

Numerical preservation of measures of ODEs and SDEs with aromatic structures

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ANR MaStoC - Manifolds and Stochastic Computations

Contents

- 1 Aromatic structures for volume-preservation
- 2 A solution from homological algebra: the aromatic complex
- 3 Aromatic structures in action

References of this talk:

- A. BL, H. Munthe-Kaas and Venkatesh G. S., The free tracial post-Lie Rinehart algebra of planar aromatic trees for the design of divergence-free Lie-group methods. *arXiv:2603.28437*.
- Z. Zhu and A. BL, Aromatic and clumped multi-indices: algebraic structure and Hopf embeddings. *arXiv:2603.13105*.
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- E. Bronasco, A. BL, Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations, *Numer. Math.*, pages 1–61 (2026).
- A. BL, The Lie derivative and Noether's theorem on the aromatic bicomplex for the study of volume-preserving numerical integrators. *Journal of Computational Dynamics*, 2024, 11(1): 10-22.
- A. BL, R. McLachlan, H. Z. Munthe-Kaas and O. Verdier, The aromatic bicomplex for the description of divergence-free aromatic forms and volume-preserving integrators. *Forum of Mathematics Sigma* 11 (2023), E69.

Contents

1 Aromatic structures for volume-preservation

2 A solution from homological algebra: the aromatic complex

3 Aromatic structures in action

Taylor expansion of the flow

Let $\varphi_t(y_0) = y(t)$ be the flow of the ODE

$$y'(t) = F(y(t)), \quad y(0) = y_0, \quad F \in \mathfrak{X}(\mathbb{R}^d).$$

Proposition

The Taylor expansion of the flow is

$$\varphi_t(y_0) = y_0 + ty'(0) + \frac{t^2}{2}y''(0) + \frac{t^3}{3!}y'''(0) + \frac{t^4}{4!}y''''(0) + \dots$$

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The Taylor expansion of the flow is

$$\varphi_t = \text{id} + tF + \frac{t^2}{2} DF \cdot F + \frac{t^3}{3!} D(DF \cdot F) \cdot F + \frac{t^4}{4!} D(D(DF \cdot F) \cdot F) \cdot F + \dots$$

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$$\varphi_t = \text{id} + tF + \frac{t^2}{2}F \triangleright F + \frac{t^3}{3!}F \triangleright (F \triangleright F) + \frac{t^4}{4!}F \triangleright (F \triangleright (F \triangleright F)) + \dots$$

where $F \triangleright G = DG \cdot F = G'F = \langle \nabla G, F \rangle$.

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where $F \triangleright G = DG \cdot F = G'F = \langle \nabla G, F \rangle$.

The Hessian is symmetric (**pre-Lie identity**):

$$\begin{aligned} D^2F(G, H) &= H \triangleright (G \triangleright F) - (H \triangleright G) \triangleright F \\ &= G \triangleright (H \triangleright F) - (G \triangleright H) \triangleright F. \end{aligned}$$

Question: How to understand the elements generated by $(\{F\}, \triangleright)$?

$$\text{Span}_{\mathbb{R}}(F, \quad F \triangleright F, \quad F \triangleright (F \triangleright F), \quad (F \triangleright F) \triangleright F, \dots)$$

The free pre-Lie algebra of Butcher trees

Idea: We have an **object** and a **product** .

The free pre-Lie algebra of Butcher trees

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Definition

A Butcher tree $\tau \in T$ is defined by induction as

$$\bullet \in T, \quad (\tau_1 \cdots \tau_n) \curvearrowright \bullet \in T, \quad \tau_1, \dots, \tau_n \in T,$$

The grafting product $\curvearrowright$ yields: $\circ \curvearrowright \bullet = \bullet + \circ \bullet$, $\circ \curvearrowright \bullet = \bullet + \circ \bullet$.

The first trees are $T = \{\bullet, \bullet, \bullet, \circ, \bullet, \circ, \bullet, \circ, \bullet, \circ, \dots\}$.

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Theorem (Chapoton, Livernet, 2001)

The free **pre-Lie** algebra is $(T, \curvearrowright)$:

"any **pre-Lie** structure $(X, \curvearrowright)$ can be represented using trees".

The free pre-Lie algebra of Butcher trees

Example: the map $\mathbb{F}^{tF} : T \rightarrow \mathfrak{X}(\mathbb{R}^d)$ translates between structures:

F	
$F \triangleright F$	
$F \triangleright (F \triangleright F)$	
$(F \triangleright F) \triangleright F$	

Application: The flow satisfies

$$\begin{aligned}
 \varphi_t &= \text{id} + tF + \frac{t^2}{2} F \triangleright F + \frac{t^3}{3!} F \triangleright (F \triangleright F) + \frac{t^4}{4!} F \triangleright (F \triangleright (F \triangleright F)) + \dots \\
 &= \text{id} + \mathbb{F}^{tF} \left(\bullet + \frac{1}{2} \text{node} + \frac{1}{6} (\text{node} + \text{node}) + \frac{1}{24} (\text{node} + \text{node} + 3 \text{node} + \text{node}) + \dots \right) \\
 &= \text{id} + tF + \frac{t^2}{2} DF \cdot F + \frac{t^3}{6} (DF \cdot DF \cdot F + D^2 F(F, F)) + \dots
 \end{aligned}$$

Most numerical methods have a Taylor expansion that writes with trees.

Volume-preserving integrators

Consider a "tree numerical method" for solving $y' = F(y)$:

$$y_{n+1} = \Phi_h(y_n) = y_n + \mathbb{F}^{hF}(\bullet + \alpha \mathbf{I} + \beta \mathbf{V} + \cdots)(y_n).$$

Example: explicit Euler method $y_{n+1} = y_n + hF(y_n)$.

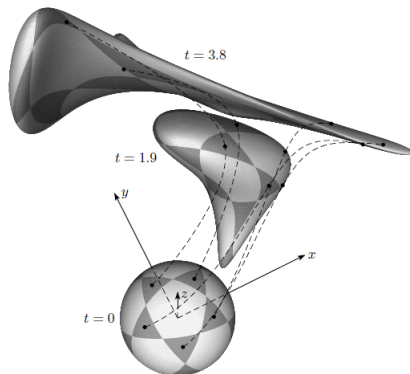


Figure: (from Hairer, Lubich, Wanner, Geometric Numerical Integration)

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Backward error analysis: the integrator is the **exact solution** of a **modified ODE**

$$\tilde{y}'(t) = \tilde{F}_h(\tilde{y}(t)), \quad h\tilde{F}_h = \mathbb{F}^{hF}(\bullet + \alpha \mathbf{!} + \beta \mathbf{V} + \cdots) = hF + \alpha h^2 F \triangleright F + \cdots$$

Proposition

A **tree method** is volume preserving if and only if $\text{Div}(\tilde{F}_h) = \text{Div}(F) = 0$.

Volume-preserving integrators

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Theorem (Iserles, Quispel, Tse, 2007; Chartier, Murua, 2007)

*The only consistent volume-preserving **tree method** is the exact flow.*

Question (Munthe-Kaas, Verdier, 2016): does there exists a non-trivial volume-preserving "**aromatic tree method**"?

Aromatic trees

We now have two bricks:  and .

¹Chartier, Murua, 07; Iserles, Quispel, Tse, 07; Bogfjellmo, 19.

Aromatic trees

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$\text{div}(F) = \partial_i F^i$	$d_{\bullet} = \bigcirc^i$
$\text{div}(F \triangleright F) = \partial_{ij} F^i \cdot F^j + \partial_j F^i \cdot \partial_i F^j$	$d_{\bullet}^j = \bigcirc^i + \bigcirc^i \bigcirc^j$
$F \triangleright \text{div}(F) = \partial_{ij} F^i \cdot F^j$	$\bullet_j \curvearrowright \bigcirc^i = \bigcirc^i$
$\text{div}(F)^2 = \partial_i F^i \cdot \partial_j F^j$	$\bigcirc^i \bigcirc^j$

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Let the aromatic trees¹

$$\mathcal{AT} = \mathcal{A} \otimes \mathcal{T} = \text{Span}_{\mathbb{R}}(\bullet, \bullet^i, \bigcirc^i, \bullet^i \bigcirc^j, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^i, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^i, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^i, \dots)$$

Theorem (Fløystad, Manchon, Munthe-Kaas, 2019)

The free *pre-Lie-Rinehart* algebra "almost" is $(\mathcal{AT}, \curvearrowright, d)$.

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$$\mathcal{AT} = \mathcal{A} \otimes \mathcal{T} = \text{Span}_{\mathbb{R}}(\bullet, \bullet^i, \bigcirc^i, \bullet^i \bigcirc^j, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^j, \bigcirc^i \bigcirc^j, \dots)$$

Theorem (Fløystad, Manchon, Munthe-Kaas, 2019)

The free *pre-Lie-Rinehart* algebra "almost" is $(\mathcal{AT}, \curvearrowright, d)$.

Goal of volume preservation: Find $\text{Ker}(\text{Div})$ on *trees* and *aromatic trees*.

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Ker() is non-trivial

Proposition

The simplest element of $\text{Ker}(d)$ is  $\bullet$ +  $\bullet$ -  - , that is,

$$\text{Div} (F^k \cdot \partial_{jk} F^j \cdot F + \partial_j F^k \cdot \partial_k F^j \cdot F - \partial_k F^k \cdot F^j \cdot \partial_j F - F^k \cdot F^j \cdot \partial_{jk} F) = 0.$$

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The simplest element of $\text{Ker}(d)$ is  $\cdot$ +  $\cdot$ -  $\cdot$ -  $\cdot$, that is,

$$\text{Div} (F^k \cdot \partial_{jk} F^j \cdot F + \partial_j F^k \cdot \partial_k F^j \cdot F - \partial_k F^k \cdot F^j \cdot \partial_j F - F^k \cdot F^j \cdot \partial_{jk} F) = 0.$$

Proof.

A calculation gives

$$\begin{aligned} d \text{circle with one dot} \cdot &= \text{V-shape with two dots} \cdot + \text{circle with one dot and one dot} \cdot + \text{circle with one dot and two dots} \cdot, \\ d \text{circle with two dots} \cdot &= 2 \text{circle with two dots and one dot} \cdot + \text{circle with two dots and two dots} \cdot, \\ d \text{circle with two dots and a vertical line} \cdot &= \text{circle with one dot and one dot} \cdot + \text{circle with one dot and two dots} \cdot + \text{circle with one dot and three dots} \cdot, \\ d \text{V-shape with two dots} \cdot &= 2 \text{circle with two dots and one dot} \cdot + \text{V-shape with two dots} \cdot. \end{aligned}$$

Hence the result. □

Aromatic forms

Idea: the *De Rham complex* is **exact**: $\operatorname{div}(X) = 0 \Leftrightarrow X = \operatorname{curl}(Y)$.

$$\Omega_0(\mathbb{R}^3) \xrightarrow{\nabla} \Omega_1(\mathbb{R}^3) \xrightarrow{\operatorname{curl}} \Omega_2(\mathbb{R}^3) \xrightarrow{\operatorname{div}} \Omega_3(\mathbb{R}^3)$$

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Definition (Aromatic forms)

Let aromatic forms in $\Omega^p = \mathcal{A} \otimes \Lambda^p(\mathcal{T})$ and their differential:

$$a\tau_1 \wedge \cdots \wedge \tau_p = \frac{1}{p!} \sum_{\sigma \in \mathcal{S}_p} \varepsilon(\sigma) a\tau_{\sigma(1)} \otimes \cdots \otimes \tau_{\sigma(p)},$$

$$da\tau_1 \otimes \cdots \otimes \tau_p = d(a\tau_p)\tau_1 \otimes \cdots \otimes \tau_{p-1} + \sum_{i=1}^{p-1} a\tau_1 \otimes \cdots \otimes (\tau_p \curvearrowright \tau_i) \otimes \cdots \otimes \tau_{p-1}.$$

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$$\begin{aligned}\tau_1 \wedge \tau_2 &= \frac{1}{2} \left(\tau_1 \otimes \tau_2 - \tau_2 \otimes \tau_1 \right), \\ d\tau_1 \otimes \tau_2 &= d(\tau_2)\tau_1 + \tau_2 \curvearrowright \tau_1.\end{aligned}$$

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Example

For the aromatic form $\bullet \wedge \mathfrak{I}$, we find

$$d\bullet \wedge \mathfrak{I} = \frac{1}{2} \left(\begin{array}{c} \bullet \\ \circ \end{array} \bullet + \begin{array}{c} \bullet \quad \bullet \\ \circ \end{array} \bullet - \begin{array}{c} \bullet \quad \bullet \\ \circ \end{array} \mathfrak{I} - \begin{array}{c} \bullet \quad \bullet \\ \vee \end{array} \right).$$

The aromatic complex²

Theorem (BL, McLachlan, Munthe-Kaas, Verdier, 2023)

The exterior derivative d satisfies $d^2 = 0$, and the **aromatic complex** is exact.

$$\dots \xrightarrow{d} \Omega^3 \xrightarrow{d} \Omega^2 \xrightarrow{d} \Omega^1 = \mathcal{AT} \xrightarrow{d} \Omega^0 = \mathcal{A}$$

²See also Dotsenko, Laubie, 2025.

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Example

The first elements of $\text{Ker}(\text{Div})$ are

$$2d_{\bullet} \wedge \text{I} = \text{I} \bullet + \text{I} \bullet - \text{I} \bullet - \text{V}$$

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$$2d_{\bullet} \wedge \text{V} = \text{V} \bullet + 2\text{I} \bullet + \text{V} - \text{I} \bullet - 2\text{V} - \text{V}$$

$$2d_{\text{I}} \wedge \text{I} = \text{I} \bullet + \text{I} \bullet + \text{I} \bullet - \text{I} \bullet - \text{I} \bullet - \text{I} \bullet$$

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Applications:

- The aromatic complex is an infinite-dimensional generalisation of the De Rham complex on jet spaces.
- The quotiented complex is "almost" exact:

$$\dots \xrightarrow{d} \Omega^2 / \text{Div}(F) \xrightarrow{d} \Omega^1 / \text{Div}(F) \xrightarrow{d} \Omega^0 / \text{Div}(F)$$

Corollary (BL, McLachlan, Munthe-Kaas, Verdier, 2023)

An aromatic Runge-Kutta method cannot be volume-preserving.

- To preserve the volume exactly, one must start with an **ansatz that is exact for linear problems**, such as exponential methods.

²See also Dotsenko, Laubie, 2025.

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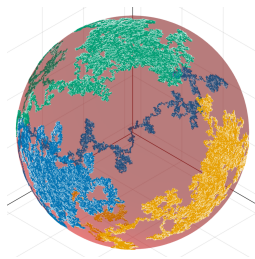
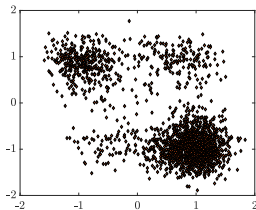
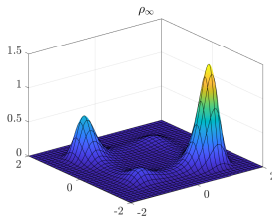
Application: exact samplers for ergodic SDEs?

Overdamped Langevin dynamics in $\mathbb{R}^d$:

$$dY(t) = -\nabla V(Y(t))dt + dW(t).$$

Ergodicity property:

$$\lim_{T \rightarrow +\infty} \frac{1}{T} \int_0^T \phi(X(s))ds = \int_{\mathbb{R}^d} \phi(y) \rho_\infty(y) dy \quad \text{almost surely.}$$



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Shardlow, 2006: **there is no stochastic backward error analysis!**

BUT, for ergodic dynamics, the integrator behaves in long time according to the **invariant measure**³ of a modified SDE:

$$d\tilde{Y}(t) = \tilde{F}_h(\tilde{Y}(t))dt + dW(t).$$

³References: Zygalakis, 11; Abdulle, Cohen, Vilmart, Zygalakis, 12; Debussche, Faou, 12; Kopec, 15; BL, Macé, 26.

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Theorem (BL, 2020; Bronasco, BL, 2026)

The modified vector field $\tilde{F}_h$ is built with  and .

A method is invariant-measure-preserving if $(\text{Div} + \langle \cdot, F \rangle)(\tilde{F}_h) = 0$.

Application: exact samplers for ergodic SDEs?

Overdamped Langevin dynamics in $\mathbb{R}^d$:

$$dY(t) = -\nabla V(Y(t))dt + dW(t).$$

Remark: Four universal building blocks of stochastic geometric integration

	Tree		ODE	GL-equivariant ³
	Aromatic		Volume pres.	GL-equivariant
	Exotic		SDE	O-equivariant ⁴
	Stolonic		Ergodic pres.	O-equivariant

Goal of ergodic preservation (ongoing): Find $\text{Ker}(\text{Div} + \text{F})$
on exotic trees and aromatic stolonic exotic trees.

³Munthe-Kaas, Verdier, 2016

⁴BL, Munthe-Kaas, 2023

Aromatic Novikov algebra (BL, Manchon, Zhu, 2026)

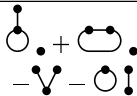
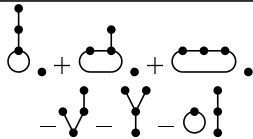
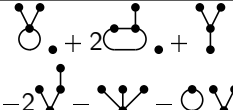
Fertility map: from aromatic trees to multi-indices

$$\Phi\left(\begin{array}{c} \bullet^0 \\ \diagup \quad \diagdown \\ \bullet^0 \quad \bullet^1 \\ \diagdown \quad \diagup \\ \bullet^2 \end{array}\right) = x_{-1}^2 x_0 x_1, \quad \Phi\left(\begin{array}{c} \bullet^0 \\ \diagup \quad \diagdown \\ \bullet^1 \quad \bullet^2 \\ \diagdown \quad \diagup \\ \bullet^2 \end{array}\right) = x_{-1} x_0 x_1.$$

2 possibilities: Novikov or *aromatic Novikov*

$$\Phi(a_1 \cdots a_n t) := \Phi(a_1) \cdots \Phi(a_n) \Phi(t) \quad \Phi: \mathcal{AT} \rightarrow M_{-1}$$

$$\Phi^\odot(a_1 \cdots a_n t) := \Phi(a_1) \odot \cdots \odot \Phi(a_n) \odot \Phi(t) \quad \Phi^\odot: \mathcal{AT} \rightarrow S(M_0) \otimes M_{-1}$$

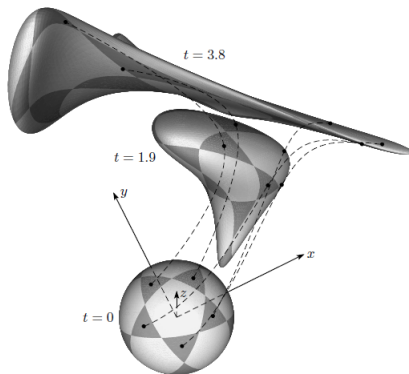
$\omega \in \text{Ker}(d)$	$\Phi^\odot(\omega)$	$\Phi(\omega)$
	$x_{-1} x_1 \odot x_{-1} + x_0^2 \odot x_{-1} - x_{-1}^2 x_1 - x_0 \odot x_{-1} x_0$	0
	$2x_{-1} x_0 x_1 \odot x_{-1} + x_0^3 \odot x_{-1} - 2x_{-1}^2 x_0 x_1 - x_0 \odot x_{-1} x_0^2$	0
	$x_{-1}^2 x_2 \odot x_{-1} + 2x_{-1} x_0 x_1 \odot x_{-1} - x_{-1}^2 x_0 x_1 - x_{-1}^3 x_2 - x_0 \odot x_{-1}^2 x_1$	0

Aromatic structures on manifolds (BL, Munthe-Kaas, Venkatesh, 2026)

ODE on a manifold $\mathcal{M}$ with frame (E_i) :

$$y'(t) = F(y(t)), \quad F = f^i E_i \in \mathfrak{X}(\mathcal{M}), \quad \operatorname{div}(F) = 0$$

Lie-Euler method: $y_{n+1} = \exp(hf^d(y_n)E_d)y_n$

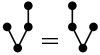
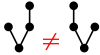


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	Aromatic	Planar Aromatic
Geometry	Euclidean	Local Lie group
Connection	$Y \triangleright X = Y[x^i]\partial_i$	$Y \triangleright X = Y[x^i]E_i$
Torsion	$T = 0$	$T(X, Y) = x^i y^j \llbracket E_j, E_i \rrbracket_j$
Trees = vector fields		
Aromas = functions		
Universality ⁵	Tracial pre-Lie-Rinehart	Tracial post-Lie-Rinehart
$\mathcal{A} \otimes \mathcal{U}(\operatorname{Lie}_{\mathcal{A}}(\mathcal{A}T))$	Pre-Hopf algebroid	Post-Hopf algebroid ⁶

Remark:

$$\rho(X)(\phi) = X[\phi], \quad \operatorname{div}(X) = E_i[x^i], \quad \tau(u) = u_j^i, \quad u(E_j) = u_j^i E_i.$$

⁵see also Rahm, 2026.

⁶see BL, Li, Sheng, 2025.

Aromatic structures on manifolds (BL, Munthe-Kaas, Venkatesh, 2026)

ODE on a manifold $\mathcal{M}$ with **frame** (E_i) :

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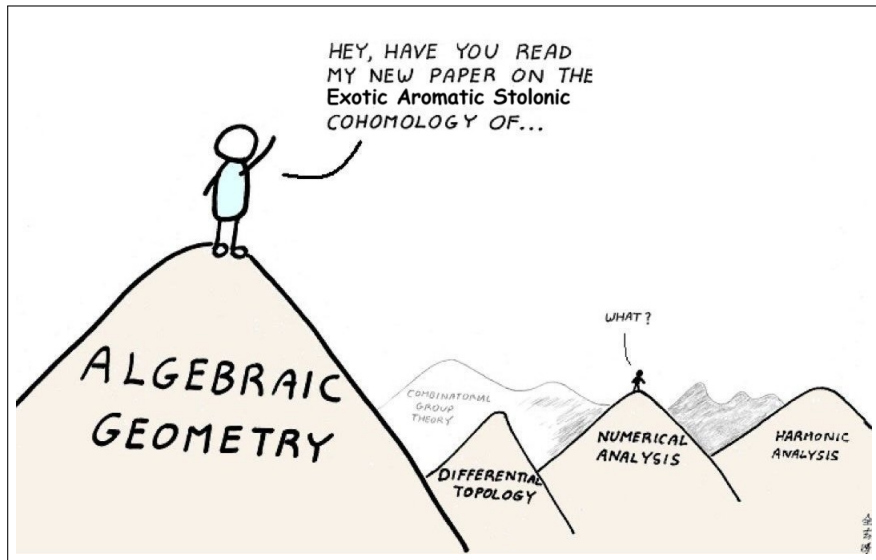
Proposition

Apply the (**order 1**) Lie-Euler method with the **preprocessed vector field**

$$\begin{aligned} h\hat{F}_h &= \mathbb{F}^{hF} \left(\bullet + \frac{1}{2} \begin{array}{c} \bullet \\ | \\ \bullet \end{array} - \frac{1}{3} \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} - \frac{1}{12} \begin{array}{c} \times \bullet \\ \diagdown \diagup \\ \bullet \end{array} \oslash \bullet - \frac{1}{12} \begin{array}{c} \times \times \\ \diagdown \diagup \\ \bullet \end{array} \oslash \bullet + \frac{1}{6} [\bullet, \bullet] \right) \\ &= hf^i E_i + \frac{h^2}{2} f^j E_j [f^i] E_i - \frac{h^3}{3} f^k E_k [f^j] E_j [f^i] E_i - \frac{h^3}{12} f^k \llbracket E_j, E_k \rrbracket_J [f^j] f^i E_i \\ &\quad - \frac{h^3}{12} E_j [f^k] E_k [f^j] f^i E_i + \frac{h^3}{6} f^k f^j E_j [f^i] \llbracket E_k, E_i \rrbracket_J. \end{aligned}$$

Then, it has **order 2 of convergence** and is **divergence-free of order 3**.

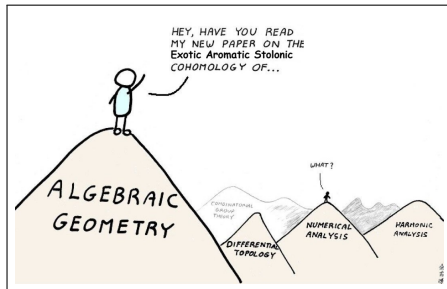
Conclusion



Conclusion

Summary:

- **Volume-preservation** is entirely characterised through **backward error analysis**, **aromatic trees**, and the **aromatic complex**.
- A volume-preserving "aromatic tree method" must be **exact on linear problems**.
- Aromatic structures extend to **many applications**, such as the challenging study of **exact discretisations** for ergodic **SDEs**, **variational calculus**, **rough paths**, **intrinsic numerics**,...



Conclusion

Outlooks:

- Aromatic structures in **different geometries** + applications (with S. Carrier),
- **Intrinsic stochastic backward error analysis** + applications (with S. Macé),
- Toward **exact sampling** (with V. Dotsenko, P. Laubie, J. Sao Joao) with **stochastic exponential Rosenbrock methods** (with S. Andersen, K. Debrabant, A. Kværnø),
- Occurrences in **diffusion models, rough paths**,... (with P. Catoire, Y. Hou, L. Trémant),
- **ANR MaStoC** (2026-2029) with S. Carrier, N. En-Nebbazi, S. Macé.

