A few open problems (for me)

Denis Talay

INRIA Saclay

QuamPROCS - Metanolin – May 2022
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
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
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:

$$\int f(x) \, d\mu - \frac{1}{K} \sum_{k=1}^{K} f(\bar{X}_k^h) = \left\{ \begin{aligned} &\int f(x) \, d\mu - \int f(x) \, d\bar{\mu}^h \\ &\quad \text{e}_d(n) \end{aligned} \right\}$$

$$+ \int f(x) \, d\bar{\mu}^h - \frac{1}{K} \sum_{k=1}^{K} f(\bar{X}_k^h) \cdot \text{e}_s(h, K)$$
Set \( u(t, x) := \mathbb{E} f(X_t(x)) \) and \( L := \text{generator of } X \). Then

\[
\frac{d}{dt} u(t, x) = L u(t, x)
\]

\[
u(0, x) = f(x)
\]

and

\[
\frac{1}{K} \sum_{k=1}^{K} f(\overline{X}_k^h) = \frac{1}{K} \sum_{k=1}^{K} u(0, \overline{X}_k^h)
\]
A Taylor expansion and the PDE lead to

\[ \mathbb{E} u(jh, X_{k+1}^h) = \mathbb{E} u((j + 1)h, X_k^h) + R_{j,k+1}^h h^2 \]

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

\[ \text{Constant} \times \mathbb{E} \left[ \psi(X_k^h) \partial_J u(jh, X_k^h + \theta(X_{k+1}^h - X_k^h)) \right] \]

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

\[ \mathbb{E}\left( \frac{1}{K} \sum_{k=1}^{K} u(0, X_k^h) \right) = \frac{1}{K} \sum_{k=1}^{K} u(kh, x) + \frac{1}{K} \sum_{k=1}^{K} \sum_{j=0}^{k-1} \mathbb{E}(R_{j,k}^h) h^2 \]

Suppose

\[ |\partial_t u(t, x)| \leq \Gamma \left( 1 + |x|^s \right) \exp(-\gamma t) \]

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

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

AND WE ARE DONE WHEN \( u(t, x) \) TENDS TO \( \int f(x) \, d\mu \)
Sufficient conditions (D.T., 1990)

(H1) the functions $b, \sigma$ are of class $C^\infty$ with bounded derivatives of any order; the function $\sigma$ is bounded

(H2) the operator $L$ is uniformly elliptic: there exists a positive constant $\alpha$ such that:

$$\forall x, \xi \in \mathbb{R}^d, \sum_{i,j} a^i_j(\xi)x_ix_j \geq \alpha |x|^2$$

(H3) there exists a strictly positive constant $\beta$ and a compact set $K$ such that:

$$\forall x \in \mathbb{R}^d - K, \ x \cdot b(x) \leq -\beta |x|^2$$
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 $\theta$, and $\int |u(t, x)|^2 \mu(dx)$ is decreasing:

$$\frac{d}{dt} \int |u(t, x)|^2 d\mu = 2 \int u(t, x) Lu(t, x) \mu(dx)$$

$$\leq - \int a^i_j(x) \partial_i u(t, x) \partial_j u(t, x) d\mu$$

$$\leq 0$$
From $u$ to $\nabla u$: 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 $\nabla u$: Second step

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

$$\frac{d}{dt}|\nabla u(t)|^2 - L(|\nabla u(t)|^2) = -a^i_j(\partial_{ik} u(t))(\partial_{jk} u(t)) + (\partial_p a^i_j)(\partial_{ij} u(t))(\partial_p u(t))$$

$$+ 2(\partial_p b^i)(\partial_i u(t))(\partial_p u(t))$$

$$\leq -C_1 |D^2 u(t)|^2 + C_2 |\nabla u(t)|^2$$

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

$$e^{\gamma T} \int |\nabla u(T)|^2 \, d\mu + C_1 \int_0^T e^{\gamma t} \left( \int |D^2 u(t)|^2 d\mu \right) dt$$

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

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

\[
\|\partial^J u(t)\|_{L^2(B)}^2 \leq C \int |\partial^J u(t, x)|^2 p(x) \, dx
\]

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**

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

**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 \( I \),

\[ |\partial_I u(t, x)| \leq \Gamma_I (1 + |x|^{s'}) \exp(-\gamma_I t) \]
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
Stochastic Hamiltonian dynamics

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

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 \( \mu \)
- The measure \( \mu \) 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 $\mu$ 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

$$
\begin{aligned}
\frac{dQ_t^u}{dt} &= \partial_p H(Q^u_t, P^u_t)dt,
\frac{dP_t^u}{dt} &= -\partial_q H(Q^u_t, P^u_t)dt - F_1(H(P^u_t, Q^u_t))\partial_p H(Q^u_t, P^u_t)dt \\
&\quad + F_2(H(P^u_t, Q^u_t))u_t dt
\end{aligned}
$$

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

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

**Theorem (D.T., 2002)**

For any integer \( m \) there exist an integer \( s_m \) and positive numbers \( C_m, \gamma_m \) 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,

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

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

  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.
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
On the convergence to equilibrium by Malliavin calculus

A representation formula in the one-dimensional case:

\[
p(t, x) = \mathbb{E} \left[ \mathbb{1}_{X_t > x} \delta \left( \frac{D \cdot X_t}{\|D \cdot X_t\|^2} \right) \right]
\]

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 \( \|D \cdot X_t\|^2 = 1 - e^{-2t} \)
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 \( t \), \( \langle M \rangle_t = \frac{1}{2} (e^{2t} - 1) \approx \frac{e^{2t}}{2} \).

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

that is, up to an explicit remaining term,

\[
p(t, x) \approx \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}
\]
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

\[ \delta \left( \frac{\exp(\int_0^t b'(X_s) \, ds)}{\int_0^t \exp(2 \int_\gamma^t b'(X_s) \, ds) \, d\gamma} \right) \]

Trick: For adapted \((u_t)\) use

\[ \delta(F \, u_\cdot) = F \, \delta(u_\cdot) - \int_0^t D_\theta F \, u_\theta \, d\theta = F \int_0^t u_s \, dW_s - \int_0^t D_\theta F \, u_\theta \, d\theta \]
Set

\[ M_t := \int_0^t \exp \left( -2 \int_0^\theta b'(X_s) \, ds \right) \, dW_\theta \]

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

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

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

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

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 $C := (C^{ij})$. 

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

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

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

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

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 $C := (C^{ij})$. 

\[ \int_0^T (Y_s^{ij})^2 \, ds < \infty \quad \mathbb{P} - \text{a.s.} \]
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 $\nabla u$ is unknown (work in slow progress)
- Berry-Esseen theorem and Edgeworth expansions (see Fukasawa under heavy assumptions):

\[
P\left(\frac{1}{\sigma \sqrt{K}} \int_0^K (f(X_s) - \int f \, d\mu) \, ds > x\right) - P(G > x) = \frac{C}{\sqrt{K}} Q(x) \exp\left(-\frac{x^2}{2}\right) + o\left(\frac{1}{\sqrt{K}}\right)
\]
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
The parabolic parabolic 2D Keller-Segel model

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

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

Under explicit constraints on \((\rho_0, c_0)\) there exists a unique solution to the two-dimensional parabolic parabolic Keller-Segel PDE and to the McKean-Vlasov non-linear SDE

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

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 \((\rho, c)\) uniquely solves the K-S PDE, where

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

Remark: The corresponding particle system is NON MARKOV.
Solutions tend to self-similar solutions

A solution is self-similar iff it writes

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

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

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

Theorem (Corrias, Escobedo, Matos)

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

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