The computation of averages from equilibrium and nonequilibrium Langevin dynamics

Gabriel STOLTZ

stoltz@cermics.enpc.fr

(CERMICS, Ecole des Ponts & MICMAC team, INRIA Rocquencourt)

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Outline

Some elements of statistical physics

- Microscopic description of physical systems
- Macroscopic description: average properties

Practical computation of average properties

- Ergodic averages using Langevin dynamics
- Discretization of Langevin dynamics

Error estimates on the computation of average properties

- A priori estimates
- How to correct for the systematic bias

Extensions

- The overdamped limit
- Error estimates on transport coefficients (nonequilibrium dynamics)

B. Leimkuhler, Ch. Matthews and G. Stoltz, The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics, *arXiv preprint* **1308.5814** (2013)

Some elements of statistical physics

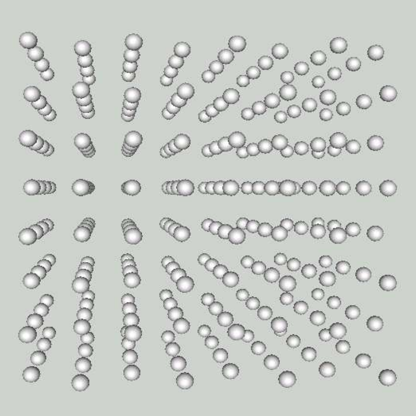
General perspective (1)

- Aims of computational statistical physics:
  - numerical microscope
  - computation of average properties, static or dynamic

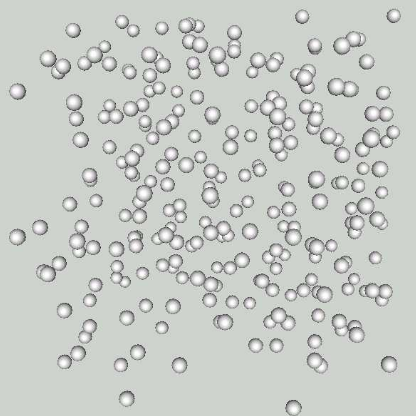
- Orders of magnitude
  - distances $\sim 1\ \mathring{A} = 10^{-10}$ m
  - energy per particle $\sim k_{\rm B}T \sim 4 \times 10^{-21}$ J at room temperature
  - atomic masses $\sim 10^{-26}$ kg
  - time $\sim 10^{-15}$ s
  - number of particles $\sim \mathcal{N}_A = 6.02 \times 10^{23}$

- "Standard" simulations
  - 10^6 particles ["world records": around 10^9 particles]
  - integration time: (fraction of) ns ["world records": (fraction of) μs]

What is the melting temperature of argon?



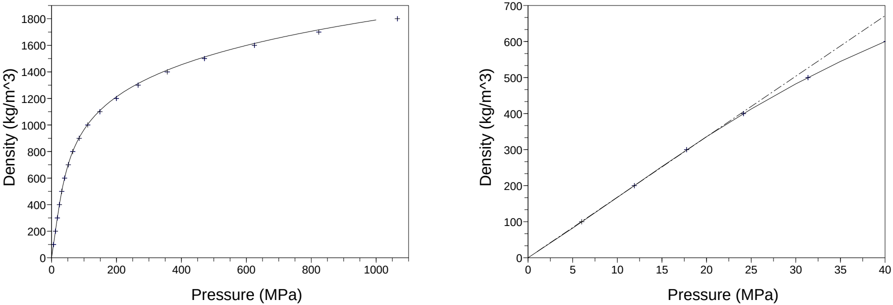
(a) Solid argon (low temperature)



(b) Liquid argon (high temperature)

General perspective (3)

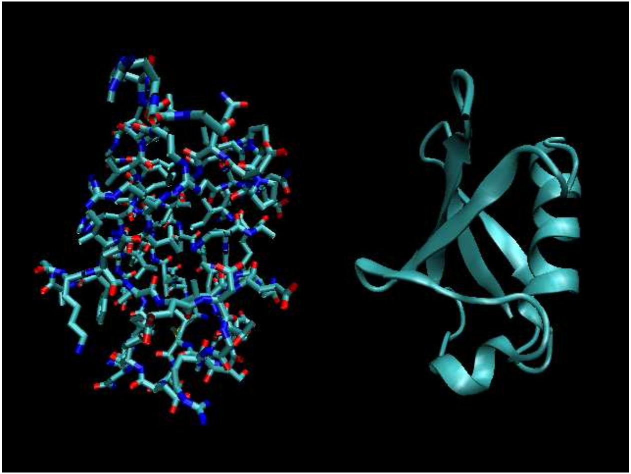
"Given the structure and the laws of interaction of the particles, what are the macroscopic properties of the matter composed of these particles?"



Equation of state (pressure/density diagram) for argon at $T = 300$ K

General perspective (4)

What is the structure of the protein? What are its typical conformations, and what are the transition pathways from one conformation to another?



Microscopic description of physical systems: unknowns

• Microstate of a classical system of N particles:

$$(q,p) = (q_1,\dots,q_N,\ p_1,\dots,p_N) \in \mathcal{E}$$

Positions q (configuration), momenta p (to be thought of as $M\dot{q}$)

• Here, periodic boundary conditions: $\mathcal{E} = \mathcal{D} \times \mathbb{R}^{3N}$ with $\mathcal{M} = (L\mathbb{T})^{3N}$

• More complicated situations can be considered: molecular constraints defining submanifolds of the phase space

• Hamiltonian $H(q,p) = E_{\mathrm{kin}}(p) + V(q)$, where the kinetic energy is

$$E_{\mathrm{kin}}(p) = \frac{1}{2}\, p^T M^{-1} p, \qquad M = \begin{pmatrix} m_1\,\mathrm{Id}_3 & & 0 \\ & \ddots & \\ 0 & & m_N\,\mathrm{Id}_3 \end{pmatrix}.$$

Microscopic description: interaction laws

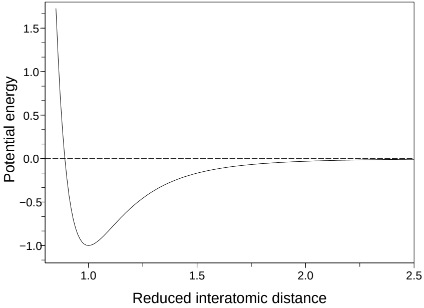
- All the physics is contained in V
  - ideally derived from quantum mechanical computations
  - in practice, empirical potentials for large scale calculations

- An example: Lennard-Jones pair interactions to describe noble gases

$$V(q_1,\ldots,q_N) = \sum_{1\leqslant i<j\leqslant N} v(|q_j-q_i|)$$

$$v(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$\text{Argon:}\quad \begin{cases} \sigma = 3.405\times 10^{-10}\ \text{m} \\ \varepsilon/k_{\rm B} = 119.8\ \ \text{K} \end{cases}$$



Average properties

- Macrostate of the system described by a probability measure

Equilibrium thermodynamic properties (pressure,...)

$$\langle A \rangle_\mu = \mathbb{E}_\mu(A) = \int_{\mathcal{E}} A(q,p)\, \mu(dq\, dp)$$

- Examples of observables:
  - Pressure $A(q,p) = \dfrac{1}{3|\mathcal{D}|} \displaystyle\sum_{i=1}^N \left(\frac{p_i^2}{m_i} - q_i \cdot \nabla_{q_i} V(q) \right)$
  - Kinetic temperature $A(q,p) = \dfrac{1}{3Nk_\mathrm{B}} \displaystyle\sum_{i=1}^N \frac{p_i^2}{m_i}$
- Canonical ensemble = measure on (q,p) (average energy fixed)

$$\mu_{\mathrm{NVT}}(dq\, dp) = Z_{\mathrm{NVT}}^{-1}\, \mathrm{e}^{-\beta H(q,p)}\, dq\, dp, \qquad \beta = \frac{1}{k_\mathrm{B} T}$$

Practical computation of average properties

Computing average properties

Main issue

Computation of high-dimensional integrals... Ergodic averages

$$\langle A \rangle_\mu = \lim_{t \to +\infty} \frac{1}{t} \int_0^t A(q_s, p_s)\, ds$$

- One possible choice: Langevin dynamics with friction parameter $\gamma > 0$

$=$ Stochastic perturbation of the Hamiltonian dynamics

$$\begin{cases} dq_t = M^{-1} p_t \, dt \\ dp_t = -\nabla V(q_t)\, dt - \gamma M^{-1} p_t \, dt + \sqrt{\dfrac{2\gamma}{\beta}}\, dW_t \end{cases}$$

- Denote by $\psi(t, q, p)$ the law of (q_t, p_t)

Convergence of the Langevin dynamics

- Irreducibility + smoothness of the transition probabilities (hypoellipticity)
- Invariance of the canonical measure
  - Evolution of the law: $\dfrac{d}{dt}\mathbb{E}\Big(f(q_t,p_t)\Big) = \mathbb{E}\Big(\mathcal{L}f(q_t,p_t)\Big)$, *i.e.*

$$\int_{\mathcal{E}} f\partial_t\psi = \int \mathcal{L}f\,\psi \qquad \text{or} \qquad \partial_t\psi = \mathcal{L}^\dagger\psi$$

  - Generator $\mathcal{L} = \mathcal{L}_{\rm ham} + \mathcal{L}_{\rm thm}$ with

$$\mathcal{L}_{\rm ham} = \frac{p}{m}\cdot\nabla_q - \nabla V(q)\cdot\nabla_p, \qquad \mathcal{L}_{\rm thm} = \gamma\left(-\frac{p}{m}\cdot\nabla_p + \frac{1}{\beta}\Delta_p\right)$$

  - A simple computation shows that $\mathcal{L}^\dagger\left(\mathrm{e}^{-\beta H}\right) = 0$
- Convergence rates: functional estimates on Banach spaces

$$\left\|\mathrm{e}^{t\mathcal{L}}h\right\| \leqslant C\mathrm{e}^{-\lambda t}\|f\|$$

Hypocoercivity: $H^1(\mu)$, Lyapunov: $\|f\|_{L^\infty_W} = \sup \dfrac{|f(q,p)|}{W(q,p)}$ with $W \geqslant 1$

Practical computation of average properties

- Numerical scheme = Markov chain characterized by evolution operator

$$P_{\Delta t}\psi(q,p) = \mathbb{E}\Big(\psi\left(q^{n+1},p^{n+1}\right)\Big|(q^n,p^n)=(q,p)\Big)$$

- Discretization of the Langevin dynamics: splitting strategy

$$A = M^{-1}p\cdot\nabla_q, \qquad B = -\nabla V(q)\cdot\nabla_p, \qquad C = -M^{-1}p\cdot\nabla_p + \frac{1}{\beta}\Delta_p$$

- First order splitting schemes: $P_{\Delta t}^{ZYX} = \mathrm{e}^{\Delta t Z}\mathrm{e}^{\Delta t Y}\mathrm{e}^{\Delta t X} \simeq \mathrm{e}^{\Delta t \mathcal{L}}$
- Example: $P_{\Delta t}^{B,A,\gamma C}$ corresponds to (with $\alpha_{\Delta t} = \exp(-\gamma M^{-1}\Delta t)$)

$$\begin{cases} \widetilde{p}^{n+1} = p^n - \Delta t\,\nabla V(q^n), \\ q^{n+1} = q^n + \Delta t\, M^{-1}\widetilde{p}^{n+1}, \\ p^{n+1} = \alpha_{\Delta t}\widetilde{p}^{n+1} + \sqrt{\dfrac{1-\alpha_{\Delta t}^2}{\beta}M}\, G^n, \end{cases} \tag{1}$$

where G^n are i.i.d. standard Gaussian random variables

Practical computation of average properties (2)

- Second order splitting $P_{\Delta t}^{ZYXYZ} = \mathrm{e}^{\Delta t Z/2}\mathrm{e}^{\Delta t Y/2}\mathrm{e}^{\Delta t X}\mathrm{e}^{\Delta t Y/2}\mathrm{e}^{\Delta t Z/2}$
- Example: $P_{\Delta t}^{\gamma C,B,A,B,\gamma C}$ (Verlet in the middle)

$$\begin{cases} \widetilde{p}^{n+1/2} = \alpha_{\Delta t/2} p^n + \sqrt{\dfrac{1-\alpha_{\Delta t}}{\beta} M}\, G^n, \\ p^{n+1/2} = \widetilde{p}^{n+1/2} - \dfrac{\Delta t}{2}\,\nabla V(q^n), \\ q^{n+1} = q^n + \Delta t\, M^{-1} p^{n+1/2}, \\ \widetilde{p}^{n+1} = p^{n+1/2} - \dfrac{\Delta t}{2}\,\nabla V(q^{n+1}), \\ p^{n+1} = \alpha_{\Delta t/2} \widetilde{p}^{n+1} + \sqrt{\dfrac{1-\alpha_{\Delta t}}{\beta} M}\, G^{n+1/2}, \end{cases}$$

- Other category: Geometric Langevin algorithms, *e.g.* $P_{\Delta t}^{\gamma C,A,B,A}$

Error estimates on the computation of average properties

Error estimates on the computation of average properties

- The ergodicity of numerical schemes can be proved ($\mathcal{M}$ bounded):

$$\frac{1}{N_{\rm iter}} \sum_{n=1}^{N_{\rm iter}} A(q^n,p^n) \xrightarrow[N_{\rm iter}\to+\infty]{} \int A(q,p)\, d\mu_{\gamma,\Delta t}(q,p)$$

- Statistical errors *vs.* systematic errors (bias)

Systematic error estimates: α order of the splitting scheme

$$\int_{\mathcal{E}} \psi(q,p)\, \mu_{\gamma,\Delta t}(dq\,dp) = \int_{\mathcal{E}} \psi(q,p)\, \mu(dq\,dp) + \Delta t^\alpha \int_{\mathcal{E}} \psi(q,p) f_{\alpha,\gamma}(q,p)\, \mu(dq\,dp) + \mathrm{O}(\Delta t^{\alpha+1})$$

- Correction function $f_{\alpha,\gamma}$ solution of an appropriate Poisson equation

$$\mathcal{L}^* f_{\alpha,\gamma} = g_\gamma$$

where g_γ depends on the numerical scheme (adjoints taken on $L^2(\mu)$)

Proof for the first-order scheme $P_{\Delta t}^{\gamma C,B,A}$ (1)

- By definition of the invariant measure, $\displaystyle\int_{\mathcal{E}} P_{\Delta t}\varphi \, d\mu_{\gamma,\Delta t} = \int_{\mathcal{E}} \varphi \, d\mu_{\gamma,\Delta t}$, so

$$\int_{\mathcal{E}} \left[\left(\frac{\mathrm{Id} - P_{\Delta t}}{\Delta t} \right) \varphi \right] d\mu_{\gamma,\Delta t} = 0$$

- In view of the BCH formula $\mathrm{e}^{\Delta t A_3}\mathrm{e}^{\Delta t A_2}\mathrm{e}^{\Delta t A_1} = \mathrm{e}^{\Delta t \mathcal{A}}$ with

$$\mathcal{A} = A_1 + A_2 + A_3 + \frac{\Delta t}{2}\Big([A_3, A_1 + A_2] + [A_2, A_1] \Big) + \dots,$$

it holds $P_{\Delta t}^{\gamma C,B,A} = \mathrm{Id} + \Delta t \mathcal{L} + \dfrac{\Delta t^2}{2} \left(\mathcal{L}^2 + S_1 \right) + \Delta t^3 R_{1,\Delta t}$ with

$$S_1 = [C, A + B] + [B, A], \qquad R_{1,\Delta t} = \frac{1}{2} \int_0^1 (1-\theta)^2 \mathcal{R}_{\theta \Delta t} \, d\theta,$$

Proof for the first-order scheme $P_{\Delta t}^{\gamma C,B,A}$ (2)

- The correction function $f_{1,\gamma}$ is chosen so that

$$\int_{\mathcal{E}} \left[\left(\frac{\mathrm{Id} - P_{\Delta t}^{\gamma C,B,A}}{\Delta t} \right) \varphi \right] (1 + \Delta t f_{1,\gamma})\, d\mu = \mathrm{O}(\Delta t^2)$$

This requirement can be rewritten as

$$\int_{\mathcal{E}} \left(\frac{1}{2} S_1 \varphi + (\mathcal{L}\varphi) f_{1,\gamma} \right) d\mu = \int_{\mathcal{E}} \varphi \left[\frac{1}{2} S_1^* \mathbf{1} + \mathcal{L}^* f_{1,\gamma} \right] d\mu,$$

which suggests to choose $\mathcal{L}^* f_{1,\gamma} = -\dfrac{1}{2} S_1^* \mathbf{1}$ (well posed equation)

- Replace φ by $\left(\dfrac{\mathrm{Id} - P_{\Delta t}^{\gamma C,B,A}}{\Delta t} \right)^{-1} \psi$? No control on the derivatives...

- Use the "nice" properties of the continuous dynamics, *i.e.* functional estimates[1] on $\mathcal{L}^{-1}$

[1] D. Talay, Stoch. Proc. Appl. (2002); M. Kopec, arxiv 1310.2599 (2013)

Proof for the first-order scheme $P_{\Delta t}^{\gamma C,B,A}$ (3)

- Introduce pseudo-inverse $Q_{1,\Delta t} = -\mathcal{L}^{-1} + \frac{\Delta t}{2}(\mathrm{Id} + \mathcal{L}^{-1} S_1 \mathcal{L}^{-1})$ with

$$\left(\frac{\mathrm{Id} - P_{\Delta t}^{\gamma C,B,A}}{\Delta t} \right) Q_{1,\Delta t} = \mathrm{Id} + \Delta t^2 Z_{1,\Delta t}$$

and replace φ by $Q_{1,\Delta t}\psi$

- Properties of one scheme carry over to other schemes

TU lemma

Consider two ergodic numerical schemes with associated evolution operators

$$P_{\Delta t} = U_{\Delta t} T_{\Delta t}, \qquad Q_{\Delta t} = T_{\Delta t} U_{\Delta t}$$

Then, for all bounded measurable functions φ,

$$\int_{\mathcal{E}} \varphi \, d\mu_{Q,\Delta t} = \int_{\mathcal{E}} (U_{\Delta t}\varphi) \, d\mu_{P,\Delta t}$$

Estimating the correction

- Standard procedure: Romberg extrapolation from the a priori estimate

$$\int_{\mathcal{E}} \psi(q,p)\, \mu_{\gamma,\Delta t}(dq\, dp) \simeq \int_{\mathcal{E}} \psi(q,p)\, \mu(dq\, dp) + C\Delta t^{\alpha}$$

- Estimate the leading order correction term $\displaystyle\int_{\mathcal{E}} \psi(q,p) f_{\alpha,\gamma}(q,p)\, \mu(dq\, dp)$?
- Use the operator identity (valid on $H^1(\mu)\backslash \mathrm{Ker}(\mathcal{L})$ for instance)

$$\mathcal{L}^{-1} = -\int_0^{+\infty} \mathrm{e}^{t\mathcal{L}}\, dt$$

to rewrite the correction as an integrated correlation function

$$\int_{\mathcal{E}} \psi(q,p) f_{\alpha,\gamma}(q,p)\, \mu(dq\, dp) = -\int_0^{+\infty} \mathbb{E}\Big(\psi(q_t,p_t) g_{\gamma}(q_0,p_0)\Big) dt$$

Estimating the correction (2)

Assume $\frac{P_{\Delta t} - \mathrm{Id}}{\Delta t} = \mathcal{L} + \Delta t S_1 + \cdots + \Delta t^{\alpha-1} S_{\alpha-1} + \Delta t^{\alpha} \widetilde{R}_{\alpha,\Delta t}$ and

$$\left\| \left(\frac{\mathrm{Id} - P_{\Delta t}}{\Delta t} \right)^{-1} \right\|_{\mathcal{B}(L^\infty_W)} \leqslant C, \qquad \int_{\mathcal{E}} \psi \, d\mu_{\Delta t} = \int_{\mathcal{E}} \psi \, d\mu + \Delta t^{\alpha} r_{\psi,\Delta t}$$

Error estimates on the Green-Kubo formula

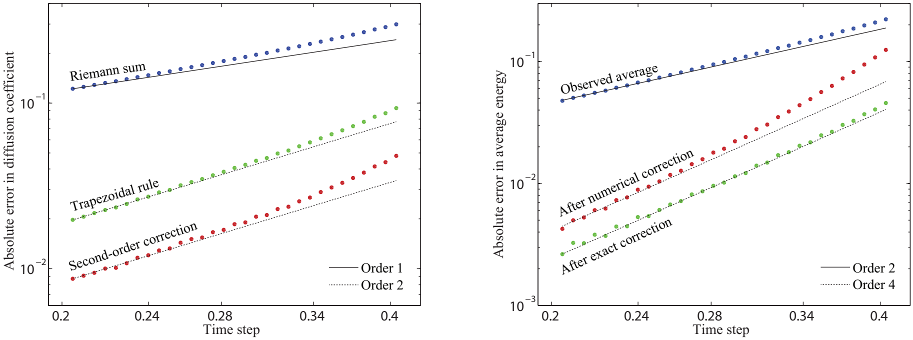
For ψ, φ with average 0 w.r.t. μ,

$$\int_0^{+\infty} \mathbb{E}\Big(\psi(q_t,p_t)\varphi(q_0,p_0)\Big)dt = \Delta t \sum_{n=0}^{+\infty} \mathbb{E}_{\Delta t}\Big(\widetilde{\psi}_{\Delta t}\left(q^n,p^n\right)\varphi\left(q^0,p^0\right)\Big) + \mathrm{O}(\Delta t^{\alpha})$$

with $\widetilde{\psi}_{\Delta t} = \Big(\mathrm{Id} + \Delta t \, S_1 \mathcal{A}^{-1} + \cdots + \Delta t^{\alpha-1} S_{\alpha-1} \mathcal{A}^{-1}\Big)\psi - \mu_{\Delta t}(\dots)$

- Reduces to trapezoidal rule for second order schemes

Numerical results



Potential $V(x,y) = 2\cos(2x) + \cos(y)$, scheme $P_{\Delta t}^{\gamma C,B,A,B,\gamma C}$ with $\beta = \gamma = 1$.

Left: Error on the integrated velocity auto-correlation.
Right: Error on the average energy.

Some extensions

The overdamped limit (1)

• Limit $\gamma \to +\infty$ with $M = \mathrm{Id}$: solution $(q_{\gamma,\gamma s}, p_{\gamma,\gamma s})_{s \geqslant 0}$ pathwise converges (finite times) to solution of overdamped Langevin dynamics

$$dQ_t = -\nabla V(Q_t)\, dt + \sqrt{\frac{2}{\beta}}\, dW_t$$

with generator $\mathcal{L}_{\mathrm{ovd}} = -\nabla V(q) \cdot \nabla_q + \frac{1}{\beta} \Delta_q$

Uniform hypocoercivity estimates

There exists a constant $K > 0$ such that, for any $\gamma \geqslant 1$,

$$\left\| \mathcal{L}_\gamma^{-1} - \gamma \mathcal{L}_{\mathrm{ovd}}^{-1} \pi - p^T \nabla_q \mathcal{L}_{\mathrm{ovd}}^{-1} \pi + \mathcal{L}_{\mathrm{ovd}}^{-1} \pi (A+B) C^{-1} (\mathrm{Id} - \pi) \right\|_{\mathcal{B}(\mathcal{H}^1)} \leqslant \frac{K}{\gamma}$$

where $\mathcal{H}^1 = \left\{ f \in H^1(\mu) \, \middle| \, \int_{\mathcal{E}} f \, d\mu = 0 \right\}$.

The overdamped limit (2)

• Invariant measure $\overline{\mu}(dq) \propto \mathrm{e}^{-\beta V(q)}\,dq$ for the continuous dynamics

• Overdamped limit well defined only for certain second order splitting schemes (A and B not intertwinned with C)

Error estimates in the overdamped limit

$$\int_{\mathcal{M}} \psi(q)\,\overline{\mu}_{\gamma,\Delta t}(dq) = \int_{\mathcal{M}} \psi\,d\overline{\mu} + \Delta t^2 \int_{\mathcal{M}} \psi\,f_{2,\infty}\,d\overline{\mu} + r_{\psi,\gamma,\Delta t},$$

with remainder of order Δt^4 up to terms exponentially small in $\gamma\Delta t$:

$$|r_{\psi,\gamma,\Delta t}| \leqslant a\Delta t^4 + b\,\mathrm{e}^{-\kappa\gamma\Delta t}$$

• Consistency of the limit for the correction terms: $f_{2,\gamma} \xrightarrow[\gamma\to+\infty]{H^1(\mu)} f_{2,\infty}$

$$\lim_{\Delta t\to 0}\lim_{\gamma\to+\infty} \frac{1}{\Delta t^2}\left(\int_{\mathcal{M}} \psi\,d\overline{\mu}_{\gamma,\Delta t} - \int_{\mathcal{M}} \psi\,d\overline{\mu}\right) = \lim_{\gamma\to+\infty}\lim_{\Delta t\to 0} \dots$$

Sketch of proof for $P_{\Delta t}^{\gamma C,A,B,A\gamma C}$

- Reduction to a limiting operator up to exponentially small terms

$$\left\| \mathrm{e}^{\gamma t C} - \pi \right\|_{\mathcal{B}(L^\infty_W)} \leqslant K \mathrm{e}^{-\alpha \gamma t}, \qquad W(q,p) = 1 + |p|^2$$

- Error estimates for the limiting operator $P_{\infty,\Delta t} = \pi P_{\mathrm{ham},\Delta t} \pi$:

$$P_{\infty,\Delta t} = \pi + h \mathcal{L}_{\mathrm{ovd}} + \frac{h^2}{2} \left(\mathcal{L}_{\mathrm{ovd}}^2 + D \right) \pi + h^3 R_{\infty,\Delta t}, \qquad h = \frac{\Delta t^2}{2}$$

corresponding to the limiting numerical scheme

$$\begin{cases} q^{n+1/2} = q^n + \dfrac{\Delta t}{2} \sqrt{\dfrac{1}{\beta}} G^n \\ p^{n+1} = \sqrt{\dfrac{1}{\beta}} G^n - \Delta t \nabla V \left(q^{n+1/2} \right) \\ q^{n+1} = q^{n+1/2} + \dfrac{\Delta t}{2} p^{n+1} \end{cases}$$

Transport coefficients: definition

- Nonequilibrium Langevin dynamics, non-gradient force $F \in \mathbb{R}^{3N}$

$\rightarrow$ Invariant measure $\mu_{\gamma,\eta}(dq\,dp)$

$$\left\{\begin{aligned} dq_t &= M^{-1}p_t\,dt \\ dp_t &= \Big(-\nabla V(q_t) + \eta F\Big)dt - \gamma M^{-1}p_t\,dt + \sqrt{\frac{2\gamma}{\beta}}\,dW_t \end{aligned}\right.$$

- Transport coefficient: mobility

$$\nu_{F,\gamma} = \lim_{\eta\to 0}\frac{1}{\eta}\int_{\mathcal{E}} F^T M^{-1} p\,\mu_{\gamma,\eta}(dq\,dp) = \int_{\mathcal{E}} F^T M^{-1} p\, f_{0,1,\gamma}(q,p)\,\mu(dq\,dp)$$

where the correction function satisfies $\mathcal{L}^* f_{0,1,\gamma} = -\beta F^T M^{-1} p$

- Splitting schemes obtained by replacing B with $B_\eta = B + \eta F \cdot \nabla_p$

$\rightarrow$ invariant measures $\mu_{\gamma,\eta,\Delta t}$

Error estimates on the mobility

Error estimates for nonequilibrium dynamics

There exists a function $f_{\alpha,1,\gamma} \in H^1(\mu)$ such that

$$\int_{\mathcal{E}} \psi \, d\mu_{\gamma,\eta,\Delta t} = \int_{\mathcal{E}} \psi \Big(1 + \eta f_{0,1,\gamma} + \Delta t^\alpha f_{\alpha,0,\gamma} + \eta \Delta t^\alpha f_{\alpha,1,\gamma} \Big) d\mu + r_{\psi,\gamma,\eta,\Delta t},$$

where the remainder is compatible with linear response

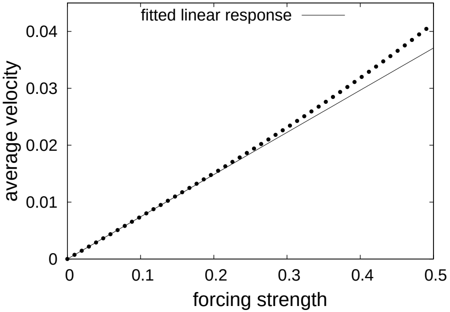
$$|r_{\psi,\gamma,\eta,\Delta t}| \leqslant K(\eta^2 + \Delta t^{\alpha+1}), \qquad |r_{\psi,\gamma,\eta,\Delta t} - r_{\psi,\gamma,0,\Delta t}| \leqslant K\eta(\eta + \Delta t^{\alpha+1})$$

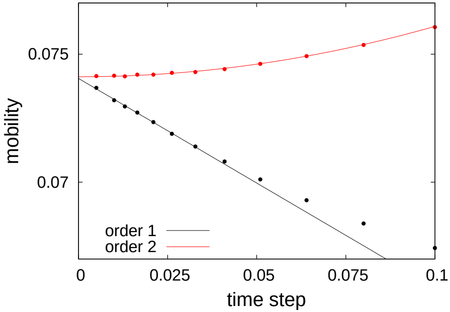
- Corollary: error estimates on the numerically computed mobility

$$\begin{aligned} \nu_{F,\gamma,\Delta t} &= \lim_{\eta \to 0} \frac{1}{\eta} \left(\int_{\mathcal{E}} F^T M^{-1} p \, \mu_{\gamma,\eta,\Delta t}(dq\,dp) - \int_{\mathcal{E}} F^T M^{-1} p \, \mu_{\gamma,0,\Delta t}(dq\,dp) \right) \\ &= \nu_{F,\gamma} + \Delta t^\alpha \int_{\mathcal{E}} F^T M^{-1} p \, f_{\alpha,1,\gamma} \, d\mu + \Delta t^{\alpha+1} r_{\gamma,\Delta t} \end{aligned}$$

- Results in the overdamped limit

Numerical results





Left: Linear response of the average velocity as a function of η for the scheme associated with $P_{\Delta t}^{\gamma C,B_\eta,A,B_\eta,\gamma C}$ and $\Delta t = 0.01, \gamma = 1$.

Right: Scaling of the mobility $\nu_{F,\gamma,\Delta t}$ for the first order scheme $P_{\Delta t}^{A,B_\eta,\gamma C}$ and the second order scheme $P_{\Delta t}^{\gamma C,B_\eta,A,B_\eta,\gamma C}$.

In conclusion...

The full content of this work

• Standard but systematic error estimates à la Talay-Tubaro for splitting schemes of the equilibrium Langevin dynamics, spectral approach

• Alternative way to estimate the correction, on-the-fly, for a single simulation (using some integrated correlation)

• Overdamped limit fully treated (uniform hypocoercivity estimates), Hamiltonian limit only partially

• Error estimates on blue transport coefficients, computed either

- through a Green-Kubo formula (general)
- or with the linear response of an appropriate nonequilibrium dynamics (demonstrated on a specific case)

• Any result for splitting schemes on unbounded position spaces? Need for an appropriate Lyapunov function...

B. Leimkuhler, Ch. Matthews and G. Stoltz, The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics, *arXiv preprint* **1308.5814** (2013)