

A few open problems (for me)

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Outline

- 1 Exponential decay of partial derivatives of solutions to strongly elliptic parabolic PDEs
- 2 Extension to Stochastic Hamiltonian Dissipative Systems
- 3 Convergence of diffusion densities to equilibrium densities: Pointwise estimates (a novel approach?)
- 4 On the parabolic parabolic 2D Keller-Segel model

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Motivation

Target result: An accurate estimate on the numerical approximation

$$\int f(x) d\mu - \frac{1}{K} \sum_{k=1}^N f(\bar{X}_k^h)$$

Decomposition of the global error:

$$\begin{aligned} \int f(x) d\mu - \frac{1}{K} \sum_{k=1}^K f(\bar{X}_k^h) &= \underbrace{\int f(x) d\mu - \int f(x) d\bar{\mu}^h}_{e_d(n)} \\ &+ \underbrace{\int f(x) d\bar{\mu}^h - \frac{1}{K} \sum_{k=1}^K f(\bar{X}_k^h)}_{e_s(h,K)}. \end{aligned}$$

Discretization error: Methodology

Set $u(t, x) := \mathbb{E}f(X_t(x))$ and $L :=$ generator of X . Then

$$\begin{aligned} \frac{d}{dt} u(t, x) &= L u(t, x) \\ u(0, x) &= f(x) \end{aligned}$$

and

$$\frac{1}{K} \sum_{k=1}^K f(\bar{X}_k^h) = \frac{1}{K} \sum_{k=1}^K u(0, \bar{X}_k^h)$$

Expansions

A Taylor expansion and the PDE lead to

$$\mathbb{E} u(jh, \bar{X}_{k+1}^h) = \mathbb{E} u((j+1)h, \bar{X}_k^h) + R_{j,k+1}^h h^2$$

and the remainder term $R_{j,k+1}^h$ is a sum of terms of the type

$$\text{Constant} \times \mathbb{E} \left[\psi(\bar{X}_k^h) \partial_J u(jh, \bar{X}_k^h + \theta(\bar{X}_{k+1}^h - \bar{X}_k^h)) \right]$$

where

- $\psi(x)$ is a polynomial of b , σ and their partial derivatives
- $0 < \theta < 1$

Thus

$$\mathbb{E}\left(\frac{1}{K} \sum_{k=1}^K u(0, \bar{X}_k^h)\right) = \frac{1}{K} \sum_{k=1}^K u(kh, x) + \frac{1}{K} \sum_{k=1}^K \sum_{j=0}^{k-1} \mathbb{E}(R_{j,k}^h) h^2$$

Suppose

$$|\partial_t u(t, x)| \leq \Gamma_t (1 + |x|^{s_t}) \exp(-\gamma_t t)$$

Then: $\exists \lambda > 0, s \in \mathbb{N}$,

$$\sum_{j=0}^{+\infty} \mathbb{E}|R_{j,k}^h| \leq \frac{C_0}{1 - e^{-\lambda h}} \mathbb{E}(1 + |\bar{X}_k^h|^s) \leq \frac{C}{h}$$

AND WE ARE DONE WHEN $u(t, x)$ TENDS TO $\int f(x) d\mu$

Sufficient conditions (D.T., 1990)

- (H1) the functions b, σ are of class C^∞ with bounded derivatives of any order ; the function σ is bounded
- (H2) the operator L is uniformly elliptic : there exists a positive constant α such that :

$$\forall x, \xi \in \mathbb{R}^d, \quad \sum_{i,j} a_j^i(\xi) x_i x_j \geq \alpha |x|^2$$

- (H3) there exists a strictly positive constant β and a compact set K such that :

$$\forall x \in \mathbb{R}^d - K, \quad x \cdot b(x) \leq -\beta |x|^2$$

Exponential decay of u

Lemma

There exist $C > 0$ and $\lambda > 0$ such that

$$\forall t > 0, \quad \int |u(t, x)|^2 d\mu \leq C \exp(-\lambda t)$$

Hint: The Markov chain $(X_{n\theta})$ is **geometrically** recurrent for any θ , and $\int |u(t, x)|^2 \mu(dx)$ is decreasing:

$$\begin{aligned} \frac{d}{dt} \int |u(t, x)|^2 d\mu &= 2 \int u(t, x) Lu(t, x) \mu(dx) \\ &\leq - \int a_j^j(x) \partial_i u(t, x) \partial_j u(t, x) d\mu \\ &\leq 0 \end{aligned}$$

From u to ∇u : First step

From

$$\frac{d}{dt}|u(t)|^2 - L(|u(t)|^2) = -a_j^i(\partial_i u(t))(\partial_j u(t))$$

it comes

$$e^{\delta t} \frac{d}{dt} \int |u(t)|^2 d\mu + C e^{\delta t} \int |\nabla u(t)|^2 d\mu \leq 0$$

Therefore,

$$\begin{aligned} e^{\delta T} \int |u(T)|^2 d\mu + C \int_0^T e^{\delta t} \left(\int |\nabla u(t)|^2 d\mu \right) dt \\ \leq \int |f|^2 d\mu + \delta \int_0^T e^{\delta t} \left(\int |u(t)|^2 d\mu \right) dt \end{aligned}$$

Now choose $\delta < \lambda$.

From u to ∇u : Second step

There exist $C_1 > 0$ and $C_2 > 0$ such that

$$\begin{aligned} \frac{d}{dt} |\nabla u(t)|^2 - L(|\nabla u(t)|^2) &= -a_j^i (\partial_{ik} u(t)) (\partial_{jk} u(t)) + (\partial_p a_j^i) (\partial_{ij} u(t)) (\partial_p u(t)) \\ &\quad + 2(\partial_p b^i) (\partial_i u(t)) (\partial_p u(t)) \\ &\leq -C_1 |D^2 u(t)|^2 + C_2 |\nabla u(t)|^2 \end{aligned}$$

Choose $\gamma < \delta$ and proceed as above. It comes:

$$\begin{aligned} e^{\gamma T} \int |\nabla u(T)|^2 d\mu + C_1 \int_0^T e^{\gamma t} \left(\int |D^2 u(t)|^2 d\mu \right) dt \\ \leq \int |\nabla f|^2 d\mu + (C_2 + \gamma) \int_0^T e^{\gamma t} \left(\int |\nabla u(t)|^2 d\mu \right) dt \end{aligned}$$

Thus,

$$\int |\nabla u(t, x)|^2 d\mu \leq C \exp(-\gamma t)$$

From L^p norm to local estimates

By induction on the order of differentiation: For any multi-index J ,
 $\exists C_J > 0$, $\lambda_J > 0$ such that

$$\int |\partial_J u(t, x)|^2 \mu(dx) \leq C_J \exp(-\lambda_J t)$$

Since μ has a density $\rho(x)$ which is **strictly positive on any ball $B = B(O, R)$** ,

$$\|\partial_J u(t)\|_{L^2(B)}^2 \leq C \int |\partial_J u(t, x)|^2 \rho(x) dx$$

By Sobolev's imbedding Theorem:

$$\forall t > 0, \forall x \in B, |u(t, x)| \leq C \exp(-\lambda t)$$

From local to global

Similarly, let

$$\pi_s(x) := \frac{1}{(1 + |x|^2)^s}$$

Lemma

$$\forall t > 0, \int |u(t, x)|^2 \pi_s(x) dx \leq C \exp(-\lambda t)$$

Hint: Compute $\frac{d}{dt}$. Split the integrals into integrals on $B(0, R)$ and $\mathbb{R}^d - B(0, R)$. On $B(0, R)$ use the preceding. On $\mathbb{R}^d - B(0, R)$ use the condition on $b(x)$.

Proceed as above. It comes:

Lemma

For any multiindex l ,

$$|\partial_l u(t, x)| \leq \Gamma_l (1 + |x|^{s_l}) \exp(-\gamma_l t)$$

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Stochastic Hamiltonian dynamics

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

where $H : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$, and $F_1, F_2 : \mathbb{R} \rightarrow \mathbb{R}$.

Problems to solve:

- Existence, uniqueness of an invariant probability measure μ
- The measure μ has a continuous and strictly positive density
- Numerical analysis

Our main assumptions

- H, F_1, F_2 are smooth functions;
- A convexity type assumption on D^2H
- $\partial_{pp}H$ 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

Ergodicity of the Hamiltonian process

To get **existence** of an invariant probability measure μ for (Q_t, P_t) :
Uniform in time upper bounds for moments

To get **uniqueness**, prove:

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

$$\begin{cases} dQ_t^u &= \partial_p H(Q_t^u, P_t^u) dt, \\ dP_t^u &= -\partial_q H(Q_t^u, P_t^u) dt - F_1(H(P_t^u, Q_t^u)) \partial_p H(Q_t^u, P_t^u) dt \\ &\quad + F_2(H(P_t^u, Q_t^u)) u_t dt \end{cases}$$

is the whole space.

Remark: the measure μ has finite moments of all order.

Exponential decay of moments of (Q_t, P_t) : the statement

Set

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

Theorem (D.T., 2002)

For any integer m there exist an integer s_m and positive numbers C_m, γ_m 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

$$\forall t > 0, \int_{B(0,R)} |u(t)|^2 d\mu \leq C \exp(-\gamma t)$$

- 2.

$$\forall t > 0, \int_{B(0,R)} |D^m u(t)|^2 d\mu \leq C \exp(-\gamma t)$$

3. By Sobolev's imbedding Theorem,

$$\forall (x, v) \in B(0, R), \quad \forall t > 0, \quad |u(t, q, p)| \leq C \exp(-\gamma t)$$

Sketch of the proof of Theorem 1 (cont.)

4. For some $C > 0$ and $\gamma > 0$,

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

where, for some integer s ,

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

5. For some new $C > 0$ and $\gamma > 0$,

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

6. Use Sobolev's imbedding Theorem

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. A similar inequality for $\left| \frac{\partial u}{\partial p}(t) - \frac{\partial u}{\partial q}(t) \right|^2$

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

Open problems

- Adapt or change the proof when the coefficients have low regularity
- Same questions when the drift coefficient satisfies a weaker assumption (cf. Pardoux et Veretennikov):

$$\exists r > 0, \exists \alpha > -1, \forall x \in \mathbb{R}^d - K, \frac{x}{|x|} \cdot b(x) \leq -r |x|^\alpha$$

Which is the right convergence rate of $|\partial_j u(t)|$ to 0?

- Same questions for models and numerical methods studied by Tony, Gabriel and their coauthors.

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On the convergence to equilibrium by Malliavin calculus

A representation formula in the one-dimensional case:

$$p(t, x) = \mathbb{E} \left[\mathbb{I}_{X_t > x} \delta \left(\frac{D_{\bullet} X_t}{\|D_{\bullet} X_t\|^2} \right) \right]$$

The particular case of the Ornstein-Uhlenbeck:

$$X_t = X_0 - \int_0^t X_s ds + \sqrt{2} W_t$$

Malliavin derivative: For $0 \leq \theta \leq t$,

$$D_{\theta} X_t = \sqrt{2} - \int_{\theta}^t D_s X_t ds$$

from which $D_{\theta} X_t = \sqrt{2} e^{\theta-t}$ and $\|D_{\bullet} X_t\|^2 = 1 - e^{-2t}$

Set $M_t := \int_0^t e^s dW_s$. Then

$$X_t = X_0 e^{-t} + \sqrt{2} e^{-t} M_t$$

Skorokhod integrals of **adapted** processes = Itô integrals, thus

$$p(t, x) = \mathbb{E} \left[\mathbb{I}_{X_0 e^{-t} + \sqrt{2} e^{-t} M_t > x} \frac{\sqrt{2} e^{-t}}{1 - e^{-2t}} M_t \right]$$

For large t , $\langle M \rangle_t = \frac{1}{2}(e^{2t} - 1) \simeq \frac{e^{2t}}{2}$.

$$p(t, x) \simeq \mathbb{E} \left[\mathbb{I}_{\frac{M_t}{\sqrt{\langle M \rangle_t}} > x} \frac{M_t}{\sqrt{\langle M \rangle_t}} \right] = \mathbb{E}[\mathbb{I}_{G > x} G]$$

that is, up to an explicit remaining term,

$$p(t, x) \simeq \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

For general one-dimensional diffusions:

After Lamperti transform,

$$X_t = X_0 + \int_0^t b(X_s) ds + W_t$$

from which for $0 \leq \theta \leq t$

$$D_\theta X_t = \exp\left(\int_\theta^t b'(X_s) ds\right)$$

One then has to consider

$$\delta\left(-\frac{e^{\int_0^t b'(X_s) ds}}{\int_0^t \exp(2 \int_\gamma^t b'(X_s) ds) d\gamma} e^{-\int_0^\bullet b'(X_s) ds}\right)$$

Trick: For adapted (u_t) use

$$\delta(F u_\bullet) = F \delta(u_\bullet) - \int_0^t D_\theta F u_\theta d\theta = F \int_0^t u_s dW_s - \int_0^t D_\theta F u_\theta d\theta$$

Set

$$M_t := \int_0^t \exp\left(-\int_0^s b'(X_s) ds\right) dW_s$$

Part of the representation formula for $p(t, x)$ becomes

$$\mathbb{E} \left[\mathbb{I}_{X_t > x} \frac{M_t}{\sqrt{\langle M \rangle_t}} \right]$$

AND NOW? UNDER WHICH CONDITIONS THE REMAINING TERMS ARE SMALL? – Work in progress

Statistical error

Poisson PDE:

$$Lu = f - \int f d\mu$$

Then

$$u(X_t) = u(X_0) + \int_0^t Lu(X_s) ds + \int_0^t \nabla u(X_s) \cdot \sigma(X_s) dW_s$$

from which

$$\frac{u(X_K)}{K} = \frac{u(X_0)}{K} + \frac{1}{K} \int_0^K (f(X_s) - \int f d\mu) ds + \frac{1}{K} \int_0^K \nabla u(X_s) \cdot \sigma(X_s) dW_s$$

For **functional extensions and numerical applications** : see
Bhattacharya, Lamberton-Pagès, Pagès and Rey, etc.

CLT Theorem (Kutoyants, ...)

Let (Y_t) be an $d \times r$ -matrix valued adapted process such that

$$\forall T > 0, \int_0^T (Y_s^{ij})^2 ds < \infty \quad \mathbb{P} - \text{a.s.}$$

Suppose there exists a non-degenerate covariance matrix \mathbf{C} s.t.

$$\forall 1 \leq i, j \leq d, \quad \frac{1}{T} \sum_{k=1}^r \int_0^T Y_s^{ik} Y_s^{jk} ds \xrightarrow{P} \mathbf{C}^{ij} \quad \text{as } T \rightarrow \infty$$

Then

$$Z_T := \frac{1}{\sqrt{T}} \int_0^T Y_s dW_s$$

weakly converges to the Gaussian distribution with mean zero and covariance matrix $\mathbf{C} := (\mathbf{C}^{ij})$.

Open problems:

- Under **weak assumptions** deduce the CLT theorem for the statistical error from the CLT for stochastic integrals
- Dynamical estimation of the variance of the normalized statistical error along the simulation since ∇u is unknown (work in slow progress)
- Berry-Esseen theorem and Edgeworth expansions (see Fukasawa under heavy assumptions):

$$\begin{aligned} \mathbb{P}\left(\frac{1}{\sigma\sqrt{K}} \int_0^K (f(X_s) - \int f d\mu) ds > x\right) &= \mathbb{P}(G > x) \\ &= \frac{C}{\sqrt{K}} Q(x) \exp\left(-\frac{x^2}{2}\right) + o\left(\frac{1}{\sqrt{K}}\right) \end{aligned}$$

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The **parabolic parabolic** 2D Keller-Segel model

Time evolution of the cell density $\rho(t, x)$ and the concentration of chemo-attractant $c(t, x)$:

$$\begin{cases} \partial_t \rho(t, x) = \nabla \cdot (\nabla \rho - \chi \rho \nabla c)(t, x), & t > 0, x \in \mathbb{R}^2, \\ \partial_t c(t, x) = \Delta c(t, x) - \lambda c(t, x) + \rho(t, x), & t > 0, x \in \mathbb{R}^2, \\ \rho(0, x) = \rho_0(x), \quad c(0, x) = c_0(x), & x \in \mathbb{R}^2 \end{cases}$$

Theorem (M. Tomasevic)

Under explicit constraints on (ρ_0, c_0) there exists a unique solution to the two-dimensional **parabolic parabolic** Keller-Segel PDE and to the McKean-Vlasov non-linear SDE

$$\left\{ \begin{array}{l} dX_t = \chi e^{-\lambda t} (G(t, \cdot) * \nabla c_0)(X_t) dt \\ \quad + \chi \left\{ \int_0^t \int_{\mathbb{R}^d} K_{t-s}(X_t - y) \rho(s, y) dy ds \right\} dt + \sqrt{2} dW_t, \\ X_0 \sim \rho_0, \quad X_t \sim \rho(t, x) dx, \end{array} \right.$$

where $K_t(x) := e^{-\lambda t} \nabla G(t, x) = e^{-\lambda t} \frac{-x}{2\pi t^2} \exp\left(-\frac{|x|^2}{2t}\right)$.

In addition (ρ, c) uniquely solves the K-S PDE, where

$$c(t, \cdot) = e^{-\lambda t} G(t, \cdot) * c_0 + \int_0^t e^{-\lambda(t-s)} G(t-s, \cdot) * \rho(s, \cdot) ds$$

Remark: The corresponding particle system is **NON MARKOV**

Solutions tend to self-similar solutions

A solution is **self-similar** iff it writes

$$\bar{\rho}(t, x) = \frac{1}{t} U\left(\frac{x}{\sqrt{t}}\right) \quad \text{and} \quad \bar{c}(t, x) = V\left(\frac{x}{\sqrt{t}}\right)$$

where the profile (U, V) satisfies the elliptic PDE

$$\begin{cases} \Delta_{\xi} U + \nabla_{\xi} \cdot (U \nabla_{\xi} \left(\frac{|\xi|^2}{4} - V\right)) = 0, \\ \Delta_{\xi} V + \frac{1}{2} \xi \cdot \nabla_{\xi} V + U = 0 \end{cases}$$

Theorem (Corrias, Escobedo, Matos)

Suppose $\lambda = 0$ and χ is large enough. If $\rho_0 \in \dot{H}(\mathbb{R}^2)$ then for all $p \geq 1$ and $r \geq 2$,

$$\lim_{t \rightarrow \infty} t^{1-\frac{1}{p}} \|\rho - \bar{\rho}\|_{L^p(\mathbb{R}^2)} = 0 \quad \text{and} \quad \lim_{t \rightarrow \infty} t^{1-\frac{1}{r}} \|\nabla c - \nabla \bar{c}\|_{L^r(\mathbb{R}^2)} = 0$$

Open problems:

- Probabilistic interpretation of the previous limit theorem
- Existence and uniqueness results for the non Markov particle system with singular interactions (work in progress, M. Tomasevic and D.T.)