High order volume preserving integrators for three kinds of divergence-free vector fields via commutators

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Abstract

In this paper, we focus on construction of high order volume preserving integrators for divergence-free vector fields of the monomial basis, exponential basis and tensor product of the monomial and exponential basis. We first prove that the commutators of *elementary divergence-free vector fields* (EDFVF) of these three kinds are still divergence-free vector fields of the same kind. For EDFVFs of these three kinds, we construct high order volume preserving integrators using the multi-commutators. Moreover, we consider ordering of EDFVFs and their commutators to reduce the error of the schemes, showing by numerical tests that the strategies in [8] work well.

Keywords: Divergence-free vector field, Volume preserving, Commutator.

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1 Introduction

In [5], Xue and Zanna proposed an approach to develop explicit volume preserving splitting methods for arbitrary polynomial divergence-free vector fields, including the negative degree, by expanding the divergence equation in terms of the monomial basis. In [7], Zanna studied explicit volume preserving splitting integrators for more general divergence-free ODEs than polynomial vector fields, by tensor-product bases decompositions, which included the polynomial case [5] and trigonometric polynomial case [4] as special cases.

In this paper, we present some notes on construction of high order volume preserving integrators for divergence-free vector fields of the monomial basis, the exponential basis and the tensor product of the monomial and exponential basis. In Sections 2 and 3, we study the properties of EDFVFs of these three kinds under the commutation. In Section 4, high order volume preserving methods are constructed via commutators. The strategies of ordering EDFVFs and their commutators are discussed and used to obtain more accurate schemes. All high order schemes are tested by Example 1. In the last section, we give some conclusions and remarks.

2 Properties of divergence-free polynomial vector fields based on diagonal and off-diagonal splitting

Consider the ordinary differential equation

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{x}_0, \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$, $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}), \ldots, f_n(\mathbf{x})]^T$, is subject to the divergence-free condition

$$\nabla \cdot \mathbf{f} = \sum_{i=1}^{n} \partial_{x_i} f_i(\mathbf{x}) = 0. \tag{2}$$

We can always decompose an arbitrary vector field $\mathbf{f}(\mathbf{x})$ into a *diagonal* and an *off-diagonal* part by

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}^{\text{diag}}(\mathbf{x}) + \mathbf{f}^{\text{offdiag}}(\mathbf{x})$$

where $f_i^{\text{diag}}(\mathbf{x})$ (component-wise) is the collection of terms in $f_i(\mathbf{x})$ that depend on x_i, that is, $\partial_{x_i} f_i^{\text{diag}}(\mathbf{x}) \neq 0$; Similarly, $\mathbf{f}^{\text{offdiag}}(\mathbf{x})$ is given by $\partial_{x_i} f_i^{\text{offdiag}}(\mathbf{x}) = 0$.

In [5], Xue and Zanna considered the *diagonal part* with the form

$$\dot{x}_i = a_i x_i \mathbf{x}^{\mathbf{j}}, \qquad i = 1, \ldots, n, \qquad \mathbf{a} = (a_1, \ldots, a_n)^T. \tag{3}$$

Here $\mathbf{j} = (j_1, j_2, \ldots, j_n) \in N^n$ is the multi-index and $\mathbf{x}^{\mathbf{j}} = x_1^{j_1} x_2^{j_2} \ldots x_n^{j_n}$. In short, one could rewrite (3) as

$$\mathbf{x} = \mathbf{F}_{\mathbf{j}}(\mathbf{x}).$$

As presented in [5], each divergence-free vector field $\mathbf{F}_{\mathbf{j}}$ is associated to a monomial basis element, and is called an *elementary divergence-free vector field* (EDFVF).

The divergence-free condition associated with (3) then becomes the algebraic relation

$$\mathbf{a}^T(\mathbf{j} + \mathbf{1}) = 0, \qquad \mathbf{1} = (1, \ldots, 1)^T. \tag{4}$$

Moreover, according to the definition of $\mathbf{f}^{\mathrm{offdiag}}$, we can write the *off-diagonal part* as

$$\dot{\mathbf{x}} = \mathbf{f}^{\mathrm{offdiag}} = \begin{pmatrix} g_1(x_2, \ldots, x_n) \\ \cdots \\ g_i(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) \\ \cdots \\ g_n(x_1, \ldots, x_{n-1}) \end{pmatrix}.$$

According to the splitting rules in [3, 5], we can always split the *off-diagonal* part into shears, where the ith has the form,

$$\begin{cases} \dot{x}_1 = 0, \\ \cdots \\ \dot{x}_{i-1} = 0, \\ \dot{x}_i = g_i(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n), i = 1, \ldots, n, \\ \dot{x}_{i+1} = 0, \\ \cdots \\ \dot{x}_n = 0. \end{cases}$$

We can rewrite the above equations as

$$\dot{\mathbf{x}} = \mathbf{g}_i^{\mathrm{offdiag}} = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ g_i(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) \\ 0 \\ \cdots \\ 0 \end{pmatrix}. \tag{5}$$

It is well known that if $\mathbf{f}$ is a divergence-free polynomial vector field, $\mathbf{f}_1$ and $\mathbf{f}_2$ are either its diagonal or off-diagonal part, we have

$$\nabla \cdot [\mathbf{f}_1, \mathbf{f}_2] = 0,$$

that is, $[\mathbf{f}_1, \mathbf{f}_2]$ is a divergence-free polynomial vector field.

For two EDFVFs, we have the following proposition.

Proposition 1 *If $\mathbf{f}_1$ and $\mathbf{f}_2$ are both EDFVFs, then $[\mathbf{f}_1, \mathbf{f}_2]$ is also an EDFVF. If $\mathbf{f}_1$ and $\mathbf{f}_2$ are two EDFVFs corresponding to multi-indices $\mathbf{j}$ and $\mathbf{k}$, then $[\mathbf{f}_1, \mathbf{f}_2]$ is an EDFVF corresponding to a multi-index $\mathbf{j} + \mathbf{k}$. Moreover, if we assume*

$$\mathbf{f}_1 : \dot{x}_i = a_i x_i \mathbf{x}^{\mathbf{j}}, \;\; \mathbf{a} = (a_1, \ldots, a_n)^T, \;\; \mathbf{a}^T(\mathbf{j} + \mathbf{1}) = 0, \tag{6}$$

$$\mathbf{f}_2 : \dot{x}_i = b_i x_i \mathbf{x}^{\mathbf{k}}, \;\; \mathbf{b} = (b_1, \ldots, b_n)^T, \;\; \mathbf{b}^T(\mathbf{k} + \mathbf{1}) = 0, \tag{7}$$

then we have

$$[\mathbf{f}_1, \mathbf{f}_2] : \dot{x}_i = [\mathbf{a}(\mathbf{b}^T\mathbf{j}) - \mathbf{b}(\mathbf{a}^T\mathbf{k})]_i x_i \mathbf{x}^{\mathbf{j}+\mathbf{k}},$$

with the divergence-free condition

$$[\mathbf{a}(\mathbf{b}^T\mathbf{j}) - \mathbf{b}(\mathbf{a}^T\mathbf{k})]^T(\mathbf{j} + \mathbf{k} + \mathbf{1}) = 0. \tag{8}$$

Proof. From direct calculation, we obtain

$$[\mathbf{f}_1, \mathbf{f}_2]_i = (\nabla \mathbf{f}_1 \cdot \mathbf{f}_2 - \nabla \mathbf{f}_2 \cdot \mathbf{f}_1)_i = [\mathbf{a}(\mathbf{b}^T \mathbf{j}) - \mathbf{b}(\mathbf{a}^T \mathbf{k})]_i x_i \mathbf{x}^{\mathbf{j}+\mathbf{k}}.$$

We can see that (8) is true after some arithmetic by using (6) and (7).

□

3 Properties of divergence-free vector fields: tensor product bases

In this section, we consider more general divergence-free vector fields than polynomial vector fields where the basis functions are the tensor product of 1D cases.

3.1 The exponential basis

In [7], Zanna supposed the basis functions $\phi_{\mathbf{j}}(\mathbf{x})$ with the form below,

$$\phi_{\mathbf{j}}(\mathbf{x}) = \phi_{j_1}(x_1) \dots \phi_{j_n}(x_n),$$

$$j_l \in \mathcal{J}_l, \ \mathbf{j} = (j_1, \dots, j_n) \in \mathcal{J} = \mathcal{J}_1 \times \cdots \times \mathcal{J}_n.$$

The choice $\phi_{j_l} = x_l^{j_l}$ and $\phi_{\mathbf{j}} = \mathbf{x}^{\mathbf{j}} = x_1^{j_1} \dots x_n^{j_n}$ is the case of the monomial basis for the polynomial vector fields, which was discussed in [5] and the previous section. We have the following proposition, see also [7].

Proposition 2 *[7] Given a divergence-free vector field $\mathbf{f}(\mathbf{x})$, consider the divergence $p(\mathbf{x}) = \nabla \cdot \mathbf{f}(\mathbf{x})$ and assume that it can be expanded in a set of basis functions $\{\phi_{\mathbf{j}}(\mathbf{x})\}_{\mathbf{j} \in \mathcal{J}}$,*

$$p(\mathbf{x}) = \sum_{\mathbf{j} \in \mathcal{J}} p_{\mathbf{j}} \phi_{\mathbf{j}}(\mathbf{x}).$$

Let $F_{\mathbf{j}}(\mathbf{x})$ be the unique vector field obtained as the collection of terms in $\mathbf{f}(\mathbf{x})$ such that

$$\nabla F_{\mathbf{j}}(\mathbf{x}) = p_{\mathbf{j}} \phi_{\mathbf{j}}(\mathbf{x}). \tag{9}$$

Then the differential equation

$$\dot{\mathbf{x}} = F_{\mathbf{j}}(\mathbf{x}) \tag{10}$$

is divergence-free and $\mathbf{f}(\mathbf{x}) = \sum_{\mathbf{j}} F_{\mathbf{j}}(\mathbf{x})$.

Now, we can extend the definition of EDFVF to a more general case, see [7] for more details.

Definition 1 *[7] Given the basis $\{\phi_{\mathbf{j}}(\mathbf{x})\}_{\mathbf{j} \in \mathcal{J}}$, a vector field $F_{\mathbf{j}}$ obeying (9) is called an EDFVF associated with the basis function $\phi_{\mathbf{j}}(\mathbf{x})$.*

In [7], we note that when the 1D function $\phi_{j_i}(x_i)$ is a monomial basis or exponential basis or mixed monomial and exponential basis, explicit volume preserving splitting integrators can be constructed. For other cases, we need to either transform them into a monomial basis or exponential basis.

Now, we study the properties of commutators of EDFVFs under the exponential basis.

Proposition 3 *Consider a vector field* $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ *and assume that it can be split into vector fields* $\mathbf{f}_1$ *and* $\mathbf{f}_2$ *corresponding to multi-indices* $\mathbf{k}$ *and* $\mathbf{l}$*. Both functions can be written in an exponential basis,*

$$\mathbf{f}_1: \quad \dot{x}_i = \mathbf{c}e^{\mathrm{i}\mathbf{k}^T\mathbf{x}}, \qquad \mathbf{f}_2: \quad \dot{x}_i = \mathbf{d}e^{\mathrm{i}\mathbf{l}^T\mathbf{x}},$$

where $\mathbf{k} = (k_1, \ldots, k_n)^T$, $\mathbf{l} = (l_1, \ldots, l_n)^T$ *and* $\mathbf{c} = (c_1, \ldots, c_n)^T$, $\mathbf{d} = (d_1, \ldots, d_n)^T$*. The divergence-free conditions give the following,*

$$\mathbf{k}^T\mathbf{c} = 0, \ \mathbf{l}^T\mathbf{d} = 0. \tag{11}$$

Then we obtain

$$\nabla \cdot [\mathbf{f}_1, \mathbf{f}_2] = 0, \tag{12}$$

which implies that $[\mathbf{f}_1, \mathbf{f}_2]$ *is still a vector field in an exponential basis. Moreover, we have*

$$[\mathbf{f}_1, \mathbf{f}_2] : \dot{\mathbf{x}} = \mathrm{i}[\mathbf{c}(\mathbf{d}^T\mathbf{k}) - \mathbf{d}(\mathbf{c}^T\mathbf{l})]e^{\mathrm{i}(\mathbf{k}+\mathbf{l})^T\mathbf{x}}, \tag{13}$$

with the divergence-free condition

$$\mathrm{i}(\mathbf{c}(\mathbf{d}^T\mathbf{k}) - \mathbf{d}(\mathbf{c}^T\mathbf{l}))^T(\mathbf{k}+\mathbf{l}) = 0. \tag{14}$$

Proof. From direct calculation, we obtain

$$\begin{aligned}[\mathbf{f}_1, \mathbf{f}_2] : \dot{x}_i &= [\nabla\mathbf{f}_1 \cdot \mathbf{f}_2 - \nabla\mathbf{f}_2 \cdot \mathbf{f}_1]_i \\ &= [\mathrm{i}(\mathbf{c}(\mathbf{d}^T\mathbf{k}) - \mathbf{d}(\mathbf{c}^T\mathbf{l}))]_i e^{\mathrm{i}(\mathbf{k}+\mathbf{l})^T\mathbf{x}}.\end{aligned}$$

This proves (13). Moreover, from the divergence-free conditions (11) for EDFVFs $\mathbf{f}_1$ and $\mathbf{f}_2$, we can obtain the divergence-free condition (14) for $[\mathbf{f}_1, \mathbf{f}_2]$. □

Formula (13) involves imaginary numbers in the coefficients. To avoid complex arithmetic, see [7] for more details.

3.2 The tensor product of the monomial and exponential basis

In this subsection, we study the case of a mixed monomial and exponential basis. We begin with the divergence-free vector field which can be written as follows,

$$\nabla \cdot \mathbf{f} = \sum_{\mathbf{j}} p_{\mathbf{j}} \mathbf{x}^{\mathbf{j}_m} \mathrm{e}^{\mathrm{i}\mathbf{j}_f^T\mathbf{x}}.$$

Now, we assume that vector field $\mathbf{f}$ can be split into two sub vector fields according to multi-indices $\mathbf{j}$ and $\mathbf{l}$,

$$\mathbf{f} = \mathbf{f}_{\mathbf{j}} + \mathbf{f}_{\mathbf{l}}.$$

For the sub vector field $\mathbf{f}_{\mathbf{j}}$, we assume the multi-index as follows,

$$\mathbf{j} = \mathbf{j}_m \oplus \mathbf{j}_f, \qquad \mathbf{j}_m = \begin{pmatrix} j_1 \\ \vdots \\ j_p \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \mathbf{j}_f = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ j_{p+1} \\ \vdots \\ j_n \end{pmatrix}.$$

According to [7], the subscript m is associated with the projection onto first p components which refer to the monomial part, while the subscript f refers to the projection onto the remaining $n-p$ components which are for the exponential part (Fourier part). A similar notation is also used in the following.

The differential equation referring to $\mathbf{f_j}(\mathbf{x})$ must have the following form,

$$\dot{\mathbf{x}} = \mathbf{f_j}(\mathbf{x}) = \mathbf{a} \otimes \begin{pmatrix} \frac{x_1}{j_1+1} \\ \vdots \\ \frac{x_p}{j_p+1} \\ \frac{1}{\mathrm{i}j_{p+1}} \\ \vdots \\ \frac{1}{\mathrm{i}j_n} \end{pmatrix} \mathbf{x}^{\mathbf{j}_m} \mathrm{e}^{\mathrm{i}\mathbf{j}_f^T \mathbf{x}} = \mathbf{c_a} \otimes \begin{pmatrix} x_1 \\ \vdots \\ x_p \\ 1 \\ \vdots \\ 1 \end{pmatrix} \mathbf{x}^{\mathbf{j}_m} \mathrm{e}^{\mathrm{i}\mathbf{j}_f^T \mathbf{x}}, \tag{15}$$

subject to

$$\begin{aligned} \mathbf{a}^T \mathbf{1} &= 0, \\ \mathbf{c_a}^T((\mathbf{j}+\mathbf{1})_m + \mathrm{i}\mathbf{j}_f) &= 0, \end{aligned} \tag{16}$$

where $\mathbf{c_a} = \begin{pmatrix} \frac{a_1}{j_1+1} \cdots \frac{a_p}{j_p+1} \; \frac{a_{p+1}}{\mathrm{i}j_{p+1}} \cdots \frac{a_n}{\mathrm{i}j_n} \end{pmatrix}^T$ and the $\otimes$ denoting the tensor (component-wise) product of two vectors. (16) are two equivalent divergence-free conditions for differential equation (15).

Similarly, for the other sub vector field $\mathbf{f_l}$, we assume that

$$\dot{\mathbf{x}} = \mathbf{f_l}(\mathbf{x}) = \mathbf{c_b} \otimes \begin{pmatrix} x_1 \\ \vdots \\ x_p \\ 1 \\ \vdots \\ 1 \end{pmatrix} \mathbf{x}^{\mathbf{l}_m} \mathrm{e}^{\mathrm{i}\mathbf{l}_f^T \mathbf{x}}, \tag{17}$$

with the divergence-free condition

$$\mathbf{c_b}^T((\mathbf{l}+\mathbf{1})_m + \mathrm{i}\mathbf{l}_f) = 0, \tag{18}$$

where $\mathbf{c_b} = \begin{pmatrix} \frac{b_1}{l_1+1} \cdots \frac{b_p}{l_p+1} \; \frac{b_{p+1}}{\mathrm{i}l_{p+1}} \cdots \frac{b_n}{\mathrm{i}l_n} \end{pmatrix}^T$.

For the case of tensor product of the exponential and monomial bases, we also obtain similar properties as the monomial and exponential basis (Fourier series) cases. We propose the following proposition.

Proposition 4 *We assume that the divergence-free vector field* $\mathbf{f}$*, which is a function expanded in tensor product of the exponential and monomial basis, can be split into two divergence-free sub vector fields* $\mathbf{f_j}$ *and* $\mathbf{f_l}$ *defined in (15) and (17). Then the commutator* $[\mathbf{f_j}, \mathbf{f_l}]$ *is also divergence-free and has the form*

$$[\mathbf{f_j},\mathbf{f_l}]:\left\{\begin{array}{l}\dot{x}_i=[\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}'})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}'})]_{1:p}\mathbf{x}^{(\mathbf{j}_m+\mathbf{l}_m+\mathbf{e}_i)}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}},i=1\ldots,p,\\ \dot{x}_i=[\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}})]_{p+1:n}\mathbf{x}^{(\mathbf{j}_m+\mathbf{l}_m)}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}},i=p+1,\ldots,n,\end{array}\right. \tag{19}$$

where $\tilde{\mathbf{j}}=(j_1,\ldots,j_p,\mathrm{i}j_{p+1},\ldots,\mathrm{i}j_n)^T$, $\tilde{\mathbf{l}}=(l_1,\ldots,l_p,\mathrm{i}l_{p+1},\ldots,\mathrm{i}l_n)^T$, $\tilde{\mathbf{j}'}=(j_1+1,\ldots,j_p+1,\mathrm{i}j_{p+1},\ldots,\mathrm{i}j_n)^T$, $\tilde{\mathbf{l}'}=(l_1+1,\ldots,l_p+1,\mathrm{i}l_{p+1},\ldots,\mathrm{i}l_n)^T$.

The divergence-free condition for vector field $[\mathbf{f_j},\mathbf{f_l}]$ *becomes*

$$\mathbf{c_{ab}}^T((\mathbf{j}+\mathbf{l}+\mathbf{1})_m+\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f))=0, \tag{20}$$

where $\mathbf{c_{ab}}=([\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}'})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}'})]_{1:p},[\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}})]_{p+1:n})^T$.

Proof. To start with, we consider the case of $m=1,n=2$, which can be extended to the arbitrary case. For $m=1$ and $n=2$, we have

$$\mathbf{f_j}:\left\{\begin{array}{l}\dot{x}_1=a_1\frac{x_1}{j_1+1}\mathbf{x}^{\mathbf{j}_1}e^{\mathrm{i}\mathbf{j}_f^T\mathbf{x}},\\ \dot{x}_2=a_2\frac{1}{\mathrm{i}j_2}\mathbf{x}^{\mathbf{j}_1}e^{\mathrm{i}\mathbf{j}_f^T\mathbf{x}},\end{array}\right.\qquad \mathbf{f_l}:\left\{\begin{array}{l}\dot{x}_1=b_1\frac{x_1}{l_1+1}\mathbf{x}^{\mathbf{l}_1}e^{\mathrm{i}\mathbf{l}_f^T\mathbf{x}},\\ \dot{x}_2=b_2\frac{1}{\mathrm{i}l_2}\mathbf{x}^{\mathbf{l}_1}e^{\mathrm{i}\mathbf{l}_f^T\mathbf{x}},\end{array}\right.$$

where $\mathbf{a}=(a_1,a_2)^T$, $\mathbf{c_a}=(\frac{a_1}{j_1+1},\frac{a_2}{\mathrm{i}j_2})$, $\mathbf{b}=(b_1,b_2)^T$, $\mathbf{c_b}=(\frac{b_1}{l_1+1},\frac{b_2}{\mathrm{i}l_2})$. Now, we have

$$\begin{aligned}[\mathbf{f_j},\mathbf{f_l}] &= \begin{pmatrix}(\frac{a_1}{j_1+1}(\frac{b_1(j_1+1)}{l_1+1}+\frac{b_2j_2}{(j_1+1)l_2})-\frac{b_1}{l_1+1}(\frac{a_1(l_1+1)}{j_1+1}+\frac{a_2l_2}{j_2}))\mathbf{x}^{\mathbf{j}_1+\mathbf{l}_1+\mathbf{e}_1}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}}\\ (\frac{a_2}{\mathrm{i}j_2}(\frac{b_1j_1}{l_1+1}+\frac{b_2j_2}{l_2})-\frac{b_2}{\mathrm{i}l_2}(\frac{a_1j_1}{j_1+1}+\frac{a_2l_2}{j_2}))\mathbf{x}^{\mathbf{j}_1+\mathbf{l}_1}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}}\end{pmatrix}\\ &= \begin{pmatrix}(\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}'})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}'}))_1\mathbf{x}^{\mathbf{j}_1+\mathbf{l}_1+\mathbf{e}_1}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}}\\ (\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}}))_2\mathbf{x}^{\mathbf{j}_1+\mathbf{l}_1}e^{\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f)^T\mathbf{x}}\end{pmatrix},\end{aligned}$$

where $\tilde{\mathbf{j}}=(j_1,\mathrm{i}j_2)^T$, $\tilde{\mathbf{l}}=(l_1,\mathrm{i}l_2)^T$, $\tilde{\mathbf{j}'}=(j_1+1,\mathrm{i}j_2)^T$ and $\tilde{\mathbf{j}'}=(l_1+1,\mathrm{i}l_2)^T$. Moreover, by calculation

$$\nabla\cdot[\mathbf{f_j},\mathbf{f}_l]=0$$

due to the divergence-free conditions $\mathbf{c_a}^T((\mathbf{j}+\mathbf{1})_1+\mathrm{i}\mathbf{j}_f)=0$ and $\mathbf{c_b}^T((\mathbf{l}+\mathbf{1})_1+\mathrm{i}\mathbf{l}_f)=0$. Therefore the differential equation $\dot{\mathbf{x}}=[\mathbf{f_j},\mathbf{f_l}]$ is divergence-free with the condition $\mathbf{c_{ab}}^T((\mathbf{j}+\mathbf{l}+\mathbf{1})_1+\mathrm{i}(\mathbf{j}_f+\mathbf{l}_f))=0$, where $\mathbf{c_{ab}}=([\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}'})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}'})]_1,[\mathbf{c_a}(\mathbf{c_b}^T\tilde{\mathbf{j}})-\mathbf{c_b}(\mathbf{c_a}^T\tilde{\mathbf{l}})]_2)^T$.

The computation for arbitrary values of m and n follows similarly but is simply more tedious. Firstly extending the vectors $\mathbf{a},\mathbf{c_a},\mathbf{b},\mathbf{c_b}$ as in (16) and (18), we define $\tilde{\mathbf{j}},\tilde{\mathbf{l}},\tilde{\mathbf{j}'},\tilde{\mathbf{l}'}$ as in Proposition 4. After similar calculation to the case $m=1,n=2$, $[\mathbf{f_j},\mathbf{f_l}]$ has the form of (19) and the divergence-free condition becomes (20). □

4 Construction of high order integrators

In this section, we construct high order volume preserving integrators for the three kinds of divergence-free vector fields discussed in the two previous sections: the monomial basis, exponential basis and tensor product of the exponential and monomial basis. Furthermore, we assume that for the monomial basis there is only the diagonal part (EDFVFs only). In the text below, when referring to divergence-free vector fields or vector fields, we mean these three kinds of divergence-free vector fields.

4.1 The fourth order scheme

Assume the divergence-free vector field can be split into two EDFVFs, A and B. Given the symmetric second order method

$$S_2(\tau) = e^{\frac{\tau}{2}A}e^{\tau B}e^{\frac{\tau}{2}A}, \tag{21}$$

we can construct a symmetric fourth order method by

$$S_4(\tau) = e^{\frac{\tau^3}{48}[A,[A,B]]}e^{-\frac{\tau^3}{24}[B,[B,A]]}e^{\frac{\tau}{2}A}e^{\tau B}e^{\frac{\tau}{2}A}e^{-\frac{\tau^3}{24}[B,[B,A]]}e^{\frac{\tau^3}{48}[A,[A,B]]}. \tag{22}$$

The well-known BCH form tells us

$$e^{\frac{\tau}{2}A}e^{\tau B}e^{\frac{\tau}{2}A} = exp(t(A+B) + t^3(-\frac{1}{24}[A,[A,B]] + \frac{1}{12}[B,[B,A]]) + \dots).$$

It is easy to see that

$$\begin{aligned} S_4(\tau) &= e^{\frac{\tau^3}{48}[A,[A,B]]}e^{-\frac{\tau^3}{24}[B,[B,A]]}e^{\frac{\tau}{2}A}e^{\tau B}e^{\frac{\tau}{2}A}e^{-\frac{\tau^3}{24}[B,[B,A]]}e^{\frac{\tau^3}{48}[A,[A,B]]} \\ &= exp(\tau(A+B) + \tau^3(-\frac{1}{24}[A,[A,B]] + \frac{1}{12}[B,[B,A]] + \frac{2}{48}[A,[A,B]] \\ &- \frac{2}{24}[B,[B,A]]) + O(\tau^5)) \\ &= exp(\tau(A+B) + O(\tau^5)), \end{aligned}$$

which implies that (22) is a fourth order method. In the following, we give an example and test the scheme of (22).

Example 1 We consider the divergence free vector field

$$\begin{aligned} \dot{x}_1 &= x_1x_2 + x_1x_3, \\ \dot{x}_2 &= -x_2^2 + x_2x_3, \\ \dot{x}_3 &= x_2x_3 - x_3^2. \end{aligned}$$

According to [5], we split it into two EDFVFs corresponding to multi-indices $\mathbf{j} = (0,1,0)^T$ and $\mathbf{k} = (0,0,1)^T$.

$$\mathbf{f}_1 : \begin{aligned} \dot{x}_1 &= x_1x_2, \\ \dot{x}_2 &= -x_2^2, \\ \dot{x}_3 &= x_3x_2, \end{aligned} \qquad \mathbf{f}_2 : \begin{aligned} \dot{x}_1 &= x_1x_3, \\ \dot{x}_2 &= x_2x_3, \\ \dot{x}_3 &= -x_3^2. \end{aligned}$$

According to Proposition 1, we have the coefficient of $[\mathbf{f}_1, \mathbf{f}_2]$: $(0,-2,2)^T$ and multi-index: $(0,1,1)^T$,

$$[\mathbf{f}_1, \mathbf{f}_2] : \begin{aligned} \dot{x}_1 &= 0, \\ \dot{x}_2 &= -2x_2^2x_3, \\ \dot{x}_3 &= 2x_2x_3^2. \end{aligned}$$

Similarly, we have

$$[\mathbf{f}_1, [\mathbf{f}_1, \mathbf{f}_2]] : \begin{aligned} \dot{x}_1 &= -2x_1x_2^2x_3, \\ \dot{x}_2 &= 2x_2^3x_3, \\ \dot{x}_3 &= -2x_2^2x_3^2, \end{aligned} \qquad [\mathbf{f}_2, [\mathbf{f}_2, \mathbf{f}_1]] : \begin{aligned} \dot{x}_1 &= -2x_1x_2x_3^2, \\ \dot{x}_2 &= -2x_2^2x_3^2, \\ \dot{x}_3 &= 2x_2x_3^3. \end{aligned}$$

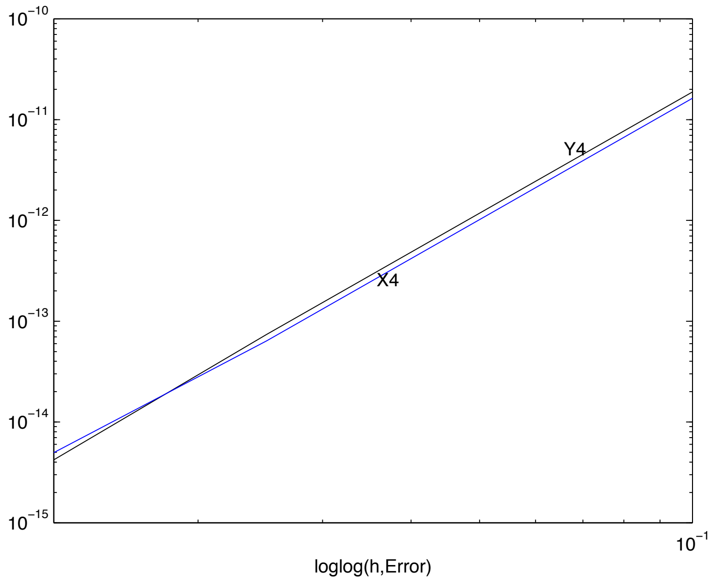

Figure 1: The settings are the same as in Table 1, X4 is obtained from (22) and Y4 is the Yoshida 4th order method in [6].

According to (22), we can construct the fourth order method (X4). We compare the error of X4 to the fourth order method proposed by Yoshida [6] (Y4). From Figure 1 and Table 1, we can see that X4 is performing better than Y4, but the error is still off the same magnitude.

h	0.1	0.05	0.025	0.0125
X4	0.1631e-10	0.0102e-10	0.0006e-10	0.00004e-10
Y4	0.1887e-10	0.0118e-10	0.0007e-10	0.00004e-10

Table 1: Error $\|\mathbf{x}_n - \mathbf{x}^*\|$ at time $T = 1$ by volume preserving implementations Y4 and X4 (at various time steps h) for Example 1. Y4 is the fourth method of Yoshida [6] and X4 is the method of (22). All the experiments are with the initial condition $\mathbf{x}_0 = [0.1, 0.1, 0.1]^T$ and the reference solution $\mathbf{x}^*$ is obtained by `ode45` imposing machine accuracy on the relative and absolute tolerance.

4.2 The composition method with an effective error

Table 1 shows that the method proposed in (22) has the same magnitude in error as Y4 in [6]. According to the experiments in [5] the fourth order method O4 in [1] has much lower error than Y4 in [6]. In order to get more accurate schemes, [1] proposed to increase the number of stages not only to just reach a given order, but also leave the space for optimizing the methods to obtain smaller error. However, increasing the number of stages is expensive. From a practical perspective, one has to balance the cost and accuracy.

Moreover, McLachlan [2] gave a systematic study with composition methods and showed that TYPE S, symmetric method (m=5) is more accurate compared to TYPE SS methods which were based on the Yoshida fourth order scheme (Y4) in [6]. Therefore, we consider second order TYPE S method (with more stages than a given order) to improve the scheme in (22). In [2], McLachlan gave a second order method (S, m=2, error:0.026, denoted as $S_2^{m=2}$) which had smaller error than the leapfrog (error: 0.070) which is exactly the form $S_2(\tau)$ in (22). In [2], $S_2^{m=2}$ can be written as

$$S_2^{m=2}(\tau) = e^{a_1\tau A}e^{b_1\tau B}e^{a_2\tau A}e^{b_1\tau B}e^{a_1\tau A}, \tag{23}$$

where

$$\begin{aligned} a_1 &= 0.1932, \\ b_1 &= 0.5, \\ a_2 &= 0.6136. \end{aligned} \tag{24}$$

Proposition 5 *Suppose the divergence-free vector field could be split into two EDFVFs, A and B. Given*

$$C_{aab} = \frac{1}{6}a_2^2 b_1 - \frac{1}{3}a_1^2 b_1 - \frac{1}{3}a_1 a_2 b_1, \tag{25}$$

$$C_{bba} = -\frac{1}{6}a_2 b_1^2 + \frac{2}{3}b_1^2 a_1, \tag{26}$$

based on (23), we can construct a symmetric fourth order method by

$$\begin{aligned} S_4^{'}(\tau) = {} & e^{-\frac{C_{aab}}{2}\tau^3[A,[A,B]]}e^{-\frac{C_{bba}}{2}\tau^3[B,[B,A]]}e^{a_1\tau A}e^{b_1\tau B}e^{a_2\tau A}e^{b_1\tau B}e^{a_1\tau A}e^{-\frac{C_{bba}}{2}\tau^3[B,[B,A]]} \\ & e^{-\frac{C_{aab}}{2}\tau^3[A,[A,B]]}. \end{aligned} \tag{27}$$

Proof. First we compute the three terms BCH form,

$$e^{b_1\tau B}e^{a_2\tau A}e^{b_1\tau B} = exp(\tau(2b_1 B + a_2 A) + \tau^3(\frac{a_2^2 b_1}{6}[A,[A,B]] - \frac{b_1^2 a_2}{6}[B,[B,A]]) + O(\tau^5)).$$

The same procedure gives

$$S_2^{m=2} = exp(\tau(2b_1 B + (2a_1 + a_2)A) + \tau^3(C_{aab}[A,[A,B]] + C_{bba}[B,[B,A]]) + O(\tau^5)),$$

where C_{aab} and C_{bba} is (25) and (26) respectively. From (24) we know that $2b_1 = 1$ and $2a_1 + a_2 = 1$, then we obtain

$$S_4^{'}(\tau) = exp(\tau(A+B) + O(\tau^5)).$$

This proves the proposition. □

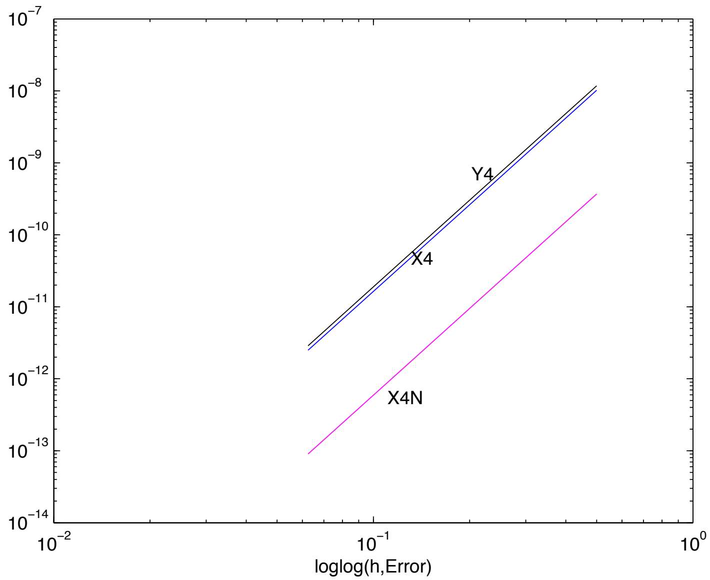

Figure 2: The settings are the same as in Table 2, X4 and Y4 are the same as Fig 1 and X4N is obtained from Proposition 5.

According to our analysis in the beginning of this subsection, the fourth order method (27) (X4N) is supposed to have smaller error than the fourth order method X4. Now, we compare them by Example 1. We use larger step sizes h, which range from 0.5 to 0.0625 and the same initial condition for all the experiments. The results are presented in Table 2 and Figure 2, where we can see that X4N has smaller error (at least 1e-1 better) compared to Y4 and X4. The CPU cost of X4N and X4 for $T = 10000$ and step size $h = 0.1$ is 0.672 and 0.564 seconds, respectively. We can see that for Example 1 there is no remarkable increase in computational cost for X4N compared to X4, but the former scheme gives us much more accurate results.

4.3 Split the vector field into more than two EDFVFs

In this subsection, we consider the case where the vector field has to be split into more than two EDFVFs. The following proposition gives the fourth order method based on the symmetric BCH formula in [8].

Proposition 6 *Assume that the vector field can be split into n EDFVFs, $\mathbf{f}_1, \ldots, \mathbf{f}_n$, the symmetric second order method can be constructed by*

$$S_2^{nv}(\tau) = e^{\frac{\tau}{2}\mathbf{f}_1} \ldots e^{\tau \mathbf{f}_n} \ldots e^{\frac{\tau}{2}\mathbf{f}_1}. \tag{28}$$

h	0.5	0.25	0.125	0.0625
X4N	0.036894e-8	0.002307e-8	0.000144e-8	0.000009e -8
X4	0.101919e-7	0.006371e-7	0.000398e-7	0.000025e-7
Y4	0.117854e-7	0.007370e-7	0.000461e-7	0.000029e-7

Table 2: Error $\|\mathbf{x}_n - \mathbf{x}^*\|$ at time $T = 1$ by volume preserving implementations Y4, X4 and X4N (at various time steps h) for Example 1. Y4 and X4 are the methods depicted above, and X4N is the method from Proposition 5. All the experiments are with the initial condition $\mathbf{x}_0 = [0.1, 0.1, 0.1]^T$ and the reference solution $\mathbf{x}^*$ is obtained by `ode45` imposing machine accuracy on the relative and absolute tolerance.

In [8], Zanna gave the symmetric BCH formula,

$$e^{\frac{\tau}{2}\mathbf{f}_1} \dots e^{\tau \mathbf{f}_n} \dots e^{\frac{\tau}{2}\mathbf{f}_1} = e^{Z(\tau)},$$

where

$$Z(\tau) = \tau \sum_{i=1}^{n} \mathbf{f}_i - \frac{\tau^3}{12} \sum_{i,j,k=1, j<i, j<k}^{n} [\mathbf{f}_i, [\mathbf{f}_j, \mathbf{f}_k]] - \frac{\tau^3}{24} \sum_{i,k=1, i<k}^{n} [\mathbf{f}_i, [\mathbf{f}_i, \mathbf{f}_k]] + O(\tau^5). \tag{29}$$

Then, we have the symmetric fourth order method by

$$\begin{aligned} S_4^{nv}(\tau) = & \textstyle\prod_{i,j,k=1,j<i,j<k}^{n} e^{\frac{\tau^3}{24}[\mathbf{f}_i,[\mathbf{f}_j,\mathbf{f}_k]]} \prod_{i,k=1,i<k}^{n} e^{\frac{\tau^3}{48}[\mathbf{f}_i,[\mathbf{f}_i,\mathbf{f}_k]]} S_2^{nv}(\tau) \prod_{i,k=n,i>k}^{1} e^{\frac{\tau^3}{48}[\mathbf{f}_i,[\mathbf{f}_i,\mathbf{f}_k]]} \\ & \textstyle\prod_{i,j,k=n,j>i,j>k}^{1} e^{\frac{\tau^3}{24}[\mathbf{f}_i,[\mathbf{f}_j,\mathbf{f}_k]]}. \end{aligned} \tag{30}$$

Proof. From (30) we have

$$S_2^{nv}(\tau) = exp(Z(\tau) + \frac{2\tau^3}{24} \sum_{i,j,k=1, j<i, j<k}^{n} [\mathbf{f}_i, [\mathbf{f}_j, \mathbf{f}_k]] + \frac{2\tau^3}{48} \sum_{i,k=1, i<k}^{n} [\mathbf{f}_i, [\mathbf{f}_i, \mathbf{f}_k]] + O(\tau^6)).$$

Together with (29) we obtain

$$S_4^{nv}(\tau) = exp(\tau \sum_{i=1}^{n} \mathbf{f}_i + O(\tau^5)). \tag{31}$$

□

4.4 Ordering of the sub vector fields and their commutators

In this subsection we study ordering of the vector fields. Here, we use the strategies in [8], where Zanna observed from the symmetric BCH formula that collecting the commuting vector fields decreases the number of error terms. However, when the vector fields do not commute, we try a strategy by minimizing the commutators.

We obtain a new scheme by ordering the sub vector fields and their commutators $(A, B, [A, [A, B]]$ and $[B, [B, A]])$ in (22) as follows.

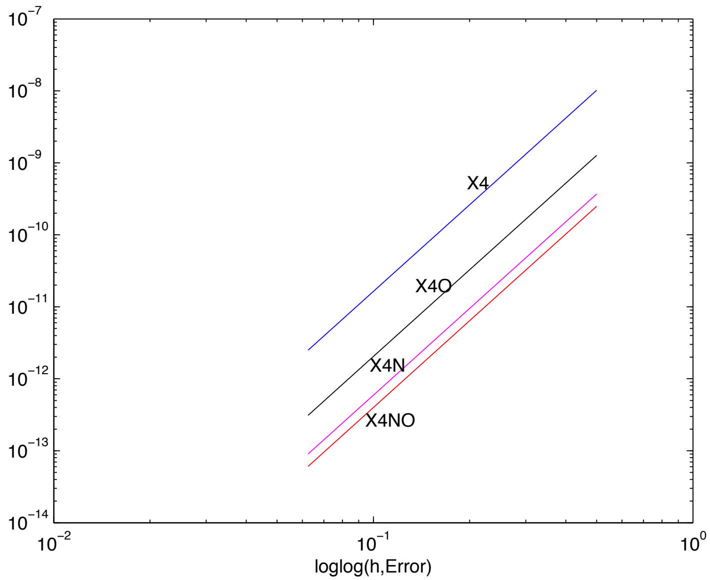

Figure 3: The settings are the same as in Table 3

Proposition 7 *Assume that the vector field could be split into two EDFVFs, A and B. We obtain the symmetric fourth order method by*

$$S_4(\tau) = e^{\frac{\tau^3}{48}[A,[A,B]]} e^{\frac{\tau}{2}A} e^{-\frac{\tau^3}{24}[B,[B,A]]} e^{\tau B} e^{-\frac{\tau^3}{24}[B,[B,A]]} e^{\frac{\tau}{2}A} e^{\frac{\tau^3}{48}[A,[A,B]]}. \tag{32}$$

From (32) we can minimize the term by computing $e^{-\frac{\tau^3}{24}[B,[B,A]]} e^{\tau B} e^{-\frac{\tau^3}{24}[B,[B,A]]}$, by comparing other vector fields, vector field B can minimize the commutator $[B,[B,A]]$. Then we similarly obtain (32) which has smaller error terms than (22). Moreover, we show this by the numerical results in Table 3.

We could also optimize Proposition 5 by the same strategy and obtain a better fourth order method with smaller error.

Proposition 8 *Assuming the same conditions as in Proposition 5, we construct the symmetric fourth order method as*

$$\begin{aligned} S_4'(\tau) = {} & e^{a_1\tau A} e^{-\frac{C_{bba}}{2}\tau^3[B,[B,A]]} e^{b_1\tau B} e^{-\frac{C_{aab}}{2}\tau^3[A,[A,B]]} e^{a_2\tau A} e^{-\frac{C_{aab}}{2}\tau^3[A,[A,B]]} \\ & e^{b_1\tau B} e^{-\frac{C_{bba}}{2}\tau^3[B,[B,A]]} e^{a_1\tau A}. \end{aligned} \tag{33}$$

We test Proposition 7 (X4O) and Proposition 8 (X4NO) using Example 1. The results are presented in Table 3 and Table 3. We compare the results with Table 2. From Table 3 and Figure 3 we can see that the ordering strategies give us much better results. X4O is at least 10 times more accurate than X4 and X4NO is also more accurate than X4N.

h	0.5	0.25	0.125	0.0625
X4N	0.036894e-8	0.002307e-8	0.000144e-8	0.000009e-8
X4NO	0.024912e-8	0.001557e-8	0.000097e-8	0.000006e-8
X4	0.101919e-7	0.006371e-7	0.000398e-7	0.000025e-7
X4O	0.127177e-8	0.007951e-8	0.000497e-8	0.000031e-8

Table 3: Error $\|\mathbf{x}_n - \mathbf{x}^*\|$ at time $T = 1$ by volume preserving implementations X4, X4O, X4N and X4NO (at various time steps h) for Example 1. All the experiments are with the initial condition $\mathbf{x}_0 = [0.1, 0.1, 0.1]^T$ and the reference solution $\mathbf{x}^*$ is obtained by `ode45` imposing machine accuracy on the relative and absolute tolerance. X4, X4N are defined from before, while X4O is defined by Proposition 7 and X4NO is defined by Proposition 8

5 Conclusion and remarks

In this paper, we have studied the properties of three kinds of divergence-free vector fields: the monomial basis, exponential basis and tensor product of both. For EDFVFs of these three kinds, their commutators are still divergence-free vector fields of the same kind.

In general, we can obtain a second order method by symmetrization. For instance, we use the $\phi_{A,h}$ and $\phi_{B,h}$ to represent the first order methods for the vector fields A and B, respectively. Then the second order symmetric method is simply obtained by

$$S_2(h) = \phi_{A,h/2} \circ \phi_{B,h} \circ \phi_{A,h/2}$$

which is exactly (21). We can apply Yoshida technique [6] to construct the fourth order method Y4 by using the symmetric second order method S_2

$$Y4(h) = S_2(\alpha h) S_2(\beta h) S_2(\alpha h)$$

where $\alpha = \frac{1}{2-2^{1/3}}$ and $\beta = -\frac{2^{1/3}}{2-2^{1/3}}$.

In this paper, we used the multi-commutators $h^3[A, [A, B]]$, $h^3[B, [B, A]]$ as well as the two vector fields hA and hB to obtain a fourth order method instead of Yoshida technique [6] or the technique in [1]. Based on the symmetric second order method S_2, we constructed the fourth order method X4 in (22) by using BCH form and simple algebraic calculation. From results in Table 2 for Example 1, we know that although X4 is better than Y4, the error is still off the same magnitude.

Next, we used the more effective second order method $S_2^{m=2}$ proposed by McLachlan [2] instead of the symmetric second order method S_2. The fourth order method X4N based on $S_2^{m=2}$ behaved numerically much better than X4 in Example 1.

Later on, we studied ordering of the vector fields by considering the strategies in [8], that is, collecting the commuting vector fields or minimizing the commutators when the vector fields do not commute. Numerical results showed that the strategies in [8] work well.

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