Discretization of Stochastic Differential Systems With Singular Coefficients Part I

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Outline

Introduction

Monte Carlo Methods For Linear PDEs

Discretization of Stochastic Hamiltonian Dissipative Systems

Stochastic Lagrangian Models for Turbulent Flows

Conclusion
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Monte Carlo Methods For Linear PDEs

Discretization of Stochastic Hamiltonian Dissipative Systems

Stochastic Lagrangian Models for Turbulent Flows

Conclusion
Why is Probability useful?

THE WORLD IS COMPLEX

- The physical model is badly calibrated (e.g., MEG or electrical neuronal activity: few sensors),
- The physical law is not completely known (e.g., turbulence, meteorology, . . . ),
- There is no physical law (e.g., finance).

THE PARTIAL DIFFERENTIAL EQUATIONS ARE COMPLEX

- Mathematical analysis (existence, uniqueness, smoothness),
- Probabilistic analysis of deterministic numerical methods (cf. Kushner, or domain decompositions, or artificial boundary conditions),
- Probabilistic numerical methods for high dimensional problems and/or equations in domains with possibly complex geometries and/or small viscosities (high Reynolds numbers), . . . ).
SUMMARY:

- Probability theory (in particular, stochastic integration theory) is used to solve problems which, by nature, are deterministic or ‘stochastic’,
- Probabilistic models and numerical methods are used when deterministic ones are unefficient.
- In all cases, one seeks a statistical information on the model: classical numerical analysis needs to be deeply adapted.

Remarks:

- For physicists, Stochastic PDEs often are PDEs with random coefficients,
- Stochastic collocation methods are not stochastic.
General parabolic PDEs

Let $b : \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma_j : \mathbb{R}^d \to \mathbb{R}^d$, $(1 \leq j \leq r)$. Consider the elliptic operator

$$L\psi(x) := \sum_{i=1}^{d} b^i(x) \partial_i \psi(x) + \frac{1}{2} \sum_{i,j=1}^{d} a_{ij}^t(x) \partial_{ij} \psi(x),$$

where

$$a(x) := \sigma(x) \sigma(x)^t,$$

and the evolution problem

$$\begin{cases} 
\frac{\partial u}{\partial t}(t, x) = Lu(t, x), & t > 0, \ x \in \mathbb{R}^d, \\
\quad u(0, x) = f(x), & x \in \mathbb{R}^d.
\end{cases}$$
The Euler scheme for SDEs

Let \((G^j_p)\) be i.i.d. \(\mathcal{N}(0, 1)\) and \(h > 0\) be the discretization step.

\[
\begin{align*}
\bar{X}^h_0(x) &= x, \\
\bar{X}^h_{(p+1)h}(x) &= \bar{X}^h_{ph}(x) + b(\bar{X}^h_{ph}(x)) \cdot h \\
&\quad + \sum_{j=1}^{r} \sigma_j(\bar{X}^h_{ph}(x)) \cdot \sqrt{h} \cdot G^j_{p+1}.
\end{align*}
\]

- Easy to simulate (even for Lévy driven SDEs).
- Discretizes the stochastic differential equation

\[
X_t(x) = x + \int_0^t b(X_s(x)) \, ds + \int_0^t \sigma(X_s(x)) \, dW_s.
\]
Moments of the Euler scheme

$$
\mathbb{E} \left\{ \bar{X}^h_{(p+1)h}(x) - \bar{X}^h_{ph} \right\} = \mathbb{E} b(\bar{X}^h_{ph}(x)) \ h,
$$

$$
\mathbb{E} \left\{ (\bar{X}^h_{(p+1)h}(x) - \bar{X}^h_{ph}) \cdot (\bar{X}^h_{(p+1)h}(x) - \bar{X}^h_{ph})^t \right\} = \mathbb{E} a(\bar{X}^h_{ph}) \ h + \mathcal{O}(h^2). 
$$
Moments of the Euler scheme

\[ \mathbb{E} \{ \bar{X}_{(p+1)h}^h(x) - \bar{X}_{ph}^h \} = \mathbb{E} b(\bar{X}_{ph}^h(x)) \cdot h, \]
\[ \mathbb{E} \{ (\bar{X}_{(p+1)h}^h(x) - \bar{X}_{ph}^h) \cdot (\bar{X}_{(p+1)h}^h(x) - \bar{X}_{ph}^h)^t \} = \mathbb{E} a(\bar{X}_{ph}^h) \cdot h + \mathcal{O}(h^2). \]
Probabilistic interpretation of parabolic PDEs

\[ \mathbb{E} f(\tilde{X}_T^h(x)) - u(T, x) \]
\[ = \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p+1)h, \tilde{X}_{(p+1)h}^h(x) \right) - u \left( T - ph, \tilde{X}_{ph}^h(x) \right) \right] \]
\[ = \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p+1)h, \tilde{X}_{ph}^h(x) \right) - u \left( T - ph, \tilde{X}_{ph}^h(x) \right) \right] \]
\[ + h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - (p+1)h, \tilde{X}_{ph}^h(x) \right) \right] + \sum_{p=0}^{T/h-1} \mathcal{O} (h^2) \]
\[ = h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - ph, \tilde{X}_{ph}^h(x) \right) - \frac{\partial u}{\partial t} \left( T - ph, \tilde{X}_{ph}^h(x) \right) \right] + \mathcal{O} (h) \]
\[ = \mathcal{O} (h), \]

since \( \frac{\partial u}{\partial t} (t, x) = Lu(t, x) \).
Probabilistic interpretation of parabolic PDEs

\[ \mathbb{E} f(\bar{X}_T^h(x)) - u(T, x) \]

\[ = \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p + 1)h, \bar{X}_{(p+1)h}(x) \right) - u \left( T - ph, \bar{X}_{ph}(x) \right) \right] \]

\[ + h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - (p + 1)h, \bar{X}_{ph}(x) \right) \right] + \sum_{p=0}^{T/h-1} O(h^2) \]

\[ = h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - ph, \bar{X}_{ph}(x) \right) - \frac{\partial u}{\partial t} \left( T - ph, \bar{X}_{ph}(x) \right) \right] + O(h) \]

\[ = O(h) , \]

since \( \frac{\partial u}{\partial t}(t, x) = Lu(t, x) \).
Probabilistic interpretation of parabolic PDEs

\[ E f(\tilde{X}_T^h(x)) - u(T, x) \]

\[ = \sum_{p=0}^{T/h-1} E \left[ u \left( T - (p + 1)h, \tilde{X}_{(p+1)h}(x) \right) - u \left( T - ph, \tilde{X}_{ph}(x) \right) \right] \]

\[ = \sum_{p=0}^{T/h-1} E \left[ u \left( T - (p + 1)h, \tilde{X}_{ph}(x) \right) - u \left( T - ph, \tilde{X}_{ph}(x) \right) \right] \]

\[ + h \sum_{p=0}^{T/h-1} E \left[ Lu \left( T - (p + 1)h, \tilde{X}_{ph}(x) \right) \right] + \sum_{p=0}^{T/h-1} O(h^2) \]

\[ = h \sum_{p=0}^{T/h-1} E \left[ Lu \left( T - ph, \tilde{X}_{ph}(x) \right) - \frac{\partial u}{\partial t} \left( T - ph, \tilde{X}_{ph}(x) \right) \right] + O(h) \]

\[ = O(h), \]

since \( \frac{\partial u}{\partial t}(t, x) = Lu(t, x) \).
Probabilistic interpretation of parabolic PDEs

\[ \mathbb{E} f(\bar{X}_T^h(x)) - u(T, x) \]
\[ = \frac{T}{h} - 1 \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p + 1)h, \bar{X}_{(p+1)h}^h(x) \right) - u \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] \]
\[ = \frac{T}{h} - 1 \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p + 1)h, \bar{X}_{ph}^h(x) \right) - u \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] \]
\[ + h \frac{T}{h} - 1 \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - (p + 1)h, \bar{X}_{ph}^h(x) \right) \right] + \sum_{p=0}^{T/h-1} O(h^2) \]
\[ = h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - ph, \bar{X}_{ph}^h(x) \right) - \frac{\partial u}{\partial t} \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] + O(h) \]
\[ = O(h), \]

since \( \frac{\partial u}{\partial t}(t, x) = Lu(t, x). \)
Probabilistic interpretation of parabolic PDEs

\[ \mathbb{E} f(\bar{X}_T^h(x)) - u(T, x) \]
\[ = \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p + 1)h, \bar{X}_{(p+1)h}^h(x) \right) - u \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] \]
\[ = \sum_{p=0}^{T/h-1} \mathbb{E} \left[ u \left( T - (p + 1)h, \bar{X}_{ph}^h(x) \right) - u \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] \]
\[ + h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - (p + 1)h, \bar{X}_{ph}^h(x) \right) \right] + \sum_{p=0}^{T/h-1} \mathcal{O} \left( h^2 \right) \]
\[ = h \sum_{p=0}^{T/h-1} \mathbb{E} \left[ Lu \left( T - ph, \bar{X}_{ph}^h(x) \right) - \frac{\partial u}{\partial t} \left( T - ph, \bar{X}_{ph}^h(x) \right) \right] + \mathcal{O} \left( h \right) \]
\[ = \mathcal{O} \left( h \right), \]

since \( \frac{\partial u}{\partial t} (t, x) = Lu(t, x). \)
Convergence rate

Let $F(\cdot)$ be a functional on the path space. The global error of a Monte Carlo method is

$$
\mathbb{E} F(X) - \frac{1}{N} \sum_{k=1}^{N} \mathbb{E} F(\bar{X}^{h,k}) = \mathbb{E} F(X) - \mathbb{E} F(\bar{X}^{h}) =: \epsilon_d(h)
$$

$$
\mathbb{E} F(\bar{X}^{h}) - \frac{1}{N} \sum_{k=1}^{N} F(\bar{X}^{h,k}) =: \epsilon_s(h,N)
$$

The statistical error satisfies

$$
\exists \, C > 0, \quad \mathbb{E} |\epsilon_s(h)| \leq \frac{C}{\sqrt{N}} \quad \text{for all } h.
$$
Concerning the discretization error: Suppose that $f$ has a polynomial growth at infinity. Under hypoellipticity conditions, or when all the functions of the problem are smooth, one has (T.-Tubaro, Bally-T. etc.)

$$e_d(h) = C_f(T, x) \ h + Q_h(f, T, x) \ h^2,$$

where

$$|C_f(T, x)| + \sup_h |Q_h(f, T, x)| \leq C (1 + \|x\|^Q)^{1 + K(T)} \frac{1}{T^q}.$$

Thus, Romberg extrapolation techniques can be used:

$$\mathbb{E} \left\{ \frac{2}{N} \sum_{k=1}^{N} f(\bar{X}_T^{h/2, k}) - \frac{1}{N} \sum_{k=1}^{N} f(\bar{X}_T^{h, k}) \right\} = O(h^2).$$

Remark: The technique used in the proofs is purely probabilistic (stochastic flows of diffeomorphisms, Malliavin variations calculus).
Dirichlet boundary conditions

For

\[
\begin{aligned}
  \frac{\partial u}{\partial t}(t, x) &= Lu(t, x), \ t > 0, \ x \in D, \\
  u(0, x) &= f(x), \ x \in D, \\
  u(t, x) &= g(x), \ x \in \partial D,
\end{aligned}
\]

one has

\[
 u(t, x) = \mathbb{E} f(X_t(x)) \mathbb{1}_{t < \tau} + \mathbb{E} g(X_{\tau}(x)) \mathbb{1}_{t \geq \tau},
\]

where \( \tau := \text{‘first boundary hitting time of } (X_t) \text{’} \).

The stopped Euler scheme is defined as

\[
\bar{X}^h_{p(h \wedge \tau)}(x),
\]

where \( \tau^h := \text{‘first boundary hitting time of the Euler scheme’} \).

For a convergence rate analysis, see Gobet, Menozzi, etc.
Neumann boundary conditions

For

\[
\begin{align*}
\frac{\partial u}{\partial t}(t, x) &= Lu(t, x), \quad t > 0, \quad x \in D, \\
u(0, x) &= f(x), \quad x \in D, \\
\nabla u(t, x) \cdot n(x) &= 0, \quad x \in \partial D,
\end{align*}
\]

one has

\[u(t, x) = \mathbb{E} f(X_t(x))\]

where \(X:= \text{‘reflected diffusion process’}\):

\[X_t(x) = x + \int_0^t b(X_s(x)) \, ds + \int_0^t \sigma(X_s(x)) \, dW_s + \int_0^t n(X_s) \, dL_s(X).
\]

Here, \((L_t(X))\) is an increasing process, namely the local time of \(X\) at the boundary.

The reflected Euler scheme is defined in such a way that the simulation of the local time is avoided.
Consider a domain $D \subset \mathbb{R}^d$, with smooth boundary. Let $n(s)$ denote the unit inward normal vector at $s \in \mathcal{D}$. Suppose that the vector field $\gamma$ defining the reflection direction is uniformly non tangent to the boundary.

Consider the reflected S.D.E. with smooth coefficients and strictly uniformly elliptic generator

$$X_t = x + \int_0^t b(X_s) ds + \int_0^t \sigma(X_s) dW_s + \int_0^t \gamma(X_s) dk_s,$$

where

$$k_t = \int_0^t \mathbb{1}_{X_s \in \mathcal{D}} dk_s.$$

To discretize the above reflected SDE, start at $x \in D$ at time 0, and assume that one has obtained $\hat{X}_{ph}^h \in \overline{D}$. Then observe that for all $x$ in a neighborhood of $D$, there exist a unique pair of functions $\pi_{\partial D}^\gamma$ taking values in $\partial D$ and $F^\gamma$ taking values in $\mathbb{R}$ such that

$$x = \pi_{\partial D}^\gamma(x) + F^\gamma(x)\gamma(\pi_{\partial D}^\gamma(x)).$$
Then,

- For $t \in [t_i^n, t_{i+1}^n]$, set
  \[
  \tilde{Y}_t^i := \tilde{X}_{ph}^h + b(\tilde{X}_{ph}^h)(t - t_i^n) + \sigma(\tilde{X}_{ph}^h)(W_t - W_{t_i^n}).
  \]

- i) If $\tilde{Y}_{(p+1)h}^i \not\in \overline{D}$, set
  \[
  \tilde{X}_{(p+1)h}^i = \pi^\gamma_{\partial D}(\tilde{Y}_{(p+1)h}^i) - F^\gamma(\tilde{Y}_{(p+1)h}^i)\gamma(\tilde{Y}_{(p+1)h}^i).
  \]

  ii) If $\tilde{Y}_{(p+1)h}^i \in \overline{D}$, $\tilde{X}_{(p+1)h}^i = \tilde{Y}_{(p+1)h}^i$.

Let $f$ be a function of class $C^5_b(\overline{D}, \mathbb{R})$ which satisfies the compatibility condition

\[
\forall z \in \partial D, \quad [\nabla f \gamma](z) = [\nabla (Lf) \gamma](z) = 0.
\]

**Theorem.** (Bossy–Gobet–T.) One has

\[
|E(f(\tilde{X}_T^h)) - E(f(X_T))| \leq \frac{K(T)}{n} \sum_{\alpha:|\alpha| \leq 5} \|\partial_x^\alpha f\|_\infty
\]

for some constant $K(T)$ uniform w.r.t. $x$ and $f$. 
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Stochastic Hamiltonian dynamics

\[
\begin{aligned}
\begin{cases}
  dQ_t &= \partial_p H(Q_t, P_t) dt, \\
  dP_t &= -\partial_q H(Q_t, P_t) dt - F_1(H(P_t, Q_t))\partial_p H(Q_t, P_t) dt + F_2(H(P_t, Q_t))dW_t,
\end{cases}
\end{aligned}
\]

where \( H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \), and \( F_1, F_2 : \mathbb{R} \to \mathbb{R} \).

Problems to solve:

- Existence, uniqueness of an invariant probability measure \( \mu \);
- The measure \( \mu \) has a continuous and strictly positivite density;
- Construction of an approximate ergodic process \( (\bar{Q}^n, \bar{P}^n) \);
- Precise estimate on the global error

\[
\int f(q, p) d\mu - \frac{1}{K} \sum_{k=1}^{K} f(\bar{Q}_{k/n}^n, \bar{P}_{k/n}^n).
\]
Our main assumptions

- $H, F_1, F_2$ are smooth functions;
- A convexity type assumption on $D^2 H$;
- $\partial_{pp} H$ is bounded;
- $\exists R > 0, \exists C_0 > 0, F_1(x) \geq C_0$ for $x \geq R$;
- $\exists C_0 > 0, F_2(x) \geq C_0$;
- Boundedness conditions on the derivatives of $F^2$. 
The implicit Euler scheme

The explicit Euler scheme may have moments not uniformly bounded in time (counterexamples…).

**The implicit Euler scheme:**
Choose an arbitrary $0 < \rho < 1$.

\[
\begin{align*}
\tilde{Q}_{k+1}^n &= \tilde{Q}_k^n + \partial_p H(\tilde{Q}_{k+1}^n, \tilde{P}_{k+1}^n) \frac{\rho}{n}, \\
\tilde{P}_{k+1}^n &= \tilde{P}_k^n - \partial_q H(\tilde{Q}_{k+1}^n, \tilde{P}_{k+1}^n) \frac{\rho}{n} - F_1 \circ H(\tilde{Q}_{k+1}^n, \tilde{P}_{k+1}^n) \frac{\rho}{n} \\
&
+ F_2 \circ H(\tilde{Q}_k^n, \tilde{P}_k^n) \left( W_{(k+1)\rho/n} - W_{k\rho/n} \right).
\end{align*}
\]

Remark: using $H + 1$ as a Lyapunov function, one can prove that the implicit Euler scheme has moments uniformly bounded in time.
Ergodicity of the implicit Euler scheme

Uniform in time upper bounds for the moments $\Rightarrow$ existence of an invariant probability measure $\bar{\mu}^n$ for the implicit Euler scheme. To get uniqueness, prove that the chain is positive Harris recurrent owing to sufficient conditions found in Meyn and Tweedie:

- Prove that the chain is forward accessible and 0 is a global attracting state, which provides the irreducibility of the chain;
- Check that the chain is a T-chain; for an irreducible T-chain, every compact set is a petite set; thus, there obviously exists a petite set $\mathcal{K}$ such that

$$
\mathbb{E} \left[ H(\bar{Q}_1^n, \bar{P}_1^n) \mid (\bar{Q}_0^n, \bar{P}_0^h) = (q, p) \right] - H(q, p) 
\leq -1 + b \mathbb{I}_\mathcal{K}(q, p), \quad \forall (q, p) \in \mathbb{R}^{2d}.
$$

For similar results: see Shardlow & Stuart (1999), Higham & Mattingly & Stuart (1999).
Ergodicity of the Hamiltonian process

Uniform in time upper bounds for the moments $\implies$ existence of an invariant probability measure $\mu$ for $(Q_t, P_t)$.
To get uniqueness, prove:

- The law of $(Q_t, P_t)$ has a smooth density $\pi(t, q, p)$ for all $t > 0$: this results, e.g., from hypoellipticity and a localization technique (the latter argument is used because of the possible unboundedness of $\partial_{pq}H, \partial_{qq}H$);
- The density $\pi(t, q, p)$ is strictly positive everywhere: this results from Michel & Pardoux’s controllability argument, since the reachibility set of the system

$$
\begin{align*}
\left\{ dQ_t^u &= \partial_p H(Q_t^u, P_t^u)dt, \\
 dP_t^u &= -\partial_q H(Q_t^u, P_t^u)dt - F_1(H(P_t^u, Q_t^u))\partial_p H(Q_t^u, P_t^u)dt + F_2(H(P_t^u, Q_t^u))u_t dt
\right.
\end{align*}
$$

is the whole space.

Remark: the measure $\mu$ has finite moments of all order.
Exponential decay of moments of \((Q_t, P_t)\): the statement

Set

\[
u(t, x, v) := \mathbb{E} \left[ f(X_t, V_t) \middle| (X_0, V_0) = (x, v) \right] - \int_{\mathbb{R}^{2d}} f \, d\mu.
\]

**Theorem 1**

Suppose that \(f\) is a smooth function, and that all its derivatives have a growth at most polynomial at infinity. Let \(D^m u(t)\) denote the vector of the derivatives of order \(m\) of the mapping

\[(q, p) \mapsto u(t, q, p).\]

For all integer \(m\) there exist an integer \(s_m\) and \(C_m > 0, \gamma_m > 0\) such that

\[|D^m u(t)| \leq C_m (1 + |q|^{s_m} + |p|^{s_m}) \exp(-\gamma_m t), \quad \forall \, t > 0, \quad \forall (q, p) \in \mathbb{R}^{2d}.
\]
Sketch of the proof of Theorem 1

1. Prove that, for any ball $B$ in $\mathbb{R}^{2d}$, there exist $C > 0$ and $\lambda > 0$ such that

$$\int_B |u(t)|^2 d\mu \leq C \exp(-\gamma t), \ \forall t > 0.$$ 

2. Show that the preceding inequality also holds for any spatial derivative of $u(t)$ (possibly with different real numbers $C$ and $\gamma$). As $\mu$ has a smooth and strictly positive density w.r.t. Lebesgue's measure, deduce from the Sobolev imbedding Theorem that, for any ball $B$ in $\mathbb{R}^{2d}$, there exist $C > 0$ and $\gamma > 0$ such that

$$\forall (x, v) \in B, \ |u(t, q, p)| \leq C \exp(-\gamma t), \ \forall t > 0.$$
3. Then show that there exist $C > 0$ and $\gamma > 0$ such that

$$\int |u(t)|^2 \pi_s(q, p) \, dq \, dp \leq C \exp(-\gamma t), \quad \forall t > 0,$$

where

$$\pi_s(q, p) := \frac{1}{(H(q, p) + 1)^s}$$

for some integer $s$.

4. Finally, prove that the preceding inequality also holds for any spatial derivative of $u(t)$ (possibly with different real numbers $s, C$ and $\gamma$). Then conclude by using the Sobolev imbedding Theorem again.
Sketch of the proof of Theorem 1 (end)

Main step: in spite of the degeneracy of the generator $L$ of $(Q_t, P_t)$, one has

A. $\exists C > 0, \exists \gamma_0 > 0, \int |u(t)|^2 d\mu \leq C \exp(-\gamma_0 t), \forall t \geq 0,$

B. $\exists C_{kl} > 0, \exists \gamma_{kl} > 0, \int |u(t)|^2(|q|^k + |p|^\ell) d\mu \leq C_{kl} \exp(-\gamma_{kl} t), \forall t \geq 0,$

C. $\exp(\gamma T) \int |u(T)|^2 d\mu + \int_0^T \exp(\gamma t) \int \left| \frac{\partial u}{\partial p}(t) \right|^2 d\mu \, dt \leq C, \forall T > 0,$

D. $- \int_0^T \exp(\gamma_1 t) \int \frac{\partial u}{\partial q}(t) \frac{\partial u}{\partial p}(t)|q|^2 d\mu \, dt \leq C, \forall T > 0,$

E. $\int \left| \frac{\partial u}{\partial q}(T) \right|^2 d\mu \leq C \exp(-\gamma_2 T), \forall T > 0.$
Convergence rate of the implicit Euler scheme

Decomposition of the global error:

\[
\int f(q, p) d\mu - I_{n,K}^n = \int f(q, p) d\mu - \int_{\mathbb{R}^{2d}} f(q, p) \bar{\mu}^n(dq, dp) + \int_{\mathbb{R}^{2d}} f(q, p) \bar{\mu}^n(dq, dp) - I_{n,K}^n.
\]

- The term \(e_d(n)\) is a discretization error: we expand it in terms of \(1/\rho/n\), from which we justify Romberg-Richardson extrapolation techniques to accelerate the convergence rate.
- The term \(e_s(n, K)\) is a statistical error: we provide estimates by using classical results on the weak convergence of normalized martingales.
Convergence rate of the implicit Euler scheme (cont.)

Theorem 2

Suppose that $f$ is a smooth function, and that all its derivatives have a growth at most polynomial at infinity.

Then

$$e_d(n) = \frac{C_1}{n} + \ldots + \frac{C_m}{n^m} + \mathcal{O}\left(\frac{1}{n^{m+1}}\right), \quad \forall m \in \mathbb{N} - \{0\},$$

for some real numbers $C_j$ uniform w.r.t. $n$,

and

$$e_s(n, K) \xrightarrow[K \to +\infty]{} 0 \text{ a.s.} \quad \Rightarrow \quad \sqrt{\frac{n}{K}} e_s(n, K) \rightarrow \mathcal{N}(0, \Sigma^n),$$

with $\Sigma^n$ uniformly bounded w.r.t. $n$. 

Sketch of the proof of Theorem 2

Set

\[ \bar{Y}_k^n := (\bar{Q}_k^n, \bar{P}_k^n). \]

One has

\[ u(j\rho/n, Y_{k+1}) \equiv u(j\rho/n, Y_k^n) + Lu(j\rho/n, Y_k^n) \frac{\rho}{n} + c_0(j\rho/n, Y_k^n) \frac{\rho^2}{n^2} + r_{j,k+1} \frac{1}{n^3}. \]

As \( u(t, q, p) \) solves \( du/dt = Lu \), one deduces

\[ u(j\rho/n, \bar{Y}_{k+1}^n) \equiv u((j + 1)\rho/n, \bar{Y}_{k+1}^n) + C(j\rho/n, \bar{Y}_k^n) \frac{\rho^2}{n^2} + R_{j,k+1}^n \frac{1}{n^3}. \]

The function \( C(t, y) \) is a sum of terms of the type \( \phi(q, p)\partial_J u(t, q, p) \).

The remainder term \( R_{j,k+1}^n \) is a sum of terms of the type

\[ \mathbb{E} \left[ P(\bar{Y}_k^n)\partial_J u \left( j\rho/n, \bar{Y}_k^n + \theta(\bar{Y}_{(k+1)\rho/n} - \bar{Y}_k^n) \right) \right], \ \theta \in (0, 1). \]
Sketch of the proof of Theorem 2 (cont.)

Observe that

\[
\frac{1}{K} \sum_{k=1}^{K} f(\bar{Y}^n_k) = \frac{1}{K} \sum_{k=1}^{K} u(0, \bar{Y}^n_k) + \int_{\mathbb{R}^{2d}} f \ d\mu.
\]

Thus

\[
\frac{1}{K} \sum_{k=1}^{K} f(\bar{Y}^n_k) \overset{\mathbb{E}}{=} \int_{\mathbb{R}^{2d}} f \ d\mu + \frac{1}{K} \sum_{k=1}^{K} u(j\rho/n, \bar{Y}_0) + \frac{1}{K} \sum_{k=1}^{K} \sum_{j=0}^{k-1} c(j\rho/n, \bar{Y}^n_k) \frac{\rho^2}{n^2} + \frac{1}{K} \sum_{k=1}^{K} \sum_{j=0}^{k-1} R_n j.\]

By ergodicity,

\[
\lim_{K \to \infty} \frac{1}{K} \sum_{k=1}^{K} \mathbb{E} u(k\rho/n, \bar{Y}_0) = 0 \quad \text{and} \quad \lim_{K \to \infty} \mathbb{E} f(\bar{Y}^n_k) = \int_{\mathbb{R}^2} f \ d\bar{\mu}^n.
\]
Sketch of the proof of Theorem 2 (end)

In view of the estimates of Theorem 1,
\[ \sum_{j=0}^{+\infty} |R_{j,k+1}^n| \leq \frac{C_0}{1 - \exp(-\gamma \rho/n)} \mathbb{E} \left( 1 + |\bar{Y}_k^n|^s + |\bar{Y}_{k+1}^n|^s \right), \]
from which
\[ \sum_{j=0}^{+\infty} |R_{j,k+1}^n| \leq Cn(1 + \mathbb{E} |\bar{Y}_0^n|^s). \]

Moreover, in view of Theorem 1 again,
\[ \frac{\rho}{n} \lim_{K \to \infty} \frac{1}{K} \sum_{k=1}^{K} \sum_{j=0}^{k-1} \mathbb{E} C(j \rho/n, \bar{Y}_k^n) = \int_0^\infty \int_{\mathbb{R}^{2d}} C(t, q, p) \mu(dq, dp) \, dt + O \left( \frac{\rho}{n} \right). \]
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Conclusion
Consider a $d$-dimensional standard Brownian motion $(W_t; \ t \in [0, T])$, and $((X_t, U_t); \ t \in [0, T])$ solution of

$$
\begin{cases}
X_t = X_0 + \int_0^t U_s \, ds, \\
U_t = U_0 + \int_0^t B [X_s, U_s; \rho_s] \, ds + \int_0^t \sigma(s, X_s, U_s) \, dW_s,
\end{cases}
$$

$\rho_t$ is the density distribution of $(X_t, U_t)$ for all $t \in (0, T]$. 

(1)
Here, $B$ is the mapping from $\mathbb{R}^d \times \mathbb{R}^d \times L^1(\mathbb{R}^{2d})$ to $\mathbb{R}^d$ defined by

$$B[x, u; \gamma] = \begin{cases} 
\frac{\int_{\mathbb{R}^d} b(v, u)\gamma(x, v) \, dv}{\int_{\mathbb{R}^d} \gamma(x, v) \, dv} & \text{if } \int_{\mathbb{R}^d} \gamma(x, v) \, dv \neq 0, \\
0 & \text{elsewhere,}
\end{cases}$$

where $b : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is bounded.
Formally, the drift component of (1) involves

$$(x, u) \mapsto \mathbb{E} \left[ b(U_t, u) \Big| X_t = x \right].$$

(3)

Such nonlinearity is typical of Lagrangian stochastic models for the position $X_t$ and the velocity $U_t$ of a generic fluid-particle in a turbulent flow: see the dramatically complex Probability Density Function (PDF) methods for turbulent flows and S. Pope’s models which aim to be alternative approaches to the Navier-Stokes equations for turbulent flows.

Our objective is to show existence and uniqueness of a solution to our simplified Lagrangian model.
Lagrangian stochastic models for monophasic turbulent flows

Statistical solutions to the Navier–Stokes equation: the Reynolds decomposition of the Eulerian velocity $U$ of a turbulent flow is

$$ U(t, x, \omega) = \langle U \rangle(t, x) + u(t, x, \omega), $$

where $\langle U \rangle$ is the (ensemble) averaged part, and $u$ is the fluctuating part.

Reynolds Averaged Navier-Stokes (RANS) equations:

$$ \begin{cases} 
(\nabla_x \cdot \langle U \rangle) = 0, \\
\partial_t \langle U^{(i)} \rangle + (\langle U \rangle \cdot \nabla_x \langle U^{(i)} \rangle) = -\frac{1}{\rho} \nabla_x \langle P^{(i)} \rangle + \nu \Delta_x \langle U^{(i)} \rangle - \partial_{x_j} \langle u^{(i)} u^{(j)} \rangle, \\
\langle U \rangle(0, x) = \langle U_0 \rangle(x). 
\end{cases} $$
The gradient pressure $\nabla_x \langle P \rangle$ solves the Poisson equation:

$$-\frac{1}{\rho} \Delta_x \langle P \rangle = \partial_{x_i,x_j}^2 \langle U^{(i)} \rangle \langle U^{(j)} \rangle + \partial_{x_i,x_j}^2 \langle u^{(i)} u^{(j)} \rangle.$$ 

The **Reynolds stress tensor** stands for the covariance of velocity components:

$$\langle u^{(i)} u^{(j)} \rangle = \langle U^{(i)} U^{(j)} \rangle - \langle U^{(i)} \rangle \langle U^{(j)} \rangle.$$
The RANS equation is not closed. In Pope’s model, Lagrangian and Eulerian quantities are related as follows: for all suitable measurable function $g : \mathbb{R}^d \to \mathbb{R}^d$,

$$
\langle g(U) \rangle (t, x) = \mathbb{E} \left[ g(U_t) / X_t = x \right].
$$ (4)

The simplest model proposed by Pope (2003) is the simplified Langevin model

$$
\begin{cases}
X_t = X_0 + \int_0^t U_s \, ds, \\
U_t = U_0 - \frac{1}{\rho} \int_0^t \nabla_x \langle P \rangle (s, X_s) \, ds + \nu \int_0^t \nabla_x \langle U \rangle (s, X_s) \, ds \\
+ C_1 \int_0^t \frac{\phi(s, X_s)}{k(s, X_s)} (\langle U \rangle (s, X_s) - U_s) \, ds + \int_0^t \sqrt{C_2 \phi(s, X_s)} \, dW_s.
\end{cases}
$$
Technical difficulties in the analysis

Difficulties come from the dependency of the drift coefficient on the conditional expectation.

Related situations:

Sznitman (1986):

\[ d\zeta_t = p_t(\zeta_t) \, dt + dW_t, \]

where \( p_t \) is the Lebesgue density of \( \zeta_t \).

Oelschlager (1985):

\[ d\zeta_t = F(\zeta_t, p_t(\zeta_t)) \, dt + dW_t, \]

where \( F : \mathbb{R}^d \times \mathbb{R} \) is a bounded function, and

\[ d\zeta_t = \nabla p_t(\zeta_t) \, dt + dW_t. \]

Dermoune (2003):

\[ d\zeta_t = \mathbb{E} \left( v(\zeta_0) / \zeta_t \right) dt + dW_t, \]

where \( v : \mathbb{R}^d \rightarrow \mathbb{R}^d \) is a bounded continuous function.
Our situation drastically differs from the above:

- our drift coefficient depends on **conditional distributions** rather than the density $\rho_t$ itself;
- the infinitesimal generator of $(X_t, \mathcal{U})$ is **not strongly elliptic**.
A stochastic particle system

Consider

\[
\begin{aligned}
X^{i,\epsilon,N}_t &= X^i_0 + \int_0^t \mathcal{U}^{i,\epsilon,N}_s ds, \\
\mathcal{U}^{i,\epsilon,N}_t &= \mathcal{U}^i_0 + \int_0^t \frac{1}{N} \sum_{j=1}^N b(\mathcal{U}^{i,\epsilon,N}_s, \mathcal{U}^{i,\epsilon,N}_s) \phi_\epsilon(X^{i,\epsilon,N}_s - X^{j,\epsilon,N}_s) \\
&\quad + \int_0^t \sigma(s, X^i_s, \mathcal{U}^{i,\epsilon,N}_s) dW^i_s, \quad i = 1, \ldots, N,
\end{aligned}
\]

where \(\{\phi_\epsilon; \epsilon > 0\}\) is a family of mollifiers.
We prove that the particles propagate chaos: as $N$ tends to infinity, 
$(X^1,\epsilon,N,\mathcal{U}^1,\epsilon,N)$ converges weakly to the solution of

$$
\begin{cases}
X_\epsilon^t = X_0 + \int_0^t \mathcal{U}_s^\epsilon \, ds, \\
\mathcal{U}_\epsilon^t = \mathcal{U}_0 + \int_0^t B_\epsilon [X_s^\epsilon,\mathcal{U}_s^\epsilon,\rho_s^\epsilon] \, ds + \int_0^t \sigma(s,X_s,\mathcal{U}_s) \, dW_s,
\end{cases}
$$

\begin{equation}
\rho_t^\epsilon \text{ is the density of } (X_t^\epsilon,\mathcal{U}_t^\epsilon) \text{ for all } t \in (0,T],
\end{equation}

where the kernel $B_\varepsilon [x, u; \gamma]$ is defined by: for all nonnegative $\gamma \in L^1(\mathbb{R}^{2d})$, $(x, u) \in \mathbb{R}^{2d}$,

$$B_\varepsilon [x, u; \gamma] = \int_{\mathbb{R}^d} b(v, u) \phi_\varepsilon \ast \gamma(x, v) \, dv \frac{\int_{\mathbb{R}^d} \phi_\varepsilon \ast \gamma(x, v) \, dv + \varepsilon}{\int_{\mathbb{R}^d} \phi_\varepsilon \ast \gamma(x, v) \, dv + \varepsilon},$$

(6)

where

$$\phi_\varepsilon \ast \gamma(x, u) = \int_{\mathbb{R}^d} \phi_\varepsilon(x - y) \gamma(y, u) \, dy.$$
Our main theorem

Our assumptions.

- $b$ is a bounded continuous function.
- The velocity diffusion coefficient $\sigma$ is bounded and strongly elliptic.
- For all $1 \leq i, j \leq d$, $\sigma^{(i,j)}$ is Hölder continuous (in a reinforced sense).

Theorem.

(i) For all $\epsilon > 0$, the sequence $\{(X_{1}^{\epsilon,N}, U_{1}^{\epsilon,N}); \ N \geq 1\}$ converges weakly to a weak solution $(X_{\epsilon}^{\epsilon}, U_{\epsilon}^{\epsilon})$ of (5). This solution is unique and, if $P^{\epsilon}$ denotes the law by $(X_{\epsilon}, U_{\epsilon})$ (5), the interacting particle system is $P^{\epsilon}$-chaotic; that is, for every integer $k \geq 2$ and every finite family $\{\psi_{l}; \ l = 1, \cdots, k\}$ of $C_{b}(C([0, T]; \mathbb{R}^{2d}))$,

$$\langle P^{\epsilon,N}, \psi_{1} \otimes \cdots \psi_{k} \otimes \cdots \rangle \rightarrow \prod_{l=1}^{k} \langle P^{\epsilon}, \psi_{l} \rangle, \ \text{when} \ N \rightarrow +\infty.$$  

(ii) When $\epsilon$ tends to 0, $(X_{\epsilon}, U_{\epsilon})$ converges weakly to the unique solution $(X, U)$ of (1).
The non-linear martingale problems

**Definition.** A probability measure $P$ on $\mathcal{C}([0, T] ; \mathbb{R}^{2d})$ is said a **weak solution** to (1) or a solution to the martingale problem ($MP$) if

(i) $P \circ (x_0, u_0)^{-1} = \mu_0$.

(ii) For all $t \in (0, T]$, the time-marginal $P \circ (x_t, u_t)^{-1}$ has a positive density $\rho_t$ w.r.t. Lebesgue measure on $\mathbb{R}^{2d}$.

(iii) For all $f \in \mathcal{C}^2_b(\mathbb{R}^{2d})$, the process

$$f(x_t, u_t) - f(x_0, u_0) - \int_0^t A_{\rho_s}(f)(s, x_s, u_s) \, ds$$

is a $P$-martingale, where, for each positive $\gamma \in L^1(\mathbb{R}^{2d})$, $A_\gamma$ is defined as

$$A_\gamma(f)(t, x, u) = (u \cdot \nabla_x f(x, u)) + (B[x, u; \gamma] \cdot \nabla_u f(x, u))$$

$$+ \frac{1}{2} \sum_{i,j=1}^d (\sigma^*)^{(i,j)}(t, x, u) \partial^2_{u_i, u_j} f(x, u).$$

(9)
Definition. A probability measure $P^\epsilon$ on $C([0, T]; \mathbb{R}^{2d})$ is said a weak solution to (5) or a solution to the martingale problem $(MP^\epsilon)$ if

(i) $P^\epsilon \circ (x_0, u_0)^{-1} = \mu_0$.

(ii) For all $t \in (0, T]$, the time–marginal $P^\epsilon \circ (x_t, u_t)^{-1}$ has a density $\rho_t^\epsilon$ w.r.t. Lebesgue measure on $\mathbb{R}^{2d}$.

(iii) For all $f \in C^2_b(\mathbb{R}^{2d})$, the process

$$f(x_t, u_t) - f(x_0, u_0) - \int_0^t A^\epsilon_{\rho^\epsilon_s}(f)(s, x_s, u_s) \, ds$$

is a $P^\epsilon$-martingale where, for all $\gamma \in L^1(\mathbb{R}^{2d})$, $A^\epsilon_\gamma$ is defined as

$A^\epsilon_\gamma(f)(t, x, u) = (u \cdot \nabla_x f(x, u)) + (B_\epsilon [x, u; \gamma] \cdot \nabla_u f(x, u))$

$$+ \frac{1}{2} \sum_{i, j=1}^d (\sigma \sigma^*)(i, j)(t, x, u) \partial_{u_i, u_j}^2 f(x, u).$$
Proposition. There is at most one weak solution to Equation (1) and one weak solution to Equation (5).

Sketch of the proof:

One can easily prove existence and weak uniqueness for

\[
\begin{cases}
Y^{s,y,v}_t &= y + \int_s^t V^{s,y,v}_\theta \, d\theta, \\
V^{s,y,v}_t &= v + \int_s^t \sigma(\theta, Y^{s,y,v}_\theta, V^{s,y,v}_\theta) \, dW_\theta.
\end{cases}
\]

In addition, the transition density \( \Gamma(s, y, v; t, x, u) \) of the solution satisfies the following estimate (see Francesco and Pascucci (2006)):

\[
\sup_{(y, v) \in \mathbb{R}^2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\nabla_v \Gamma(s, y, v; t, x, u)| \, dx \, du \leq \frac{C}{\sqrt{t-s}}, \ \forall \ 0 \leq s < t \leq T.
\]
A uniqueness result

Set

\[ S_{t,s}^{*}(f)(x, u) = \int_{\mathbb{R}^{2d}} \Gamma(s, y, v; t, x, u)f(y, v) \, dy \, dv. \]

We then prove that the densities \( \rho_t \) and \( \rho_{t}^{\varepsilon} \) are the unique solutions (in appropriate spaces) to mild equations: for example,

\[ \forall t \in (0, T], \quad \rho_t = S_{t,0}^{*}(\mu_0) + \int_0^t S'_{t,s}(\rho_s(\cdot)B[\cdot ; \rho_s]) \, ds \text{ in } L^1(\mathbb{R}^{2d}). \]
An existence result

Proposition. *The martingale problem* \((M_{P, \epsilon})\) *has a unique solution* \(P_{\epsilon}\) *and, when* \(\epsilon\) *tends to 0, \(P_{\epsilon}\) *converges to a solution of \((MP)\).* The proof proceeds in two steps:

- We show that \(\{\bar{P}_{\epsilon, N}; \ N \geq 1\}\) is relatively compact and that any weakly convergent subsequence assigns full measure to the set of the solutions to the martingale problem \((M_{P, \epsilon})\).
- The probability measure \(P_{\epsilon}\), solution of the martingale problem \((M_{P, \epsilon})\), converges to the solution of the martingale problem \((MP)\).
First step

Let $\bar{\mu}^{\epsilon,N}$ be the empirical measure defined on $\mathcal{M}(C([0, T]; \mathbb{R}^{2d}))$ by

$$
\bar{\mu}^{\epsilon,N} = \frac{1}{N} \sum_{i=1}^{N} \delta_{\{X_{i,\epsilon,N},U_{i,\epsilon,N}\}}.
$$

Let $\bar{\mathbb{P}}^{\epsilon,N} = \mathbb{Q} \circ (\bar{\mu}^{\epsilon,N})^{-1}$ be the probability law of $\bar{\mu}^{\epsilon,N}$.

Easy: The sequence $\{\bar{\mathbb{P}}^{\epsilon,N}; \ N \geq 1\}$ is tight on $\mathcal{M}(C([0, T]; \mathbb{R}^{2d}))$. Let $\bar{\mathbb{P}}^{\epsilon,\infty}$ be the limit of a weakly converging sequence.

**Lemma.** $\bar{\mathbb{P}}^{\epsilon,\infty}$ assigns full measure to the set of the solutions to the martingale problem $(MP_\epsilon)$. 
Second step

The sequence

\[ \tilde{P}^c := P^c \circ ((x_t, u_t, u_t - u_0 - \int_0^t B_\epsilon[x_s, u_s; \rho_s^c] \, ds); \ t \in [0, T])^{-1} \]

is tight. The support of any accumulation point has full measure on the set of continuous functions \((\tilde{x}, \tilde{u}, \tilde{D})\) of \(C([0, T]; \mathbb{R}^{3d})\) satisfying

\[ \tilde{x}(t) = \tilde{x}(0) + \int_0^t \tilde{u}(s) \, ds, \ \forall \ t \in [0, T], \]

and there exists a bounded function \(\tilde{a}\) such that

\[ \sup_{t \in [0, T]} |\tilde{a}(t)| \leq \|b\|_\infty, \]

and

\[ \tilde{u}(t) - \tilde{u}(0) - \tilde{D}(t) = \int_0^t \tilde{a}(s) \, ds, \ \forall \ t \in [0, T]. \]
Consider the following marginal distribution $\mathbb{P}$ of $\tilde{\mathbb{P}}$ on $C([0, T]; \mathbb{R}^{2d})$:

$$
\mathbb{P} = \tilde{\mathbb{P}} \circ \left((x_t, u_t); \ t \in [0, T]\right)^{-1}.
$$

**Proposition.** $\mathbb{P}$ solves the martingale problem (MP).

**Sketch of the proof:**

- Weak convergence (but we have to make fractions converge. . . )
- Estimates by Francesco and Pascucci (2006) for ultraparabolic PDEs.
- To overcome the difficulty due to the fact that $\mathbb{P}^\epsilon$ and $B_\epsilon[\cdot; \rho^\epsilon]$ depend on $\epsilon$, we adapt a method designed by Stroock and Varadhan for the case of strongly elliptic diffusion processes:
Key lemma. For all $0 < t \leq T$, $\rho_t^\epsilon$ converges to $\rho_t$ in $L^1(\mathbb{R}^{2d})$ when $\epsilon \to 0^+.$

Key result (Stroock & Varadhan (1979)). Let $\{f_n; \ n \geq 1\}$ be a sequence of non–negative measurable functions such that $\int_{\mathbb{R}^q} f_n(z) \, dz = 1$, for all $n \geq 1$. Suppose

1. There exists a density function $f$ such that, for all $\psi \in C_c(\mathbb{R}^q)$,

   $$\lim_{n \to +\infty} \int_{\mathbb{R}^q} f_n(z) \psi(z) \, dz = \int_{\mathbb{R}^q} f(z) \psi(z) \, dz.$$

2. For all $h \in \mathbb{R}^q$,

   $$\lim_{|h| \to 0} \sup_{n \in \mathbb{N}} \int_{\mathbb{R}^q} |f_n(z + h) - f_n(z)| \, dz = 0.$$

Then $\{f_n\}$ converges towards $f$ in $L^1(\mathbb{R}^q)$. 
Complements and perspectives

- Extensions to (simplified) stochastic Lagrangian models with specular boundary conditions: see Bossy & Jabir (2008-2012).
- For numerical issues and an application to meteorology, see Bossy et al. (2008-2012).
- For the study of the Poisson equation, see Bossy and Fontbona (in progress).
- For the full treatment of Pope’s model: a challenging problem!
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Many other problems:

- McKean–Vlasov systems for Navier–Stokes equations,
- Discretization of (reflected) backward SDEs for variational inequalities (American options, Stefan problems),
- Stochastic PDEs (Gyöngy, Walsh, de Bouard–Debussche),
- Discretization of Hamilton–Jacobi–Belman equations for stochastic control (Krtlov, Barles–Jakobsen),
- Bessel–type SDEs,
- Variance reduction methods (Arouna–Lapeyre, Kebaier–Kohatsu-Higa, . . .).