

Intrinsic integrators for the weak and ergodic approximation of stochastic dynamics on manifolds

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ANR project MaStoC - Manifolds and Stochastic Computations

Contents

- 1 Intrinsic stochastic numerics on manifolds
- 2 New stochastic frozen-flow integrators
- 3 Convergence analysis
- 4 Algebraic foundations of intrinsic stochastic order theory

References of this talk:

- E. Bronasco, A. BL, Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations, *Numer. Math.* (2026).
- E. Bronasco, A. BL, B. Huguet, High order integration of stochastic dynamics on Riemannian manifolds with frozen flow methods, In revision in *FoCM*.
- A. BL, S. Macé, Post-processed frozen-flow methods for the long time sampling of ergodic dynamics on Riemannian manifolds, *arXiv:2606.06150*.

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Riemannian stochastic dynamics

Consider a Riemannian manifold $(\mathcal{M}, \nabla^{\text{LC}})$. Let $E_1, \dots, E_D$ be a smooth frame:

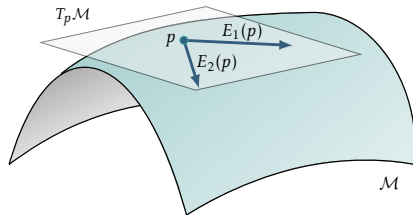
$$\text{Span}_{\mathbb{R}}(E_1(p), \dots, E_D(p)) = T_p\mathcal{M}, \quad y \in \mathcal{M}.$$

Given a vector field $F(x) = \sum_{d=1}^D f^d(x) E_d(x)$, we consider

$$dX(t) = F(X(t))dt + \sqrt{2} \sum_{d=1}^D E_d(X(t)) \circ dW_d(t).$$

Riemannian Langevin dynamics for E_d orthonormal basis:

$$dX(t) = - \sum_{d=1}^D (E_d[V]E_d + \nabla_{E_d}^{\text{LC}} E_d)(X(t))dt + \sqrt{2} \sum_{d=1}^D E_d(X(t)) \circ dW_d(t)$$



Riemannian stochastic dynamics

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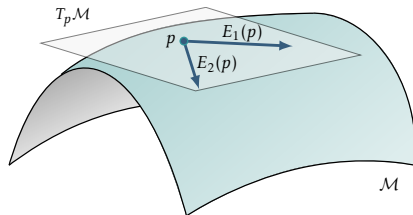
$$\text{Span}_{\mathbb{R}}(E_1(p), \dots, E_D(p)) = T_p\mathcal{M}, \quad y \in \mathcal{M}.$$

Given a vector field $F(x) = \sum_{d=1}^D f^d(x) E_d(x)$, we consider

$$dX(t) = F(X(t))dt + \sqrt{2} \sum_{d=1}^D E_d(X(t)) \circ dW_d(t).$$

Riemannian Langevin dynamics for E_d orthonormal basis:

$$dX(t) = -\nabla_{\mathcal{M}} V(X(t))dt + \sqrt{2}dW_{\mathcal{M}}(t)$$



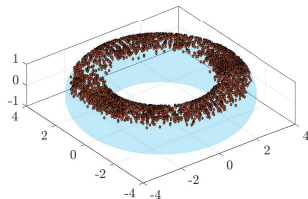
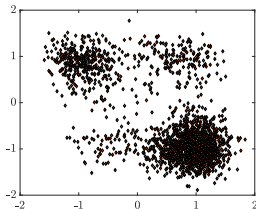
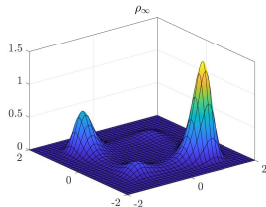
Ergodicity and applications

Weak approximations: Given a test function $\phi \in \mathcal{C}_p^\infty(\mathcal{M})$, an integrator is of weak order p if

$$|\mathbb{E}[\phi(X_n)] - \mathbb{E}[\phi(X(t_n))]| \leq Ch^p, \quad n = 0, \dots, N.$$

Ergodicity property:

$$\lim_{T \rightarrow +\infty} \frac{1}{T} \int_0^T \phi(X(s)) ds = \int_{\mathcal{M}} \phi(y) \rho_\infty(y) d \text{vol}(y) \quad \text{almost surely,} \quad \rho_\infty \propto e^{-V}.$$

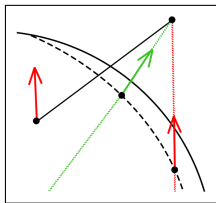


Applications of sampling on manifolds: geometric statistics, molecular dynamics, stochastic optimisation, ...

Existing stochastic integrators on manifolds

Motivations for finding intrinsic methods:

- Projection methods rely on an embedding in a bigger space, are expensive and unstable.
- The high order theory of projection methods is **difficult** (BL, 2021 - 7 pages of calculations, **no straightforward algebraic structure**, ~ 25 order conditions for order 2).



Example (Euler projection integrator)

The most popular integrator is **the Euler scheme** with **explicit** projection direction^a

$$X_{n+1} = X_n + hf(X_n) + \sqrt{2h}\xi_n + \lambda \nabla \zeta(X_n), \quad \zeta(X_{n+1}) = 0.$$

^aCiccotti, Kapral, Vanden-Eijnden, 2005; Lelièvre, Le Bris, Vanden-Eijnden, 2008; Lelièvre, Rousset, Stolz, 2010; ...

Example (From Bharath, Lewis, Sharma, Tretyakov, 2024)

The Riemannian Langevin method has order one:

$$X_{n+1} = \exp_{X_n}^{\text{Riem}}(hf(X_n) + \sqrt{2hg}^{-1/2}(X_n)\xi_n)$$

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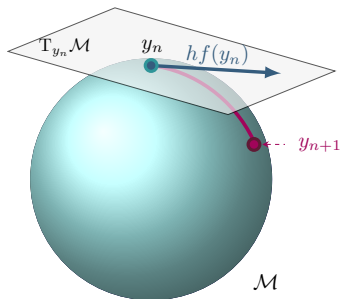
Connection and geodesic exponential

An affine **connection** $\triangleright: \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \rightarrow \mathfrak{X}(\mathcal{M})$ encodes the geometric structure we equip the manifold with.

A **geodesic** $\gamma(t) = \exp(tv)p$ is a curve on $\mathcal{M}$ satisfying

$$\gamma'(t) \triangleright \gamma'(t) = 0, \quad \gamma(0) = p \in \mathcal{M}, \quad \gamma'(0) = v \in T_p\mathcal{M}.$$

Example: the **geodesic Euler method** for $y' = F(y)$ is $y_{n+1} = \exp(hF(y_n))y_n$.



Example

Euclidean case:

$$g \triangleright f(p) = f'(p)g(p),$$

$$\exp(tv)p = p + tv.$$

Matrix Lie group:

$$\exp(tv)p = \text{Exp}(tv)p.$$

Frame and connection

Let $E_1, \dots, E_D$ be a **frame basis** (for simplicity):

$$\text{Span}_{\mathbb{R}}(E_1(p), \dots, E_D(p)) = T_p \mathcal{M}, \quad p \in \mathcal{M}.$$

Define the **Weitzenböck connection**

$$G \triangleright F = \sum_{d=1}^D G[f^d] E_d, \quad F = \sum_{d=1}^D f^d E_d,$$

and the bracket

$$[F, G] = \llbracket F, G \rrbracket_J - F \triangleright G + G \triangleright F = -T(F, G),$$

where $\llbracket F, G \rrbracket_J$ is the Jacobi bracket.

Proposition (Ebrahimi-Fard, Lundervold, Munthe-Kaas, '12)

*If the frame spans a Lie algebra, the space $(\mathfrak{X}(\mathcal{M}), [-, -], \triangleright)$ is a **post-Lie algebra**:*

$$F \triangleright [G, H] = [F \triangleright G, H] + [G, F \triangleright H],$$

$$[F, G] \triangleright H = F \triangleright (G \triangleright H) - (F \triangleright G) \triangleright H - G \triangleright (F \triangleright H) + (G \triangleright F) \triangleright H.$$

*In particular, $\triangleright$ has **constant torsion and vanishing curvature**.*

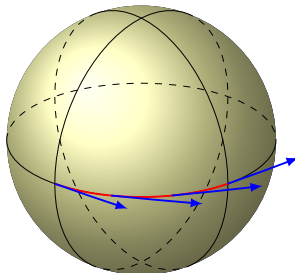
Frozen flows and frozen-flow methods

A **frozen vector field** is

$$F_x(p) = \sum_{d=1}^D f^d(x) E_d(p).$$

The **frozen-flow** $\exp(tF_x)p$ is the solution of

$$y'(t) = F_x(y(t)), \quad y(0) = p.$$



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Proposition

The *frozen-flow Euler method* for

$$dX = F(X)dt + \sqrt{2}E_d(X) \circ dW_d$$

is of weak order one and is given by

$$Y_{n+1} = \exp \left(\sum_{d=1}^D \left(hf^d(Y_n) + \sqrt{2h}\xi_n^d \right) E_d \right) Y_n, \quad \xi_n \sim \mathcal{N}(0, I_D)$$

Frozen flows and frozen-flow methods

New frozen-flow integrators¹

$$\begin{aligned} H_n^i &= \exp\left(\sum_{d=1}^D \left(h \sum_{j=1}^s Z_{i,j,K}^0 f^d(H_n^j) + \sqrt{h} Z_{i,K}^d\right) E_d\right) \dots \\ &\dots \exp\left(\sum_{d=1}^D \left(h \sum_{j=1}^s Z_{i,j,1}^0 f^d(H_n^j) + \sqrt{h} Z_{i,1}^d\right) E_d\right) Y_n, \\ Y_{n+1} &= \exp\left(\sum_{d=1}^D \left(h \sum_{i=1}^s z_{i,K}^0 f^d(H_n^i) + \sqrt{h} z_K^d\right) E_d\right) \dots \\ &\dots \exp\left(\sum_{d=1}^D \left(h \sum_{i=1}^s z_{i,1}^0 f^d(H_n^i) + \sqrt{h} z_1^d\right) E_d\right) Y_n. \end{aligned}$$

where the coefficients are **Gaussian**.

Remark: the frozen-flow methods work on **ANY smooth Riemannian manifold**.

¹in the spirit of [Crouch-Grossman and commutator-free Lie group methods](#), see Celledoni, Marthinsen, Owren and also Iserles, Munthe-Kaas, Quispel, Zanna, ~ 1990's-2006

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Convergence theorem for weak error

Theorem (Bronasco, BL, Huguet)

Taylor-Talay-Tubaro expansions:

$$\begin{aligned}\mathbb{E}[\phi(X_1)|X_0 = x] &= \phi(x) + \sum_{j=1}^p h^j \mathcal{A}_j \phi(x) + h^{p+1} R_p^h(\phi, x), \\ \mathbb{E}[\phi(X(h))|X_0 = x] &= \phi(x) + \sum_{j=1}^p \frac{h^j}{j!} \mathcal{L}^j \phi(x) + h^{p+1} R_p^h(\phi, x).\end{aligned}$$

Then, the integrator has global weak order p if $\mathcal{A}_j = \frac{1}{j!} \mathcal{L}^j$, $j = 1, \dots, p$.

New explicit frozen flow integrator of weak order two:

$$\begin{aligned}H_n &= \exp \left(\sum_{d=1}^D \left(\frac{1}{2} h f^d(Y_n) + \sqrt{h} \xi_n^{d,1} \right) E_d \right) Y_n \\ Y_{n+1} &= \exp \left(\sum_{d=1}^D \left(\left(\frac{\sqrt{2}}{2} - 1 \right) h f^d(Y_n) + (2 - \sqrt{2}) h f^d(H_n) + (1 - \sqrt{2}) \sqrt{h} \xi_n^{d,1} + \sqrt{h} \xi_n^{d,2} \right) E_d \right) \\ &\quad \exp \left(\sum_{d=1}^D \left(\left(1 - \frac{\sqrt{2}}{2} \right) h f^d(Y_n) + (\sqrt{2} - 1) h f^d(H_n) + \sqrt{2h} \xi_n^{d,1} \right) E_d \right) Y_n.\end{aligned}$$

Convergence theorem for the invariant measure²

Theorem (BL, Macé)

Let the Taylor-Talay-Tubaro expansion $\mathbb{E}[\phi(X_1)] = \phi + h\mathcal{A}_1\phi + h^2\mathcal{A}_2\phi + \dots$
Under technical assumptions, if the operators satisfy

$$\mathcal{A}_1 = \mathcal{L}, \quad \mathcal{A}_j^* \rho_\infty d\text{vol} = 0, \quad j = 2, \dots, p,$$

then the integrator has order p for the invariant measure.

Frozen-flow generalisation of the Leimkuhler-Matthews method:

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

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

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

²see also Debussche, Faou, 2012 and Abdulle, Vilmart, Zygalakis, 2014.

Numerical experiment on SO

Sampling of Riemannian Langevin dynamics with a quadratic potential:

$$dX(t) = -\nabla_{\mathcal{M}} V(X(t))dt + \sqrt{2}dW_{\mathcal{M}}(t).$$

The frame simply is

$$E_d(y) = A_d y, \quad A_d \in \mathfrak{so}.$$

Method 1 New order 2 method on SO

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

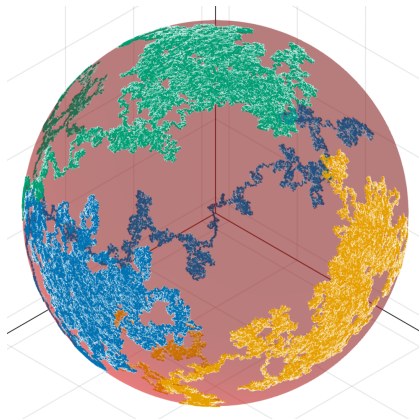
$$X_{n+1} = \text{Exp} \left(\left(\frac{5h}{4} f^d(H_n) + \frac{\sqrt{2h}}{4} \xi_n^d \right) A_d \right) \text{Exp} \left(\left(-\frac{h}{4} f^d(H_n) + \frac{3\sqrt{2h}}{4} \xi_n^d \right) A_d \right) X_n,$$

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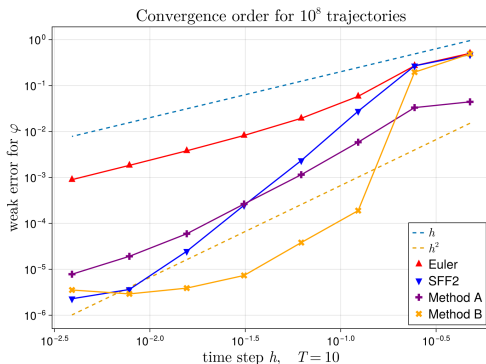
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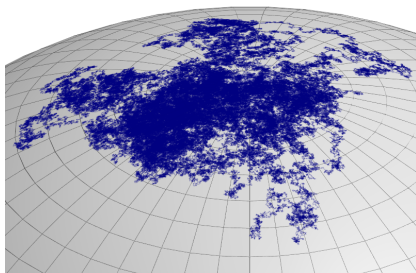


Trajectory on SO_3 with quadratic potential.

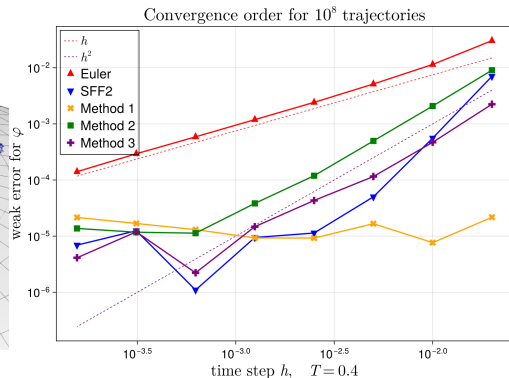


Order for the invariant measure for a quadratic potential on SO_3 .

Numerical experiment on $\mathbb{S}^2$



Sampling the Von-Mises-Fisher distribution.



Order for the invariant measure for the potential $(x, y, z) \mapsto -25z$.

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Hopf algebras over vector fields

Let the **frozen composition** in $T(\mathfrak{X}(\mathcal{M}))$ be the differential operator

$$(G \cdot F) \triangleright \phi = \sum_{i,j} g^j f^i E_j[E_i[\phi]].$$

Similarly, define the **Grossman-Larson product** (extend by Guin-Oudom)

$$(G * F) \triangleright \phi = \sum_{i,j} g^j E_j[f^i E_i[\phi]] = G \triangleright (F \triangleright \phi) = (G \triangleright F) \triangleright \phi + (G \cdot F) \triangleright \phi.$$

In $\mathbb{R}^d$, we have

$$(G \cdot F) \triangleright \phi = \phi''(G, F), \quad (G * F) \triangleright \phi = (\phi' F)' G.$$

Then, $(T(\mathfrak{X}(\mathcal{M})), \cdot, \Delta_{\sqcup}, \triangleright)$ and $(T(\mathfrak{X}(\mathcal{M})), *, \Delta_{\sqcup})$ are **Hopf algebras**.

Hopf algebras over vector fields

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Then, $(T(\mathfrak{X}(\mathcal{M})), \cdot, \Delta_{\sqcup}, \triangleright)$ and $(T(\mathfrak{X}(\mathcal{M})), *, \Delta_{\sqcup})$ are **Hopf algebras**.

Proposition

The Taylor expansions of the **geodesic and exact flow exponentials** are

$$\phi(\exp(F_p)p) = \exp \cdot (F) \triangleright \phi(p), \quad \phi(\exp(F)p) = \exp^*(F) \triangleright \phi(p),$$

where $\exp^*(F) = \text{id} + F + \frac{1}{2!} F * F + \frac{1}{3!} F * F * F + \dots$

Example of the Euler method

The Taylor expansion of the Euler frozen-flow method is

$$\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p) = \exp(hF + \sqrt{2h}\xi^d E_d) \triangleright \phi$$

³see Isserlis-Wick theorem.

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The Taylor expansion of the Euler frozen-flow method is

$$\begin{aligned}\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p) &= \exp(hF + \sqrt{2h}\xi^d E_d) \triangleright \phi \\ &= \left(\text{id} + h^{1/2}\sqrt{2}\xi^d E_d + h(F + \xi^{d_2}\xi^{d_1} E_{d_2} \cdot E_{d_1}) \right. \\ &\quad \left. + h^{3/2}\left(\frac{\sqrt{2}}{2}\xi^d F \cdot E_d + \frac{\sqrt{2}}{2}\xi^d E_d \cdot F + \frac{\sqrt{2}}{3}\xi^{d_3}\xi^{d_2}\xi^{d_1} E_{d_3} \cdot E_{d_2} \cdot E_{d_1}\right) + \dots \right) \triangleright \phi.\end{aligned}$$

³see Isserlis-Wick theorem.

Example of the Euler method

The Taylor expansion of the Euler frozen-flow method is

$$\begin{aligned}\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p) &= \exp(hF + \sqrt{2h}\xi^d E_d) \triangleright \phi \\ &= \left(\text{id} + h^{1/2} \sqrt{2} \xi^d E_d + h(F + \xi^{d_2} \xi^{d_1} E_{d_2} \cdot E_{d_1}) \right. \\ &\quad \left. + h^{3/2} \left(\frac{\sqrt{2}}{2} \xi^d F \cdot E_d + \frac{\sqrt{2}}{2} \xi^d E_d \cdot F + \frac{\sqrt{2}}{3} \xi^{d_3} \xi^{d_2} \xi^{d_1} E_{d_3} \cdot E_{d_2} \cdot E_{d_1} \right) + \dots \right) \triangleright \phi.\end{aligned}$$

Then, the expectation pairs the Gaussians together³ and yields

$$\begin{aligned}\mathbb{E}[\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p)] &= \left(\text{id} + h(F + E_d \cdot E_d) \right. \\ &\quad + h^2 \left(\frac{1}{2} F \cdot F + \frac{1}{3} F \cdot E_d \cdot E_d + \frac{1}{3} E_d \cdot F \cdot E_d + \frac{1}{3} E_d \cdot E_d \cdot F \right. \\ &\quad + \frac{1}{6} E_{d_2} \cdot E_{d_2} \cdot E_{d_1} \cdot E_{d_1} + \frac{1}{6} E_{d_2} \cdot E_{d_1} \cdot E_{d_2} \cdot E_{d_1} + \frac{1}{6} E_{d_1} \cdot E_{d_2} \cdot E_{d_2} \cdot E_{d_1} \\ &\quad \left. \left. + \dots \right) \right) \triangleright \phi.\end{aligned}$$

³see Isserlis-Wick theorem.

Elementary differential map

The elementary differential map $\mathbb{F}: \mathcal{EF} \rightarrow T(\mathcal{X}(\mathcal{M}))$ translates from exotic forests to differential operators:

$$\mathbb{F}(\bullet) = F, \quad \mathbb{F}(\textcircled{\bullet}) = F \triangleright F, \quad \mathbb{F}(\textcircled{\textcircled{\bullet}}) = E_d \cdot (E_d \triangleright F), \quad \mathbb{F}(\textcircled{\bullet} \textcircled{\bullet}) = (E_d \triangleright F) \cdot E_d.$$

Proposition

$\mathbb{F}$ is a *morphism* and $(\mathcal{EF}, \cdot, \Delta_{\sqcup})$ and $(\mathcal{EF}, \diamond, \Delta_{\sqcup})$ are *Hopf algebras*.

Example (frozen-flow Euler method)

$$\begin{aligned} \mathbb{E}[\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p)] &= \mathbb{F}\left(\mathbf{1} + h(\bullet + \textcircled{\bullet}) + h^2\left(\frac{1}{2}\bullet \bullet + \frac{1}{3}\bullet \textcircled{\bullet}\right.\right. \\ &\quad \left.\left.+ \frac{1}{3}\textcircled{\bullet} \bullet + \frac{1}{3}\textcircled{\bullet} \textcircled{\bullet} + \frac{1}{6}\textcircled{\textcircled{\bullet}} \textcircled{\textcircled{\bullet}} + \frac{1}{6}\textcircled{\textcircled{\bullet}} \textcircled{\textcircled{\bullet}} + \frac{1}{6}\textcircled{\textcircled{\bullet}} \textcircled{\textcircled{\textcircled{\bullet}}}\right) + \dots\right) \triangleright \phi(p) \\ &= \left(\text{id} + h(F + E_d \cdot E_d) + h^2\left(\frac{1}{2}F \cdot F + \frac{1}{3}F \cdot E_d \cdot E_d + \frac{1}{3}E_d \cdot F \cdot E_d\right.\right. \\ &\quad \left.\left.+ \frac{1}{3}E_d \cdot E_d \cdot F + \frac{1}{6}E_{d_2} \cdot E_{d_2} \cdot E_{d_1} \cdot E_{d_1} + \frac{1}{6}E_{d_2} \cdot E_{d_1} \cdot E_{d_2} \cdot E_{d_1} + \dots\right)\right) \triangleright \phi(p). \end{aligned}$$

Weak order conditions

Exotic forest π	Differential $\mathbb{F}(\pi)[\phi]$	Order condition $a(\pi) = e(\pi)$
$\bullet$	$f^i E_i[\phi]$	$z_{i,k_1}^0 = 1$
$\textcircled{1}\textcircled{1}$	$E_{d_1}[E_{d_1}[\phi]]$	$\sum_{k_1 \geq k_2}^! \mathbb{E}[z_{k_2}^{d_1} z_{k_1}^{d_1}] = 1$
$\bullet$ $\textcircled{1}\textcircled{1}$	$f^j E_j[f^i] E_i[\phi]$	$z_{i,k_2}^0 z_{i,j,k_1}^0 = \frac{1}{2}$
$\textcircled{1}\textcircled{1}$ $\bullet$	$E_{d_1}[E_{d_1}[f^i]] E_i[\phi]$	$\sum_{k_2 \geq k_3}^! \mathbb{E}[Z_{i,k_3}^{d_1} Z_{i,k_2}^{d_1}] z_{i,k_1}^0 = \frac{1}{2}$
$\bullet \bullet$	$f^j f^i E_j[E_i[\phi]]$	$\sum_{k_1 \geq k_2}^! z_{j,k_2}^0 z_{i,k_1}^0 = \frac{1}{2}$
$\textcircled{1}$ $\bullet \textcircled{1}$	$E_{d_1}[f^i] E_i[E_{d_1}[\phi]]$	$\sum_{k_1 \geq k_2}^! z_{i,k_2}^0 \mathbb{E}[Z_{i,k_3}^{d_1} z_{k_1}^{d_1}] = 0$
$\textcircled{1}\textcircled{1}$ $\bullet$	$E_{d_1}[f^i] E_{d_1}[E_i[\phi]]$	$\sum_{k_2 \geq k_1}^! z_{i,k_2}^0 \mathbb{E}[Z_{i,k_3}^{d_1} z_{k_1}^{d_1}] = 1$
$\bullet \textcircled{1}\textcircled{1}$	$f^i E_i[E_{d_1}[E_{d_1}[\phi]]]$	$\sum_{k_1 \geq k_2 \geq k_3}^! z_{i,k_3}^0 \mathbb{E}[z_{k_2}^{d_1} z_{k_1}^{d_1}] = \frac{1}{2}$
$\textcircled{1} \bullet \textcircled{1}$	$f^i E_{d_1}[E_i[E_{d_1}[\phi]]]$	$\sum_{k_1 \geq k_3 \geq k_2}^! z_{i,k_3}^0 \mathbb{E}[z_{k_2}^{d_1} z_{k_1}^{d_1}] = 0$
$\textcircled{1}\textcircled{1} \bullet$	$f^i E_{d_1}[E_{d_1}[E_i[\phi]]]$	$\sum_{k_3 \geq k_1 \geq k_2}^! z_{i,k_3}^0 \mathbb{E}[z_{k_2}^{d_1} z_{k_1}^{d_1}] = \frac{1}{2}$
$\textcircled{2}\textcircled{2}\textcircled{1}\textcircled{1}$	$E_{d_2}[E_{d_2}[E_{d_1}[E_{d_1}[\phi]]]]$	$\sum_{k_1 \geq k_2 \geq k_3 \geq k_4}^! \mathbb{E}[z_{k_4}^{d_2} z_{k_3}^{d_2}] \mathbb{E}[z_{k_2}^{d_1} z_{k_1}^{d_1}] = \frac{1}{2}$
$\textcircled{2}\textcircled{1}\textcircled{2}\textcircled{1}$	$E_{d_2}[E_{d_1}[E_{d_2}[E_{d_1}[\phi]]]]$	$\sum_{k_1 \geq k_2 \geq k_3 \geq k_4}^! \mathbb{E}[z_{k_4}^{d_2} z_{k_2}^{d_2}] \mathbb{E}[z_{k_3}^{d_1} z_{k_1}^{d_1}] = 0$
$\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}$	$E_{d_1}[E_{d_2}[E_{d_2}[E_{d_1}[\phi]]]]$	$\sum_{k_1 \geq k_2 \geq k_3 \geq k_4}^! \mathbb{E}[z_{k_3}^{d_2} z_{k_2}^{d_2}] \mathbb{E}[z_{k_4}^{d_1} z_{k_1}^{d_1}] = 0$

Order conditions for the invariant measure

Theorem (A. BL & S. MACÉ)

A numerical method is of **order 2 for the invariant measure** if it satisfies

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

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

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

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

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

For the third order, there are **40 equations** for the invariant measure, instead of **73 weak order conditions**.

Forest π	RED(π)
$\bullet \bullet$	$\bullet \bullet$
	$-\bullet - \textcircled{1} \textcircled{1}$
$\bullet \textcircled{1} \textcircled{1}$	$\bullet \textcircled{1} \textcircled{1}$
$\textcircled{1} \bullet \textcircled{1}$	$-\bullet - \textcircled{1} \textcircled{1}$
$\textcircled{1} \textcircled{1} \bullet$	$\bullet + \textcircled{1} \textcircled{1} - \bullet \bullet$
$\textcircled{2} \textcircled{2} \textcircled{1} \textcircled{1}$	$-\bullet \textcircled{1} \textcircled{1}$
$\textcircled{2} \textcircled{1} \textcircled{2} \textcircled{1}$	$\bullet \bullet + \textcircled{1} \textcircled{1}$
$\textcircled{1} \textcircled{2} \textcircled{2} \textcircled{1}$	$\bullet \bullet - \bullet - \textcircled{1} \textcircled{1}$

Table: Second order reductions.

Conclusion

Summary:

- We provide a **brand new class** of **intrinsic** high-order methods for solving stochastic dynamics on manifolds in the weak sense and for the invariant measure.
- We give a **Riemannian convergence analysis** in both cases.
- The order theory relies on a new formalism of **planar exotic forests**, which extends the existing deterministic works and now appears in quantum physics, in the approximation of PDEs, the study of turbulence,...

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Summary:

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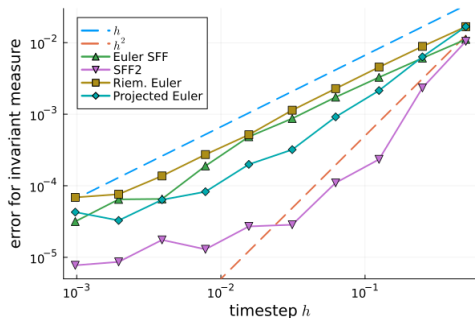
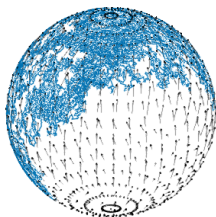
Outlooks:

- The analysis and implementation rely on an **artificial connection**. Ongoing extension of Lie-group methods to any geometry (with S. Carrier, H. Munthe-Kaas,...).
- Characterisation of **exact sampling methods** with the exotic aromatic bicomplex (with V. Dotsenko, P. Laubie, J. Sao Joao).
- Concrete applications in **electromagnetics and biology** (with S. Macé and Inria).
- **Algebraic and geometric foundations of intrinsic geometric integration** (ANR MaStoC team: S. Carrier, N. En-Nebbazi, S. Macé.)

Numerical experiment on the sphere

We now have **3 numerical approaches**:

- **Projection**: $X_{n+1} = X_n + hF(X_n) + \sqrt{2h}\xi_n + \lambda g(X_n), \quad \zeta(X_{n+1}) = 0,$
- **Riemannian**: $X_{n+1} = \exp_{X_n}^{\text{Riem}}(hF(X_n) + \sqrt{2h}\xi_n),$
- **Frozen-flow**: $X_{n+1} = \exp(hF(X_n) + \sqrt{2h}\xi_n^d E_d)X_n.$



The new second order methods outperforms the other integrators in accuracy for a similar cost. It is the **first high-order intrinsic integrator of the literature**.

Primitive elements and shuffle relations

Shuffle product:

$$\begin{aligned}\bullet \sqcup \textcircled{1}\textcircled{1} &= \bullet \textcircled{1}\textcircled{1} + \textcircled{1} \bullet \textcircled{1} + \textcircled{1}\textcircled{1} \bullet, \\ \textcircled{2}\textcircled{2} \sqcup \textcircled{1}\textcircled{1} &= 2\textcircled{2}\textcircled{2}\textcircled{1}\textcircled{1} + 2\textcircled{2}\textcircled{1}\textcircled{2}\textcircled{1} + 2\textcircled{2}\textcircled{1}\textcircled{1}\textcircled{2},\end{aligned}$$

The coefficient maps of numerical flows are **characters** of $(\mathcal{EF}, \sqcup)$:

$$a(\pi_1 \sqcup \pi_2) = a(\pi_1)a(\pi_2).$$

Following Owren, '06, we have **shuffle relations**:

$$\begin{aligned}a(\bullet)^2 &= 2a(\bullet \bullet), \\ a(\bullet)a(\textcircled{1}\textcircled{1}) &= a(\bullet \textcircled{1}\textcircled{1}) + a(\textcircled{1}\textcircled{1} \bullet) + a(\textcircled{1} \bullet \textcircled{1}), \\ a(\textcircled{1}\textcircled{1})^2 &= 2a(\textcircled{2}\textcircled{2}\textcircled{1}\textcircled{1}) + 2a(\textcircled{2}\textcircled{1}\textcircled{2}\textcircled{1}) + 2a(\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}).\end{aligned}$$

Proposition

The order conditions are indexed by the exotic forests, modulo the shuffle relations. In particular, there are 2, 8, and 73 conditions for order 1, 2, and 3 (against 2, 11, and 95 exotic forests).

Exotic MKW structure

Theorem

Let the Munthe-Kaas-Wright coproduct:

$$\Delta_{MKW}(\tau) := \sum_{\text{adm. cut } c} P^c(\tau) \otimes R^c(\tau), \quad \Delta_{MKW}(\pi) := (id \otimes B^-) \Delta_{MKW}(B^+(\pi)).$$

Then, $(\mathcal{EF}, \sqcup, \Delta_{MKW})$ is a **Hopf algebra** dual to $(\mathcal{EF}, \diamond, \Delta_{\sqcup})$. Its convolution product represents the composition of exotic series:

$$S(a) \circ S(b) = S(a * b), \quad a * b = \mu_{\mathbb{R}} \circ (a \otimes b) \circ \Delta_{MKW},$$

Example

$$\Delta_{MKW}(\textcircled{1}\textcircled{1}) = \textcircled{1}\textcircled{1} \otimes \mathbf{1} + \mathbf{1} \otimes \textcircled{1}\textcircled{1},$$

$$\Delta_{MKW}(\textcircled{1}\textcircled{1}) = \textcircled{1}\textcircled{1} \otimes \mathbf{1} + \textcircled{1}\textcircled{1} \otimes \bullet + \mathbf{1} \otimes \textcircled{1}\textcircled{1},$$

$$\begin{aligned} \Delta_{MKW}(\textcircled{1}\textcircled{1}) &= \textcircled{1}\textcircled{1} \otimes \mathbf{1} + 2\textcircled{1}\textcircled{1} \otimes \bullet + (\textcircled{1}\textcircled{1} + \textcircled{1}\textcircled{1}) \otimes \bullet + (\textcircled{1}\textcircled{1} + \textcircled{1}\textcircled{1}) \otimes \bullet \\ &\quad + (\textcircled{1}\textcircled{1} + \textcircled{1}\textcircled{1}) \otimes \bullet + 2\textcircled{1}\textcircled{1} \otimes \bullet + \mathbf{1} \otimes \textcircled{1}\textcircled{1}. \end{aligned}$$