On aromatic trees and related algebraic structures for the study of measure-preserving numerical integrators

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ANR MaStoC - Manifolds and Stochastic Computations

Contents

References of this talk:

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• Z. Zhu and A. BL, Aromatic and clumped multi-indices: algebraic structure and Hopf embeddings. *arXiv:2603.13105*.

• A. BL, Y. Li and Y. Sheng, Post-Hopf algebroids, post-Lie-Rinehart algebras and geometric numerical integration. *arXiv:2512.21971*.

• 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, 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

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

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

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

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

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

$$\mathrm{Span}_{\mathbb{R}}(F, \quad F \rhd F, \quad F \rhd (F \rhd F), \quad (F \rhd F) \rhd F, \dots)$$

The free pre-Lie algebra of Butcher trees

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

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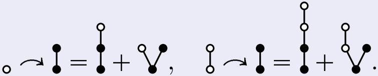
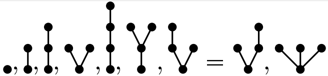
Definition

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: 

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

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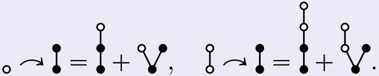
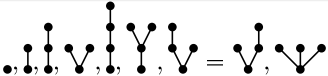
The grafting product $\curvearrowright$ yields: 

The first trees are $T = \{$  $, \ldots\}$.

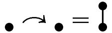
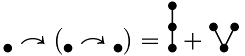
Theorem (Chapoton, Livernet, 2001)

The free pre-Lie algebra is $(\mathcal{T}, \curvearrowright)$:

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

The free pre-Lie algebra of Butcher trees

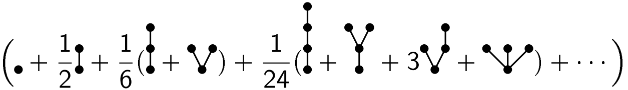
Example: the map $\mathbb{F}^{tF} : T \to \mathfrak{X}(\mathbb{R}^d)$ translates between structures:

F	
$F \rhd F$	
$F \rhd (F \rhd F)$	
$(F \rhd F) \rhd F$	

Application: The flow satisfies

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

$$= \mathrm{id} + \mathbb{F}^{tF}$$



$$= \mathrm{id} + tF + \frac{t^2}{2} DF \cdot F + \frac{t^3}{6} (DF \cdot DF \cdot F + D^2F(F,F)) + \cdots$$

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

Volume-preserving integrators

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

$$y_{n+1} = \Phi_h(y_n) = y_n + \mathbb{F}^{hF}(\bullet + \alpha [\bullet] + \beta [\bullet,\bullet] + \cdots)(y_n).$$

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

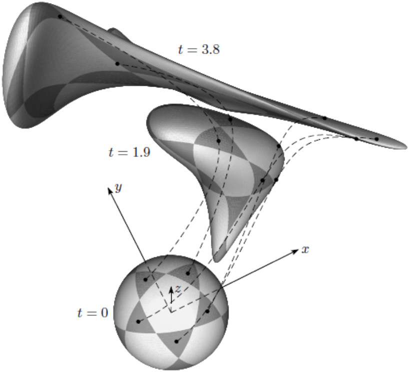


Figure: (from Hairer, Lubich, Wanner, Geometric Numerical Integration)

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

$$\tilde{y}'(t) = \tilde{F}_h(\tilde{y}(t)), \quad h\tilde{F}_h = \mathbb{F}^{hF}(\bullet + \alpha [\bullet] + \beta [\bullet\bullet] + \cdots) = hF + \alpha h^2 F \rhd F + \cdots$$

Proposition

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

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A tree method is volume preserving if and only if $\boxed{\mathrm{Div}(\widetilde{F}_h) = \mathrm{Div}(F) = 0}$.

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 

.

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

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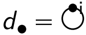
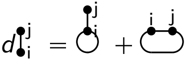
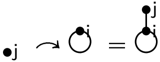
$\mathrm{div}(F) = \partial_i F^i$	
$\mathrm{div}(F \rhd F) = \partial_{ij} F^i \cdot F^j + \partial_j F^i \cdot \partial_i F^j$	
$F \rhd \mathrm{div}(F) = \partial_{ij} F^i \cdot F^j$	
$\mathrm{div}(F)^2 = \partial_i F^i \cdot \partial_j F^j$	

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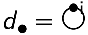
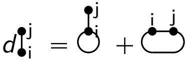
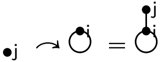
$\mathrm{div}(F) = \partial_i F^i$	
$\mathrm{div}(F \rhd F) = \partial_{ij} F^i \cdot F^j + \partial_j F^i \cdot \partial_i F^j$	
$F \rhd \mathrm{div}(F) = \partial_{ij} F^i \cdot F^j$	
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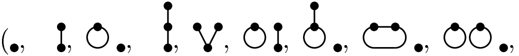
Let the aromatic trees[1]

$$\mathcal{AT} = \mathcal{A} \otimes \mathcal{T} = \mathrm{Span}_{\mathbb{R}}($$  $$)$$

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

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

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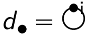
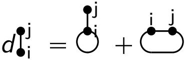
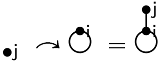
$\mathrm{div}(F) = \partial_i F^i$	
$\mathrm{div}(F \rhd F) = \partial_{ij} F^i \cdot F^j + \partial_j F^i \cdot \partial_i F^j$	
$F \rhd \mathrm{div}(F) = \partial_{ij} F^i \cdot F^j$	
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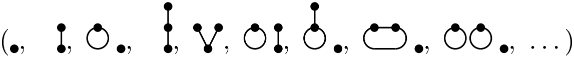
$$\mathcal{AT} = \mathcal{A} \otimes \mathcal{T} = \mathrm{Span}_{\mathbb{R}}($$  $$)$$

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

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

Goal of volume preservation: Find Ker(

) on trees and aromatic trees.

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

Contents

Ker(Div) is non-trivial

Proposition

The simplest element of $\mathrm{Ker}(d)$ *is* *, that is,*

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

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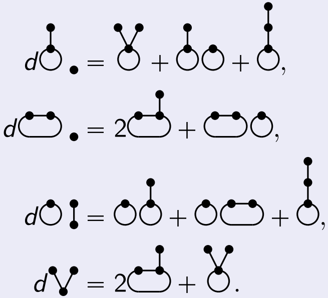
Proof.

A calculation gives



Hence the result. □

Aromatic forms

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

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

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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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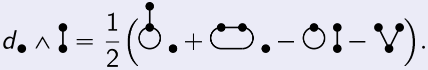
Example

For the aromatic form *, we find*



The aromatic complex[2]

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

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

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

[2] See also Dotsenko, Laubie, 2025.

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Example

The first elements of Ker(

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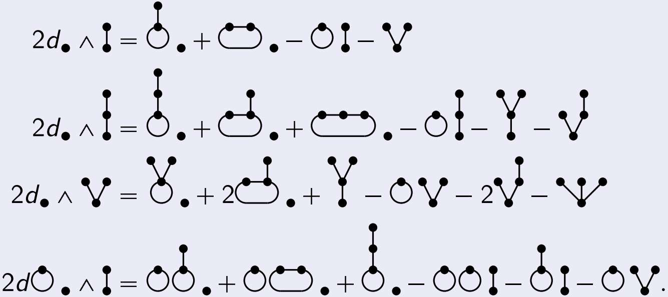

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Applications:

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

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

Corollary

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.

[2] See also Dotsenko, Laubie, 2025.

Contents

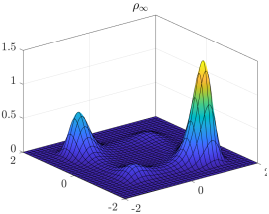
Application: exact samplers for ergodic SDEs?

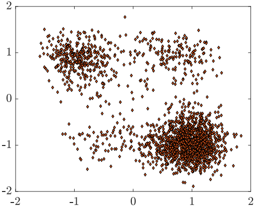
Overdamped Langevin dynamics in $\mathbb{R}^d$:

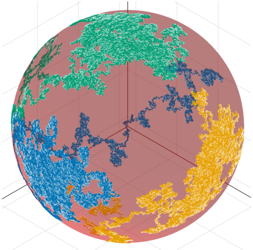
$$dY(t) = -\nabla V(Y(t))dt + dW(t).$$

Ergodicity property:

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







Application: exact samplers for ergodic SDEs?

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

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

Shardlow, 2006: there is no general strong or weak stochastic backward error analysis!

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

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

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

The modified vector field $\widetilde{F}_h$ is built with 

and 

.

A method is invariant-measure-preserving if (

$+$ 

)$(\widetilde{F}_h) = 0$.

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

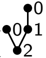
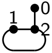
	Tree		ODE	GL-equivariant[3]
	Aromatic		Volume pres.	GL-equivariant
	Exotic		SDE	O-equivariant[4]
	Stolonic		Ergodic pres.	O-equivariant

Goal of ergodic preservation (ongoing): Find Ker( + ) on exotic trees and aromatic stolonic exotic trees.

[3] Munthe-Kaas, Verdier, 2016
[4] BL, Munthe-Kaas, 2023

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

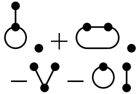
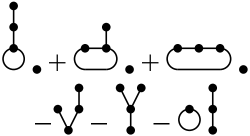
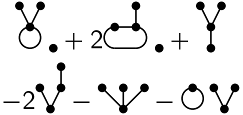
Fertility map: from aromatic trees to multi-indices

$\Phi($  $) = x_{-1}^2 x_0 x_1$, $\Phi($  $) = x_{-1} x_0 x_1$.

2 possibilities: Novikov or ***aromatic Novikov***

$$\Phi(a_1 \cdots a_n t) := \Phi(a_1)\cdots\Phi(a_n)\Phi(t) \qquad \Phi\colon \mathcal{AT} \to M_{-1}$$

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

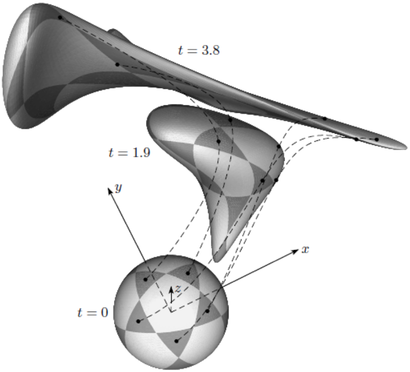
$\omega \in \mathrm{Ker}(d)$	$\Phi^{\odot}(\omega)$	$\Phi(\omega)$
	$x_{-1}x_1 \odot x_{-1} + x_0^2 \odot x_{-1}$ $-x_{-1}^2 x_1 - x_0 \odot x_{-1}x_0$	0
	$2x_{-1}x_0x_1 \odot x_{-1} + x_0^3 \odot x_{-1}$ $-2x_{-1}^2 x_0 x_1 - x_0 \odot x_{-1}x_0^2$	0
	$x_{-1}^2 x_2 \odot x_{-1} + 2x_{-1}x_0x_1 \odot x_{-1}$ $-x_{-1}^2 x_0 x_1 - x_{-1}^3 x_2 - x_0 \odot x_{-1}^2 x_1$	0

Aromatic structures on manifolds

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

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

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



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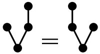
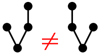
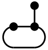
	Aromatic	**Planar** Aromatic
Geometry	Euclidean	Local Lie group
Connection	$Y \triangleright X = Y[x^i]\partial_i$	$Y \triangleright X = Y[x^i]E_i$
Torsion	$T = 0$	$T(X,Y) = x^i y^j [\![E_j, E_i]\!]_J$
Trees = vector fields		
Aromas = functions		
Universality[5]	Tracial pre-Lie-Rinehart	Tracial post-Lie-Rinehart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

Remark:

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

[5] see Rahm, 2026 and BL, Munthe-Kaas, Venkatesh, 2026.
[6] see BL, Li, Sheng, 2025.

Aromatic structures on manifolds

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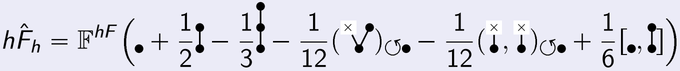
Proposition

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



$$= hf^iE_i + \frac{h^2}{2}f^jE_j[f^i]E_i - \frac{h^3}{3}f^kE_k[f^j]E_j[f^i]E_i - \frac{h^3}{12}f^k[\![E_j, E_k]\!]_J[f^j]f^iE_i$$

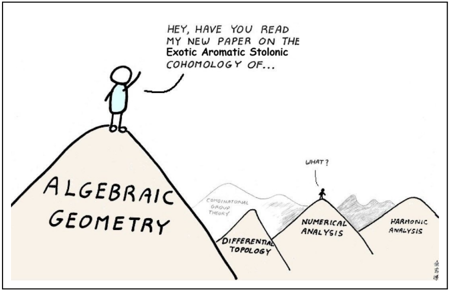
$$- \frac{h^3}{12}E_j[f^k]E_k[f^j]f^iE_i + \frac{h^3}{6}f^kf^jE_j[f^i][\![E_k, E_i]\!]_J.$$

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

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),
- Application to diffusion models, rough paths,... (with P. Catoire, Y. Hou, L. Trémant),
- **ANR MaStoC** (2026-2029) with S. Carrier, N. En-Nebbazi, S. Macé.