

Postprocessed frozen-flow methods for the long time sampling of ergodic dynamics on Riemannian manifolds

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Joint work with A. Busnot Laurent

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Equation: $dX(t) = -\nabla V(X(t))dt + \sqrt{2}dB_{\mathcal{M}}(t)$ on $\mathcal{M}$

The Euclidian space $\mathbb{R}^d$

Consider the differential equation: $X'(t) = F(X(t))$. The **explicit Euler** method relies on the finite differences approximation:

$$X'(t) \sim \frac{X(t + \delta t) - X(t)}{\delta t} \text{ becomes } X_{n+1} = X_n + hF(X_n).$$

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Generalization to manifolds

The vector $X_n + hF(X_n)$ does not belong on $\mathcal{M}$ but on the tangent space $T_{X_n}\mathcal{M}$.

Question

How to sample the long time behaviour of **ergodic dynamic** on a **Riemannian manifold**?

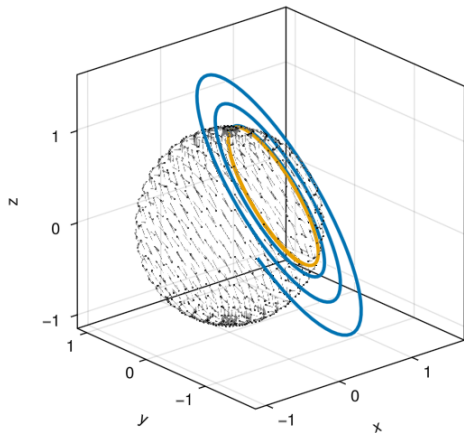


Figure 1: The trajectory does not stay on the sphere.

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- 3 Numerical experiments
- 4 Algebraic operator on $\mathcal{EF}$

Reference of this talk:

- A. Busnot Laurent, S. Macé, Postprocessed frozen-flow methods for the long time sampling of ergodic dynamics on Riemannian manifolds, *In preparation*.

Butcher series for ODEs on $\mathbb{R}^d$ (A. Cayley: 1857; J. Butcher: 1963)

We consider the problem $X' = F(X), \quad X(0) = x$ with $X : \mathbb{R}_+ \rightarrow \mathbb{R}^d$ and $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$. A Taylor expansion at the order p yields,

$$X(t) = x + tX'(0) + \frac{t^2}{2}X''(0) + \frac{t^3}{6}X^{(3)}(0) + \dots + \mathcal{O}(t^{p+1}).$$

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However, the ODE allows us to replace the derivatives of X by the ones of F evaluated on x :

$$\begin{aligned} X'(0) &= F(x) & \left| \quad X''(0) &= (F \circ X)'(0) \right| & X^{(3)}(0) &= (F \circ X)^{(2)}(0) \\ & & &= dF(x) \cdot F(x) & &= dF(x) \cdot dF(x) \cdot F(x) + d^2F(x) \cdot (F(x), F(x)) \end{aligned}$$

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However, the ODE allows us to replace the derivatives of X by the ones of F evaluated on x :

$$\begin{array}{lcl} X'(0) & = & F(x) \\ & = & \bullet \end{array} \quad \left| \quad \begin{array}{lcl} X''(0) & = & dF(x) \cdot F(x) \\ & = & \begin{array}{c} \bullet \\ | \\ \bullet \end{array} \end{array} \quad \left| \quad \begin{array}{lcl} X^{(3)}(0) & = & dF(x) \cdot dF(x) \cdot F(x) + d^2F(x) \cdot (F(x), F(x)) \\ & = & \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} + \begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \quad \bullet \end{array} \end{array}$$

Express each differential terms by trees:

$$X(t) = x + t \bullet + \frac{t^2}{2} \begin{array}{c} \bullet \\ | \\ \bullet \end{array} + \frac{t^3}{6} \left(\begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} + \begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \quad \bullet \end{array} \right) + \frac{t^4}{24} \left(\begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} + \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \diagup \bullet \diagdown \end{array} + 2 \begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \quad \bullet \end{array} + \begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \diagup \bullet \diagdown \end{array} + \begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \diagdown \bullet \diagup \end{array} \right) + \dots + \mathcal{O}(t^{p+1}).$$

Remark

Note that on $\mathbb{R}^d$, the differential operators commute and $\begin{array}{c} \bullet \diagup \bullet \diagdown \\ | \quad | \\ \bullet \quad \bullet \end{array} = \begin{array}{c} \bullet \diagdown \bullet \diagup \\ | \quad | \\ \bullet \quad \bullet \end{array}$.

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We focus on the weak convergence, that is, on the approximation of $\varphi(X)$ for all test function $\varphi \in C_P^\infty(\mathcal{M})$, we apply the same formalism¹,

$$\varphi(X(t)) = \mathbb{1} + t \bullet + \frac{t^2}{2} (\begin{array}{c} \bullet \\ \mid \\ \bullet \end{array} + \bullet \bullet) + \frac{t^3}{6} \left(\begin{array}{c} \bullet \\ \mid \\ \bullet \end{array} + \begin{array}{c} \bullet \quad \bullet \\ \diagdown \quad \diagup \\ \bullet \end{array} + 2 \bullet \begin{array}{c} \bullet \\ \mid \\ \bullet \end{array} \bullet + \bullet \bullet \bullet \right) + \dots + \mathcal{O}(t^{p+1}).$$

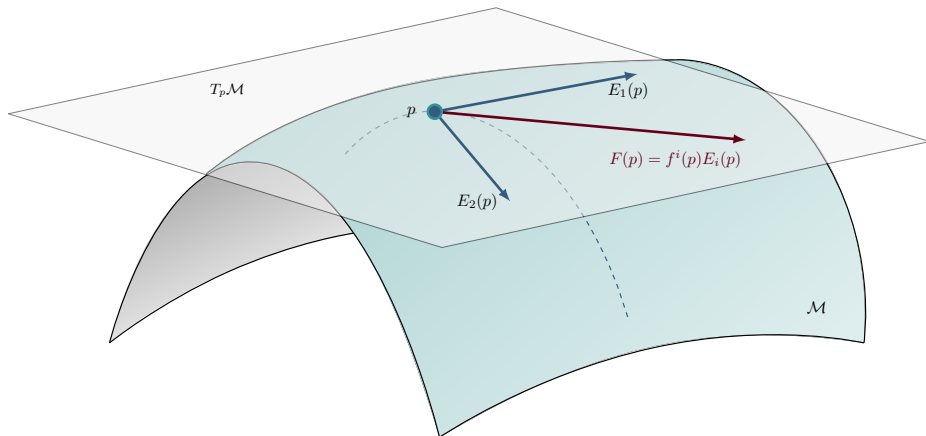
¹The unique node associated to φ being at the root, it is implicit.

S-series for ODEs on $(\mathcal{M}, g)$ (H. Munthe-Kaas: 1999)

Let $E_1, \dots, E_D$ be an **orthonormal frame** of a Riemannian manifold $(\mathcal{M}, g)$. General ODEs are of the form:

$$X'(t) = F(X(t)), \quad X(0) = x \in \mathcal{M}.$$

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For all φ , we denote by $v[\varphi]$ **the differential** $d\varphi \cdot v$.

The **Weitzenböck affine connection** $\triangleright$ is defined on vector fields by

$$X \triangleright Y = (X \triangleright y^d) E_d, \quad X \triangleright \varphi = X[\varphi].$$

Differential operators act on functions φ by:

$$(X_1 \cdots X_n) \triangleright \varphi = x_1^{i_1} \cdots x_n^{i_n} E_{i_1}[\dots E_{i_n}[\varphi] \dots], \quad X_j = \sum_{i_j=1}^D x_j^{i_j} E_{i_j}.$$

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A Taylor expansion at the order p yields,

$$\varphi(X(t)) = \varphi(x) + t f^i(x) E_i \triangleright \varphi(x) + \frac{t^2}{2} \left(f^j(x) E_j [f^i(x)] E_i + f^i(x) f^j(x) (E_i \cdot E_j) \right) \triangleright \varphi(x) + \cdots + \mathcal{O}(t^{p+1}).$$

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We apply our algebraic framework,

$$\varphi(X(t)) = \mathbb{1} + t \bullet + \frac{t^2}{2} (\mathfrak{I} + \bullet \bullet) + \frac{t^3}{6} \left(\mathfrak{I} + \mathfrak{V} + 2 \bullet \mathfrak{I} + \mathfrak{I} \bullet + \bullet \bullet \bullet \right) + \cdots + \mathcal{O}(t^{p+1}).$$

S-series for SDEs on $(\mathcal{M}, g)$ (A. B. Laurent and G. Vilmart: 2022)

General stochastic differential equations with an additive noises are of the form:

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

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The generator $\mathcal{L}$ of the SDE (2) is defined by

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We are, in particular, interested in the case where $F = -\nabla V - \nabla_{E_p} E_p$, $f^i = -E_i[V] - \langle \nabla_{E_p} E_p | E_i \rangle$ for a certain potential V . Hence equation (2) becomes, by denoting $B_{\mathcal{M}}(t)$ a Brownian motion on $\mathcal{M}$, the **Riemannian Langevin equation**

$$dX(t) = -\nabla V(X(t))dt + \sqrt{2} dB_{\mathcal{M}}(t), \quad X(0) = X_0 \in \mathcal{M}. \quad (3)$$

Exotic forests algebra

Definition (Exotic forest and order)

An **exotic forest** is a planar decorated forest with the decorations $D = \{\bullet\} \cup \mathbb{N}$, $\mathbb{N} = \{1, 2, \dots\}$ satisfying **if an integer is used as decoration then it must decorate exactly two leaves**. Two pairly decorated nodes are call lianas. The set of exotic forests is $\mathcal{EF}$, the associated vector space is $\mathcal{EF} = \text{Span}_{\mathbb{R}}(\mathcal{EF})$.

The **order of a forest** $\pi \in \mathcal{EF}$ is defined by the order of the associated differential operators.

Examples

Consider these examples.

$$f^i(E_i \triangleright \varphi) \mapsto \bullet, \quad (E_{d_1} \cdot E_{d_1}) \triangleright \varphi \mapsto \textcircled{1}\textcircled{1},$$

$$f^k(E_{d_2} \triangleright f^j)((E_k \cdot E_{d_1}) \triangleright f^i)((E_{d_1} \cdot E_i \cdot E_{d_2} \cdot E_j) \triangleright \varphi) \mapsto \textcircled{1}\textcircled{2}$$

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There are ?? exotic forests of order 3.

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There are 95 exotic forests of order 3.

Frozen flow of the differential equation $X'(t) = F(X(t))$ on $\mathcal{M}$

Definition (Frozen flow method)

We freeze the vector field, using an approximation α_n^d of f^d in the segment of $[X_n, X_{n+1}]$,

$$Y'(t) = \alpha_n^d E_d(Y(t)), \quad Y(0) = X_n.$$

Then let $\exp(h\alpha_n^d E_d)$ be the flow of the solution and we denote $X_{n+1} = \exp(h\alpha_n^d E_d) X_n$.

Frozen flow on $\mathbb{R}^D$

With $\alpha_n^d = f^d(X_n)$, we recover the **explicit Euler method**

$$X_{n+1} = X_n + hf^d(X_n)e_d,$$

and with

$$\alpha_n^d = \frac{1}{2} \left(f^d(X_n) + f^d(X_n + hf^d(X_n)e_d) \right),$$

we recover the **Heun method**,

$$H_n = X_n + hf^d(X_n)e_d,$$

$$X_{n+1} = X_n + \frac{h}{2} \left(f^d(X_n) + f^d(H_n) \right) e_d.$$

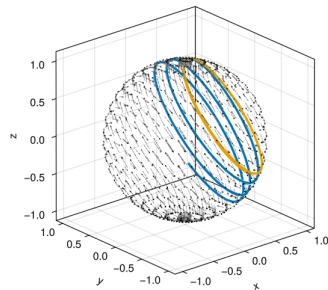


Figure 2: The trajectory does stay on the sphere.

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The easiest method to solve the SDE (2) is called **frozen flow Euler method**

$$X_{n+1} = \exp\left(\left(hf^d(X_n) + \sqrt{2h}\xi_n^d\right) E_d\right) X_n, \quad \xi_n^d \sim \mathcal{N}(0, 1).$$

In the case of the **Riemannian Langevin equation** (3), K. BHARATH, A. LEWIS, A. SHARMA, and M. V. TRETYAKOV, 2023; proposes an alternate approach, based on the Levi-Civita connection called Riemannian Langevin method:

$$X_{n+1} = \exp^{Riem}\left(-h\nabla V(X_n) + \sqrt{2h}\xi_n^d E_d\right) X_n, \quad \xi_n^d \sim \mathcal{N}(0, 1).$$

Invariant measure

Definition (Processus ergodique)

A process X is ergodic if there exists $d\mu_\infty$ a unique invariant measure with density function ρ_∞ with respect to the measure $d\text{vol}_\mathcal{M}$, such that for all test function φ and all initial data $X(0) = x$, the time average of $\varphi(X)$ converge, that is,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \varphi(X(s)) ds = \int_{\mathcal{M}} \varphi(y) d\mu_\infty(y) \text{ almost surely.}$$

A method is of **order $p \geq 1$ for the invariant measure** if $|e(\varphi, h)| \leq Ch^r$, where

$$e(\varphi, h) := \lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{n=0}^N \varphi(X_n) - \int_{\mathcal{M}} \varphi(y) d\mu_\infty(y).$$

In the case of the **Riemannian Langevin dynamics**,

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

we recover the **Gibbs measure**: $\rho_\infty \propto \exp(-V)$.

Characterization of the higher order for the invariant measure

Theorem (A. BUSNOT LAURENT & S. MACÉ)

We consider the SDE (3) on $\mathcal{M}$. Suppose some technical assumption and that the SDE is solved by a consistent ergodic numerical method satisfying, for all test function φ ,

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

In that case, if the method satisfies

$$A_j^* d\mu_\infty = 0, \quad j = 2 \dots p,$$

then the method is of **order p for the invariant measure**. 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 :

$$e(\varphi, h) = h^p \int_0^\infty \int_{\mathcal{M}} u(x, t) A_{p+1}^* d\mu_\infty(x) + \mathcal{O}_{h \rightarrow 0}(h^{p+1}).$$

In the spirit of A. DEBUSSCHE & E. FAOU, 2012; A. ABDULLE & G. VILMART & K. C. ZYGALAKIS, 2014.

New post processed second order frozen flow method

General method (extending B. OWREN & A. MARTHINSEN, 1999; A. RÖSSLER, 2006)

$$H_n = \exp \left(\left(h\alpha f^d(X_n) + \sqrt{h}\beta\xi_n^d \right) E_d \right) X_n,$$

$$X_{n+1} = \exp \left(\left(h\alpha_2 f^d(X_n) + h\gamma_2 f^d(H_n) + \sqrt{h}\beta_2\xi_n^d \right) E_d \right) \exp \left(\left(h\alpha_1 f^d(X_n) + h\gamma_1 f^d(H_n) + \sqrt{h}\beta_1\xi_n^d \right) E_d \right) X_n.$$

Consider post processed methods, where the postprocessor $X \mapsto \bar{X}$ is build as a perturbation of the identity of $\mathcal{M}$,

$$X_0 \in \mathcal{M}, \quad X_{n+1} = \Psi_h(X_n), \quad 0 \leq n \leq N-1, \quad \bar{X}_N = \bar{\Psi}_h(X_N). \quad (4)$$

General post processed method (extending G. VILMART, 2015)

$$H_n = \exp \left(\left(\sqrt{h}\beta\xi_n^d \right) E_d \right) X_n,$$

$$X_{n+1} = \exp \left(\left(h\gamma_2 f^d(H_n) + \sqrt{h}\beta_2\xi_n^d \right) E_d \right) \exp \left(\left(h\gamma_1 f^d(H_n) + \sqrt{h}\beta_1\xi_n^d \right) E_d \right) X_n.$$

$$\bar{X}_N = \exp \left(\left(\sqrt{h}\beta\xi_N^d \right) E_d \right) X_N.$$

New post processed second order frozen flow method

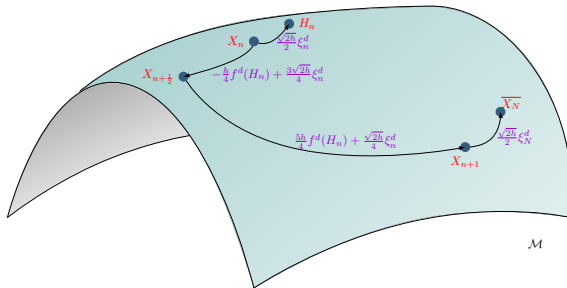
Theorem (A. BUSNOT LAURENT & S. MACÉ)

Assume some technical assumptions from A. ABDULLE, G. VILMART, & K. C. ZYGALAKIS, 2015. Assume that the SDE is solved by a consistent numerical method with postprocessor satisfying, for all test function,

$$A_{j+1}^* d\mu_\infty = \overline{A}_j^* d\mu_\infty = 0 \text{ for } j = 1 \dots p-1, \quad \left(A_{p+1} + [\mathcal{L}, \overline{A}_p] \right)^* d\mu_\infty = 0.$$

Then the method is of **order $p+1$ for the invariant measure**.

This theorem is a generalization of A. ABDULLE, G. VILMART, & K. C. ZYGALAKIS, 2015; to Riemannian manifolds.



New post processed second order frozen flow method

Method 1 Post processed frozen-flow method for equation (3)

$$H_n = \exp\left(\frac{\sqrt{2h}}{2}\xi_n^d E_d\right) X_n$$

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

$$\overline{X_N} = \exp\left(\frac{\sqrt{2h}}{2}\xi_N^d E_d\right) X_N.$$

Corollary (A. BUSNOT LAURENT & S. MACÉ)

The method 1 is of **weak order 1** and of **second order for the invariant measure**.

Remark

In the Euclidian case $\mathcal{M} = \mathbb{R}^D$, we recover the Leimkuhler-Matthews method, B. LEIMKUHLER & C. MATTHEWS, 2013; with the post processed formalism from G. VILMART, 2015;.

Second order frozen flow methods

We propose two alternative scheme, without post processor, for the sake of comparison.

Method 2 Stochastic frozen-flow Heun method for equation (3)

$$\begin{aligned} H_n &= \exp \left(\left(h f^d(X_n) + \sqrt{2h} \xi_n^d \right) E_d \right) X_n \\ X_{n+1} &= \exp \left(\left(\frac{h}{2} f^d(H_n) E_d \right) \exp \left(\left(\frac{h}{2} f^d(X_n) + \sqrt{2h} \xi_n^d \right) E_d \right) X_n \right) \end{aligned}$$

Method 3 2-steps frozen-flow Runge-Kutta method for equation (3)

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

Corollary (A. BUSNOT LAURENT & S. MACÉ)

Methods 2 and 3 are of **weak order 1** and of **second order for the invariant measure**.

Two potentials on $\mathcal{M} = SO_q$

Let $\mathcal{M} = SO_q$ be the compact Lie group of special orthogonal matrices and $(A_d)_{d=1,\dots,D}$ be a basis of the skew-symmetric matrices. As the manifold is smooth and compact, the assumptions of our theorems are satisfied and our analysis applied.

Proposition

Let $\mathcal{M}$ be a matrix Lie group and let $(A_d)_{d=1,\dots,D}$ be an orthonormal basis of its Lie algebra $\mathfrak{m} = T_e \mathcal{M}$. The associated orthonormal frame on $\mathcal{M}$ is

$$E_d(y) = A_d y, \quad d = 1, \dots, D.$$

Method 1 Postprocessed frozen-flow method for equation (3)

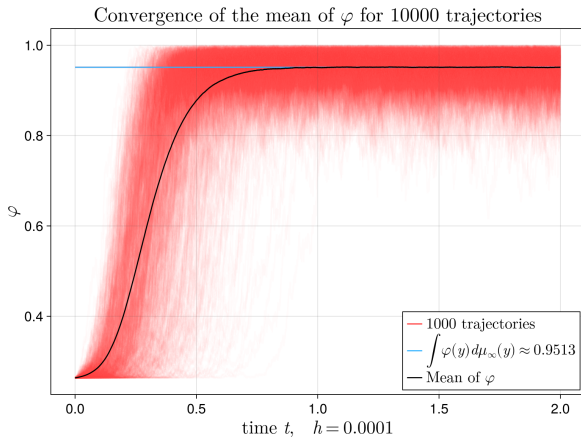
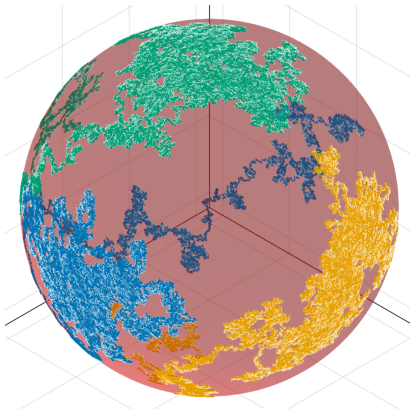
$$H_n = \text{Exp} \left(\sqrt{\frac{h}{2}} \xi_n^d A_d \right) X_n,$$

$$X_{n+1} = \text{Exp} \left(\left(\frac{5h}{4} f^d(H_n) + \frac{\sqrt{2h}}{4} \xi_n^d \right) A_d \right) \text{Exp} \left(\left(-\frac{h}{4} f^d(H_n) + \frac{3\sqrt{2h}}{4} \xi_n^d \right) A_d \right) X_n,$$

$$\overline{X_N} = \text{Exp} \left(\sqrt{\frac{h}{2}} \xi_N^d A_d \right) X_N.$$

We compare a quadratic potential well and a sextic potential barrier on $\mathcal{M} = SO_3$ to confirm our analysis.

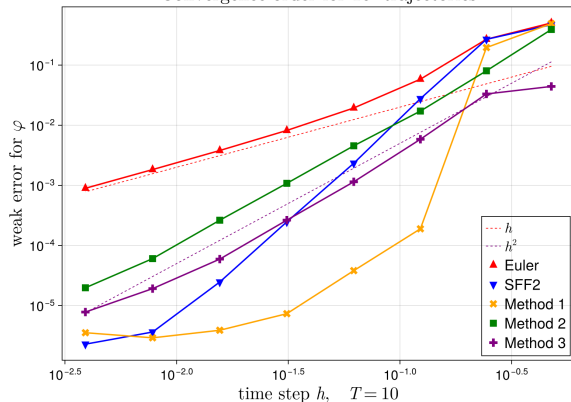
Two potentials on $\mathcal{M} = SO_q$



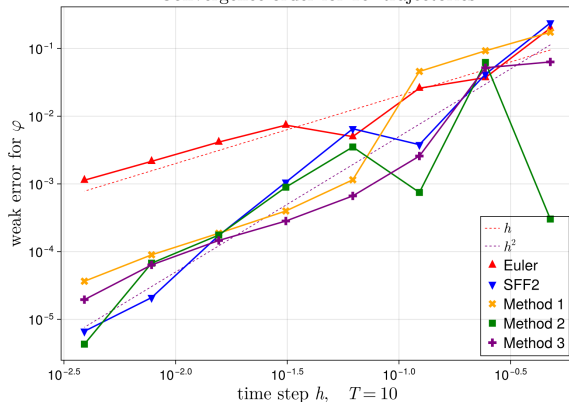
Trajectory on SO_3 for the quadratic potential with $T = 2$ and $h = 10^{-5}$ (Left). Ergodic convergence computed with 10^4 trajectories and $h = 10^{-4}$ for the quadratic potential. (Right).

Two potentials on $\mathcal{M} = SO_q$

Convergence order for 10^8 trajectories



Convergence order for 10^8 trajectories



Order of convergence for both potentials. The mean is at time $T = 10$ on 10^8 trajectories.

Von Mises Fisher dynamic on the sphere $\mathbb{S}^2$

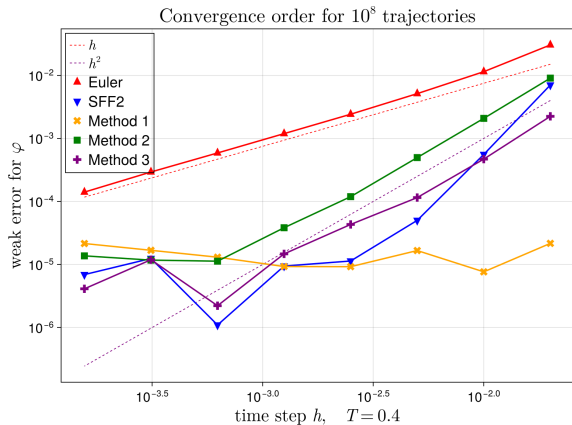
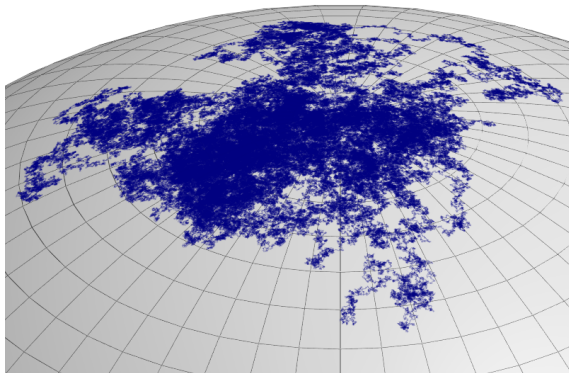


Figure 3: Order of convergence for the potential $(x, y, z) \mapsto -25z$ on the sphere $\mathbb{S}^2$. The mean is at time $T = 0.4$ on 10^8 trajectories and the test function is $\varphi : (x, y, z) \mapsto z^2$.

Integration by parts

Goal: Express A_n^* and derive conditions for higher orders of $d\mu_\infty$.

Proposition

For $\varphi, \psi \in C_p^\infty(\mathcal{M})$ the integration by parts with respect to the Gibbs measure associated to the equation (3) ensures that

$$\int_{\mathcal{M}} E_i[\varphi] \psi d\mu_\infty = - \int_{\mathcal{M}} \varphi E_i[\psi] d\mu_\infty - \int_{\mathcal{M}} \varphi \psi f^i d\mu_\infty,$$

where $F = f^i E_i$ is given by $f^i = -E_i[V] - \langle \nabla_{E_p} E_p | E_i \rangle$.

Example: $\int_{\mathcal{M}} E_{d_1}[f^i] E_{d_1}[E_i[\varphi]] d\mu_\infty = - \int_{\mathcal{M}} E_{d_1}[E_{d_1}[f^i]] E_i[\varphi] d\mu_\infty - \int_{\mathcal{M}} E_{d_1}[f^i] f^{d_1}[E_i[\varphi]] d\mu_\infty$, ie $\textcircled{1} \bullet \sim - \textcircled{1} \textcircled{1} - \textcircled{1}$.

Remark

Note that the application of Proposition 9 does not always rely on exotic forests. If we replace E_i by the vector field F , ie $\psi = f^i$, then a $E_i[f^i]$ appears and cannot be solely expressed by exotic forests,

$$\int_{\mathcal{M}} f^i (E_i \triangleright \varphi) d\mu_\infty = - \int_{\mathcal{M}} (E_i \triangleright f^i) \varphi d\mu_\infty - \int_{\mathcal{M}} f^i f^i \varphi d\mu_\infty.$$

Integration by parts

Definition (Irreducible forests)

The set of irreducible forests $\mathcal{I}_{\mathcal{R}}$ is the set of exotic forest whose first tree is not a numbered node. We denote $\mathcal{I}_{\mathcal{R}} = \text{Span}_{\mathcal{R}}(\mathcal{I}_{\mathcal{R}})$.

Definition (IBP and RED)

Define the linear operator $\text{IBP} : \mathcal{EF} \rightarrow \mathcal{EF}$ by $\text{IBP}|_{\mathcal{I}_{\mathcal{R}}} \equiv 0$ and else

$$\text{IBP}(\odot \tilde{\pi}) = -\tilde{\pi}|_{\odot \rightarrow \bullet} - \sum_{v \in V_{\bullet}} \tilde{\pi}|_{\odot \curvearrowright v}.$$

where $\tilde{\pi}|_{\odot \rightarrow \bullet}$ is the exotic forest obtained by substituting the unique $\odot$ of $\tilde{\pi}$ by $\bullet$ and $\tilde{\pi}|_{\odot \curvearrowright v}$ is the exotic forest obtained by grafting a node $\odot$ on the left of the node v of $\tilde{\pi}$.

Define the linear operator $\text{RED} : \mathcal{EF} \rightarrow \mathcal{I}_{\mathcal{R}}$ by applying IBP on each reducible forest until it remains only irreducible forests, that is

$$\text{RED} = \lim_{n \rightarrow \infty} (\text{id}_{\mathcal{I}_{\mathcal{R}}} + \text{IBP})^n,$$

where RED is well defined as the limit of a stationary sequence, as $(\text{id}_{\mathcal{I}_{\mathcal{R}}} + \text{IBP})^{2|\pi|} \pi \in \mathcal{I}_{\mathcal{R}}$.

Integration by parts

Examples

$$\text{IBP}(\bullet + \textcircled{1}\textcircled{1}) = -\bullet, \quad \text{IBP}(\textcircled{1} \textcircled{1}) = -(\textcircled{1}\textcircled{1} + \textcircled{1}), \quad \text{IBP}(\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}) = -\textcircled{2}\textcircled{2}\bullet,$$

$$\text{RED}(\bullet + \textcircled{1}\textcircled{1}) = 0, \quad \text{RED}(\textcircled{1} \textcircled{1}) = -(\textcircled{1}\textcircled{1} + \textcircled{1}), \quad \text{RED}(\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}) = \bullet\bullet - \textcircled{2}\textcircled{2} - \textcircled{1},$$

$$\text{IBP}(\textcircled{2}\textcircled{1} \textcircled{1}\textcircled{2}) = -(\textcircled{2}\textcircled{1}\textcircled{2} + \textcircled{1}\textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{1}\textcircled{1})$$

$$\text{RED}(\textcircled{2}\textcircled{1} \textcircled{1}\textcircled{2}) = \textcircled{1}\textcircled{2}\textcircled{1}\textcircled{2} + \textcircled{2}\textcircled{1}\textcircled{1}\textcircled{2} + \textcircled{1}\textcircled{1}\textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{1}\textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{1}\textcircled{1} + \textcircled{1}\textcircled{1}\textcircled{2} + \textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{2}\textcircled{2} + \textcircled{1}\textcircled{1}\textcircled{1}.$$

Then we can express the adjoint.

Proposition

For all $\pi \in \mathcal{EF}$, π and $\text{RED}(\pi)$ represent the same adjoint operator, that is,

$$\pi^* d\mu_\infty = \text{RED}(\pi)^* d\mu_\infty.$$

Second order conditions for $A_2 = \sum_{\pi \in \text{EF}} a(\pi) \pi$

Applying RED to $A_2 \varphi = \sum_{\pi \in \text{EF}_2} a(\pi) \mathbb{F}^F(\pi) \triangleright \varphi$ gives us

$$\begin{aligned}
 \int_{\mathcal{M}} A_2 \varphi d\mu_{\infty} &= \sum_{\pi \in \text{EF}_2} a(\pi) \int_{\mathcal{M}} \mathbb{F}^F(\text{RED}(\pi)) \triangleright \varphi d\mu_{\infty} \\
 &= a \left(\begin{array}{c} \textcircled{1} \\ | \\ \bullet - \textcircled{1} \bullet + \textcircled{1} \textcircled{1} \bullet - \textcircled{1} \textcircled{2} \textcircled{2} \textcircled{1} \end{array} \right) \int_{\mathcal{M}} \mathbb{F}^F \left(\begin{array}{c} \textcircled{1} \\ | \\ \bullet \end{array} \right) \triangleright \varphi d\mu_{\infty} \\
 &\quad + a \left(\begin{array}{c} \textcircled{1} \textcircled{1} \\ \vee \\ \bullet - \textcircled{1} \bullet + \textcircled{1} \textcircled{1} \bullet - \textcircled{1} \textcircled{2} \textcircled{2} \textcircled{1} \end{array} \right) \int_{\mathcal{M}} \mathbb{F}^F \left(\begin{array}{c} \textcircled{1} \textcircled{1} \\ \vee \\ \bullet \end{array} \right) \triangleright \varphi d\mu_{\infty} \\
 &\quad + a \left(\bullet \bullet - \textcircled{1} \bullet \textcircled{1} - \textcircled{1} \textcircled{1} \bullet + \textcircled{2} \textcircled{1} \textcircled{2} \textcircled{1} + \textcircled{1} \textcircled{2} \textcircled{2} \textcircled{1} \right) \int_{\mathcal{M}} \mathbb{F}^F(\bullet \bullet) \triangleright \varphi d\mu_{\infty} \\
 &\quad + a \left(\begin{array}{c} \textcircled{1} \\ | \\ \bullet \textcircled{1} - \textcircled{1} \bullet \textcircled{1} + \textcircled{2} \textcircled{1} \textcircled{2} \textcircled{1} \end{array} \right) \int_{\mathcal{M}} \mathbb{F}^F \left(\begin{array}{c} \textcircled{1} \\ | \\ \bullet \textcircled{1} \end{array} \right) \triangleright \varphi d\mu_{\infty} \\
 &\quad + a \left(\bullet \textcircled{1} \textcircled{1} - \textcircled{2} \textcircled{2} \textcircled{1} \textcircled{1} \right) \int_{\mathcal{M}} \mathbb{F}^F(\bullet \textcircled{1} \textcircled{1}) \triangleright \varphi d\mu_{\infty}.
 \end{aligned}$$

Second order conditions for $A_2 = \sum_{\pi \in \text{EF}} a(\pi)\pi$

Theorem (A. BUSNOT LAURENT & S. MACÉ)

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

$$a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) = a \left(\begin{array}{cc} (1) & (1) \\ & \bullet \end{array} \right),$$

$$a(\bullet \textcircled{1} \textcircled{1}) = a(\textcircled{2} \textcircled{2} \textcircled{1} \textcircled{1}),$$

$$a\left(\begin{array}{c} \textcircled{1} \\ \bullet \\ \textcircled{1} \end{array}\right) + a(\textcircled{2}\textcircled{1}\textcircled{2}\textcircled{1}) = a(\textcircled{1} \bullet \textcircled{1})$$

$$a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) + a \left(\begin{array}{c} \textcircled{1} \textcircled{1} \bullet \end{array} \right) = a \left(\begin{array}{c} \textcircled{1} \\ | \\ \textcircled{1} \bullet \end{array} \right) + a \left(\begin{array}{c} \textcircled{1} \textcircled{2} \textcircled{2} \textcircled{1} \end{array} \right),$$

$$a(\bullet \bullet) + a(\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}) = a\left(\begin{array}{c} \textcircled{1} \\ \bullet \\ \textcircled{1} \end{array}\right) + a(\textcircled{1}\textcircled{1} \bullet).$$

For the third order, there are **40 equations and with 95 variables**. We recall from E. BRONASCO & A. BUSNOT LAURENT & B. HUGUET, 2025; that for the weak error, there are **8 equations for the order 2** and **73 for the order 3**.

[illegible]

Table 1: Second order reductions.

Future works

- Application of our construction to Runge-Kutta-Munthe-Kaas methods on Lie groups
- Intrinsic stochastic backward error analysis to modify the equation to reach higher order
- Application to multiscale context
- Extension to fully Riemannian method: $\exp^{Riem}$
- Extension to general ergodic SDEs on manifolds (work in progress)

