Frozen-flow methods for the long time sampling of SDEs on manifolds

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Geometric numerical integration of the Riemannian Langevin equation

The goal is to approximate the **invariant measure** $d\mu_\infty = \rho_\infty d\,\mathrm{vol}_{\mathcal{M}}$, the unique solution to

$$\mathcal{L}^* \mu_\infty = 0.$$

Definition . The method is of order $r \geq 1$ for μ_∞ if there exists $h_0 > 0$ and $C_\varphi > 0$ which depends on h_0 and the test function φ such that for all $h \in (0, h_0)$,

$$|e(\varphi, h)| \leq C_\varphi h^r \text{ with } e(\varphi, h) := \lim_{N\to\infty} \frac{1}{N+1}\sum_{n=0}^{N} \varphi(X_n) - \int_{\mathcal{M}} \varphi(y)\rho_\infty(y) d\,\mathrm{vol}_{\mathcal{M}}(y).$$

Let $(\mathcal{M}, g)$ be a smooth **Riemannian manifold** of dimension D endowed with a metric g. Let $E_1, \ldots, E_D$ be an orthonormal frame basis.
We denote by $v[\varphi](x)$ or $v \rhd \varphi(x)$ the differential $d\varphi(x) \cdot v$ of φ in the direction of $v \in T_x\mathcal{M}$ at the point $x \in \mathcal{M}$.
For $F : x \mapsto \sum_{d=1}^{D} f^d(x) E_d(x)$, a smooth and Lipschitz vector field on $\mathcal{M}$, general stochastic differential equations with an additive noise are of the form:

$$dX(t) = F(X(t))dt + \sqrt{2}E_d(X(t)) \circ dW_d(t), \quad X(0) = x \in \mathcal{M}. \tag{1}$$

Definition . The generator $\mathcal{L}$ of the SDE (1) is defined by $\mathcal{L}\varphi = F[\varphi] + E_d[E_d[\varphi]]$.
We are especially interested in the case where $F = -\nabla V - \nabla_{E_p} E_p$ for a certain potential V. Hence equation (1) becomes, by denoting $B_{\mathcal{M}}(t)$ a Brownian motion on $\mathcal{M}$, the **Riemannian Langevin equation**:

$$dX(t) = -\nabla V(X(t))dt + \sqrt{2}dB_{\mathcal{M}}(t), \quad X(0) = X_0 \in \mathcal{M}. \tag{2}$$

Definition . The considered numerical methods are post-processed methods, where the post-processors $X \mapsto \overline{X}$ is built as a random perturbation of the identity on $\mathcal{M}$,

$$X_0 \in \mathcal{M}, \quad X_{n+1} = \Psi_h(X_n), \quad \overline{X}_N = \overline{\Psi}_h(X_N). \tag{3}$$

Characterization of the order for the invariant measure

Let us introduce the Taylor-Talay-Tubaro expansion of the numerical method.

Proposition . For all function $\varphi \in C_P^\infty(\mathcal{M})$ and h small enough, the expansion holds

$$\mathbb{E}\left[\varphi(X_1) | X_0 = x\right] = \varphi(x) + \sum_{j=1}^{p} h^j A_j \varphi(x) + h^{p+1} R_p^h(\varphi, x).$$

In the case of post-processed method (3), the expansion is of the same form.
Let us now state one of the central results of this work: the characterization of the invariant measure, adapted from [AVZ14]. The analysis of [DF12] is generalized for designing the high-order numerical schemes.

Theorem . Consider the SDE (2) on $\mathcal{M}$ satisfying technical assumptions and solved by an ergodic numerical method with $\overline{\Psi}_h = id_{\mathcal{M}}$ satisfying

$$A_j^* \rho_\infty = 0 \text{ for } j = 2 \ldots r.$$

Then **the method is of order** r **for the invariant measure for equation** (2). More precisely, the error of the invariant measure $e(\varphi, h)$ satisfies for all $\varphi \in C_P^\infty$ and all $h \in [0, h_0]$ for a small h_0:

$$e(\varphi, h) = h^r \int_0^\infty \int_{\mathcal{M}} u(t,x) A_{r+1}^* \rho_\infty(x) d\,\mathrm{vol}_{\mathcal{M}}(x) dt + \mathcal{O}(h^{r+1}).$$

This characterization is generalized by adapting a result from [Vil15], to post-processed methods (3), as the following.

Theorem 2. Under technical assumptions, a numerical consistent ergodic post-processed method (3) which satisfies

$$A_j^* \rho_\infty = 0 \text{ and } \overline{A_{j-1}}^* \rho_\infty = 0 \text{ for } j = 2 \ldots p \text{ and } \left(A_{p+1} + [\mathcal{L}, \overline{A_p}]\right)^* \rho_\infty = 0.$$

Then **the post-processed method** (3) **is at least of order** $p+1$ **for the invariant measure for equation** (2).

New methods of order two for the invariant measure

The following methods, in the spirit of post-processed methods [Vil15, LM13], are of first order for the weak error and of second order for the invariant measure $\rho_\infty d\,\mathrm{vol}_{\mathcal{M}}$. They use second order conditions (4).

Method A: second order method for sampling a_{μ_∞} without postprocessors for Riemannian Langevin

$$H_n = \exp\left(\left(\tfrac{h}{4} f^d(X_n) + \tfrac{\sqrt{2h}}{2}\xi_n^d\right) E_d\right) X_n$$
$$X_{n+1} = \exp\left(\left(\tfrac{h}{6} f^d(X_n) + \tfrac{2h}{3} f^d(H_n) + \tfrac{\sqrt{2h}}{2}\xi_n^d\right) E_d\right) \exp\left(\left(\tfrac{h}{6} f^d(X_n) + \tfrac{\sqrt{2h}}{2}\xi_n^d\right) E_d\right) X_n$$

The second method generalizes the Leimkuhler-Matthews method to manifolds and uses only one evaluation of F per step.

Method B: second order post-processed method for sampling a_{μ_∞} for Riemannian Langevin

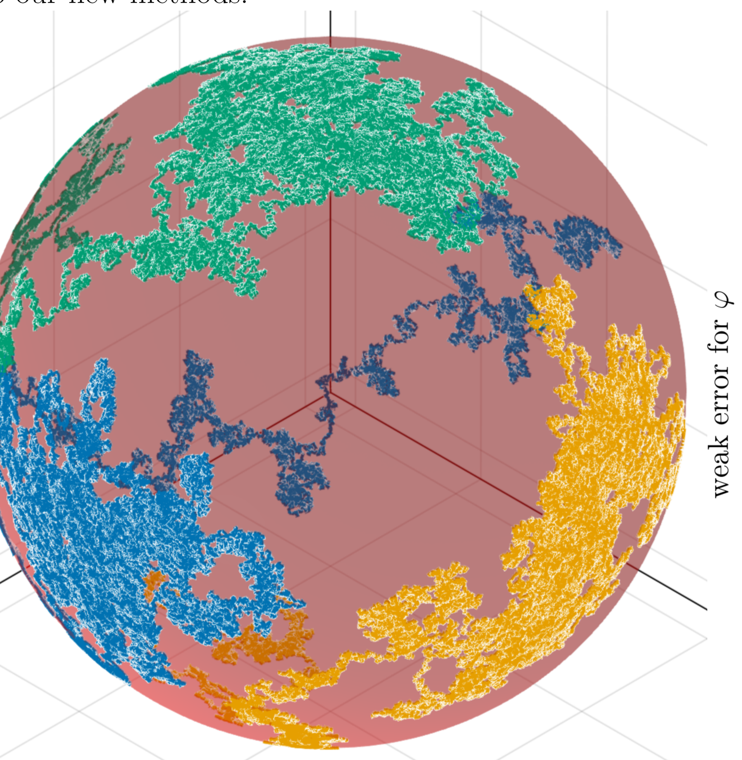
$$H_n = \exp\left(\left(\tfrac{\sqrt{2h}}{2}\xi_n^d\right) E_d\right) X_n$$
$$X_{n+1} = \exp\left(\left(\tfrac{5h}{4} f^d(H_n) + \tfrac{\sqrt{2h}}{4}\xi_n^d\right) E_d\right) \exp\left(\left(-\tfrac{h}{4} f^d(H_n) + \tfrac{3\sqrt{2h}}{4}\xi_n^d\right) E_d\right) X_n$$
$$\overline{X_N} = \exp\left(\tfrac{\sqrt{2h}}{2}\overline{\xi_N^d} E_d\right) X_N.$$

Remark . On $\mathcal{M} = \mathbb{R}^D$, it gives back the Leimkuhler-Matthews method [LM13] presented in [Vil15].

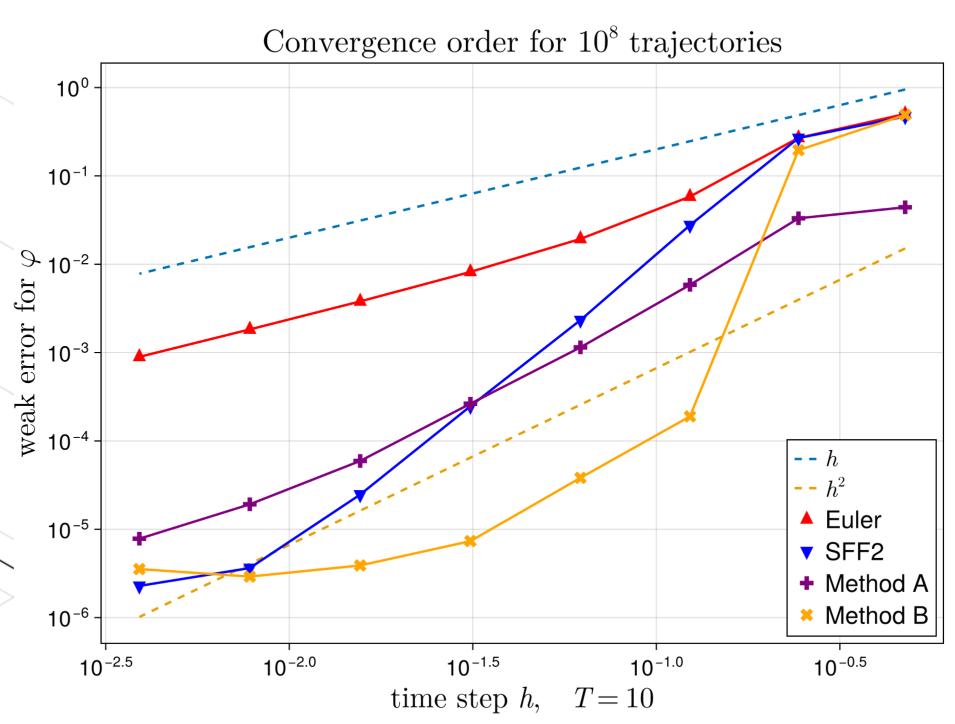
$$H_N = X_n + \frac{\sqrt{2h}}{2}\xi_n, \quad X_{n+1} = X_n + hf(H_n) + \sqrt{2h}\xi_n, \quad \overline{X_N} = X_N + \frac{\sqrt{2h}}{2}\overline{\xi_N}.$$

Numerical experiment

We recall the results from [BBLH25] on the orthogonal group and we generalize it using our new methods for the invariant measure. We compare the frozen-flow Euler method and the SFF2 method [BBLH25], which uses two random variables and is of weak order 2, to our new methods.



Trajectory on SO_3 with quadratic potential, $T = 2$, and $N = 2^{16}$ steps.



Order for the invariant measure for a quadratic potential on SO_3.

Exotic forests algebra and integration by parts

RED(• + ①②) = 0, RED(① •①) = −(①① V + •|•),
RED(① •①V② ②•) = −(...), RED(②① •① ②) = ...

Definition . An exotic forest is a planar decorated forest with the decorations $D = \{\bullet\} \cup \mathbb{N}$, $\mathbb{N} = \{1, 2, \ldots\}$ which follows the following rule: if an integer is used as decoration then it must decorate exactly two leaves.

$$\mathbb{F}^F(\bullet) = F \rhd \varphi, \quad \mathbb{F}^F(①①) = (E_d \cdot E_d) \rhd \varphi, \quad \mathcal{L} = \mathbb{F}^F(\bullet + ①①) \text{ and}$$
$$\mathbb{F}^F(\pi) = f^k(E_{d_2} \rhd f^j)((E_k \cdot E_{d_1}) \rhd f^i)((E_{d_1} \cdot E_i \cdot E_{d_2} \cdot E_j) \rhd \varphi).$$

The operation $X \rhd Y = (X \rhd Y^d)E_d$ is an affine connection, **the connection of Weitzenböck**.

Definition . We define the (non-symmetric) Hessian of φ:

$$(X \cdot Y) \rhd \varphi := X \rhd (Y \rhd \varphi) - (X \rhd Y) \rhd \varphi.$$

Proposition . The exotic forests $\mathcal{EF}$ generates a Hopf algebra.

Theorem . There exists an operation RED on $\mathcal{EF}$ which reduces a forest into a linear combinaison of forests without numbered roots in first position. This operation relies on the integration by parts with respect to the invariant measure.

Reduction of differential operators

Theorem . The expansion of the method (3) as an exotic S-series at the first order ensures that the coefficient of $f^i E_i[\varphi]$ is $\sum_k z_{i,k}^0$ and of $E_{d_1}[E_{d_1}[\varphi]]$ is $\sum^!_{k_2 \leq k_1} z_{k_1}^{d_1} z_{k_2}^{d_1}$. For the second order, the expression of coefficients is given in Table 1.

Forest π	Differential operator $\mathbb{F}^F(\pi) \rhd \varphi$	S-series coefficient $a(\pi)$	RED(π)
•|•	$f^j E^j[f^i] E_i[\varphi]$	$\sum_k z_{i,k}^0 Z_{i,j,k}^0$	•|•
①①V	$E_{d_1}[E_{d_1}[f^i]] E_i[\varphi]$	$\sum_k \sum^!_{k_2 \leq k_1} z_{i,k}^0 Z_{i,k_2}^{d_1} Z_{i,k_1}^{d_1} + \left(\sum_k \bar{z}_{i,k}^0 - \sum^!_{k_2 \leq k_1} \bar{z}_{k_1}^{d_1} \bar{z}_{k_2}^{d_1}\right)$	①①V
• •	$f^j f^i E_j[E_i[\varphi]]$	$\sum^!_{k_2 \leq k_1} z_{j,k_2}^0 z_{i,k_1}^0$	• •
①|• ①	$E_{d_1}[f^i] E_i[E_{d_1}[\varphi]]$	$\sum_k \sum^!_{k_2 \leq k_1} (z_{i,k}^{d_1} z_{i,k_2}^0) z_{k_1}^{d_1}$	①|• ①
① ①|•	$E_{d_1}[f^i] E_{d_1}[E_i[\varphi]]$	$\sum_k \sum^!_{k_2 \leq k_1} z_{k_2}^{d_1}(z_{i,k}^{d_1} z_{i,k_1}^0) + 2\left(\sum_k \bar{z}_{i,k}^0 - \sum^!_{k_2 \leq k_1} \bar{z}_{k_1}^{d_1} \bar{z}_{k_2}^{d_1}\right)$	$-$•|• $-$ ①①V
• ①①	$f^i E_i[E_{d_1}[E_{d_1}[\varphi]]]$	$\sum^!_{k_3 \leq k_2 \leq k_1} z_{i,k_3}^0 z_{k_2}^{d_1} z_{k_1}^{d_1} - \left(\sum_k \bar{z}_{i,k}^0 - \sum^!_{k_2 \leq k_1} \bar{z}_{k_1}^{d_1} \bar{z}_{k_2}^{d_1}\right)$	• ①①
① • ①	$f^i E_{d_1}[E_i[E_{d_1}[\varphi]]]$	$\sum^!_{k_3 \leq k_2 \leq k_1} z_{k_3}^{d_1} z_{i,k_2}^0 z_{k_1}^{d_1}$	$-$• • $-$ ①|• ①
①① •	$f^i E_{d_1}[E_{d_1}[E_i[\varphi]]]$	$\sum^!_{k_3 \leq k_2 \leq k_1} z_{k_3}^{d_1} z_{k_2}^{d_1} z_{i,k_1}^0 + \left(\sum_k \bar{z}_{i,k}^0 - \sum^!_{k_2 \leq k_1} \bar{z}_{k_1}^{d_1} \bar{z}_{k_2}^{d_1}\right)$	•|• + ①①V $-$ • •
②②①①	$E_{d_2}[E_{d_2}[E_{d_1}[E_{d_1}[\varphi]]]]$	$\sum^!_{k_4 \leq k_3 \leq k_2 \leq k_1} z_{k_4}^{d_2} z_{k_3}^{d_2} z_{k_2}^{d_1} z_{k_1}^{d_1}$	$-$• ①①
②①②①	$E_{d_2}[E_{d_1}[E_{d_2}[E_{d_1}[\varphi]]]]$	$\sum^!_{k_4 \leq k_3 \leq k_2 \leq k_1} z_{k_4}^{d_2} z_{k_3}^{d_1} z_{k_2}^{d_2} z_{k_1}^{d_1}$	• • + ①|• ①
①②②①	$E_{d_1}[E_{d_2}[E_{d_2}[E_{d_1}[\varphi]]]]$	$\sum^!_{k_4 \leq k_3 \leq k_2 \leq k_1} z_{k_4}^{d_1} z_{k_3}^{d_2} z_{k_2}^{d_2} z_{k_1}^{d_1}$	• • $-$ •|• $-$ ①①V

Table 1: Coefficient of $A_2\varphi = \sum_{\substack{\pi \in \mathcal{EF} \\ |\pi| = 2}} a(\pi) \mathbb{F}^F(\pi) \rhd \varphi$ for the method (3).

Updated high order conditions

For the first order the condition is $a(\bullet) = a(①①)$.
We impose $a(\bullet) = a(①①) = 1$ to be consistent.

A method (3) for solving equation (2) is of order 2 for the invariant measure if the method satisfies

$$\boxed{\begin{array}{c} a(•|•) = a(①①V), \quad a(•①①) = a(②②①①), \quad a(①|•①) + a(②①②①) = a(①•①), \\ a(•|•) + a(①①•) = a(①①|•) + a(①②②①), \quad a(••) + a(①②②①) = a(①|•①) + a(①①•). \end{array}} \tag{4}$$

For Method A, we have

$$a(•|•) = \tfrac{1}{6}, \quad a(①①V) = \tfrac{1}{6}, \quad a(••) = \tfrac{1}{2}, \quad a(①|•①) = \tfrac{1}{6}, \quad a(①①|•) = \tfrac{1}{2},$$
$$a(•①①) = \tfrac{1}{6}, \quad a(①•①) = \tfrac{1}{3}, \quad a(①①•) = \tfrac{1}{2} \quad a(②②①①) = a(②①②①) = a(①②②①) = \tfrac{1}{6}.$$

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