + \int_0^t \hat{K}_\epsilon[Y_s^{i,N}; \mu_s^N]ds + \sigma w_t^i, \quad \mu_t^N = \sum_{i=1}^N \delta_{Y_t^{i,N}}$$

with $\hat{K}_\epsilon[x;\gamma] := \|\rho_t\| \wedge K_\epsilon[x;\gamma] \vee -\|\rho_t\|$

**Lemma**

Assume that $\rho_0(\cdot) \in C_K^2(\mathbb{R})$, for a 2-order cut-off $\phi(x)$, $\forall\, k \leq K$,

$$\mathbb{E}\|\phi_\varepsilon * \mu_t^N - \rho_t\|_{L^1(\mathbb{R}) \text{ or } L^\infty(\mathbb{R})} \leq C_{b,\sigma,T,\rho_0}\left(\frac{1}{\varepsilon\sqrt{N}} + \varepsilon^2\right).$$

# Go back to McKean kinetic particle system

$(X_t^i, U_t^i, t \leq T, i = 1, \ldots, N)$ are the strong solution of

$$\begin{cases} X_t^i = \left[X_0^i + \int_0^t U_s^i \, ds\right] \mod 1 \\ U_t^i = U_0^i + \int_0^t B[X_s^i, \rho_s] \, ds + W_t^i, \quad \rho_t = \mathcal{L}(X_t^i, U_t^i), \quad \text{for all } t \leq T, \end{cases}$$

where we recall that $(X_0^i, U_0^i, i = 1, \ldots, N)$ are i.i.d. with density $\rho_0$.
$(X_t^{i,\epsilon}, U_t^{i,\epsilon}, t \leq T, i = 1, \ldots, N)$ are the strong solution of

$$\begin{cases} X_t^{i,\epsilon} = \left[X_0^i + \int_0^t U_s^{i,\epsilon} \, ds\right] \mod 1 \\ U_t^{i,\epsilon} = U_0^i + \int_0^t B_\epsilon[X_s^{i,\epsilon}, \rho_s^\epsilon] \, ds + W_t^i, \quad \rho_t^\epsilon = \mathcal{L}(X_t^{i,\epsilon}, U_t^{i,\epsilon}), \quad \text{for all } t \leq T, \end{cases}$$

$$\begin{cases} X_t^{i,N} = X_0^i + \int_0^t U_s^{i,N} ds, \\ U_t^{i,N} = U_0^i + \int_0^t \underbrace{\frac{\frac{1}{N}\sum_{j=1}^N b(U_s^{j,N}) K_\epsilon(X_s^{i,N} - X_s^{j,N})}{\frac{1}{N}\sum_{j=1}^N K_\epsilon(X^{i,N} - X_s^{j,N})}}_{\text{Nadaraya-Watson estimator at } X_s^{i,N}} ds + W_t^i, \quad \text{for all } t \leq T. \end{cases}$$

- **Control the error seen by the particles :** $\mathbb{E}\left|F[X_t^1; \rho_t] - F_\epsilon[X_t^{1,N}; \mu_t^N]\right|$.

# Rate of convergence

For any $f$ measurable bounded on $\mathbb{R}^d$, we set the kernel regression version of the conditional expectation :

$$(x,t) \mapsto F[x;\rho_t] = \mathbb{E}[f(U_t)|X_t = x],$$

$$(x,t) \mapsto F_\epsilon[x;\rho_t] = \frac{\int_{\mathbb{R}^d\times\mathbb{R}^d} f(v) K_\epsilon(x-y)\,\rho_t(dy,dv)}{\int_{\mathbb{R}^d\times\mathbb{R}^d} K_\epsilon(x-y)\,\rho_t(dy,dv)} = \frac{\mathbb{E}[f(U_t)K_\epsilon(x-X_t)]}{\mathbb{E}[K_\epsilon(x-X_t)]}$$

Assume that $f$ and $b$ smooth and bounded function with bounded derivatives; $K > 0$ Lipschitz bounded, with compact support.

**Theorem** (Bossy and Violeau, preprint)

[Measure discretization error] For any $1 < p < 1 + \dfrac{1}{1+3d}$ and $c > 0$, there exists a constant $C$ such that for all $\alpha > 0$, $\epsilon > 0$ and $N > 1$ satisfying $\dfrac{1}{\alpha^2 \epsilon^d N^{\frac{1}{p}}} \leq c$, we bound the error seen by the particles by

$$\mathbb{E}\left|F[X_t^1;\rho_t] - F_\epsilon[X_t^{1,N};\mu_t^N]\right| \leq C\left(\epsilon + \frac{1}{\alpha\epsilon^d N} + \frac{1}{\epsilon^{(d+1)p}N} + \frac{1}{(\epsilon^d N)^{\frac{1}{p}}} + \frac{1}{\epsilon^{\frac{dp}{2}}\sqrt{N}}\right).$$

If we choose $\alpha = \epsilon$, the optimal rate of convergence is achieved for $N = \epsilon^{-(d+2)p}$ and

$$\mathbb{E}\left[\left|F[X_t^1;\rho_t] - F_\epsilon[X_t^{1,N};\mu_t^N]\right|\right] \leq N^{-\frac{1}{(d+2)p}}.$$

# Nonparametric regression estimate

Let $(X_i, U_i)$ be an **i.i.d** sequence of $n$ random variables.

## Local averaging estimate :

approximate $F(x) = \mathbb{E}[f(U)|X = x]$ with:

$$F_n(x) = \sum_{i=1}^{n} W_{n,i}(x) \cdot f(U_i),$$

where the weight $W_{n,i}$ depends only on $x$ and $(X_j, f(U_j))$, $j \leq n$.

## Kernel estimate :

$$W_{n,i}(x) = \frac{K_\epsilon(x - X_i)}{\sum_{j=1}^{n} K_\epsilon(x - X_j)},$$

where $K_\epsilon(x) = K(\frac{x}{\epsilon})$. Related to the minimization:

$$F_n(x) = \arg\min_c \left\{ \frac{1}{n} \sum_{i=1}^{n} K_\epsilon(x - X_i)(f(U_i) - c)^2 \right\}.$$

# Nonparametric regression estimate

## Partitioning estimate :

Let $\mathcal{P}_n = \{A_{n,1}, A_{n,2}, \dots\}$ be a partition of the domain. Set

$$W_{n,i}(x) = \frac{\mathbb{1}_{\{X_i \in A_{n,j}\}}}{\sum_{i=1}^n \mathbb{1}_{\{X_i \in A_{n,j}\}}}, \quad \text{for } x \in A_{n,j}.$$

Related to the least squares estimate:

$$F_n = \arg\min_{f_n} \left\{ \frac{1}{n} \sum_{i=1}^n (f(U_i) - f_n(X_i))^2 \right\},$$

where the $\arg\min$ is taken on the set of piecewise constant functions adapted to $\mathcal{P}_n$.

Also: local modeling estimates (e.g. local polynomial estimates), global modeling/least squares estimates, penalized modeling...

# Convergence rate of the nonparametric estimates

- Consider the mean $L^2$ error:

$$\mathbb{E}\Big[\int_{\mathcal{D}} \big|F(x) - F_n(x)\big|^2 \rho(x)\, dx\Big].$$

- Variance-Bias decomposition:

$$\mathbb{E}\Big[\int_{\mathcal{D}} \big|F(x) - F_n(x)\big|^2 \rho(x)\, dx\Big] = \int \mathrm{Var}\, F_n(x)\rho(x)\, dx + \int |\text{bias}(x)|^2 \rho(x)\, dx.$$

- The previous estimators are weakly universally consistent (Stone's theorem).
- For $(p, C)$ smooth conditional expectations, the lower optimal convergence rate is of order $n^{-\frac{2p}{2p+d}}$.

**Theorem** (Bossy and Violeau, preprint)

For Lipschitz continuous regression functions, we have

$$E\|F_n - F\|^2 \leq C\frac{1}{n\epsilon^d} + dC\epsilon^2,$$

for both partitioning estimate and kernel estimate (with naive kernel).
This gives an optimal rate of $n^{-\frac{2}{d+2}}$.

# Local averaging based particle algorithm

## Particle algorithm :

1. **Initialization** of $(X_0^i, U_0^i)$ for $1 \leq i \leq n$
2. **Time loop** : for $t_k = k\Delta_t$ up to $T$ :
   - for each particle $1 \leq i \leq n$ :
     - 2.1 update the position : $X_k^{i,n} = X_{k-1}^{i,n} + U_{k-1}^{i,n}$
     - 2.2 add gaussian noise: $U_k^{i,n} = U_{k-1}^{i,n} + (W_k^i - W_{k-1}^i)$
     - 2.3 drift computation : loop over each particle to calculate the $W_{n,j}(X_{k-1}^{i,n})$:

$$U_k^{i,n} += \frac{\sum_{j=1}^{N} b(U_{k-1}^{j,n}) K_n(X_{k-1}^{i,n} - X_{k-1}^{j,n})}{\sum_{j=1}^{N} K_n(X_{k-1}^{i,n} - X_{k-1}^{j,n})} \Delta_t$$

   - End loop particles
3. **Final mean field evaluation at** $x$: Loop on all particles

$$\frac{\sum_{j=1}^{n} f(U_T^{j,n}) K_n(x - X_T^{j,n})}{\sum_{j=1}^{n} K_n(x - X_T^{j,n})}$$

Complexity up to $\mathcal{O}(n^2)$ for kernel estimates,
and only $\mathcal{O}(n)$ for partitioning estimates.

# Numerical simulation

For $d = 2$

## Test case

$$dU_t = C dt - \underbrace{\nabla V(X_t) dt}_{\text{“pressure”}} + \underbrace{(\langle U_t \rangle - 2U_t) dt}_{\text{conditional drift}} + dW_t,$$

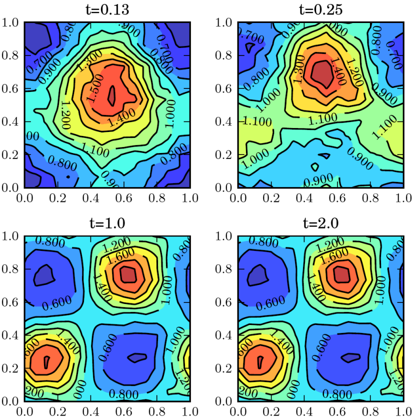
with

$$V(x, y) = \frac{1}{2\pi} \cos(2\pi\, x) \sin(2\pi\, y) - \frac{1}{2} x,$$

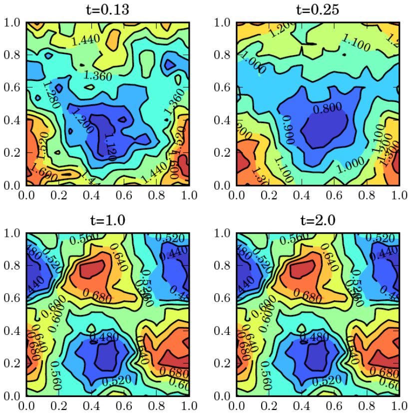
$$X_0 = \sigma Z \text{ with } \mathcal{L}(Z) = \mathcal{N}(0, 1), \quad \mathcal{L}(U_0) = \mathcal{N}(0, 1), \quad \sigma = 0.3.$$

## Reference simulation

Regression estimate implemented with Epanechnikov kernel
$T = 2$, 128 times step,
$\bar{N} = 10^5$ particles, $\underline{\epsilon} = \frac{1}{16}$.




(a) Density




(b) Turbulent kinetic energy

We want to observe the error of the scheme as

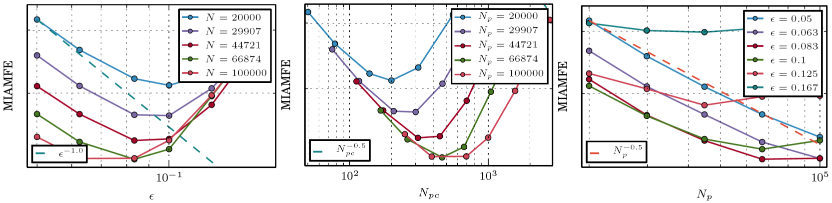
$$\int_{\mathcal{D}} |F[x;\rho_T] - F_\epsilon[x;\mu_T^{\epsilon,N}]|\rho_T(x)\,dx,$$

First we approximate the mean field $F[x;\rho_T]$ by

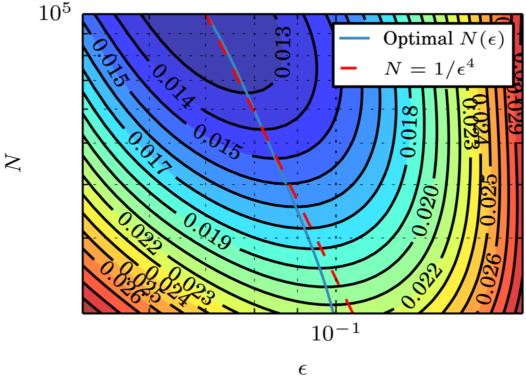
$$\overline{F_{\underline{\epsilon}}[x;\mu^{\underline{\epsilon},\bar{N}}]} := \frac{1}{N_{mc}}\sum_{k=1}^{N_{mc}} F_{\underline{\epsilon}}[x;\mu^{\underline{\epsilon},\bar{N}}(\omega_k)],$$

Using spline interpolation on a mesh of size $\Delta x$, we observe the approximate $L^1$error

$$\frac{1}{N_{mc}}\sum_{k=1}^{N_{mc}}\int_{\mathcal{D}} \left|\overline{F_{\underline{\epsilon}}[x;\mu^{\underline{\epsilon},\bar{N}}]}^{\Delta x} - F_\epsilon^{\Delta x}[x;\mu^{\epsilon,N}(\omega_k)]\right|\bar{\rho}^{\Delta x}(x)\,dx.$$



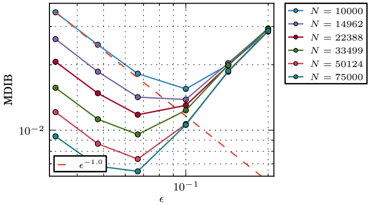
Observe the approximate $L^1$ error:



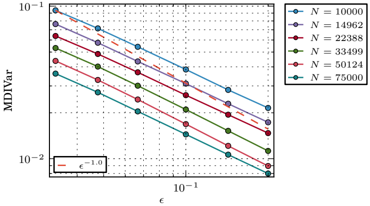

in-line with what we expected from the theoretical rate where the optimal value of window size is given by $\frac{1}{N^{\frac{1}{d+2}}}$.

# Observe the kernel regression estimation error

$$\text{bias}: \quad \int_{\mathcal{D}} \left| \overline{F_\epsilon\left[x;\mu^{\epsilon,N}\right]}^{\Delta x} - \overline{F_\epsilon\left[x;\mu^{\epsilon,\bar{N}}\right]}^{\Delta x} \right|^2 \bar{\rho}_\epsilon^{\Delta x}(x)\,dx,$$

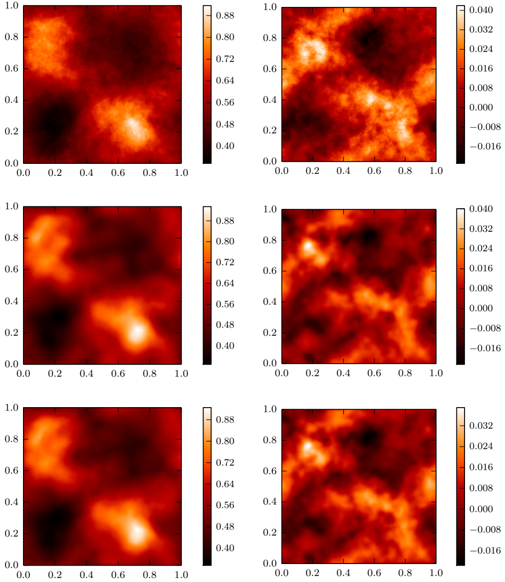



$$\text{variance}: \quad \frac{1}{N_{mc}} \sum_{j=1}^{N_{mc}} \int_{\mathcal{D}} \left| \overline{F_\epsilon\left[x;\mu^{\epsilon,N}\right]}^{\Delta x} - F_\epsilon^{\Delta x}\left[x;\mu^{\epsilon,N}(\omega_j)\right] \right|^2 \bar{\rho}_\epsilon^{\Delta x}(x)\,dx.$$



# Impact of the choice of the kernel

Velocity field and its error

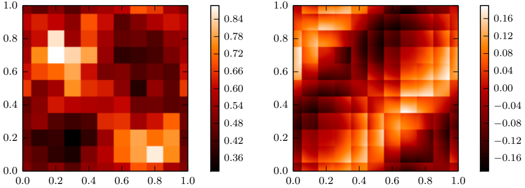



Regression kernels :

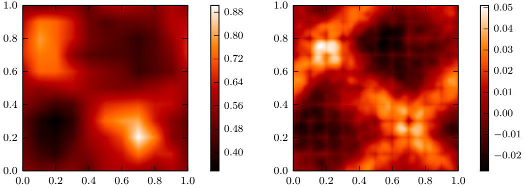
hat kernel

triangle kernel

epanechnikov kernel




Indicator function (NGP)




Hat function (CIC)

# Thank you for your attention

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