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# Numerical methods for the linear response of nonequilibrium stochastic dynamics

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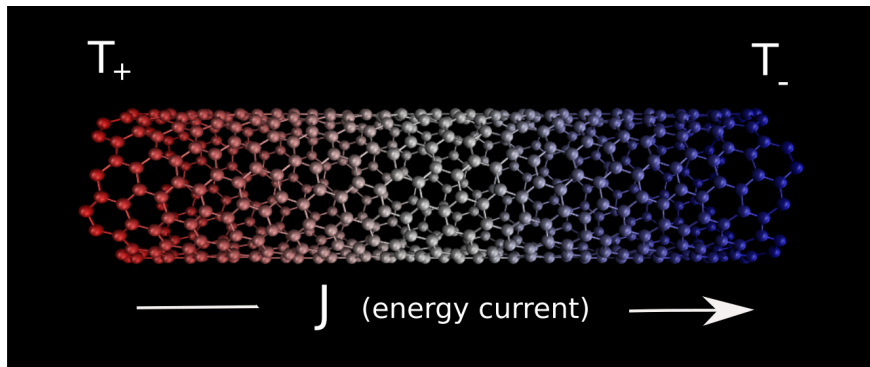
- **Linear response for steady-state nonequilibrium dynamics**
  - Equilibrium dynamics and their perturbations
  - Definition of transport coefficients
- **Error estimates (variance, bias)**
  - Nonequilibrium molecular dynamics (NEMD)
  - Green–Kubo formulas
- **Perspectives**
  - Variance reduction strategies
  - Alternative numerical approaches

# Linear response for steady-state nonequilibrium dynamics

# Physical context and motivations

**Transport coefficients** (e.g. thermal conductivity): **quantitative** estimates

$$J = -\kappa \nabla T \quad (\text{Fourier's law})$$



Slow convergence due to **large noise to signal ratio**

**Long computational times** to estimate  $\kappa$  (up to several weeks/months)

# Reference equilibrium dynamics

Positions  $q \in \mathcal{D}$  and momenta  $p \in \mathbb{R}^d$ , phase-space  $\mathcal{E} = \mathcal{D} \times \mathbb{R}^d$

**Hamiltonian**  $H(q, p) = V(q) + \frac{1}{2}p^T M^{-1}p$

**Langevin dynamics** (for given  $\gamma > 0$ )

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

Generator  $\mathcal{L} = \mathcal{L}_{\text{ham}} + \gamma\mathcal{L}_{\text{FD}}$  with

$$\mathcal{L}_{\text{ham}} = p^T M^{-1} \nabla_q - \nabla V^T \nabla_p, \quad \mathcal{L}_{\text{FD}} = -p^T M^{-1} \nabla_p + \frac{1}{\beta} \Delta_p$$

Unique invariant measure  $\mu(dq dp) = Z^{-1} e^{-\beta H(q,p)} dq dp = \nu(dq) \kappa(dp)$

# Ergodicity results for Langevin dynamics (1)

Almost-sure convergence<sup>1</sup> of **ergodic averages**  $\widehat{\varphi}_t = \frac{1}{t} \int_0^t \varphi(q_s, p_s) ds$

**Asymptotic variance** of ergodic averages (with  $\Pi_0\varphi = \varphi - \mathbb{E}_\mu(\varphi)$ )

$$\sigma_\varphi^2 = \lim_{t \rightarrow +\infty} t \text{Var} [\widehat{\varphi}_t^2] = 2 \int_{\mathcal{E}} (-\mathcal{L}^{-1} \Pi_0 \varphi) \Pi_0 \varphi d\mu$$

**Central limit theorem**<sup>2</sup> when Poisson equation can be solved in  $L^2(\mu)$

$$-\mathcal{L}\Phi = \Pi_0\varphi$$

Well-posedness for  $\mathcal{L}$  invertible on subsets of  $L_0^2(\mu) = \Pi_0 L^2(\mu)$

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

<sup>1</sup>Kliemann, *Ann. Probab.* **15**(2), 690-707 (1987)

<sup>2</sup>Bhattacharya, *Z. Wahrsch. Verw. Gebiete* **60**, 185-201 (1982)

## Ergodicity results for Langevin dynamics (2)

Prove **exponential convergence** of the semigroup  $e^{t\mathcal{L}}$  on  $E \subset L_0^2(\mu)$

- **Lyapunov** techniques<sup>3</sup>  $L_W^\infty(\mathcal{E}) = \left\{ \varphi \text{ measurable, } \sup \left| \frac{\varphi}{W} \right| < +\infty \right\}$
- standard **hypocoercive**<sup>4</sup> setup  $H^1(\mu)$
- $E = L^2(\mu)$  after hypoelliptic regularization<sup>5</sup> from  $H^1(\mu)$
- Direct transfer from  $H^1(\mu)$  to  $E = L^2(\mu)$  by spectral argument<sup>6</sup>
- Directly<sup>7</sup>  $E = L^2(\mu)$  (recently<sup>8</sup> Poincaré using  $\partial_t - \mathcal{L}_{\text{ham}}$ )
- **coupling** arguments<sup>9</sup>
- Direct estimates on the resolvent using Schur complements<sup>10</sup>

Rate of convergence  $\min(\gamma, \gamma^{-1})$  in all cases

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<sup>3</sup>Wu ('01); Mattingly/Stuart/Higham ('02); Rey-Bellet ('06); Hairer/Mattingly ('11)

<sup>4</sup>Villani (2009) and before Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004),...

<sup>5</sup>F. Hérau, *J. Funct. Anal.* (2007)

<sup>6</sup>G. Deligiannidis, D. Paulin and A. Doucet, *Ann. Appl. Probab.* (2020)

<sup>7</sup>Hérau (2006), Dolbeaut/Mouhot/Schmeiser (2009, 2015)

<sup>8</sup>Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)

<sup>9</sup>A. Eberle, A. Guillin and R. Zimmer, *Ann. Probab.* (2019)

<sup>10</sup>E. Bernard, M. Fathi, A. Levitt, G. Stoltz, *Annales Henri Lebesgue* (2022)

# Definition of transport coefficients (1)

Linear response of **nonequilibrium dynamics**

**Example:**  $\mathcal{D} = (L\mathbb{T})^d$ , **non-gradient** force  $F \in \mathbb{R}^{3N}$

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

Existence and uniqueness of invariant measure (Lyapunov techniques)

Generator  $\mathcal{L} + \eta \tilde{\mathcal{L}}$ , **invariant measure**  $f_\eta \mu$  with  $(\mathcal{L}^* + \eta \tilde{\mathcal{L}}^*) f_\eta = 0$

$$f_\eta = 1 + \eta f_1 + \eta^2 f_2 + \dots, \quad -\mathcal{L}^* f_1 = \tilde{\mathcal{L}}^* \mathbf{1} = \Pi_0 \tilde{\mathcal{L}}^* \mathbf{1}.$$

where adjoints are taken on  $L^2(\mu)$  and  $\Pi_0 \varphi = \varphi - \int_{\mathcal{E}} \varphi d\mu$



## Definition of transport coefficients (2)

**Response property**  $R \in L^2_0(\mu) = \Pi_0 L^2_0(\mu)$ , conjugated response  $S = \tilde{\mathcal{L}}^* \mathbf{1}$ :

$$\begin{aligned}\alpha &= \lim_{\eta \rightarrow 0} \frac{\mathbb{E}_\eta(R)}{\eta} = \int_{\mathcal{E}} R \mathfrak{f}_1 d\mu = \int_{\mathcal{E}} R \left[ (-\mathcal{L}^*)^{-1} S \right] d\mu = \int_{\mathcal{E}} (-\mathcal{L}^{-1} R) S d\mu \\ &= \int_0^{+\infty} \mathbb{E}_0 \left( R(q_t, p_t) S(q_0, p_0) \right) dt\end{aligned}$$

**In practice:**

- Identify the **response** function
- Construct a physically meaningful **perturbation** (bulk or boundary driven)
- Obtain the transport coefficient  $\alpha$  (thermal cond., shear viscosity,...)

For the previous example, definition of **mobility** with  $R(q, p) = F^T M^{-1} p$

$$\lim_{\eta \rightarrow 0} \frac{\mathbb{E}_\eta (F^T M^{-1} p)}{\eta} = \beta F^T D F, \quad D = \int_0^{+\infty} \mathbb{E}_0 \left( (M^{-1} p_t) \otimes (M^{-1} p_0) \right) dt$$

# Error estimates for NEMD

# Principle of nonequilibrium molecular dynamics

**Example:**  $\mathcal{D} = (L\mathbb{T})^d$ , non-gradient force  $F \in \mathbb{R}^{3N}$

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

Estimator of linear response (observable  $R$  with equilibrium average 0)

$$\widehat{A}_{\eta,t} = \frac{1}{\eta t} \int_0^t R(q_s^\eta, p_s^\eta) ds \xrightarrow[t \rightarrow +\infty]{\text{a.s.}} \alpha_\eta := \frac{1}{\eta} \int_{\mathcal{E}} R f_\eta d\mu = \alpha + O(\eta)$$

## Issues with linear response methods:

- Statistical error with **asymptotic variance**  $O(\eta^{-2})$
- Bias  $O(\eta)$  due to  $\eta \neq 0$
- Bias from finite integration time
- **Timestep discretization bias**

# Analysis of variance / finite integration time bias

- **Statistical error** dictated by **Central Limit Theorem**:

$$\sqrt{t} \left( \widehat{A}_{\eta,t} - \alpha_{\eta} \right) \xrightarrow[t \rightarrow +\infty]{\text{law}} \mathcal{N} \left( 0, \frac{\sigma_{R,\eta}^2}{\eta^2} \right), \quad \sigma_{R,\eta}^2 = \sigma_{R,0}^2 + O(\eta)$$

so  $\widehat{A}_{\eta,t} = \alpha + O\left(\frac{1}{\eta\sqrt{t}}\right) \rightarrow$  requires **long simulation times**  $t \sim \eta^{-2}$

- **Finite time integration bias**:  $\left| \mathbb{E} \left( \widehat{A}_{\eta,t} \right) - \alpha_{\eta} \right| \leq \frac{K}{\eta t}$

Bias due to  $t < +\infty$  is  $O\left(\frac{1}{\eta t}\right) \rightarrow$  typically **smaller than statistical error**

- Key equality for the proofs: introduce  $-\left(\mathcal{L} + \eta\tilde{\mathcal{L}}\right) \mathcal{R}_{\eta} = R - \int_{\mathcal{E}} R f_{\eta} d\mu$

$$\widehat{A}_{\eta,t} - \frac{1}{\eta} \int_{\mathcal{E}} R f_{\eta} d\mu = \frac{\mathcal{R}_{\eta}(q_0^{\eta}, p_0^{\eta}) - \mathcal{R}_{\eta}(q_t^{\eta}, p_t^{\eta})}{\eta t} + \frac{\sqrt{2\gamma}}{\eta t \sqrt{\beta}} \int_0^t \nabla \mathcal{R}_{\eta}(q_s^{\eta}, p_s^{\eta})^T dW_s$$

# Analysis of the timestep discretization bias (1)

- **Numerical scheme:** **Markov chain** characterized by evolution operator

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

- Discretization of the Langevin dynamics: **splitting** strategy

$$A = M^{-1}p \cdot \nabla_q, \quad B_\eta = (-\nabla V(q) + \eta F) \cdot \nabla_p, \quad C = -M^{-1}p \cdot \nabla_p + \beta^{-1} \Delta_p$$

First and second order splittings, determined by order of operators

- **Example:**  $P_{\Delta t}^{B_\eta, A, \gamma C}$  corresponds to (with  $\alpha_{\Delta t} = \exp(-\gamma M^{-1} \Delta t)$ )

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

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

## Analysis of the timestep discretization bias (2)

Invariant measure  $\mu_{\gamma,\eta,\Delta t}$  of the numerical scheme;  $a \geq$  weak order

$$\int_{\mathcal{E}} R d\mu_{\gamma,\eta,\Delta t} = \int_{\mathcal{E}} R \left( 1 + \eta f_{0,1,\gamma} + \Delta t^a f_{a,0,\gamma} + \eta \Delta t^a f_{a,1,\gamma} \right) d\mu + r_{\varphi,\gamma,\eta,\Delta t},$$

where the remainder is compatible with linear response

$$|r_{\varphi,\gamma,\eta,\Delta t}| \leq K(\eta^2 + \Delta t^{a+1}), \quad |r_{\varphi,\gamma,\eta,\Delta t} - r_{\varphi,\gamma,0,\Delta t}| \leq K\eta(\eta + \Delta t^{a+1})$$

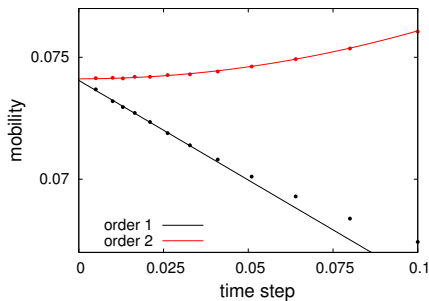
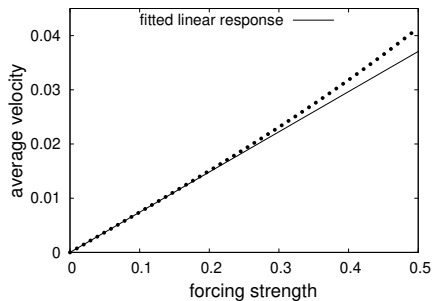
**Corollary:** error estimates on the **numerically computed mobility**

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

Results in the **overdamped** limit  $\gamma \rightarrow +\infty$

B. Leimkuhler, Ch. Matthews and G. Stoltz, The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics, *IMA J. Numer. Anal.* **36**(1), 13-79 (2016)

# Numerical results



**Left:** Linear response of the average velocity as a function of  $\eta$  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  $P_{\Delta t}^{\gamma C, B_\eta, A, B_\eta, \gamma C}$ .

# Error estimates for Green–Kubo formulas



# Error estimates on the Green-Kubo formula (1)

- Aim: approximate  $\alpha = \int_0^{+\infty} \mathbb{E}_0 \left( R(q_t, p_t) S(q_0, p_0) \right) dt$
- **Issues with Green-Kubo formula:**
  - Truncature of time (exponential convergence of  $e^{t\mathcal{L}}$ )
  - The **statistical error** for correlations increases a lot with time lag<sup>11</sup>
  - **Timestep bias and quadrature formula**

Possible benefits from...

- Fourier approaches and time series analysis<sup>12</sup>
- importance sampling on trajectory space<sup>13</sup>

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<sup>11</sup>de Sousa Oliveira/Greaney, *Phys. Rev. E* **95** (2017)

<sup>12</sup>Ercole/Marcolongo/Baroni, *Sci. Rep.* **7** (2017)

<sup>13</sup>Donati/Hartmann/Keller, *J. Chem. Phys.* **146** (2017)

# Truncation of time and statistical error

“Natural” estimator  $\hat{A}_{K,T} = \frac{1}{K} \sum_{k=1}^K \int_0^T R(q_t^k, p_t^k) S(q_0^k, p_0^k) dt$

- **Truncation bias:** **small** due to generic exponential decay of correlations

$$\left| \mathbb{E} \left( \hat{A}_{K,T} \right) - \alpha \right| \leq C e^{-\kappa T}$$

- **Statistical error:** **large**, increases with the integration time

$$\forall T \geq 1, \quad \text{Var} \left( \hat{A}_{K,T} \right) \leq C \frac{T}{K}$$

Proof based on the following equality, with  $-\mathcal{L}\mathcal{R} = R$ :

$$\int_0^T R(q_t, p_t) dt = \mathcal{R}(q_0, p_0) - \mathcal{R}(q_T, p_T) + \sqrt{\frac{2\gamma}{\beta}} \int_0^T \nabla \mathcal{R}(q_t, p_t) \cdot dW_t$$

# Timestep bias for Green–Kubo formulas

Generic stochastic dynamics satisfying certain technical conditions:

- **uniform-in- $\Delta t$  convergence** (relies on  $P_{\Delta t}^{\lceil T/\Delta t \rceil}(X_0, dX) \geq a m(dX)$ )
- error on the invariant measure of order  $\Delta t^a$
- $P_{\Delta t} = \text{Id} + \Delta t \mathcal{L} + \Delta t^2 S_1 + \dots + \Delta t^a S_{a-1} + \dots$

## Riemann–like formula

For  $R, S$  with average 0 w.r.t.  $\mu$ ,

$$\int_0^{+\infty} \mathbb{E} \left( R(X_t) S(X_0) \right) dt = \Delta t \sum_{n=0}^{+\infty} \mathbb{E}_{\Delta t} \left( \tilde{R}_{\Delta t}(X^n) S(X^0) \right) + O(\Delta t^a)$$

with  $\tilde{R}_{\Delta t} = \left( \text{Id} + \Delta t S_1 \mathcal{L}^{-1} + \dots + \Delta t^{a-1} S_{a-1} \mathcal{L}^{-1} \right) R - \mu_{\Delta t}(\dots)$

Reduces to **trapezoidal** rule for **second** order schemes

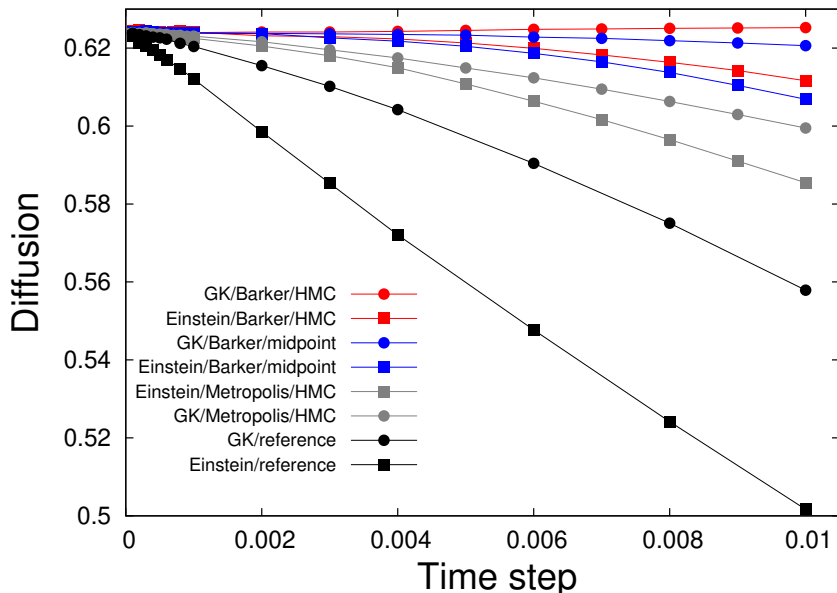
Side result: statistical error for numerical schemes  $\approx$  continuous process

B. Leimkuhler, Ch. Matthews and G. Stoltz, *IMA J. Numer. Anal.* **36**(1), 13-79 (2016)

T. Lelièvre and G. Stoltz, *Acta Numerica* **25** (2016)

A. Durmus, A. Enfroy, E. Moulines, G. Stoltz, *arXiv preprint* **2107.14542**

# 1D overdamped Langevin, $R = S = V'$ , cosine potential



# Variance reduction techniques and alternative dynamics

# Variance reduction for NEMD and Einstein methods

- **Control variate approach:** reduce variance by subtracting a quantity with known average, correlated (in a good way) with the target quantity
- Some instances of control variate techniques for transport coefficients<sup>14</sup>
- In the NEMD context, consider

$$\frac{\mathbb{E}_\eta(R)}{\eta} = \frac{\mathbb{E}_\eta(R - \mathcal{L}_\eta \Phi)}{\eta} \quad \text{with} \quad \text{Var}_\eta(R - \mathcal{L}_\eta \Phi) \ll \text{Var}_\eta(R)$$

Zero variance control variate  $\Phi_\eta = \mathcal{L}_\eta^{-1}(R - \mu_\eta(R))$

More practical choice<sup>15</sup>  $-\mathcal{L}_0 \Phi = R$  for some approximate operator  $\mathcal{L}_0$

Variance of order  $\eta^2$  when  $\mathcal{L}_0 = \mathcal{L} \rightarrow$  relative error  $O(1)$

- Extension to time-dependent quantities (Einstein formula)<sup>16</sup>

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<sup>14</sup>Ciccotti/Jacucci (1975); Mangaud/Rotenberg (2020); ...

<sup>15</sup>Roussel/Stoltz, *SIAM MMS* (2019)

<sup>16</sup>G. Pavliotis, G. Stoltz, U. Vaes (2022)

# Sensitivity estimator: motivation

**General non-degenerate stochastic dynamics** on  $\mathcal{D} = \mathbb{T}^d$

- **Reference dynamics**  $dX_t^0 = b(X_t^0) dt + \sigma(X_t^0) dW_t$
- **Perturbed dynamics**  $dX_t^\eta = (b(X_t^\eta) + \eta F(X_t^\eta)) dt + \sigma(X_t^\eta) dW_t$
- Assume  $\sigma\sigma^T$  positive definite  $\rightarrow$  unique invariant measure  $\nu_\eta$

**Estimator of the linear response**

$$\alpha = \lim_{\eta \rightarrow 0} \frac{\nu_\eta(R) - \nu_0(R)}{\eta} = \lim_{t \rightarrow \infty} \mathbb{E}_0 \left\{ \left( \frac{1}{t} \int_0^t (R(X_s^0) - \nu_0(R)) ds \right) Z_t \right\}$$

with  $Z_t = \int_0^t U(X_s^0) \cdot dW_s$  and  $\sigma U = F$

Motivation: Girsanov theorem, linearization, and longtime limit (formal)

$$\mathbb{E}_\eta \left[ \frac{1}{t} \int_0^t R(X_s^\eta) ds \right] = \mathbb{E}_0 \left[ \left( \frac{1}{t} \int_0^t R(X_s^0) ds \right) \exp \left( \eta \int_0^t U(X_s^0)^T dW_s - \frac{\eta^2}{2} \int_0^t |U(X_s^0)|^2 ds \right) \right]$$

# Sensitivity estimator: proof

**Proof of consistency:** Generator  $\mathcal{L} + \eta\tilde{\mathcal{L}}$ , Poisson equation  $-\mathcal{L}\hat{R} = \Pi_0 R$  (well posed)

Rewrite the time integral as a martingale, up to remainder terms

$$\int_0^t \Pi_0 R(X_s^0) ds = M_t + \hat{R}(X_0^0) - \hat{R}(X_t^0), \quad M_t = \int_0^t \nabla \hat{R}(X_s)^T \sigma(X_s^0) dW_s$$

and use Itô isometry to write  $\frac{1}{t} \mathbb{E}(M_t Z_t)$  as

$$\frac{1}{t} \int_0^t \mathbb{E} \left( U(X_s^0)^T \sigma(X_s^0)^T \nabla \hat{R}(X_s^0) \right) ds \xrightarrow[t \rightarrow +\infty]{} \int_{\mathcal{D}} F^T \nabla \hat{R} d\nu_0 = \alpha$$

**Variance uniformly bounded in time:** by similar manipulations,

$$\forall t > 0, \quad \text{Var} \left\{ \left( \frac{1}{t} \int_0^t (R(X_s^0) - \nu_0(R)) ds \right) Z_t \right\} \leq C$$



# Sensitivity estimator: discretization

## Discrete sensitivity estimator (slightly idealized)

$$\mathcal{M}_{\Delta t, N_{\text{iter}}}^{[1]}(R) = \frac{1}{N_{\text{iter}}} \sum_{n=0}^{N_{\text{iter}}-1} (R(X^n) - \mathbb{E}_{\Delta t}(R)) Z^{N_{\text{iter}}}$$

$$\text{with } Z^{N_{\text{iter}}} = \sum_{n=0}^{N_{\text{iter}}-1} (\sigma(X^n)^{-1} F(X^n))^T G^n$$

$$\left| \mathbb{E}_{\Delta t} \left\{ \mathcal{M}_{\Delta t, N_{\text{iter}}}^{[1]}(R) \right\} - \alpha \right| \leq C \left( \Delta t + \frac{1}{\sqrt{N_{\text{iter}} \Delta t}} \right)$$
$$\text{Var}_{\Delta t} \left\{ \mathcal{M}_{\Delta t, N_{\text{iter}}}^{[1]}(R) \right\} \leq C_1 + C_2 \left( \Delta t + \frac{1}{N_{\text{iter}} \Delta t} \right)$$

Finite-time bias  $O(\text{time}^{-1/2})$  ( $\text{time}^{-1}$  for standard time averages)

Extension to Langevin dynamics; **not yet used in actual MD simulations**

P. Plechac, G. Stoltz and T. Wang, *M2AN* **55** (2021)

P. Plechac, G. Stoltz, T. Wang, *arXiv preprint* **2112.00126**

# Extensions and future work

# Study of alternative approaches: several year workplan!

- **Alternative approaches**, possibly with some **blending**
  - Rely on tangent dynamics<sup>17</sup>
  - Resort to efficient **coupling methods** such as sticky coupling<sup>18</sup>
  - Optimize **synthetic forcings**<sup>19</sup>
  - Large deviation techniques to estimate second order cumulants<sup>20</sup>
  - Consider using transient dynamics
  - ... other options too prospective to be mentioned...
- For all methods...
  - **quantify variance and bias** (related to  $\Delta t, \eta, \dots$ )
  - Application to model systems (atom chains, LJ fluid)

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<sup>17</sup> Assaraf/Jourdain/Lelièvre/Roux, *Stoch. Partial Differ. Equ. Anal. Comput.* (2018)

<sup>18</sup> Eberle/Zimmer (2019); Durmus/Eberle/Enfroy/Guillin/Monmarché (2021)

<sup>19</sup> Evans/Morriss (2008); work in progress with Renato Spacek

<sup>20</sup> Limmer/Gao/Poggioli, *Eur. Phys. J. B* (2021)