Sticky Coupling as a Control Variate for Computing Transport Coefficients

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Project funded by ANR SINEQ

(Non)equilibrium Molecular Dynamics: Algorithms, Analysis, and Applications

Outline

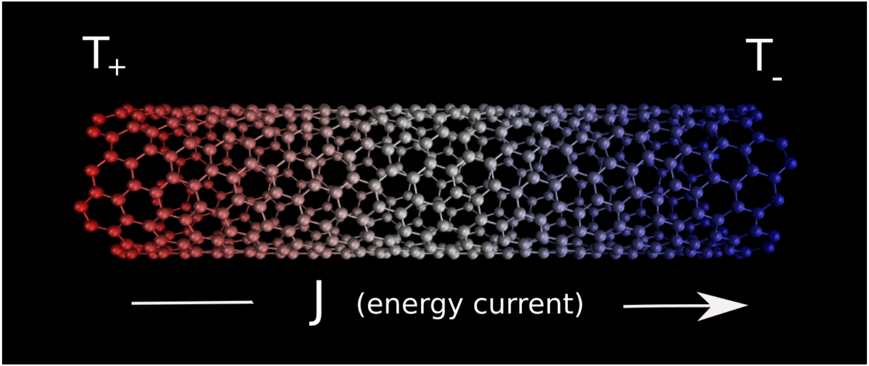
- **Linear response for steady-state nonequilibrium dynamics**
  - Equilibrium dynamics and their perturbations
  - Definition of transport coefficients
  - Variance & bias of NEMD estimator
- **Couplings based estimators**
  - Couplings based estimators
  - Synchronous coupling
  - Sticky coupling
- **Numerical Illustrations**
- **Extensions and perspectives**

Linear response for steady-state nonequilibrium dynamics

Physical context and motivations

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

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



Slow convergence due to large noise to signal ratio

Long computational times to estimate κ (up to several weeks/months)

Nonequilibrium stochastic dynamics

Consider the following family of SDEs with values in $\mathbb{R}^d$ and additive noise:

$$dX_t^\eta = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

where $b, F : \mathbb{R}^d \to \mathbb{R}^d$ are smooth and $\eta \in \mathbb{R}$. The above dynamics has generator

$$\mathcal{L}_\eta = \mathcal{L} + \eta\tilde{\mathcal{L}}, \quad \widetilde{\mathcal{L}} = F \cdot \nabla, \quad \mathcal{L} = b \cdot \nabla + \frac{1}{\beta}\Delta,$$

and we assume that for each η the above dynamics admits a unique invariant measure ν_η. We further assume that the drift is *contractive at infinity*, i.e.

Assumption

There exists $M \geqslant 0$ and $m > 0$ such that

$$\langle x - y, b(x) - b(y) \rangle \leqslant -m\left|x - y\right|^2, \qquad \text{if } |x - y| \geqslant M.$$

Technical Assumptions

We need the following technical assumption to ensure that our arguments based on the solutions to the Poisson equation are justified. Let $\mathscr{S}$ be the space of smooth function who grow at most polynomially along with their derivatives. Denoting by $\partial^k = \partial_{x_1}^{k_1} \cdots \partial_{x_d}^{k_d}$ for $k = (k_1, \ldots, k_d) \in \mathbb{N}^d$ and $\mathcal{K}_n(x) = 1 + |x|^n$,

$$\mathscr{S} := \left\{ \varphi \in C^\infty(\mathbb{R}^d) \,\middle|\, \forall k \in \mathbb{N}^d \, \exists C > 0, \exists n \in \mathbb{N} \, \text{s.t.} \, \left| \partial^k \varphi \right| \leqslant C \mathcal{K}_n \right\}$$

Assumption

Assume that $b, F \in \mathscr{S}$ and for any $\eta_* > 0$ there exists $\lambda_{\eta_*} > 0$ such that

$$\nabla \left(b(x) + \eta F(x) \right) \cdot (h, h) \leqslant \lambda_{\eta_*} \left| h \right|^2, \qquad \forall \eta \in \left[-\eta_*, \eta_* \right], \forall x, h \in \mathbb{R}^d$$

The two assumption are satisfied if $b(x) = -V_1(x) - V_2(x)$, where V_1 is a strongly convex confining potential and V_2 is a compactly supported potential modeling the local interactions.

Definition of transport coefficients

Perturbative regime: invariant measure $\nu_\eta = f_\eta \nu_0$ with $f_\eta = 1 + \mathrm{O}(\eta)$

$$\forall \varphi, \qquad 0 = \int_{\mathbb{R}^d} \left[\left(\mathcal{L} + \eta \widetilde{\mathcal{L}} \right) \varphi \right] f_\eta \, d\nu_0 = \int_{\mathbb{R}^d} \varphi \left[\left(\mathcal{L} + \eta \widetilde{\mathcal{L}} \right)^* f_\eta \right] d\nu_0$$

* = adjoints on $L^2(\nu_0)$

Fokker–Planck equation

$$\left(\mathcal{L} + \eta \widetilde{\mathcal{L}} \right)^* f_\eta = 0$$

By identifying powers of η (and denoting by $\Pi_0 \varphi := \varphi - \nu_0(\varphi)$)

$$f_\eta = 1 + \eta \mathfrak{f}_1 + \eta^2 \mathfrak{f}_2 + \dots, \qquad \mathfrak{f}_1 = \left(-\mathcal{L}^* \right)^{-1} \widetilde{\mathcal{L}}^* \mathbf{1}$$

Response property $R \in L_0^2(\nu_0) = \Pi_0 L^2(\nu_0)$, the transport coefficient α_R satisfies:

$$\alpha_R = \lim_{\eta \to 0} \frac{\mathbb{E}_\eta(R)}{\eta} = \int_{\mathbb{R}^d} R \mathfrak{f}_1 \, d\nu_0$$

Error estimates for NEMD

Principle of nonequilibrium molecular dynamics

Estimator of linear response (observable R average 0 with respect to ν_0)

$$\widehat{\Phi}_{\eta,t} = \frac{1}{\eta t}\int_0^t R(X_t^\eta)\,ds \xrightarrow[t\to+\infty]{\text{a.s.}} \alpha_{R,\eta} := \frac{1}{\eta}\int_{\mathbb{R}^d} R\,d\nu_\eta = \alpha_R + \mathrm{O}(\eta)$$

Issues with linear response methods:

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

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Analysis of variance / finite integration time bias

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

$$\sqrt{t}\left(\widehat{\Phi}_{\eta,t} - \alpha_\eta\right) \xrightarrow[t\to+\infty]{\text{law}} \mathcal{N}\left(0, \frac{\sigma^2_{R,\eta}}{\eta^2}\right), \qquad \sigma^2_{R,\eta} = \sigma^2_{R,0} + \mathrm{O}(\eta)$$

so $\widehat{\Phi}_{\eta,t} = \alpha_\eta + \mathrm{O}_{\mathrm{P}}\left(\frac{1}{\eta\sqrt{t}}\right)$ → requires long simulation times $t \sim \eta^{-2}$

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

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

- Key equality for the proofs: introduce $-\mathcal{L}_\eta \widehat{R}_\eta = R - \int_{\mathbb{R}^d} R\, d\nu_\eta$

$$\widehat{\Phi}_{\eta,t} - \frac{1}{\eta}\int_{\mathbb{R}^d} R\, d\nu_\eta = \frac{\widehat{R}_\eta(X_0^\eta) - \widehat{R}_\eta(X_t^\eta)}{\eta t} + \frac{\sqrt{2}}{\eta t\sqrt{\beta}} \int_0^t \nabla \widehat{R}_\eta(X_s^\eta)\cdot dW_s$$

Couplings Based Estimators

Couplings Based Estimator

Definition

A coupling of two random variables X and Y is a couple $\left(\widetilde{X}, \widetilde{Y}\right)$ of random variables such that $\widetilde{X} \overset{\text{Law}}{=} X$ and $\widetilde{Y} \overset{\text{Law}}{=} Y$

Idea: Use the reference dynamics to reduce the variance and bias of the estimator:

$$\widehat{\Psi}_{\eta,t} = \frac{1}{\eta t} \int_0^t \left[R\left(X_s^\eta\right) - R\left(Y_s^0\right) \right] ds, \tag{1}$$

with $(X_t^\eta, Y_t^\eta)_{t \geqslant 0}$ the solution of

$$dX_t^\eta = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

$$dY_t^0 = b\left(Y_t^0\right) dt + \sqrt{\frac{2}{\beta}} d\widetilde{W}_t,$$

where the driving noises $\left(W_t, \widetilde{W}_t\right)_{t \geqslant 0}$ are cleverly coupled.

Synchronous Coupling

By choosing $W = \widetilde{W}$, we can *synchronously* couple the X^η and Y^0, giving

$$d\left(X_t^\eta - Y_t^0\right) = \left(b\left(X_t^\eta\right) - b\left(Y_t^0\right) + \eta F\left(X_t^\eta\right)\right) dt.$$

If the drift is strongly contractive everywhere, i.e.

$$\langle x - y, b(x) - b(y) \rangle \leqslant -m \left| x - y \right|^2, \quad \forall x, y \in \mathbb{R}^d, \tag{2}$$

then we have pointwise control over the distance between the coupled trajectories:

$$\left| X_t^\eta - Y_t^0 \right| \leqslant \left(\left| X_0^\eta - Y_0^0 \right| - \frac{\eta \left\| F \right\|_\infty}{2m} \right) \mathrm{e}^{-mt} + \frac{\eta \left\| F \right\|}{2m}.$$

As a consequence,

$$\mathbb{E}\left[\left| \widehat{\Psi}_{\eta,t}^{\mathrm{sync}} \right|^p \right] \leqslant C \left(\frac{\left| X_0^\eta - Y_0^0 \right|^p}{\eta^p} \mathrm{e}^{-pmt} + \left(1 - e^{-p\lambda t}\right)^p \left(\frac{\eta \left\| F \right\|}{2m} \right)^p \right),$$

and a fortiori bounded variance and bias as $\eta \downarrow 0$ if $\left| X_0^\eta - Y_0^0 \right|^p = O\left(\eta^p\right)$.

Synchronous Coupling

In fact long as we have sufficient contractivity, say due to sufficiently high temperature[1] or in the underdamped case[2], we can control the moments of the estimator as

$$\mathbb{E}\left[\left|\widehat{\Psi}^{\mathrm{sync}}_{\eta,t}\right|^p\right] \leqslant C\left(\frac{\left|X_0^\eta - Y_0^0\right|^p}{\eta^p}\mathrm{e}^{-pmt} + \left(1 - e^{-p\lambda t}\right)^p\left(\frac{\eta\,\|F\|}{2m}\right)^p\right),$$

Moral: When there is enough strong contractivity, synchronous coupling is hard to beat.

What to do when we do not have enough strong contractivity?

[1] P. Monmarché (2022) *Wasserstein contraction and Poincaré inequalities for elliptic diffusions at high temperature*

[2] P. Monmarché (2023) *Almost sure contraction for diffusions on $\mathbb{R}^d$. Applications to generalized Langevin diffusions.*

Sticky Coupling

One can constructed a coupling[3] such that $\left(X_t^\eta - Y_t^0\right)_{t\geqslant 0}$ is *sticky at 0* in the sense that they the difference is controlled by a one-dimensional process $(r_t^\eta)_{t\geqslant 0}$ that spends a positive amount of time at 0

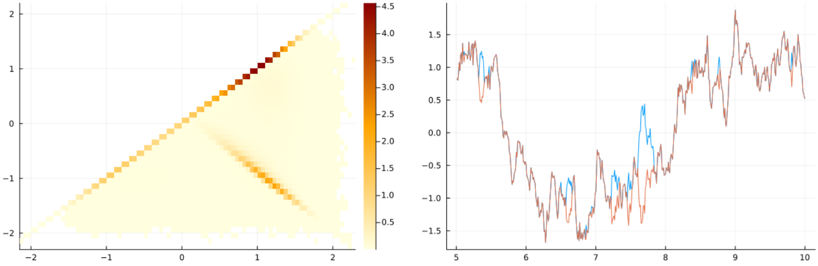


Figure: Sticky coupling of a 1D particle in a double well potential perturbed by a constant force to the right. **Left:** histogram of coupled process; **Right:** segment of trajectory of coupled process

[3] A. Eberle, R. Zimmer (2019) *Sticky couplings of multidimensional diffusions with different drifts*

Difficulties with Continuous-Time Sticky Coupling

- Non-explicit construction—constructed as the limit point of a tight family of processes
- Long-time properties of sticky coupled process are unclear. Unknown if it is ergodic, admits a unique invariant measure, etc.
- Convergence of discrete approximations also unclear

These difficulties arise because the limit object is highly degenerate. If it satisfied an SDE, the equation would have discontinuous coefficients and likely could not admit a strong solution. Furthermore $\left\{t \geqslant 0 : X_t^\eta = Y_t^0\right\}$ is random fat Cantor set: for any $T > 0$

$$\mathbb{P}\left(\left|\left\{t \in [0,T] : X_t^\eta = Y_t^0\right\}\right| > 0\right) > 0,$$

but

$$\mathbb{P}\left(\exists a < b, \text{ s.t. } [a,b] \subset \left\{t \in [0,T] : X_t^\eta = Y_t^0\right\}\right) = 0.$$

Discrete-Time Sticky Coupling

Lets work with the discrete version of sticky coupling [4] instead. Consider the estimator

$$\widehat{\Psi}_{\eta,N}^{\Delta t} = \frac{1}{\eta N} \sum_{k=0}^{N-1} \left[R\left(X_k^{\eta,\Delta t}\right) - R\left(Y_k^{0,\Delta t}\right) \right]$$

with $\left\{ X_k^{\eta,\Delta t}, Y_k^{0,\Delta t} \right\}_{k\in\mathbb{N}}$ the discrete sticky coupling of the Euler-Maruyama discretizations of $(X_t^\eta)_{t\geqslant 0}$ and $\left(Y^0\right)_{t\geqslant 0}$.
Let $\{G_k\}_{k\geqslant 1}$ and $\{U_k\}_{k\geqslant 1}$ be i.i.d sequences of Gaussian and uniform random variables respectively. The evolution is given by

$$X_{k+1}^{\eta,\Delta t} = X_k^{\eta,\Delta t} + \Delta t \left[b\left(X_k^{\eta,\Delta t}\right) + \eta F\left(X_k^{\eta,\Delta t}\right) \right] + \sqrt{\frac{2\Delta t}{\beta}} G_{k+1},$$

$$Y_{k+1}^{0,\Delta t} = X_{k+1}^{\eta,\Delta t} B_{k+1} + (1 - B_{k+1}) H_{\Delta t}\left(X_k^{\eta,\Delta t}, Y_k^{0,\Delta t}, G_{k+1}\right),$$

[4] A. Durmus, A. Eberle, A. Enfroy, A. Guillin, P. Monmarché (2021) *Discrete sticky couplings of functional autoregressive processes*

Discrete-Time Sticky Coupling

with $B_{k+1} = \mathbf{1}_{[0,1]}\left(p_{\Delta t,\beta}\left(X_k^{\eta,\Delta t}, Y_k^{0,\Delta t}, G_{k+1}\right) - U_{k+1}\right)$ and

$$H_{\Delta t}(x,y,z) = y + \Delta t b(y) + \sqrt{\frac{2\Delta t}{\beta}}\left[\mathrm{Id} - 2\mathbf{e}(x,y)\,\mathbf{e}(x,y)^T\right] z,$$

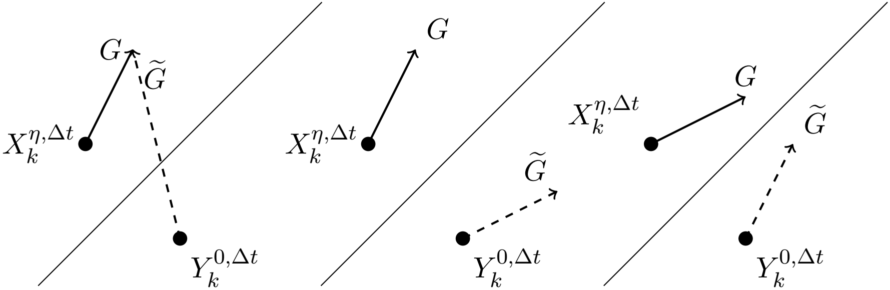
$$\mathbf{E}(x,y) = y - x + \Delta t\left[b(y) - b(x) - \eta F(x)\right],$$

$$\mathbf{e}(x,y) = \begin{cases} \dfrac{\mathbf{E}(x,y)}{|\mathbf{E}(x,y)|} & \text{if } \mathbf{E}(x,y) \neq 0 \\ \mathbf{e}_0 & \text{otherwise,} \end{cases}$$

$$p_{\Delta t,\beta}(x,y,z) = \min\left\{1, \frac{\varphi\left(\sqrt{\frac{\beta}{2\Delta t}}\,|\mathbf{E}(x,y)| - \langle \mathbf{e}(x,y), z\rangle\right)}{\varphi\left(\langle \mathbf{e}(x,y), z\rangle\right)}\right\},$$

We denote by $T^{\eta,\Delta t}$ the Markov kernel of the coupled process

Discrete-Time Sticky Coupling



(a) Collision

(b) Reflection resulting in separation

(c) Reflection resulting in contraction

Discrete-Time Sticky Coupling

Proposition

If b is strongly contractive at infinity and Δt sufficiently small, the discrete-time sticky coupled process $\left\{X_k^\eta, Y_k^0\right\}_{k\in\mathbb{N}}$ admits a unique invariant measure, $\mu_{\eta,\Delta t}$. Furthermore it is geometrically ergodic wrt to this measure.

Proof: Use Hairer & Mattingly strategy[5]
Strong contractivity implies that $e^{c|x|^2} + e^{c|y|^2}$ is a Lyapunov function. Furthermore $p_{\Delta t,\beta}(x,y,z) > 0$ implies that there is always strictly positive probability of the process returning to the diagonal. Thus for any $K > 0$ there exists $\rho_{K,\Delta} \in (0,1)$ such that

$$\inf_{\max\{|x|,|y|\}\leqslant K} T^{\eta,\Delta t}\left((x,y)\,,\cdot\right) \geqslant \rho_{K,\Delta}\xi_K\left(\cdot\right)$$

with ξ_K the uniform probability on $\{x=y\}\cap\{\max\{|x|,|y|\}\leqslant K\}$

[5] M. Hairer and J. Mattingly *Yet another look at Harris's ergodic theorem for Markov chains*

Performance of the Sticky Coupling Based Estimator

The coupling based estimator improves upon the bias and variance of the NEMD estimator by a factor of η^{-1}:

Theorem

Let $\eta_* > 0$ and $R \in \mathscr{S}$ such that $\nu_0(R) = 0$. Assume that X^η and Y^0 have the same initial value. If the two previously stated assumptions hold and Δt small enough, then $\left\{X_k^{\eta,\Delta t}, Y_k^{0,\Delta t}\right\}_{k\in\mathbb{N}}$ satisfies a CLT and there exists K_1, K_2 such that

$$\forall \eta \in [-\eta_*, \eta_*], \quad \lim_{N\to\infty} N \mathrm{Var}\left(\widehat{\Psi}_{\eta,N}^{\Delta t}\right) \leqslant K_1 \left(\frac{1+\Delta t}{\eta} + \Delta t\right), \tag{3}$$

and

$$\left|\mathbb{E}\left[\widehat{\Psi}_{\eta,N}^{\Delta t}\right] - \alpha_{R,\eta}\right| \leqslant K_2 \left(\frac{1}{N} + \Delta t\right). \tag{4}$$

Ideas of Proof (1)

Denote by $\nu_{\eta,\Delta t}$, and $\nu_{0,\Delta t}$ the invariant measures of the respective discrete marginal processes and let $\Pi_{\eta,\Delta t}$ and $\Pi_{0,\Delta t}$ be the operators that center function with respect to these measures. Denote by $P^{\eta,\Delta t}$ and $P^{0,\Delta}$ their Markov kernels.

The CLT follows ergodicity, constructing an explicit solution to the discrete Poisson equation

$$\Delta t^{-1}\left(\mathrm{Id} - T^{\eta,\Delta t}\right) u(x,y) = \Pi_{\eta,\Delta t} R(x) - \Pi_{0,\Delta t} R(y),$$

and a CLT for Markov chains[6]. This further gives an expression for the asymptotic variance, $\sigma^2_{R,\eta,\Delta t}$ in terms of the

$$\widehat{R}_{\eta,\Delta t} = \Delta t \left(\mathrm{Id} - P^{\eta,\Delta t}\right)^{-1} \Pi_{\eta,\Delta t} R,$$

and

$$\widehat{R}_{0,\Delta t} = \Delta t \left(\mathrm{Id} - P^{0,\Delta t}\right)^{-1} \Pi_{0,\Delta t} R.$$

[6] R. Douc et. al (2018) *Markov Chains*

Ideas of Proof (2)

A long computation adapting the strategies of Leimkuhler, et. al (2015)[7] and Plechac, et. al (2021)[8] lets us bound the bias and variance with terms of the form

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{K}_n(x) + \mathcal{K}_n(y)) \, \mathbf{1}_{\{x \neq y\}} \, d\mu_{\eta,\Delta t} \, (dx \, dy) \, ,$$

and higher order terms. (Recall $\mathcal{K}_n = 1 + |x|^n$). It only remains to control this integral.

[7] B. Leimkuhler, C. Matthews, and G. Stoltz *The computation of averages from equilibrium and non-equilibrium Langevin molecular dynamics*

[8] P. Plechac, G. Stoltz, and T. Wang *Convergence of the likelihood ratio method for linear response of non-equilibrium stationary states*

Ideas of Proof (3)

Proposition

Under the same hypothesis as the theorem,

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{K}_n(x) + \mathcal{K}_n(y)) \mathbf{1}_{\{x \neq y\}} \, d\mu_{\eta,\Delta t}(dx\, dy) \leqslant C\eta \left(\nu_{\eta,\Delta t}(\mathcal{K}_n) + \nu_{0,\Delta t}(\mathcal{K}_n)\right).$$

Heuristic "proof" of proposition

$$\begin{aligned} &\int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{K}_n(x) + \mathcal{K}_n(y)) \mathbf{1}_{\{x \neq y\}} \, d\mu_{\eta,\Delta t}(dx\, dy) \\ &\leqslant \mu_{\eta,\Delta t}(\{x \neq y\}) \int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{K}_n(x) + \mathcal{K}_n(y)) \, d\mu_{\eta,\Delta t}(dx\, dy), \end{aligned} \tag{5}$$

The sticky coupled process spends an $O(\eta)$ proportion of time off the diagonal. Furthermore $\mu_{\eta,\Delta t}$ is clearly a coupling of $\nu_{\eta,\Delta t}$ and $\nu_{0,\Delta t}$.

Numerical Illustrations: Strongly Convex Potential

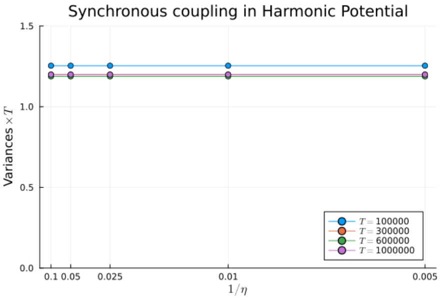
Consider a 2-dimensional Ornstein-Uhlenbeck process

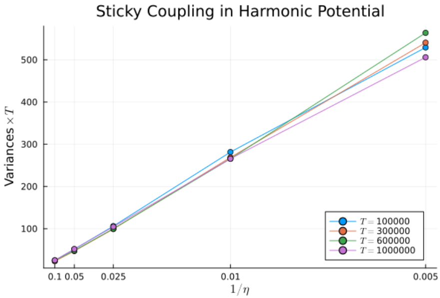
$$dX_t^\eta = -\begin{bmatrix} 1 & -\eta \\ 0 & 1 \end{bmatrix} X_t^\eta dt + \sqrt{\frac{2}{\beta}} dW_t;$$

here $b(x) = -\nabla U = -x$ and $F(x) = [x_2 \; 0]^T$. We choose as response function the covariance between the components. In this case α_R is explicitly calculable.

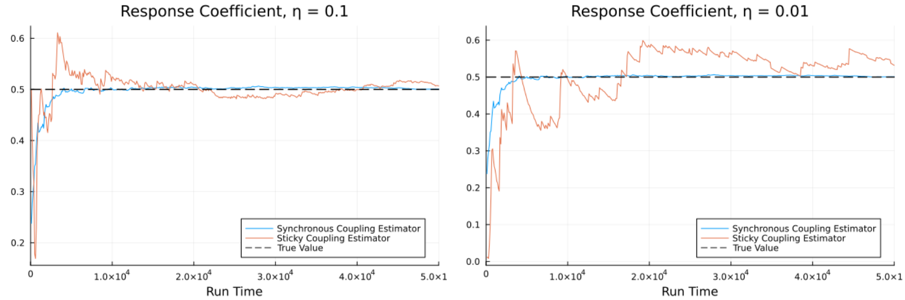
$$R(x) = x_1 x_2, \qquad \alpha_R = \frac{1}{2\beta}$$

Numerical Illustrations: Strongly Convex Potential





Numerical Illustrations: Strongly Convex Potential



Numerical Illustrations: Lennard-Jones Fluid

For less trivial example, we consider an 18 particles 2-D Lennard-Jones fluid. For $x = \left(x_1^1, x_2^1, x_1^2, x_2^2, \dots, x_1^{18}, x_2^{18}\right)$, the interaction is given by

$$U_1(x) = \sum_{i \geqslant j} \left[\left(\frac{1}{|r_{ij}|} \right)^{12} - 2 \left(\frac{1}{|r_{ij}|} \right)^{6} \right],$$

with $r_{ij} = |x^i - x^j|$ if $i < j$ and $r_{ii} = |x^i|$. The confinement is give by

$$U_2(x) = \sum_{i=1}^{18} \left[\max\left\{ |x_1^i| - 5, 0 \right\}^2 + \max\left\{ |x_2^i| - 5, 0 \right\}^2 \right].$$

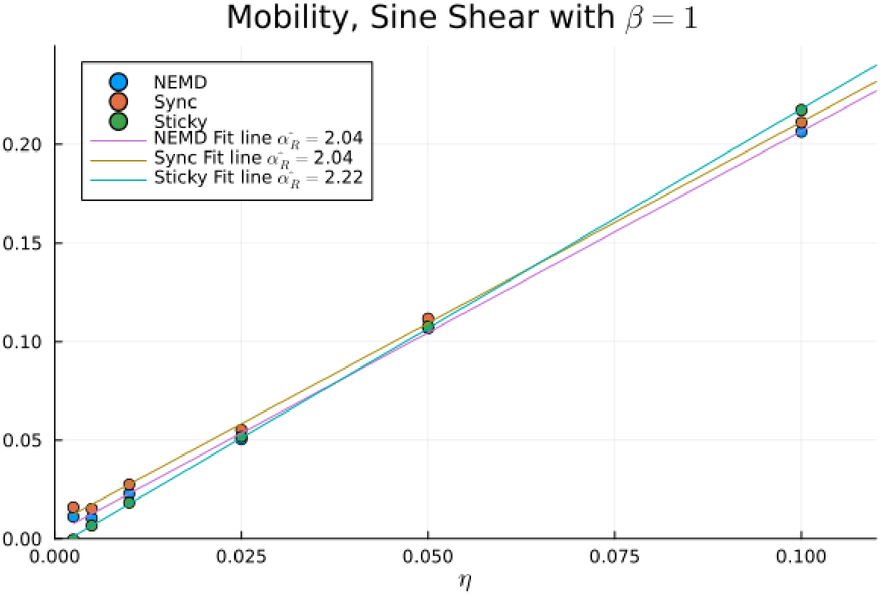
Thus $b(x) = -\nabla U = -\nabla(U_1 + U_2)$. For F we use sine shear

$$(F(x))_i = \begin{cases} \sin(\pi x_2^k / 5) & \text{if } i = 2k - 1 \\ 0 & \text{otherwise} \end{cases}$$

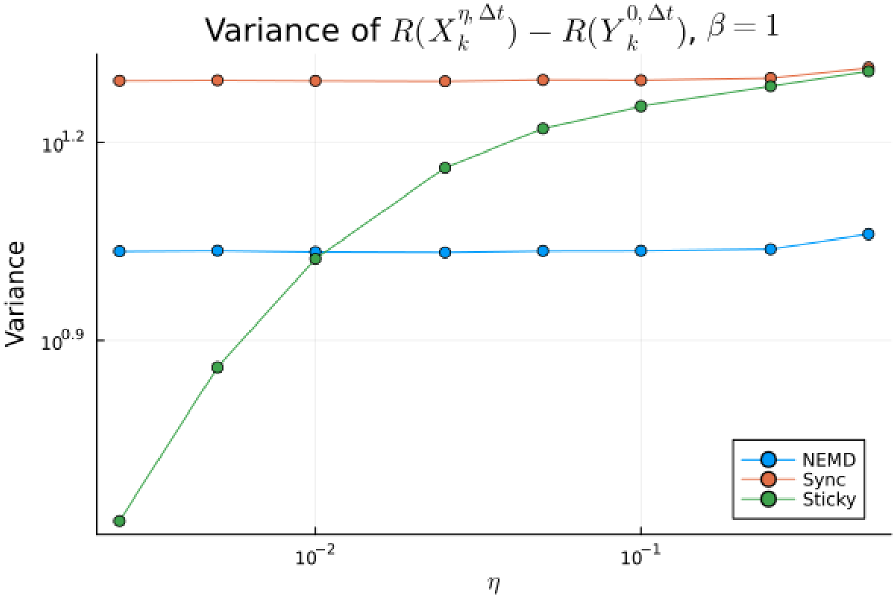
and we measure the mobility response

$$R(x) = F(x)^T \nabla V(x)$$

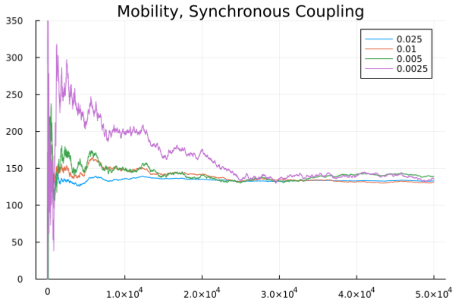
Numerical Illustrations: Lennard-Jones Fluid Sine Shear

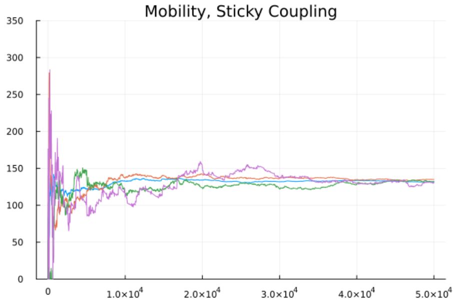


Numerical Illustrations: Lennard-Jones Fluid Sine Shear

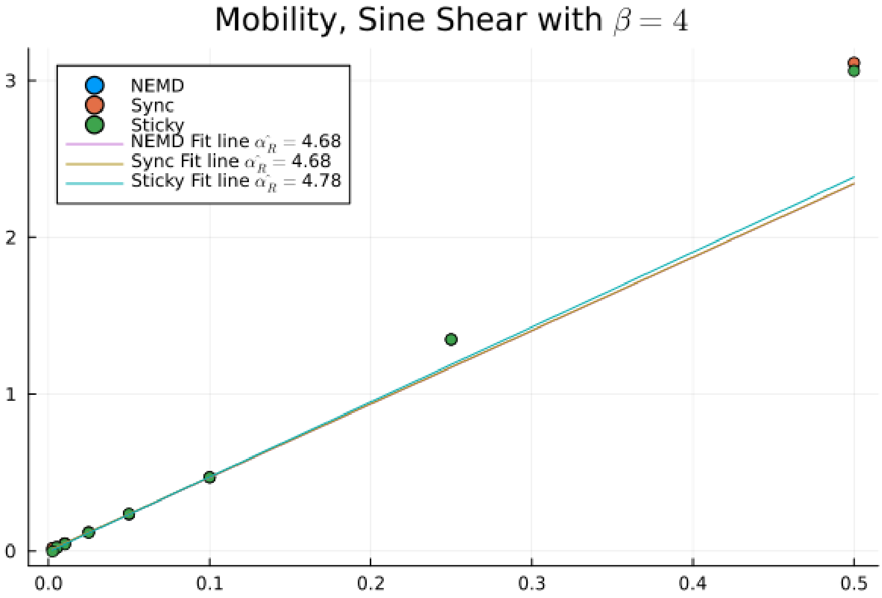


Numerical Illustrations: Lennard-Jones Fluid Sine Shear

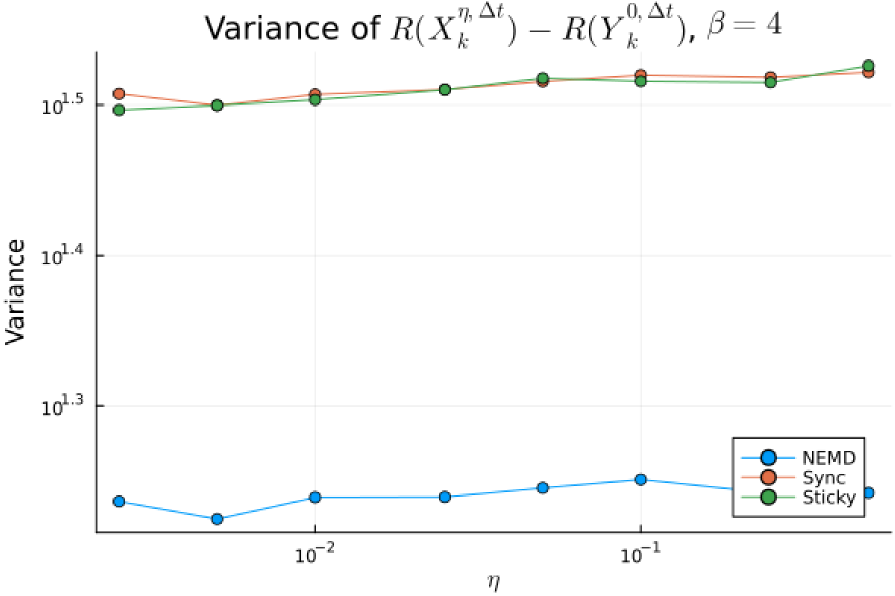




Numerical Illustrations: Lennard-Jones Fluid Sine Shear



Numerical Illustrations: Lennard-Jones Fluid Sine Shear



Extensions and perspectives

Extension to Kinetic Langevin Dynamics

For kinetic Langevin Dynamics the noise only effects the momentum.

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

The coordinate change[9][10] hints at what the coupling should do: let $\left(Z_t^\eta, Q_t^\eta\right) = \left(q_t^\eta - q_t^0, q_t^\eta - q_t^0 + \gamma^{-1}\left(p_t^\eta - p_t^0\right)\right)$, then

$$dZ_t^\eta = -\gamma M^{-1} Z_t^\eta dt + \gamma M^{-1} Q_t^\eta dt,$$
$$dQ_t^\eta = -\gamma^{-1}\left(\nabla U\left(q_t^\eta\right) - \nabla U\left(q_t^0\right)\right) dt + \gamma^{-1} \eta F\left(q_t^\eta\right) dt + \sqrt{\frac{2}{\gamma\beta}} d(W - \widetilde{W})_t.$$

Z^η is contractive whenever $\|Z_t^\eta\|_\infty \geqslant \|Q_t^\eta\|_\infty$.

[9] A. Eberle, A. Guillin, R. Zimmer (2019) *Couplings and quantitative contraction rates for Langevin dynamics*

[10] N. Bou-Rabee, A. Eberle, R. Zimmer (2020) *Coupling and Convergence for Hamiltonian Monte Carlo*

Sticky Coupling on a Manifold

Morally one should be able to extend sticky coupling to processes that take values on a manifold. The reflection part of sticky coupling can be extended to manifold-valued processes using the Kendall-Cranston[11]

If the manifold is compact can we make the coupling work for an arbitrary potential? Example: Lennard-Jones fluids with periodic boundary conditions.

[11] A. Eberle (2016) Reflection couplings and contraction rates for diffusions

Hybrid Coupling

In contractive regions of the phase space, synchronous coupling (i.e choosing $\widetilde{W} = W$) is more effective at bring the coupled trajectories together than reflection coupling.

On the other hand, reflective coupling can separate trajectories just as easily as it can bring them together—MR coupling has a long "tail".

This suggests a hybrid approach of mixing MR coupling and synchronous coupling.