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

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

Decomposition of the global error:

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

Discretization error: Methodology

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

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

and

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

Expansions

A Taylor expansion and the PDE lead to

$$\mathbb{E}\, u(jh, \overline{X}^h_{k+1}) = \mathbb{E}\, u((j+1)h, \overline{X}^h_k) + R^h_{j,k+1} h^2$$

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

$$\text{Constant} \times \mathbb{E}\left[\psi(\overline{X}^h_k)\, \partial_J u(jh, \overline{X}^h_k + \theta(\overline{X}^h_{k+1} - \overline{X}^h_k)\right]$$

where

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

Thus

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

Suppose

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

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

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

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 $\mathcal{C}^\infty$ 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 :

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

(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:

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

From u to ∇u: First step

From

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

it comes

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

Therefore,

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

Now choose $\delta < \lambda$.

From u to ∇u: Second step

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

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

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

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

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

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

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

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

By Sobolev's imbedding Theorem:

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

From local to global

Similarly, let

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

Lemma

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

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 I,

$$|\partial_I u(t,x)| \leq \Gamma_I (1 + |x|^{s_I}) \exp(-\gamma_I t)$$

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

Problems to solve:

- Existence, uniqueness of an invariant probability measure μ
- The measure μ has a continuous and strictly positivite 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 reachibility 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

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

Theorem (D.T., 2002)

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

$$|D^m u(t)| \leq C_m(1+|q|^{s_m}+|p|^{s_m})\exp(-\gamma_m t), \ \forall t>0, \ \forall (q,p)\in\mathbb{R}^{2d}$$

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

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

where, for some integer s,

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

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

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

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

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):

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

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 $0 \le \theta \le t$,

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

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

Set $\boxed{M_t := \int_0^t e^s \, dW_s}$. 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,

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

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

$$M_t := \int_0^t \exp\Big(-2 \int_0^\theta b'(X_s)\, ds \Big)\, dW_\theta$$

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

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

Suppose there exists a non-degenerate covariance matrix **C** s.t.

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

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):

$$\mathbb{P}\Big(\frac{1}{\sigma\sqrt{K}}\int_0^K (f(X_s) - \int f\, d\mu)\, ds > x\Big) - \mathbb{P}(G > x) = \frac{C}{\sqrt{K}}\, Q(x)\, exp(-\tfrac{x^2}{2}) + o(\frac{1}{\sqrt{K}})$$

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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 $c(t,x)$:

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

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 theMcKean-Vlasov non-linear SDE

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

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

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

$$\boxed{\overline{\rho}(t,x) = \frac{1}{t}\,U\Big(\frac{x}{\sqrt{t}}\Big) \quad \text{and} \quad \overline{c}(t,x) = V\Big(\frac{x}{\sqrt{t}}\Big)}$$

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

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

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 $r \geq 2$,

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

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.)