PDE methods for statistical physics

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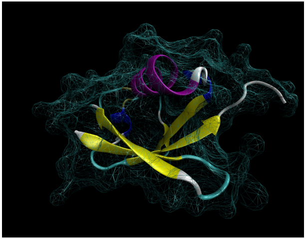
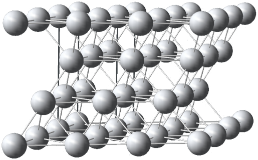
The Overdamped Langevin dynamics





N particles at positions $q_t = (q_1, \cdots, q_N) \in \mathcal{D}$

$$\mathrm{d}q_t = -\nabla V(q_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t$$

$\mathrm{d}W_t$: Brownian motion
$V(q)$: potential, for example $V(q) = \sum_{1\leq i<j\leq N} v(|q_i - q_j|)$
$\beta^{-1} = k_B T$ is fixed

Invariant measure

Maxwell-Boltzmann distribution:

$$\nu(\mathrm{d}q) = Z_\nu^{-1} \mathrm{e}^{-\beta V(q)} \mathrm{d}q \tag{1}$$

Unique invariant measure :

$$\forall \varphi, \ \mathbb{E}[\varphi(q_t) \mid q_0 \sim \nu] = \mathbb{E}_\nu[\varphi] = \int_{\mathcal{D}} \varphi(q) \, \mathrm{d}\nu(q) \tag{2}$$

Generator of the dynamics

Let φ and $q \in \mathcal{D}$, the generator $\mathcal{L}$ is defined by

$$\begin{aligned}(\mathcal{L}\varphi)(q) &:= \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\varphi(q_t) \mid q_0 = q] \\ &= \beta^{-1}\Delta\varphi(q) - \nabla V \cdot \nabla\varphi(q)\end{aligned} \tag{3}$$

using Itô calculus. Denoting

$$\langle \varphi, \psi \rangle = \int_{\mathcal{D}} \varphi \, \psi \, \mathrm{d}\nu \tag{4}$$

the scalar product on $\mathrm{L}^2(\nu)$ and $*$ the associated adjoint

$$\langle \varphi, \mathcal{L}\psi \rangle = \int_{\mathcal{D}} \varphi \, \mathcal{L}\psi \, \mathrm{d}\nu = \int_{\mathcal{D}} -\beta^{-1}\nabla\varphi \cdot \nabla\psi \, \mathrm{d}\nu. \tag{5}$$

We denote $\mathcal{L} = -\beta^{-1}\nabla^*\nabla$, it is self-adjoint in $\mathrm{L}^2(\nu)$.

Proof: Uniqueness of the invariant measure

Let us prove that ν is the **unique** invariant measure. Let f a density of probability such that

$$\begin{aligned}\forall\varphi, 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\varphi(q_t) \mid q_0 \sim f] = \int_{\mathcal{D}} \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\varphi(q_t) \mid q_0 = q]\ f(q)\mathrm{d}q \\ &= \int_{\mathcal{D}} \mathcal{L}\varphi(q)\ f(q)\mathrm{d}q = \left\langle \mathcal{L}\varphi, \frac{f}{\nu} \right\rangle\end{aligned} \tag{6}$$

then $0 = \mathcal{L}^*\left(\frac{f}{\nu}\right) = \mathcal{L}\left(\frac{f}{\nu}\right)$

ie. $0 = \left\langle \frac{f}{\nu}, \mathcal{L}\left(\frac{f}{\nu}\right)\right\rangle = -\beta^{-1}\left\|\nabla\left(\frac{f}{\nu}\right)\right\|^2$

so $f = \nu$ since they are normalized.

Convergence of empirical averages

Let $\widetilde{\varphi}_t = \frac{1}{t}\int_0^t \varphi(q_s)\,\mathrm{d}s$ the empirical mean of φ.
The dynamics can be shown to be ergodic

$$\widetilde{\varphi_t} \xrightarrow[t\to\infty]{} \mathbb{E}_\nu[\varphi] \text{ a.s.} \tag{7}$$

and Central Limit Theorem :

$$\sqrt{t}\,(\widetilde{\varphi_t} - \mathbb{E}_\nu[\varphi]) \xrightarrow[t\to\infty]{\mathcal{L}} \mathcal{N}\left(0, \sigma_\varphi^2\right) \tag{8}$$

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But what is σ_φ ?

Calculus: Asymptotic variance

Suppose $\mathbb{E}_\nu[\varphi] = 0$, then the asymptotical variance of φ is

$$\sigma_\varphi^2 = \lim_{t\to\infty} t\mathbb{E}[\widetilde{\varphi_t}^2]. \tag{9}$$

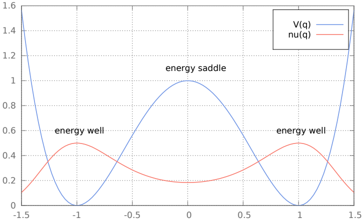
where

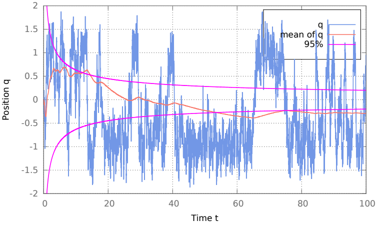
$$\begin{aligned} t\mathbb{E}[\widetilde{\varphi_t}^2] &= \frac{1}{t}\int_0^t \int_0^t \mathbb{E}[\varphi(q_s)\varphi(q_{s'})]\,\mathrm{d}s\mathrm{d}s' = 2\int_0^t \left(1 - \frac{s}{t}\right)\mathbb{E}[\varphi(q_0)\varphi(q_s)]\,\mathrm{d}s \\ &\xrightarrow[t\to\infty]{} 2\int_0^\infty \mathbb{E}[\varphi(q_0)\varphi(q_s)]\,\mathrm{d}s = 2\int_0^t \mathbb{E}[\varphi(q_0)\mathrm{e}^{s\mathcal{L}}\varphi(q_0)]\,\mathrm{d}s \\ &= 2\int_0^t \left\langle \varphi(q_0), \mathrm{e}^{s\mathcal{L}}\varphi(q_0)\right\rangle\,\mathrm{d}s \end{aligned}$$

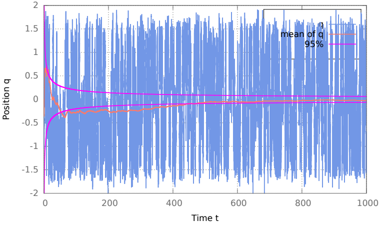
so

$$\sigma_\varphi^2 = -2\left\langle \varphi, \mathcal{L}^{-1}\varphi\right\rangle. \tag{10}$$

Application







Coercivity of the generator

Decompose the function space into an orthogonal direct sum

$$\mathrm{L}^2(\nu) = \mathrm{L}^2_0(\nu) \oplus \mathbb{R}\mathbf{1}, \quad \text{with } \mathrm{L}^2_0(\nu) = \left\{ \varphi \in \mathrm{L}^2(\nu) \mid \mathbb{E}_\nu[\varphi] = 0 \right\} \tag{11}$$

Reminder : $\mathcal{L}(\mathbf{1}) = 0$

Poincaré-Wirtinger for $\varphi \in \mathrm{L}^2_0(\nu)$:

$$-\langle \varphi, \mathcal{L}\varphi \rangle = \beta^{-1} \|\nabla \varphi\|^2 \geq \frac{1}{C\beta} \|\varphi\|^2 \tag{12}$$

$-\mathcal{L}$ is coercive so invertible on $\mathrm{L}^2_0(\nu)$. Therefore $\sigma^2_\varphi \leq C\beta \|\varphi\|^2$.

Exponential decay and inversibility

Take $\varphi_0 \in \mathrm{L}^2_0(\mu)$ and $\varphi(t) = \mathrm{e}^{t\mathcal{L}}\varphi_0$, and define $\mathscr{H}(t) = \frac{1}{2}\|\varphi(t)\|^2$

$$\mathscr{H}'(t) = \langle \mathcal{L}\varphi(t), \varphi(t) \rangle \leq -\frac{1}{C\beta}\|\varphi(t)\|^2 = -\frac{2}{C\beta}\mathscr{H}(t). \qquad (13)$$

By Gronwall

$$\mathscr{H}(t) \leq \mathrm{e}^{-2t/C\beta}\mathscr{H}(0) \quad \textit{ie.} \quad \|\mathrm{e}^{t\mathcal{L}}\|_{\mathcal{B}(\mathrm{L}^2_0(\mu))} \leq \mathrm{e}^{-t/C\beta}, \qquad (14)$$

so on $\mathrm{L}^2_0(\mu)$

$$\mathcal{L}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}} \quad \text{and} \quad \|\mathcal{L}^{-1}\|_{\mathcal{B}(\mathrm{L}^2_0(\mu))} \leq C\beta. \qquad (15)$$

The Langevin dynamics

$$N \text{ particles at } \begin{cases} \text{positions } q_t = (q_1, \cdots, q_N) \in \mathcal{D} \\ \text{momenta } p_t = (p_1, \cdots, p_N) \in \mathbb{R}^D \end{cases}$$

$$\begin{cases} \mathrm{d}q_t &= p_t \, \mathrm{d}t \\ \mathrm{d}p_t &= -\nabla V(q_t) \, \mathrm{d}t - \gamma p_t \, \mathrm{d}t + \sqrt{2\gamma\beta^{-1}} \, \mathrm{d}W_t \end{cases}$$

$\mathrm{d}W_t$: Brownian motion
$V(q)$: potential, for example $V(q) = \sum_{1 \leq i < j \leq N} v(|q_i - q_j|)$
$\beta^{-1} = k_B T$ is fixed
γ friction fixed

Invariant measure

Maxwell-Boltzmann distribution $\mu(\mathrm{d}q, \mathrm{d}p) = Z_\mu^{-1} \mathrm{e}^{-\beta H(q,p)} \mathrm{d}q$ is the unique invariant measure $\mu(\mathrm{d}q, \mathrm{d}p) = \nu(\mathrm{d}q)\ \kappa(\mathrm{d}p)$.

$$\text{Hamiltonian}: \ H(q,p) = V(q) + \frac{1}{2}|p|^2 \tag{16}$$

Limit $\gamma \to 0$: Hamiltonian system
Limit $\gamma \to \infty$ + time scaling : Overdamped

Generator of the dynamics

Let φ and $q \in \mathcal{D}$, the generator $\mathcal{L}$ is defined by

$$\begin{aligned}(\mathcal{L}\varphi)(q) &:= \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\varphi(q_t) \mid q_0 = q] \\ &= p\nabla_q - \nabla V^\top \nabla_p - \gamma\beta^{-1}\nabla_p^*\nabla_p \\ &= \mathcal{L}_{\mathrm{ham}} + \gamma\mathcal{L}_{\mathrm{FD}}\end{aligned} \tag{17}$$

using Itô calculus.

- Antisymetric transport part $\mathcal{L}_{\mathrm{ham}}^* = -\mathcal{L}_{\mathrm{ham}}$
- Symmetric fluctuation-dissipation part ${\mathcal{L}_{\mathrm{FD}}}^* = \mathcal{L}_{\mathrm{FD}}$

Kernel of the generator

Let φ such that $\mathcal{L}\varphi = 0$. Then

$$0 = \langle \varphi, \mathcal{L}\varphi \rangle = \langle \varphi, \mathcal{L}_{\mathrm{FD}}\varphi \rangle = -\beta^{-1}\|\nabla_p \varphi\|^2 \Rightarrow \varphi = \varphi(q) \qquad (18)$$

so $0 = \mathcal{L}\varphi = p^\top \nabla_q \varphi \Rightarrow \varphi \in \mathbb{R}\mathbf{1}$.
Therefore $\mathrm{Ker}(\mathcal{L}) = \mathrm{Ker}(\mathcal{L}^*) = \mathbb{R}\mathbf{1}$.

But not coercive

$$\langle \varphi, -\mathcal{L}\varphi \rangle = \beta^{-1}\|\nabla_p \varphi\|^2 \not\gtrsim \|\varphi\|^2 \qquad (19)$$

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$$\langle \varphi, -\mathcal{L}\varphi \rangle = \beta^{-1} \|\nabla_p \varphi\|^2 \not\gtrsim \|\varphi\|^2 \tag{19}$$

So is it invertible ?

Hypocoercivity

It suffices to show

$$\forall \varphi \in \mathrm{L}_0^2(\mu),\ \forall t \geq 0,\ \|\mathrm{e}^{t\mathcal{L}}\varphi\| \leq C\mathrm{e}^{-\alpha t}\|\varphi\| \tag{20}$$

to have on $\mathrm{L}_0^2(\mu)$

$$\mathcal{L}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t, \quad \text{and} \quad \|\mathcal{L}^{-1}\| \leq \frac{C}{\alpha}. \tag{21}$$

Proof: Hypocoercivity

- Define $\mathcal{H}[\varphi] = \frac{1}{2}\|\varphi\|^2 - \varepsilon \langle \varphi, A\varphi \rangle$ where

$$\begin{cases} A = (1 + (\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p))^{-1} (\mathcal{L}_{\mathrm{ham}}\Pi_p)^* \\ \Pi_p\varphi = \int_{\mathbb{R}^D} \varphi(q,p)\mathrm{d}\kappa(p) \end{cases} \tag{22}$$

- *Check* $\| \cdot \|^2 \sim \mathcal{H}[\,\cdot\,]$
- Prove $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[\mathrm{e}^{t\mathcal{L}}\varphi] \leq \alpha' \|\varphi\|^2 \leq \frac{2\alpha'}{1+\varepsilon}\mathcal{H}[\varphi]$
- Conclude using the Gronwall lemma and the norm equivalence

One more detail

$\mathscr{H}'(t) = -D[\varphi(t)]$ where

$$D[\varphi] = \langle -\gamma \mathcal{L}_{\mathrm{FD}} \varphi, \varphi \rangle + \varepsilon \langle A \mathcal{L}_{\mathrm{ham}} \Pi_p \varphi, \varphi \rangle + \varepsilon \langle A \mathcal{L}_{\mathrm{ham}} (1 - \Pi_p) \varphi, \varphi \rangle + \varepsilon \langle \mathcal{L}_{\mathrm{ham}} A \varphi, \varphi \rangle + \varepsilon \langle A \gamma \mathcal{L}_{\mathrm{FD}} \varphi, \varphi \rangle \qquad (23)$$

- $\langle -\gamma \mathcal{L}_{\mathrm{FD}} \varphi, \varphi \rangle \geq C_\kappa \|(1 - \Pi_p)\varphi\|^2$
- $\langle A \mathcal{L}_{\mathrm{ham}} \Pi_p \varphi, \varphi \rangle = \left\langle (1 + B^* B)^{-1} B^* B \varphi, \varphi \right\rangle \geq \frac{1}{2} \|B\varphi\|^2 \geq C_\nu \|\Pi_p \varphi\|^2$
- Other terms small enough

Galerkin method

Can we solve the Poisson problem

$$-\mathcal{L}\varphi = R \tag{24}$$

using a Galerkin method in $V_M \in \mathrm{L}^2_0(\mu)$?

$$\begin{aligned} &\text{Find } \varphi_M \in V_M \text{ such that} \\ &\forall \psi_M \in V_M, \langle \mathcal{L}\varphi_M, \psi_M \rangle = \langle R, \psi_M \rangle \end{aligned} \tag{25}$$

We need first to prove that $\Pi_M \mathcal{L} \Pi_M$ invertible on V_M.

Discrete hypocoercivity

Take $\varphi = \mathrm{e}^{t\Pi_M \mathcal{L} \Pi_M} \varphi_0$ and compute for $\varphi \in V_M$

$$\begin{aligned} D_M[\varphi] &= \langle \mathcal{L}\varphi, \varphi \rangle + \varepsilon \langle A \Pi_M \mathcal{L}\varphi, \varphi \rangle + \varepsilon \langle \Pi_M \mathcal{L}\varphi, A\varphi \rangle \\ &= D[\varphi] + \varepsilon \langle A(1-\Pi_M)\mathcal{L}\varphi, \varphi \rangle + \varepsilon \langle A^*(1-\Pi_M)\mathcal{L}\varphi, \varphi \rangle \\ &\geq (\alpha - \varepsilon \delta_M) \|\varphi\|^2 \end{aligned} \tag{26}$$

with $\delta_M \xrightarrow[M \to \infty]{} 0$.