The aromatic bicomplex for the study of volume-preserving integrators

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Joint work with H. Z. Munthe-Kaas and R. McLachlan

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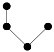
Aromatic Butcher-series

Butcher trees $\mathcal{T}$ used for numerical analysis: Butcher, 1972 and Hairer, Wanner, 1974 (see also Hairer, Wanner, Lubich, 2006 and Butcher, 2021).
The Butcher trees are used to represent Taylor expansions of numerical methods and exact flows of ODEs. $F(\gamma)(f)$ is the elementary differential of a tree γ:

$F($  $)(f) = \sum_{i,j} f^i_j f^j \partial_i = f'f, \quad F($  $)(f) = f''(f,f), \quad F($  $)(f) = f''(f'f,f).$

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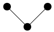
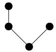
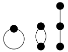
$F($$)(f) = \sum_{i,j} f^i_j f^j \partial_i = f' f,$ $F($$)(f) = f''(f, f),$ $F($$)(f) = f''(f' f, f).$

Aromatic trees $\mathcal{AT}$: introduced by Chartier, Murua and Iserles, Quispel, Tse in 2007 (See also Bogfjellmo, 2019)
In order to compute the divergence of trees, we allow loops. The connected components are called aromas.

$F($$)(f) = \sum_{i,j} f^j_j f^i \partial_i = \mathrm{div}(f) f,$ $F($$)(f) = \mathrm{div}(f)\Big(\sum_{i,j} f^i_j f^j_i\Big) f' f' f.$

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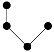
$F($$)(f) = \sum_{i,j} f^i_j f^j \partial_i = f'f,$ $F($$)(f) = f''(f,f),$ $F($$)(f) = f''(f'f,f).$

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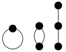
$F($$)(f) = \sum_{i,j} f^j_j f^i \partial_i = \mathrm{div}(f) f,$ $F($$)(f) = \mathrm{div}(f)\Big(\sum_{i,j} f^i_j f^j_i\Big) f'f'f.$

Aromatic B-series: Given a coefficient map $a\colon \mathcal{AT} \to \mathbb{R}$, and aromatic B-series is a formal sum of the form

$$B(a) = \sum_{\tau \in \mathcal{AT}} \frac{a(\tau)}{\sigma(\tau)} \tau.$$

Volume-preserving integrators

Consider a B-series method:

$$y_{n+1} = \Phi(y_n, h) = y_n + F(B(a))(hf)(y_n).$$

Example: explicit Euler method

$$y_{n+1} = y_n + hf(y_n) = y_n + F(\bullet)(hf)(y_n).$$

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

$$\widetilde{y}'(t) = \widetilde{f}(\widetilde{y}(t)), \quad h\widetilde{f} = B(b)(hf), \quad a = b \star e.$$

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A B-series method is volume preserving if and only if $\operatorname{div}(\widetilde{f}) = 0$.

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

The only consistent volume-preserving B-series method is the exact flow.

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

Divergence of trees and solenoidal trees

The divergence d_H is directly computed on $\mathcal{AT}$ by

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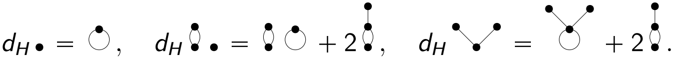
Example: 

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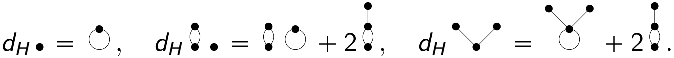
Example: 

Divergence-free context: the assumption $\mathrm{div}(f) = 0$ translates into "Every tree with a 1-loop is sent to 0."

A goal of this work: identify $\mathrm{Ker}(d_H)$ and $\mathrm{Im}(d_H)$ in the standard context and in the divergence-free context.

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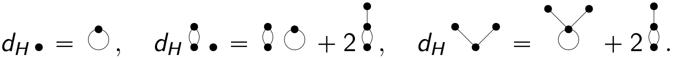
Example: 

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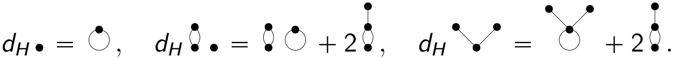
Example: 

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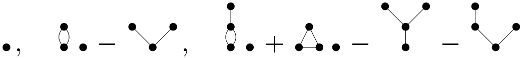
A goal of this work: identify $\mathrm{Ker}(d_H)$ and $\mathrm{Im}(d_H)$ in the standard context and in the divergence-free context.

- The only combination of trees in $\mathrm{Ker}(d_H)$ is $\bullet$.
- There are plenty of combinations of aromatic trees in $\mathrm{Ker}(d_H)$.

Example:  $\in \mathrm{Ker}(d_H)$.

Contents

Reference of this talk:

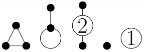
A. Laurent, H. Z. Munthe-Kaas, and R. McLachlan. The aromatic bicomplex for the characterization of volume-preserving aromatic B-series methods. *Submitted*, 41 pages.

Contents

Aromatic forms

Definition

An aromatic forest in $\mathcal{F}_{n,p}$ is a collection of unordered aromas with n ordered trees and p numbered covertices. The elementary differential extends to $\mathcal{F}_{n,p}$ and is a (n,p) tensor. Note that $\mathcal{F}_{1,0} = \mathcal{AT}$.

Example: the aromatic forest $\gamma =$ 

$\in \mathcal{F}_{3,2}$ satisfies

$$F(\gamma)(f) = \Big(\sum_{j,k,l=1}^{d} f_j^k f_k^l f_l^j \Big) \operatorname{div}(f)' f \sum_{i_{r_1}, i_{r_2}, i_{r_3}, j, k=1}^{d} f_j^{i_{r_1}} f^k f^{i_{r_2}} dx^{i_{r_1}} \otimes dx^{i_{r_2}} \otimes dx^{i_{r_3}} \otimes \theta^{i_{r_3}} \otimes \theta_k^j.$$

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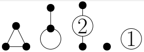
Example: the aromatic forest $\gamma =$  $\in \mathcal{F}_{3,2}$ satisfies

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Definition

For $\gamma \in \mathcal{F}_{n,p}$, the wedge $\wedge\gamma \in \mathrm{Span}(\mathcal{F}_{n,p})$ is the alternate sum of permutations of the roots and covertices of γ. The aromatic forms are in $\Omega_{n,p} = \wedge\,\mathrm{Span}(\mathcal{F}_{n,p})$.

Example: We have $\wedge$  $= \frac{1}{2}($  $-$  $)$.

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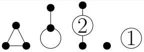
Example: the aromatic forest $\gamma =$  $\in \mathcal{F}_{3,2}$ satisfies

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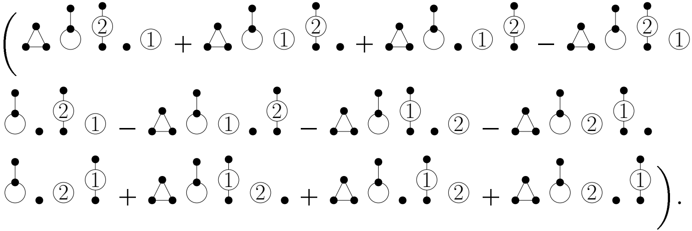
$\wedge\gamma = \frac{1}{12}$ 

Horizontal and vertical derivatives

Definition

The horizontal derivative $d_H\colon \Omega_{n,p} \to \Omega_{n-1,p}$ and the vertical derivative $d_V\colon \Omega_{n,p} \to \Omega_{n,p+1}$ are

$$d_H\gamma = \sum_{v\in V} D^{r_n \to v}\gamma, \quad d_V\gamma = \wedge \sum_{v\in V^\bullet} \gamma_{v\to \textcircled{p+1}}.$$

Example: The derivatives of $\bullet \in \Omega_{1,0}$ and $\wedge \bullet \,\text{\textbullet\!\!|\!\!\textbullet} \in \Omega_{2,0}$ are

$$d_H \bullet = \circlearrowleft\!\!\!\bullet \in \Omega_{0,0}, \quad d_V \bullet = \textcircled{1} \in \Omega_{1,1},$$

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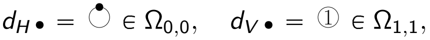

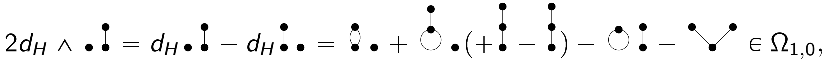

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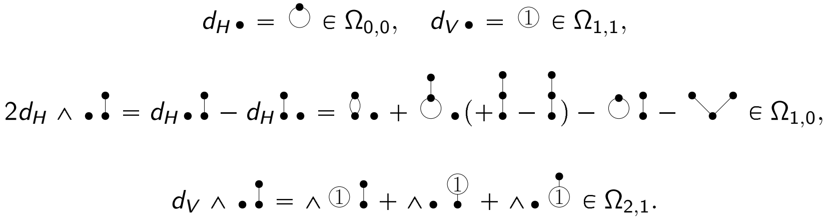

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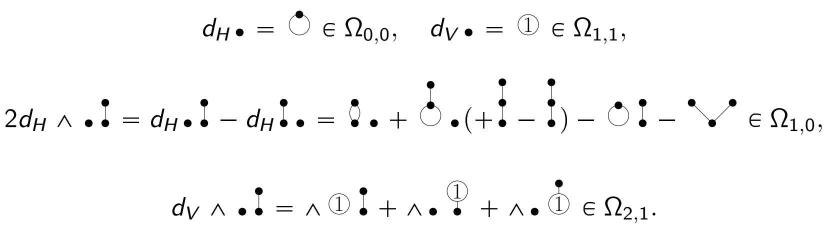

Proposition

The horizontal and vertical derivatives satisfy $d_H^2 = 0$ and $d_V^2 = 0$ on $\Omega_{n,p}$.

The aromatic bicomplex

The aromatic bicomplex is the following diagram:

$$
\begin{array}{ccccccc}
 & & \vdots & & \vdots & & \vdots \\
 & & \uparrow{\scriptstyle d_V} & & \uparrow{\scriptstyle d_V} & & \uparrow{\scriptstyle d_V} \\
\dots & \xrightarrow{d_H} & \Omega_{2,2} & \xrightarrow{d_H} & \Omega_{1,2} & \xrightarrow{d_H} & \Omega_{0,2} \\
 & & \uparrow{\scriptstyle d_V} & & \uparrow{\scriptstyle d_V} & & \uparrow{\scriptstyle d_V} \\
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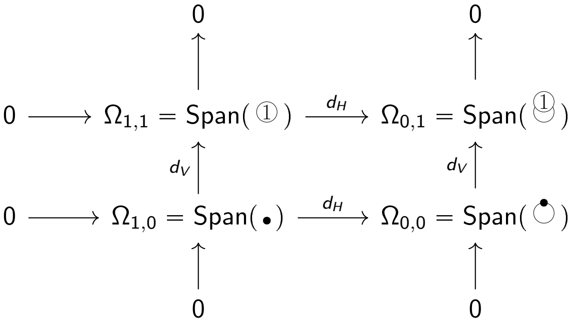
 & & \uparrow & & \uparrow & & \uparrow \\
 & & 0 & & 0 & & 0
\end{array}
$$

Remark: The elementary differential sends the aromatic bicomplex to a subcomplex of the variational bicomplex (see the textbook: Anderson, 1989). The aromatic bicomplex does not involve the dimension of the problem.

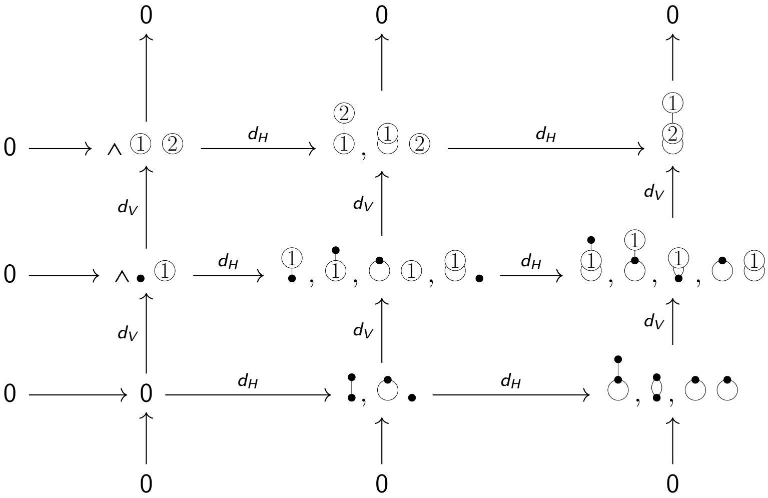
Examples

$N = 1$ nodes:



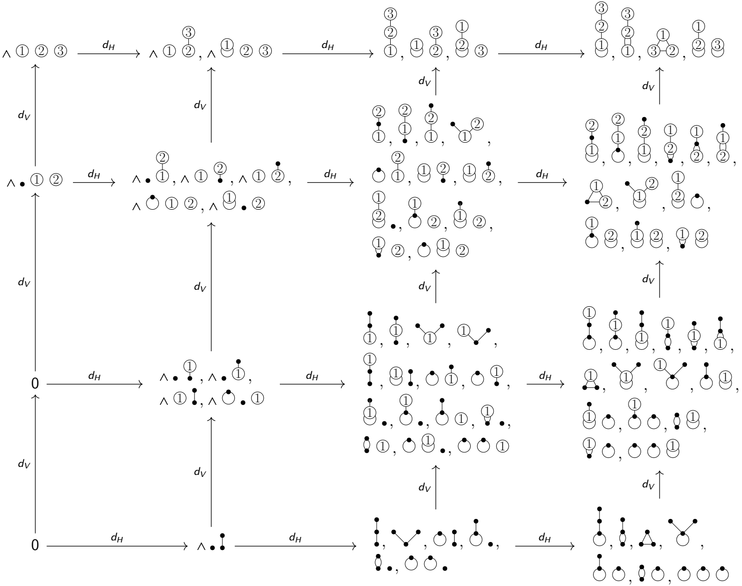
Examples

$N = 2$ nodes:



Examples

$N = 3$ nodes:



Exactness of the aromatic bicomplex

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Theorem

The horizontal and vertical sequences of the aromatic bicomplex are exact:

$$\mathrm{Im}(d_H|_{\Omega_{n+1,p}}) = \mathrm{Ker}(d_H|_{\Omega_{n,p}}), \quad \mathrm{Im}(d_V|_{\Omega_{n,p}}) = \mathrm{Ker}(d_V|_{\Omega_{n,p+1}}).$$

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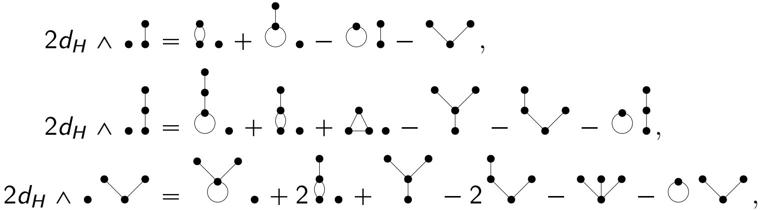
Application: we find an explicit basis of all combinations of trees of vanishing divergence. The first elements are



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The aromatic bicomplex in the divergence-free context

We write $\widetilde{\Omega}_{n,p} = \Omega_{n,p}/\{$ , , , $\cdots = 0\}$. The divergence-free aromatic bicomplex with N nodes (left) is

$$
\begin{array}{ccccccc}
 & & \vdots & & \vdots & & \vdots \\
 & & \uparrow d_V & & \uparrow d_V & & \uparrow d_V \\
\dots & \xrightarrow{d_H} & \widetilde{\Omega}^N_{2,2} & \xrightarrow{d_H} & \widetilde{\Omega}^N_{1,2} & \xrightarrow{d_H} & \widetilde{\Omega}^N_{0,2} \\
 & & \uparrow d_V & & \uparrow d_V & & \uparrow d_V \\
\dots & \xrightarrow{d_H} & \widetilde{\Omega}^N_{2,1} & \xrightarrow{d_H} & \widetilde{\Omega}^N_{1,1} & \xrightarrow{d_H} & \widetilde{\Omega}^N_{0,1} \\
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\end{array}
$$

$$
\begin{array}{ccc}
\widetilde{\Omega}^1_{1,1} = \mathrm{Span}(\textcircled{1}) & \xrightarrow{d_H} & \widetilde{\Omega}^1_{0,1} = 0 \\
\uparrow d_V & & \uparrow d_V \\
\widetilde{\Omega}^1_{1,0} = \mathrm{Span}(\bullet) & \xrightarrow{d_H} & \widetilde{\Omega}^1_{0,0} = 0
\end{array}
$$

The aromatic bicomplex in the divergence-free context

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\uparrow d_V & & \uparrow d_V \\
\widetilde{\Omega}^1_{1,0} = \mathrm{Span}(\bullet) & \xrightarrow{d_H} & \widetilde{\Omega}^1_{0,0} = 0
\end{array}
$$

Problem: The bicomplex is not exact: $\bullet \in \mathrm{Ker}(d_H)$ and $\bullet \notin \mathrm{Im}(d_H)$!

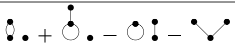
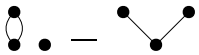
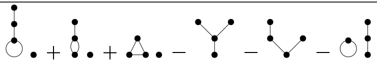
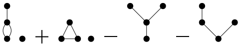
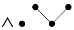
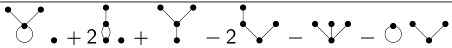
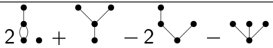
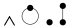
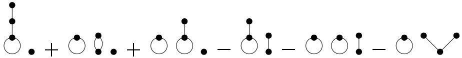
Exactness in the divergence-free context

Theorem

The divergence-free aromatic bicomplex with N nodes is exact if and only if $N \neq 1$. For $N \neq 1$, the solenoidal forms satisfies

$$\mathrm{Ker}(d_H|_{\tilde{\Omega}^N_{n,p}}) = \mathrm{Ker}(d_H|_{\Omega^N_{n,p}})/\{$$  $$, \cdots = 0\}.$$

Application:

$\gamma \in \Omega_{2,0}$	$2d_H\gamma \in \mathrm{Ker}(d_H\|_{\Omega_{1,0}})$	$2d_H\gamma \in \mathrm{Ker}(d_H\|_{\tilde{\Omega}_{1,0}})$
		
		
		
		
		0

Exactness in the divergence-free context

Theorem

The divergence-free aromatic bicomplex with N nodes is exact if and only if $N \neq 1$. For $N \neq 1$, the solenoidal forms satisfies

$$\mathrm{Ker}(d_H|_{\tilde{\Omega}^N_{n,p}}) = \mathrm{Ker}(d_H|_{\Omega^N_{n,p}})/\{$$

$$, \cdots = 0\}.$$

Application:

N	1	2	3	4	5	6	7	8	9	10
$\lvert\Omega_1^N\rvert$	1	2	6	16	45	121	338	929	2598	7261
$\lvert\mathring{\Omega}_0^N\rvert$	1	2	5	13	34	90	243	660	1818	5045
$\lvert\mathrm{Ker}(d_H\|_{\Omega^N_{n,p}})\rvert$	0	0	1	3	11	31	95	269	780	2216
$\lvert\mathrm{Ker}(d_H\|_{\tilde{\Omega}^N_{n,p}})\rvert$	1	0	1	2	7	16	48	123	346	937

Contents

B-series of a volume-preserving method

Theorem

Let $B(a)$ be a consistent volume-preserving B-series method, then there exists $\eta \in \widetilde{\Omega}_2$ such that

$$B(a) = (\bullet + d\eta) \rhd B(e).$$

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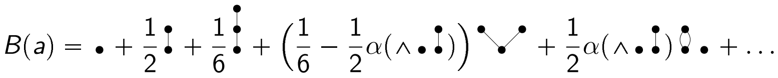

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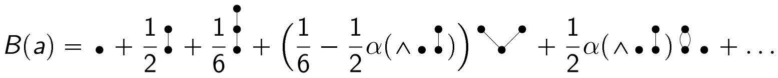


Theorem

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

Application: the methods proposed in Munthe-Kaas, Verdier, 2016 and Bogfjellmo, 2019 can yield pseudo-volume-preserving methods of high order, but cannot exactly preserve volume.

Conclusion and outlook

Summary:

- We introduced and proved the exactness of a new algebraic object, called the aromatic bicomplex, for the study of aromatic and solenoidal forms.
- We gave an explicit description of the consistent volume-preserving aromatic B-series methods.
- We introduced the Euler operators, homotopy operators, and the augmented bicomplex.
- Python package to manipulate the bicomplex.

Outlooks and future works:

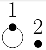
- Work in progress: volume-preserving exponential aromatic B-series methods (with G. Bogfjellmo and M. Naesan Menla Ali).
- Work in progress: integration by parts of (exotic) aromatic forests, structure of (exotic) aromatic forests (with E. Bronasco).
- Translation of differential geometry results for aromatic forms: Noether's theorems, study of the Laplace-De Rham operator $\Delta = d_H d_H^* + d_H^* d_H$, ...

The Euler operators[1]

Definition

The Euler operators are

$$\mathcal{E}^q\gamma = \sum_{v\in V}(-1)^{|\Pi(v)|-q}(D^{|\Pi(v)|-q}\gamma_{v^\diamond})^\diamond.$$

Example: Consider $\gamma =$ , then

$\gamma_{1^\diamond} =$ , $\quad (D\gamma_{1^\diamond})^\diamond =$ , $\quad D(\gamma_{1^\diamond})^\diamond =$  $+$ .

[1] References: Anderson, 1989 and Olver, 1993 (see also Hereman, Poole, 2005-2010)

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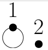
Example: Consider $\gamma =$ , then

$\gamma_{1^\diamond} =$ , $\quad (D\gamma_{1^\diamond})^\diamond =$ , $\quad D(\gamma_{1^\diamond})^\diamond =$  $+$ .

Theorem

$$\gamma = \frac{1}{|\gamma|}\sum_{q=0}^{\infty} D^q\mathcal{E}^q\gamma = \frac{1}{|\gamma|}\mathcal{E}\gamma + d_H\Big(\frac{1}{|\gamma|}\sum_{q=1}^{\infty}\frac{1}{q}D^{q-1}\mathcal{E}^q\gamma\Big).$$

The variational complex is exact.

$$\Omega_{1,0} \xrightarrow{d_H} \Omega_{0,0} \xrightarrow{\mathcal{E}} \Omega_{0,0}$$

[1] References: Anderson, 1989 and Olver, 1993 (see also Hereman, Poole, 2005-2010)

Homotopy operators and exactness

Theorem

Define

$$h_V\gamma = \frac{p}{|\gamma|}\gamma_{\textcircled{p}\to\bullet},\quad h_H\gamma = \frac{1}{|\gamma|}\sum_{q=0}^{\infty}\frac{n+1}{q+n+1}\wedge D^q\mathcal{E}^{q+1}\gamma,$$

then the aromatic bicomplex is exact and

$$(d_V h_V + h_V d_V)\gamma = \gamma,\quad (d_H h_H + h_H d_H)\gamma = \gamma.$$

Homotopy operators and exactness

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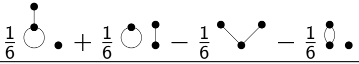
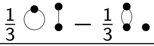
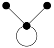
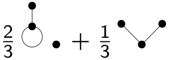
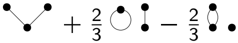
$$h_V\gamma = \frac{p}{|\gamma|}\gamma_{\textcircled{p}\to\bullet}, \quad h_H\gamma = \frac{1}{|\gamma|}\sum_{q=0}^{\infty}\frac{n+1}{q+n+1} \wedge D^q\mathcal{E}^{q+1}\gamma,$$

then the aromatic bicomplex is exact and

$$(d_V h_V + h_V d_V)\gamma = \gamma, \quad (d_H h_H + h_H d_H)\gamma = \gamma.$$

Remark: the integration by parts process from Laurent, Vilmart, 2020 yields an alternative horizontal homotopy operator $\widehat{h}_H$ on $\Omega_{0,p}$.

$\gamma \in \Omega_{0,0}$	$h_H\gamma$	$\widehat{h}_H\gamma$
		
		
		

Homotopy operators and exactness

Theorem

Define

$$h_V\gamma = \frac{p}{|\gamma|}\gamma_{\textcircled{p}\to\bullet}, \quad h_H\gamma = \frac{1}{|\gamma|}\sum_{q=0}^{\infty}\frac{n+1}{q+n+1}\wedge D^q\mathcal{E}^{q+1}\gamma,$$

then the aromatic bicomplex is exact and

$$(d_V h_V + h_V d_V)\gamma = \gamma, \quad (d_H h_H + h_H d_H)\gamma = \gamma.$$

Theorem

Define

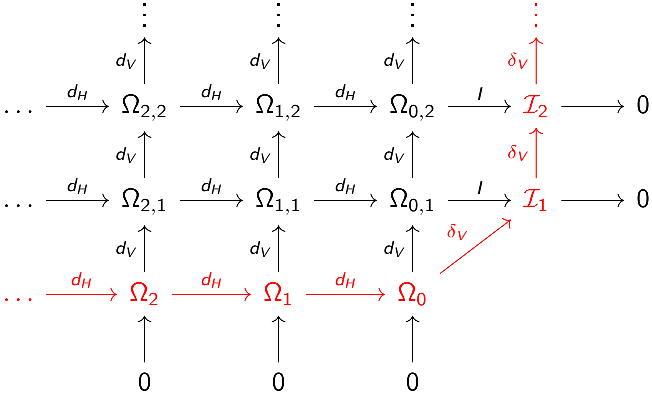
$$\widetilde{h}_H\gamma = \frac{1}{|\gamma|}\sum_{v\in V}\sum_{q=0}^{\infty}\frac{n+1}{q+n+\mathbb{1}_{v\notin R}}\wedge D^q\mathcal{E}_v^{q+1}\gamma,$$

then the divergence-free aromatic bicomplex is exact and

$$(d_H\widetilde{h}_H + \widetilde{h}_H d_H)\gamma = \gamma, \quad n>1; \quad (d_H\widetilde{h}_H + \widetilde{h}_H d_H)\gamma = \gamma - \frac{1}{|\gamma|}\mathcal{E}_r\gamma, \quad n=1.$$

Augmented bicomplex

Define $I\gamma = \wedge\mathcal{E}_{\circled{p}}\gamma = (-1)^{|\Pi(\circled{p})|} \wedge (D^{|\Pi(\circled{p})|}\gamma_{\circled{p}^\diamond})^\diamond$, $\mathcal{I}_p = I(\Omega_{0,p})$, and $\delta_V = I \circ d_V$, then the augmented aromatic bicomplex is



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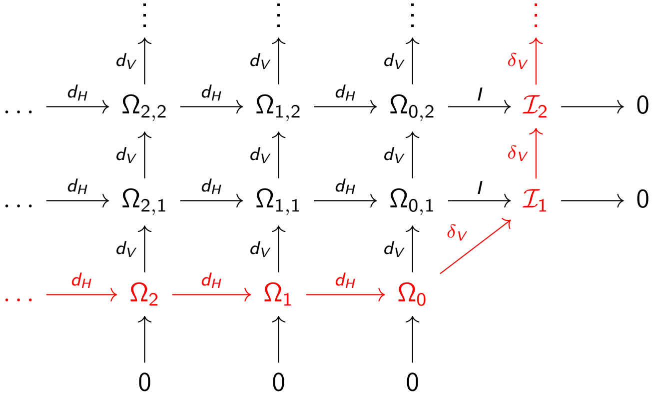

Theorem

The augmented bicomplex and the Euler-Lagrange complex are exact.

Example for $N = 3$