

# Composing exponentials and intrinsic numerical integration on manifolds

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Project MaStoC - Manifolds and Stochastic Computations



# Motivation: ODE $y' = F(y)$ , $F \in \mathfrak{X}(\mathcal{M})$

Dynamics on a manifold  $\mathcal{M}$ : .

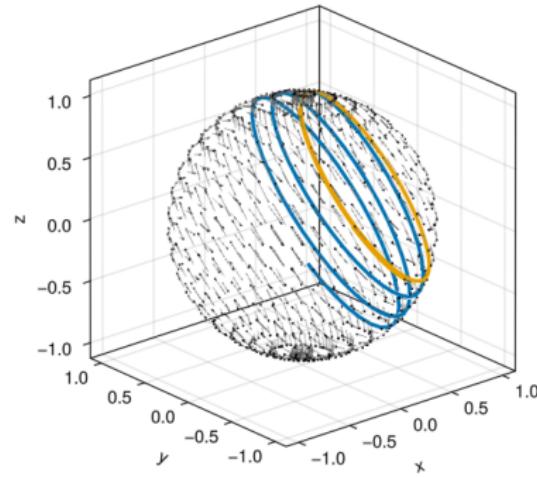
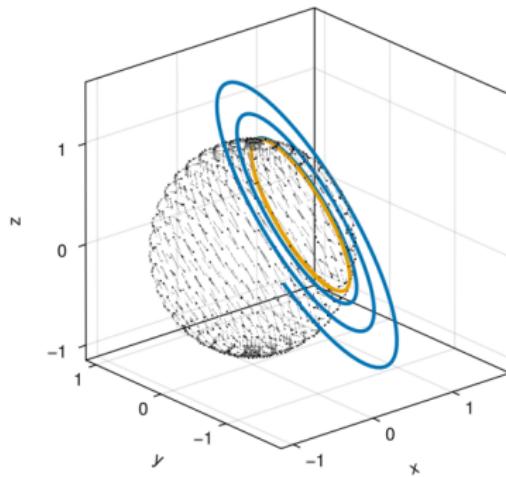
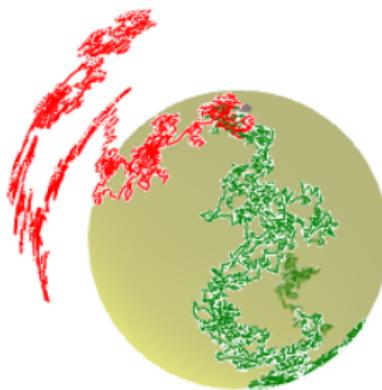


Figure: Non-geometric versus geometric methods for  $y' = A(y)y$ ,  $A^T = -A$ .

**Idea:** dynamics come with geometric invariants and the **numerical methods should try to preserve invariants as much as possible.**

**Challenge:** a geometry is not just a manifold. The numerical approaches have to satisfy that **their definition, convergence analysis, and implementation all rely on the same geometric framework as the model.**

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**Figure:** Numerical simulations of a Brownian motion on the sphere.

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# Contents

- 1 Composition of exponentials with Lie algebras and Lie group methods
- 2 Notions of differential geometry
- 3 From Lie-group methods to general methods on manifolds

## References of this talk:

- K. Beauchard, A. BL, F. Marbach, Control theory and splitting methods, arXiv:2407.02127.
- E. Bronasco, A. BL, B. Huguet, High order integration of stochastic dynamics on Riemannian manifolds with frozen flow methods, arXiv:2503.21855.
- A. BL, E. Grong, H. Munthe-Kaas, General RKM methods, *Ongoing*.

# Contents

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# Lie algebras and adjoint map

## Definition

A **Lie algebra** is

- A vector space  $\mathfrak{g}$
- A bilinear  $[-, -]: \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$  satisfying

$$[a, b] = -[b, a], \quad [a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0.$$

The smallest Lie algebra spanned by a set  $A$  is  $\text{Lie}(A)$ . The **adjoint representation** is

$$\text{ad}_\omega(x) = [\omega, x].$$

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## Example

Let an alphabet  $A = \{a, b, c, \dots\}$  and an associative product  $\cdot$ . Then  $(\text{Span}(A), [-, -])$  is a Lie algebra, where

$$[a, b] = a \cdot b - b \cdot a.$$

The words algebra  $\mathcal{W} = T(A) = \mathcal{U}(\text{Lie}(A))$  is generated by words:  $abc = a \cdot b \cdot c$ .

# The BCH formula

## Theorem (Baker-Campbell-Hausdorff formula)

Let  $a, b \in \text{Lie}(A)$ , then the **product of exponentials** satisfies

$$\exp^{\cdot}(a) \cdot \exp^{\cdot}(b) = \exp^{\cdot}(\text{BCH}(a, b)), \quad \exp^{\cdot}(x) = \sum \frac{1}{n!} x^{\cdot n}$$

where  $\text{BCH}: \text{Lie}(A) \times \text{Lie}(A) \rightarrow \text{Lie}(A)$  is the solution  $\text{BCH}(a, b) = \omega(1)$  of the ODE

$$\omega'(t) = d_{\omega(t)} \exp^{\cdot -1}(ta), \quad \omega(0) = b.$$

## Example

The first terms are

$$\begin{aligned} \text{BCH}(a, b) = & a + b + \frac{1}{2}[a, b] + \frac{1}{12}([a, [a, b]] + [b, [b, a]]) - \frac{1}{24}[b, [a, [a, b]]] \\ & - \frac{1}{720}([b, [b, [b, [b, a]]]] + [a, [a, [a, [a, b]]]]) \\ & + \frac{1}{360}([a, [b, [b, [b, a]]]] + [b, [a, [a, [a, b]]]]) + \dots \end{aligned}$$

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## Proof.

Let  $\omega(t) = \text{BCH}(ta, b)$  satisfy  $\exp^{\cdot}(\omega(t)) = \exp^{\cdot}(ta) \cdot \exp^{\cdot}(b)$ . Then we find

$$d_{\omega(t)} \exp^{\cdot}(\omega'(t)) \cdot \exp^{\cdot}(\omega(t)) = d_{ta} \exp^{\cdot}(a) \cdot \exp^{\cdot}(ta) \cdot \exp^{\cdot}(b) = ta \cdot \exp^{\cdot}(\omega(t)).$$

Hence the result. □

## A word on the map $d \exp$

The **derivative of the exponential**  $d \exp$  satisfies (see e.g. Reutenauer, 1993)

$$d_\omega \exp \cdot = \sum_{n=0} \frac{1}{(n+1)!} \text{ad}_\omega^n = \frac{e^z - 1}{z} \Big|_{z=\text{ad}_\omega}.$$

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Moreover,  $d_\omega \exp^{\cdot}$  is invertible as a formal series and satisfies

$$d_\omega \exp^{\cdot -1} = \sum_{n=0} \frac{B_n}{n!} \text{ad}_\omega^n = \frac{z}{e^z - 1} \Big|_{z=\text{ad}_\omega},$$

where the  $B_n$  are the Bernoulli numbers:

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = 0, \quad B_4 = -\frac{1}{30}, \quad B_5 = 0, \quad B_6 = \frac{1}{42}, \dots$$

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### Remark

*The BCH formula is used in the high order theory of splitting methods (see, for instance, Blanes, Casas, 2024), in control theory, ...*

# Lie group methods - RKM<sup>K</sup> approach<sup>1</sup>

## Proposition

Consider the **ODE on a matrix Lie group**

$$y'(t) = A(y(t))y(t), \quad A: G \rightarrow \mathfrak{g}, \quad y_0 \in G.$$

Then,  $y(t) = \text{Exp}(\Omega(t))y_0$ , where the dynamics on  $\mathfrak{g}$  is

$$\Omega'(t) = d \text{Exp}_{\Omega(t)}^{-1}(A(y(t))), \quad \Omega(0) = 0. \quad (*)$$

## Proof.

We find on one hand

$$y'(t) = A(y(t))y(t) = A(y(t)) \text{Exp}(\Omega(t))y_0.$$

On the second hand, we have

$$y'(t) = d \text{Exp}_{\Omega(t)}(\Omega'(t)) \text{Exp}(\Omega(t))y_0.$$

□

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<sup>1</sup>See also frozen-flow methods (Celledoni, Crouch, Grossman, Marthinsen, Owren,...).

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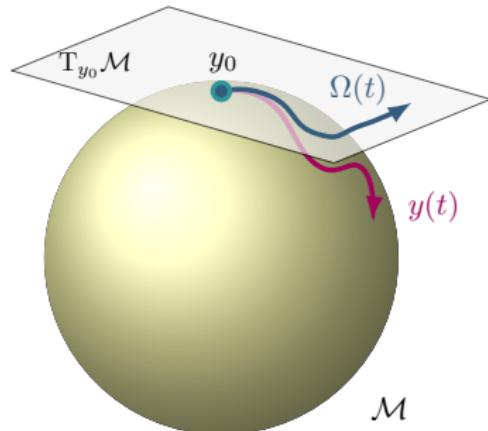
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A RKM<sup>K</sup> method is a Runge-Kutta method applied to the lifted dynamics (\*):

$$\Omega_n = \text{RK}((*)), \quad y_{n+1} = \text{Exp}(\Omega_n)y_n.$$

## Remark

One can truncate  $d \text{Exp}^{-1}$  or use retractions.

<sup>1</sup>See also frozen-flow methods (Celledoni, Crouch, Grossman, Marthinsen, Owren,...).

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# Basics in differential geometry

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We have

- A manifold  $\mathcal{M}$
- Functions  $\phi \in \mathcal{C}^\infty(\mathcal{M})$
- Smooth vector fields  $f \in \mathfrak{X}(\mathcal{M})$ , that is,  $f(p) \in T_p\mathcal{M}$ .

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## Lemma

Let the Jacobi bracket

$$[f, g]_J \triangleright \phi := f \triangleright (g \triangleright \phi) - g \triangleright (f \triangleright \phi).$$

Then  $(\mathfrak{X}(\mathcal{M}), [-, -]_J)$  is a Lie algebra.

A vector field  $f \in \mathfrak{X}(\mathcal{M})$  defines the flow of the ODE  $y' = f(y)$  on  $\mathcal{M}$ .

# Connection

## Definition

An **affine connection** is a bilinear mapping of vector fields

$$\triangleright: \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \rightarrow \mathfrak{X}(\mathcal{M}),$$

satisfying

$$(\phi f) \triangleright g = \phi(f \triangleright g), \quad f \triangleright (\phi g) = f[\phi]g + \phi f \triangleright g.$$

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## Example

In  $\mathbb{R}^D$ , the standard Euclidean connection is

$$f \triangleright g = f^i \partial_i [g^j] \partial_j = g' f = \langle \nabla g, f \rangle.$$

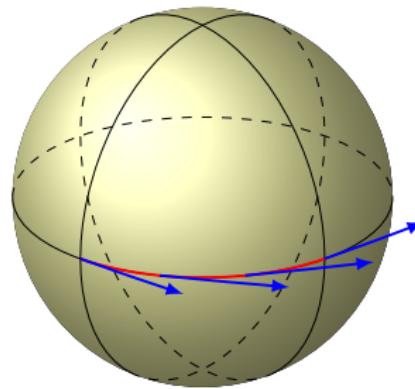
Given a frame basis  $E_i$ ,  $i = 1, \dots, D$ , the **Weitzenböck connection** is given by

$$f \triangleright g = f[g^i] E_i, \quad g = g^i E_i.$$

# Parallel transport

## Definition (Geodesic)

A parallel vector field  $f \triangleright f = 0$  defines a geodesic curve  $y(t)$  as  $y'(t) = f(y(t))$ .  
We write  $\exp_p(tv)$ .



# Parallel transport

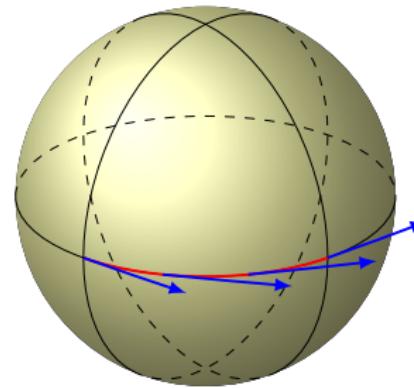
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## Definition (Parallel transport along geodesics)

The *parallel transport along geodesics*:

$$\Gamma_{tv}: T_p \mathcal{M} \rightarrow T_{\exp_p(tv)} \mathcal{M}, \quad p \in \mathcal{M}, \quad v \in T_p \mathcal{M}, \quad \Gamma_{tf}^{-1} = \exp(tf \triangleright).$$



# Torsion and curvature

## Definition

Torsion:

$$T(f, g) = f \triangleright g - g \triangleright f - [f, g]_J.$$

Curvature:

$$R(f, g)h = f \triangleright (g \triangleright h) - g \triangleright (f \triangleright h) - [f, g]_J \triangleright h.$$

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## Proposition (Bianchi identities)

*The torsion and curvature of any affine connection on any manifold satisfy:*

$$\sum_{\mathcal{O}X, Y, Z} T(T(X, Y), Z) + (X \triangleright T)(Y, Z) - R(X, Y)Z = 0,$$

$$\sum_{\mathcal{O}X, Y, Z} (X \triangleright R)(Y, Z) - R(X, T(Y, Z)) = 0.$$

## Examples of geometries

**Euclidean space**  $\mathbb{R}^d$ :  $T = 0, R = 0$ .

**Lie group**:  $\nabla T = 0, R = 0$ .

### Lemma

*If  $\nabla T = 0, R = 0$ ,  $(\mathfrak{X}(\mathcal{M}), T)$  is a Lie algebra.*

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Nomizu classification of invariant connections (1954):

Geometry	Connection	Connection algebra
Local Abelian Lie group	$T = 0, R = 0$	pre-Lie
Local Lie group	$\nabla T = 0, R = 0$	post-Lie
Local symmetric space	$T = 0, \nabla R = 0$	Lie admissible triple
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Main problem of current numerics on manifolds:

**Riemannian**:  $T = 0$ , Levi-Civita connection.

**Almost all geometries in numerics**:  $R = 0$ , Weitzenböck connection.

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# Jacobi fields

## Definition

Given a geodesic  $\gamma_t = \exp_p(tv)$  defined in a neighbourhood of  $p$ , a **Jacobi field**  $J$  is a vector field of the form

$$J(\gamma_t) = d_{tv} \exp_p(tw).$$

Equivalently,  $J$  satisfies

$$J(\gamma_t) = \frac{d}{ds}|_{s=0} \exp_p(tv + tsw).$$

## Lemma (see Kobayashi, Nomizu)

*The Jacobi field satisfies the equation*

$$(\dot{\gamma}_t \cdot \dot{\gamma}_t) \triangleright J(\gamma_t) = \dot{\gamma}_t \triangleright (T_{\gamma_t}(\dot{\gamma}_t, J(\gamma_t))) + R_{\gamma_t}(\dot{\gamma}_t, J(\gamma_t))\dot{\gamma}_t.$$

# The equivalent of $d \exp$

Define the trivialised differential of the exponential for  $p \in \mathcal{M}$ ,  $v, w \in T_p \mathcal{M}$ ,

$$\mathcal{E}_p: T_p \mathcal{M} \rightarrow \text{End}_{\mathbb{R}}(T_p \mathcal{M}), \quad \mathcal{E}_p(v)w = \Gamma_v^{-1} d_v \exp_p(w).$$

## Lemma

The operator  $\mathcal{E}_p(tv)$  satisfies

$$t \frac{d^2}{dt^2} (t \mathcal{E}_p(tv)) - t \frac{d}{dt} (\mathcal{T}_p(tv) \mathcal{E}_p(tv)) = \mathcal{R}_p(tv) \mathcal{E}_p(tv),$$

where

$$\mathcal{T}_p(v)w = (\Gamma_{tv}^{-1} \mathcal{T}_{\gamma_t})(v, w), \quad \mathcal{R}_p(v)w = (\Gamma_v^{-1} R_{\exp_p(v)})(v, w)v.$$

## Lemma (Lie Polynomials)

Let  $t_n(v): w \rightarrow (v \cdot^n \triangleright T_p)(v, w)$  and  $r_n(v): w \rightarrow (v \cdot^n \triangleright R_p)(v, w)v$ , then

$$\mathcal{T}_p(tv) = \sum_{n \geq 1} \frac{t^n}{(n-1)!} t_{n-1}(v), \quad \mathcal{R}_p(tv) = \sum_{n \geq 2} \frac{t^n}{(n-2)!} r_{n-2}(v).$$

# Expansion of $\mathcal{E}_p(tv)$

Theorem (Generalisation of Gavrilov, 2012)

The Taylor expansion of  $\mathcal{E}_p(v)w = \Gamma_v^{-1}d_v \exp_p(w)$  satisfies

$$\mathcal{E}_p(tv) = \sum_{n \geq 0} \frac{t^n}{(n+1)!} \sum_{P \in \text{LiePol}, |P|=n} c_P P(v),$$

where

$$t_n(v)w = (v \cdot^n \triangleright T_p)(v, w), \quad r_n(v)w = (v \cdot^n \triangleright R_p)(v, w)v,$$

and

$$c_{t_p P} = \binom{p+1+|P|}{p} c_P, \quad c_{r_p P} = \binom{p+1+|P|}{p} c_P, \quad c_{\text{id}} = 1.$$

First terms:

$$\begin{aligned} \mathcal{E}_p(tv) &= \text{id} + \frac{t}{2} t_0(v) + \frac{t^2}{3!} \left( 2t_1 + r_0 + t_0^2 \right) (v) \\ &\quad + \frac{t^3}{4!} \left( 3t_2 + 2r_1 + 3t_1 t_0 + 2t_0 t_1 + t_0 r_0 + r_0 t_0 + t_0^3 \right) (v) + \dots \end{aligned}$$

# The case of invariant connections

## Corollary

Let an invariant affine connection  $\triangleright$ , then we find

$$\begin{aligned}\mathcal{E}_p(tv) &= \sum_{n \geq 0} \frac{t^n}{(n+1)!} \sum_{P \in \text{LiePol}_0, |P|=n} P(v) \\ &= \text{id} + \frac{t}{2} t_0(v) + \frac{t^2}{3!} \left( r_0 + t_0^2 \right)(v) + \frac{t^3}{4!} \left( t_0 r_0 + r_0 t_0 + t_0^3 \right)(v) \\ &\quad + \frac{t^4}{5!} \left( r_0^2 + t_0^2 r_0 + t_0 r_0 t_0 + r_0 t_0^2 + t_0^4 \right)(v) \\ &\quad + \frac{t^5}{6!} \left( t_0 r_0^2 + r_0 t_0 r_0 + r_0^2 t_0 + t_0^3 r_0 + t_0^2 r_0 t_0 + t_0 r_0 t_0^2 + r_0 t_0^3 + t_0^5 \right)(v) + \dots\end{aligned}$$

In particular for  $\nabla T = 0$ ,  $R = 0$ , we recover the expansion of  $d \exp$  in the matrix case

$$\mathcal{E}_p(tv) = \sum_{n \geq 0} \frac{t^n}{(n+1)!} T(v, -)^{\circ n}.$$

# General BCH formula<sup>2</sup>

## Corollary

Let an invariant affine connection  $\triangleright$ , then

$$\begin{aligned}\mathcal{E}_p(tv)^{-1} &= \text{id} - \frac{t}{2}t_0(v) + t^2\left(-\frac{1}{6}r_0 + \frac{1}{12}t_0^2\right)(v) + t^3\left(\frac{1}{24}t_0r_0 + \frac{1}{24}r_0t_0\right)(v) \\ &+ t^4\left(\frac{7}{360}r_0^2 - \frac{1}{720}t_0^2r_0 - \frac{1}{120}t_0r_0t_0 - \frac{1}{720}r_0t_0^2 - \frac{1}{720}t_0^4\right)(v) + \dots\end{aligned}$$

## Theorem

The composition of geodesics satisfies

$$\exp_{\exp_p(v)}(\Gamma_v u) = \exp_p(BCH(u, v)),$$

where  $BCH(u, v) = \omega(1)$  and

$$\omega'(t) = \mathcal{E}_p(\omega(t))^{-1}\Gamma_{\omega(t)}^{-1}\Gamma_{\Gamma_v tu}\Gamma_v u, \quad \omega(0) = v.$$

The case  $\nabla T = 0, R = 0$  gives back the standard BCH formula.

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<sup>2</sup>See also Gavrilov's double exponentials and Al-Kaabi, Ebrahimi-Fard, Manchon, Munthe-Kaas, 2025.

# Lifting ODEs in general geometry

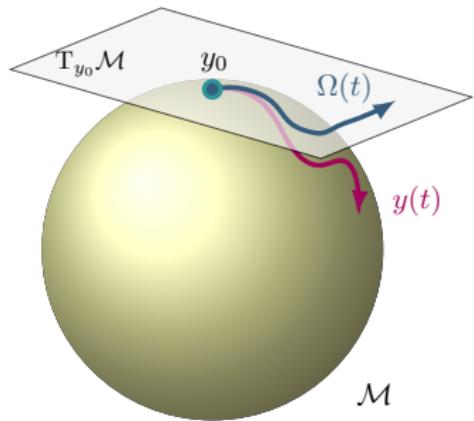
## Theorem

Consider the ODE

$$y'(t) = f(y(t)), \quad y_0 = p, \quad f \in \mathfrak{X}(\mathcal{M}).$$

Then  $y(t) = \exp_p(\Omega(t))$ , where

$$\Omega'(t) = \mathcal{E}_p(\Omega(t))^{-1} \Gamma_{\Omega(t)}^{-1} f(y(t)), \quad \Omega(0) = 0.$$



The map  $\Gamma_{\Omega}^{-1} f(y)$  is called the trivialisation of  $f$  in Lie-group methods.

If  $f(y) = A(y)y$ ,  $\Gamma_{\Omega}^{-1} f(y) = A(y)$

# RKMK in any geometry

RKMK on Lie groups were introduced by H. Munthe-Kaas in the 90's, extended on symmetric spaces ( $T = 0, \nabla R = 0$ ) in 2024.

## Definition (General RKMK)

Let  $\hat{f}(\exp_y(v)) = \Gamma_v^{-1}f(\exp_y(v))$ . The new methods are

$$\theta^i = \sum_{j=1}^s a_{ij} \Omega^j,$$

$$\Omega^i = h \mathcal{E}_p(\theta^i)^{-1} \hat{f}(\exp_y(\theta^i)),$$

$$\psi_h(y) = \exp_y\left(\sum_{i=1}^s b_i \Omega^i\right).$$

## Theorem

If the coefficients correspond to a **Euclidean** order  $p$  RK method, the RKMK method is of order  $p$ .

# Conclusion

## Summary:

- We provide a new fully general class of **intrinsic** methods for solving differential equations on manifolds.
- The approach is **versatile** and can be extended for solving deterministic and stochastic evolutionary problems.
- Ongoing **numerical experiments**.

## Outlooks:

- Study of the algebra of Lie polynomials for constructing the simplest RKMK methods: **Opening position in algebra/operads/numerics in 2026**. Study of the algebraic structures appearing in general intrinsic integration.
- Creation of efficient **high-order intrinsic sampling method** on Riemannian manifolds (thesis of Sébastien Macé).
- Implementation of the new methods in **Manifolds.jl** (with P. Navaro and R. Bergmann).
- **Multiscale dynamics on manifolds** (for electromagnetics, ML, molecular dynamics).