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Volume-preserving exponential integrators and their applications ☆

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ABSTRACT

It is well known that various dynamical systems preserve volume in phase space such as all Hamiltonian systems. This qualitative geometrical property of the analytical solution should be respected in the sense of Geometric Integration. This paper studies the volume-preserving property of exponential integrators for different vector fields. For exponential integrators, we first derive a necessary and sufficient condition of volume preservation. Then based on this condition, volume-preserving exponential integrators are discussed in detail for four kinds of vector fields. It is shown that symplectic exponential integrators can be volume preserving for a much larger class of vector fields than Hamiltonian systems. On the basis of the analysis, some applications of volume-preserving exponential integrators are discussed. For solving highly oscillatory second-order systems, novel volume-preserving exponential integrators are derived, and for separable partitioned systems, extended Runge–Kutta–Nyström (ERKN) integrators of volume preservation are presented. Moreover, the volume preservation of Runge–Kutta–Nyström (RKN) methods is also discussed. Five illustrative numerical experiments are carried out to demonstrate the notable superiority of volume-preserving exponential integrators in comparison with volume-preserving Runge-Kutta methods.

1. Introduction

In recent decades, geometric integrators (also called as structure-preserving algorithms) have been an active area of great interest. The main advantage of such methods for solving ordinary differential equations (ODEs) is that they can exactly preserve some qualitative geometrical property of the analytical solution, such as the symplecticity, energy preservation, and symmetry. Various geometric integrators have been designed and researched recently and the reader is referred to [2,3,5,9,10,12,19,21,25,27,28] for some examples of this topic. For a good theoretical foundation of geometric numerical integration for ODEs, we refer the reader to [7,13]. Surveys of structure-preserving algorithms for oscillatory differential equations are referred to [32,34].

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It is well known that volume preservation is an important property of several dynamical systems. By the classical theorem due to Liouville, it is clear that all Hamiltonian systems are volume preserving. In the sense of geometric integrators, the structure of volume preservation should also be respected in the numerical approximation. Some methods have been proposed and shown to be (or not to be) volume preserving (see, e.g. [1,4,8,14,18,20,24,36] and references therein). It has been shown that all symplectic methods are volume preserving for Hamiltonian systems. However, this result does not hold for the system beyond Hamiltonian systems (see [4,8,18]). The authors in [22] have pointed out that the derivation of efficient volume-preserving (VP) methods is still an open problem in the geometric numerical integration. Recently, various VP methods have been constructed and analysed, such as splitting methods (see [20,36]), Runge-Kutta (RK) methods (see [1]) and the methods using generating functions (see [24,37]).

On the other hand, exponential integrators have been developed and researched as an efficient approach to integrating ODEs/PDEs. The reader is referred to [15–17,30] for some examples of exponential integrators. In comparison with RK methods, exponential integrators exactly solve the linear system corresponding to the underlying ODEs. Consequently, exponential integrators are expected to perform better than RK methods when solving highly oscillatory systems and the results of many numerical experiments (see [16,30]) have shown this point numerically. However, it seems that volume-preserving exponential integrators have not been researched yet in the literature, which motivates this paper.

In this paper, we will study the volume preservation of exponential integrators for solving the first-order ODEs

$$y'(t) = Ky(t) + g(y(t)) := f(y(t)), \quad y(0) = y_0 \in \mathbb{R}^n, \tag{1}$$

where K is an $n \times n$ matrix which is assumed to satisfy $\left|e^{hK}\right| \neq -1$ for $0 < h < 1$, and $g : \mathbb{R}^n \to \mathbb{R}^n$ is a differentiable nonlinear function. In this paper, $|\cdot|$ denotes the determinant. The function f is assumed to be divergence free such that this system is volume preserving. It is well known that the exact solution of (1) can be represented by the variation-of-constants formula

$$y(t) = e^{tK} y_0 + t \int_0^1 e^{(1-\tau)tK} g(y(\tau t)) d\tau. \tag{2}$$

The main contributions of this paper are to derive the volume-preserving condition for exponential integrators and analyse their volume preservations for larger classes of vector fields than Hamiltonian systems. Furthermore, based on the analysis, volume-preserving adapted exponential integrators are formulated for highly oscillatory second-order systems and volume-preserving extended Runge–Kutta–Nyström (ERKN) integrators are derived for separable partitioned systems. We also discuss the volume preservation of Runge–Kutta–Nyström (RKN) methods by considering them as a special class of ERKN integrators. *To our knowledge, it seems that this is the first work that rigorously studies the volume-preserving properties of exponential integrators and ERKN/RKN integrators.*

We organise the remainder of this paper as follows. In Section 2, the scheme of exponential integrators is presented and some useful results of these integrators are summarised. Then a necessary and sufficient condition for exponential integrators to be volume preserving is derived in Section 3. On the basis of this condition, we study the volume-preserving properties of exponential integrators for four kinds of vector fields in Section 4. Section 5 discusses the applications of the analysis to various problems including highly oscillatory second-order systems and separable partitioned systems. Five illustrative numerical experiments are implemented in Section 6 and the concluding remarks are included in Section 7.

2. Exponential integrators

In order to solve (1) effectively, we approximate the integral appearing in (2) by a quadrature formula with suitable nodes $c_1, c_2, \dots, c_s$. This leads to the following definition of exponential integrators.

Definition 2.1. (See [16].) An s-stage exponential integrator for numerically solving (1) is defined by

$$\begin{cases} k_i = e^{c_i hK} y_n + h \sum\limits_{j=1}^{s} \bar{a}_{ij}(hK) g(k_j), \quad i = 1, 2, \dots, s, \\ y_{n+1} = e^{hK} y_n + h \sum\limits_{i=1}^{s} \bar{b}_i(hK) g(k_i), \end{cases} \tag{3}$$

where h is a stepsize, c_i are real constants for $i = 1, \dots, s$, and $\bar{b}_i(hK)$ and $\bar{a}_{ij}(hK)$ are matrix-valued functions of hK for $i, j = 1, \dots, s$.

This kind of exponential integrators has been successfully used for solving different kinds of ODEs/PDEs (see [15–17,30]). The coefficients of the integrator can be displayed in a Butcher tableau (omit (hK) for brevity):

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b}^{\intercal} \end{array} = \begin{array}{c|ccc} c_1 & \bar{a}_{11} & \dots & \bar{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1} & \cdots & \bar{a}_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \end{array}$$

It is noted that when $K = \mathbf{0}$, this integrator reduces to a classical s-stage RK method represented by the Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\intercal} \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

In this paper, we consider a kind of special and important exponential integrators which was firstly proposed in [23].

Definition 2.2. (See [23].) Define a kind of s-stage exponential integrators by

$$\bar{a}_{ij}(hK) = a_{ij} e^{(c_i - c_j)hK}, \;\; \bar{b}_i(hK) = b_i e^{(1-c_i)hK}, \;\; i, j = 1, \dots, s, \tag{4}$$

where

$$c = (c_1, \dots, c_s)^{\intercal}, \;\; b = (b_1, \dots, b_s)^{\intercal}, \;\; A = (a_{ij})_{s\times s} \tag{5}$$

are the coefficients of an s-stage Runge-Kutta (RK) method.

With regard to this kind of exponential integrators, two useful properties are shown in [23] and we summarise them as follows.

Theorem 2.3. *(See [23].) If an Runge-Kutta method with the coefficients (5) is of order m, then the exponential integrator given by (4) is also of order m.*

Theorem 2.4. *(See [23].) The exponential integrator defined by (4) is symplectic if the corresponding Runge-Kutta method (5) is symplectic.*

In this paper, we supplement an additional requirement for b and use the following two abbreviations.

Definition 2.5. An s-stage exponential integrator (4) is called as symplectic exponential integrator (SEI) if the RK method (5) is symplectic. Moreover, we call the integrator (4) as special symplectic exponential integrator (SSEI) if $b_j \neq 0$ for all $j = 1, \dots, s$ and $BA + A^T B - bb^T = 0$ with $B = \mathrm{diag}(b)$.

Remark 2.6. We note that a kind of special symplectic RK (SSRK) methods has been considered in [1] and our SSEI integrators reduce to the SSRK methods when $K = \mathbf{0}$.

3. VP condition of exponential integrators

For each stepsize h, denote the s-stage exponential integrator (3) by a map $\varphi_h : \mathbb{R}^n \to \mathbb{R}^n$, which is

$$\begin{cases} \varphi_h(y) = e^{hK} y + h \sum\limits_{i=1}^{s} \bar{b}_i(hK) g(k_i(y)), \\ k_i(y) = e^{c_i hK} y + h \sum\limits_{j=1}^{s} \bar{a}_{ij}(hK) g(k_j(y)), \;\; i = 1, 2, \dots, s. \end{cases} \tag{6}$$

We first derive the Jacobian matrix of φ_h and then present the result of its determinant.

Lemma 3.1. *The Jacobian matrix of the exponential integrator (6) can be expressed as*

$$\varphi_h'(y) = e^{hK} + h\bar{b}^{\intercal} F (I_s \otimes I - h\bar{A}F)^{-1} e^{chK},$$

where $F = \mathrm{diag}(g'(k_1), \dots, g'(k_s))$, I_s and I are the $s \times s$ and $n \times n$ identity matrices, respectively, and $e^{chK} = (e^{c_1 hK}, \dots, e^{c_s hK})^{\intercal}$. Its determinant reads

$$\left|\varphi_h'(y)\right| = \frac{\left|e^{hK}\right| \left|I_s \otimes I - h(\bar{A} - e^{(c-\mathbf{1})hK}\bar{b}^\intercal)F\right|}{\left|I_s \otimes I - h\bar{A}F\right|}, \tag{7}$$

where $e^{(c-\mathbf{1})hK} = (e^{(c_1-1)hK}, \dots, e^{(c_s-1)hK})^\intercal$. Here we make use of the Kronecker product $\otimes$ throughout this paper.

Proof. The proof is similar to that of Lemma 2.1 in [1] but with some modifications. According to the first formula of (6), we obtain

$$\varphi_h'(y) = e^{hK} + h\sum_{i=1}^{s} \bar{b}_i g'(k_i(y))k_i'(y) = e^{hK} + h\bar{b}^\intercal F(k_1', \dots, k_s')^\intercal. \tag{8}$$

Likewise, it follows from $k_i(y)$ in (6) that

$$\begin{pmatrix} I - h\bar{a}_{11}g'(k_1) & -h\bar{a}_{12}g'(k_2) & \cdots & -h\bar{a}_{1s}g'(k_s) \\ -h\bar{a}_{21}g'(k_1) & I - h\bar{a}_{22}g'(k_2) & \cdots & -h\bar{a}_{2s}g'(k_s) \\ \vdots & \vdots & \vdots & \vdots \\ -h\bar{a}_{s1}g'(k_1) & -h\bar{a}_{s2}g'(k_2) & \cdots & I - h\bar{a}_{ss}g'(k_s) \end{pmatrix} \begin{pmatrix} k_1' \\ k_2' \\ \vdots \\ k_s' \end{pmatrix} = e^{chK},$$

which can be rewritten as

$$(I_s \otimes I - h\bar{A}F)(k_1', \dots, k_s')^\intercal = e^{chK}. \tag{9}$$

Substituting (9) into (8) yields the first statement of this lemma.

For the second statement, we will use the following block determinant identity (see [1,13]):

$$|U|\left|X - WU^{-1}V\right| = \begin{vmatrix} U & V \\ W & X \end{vmatrix} = |X|\left|U - VX^{-1}W\right|,$$

which is yielded from Gaussian elimination. By letting

$$X = e^{hK},\ W = -h\bar{b}^\intercal F,\ U = I_s \otimes I - h\bar{A}F,\ V = e^{chK},$$

one arrives at

$$\begin{aligned} \left|I_s \otimes I - h\bar{A}F\right|\left|\varphi_h'(y)\right| &= \left|e^{hK}\right|\left|I_s \otimes I - h\bar{A}F + he^{chK}e^{-hK}\bar{b}^\intercal F\right| \\ &= \left|e^{hK}\right|\left|I_s \otimes I - h(\bar{A} - e^{(c-\mathbf{1})hK}\bar{b}^\intercal)F\right|, \end{aligned}$$

which leads to the result (7). $\square$

By Lemma 3.1, a necessary and sufficient condition for the SSEI methods to be volume preserving is shown in the following lemma.

Lemma 3.2. *An s-stage SSEI method defined in Definition 2.5 is volume preserving if and only if the following VP condition is satisfied*

$$|I_s \otimes I - h(A \otimes I. * E(hK))F| = \left|e^{hK}\right| \left|I_s \otimes I + h(A^\intercal \otimes I. * E(hK))F\right|, \tag{10}$$

where $E(hK)$ is a block matrix defined by

$$E(hK) = (E_{i,j}(hK))_{s\times s} = \begin{pmatrix} I & e^{(c_1-c_2)hK} & \cdots & e^{(c_1-c_s)hK} \\ e^{(c_2-c_1)hK} & I & \cdots & e^{(c_2-c_s)hK} \\ \vdots & \vdots & \ddots & \vdots \\ e^{(c_s-c_1)hK} & e^{(c_s-c_2)hK} & \cdots & I \end{pmatrix}, \tag{11}$$

and $.*$ denotes the element-wise multiplication of two matrices.

Proof. In terms of the choice (4) of the coefficients, it is computed that

$$\begin{aligned} &\bar{A} - e^{(c-\mathbf{1})hK}\bar{b}^\intercal \\ =\ &(A \otimes I). * E(hK) - (e^{(c_1-1)hK}, \dots, e^{(c_s-1)hK})^\intercal(b_1e^{(1-c_1)hK}, \dots, b_se^{(1-c_s)hK}) \\ =\ &(A \otimes I). * E(hK) - (\mathbf{1}b^\intercal \otimes I). * E(hK) \\ =\ &(A - \mathbf{1}b^\intercal) \otimes I. * E(hK). \end{aligned}$$

Thus, we obtain

$$\left|\varphi_h'(y)\right| = \frac{\left|e^{hK}\right| \left|I_s \otimes I - h(A - \mathbf{1}b^\top) \otimes I. * E(hK)F\right|}{\left|I_s \otimes I - h\bar{A}F\right|}. \tag{12}$$

Moreover, with careful calculations, it can be verified that for $B = \mathrm{diag}(b_1, \ldots, b_s)$, the following result holds

$$\begin{aligned} &\left|I_s \otimes I - h(A - \mathbf{1}b^\top) \otimes I. * E(hK)F\right| \\ =& \left|I_s \otimes I - h(B \otimes I)(A - \mathbf{1}b^\top) \otimes I. * E(hK)F(B^{-1} \otimes I)\right| \\ =& \left|I_s \otimes I - h(B \otimes I)(A - \mathbf{1}b^\top) \otimes I. * E(hK)(B^{-1} \otimes I)F\right| \\ =& \left|I_s \otimes I - hB(A - \mathbf{1}b^\top)B^{-1} \otimes I. * E(hK)F\right|. \end{aligned} \tag{13}$$

Since the RK method is symplectic, one has that $BA + A^\top B - bb^\top = 0$ (see [13]), which leads to $B(A - \mathbf{1}b^\top)B^{-1} = -A^\top$. Therefore, the result (13) can be simplified as

$$\left|I_s \otimes I - h(A - \mathbf{1}b^\top) \otimes I. * E(hK)F\right| = \left|I_s \otimes I + h(A^\top \otimes I. * E(hK))F\right|.$$

The proof is complete by considering (12). $\square$

Remark 3.3. It is noted that when $K = \mathbf{0}$, the VP condition (10) reduces to the condition of RK methods presented in [1]. Consequently, the condition (10) can be regarded as a generalisation of that of RK methods.

4. VP results for different vector fields

In this section, we study the volume-preserving properties of exponential integrators for the following four kinds of vector fields.

Definition 4.1. (See [1]) Define the following four classes of vector fields on Euclidean space using vector fields $f(y)$

$$\begin{aligned} \mathcal{H} &= \{f(y)|\ \text{there exists } \textit{a matrix } P \text{ such that for all } y,\ Pf'(y)P^{-1} = -f'(y)^\top\}, \\ \mathcal{S} &= \{f(y)|\ \text{there exists } \textit{a matrix } P \text{ such that for all } y,\ Pf'(y)P^{-1} = -f'(y)\}, \\ \mathcal{F}^{(\infty)} &= \{f(y_1, y_2) = (u(y_1), v(y_1, y_2))^\top \text{ where } u \in \mathcal{H} \cup \mathcal{F}^{(\infty)}|\ \text{there exists } \textit{a matrix } P \\ &\qquad \text{such that for all } y_1, y_2,\ P\partial_{y_2} v(y_1, y_2)P^{-1} = -\partial_{y_2} v(y_1, y_2)^\top\}, \\ \mathcal{F}^{(2)} &= \{f(y_1, y_2) = (u(y_1), v(y_1, y_2))^\top \text{ where } u \in \mathcal{H} \cup \mathcal{S} \cup \mathcal{F}^{(2)}|\ \text{there exists } \textit{a matrix } P \\ &\qquad \text{such that for all } y_1, y_2,\ \text{either } P\partial_{y_2} v(y_1, y_2)P^{-1} = -\partial_{y_2} v(y_1, y_2)^\top, \\ &\qquad \text{or } P\partial_{y_2} v(y_1, y_2)P^{-1} = -\partial_{y_2} v(y_1, y_2)\}. \end{aligned}$$

Remark 4.2. It has been proved in [1] that all these fields are equal to divergence free vector fields. The relationships of these vector fields are also given in [1] as

$$\mathcal{H} \subset \mathcal{F}^{(\infty)} \subset \mathcal{F}^{(2)} \text{ and } \mathcal{S} \subset \mathcal{F}^{(\infty)} \subset \mathcal{F}^{(2)}.$$

According to Lemma 3.2 of [1], we know that the set $\mathcal{H}$ contains all Hamiltonian systems. Denote the set of Hamiltonian systems by H. See Fig. 1 for the Venn diagram illusting the relationships. It can be seen from this figure that the sets $\mathcal{H}$, $\mathcal{F}^{(\infty)}$ and $\mathcal{F}^{(2)}$ are larger classes of vector fields than Hamiltonian systems. It is noted that the volume-preserving properties of RK methods for these vector fields have been researched in [1]. Following this work and in what follows, we consider extending those results for exponential integrators.

4.1. Vector fields in $\mathcal{H}$

Theorem 4.3. *All SSEI methods for solving (1) are volume preserving for vector fields f and g in $\mathcal{H}$ with the same P.*

Proof. For vector fields f and g in $\mathcal{H}$ with the same P, we obtain that $Pf'(y)P^{-1} = -f'(y)^\top$ and $Pg'(y)P^{-1} = -g'(y)^\top$. According to these conditions and the expression $f(y) = Ky + g(y)$, one has that $PKP^{-1} = -K^\top$. Thus it is easily obtained that $Pe^{hK}P^{-1} = e^{-hK^\top}$. In the light of this result, we have

$$\left|Pe^{hK}P^{-1}\right| = \left|e^{hK}\right| = \left|e^{-hK^\top}\right| = \left|e^{-hK}\right| = \left|(e^{hK})^{-1}\right| = \frac{1}{\left|e^{hK}\right|},$$

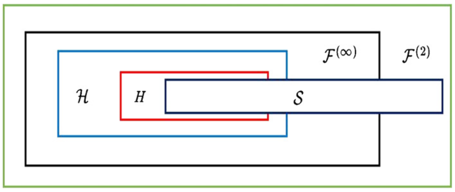

Fig. 1. Venn diagram illusting the relationships. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

which yields $\left|e^{hK}\right| = 1$ (it is assumed that $\left|e^{hK}\right| \neq -1$ in the introduction of this paper). We then compute the left-hand side of (10) as follows

$$\begin{aligned}
& |I_s \otimes I - h(A \otimes I. * E(hK))F| \\
= & \left|(I_s \otimes P)(I_s \otimes P^{-1}) - h(I_s \otimes P)(A \otimes I. * E(hK))(I_s \otimes P^{-1})(I_s \otimes P)F(I_s \otimes P^{-1})\right| \\
= & \left|I_s \otimes I + h(I_s \otimes P)(A \otimes I. * E(hK))(I_s \otimes P^{-1})F^\intercal\right| \\
= & |I_s \otimes I + h(A \otimes I. * E(-hK^\intercal))F^\intercal| \\
= & |I_s \otimes I + hF(A^\intercal \otimes I. * E(-hK^\intercal)^\intercal)| \text{ (transpose)} \\
= & |I_s \otimes I + h(A^\intercal \otimes I. * E(-hK^\intercal)^\intercal)F| \text{ (Sylvester's law).}
\end{aligned}$$

It follows from the definition (11) that

$$E(-hK^\intercal)^\intercal = (E_{i,j}(-hK^\intercal))^\intercal_{s\times s} = (E_{j,i}(-hK))_{s\times s} = (E_{i,j}(hK))_{s\times s} = E(hK). \tag{14}$$

Therefore, one arrives at

$$|I_s \otimes I - h(A \otimes I. * E(hK))F| = \left|I_s \otimes I + h(A^\intercal \otimes I. * E(hK))F\right|,$$

which shows the statement of this theorem by considering Lemma 3.2. $\square$

4.2. Vector fields in $\mathcal{S}$

Theorem 4.4. *All one-stage SSEI methods and all two-stage SSEI methods with*

$$e^{(c_2-c_1)hK} g'(k_2) e^{(c_1-c_2)hK} g'(k_1) = e^{(c_1-c_2)hK} g'(k_2) e^{(c_2-c_1)hK} g'(k_1) \tag{15}$$

(and any composition of such methods) are volume preserving for vector fields f and g in $\mathcal{S}$ with the same P.

Proof. Similarly to the proof of last theorem, we obtain that $PKP^{-1} = -K$. Thus it is true that $Pe^{hK}P^{-1} = e^{-hK}$ and $\left|e^{hK}\right| = 1$.

For the one-stage SSEI methods, according to Lemma 3.2, it is volume preserving if and only if

$$\left|I - ha_{11}g'(k_1)\right| = \left|I + ha_{11}g'(k_1)\right|,$$

which can be verified by considering

$$\left|I - ha_{11}g'(k_1)\right| = \left|PP^{-1} - ha_{11}Pg'(k_1)P^{-1}\right| = \left|I + ha_{11}g'(k_1)\right|.$$

For a two-stage SSEI method, according to Lemma 3.2 again, this two-stage SSEI method is volume preserving if and only if

$$\begin{vmatrix} I - ha_{11}g'(k_1) & -ha_{12}e^{(c_1-c_2)hK}g'(k_2) \\ -ha_{21}e^{(c_2-c_1)hK}g'(k_1) & I - ha_{22}g'(k_2) \end{vmatrix}
= \begin{vmatrix} I + ha_{11}g'(k_1) & ha_{21}e^{(c_1-c_2)hK}g'(k_2) \\ ha_{12}e^{(c_2-c_1)hK}g'(k_1) & I + ha_{22}g'(k_2) \end{vmatrix},$$

which gives the condition

$$\begin{aligned}
& |I - ha_{11}g'(k_1) - ha_{22}g'(k_2) + h^2 a_{11}a_{22}g'(k_1)g'(k_2) \\
& -h^2 a_{12}a_{21}e^{(c_1-c_2)hK}g'(k_2)e^{(c_2-c_1)hK}g'(k_1)| \\
= & |I + ha_{11}g'(k_1) + ha_{22}g'(k_2) + h^2 a_{11}a_{22}g'(k_1)g'(k_2) \\
& -h^2 a_{12}a_{21}e^{(c_1-c_2)hK}g'(k_2)e^{(c_2-c_1)hK}g'(k_1)|.
\end{aligned} \tag{16}$$

It also can be verified that

$$
\begin{aligned}
&\text{the left hand side of (16)}\\
=\ & |\,PP^{-1}-ha_{11}Pg'(k_1)P^{-1}-ha_{22}Pg'(k_2)P^{-1}+h^2a_{11}a_{22}Pg'(k_1)g'(k_2)P^{-1}\\
&-h^2a_{12}a_{21}Pe^{(c_1-c_2)hK}g'(k_2)e^{(c_2-c_1)hK}g'(k_1)P^{-1}\,|\\
=\ & |\,I+ha_{11}g'(k_1)+ha_{22}g'(k_2)+h^2a_{11}a_{22}Pg'(k_1)P^{-1}Pg'(k_2)P^{-1}\\
&-h^2a_{12}a_{21}Pe^{(c_1-c_2)hK}P^{-1}Pg'(k_2)P^{-1}Pe^{(c_2-c_1)hK}P^{-1}Pg'(k_1)P^{-1}\,|\\
=\ & |\,I+ha_{11}g'(k_1)+ha_{22}g'(k_2)+h^2a_{11}a_{22}g'(k_1)g'(k_2)\\
&-h^2a_{12}a_{21}e^{(c_2-c_1)hK}g'(k_2)e^{(c_1-c_2)hK}g'(k_1)\,|\,.
\end{aligned}
$$

Under the assumption (15), this result becomes

$$|\,I+ha_{11}g'(k_1)+ha_{22}g'(k_2)+h^2a_{11}a_{22}g'(k_1)g'(k_2)-h^2a_{12}a_{21}e^{(c_1-c_2)hK}g'(k_2)e^{(c_2-c_1)hK}g'(k_1)\,|\,.$$

Thus (16) is obtained immediately, and then all two-stage SSEI methods with (15) are volume preserving. □

Remark 4.5. It is noted that for the vector fields in $\mathcal{S}$ and two-stage SSEI methods, the condition (15) can be true for many special cases such as for some special matrix K or some special function g. The same situation will happen in the analysis of Subsection 4.4.

4.3. Vector fields in $\mathcal{F}^{(\infty)}$

For vector fields in $\mathcal{F}^{(\infty)}$, if the function $f(y):=Ky+g(y)$ has the pattern $(u(y_1),v(y_1,y_2))^\intercal$, this means that K and g can be expressed in blocks as

$$K=\begin{pmatrix}K_{11} & 0\\ 0 & K_{22}\end{pmatrix},\quad g(y)=\begin{pmatrix}g_1(y_1)\\ g_2(y_1,y_2)\end{pmatrix}. \tag{17}$$

Then the following relation is true

$$u(y_1)=K_{11}y_1+g_1(y_1),\quad v(y_1,y_2)=K_{22}y_2+g_2(y_1,y_2). \tag{18}$$

Theorem 4.6. *Consider an s-stage SSEI method for solving $y_1'=u(y_1)$ that is volume preserving for the vector field $u(y_1):\mathbb{R}^m\to\mathbb{R}^m$. Let $v(y_1,y_2):\mathbb{R}^{m+n}\to\mathbb{R}^{m+n}$ and assume that there exists an invertible matrix P such that for all y_1,y_2,*

$$P\partial_{y_2}v(y_1,y_2)P^{-1}=-\partial_{y_2}v(y_1,y_2)^\intercal,\quad P\partial_{y_2}g_2(y_1,y_2)P^{-1}=-\partial_{y_2}g_2(y_1,y_2)^\intercal.$$

Then the SSEI method is volume preserving for vector fields $f(y_1,y_2)=(u(y_1),v(y_1,y_2))^\intercal$ in $\mathcal{F}^{(\infty)}$.

Proof. From the property of v, it follows that $PK_{22}P^{-1}=-K_{22}^\intercal$ and $|e^{hK_{22}}|=1$. Thus $|e^{hK}|=|e^{hK_{11}}||e^{hK_{22}}|=|e^{hK_{11}}|$. The Jacobian matrix of $g(y)$ is block triangular as follows

$$g'(y_1,y_2)=\begin{pmatrix}\partial_{y_1}g_1(y_1) & 0\\ * & \partial_{y_2}g_2(y_1,y_2)\end{pmatrix}.$$

In what follows, we prove the condition (10). Using the block transformation, we can bring the left-hand side of (10) to the block form

$$|I_s\otimes I-h(A\otimes I.*E(hK))F|=\begin{pmatrix}\Phi_1 & 0\\ * & \Phi_2\end{pmatrix},$$

where

$$\Phi_1=\begin{pmatrix}I-h\bar{a}_{11}(hK_{11})\partial_{y_1}g_1(k_1) & \cdots & -h\bar{a}_{1s}(hK_{11})\partial_{y_1}g_1(k_s)\\ \vdots & \ddots & \vdots\\ -h\bar{a}_{s1}(hK_{11})\partial_{y_1}g_1(k_1) & \cdots & I-h\bar{a}_{ss}(hK_{11})\partial_{y_1}g_1(k_s)\end{pmatrix},$$

$$\Phi_2=\begin{pmatrix}I-h\bar{a}_{11}(hK_{22})\partial_{y_2}g_2(k_1) & \cdots & -h\bar{a}_{1s}(hK_{22})\partial_{y_2}g_2(k_s)\\ \vdots & \ddots & \vdots\\ -h\bar{a}_{s1}(hK_{22})\partial_{y_2}g_2(k_1) & \cdots & I-h\bar{a}_{ss}(hK_{22})\partial_{y_2}g_2(k_s)\end{pmatrix}.$$

Let $F_1=\mathrm{diag}(\partial_{y_1}g_1(k_1),\ldots,\partial_{y_1}g_1(k_s))$ and $F_2=\mathrm{diag}(\partial_{y_2}g_2(k_1),\ldots,\partial_{y_2}g_2(k_s))$. The above result can be simplified as

$$\begin{aligned} & |I_s \otimes I - h(A \otimes I .* E(hK))F| \\ = & |I_s \otimes I - h(A \otimes I .* E(hK_{11}))F_1| \, |I_s \otimes I - h(A \otimes I .* E(hK_{22}))F_2| . \end{aligned}$$

Since the SSEI method is volume preserving for the vector field $u(y_1)$, the following condition is true

$$|I_s \otimes I - h(A \otimes I .* E(hK_{11}))F_1| = \left|e^{hK_{11}}\right| \left|I_s \otimes I + h(A^\intercal \otimes I .* E(hK_{11}))F_1\right| .$$

On the other hand, we compute

$$\begin{aligned} & |I_s \otimes I - h(A \otimes I .* E(hK_{22}))F_2| \\ = & \left|(I_s \otimes P)(I_s \otimes P^{-1}) - h(I_s \otimes P)(A \otimes I .* E(hK_{22}))(I_s \otimes P^{-1})(I_s \otimes P)F(I_s \otimes P^{-1})\right| \\ = & \left|I_s \otimes I + h(I_s \otimes P)(A \otimes I .* E(hK_{22}))(I_s \otimes P^{-1})F_2^\intercal\right| \\ = & \left|I_s \otimes I + h(A \otimes I .* E(-hK_{22}^\intercal))F_2^\intercal\right| \\ = & \left|I_s \otimes I + hF_2(A^\intercal \otimes I .* E(-hK_{22}^\intercal)^\intercal)\right| \text{ (transpose)} \\ = & \left|I_s \otimes I + h(A^\intercal \otimes I .* E(-hK_{22}^\intercal)^\intercal)F_2\right| \text{ (Sylvester's law)} \\ = & |I_s \otimes I + h(A^\intercal \otimes I .* E(hK_{22}))F_2| \text{ (property (14))}. \end{aligned}$$

Therefore, the VP condition (10) holds and the SSEI method is volume preserving for vector fields in $\mathcal{F}^{(\infty)}$. □

4.4. Vector fields in $\mathcal{F}^{(2)}$

Suppose that the function $f(y)$ of (1) falls into $\mathcal{F}^{(2)}$. Under this situation, (17) and (18) are still true. We obtain the following result about the VP property of SSEI methods.

Theorem 4.7. *Consider a one-stage or two-stage SSEI with (15) (or a composition of such method) that is volume preserving for the vector field $u(y_1) : \mathbb{R}^m \to \mathbb{R}^m$. Letting $v(y_1, y_2) : \mathbb{R}^{m+n} \to \mathbb{R}^{m+n}$, we assume that there exists an invertible matrix P such that for all y_1, y_2,*

$$P\partial_{y_2} v(y_1, y_2)P^{-1} = -\partial_{y_2} v(y_1, y_2), \quad P\partial_{y_2} g_2(y_1, y_2)P^{-1} = -\partial_{y_2} g_2(y_1, y_2).$$

Then the SSEI method is volume preserving for the vector fields $f(y_1, y_2) = (u(y_1), v(y_1, y_2))^\intercal$ in $\mathcal{F}^{(2)}$.

Proof. It follows from the conditions of this theorem that $PK_{22}P^{-1} = -K_{22}$ and $\left|e^{hK_{22}}\right| = 1$.

For the one-stage SSEI, the condition for volume preservation is

$$\left|I - ha_{11}g'(k_1)\right| = \left|I + ha_{11}g'(k_1)\right| ,$$

which can be rewritten as

$$\left|I - ha_{11}\partial_{y_1}g_1\right| \left|I - ha_{11}\partial_{y_2}g_2\right| = \left|I + ha_{11}\partial_{y_1}g_1\right| \left|I + ha_{11}\partial_{y_2}g_2\right| . \tag{19}$$

Since the method is volume preserving for the vector field $u(y_1)$, we have

$$\left|I - ha_{11}\partial_{y_1}g_1\right| = \left|I + ha_{11}\partial_{y_1}g_1\right| .$$

On the other hand,

$$\left|I - ha_{11}\partial_{y_2}g_2\right| = \left|PP^{-1} - ha_{11}P\partial_{y_2}g_2P^{-1}\right| = \left|I + ha_{11}\partial_{y_2}g_2\right| .$$

Thus (19) is proved.

For the two-stage SSEI, it is volume preserving if and only if (16) is true. According to the special result of g', one has

$$\begin{aligned} & \text{the left hand side of (16)} \\ = & |I - ha_{11}\partial_{y_1}g_1(k_1) - ha_{22}\partial_{y_1}g_1(k_2) + h^2a_{11}a_{22}\partial_{y_1}g_1(k_1)\partial_{y_1}g_1(k_2) \\ & -h^2a_{12}a_{21}\partial_{y_1}g_1(k_2)\partial_{y_1}g_1(k_1)| \\ & |I - ha_{11}\partial_{y_2}g_2(k_1) - ha_{22}\partial_{y_2}g_2(k_2) + h^2a_{11}a_{22}\partial_{y_2}g_2(k_1)\partial_{y_2}g_2(k_2) \\ & -h^2a_{12}a_{21}\partial_{y_2}g_2(k_2)\partial_{y_2}g_2(k_1)| \\ = & |I + ha_{11}\partial_{y_1}g_1(k_1) + ha_{22}\partial_{y_1}g_1(k_2) + h^2a_{11}a_{22}\partial_{y_1}g_1(k_1)\partial_{y_1}g_1(k_2) \\ & -h^2a_{12}a_{21}\partial_{y_1}g_1(k_2)\partial_{y_1}g_1(k_1)| \\ & |I - ha_{11}\partial_{y_2}g_2(k_1) - ha_{22}\partial_{y_2}g_2(k_2) + h^2a_{11}a_{22}\partial_{y_2}g_2(k_1)\partial_{y_2}g_2(k_2) \\ & -h^2a_{12}a_{21}\partial_{y_2}g_2(k_2)\partial_{y_2}g_2(k_1)|. \end{aligned}$$

It then can be verified that

$$\begin{aligned}
& |I - ha_{11}\partial_{y_2} g_2(k_1) - ha_{22}\partial_{y_2} g_2(k_2) + h^2 a_{11}a_{22}\partial_{y_2} g_2(k_1)\partial_{y_2} g_2(k_2) \\
& \quad -h^2 a_{12}a_{21}\partial_{y_2} g_2(k_2)\partial_{y_2} g_2(k_1)| \\
= & \ |PP^{-1} - ha_{11}P\partial_{y_2} g_2(k_1)P^{-1} - ha_{22}P\partial_{y_2} g_2(k_2)P^{-1} + h^2 a_{11}a_{22}P\partial_{y_2} g_2(k_1)P^{-1} \\
& \quad P\partial_{y_2} g_2(k_2)P^{-1} - h^2 a_{12}a_{21}P\partial_{y_2} g_2(k_2)P^{-1}P\partial_{y_2} g_2(k_1)P^{-1}| \\
= & \ |\, I + ha_{11}\partial_{y_2} g_2(k_1) + ha_{22}\partial_{y_2} g_2(k_2) + h^2 a_{11}a_{22}\partial_{y_2} g_2(k_1)\partial_{y_2} g_2(k_2) \\
& \quad -h^2 a_{12}a_{21}\partial_{y_2} g_2(k_2)\partial_{y_2} g_2(k_1)\,| \,.
\end{aligned}$$

Consequently,

$$\begin{aligned}
& \text{the left hand side of (16)} \\
= & \ |I + ha_{11}\partial_{y_1} g_1(k_1) + ha_{22}\partial_{y_1} g_1(k_2) + h^2 a_{11}a_{22}\partial_{y_1} g_1(k_1)\partial_{y_1} g_1(k_2) \\
& \quad -h^2 a_{12}a_{21}\partial_{y_1} g_1(k_2)\partial_{y_1} g_1(k_1)| \\
& |I + ha_{11}\partial_{y_2} g_2(k_1) + ha_{22}\partial_{y_2} g_2(k_2) + h^2 a_{11}a_{22}\partial_{y_2} g_2(k_1)\partial_{y_2} g_2(k_2) \\
& \quad -h^2 a_{12}a_{21}\partial_{y_2} g_2(k_2)\partial_{y_2} g_2(k_1)| \\
= & \ \text{the right hand side of (16).}
\end{aligned}$$

Therefore, all two-stage SSEI methods with (15) are volume preserving. □

Remark 4.8. We note that when $K = \mathbf{0}$, all the results given in this section reduce to those proposed in [1], which demonstrate the wider applications of the analysis. Moreover, based on these results of exponential integrators, we will formulate and study different volume-preserving methods for different problems in the next section.

5. Applications to various problems

This section is devoted to the applications of the SSEI methods to various problems. By using the analysis given in Section 4, we will show the volume preservation of different integrators.

5.1. Highly oscillatory second-order systems

Consider the following first-order systems

$$y'(t) = J^{-1}My(t) + J^{-1}\nabla V(y(t)), \tag{20}$$

where the matrix J is constant and invertible, M is a symmetric matrix and V is a differentiable function.

Corollary 5.1. *All SSEI methods are volume preserving for solving the system* (20)*.*

Proof. This system is the exact pattern (1) with

$$K = J^{-1}M, \quad g(y(t)) = J^{-1}\nabla V(y(t)). \tag{21}$$

It can be verified that

$$Jg'(y)J^{-1} = JJ^{-1}\nabla^2 V(y)J^{-1} = \nabla^2 V(y)J^{-1} = -g'(y)^{\intercal}$$

and

$$J(K + g'(y))J^{-1} = -(K + g'(y))^{\intercal}.$$

This shows that the set $\mathcal{H}$ contains all vector fields of (20) with the same $P = J$. Thus in the light of Theorem 4.3, the result is proved. □

Remark 5.2. When $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$, the system (20) is a Hamiltonian system $y'(t) = J^{-1}\nabla H(y(t))$ with the Hamiltonian $H(y) = \dfrac{1}{2}y^{\intercal}My + V(y)$. Corollary 5.1 shows that all SSEI methods are volume preserving for this Hamiltonian system. This is another explanation of the fact that symplectic exponential integrators are volume preserving for Hamiltonian systems.

Consider another special and important case of (20) by choosing

$$y=\begin{pmatrix} q \\ p \end{pmatrix},\quad J^{-1}=\begin{pmatrix} 0 & I \\ -I & N \end{pmatrix},\quad M=\begin{pmatrix} \Omega & 0 \\ 0 & I \end{pmatrix},\quad V(y)=V_1(q),$$

which gives the following second-order ODE

$$q''-Nq'+\Omega q=-\nabla V_1(q). \tag{22}$$

This system stands for highly oscillatory problems and many problems fall into this kind of equation such as the dissipative molecular dynamics, the (damped) Duffing, charged-particle dynamics in a constant magnetic field and semi-discrete nonlinear wave equations. Applying the SSEI methods to (22) and considering Theorem 4.3, we obtain the following corollary.

Corollary 5.3. *The following s-stage adapted exponential integrator*

$$\begin{cases} k_i=\exp^{11}(c_ihK)q_n+\exp^{12}(c_ihK)q_n'-h\sum\limits_{j=1}^{s}a_{ij}\exp^{12}((c_i-c_j)hK)\nabla V_1(k_j), \qquad i=1,2,\ldots,s, \\ q_{n+1}=\exp^{11}(hK)q_n+\exp^{12}(hK)q_n'-h\sum\limits_{i=1}^{s}b_i\exp^{12}((1-c_i)hK)\nabla V_1(k_i), \\ q_{n+1}'=\exp^{21}(hK)q_n+\exp^{22}(hK)q_n'-h\sum\limits_{i=1}^{s}b_i\exp^{22}((1-c_i)hK)\nabla V_1(k_i) \end{cases} \tag{23}$$

are volume preserving for the second-order highly oscillatory equation (22), where $\exp(hK)$ *is partitioned into* $\begin{pmatrix} \exp^{11}(hK) & \exp^{12}(hK) \\ \exp^{21}(hK) & \exp^{22}(hK) \end{pmatrix}$ *and the same denotations are used for other matrix-valued functions. Here* $(c_1,\ldots,c_s)^{\intercal}$, $(b_1,\ldots,b_s)^{\intercal}$ *and* $(a_{ij})_{s\times s}$ *are given in Definition 2.2. If N commutes with* Ω, *the results of* $\exp^{ij}$ *for* $i,j=1,2$ *can be expressed explicitly:*

$$\begin{aligned} &\exp^{11}(hK)=e^{\frac{h}{2}N}\Big(\cosh\big(\tfrac{h}{2}\sqrt{N^2-4\Omega}\big)-N\sinh\big(\tfrac{h}{2}\sqrt{N^2-4\Omega}\big)(\sqrt{N^2-4\Omega})^{-1}\Big), \\ &\exp^{12}(hK)=2e^{\frac{h}{2}N}\sinh\big(\tfrac{h}{2}\sqrt{N^2-4\Omega}\big)(\sqrt{N^2-4\Omega})^{-1}, \\ &\exp^{21}(hK)=-\Omega\exp^{12}(hK), \\ &\exp^{22}(hK)=e^{\frac{h}{2}N}\Big(\cosh\big(\tfrac{h}{2}\sqrt{N^2-4\Omega}\big)+N\sinh\big(\tfrac{h}{2}\sqrt{N^2-4\Omega}\big)(\sqrt{N^2-4\Omega})^{-1}\Big). \end{aligned} \tag{24}$$

These results are still true if we replace h by kh with any $k\in\mathbb{R}$.

If we further assume that $\Omega=\mathbf{0}$, the equation (22) becomes

$$q''=Nq'-\nabla V_1(q). \tag{25}$$

One typical example of this system is charged-particle dynamics in a constant magnetic field (see [11])

$$x''=x'\times B+F(x). \tag{26}$$

Here $x(t)\in\mathbb{R}^3$ describes the position of a particle moving in an electro-magnetic field, $F(x)=-\nabla_x U(x)$ is an electric field with the scalar potential $U(x)$, and $B=\nabla_x\times A(x)$ is a constant magnetic field with the vector potential $A(x)=-\frac{1}{2}x\times B$.

Under the condition that $\Omega=0$, (24) can be rewritten more succinctly as:

$$\exp^{11}(hK)=I,\quad \exp^{12}(hK)=h\varphi_1(hN),\quad \exp^{21}(hK)=0,\quad \exp^{22}(hK)=\varphi_0(hN),$$

where the φ-functions are defined by (see [16,17])

$$\varphi_0(z)=e^z,\quad \varphi_k(z)=\int_0^1 e^{(1-\sigma)z}\frac{\sigma^{k-1}}{(k-1)!}d\sigma,\quad k=1,2,\ldots. \tag{27}$$

We then get the following volume-preserving methods for the special and important second-order system (25).

Corollary 5.4. *The following s-stage integrator*

$$\begin{cases} k_i = q_n + c_i h\varphi_1(c_i hN)q_n' - h^2 \sum\limits_{j=1}^{s} a_{ij}(c_i - c_j)\varphi_1((c_i - c_j)hN)\nabla V_1(k_j), \quad i = 1, 2, \ldots, s, \\ q_{n+1} = q_n + h\varphi_1(hN)q_n' - h^2 \sum\limits_{i=1}^{s} b_i(1 - c_i)\varphi_1((1 - c_i)hN)\nabla V_1(k_i), \\ q_{n+1}' = \varphi_0(hN)q_n' - h\sum\limits_{i=1}^{s} b_i\varphi_0((1 - c_i)hN)\nabla V_1(k_i) \end{cases} \tag{28}$$

are volume preserving for the highly oscillatory second-order system (25), where $(c_1, \ldots, c_s)^\intercal$, $(b_1, \ldots, b_s)^\intercal$ and $(a_{ij})_{s\times s}$ are given in Definition 2.2.

Remark 5.5. It is noted that the above two corollaries are new discoveries which are of great importance to Geometric Integration for second-order highly oscillatory problems.

5.2. Separable partitioned systems

It has been proved in [1] that the set $\mathcal{S}$ contains all separable partitioned systems. As an example, we consider

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} p \\ -\Omega q + \tilde{g}(q) \end{pmatrix} = \begin{pmatrix} 0 & I \\ -\Omega & 0 \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ \tilde{g}(q) \end{pmatrix}, \tag{29}$$

which is exactly the system (1) with

$$K = \begin{pmatrix} 0 & I \\ -\Omega & 0 \end{pmatrix}, \; g = \begin{pmatrix} 0 \\ \tilde{g}(q) \end{pmatrix}, \; f = \begin{pmatrix} p \\ -\Omega q + \tilde{g}(q) \end{pmatrix}.$$

It can be checked that f and g both fall into $\mathcal{S}$ with the same $P = \operatorname{diag}(I, -I)$. For this special matrix K, it is clear that

$$e^{xK} = \begin{pmatrix} \phi_0(x^2\Omega) & x\phi_1(x^2\Omega) \\ -x\Omega\phi_1(x^2\Omega) & \phi_0(x^2\Omega) \end{pmatrix} \quad \text{for} \quad x \in \mathbb{R}, \tag{30}$$

where $\phi_i(\Omega) := \sum\limits_{l=0}^{\infty} \dfrac{(-1)^l\Omega^l}{(2l+i)!}$ for $i = 0, 1$. Thus the exponential integrator (3) has a special form and we present it by the following definition.

Definition 5.6. (See [35].) An s-stage ERKN integrator for solving (29) is defined by

$$\begin{cases} Q_i &= \phi_0(c_i^2 V)q_n + hc_i\phi_1(c_i^2 V)p_n + h^2 \sum\limits_{j=1}^{s} \bar{a}_{ij}(V)\tilde{g}(Q_j), \quad i = 1, \ldots, s, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)p_n + h^2 \sum\limits_{i=1}^{s} \bar{b}_i(V)\tilde{g}(Q_i), \\ p_{n+1} &= -h\Omega\phi_1(V)q_n + \phi_0(V)p_n + h\sum\limits_{i=1}^{s} b_i(V)\tilde{g}(Q_i), \end{cases}$$

where c_i for $i = 1, \ldots, s$ are real constants, and $b_i(V)$, $\bar{b}_i(V)$ and $\bar{a}_{ij}(V)$ for $i, j = 1, \ldots, s$ are matrix-valued functions of $V \equiv h^2\Omega$.

ERKN integrators were firstly proposed in [35]. Further discussions about ERKN integrators have been given recently, including symmetric integrators (see [31]), symplectic integrators (see [34]), energy-preserving integrators (see [33]) and other kinds (see [26,29]). However, to our knowledge, the volume-preserving property of ERKN integrators has not been researched yet in the literature. With the analysis given in this paper, we get the following VP result of ERKN integrators.

Corollary 5.7. *Consider a kind of s-stage ERKN integrators*

$$\begin{cases} Q_i &= \phi_0(c_i^2 V)q_n + hc_i\phi_1(c_i^2 V)p_n + h^2 \sum\limits_{j=1}^{s} a_{ij}(c_i - c_j)\phi_1((c_i - c_j)^2 V)\tilde{g}(Q_j), \quad i = 1, \ldots, s, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)p_n + h^2 \sum\limits_{i=1}^{s} b_i(1 - c_i)\phi_1((1 - c_i)^2 V)\tilde{g}(Q_i), \\ p_{n+1} &= -h\Omega\phi_1(V)q_n + \phi_0(V)p_n + h\sum\limits_{i=1}^{s} b_i\phi_0((1 - c_i)^2 V)\tilde{g}(Q_i), \end{cases} \tag{31}$$

where $(c_1, \dots, c_s)^\intercal$, $(b_1, \dots, b_s)^\intercal$ *and* $(a_{ij})_{s\times s}$ *are given in Definition 2.2. Under the condition that* $b_j \neq 0$ *for* $j = 1, \dots, s$, *all one-stage and two-stage (with (15)) ERKN integrators (31) (and any composition of these methods) are volume preserving for solving the separable partitioned system (29).*

Proof. In the light of Definition 2.2 and the result (30), we adapt the SSEI methods to the system (29) and then get the scheme (31). Based on Theorem 4.4, the volume-preserving result of (31) is immediately obtained. □

Remark 5.8. We note that this is a novel result which studies the volume-preserving ERKN integrators for (29). Moreover, it can be observed from the scheme (31) that all one-stage ERKN integrators are explicit, which means that explicit volume preserving ERKN integrators are obtained for the separable partitioned system (29).

Remark 5.9. If Ω is a symmetric and positive semi-definite matrix and $\tilde{g}(q) = -\nabla U(q)$, the system (29) is an oscillatory Hamiltonian system $\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \nabla H(q, p)$ with the Hamiltonian

$$H(q, p) = \frac{1}{2} p^\intercal p + \frac{1}{2} q^\intercal \Omega q + U(q). \tag{32}$$

It has been noted in Subsection 5.1 that this vector field falls into the set $\mathcal{H}$. Thus Theorem 4.3 provides another way to prove the well-known fact that all symplectic ERKN integrators (31) are volume preserving for the oscillatory Hamiltonian system (32).

In what follows, we study the volume-preserving property of RKN methods for second-order ODEs. Consider $\Omega = \mathbf{0}$ for the above analysis and under this situation, ERKN integrators reduce to RKN methods. Therefore, we are now in a position to present the following volume-preserving property for RKN methods.

Corollary 5.10. *Consider the following s-stage RKN methods*

$$\begin{cases} Q_i &= q_n + hc_i q_n' + h^2 \sum\limits_{j=1}^{s} a_{ij}(c_i - c_j)\tilde{g}(Q_j), \quad i = 1, \dots, s, \\ q_{n+1} &= q_n + hq_n' + h^2 \sum\limits_{i=1}^{s} b_i(1 - c_i)\tilde{g}(Q_i), \\ q_{n+1}' &= q_n' + h \sum\limits_{i=1}^{s} b_i \tilde{g}(Q_i) \end{cases} \tag{33}$$

with the coefficients $c = (c_1, \dots, c_s)^\intercal$, $b = (b_1, \dots, b_s)^\intercal$ *and* $A = (a_{ij})_{s\times s}$ *of an s-stage RK method. If this RK method is symplectic and* $b_j \neq 0$ *for all* $j = 1, \dots, s$, *then all one-stage and two-stage RKN methods (33) (and compositions thereof) are volume preserving for solving the second-order system* $q'' = \tilde{g}(q)$.

Remark 5.11. It is noted that the fact of this corollary can be derived in a different way. Hairer, Lubich and Wanner have proved in [13] that any symplectic RK method with at most two stages (and any composition of such methods) is volume preserving for separable divergence free vector fields. Rewriting the second-order equation $q'' = \tilde{g}(q)$ as a first-order system and applying symplectic RK methods to it implies the result of Corollary 5.10. It is seen that the analysis of volume-preserving ERKN integrators provides an alternative derivation of the volume-preserving RKN methods.

5.3. Other applications

It has been shown in [1] that $\mathcal{F}^{(\infty)}$ contains the affine vector fields $f(y) = Ly + d$ such that $\left|I + \frac{h}{2}L\right| = \left|I - \frac{h}{2}L\right|$ for all $h > 0$. For solving the system in the affine vector fields, the exponential integrator (3) becomes

$$\begin{cases} k_i = e^{c_i hL} y_n + h \sum\limits_{j=1}^{s} \bar{a}_{ij}(hL)d, \quad i = 1, 2, \dots, s, \\ y_{n+1} = e^{hL} y_n + h \sum\limits_{i=1}^{s} \bar{b}_i(hL)d. \end{cases}$$

In the light of Theorem 4.6, this SSEI method is volume preserving for the affine vector fields.

It was also noted in [1] that $\mathcal{F}^{(\infty)}$ contains the vector fields $f(y)$ such that $f'(y) = JS(y)$ with a skew-symmetric matrix J and the symmetric matrix $S(y)$. Assume that

$$K = JM, \quad g'(y) = JS(y), \tag{34}$$

where M is a symmetric matrix. The system (1) with the vector field (34) falls into $\mathcal{F}^{(\infty)}$. Thus all SSEI methods are volume preserving for the vector field (34).

6. Numerical examples

In order to show the performance of SSEI methods, the solvers chosen for comparison are:

- SSRK1: the Gauss-Legendre method of order two whose coefficients are given as

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

- SSEI1: the one-stage SSEI method of order two with the coefficients

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & e^{\frac{1}{2}hK} \end{array}$$

- SSRK2: the Gauss-Legendre method of order four whose coefficients are given as

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2\sqrt{3}}{12} \\ \frac{3+\sqrt{3}}{6} & \frac{3+2\sqrt{3}}{12} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

- SSEI2: the two-stage SSEI method of order four with the coefficients

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2\sqrt{3}}{12}e^{-\frac{\sqrt{3}}{3}hK} \\ \frac{3+\sqrt{3}}{6} & \frac{3+2\sqrt{3}}{12}e^{\frac{\sqrt{3}}{3}hK} & \frac{1}{4} \\ \hline & \frac{1}{2}e^{\frac{3+\sqrt{3}}{6}hK} & \frac{1}{2}e^{\frac{3-\sqrt{3}}{6}hK} \end{array}$$

It is noted that all these methods are general implicit and we use fixed-point iteration here. We set 10^{-16} as the error tolerance and 100 as the maximum number of each fixed-point iteration.

Problem 1. As the first numerical example, we consider the Duffing equation

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -\omega^2 - k^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ 2k^2q^3 \end{pmatrix}, \quad \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = \begin{pmatrix} 0 \\ \omega \end{pmatrix}.$$

The exact solution of this system is $q(t) = sn(\omega t; k/\omega)$ with the Jacobi elliptic function sn. Since it is a Hamiltonian system, all the methods chosen for comparison are volume preserving. For this problem, we choose $k = 0.07$ and $\omega = 20$ and then solve it on the interval $[0, 100]$ with different stepsizes $h = 1/2, 1/10, 1/50, 1/200$. The numerical flows at the time points $\{\frac{1}{2}i\}_{i=1,\dots,200}$ of the four methods are given in Fig. 2. From the results, it can be observed clearly that the integrators SSEI1 and SSEI2 perform better than Runge-Kutta methods since they present a uniform result for every different stepsizes. Finally, we integrate this problem in $[0, t_{\text{end}}]$ with $h = 0.1/2^i$ for $i = 1, \dots, 4$. The relative global errors for different t_{end} are presented in Fig. 3. These results show clearly again that exponential integrators have better accuracy than Runge-Kutta methods. It is noted that in Fig. 3, some methods do not show the correct convergence. The reason for this observation might be that we set 10^{-16} as the error tolerance and 100 as the maximum number of each fixed-point iteration, and implicit iterations converge not very well for these methods.

Problem 2. Consider the following divergence free ODEs

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}' = \begin{pmatrix} 0 & -\omega & 0 \\ \omega & 0 & -\omega \\ 0 & \omega & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \sin(x-z) \\ 0 \\ \sin(x-z) \end{pmatrix}.$$

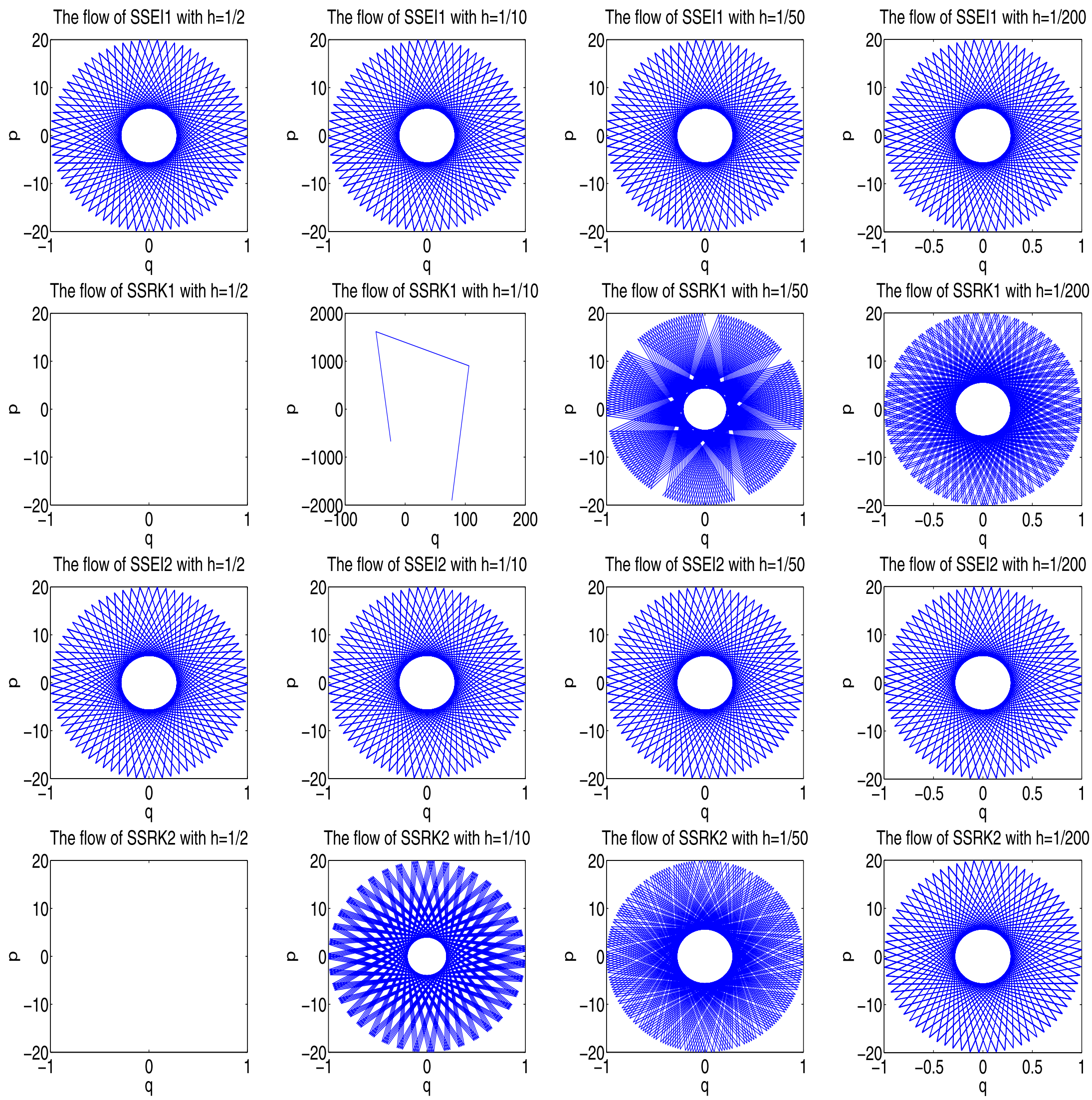

Fig. 2. Problem 1: the flows of different methods.

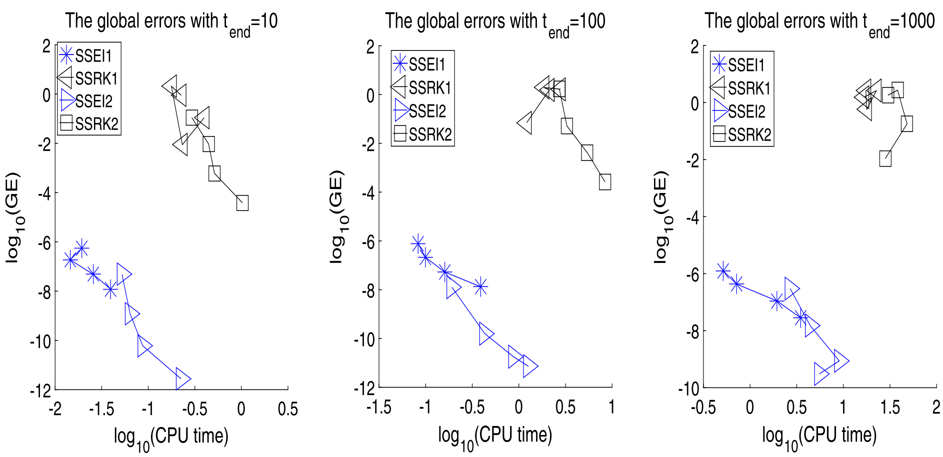

Fig. 3. Problem 1: the relative global errors.

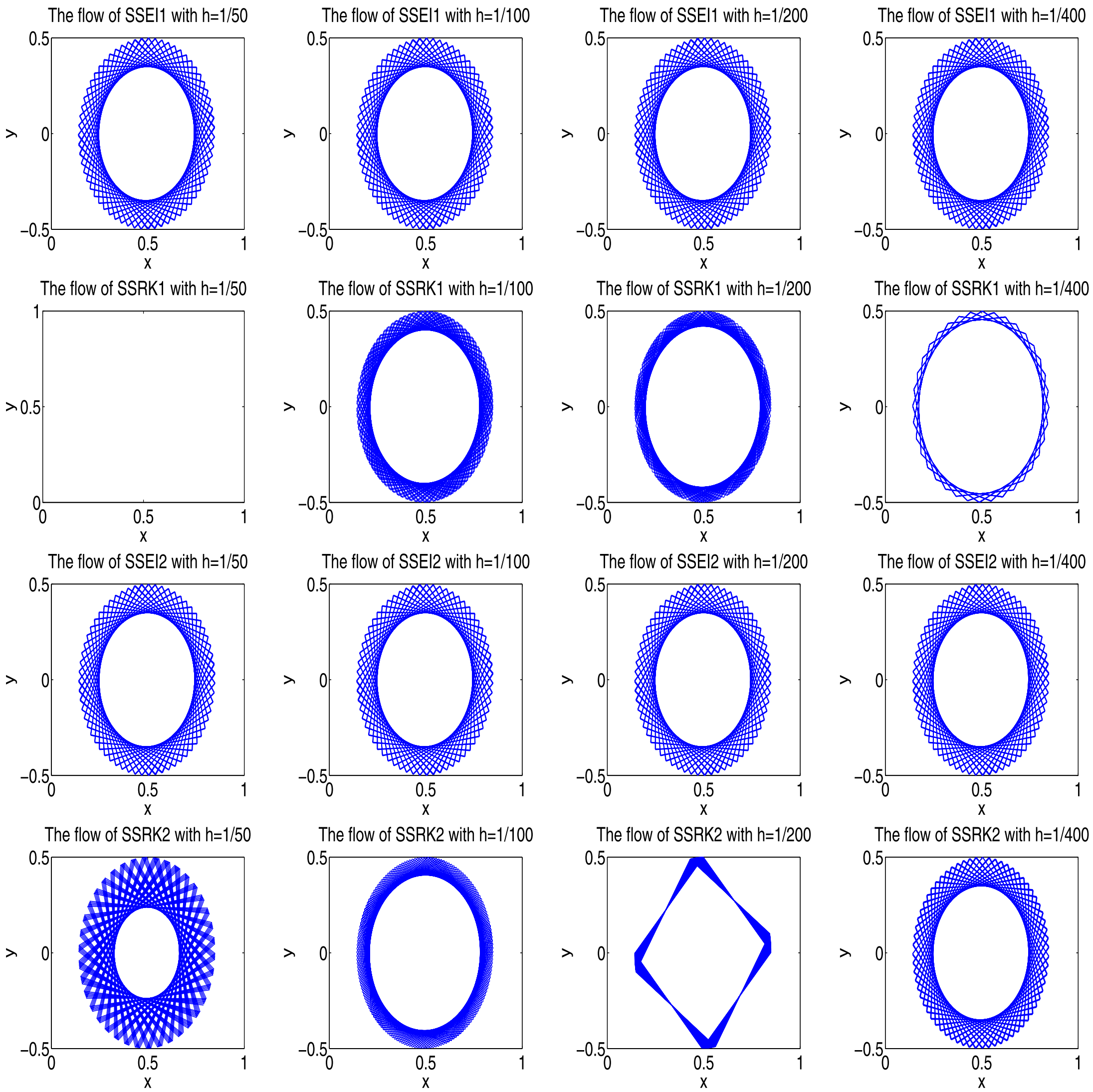

Fig. 4. Problem 2: the flows of different methods.

By choosing $P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$, it can be checked that the vector field of this problem falls into $\mathcal{S}$. We consider $\omega = 100$ and $(0.5, 0.5, 0.5)^\intercal$ as the initial value. This problem is firstly integrated in $[0, 100]$ with $h = 1/50, 1/100, 1/200, 1/400$ and the numerical flows x and y at the time points $\{\frac{1}{2}i\}_{i=1,\ldots,200}$ are shown in Fig. 4. Then the relative global errors for different t_{end} with $h = 0.1/2^i$ for $i = 2, \ldots, 5$ are given in Fig. 5. These results demonstrate clearly again that SSEI methods perform better than SSRK methods.

Problem 3. Consider the damped Helmholtz-Duffing oscillator (see [6])

$$q'' + 2\upsilon q' + Aq = -Bq^2 - \varepsilon q^3,$$

where q denotes the displacement of the system, A is the natural frequency, ε is a non-linear system parameter, υ is the damping factor, and B is a system parameter independent of time. It is well known that the dynamical behaviour of eardrum oscillations, elasto-magnetic suspensions, thin laminated plates, graded beams, and other physical phenomena all fall into this kind of equations. We choose the parameters

$$\upsilon = 0.01, \;\; A = 200, \;\; B = -0.5, \;\; \varepsilon = 1$$

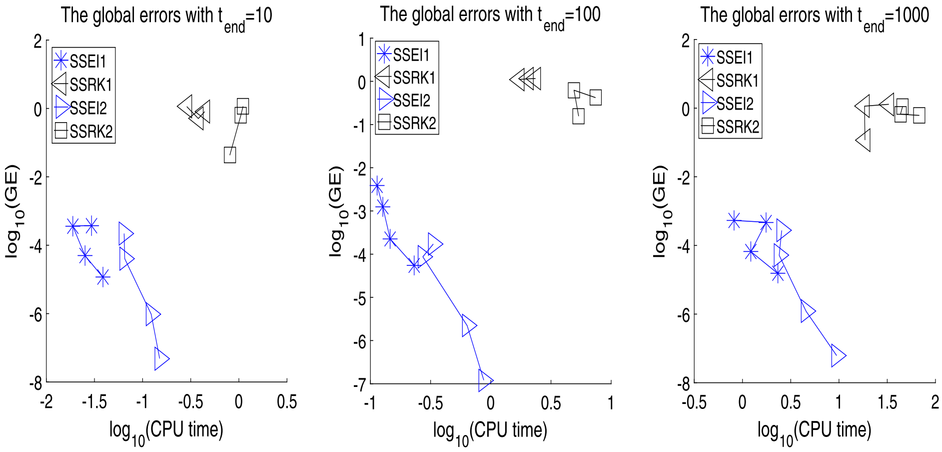

Fig. 5. Problem 2: the relative global errors.

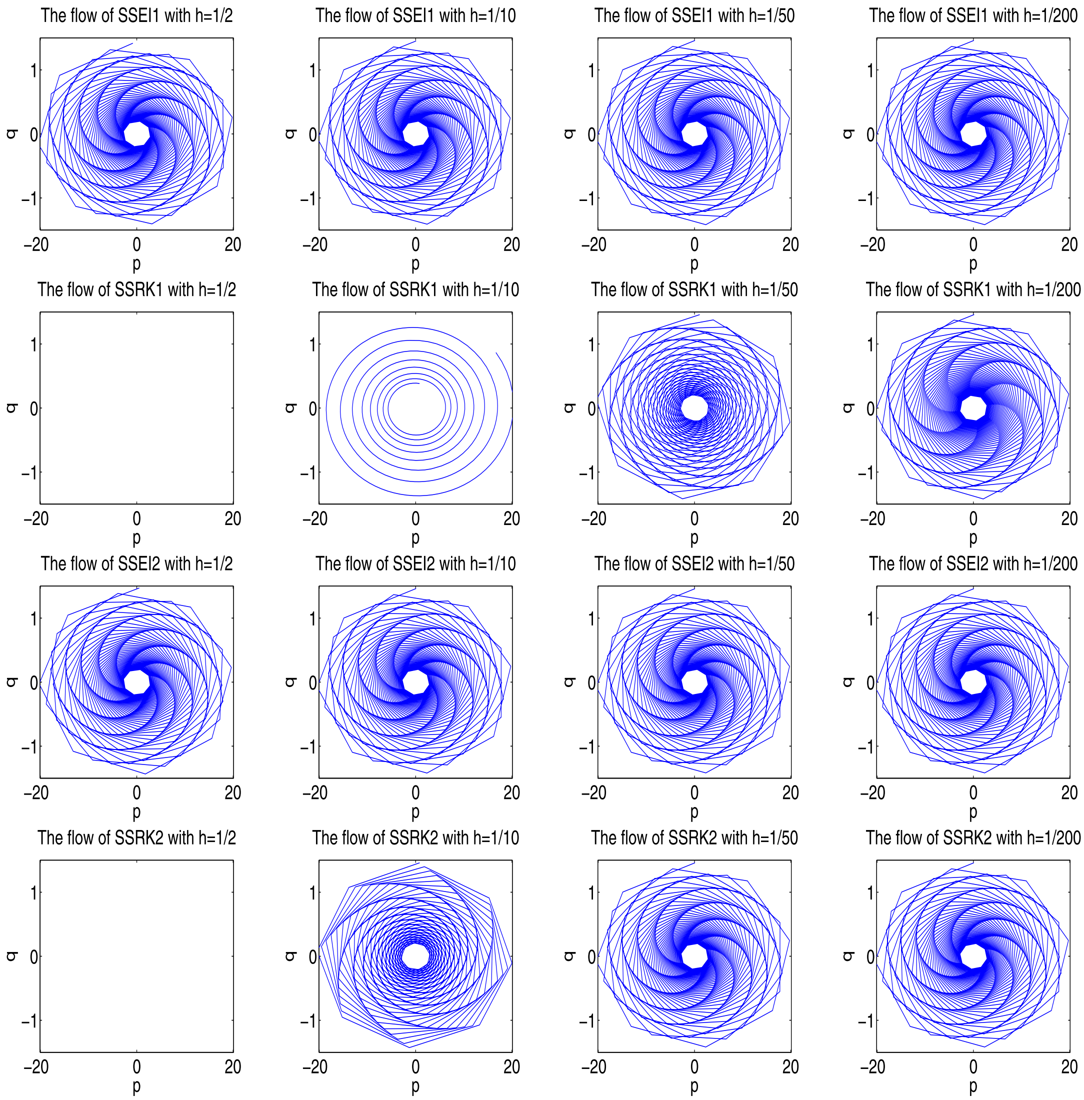

Fig. 6. Problem 3: the flows of different methods.

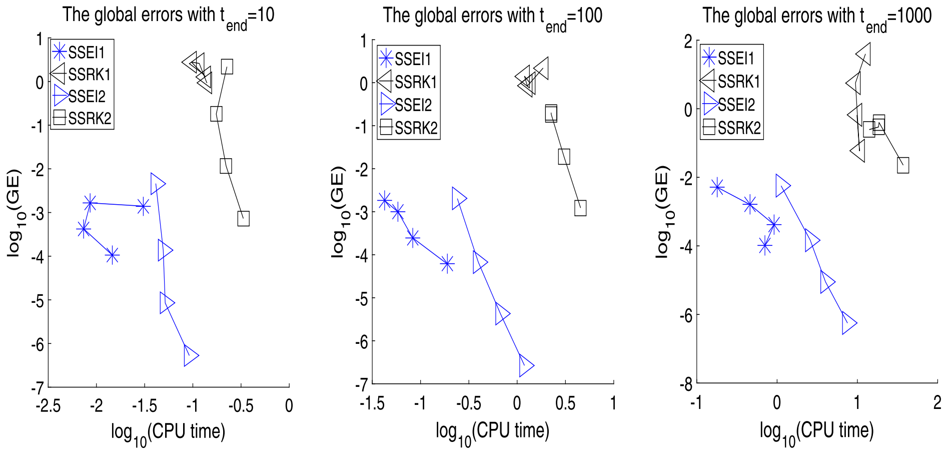

Fig. 7. Problem 3: the relative global errors.

and the initial value $q(0) = 1$ and $q'(0) = 15.199$. This problem is firstly integrated on $[0, 200]$ with $h = 1/2, 1/10, 1/50, 1/200$. We present the numerical flows q and $p = q'$ at the time points $\{\frac{1}{2}i\}_{i=1,\dots,400}$ in Fig. 6. We then solve the problem with different $t_{\text{end}} = 10, 100, 1000$ and $h = 0.1/2^i$ for $i = 0, \dots, 3$. The relative global errors are shown in Fig. 7. It follows again from the results that SSEI methods perform much better than SSRK methods.

Problem 4. This numerical experiment is concerned with the charged particle system with a constant magnetic field (see [11]). The system can be given by (26) with the potential $U(x) = \frac{1}{100\sqrt{x_1^2+x_2^2}}$ and the constant magnetic field $B = (0, 0, 10)^\intercal$. The initial values are chosen as $x(0) = (0.7, 1, 0.1)^\intercal$ and $x'(0) = (0.9, 0.5, 0.4)^\intercal$. We firstly integrate this system on $[0, 100]$ with $h = 1/2, 1/10, 1/50, 1/200$ and show the numerical flows x_2 and $v_2 = x_2'$ at the time points $\{\frac{1}{2}i\}_{i=1,\dots,200}$ in Fig. 8. Then the problem is solved with $t_{\text{end}} = 10, 100, 1000$ and $h = 0.1/2^i$ for $i = 0, \dots, 3$ and the relative global errors are shown in Fig. 9. The SSEI methods are also shown to be robust to this problem. Here, it is important to note that our SSEI1 method is explicit (see (28)) when applied to this problem, whereas, the SSRK1 method is implicit and the iteration is required for solving this problem. This fact shows another advantage of our volume-preserving exponential integrators in comparison with volume-preserving RK methods.

Problem 5. The last numerical experiment is devoted to the dynamical system for investigating fluid particle motion (see [36])

$$\begin{aligned}
\dot{x}_1 &= \tfrac{1}{2}(w_2x_3 - w_3x_2) + \tfrac{1}{2}\Big[(5r^2-3)\tfrac{x_1}{1+\alpha} - 2x_1\big(\tfrac{x_1^2}{1+\alpha} + \tfrac{\alpha x_1^2}{1+\alpha} - x_3^2\big)\Big],\\
\dot{x}_2 &= \tfrac{1}{2}(w_3x_1 - w_1x_3) + \tfrac{1}{2}\Big[(5r^2-3)\tfrac{\alpha x_2}{1+\alpha} - 2x_2\big(\tfrac{x_1^2}{1+\alpha} + \tfrac{\alpha x_1^2}{1+\alpha} - x_3^2\big)\Big],\\
\dot{x}_3 &= \tfrac{1}{2}(w_1x_2 - w_2x_1) + \tfrac{1}{2}\Big[-(5r^2-3)x_3 - 2x_3\big(\tfrac{x_1^2}{1+\alpha} + \tfrac{\alpha x_1^2}{1+\alpha} - x_3^2\big)\Big]
\end{aligned}$$

with $\alpha = 1$ and $(w_1, w_2, w_3) = (300, 500, 400)$. We choose the initial value by $(-0.1689, 0, -0.0437)^\intercal$ and solve this problem on $[0, 1000]$ with $h = 1/50, 1/200, 1/500, 1/1000$. The numerical flows through the (x_1, x_3) plane at the time points $\{\frac{1}{50}i\}_{i=1,\dots,1000}$ are given in Fig. 10. Then the problem is integrated with $t_{\text{end}} = 10, 100, 1000$ and $h = 0.01/2^i$ for $i = 0, \dots, 3$ and we show the relative global errors in Fig. 11.

Counterexample. In what follows, we present a counterexample where higher-order methods do not preserve the volume of the phase space for some vector fields. Let's consider the following problem

$$\begin{aligned}
&\dot{x} = -y + \sin(z),\\
&\dot{y} = -x + z + \cos(z),\\
&\dot{z} = y + \cos(x) + \sin(y)
\end{aligned}$$

with the initial value $(0, 0, 0)^\intercal$. This problem is solved on $[0, 10]$ with $h = 0.1$. The determinant of the derivative of the numerical flow as a function of time is given in Fig. 12. It follows from the results clearly that only the second-order method SSEI1 is volume-preserving while the fourth-order method SSEI2 does not preserve the volume. It is noted here that for higher-order methods, the volume-preserving property is more likely to fail than low order methods and one should be more careful when studying the volume preservation of higher-order methods.

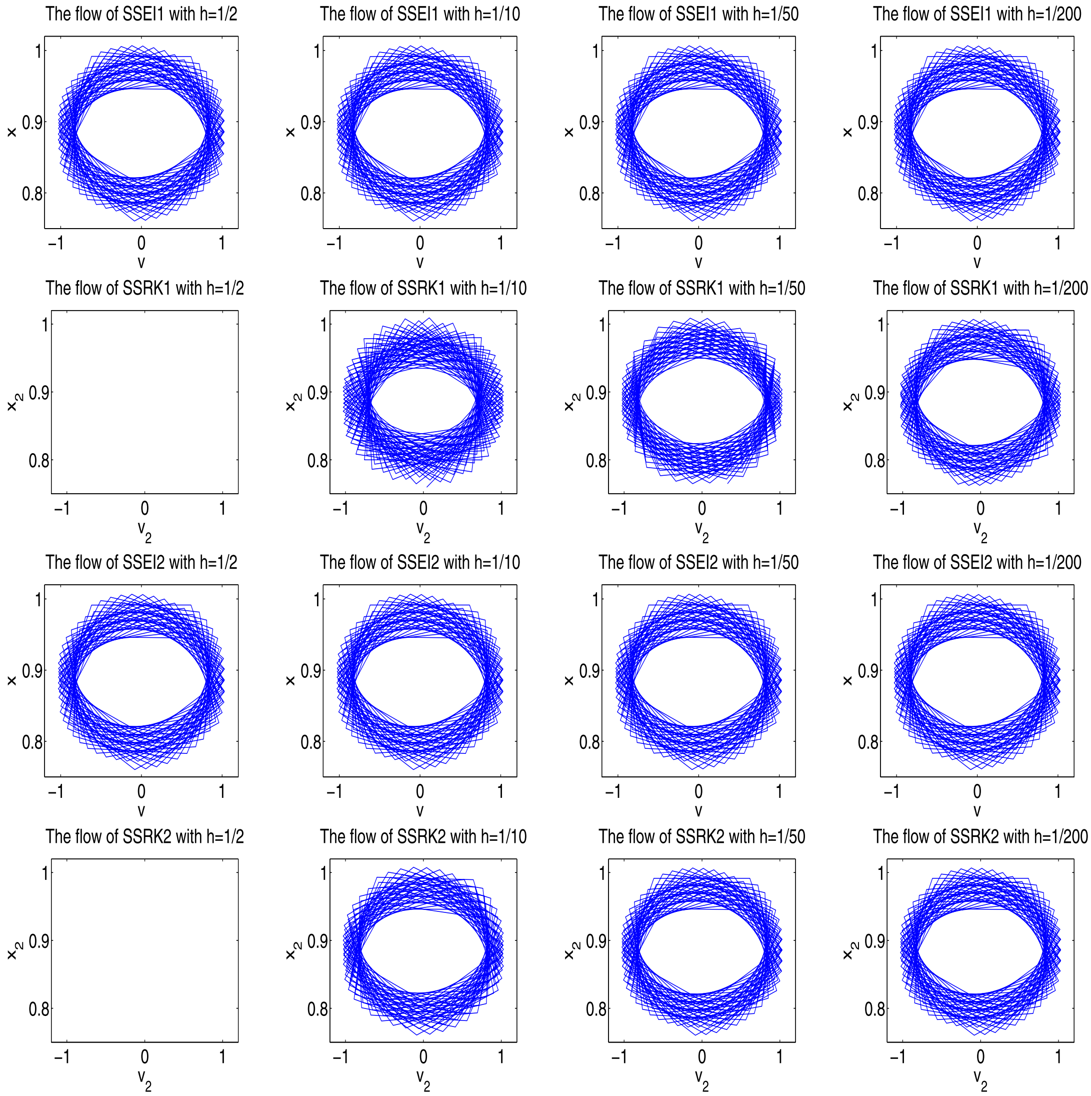

Fig. 8. Problem 4: the flows of different methods.

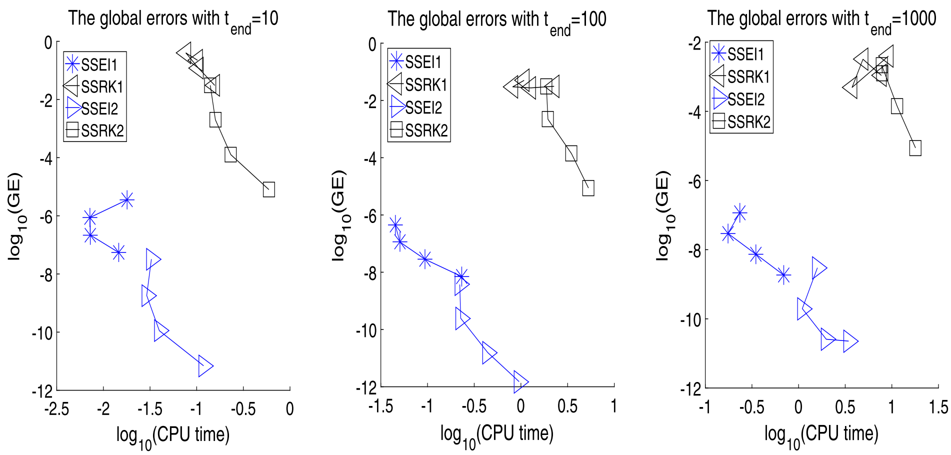

Fig. 9. Problem 4: the relative global errors.

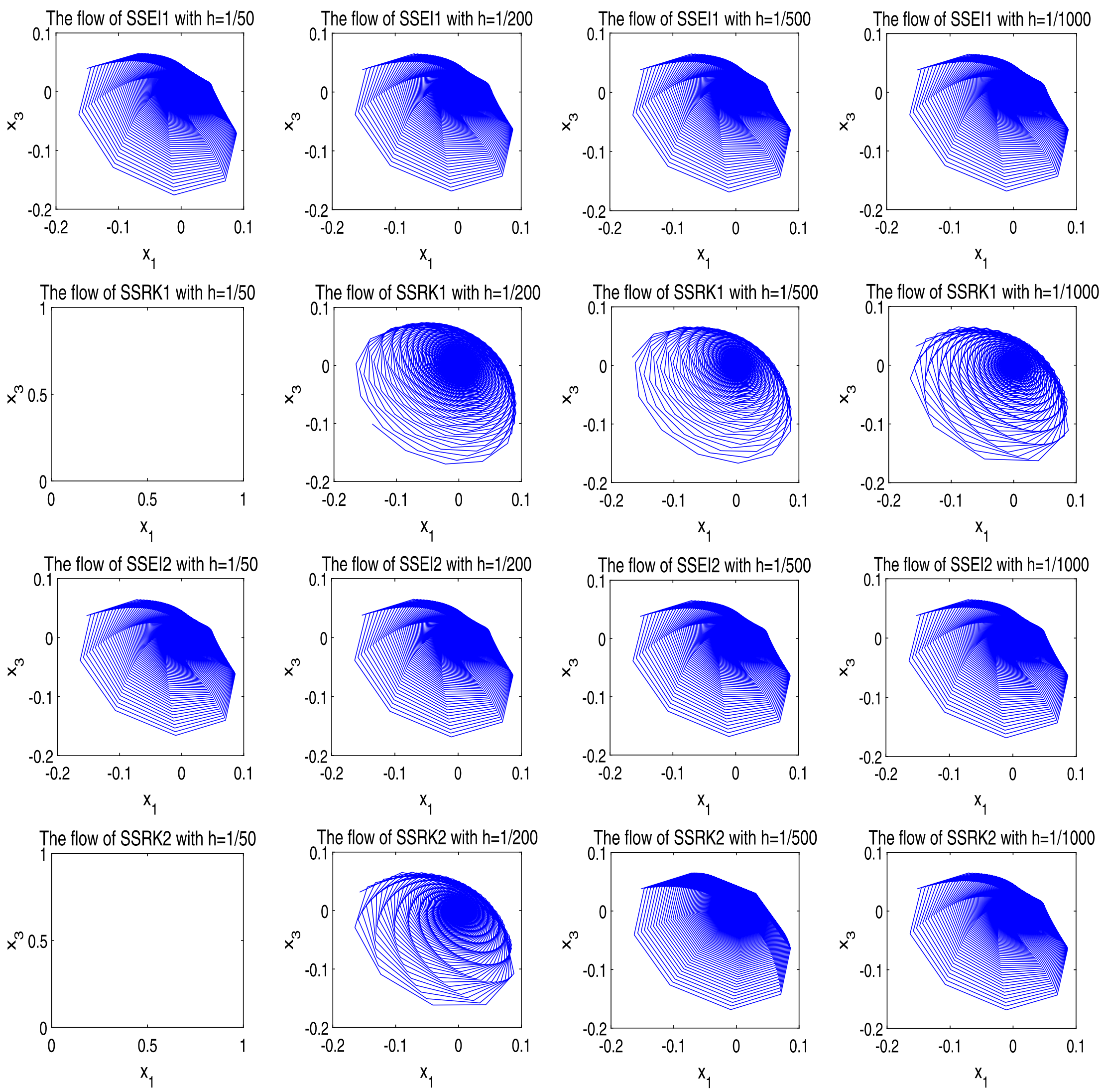

Fig. 10. Problem 5: the flows of different methods.

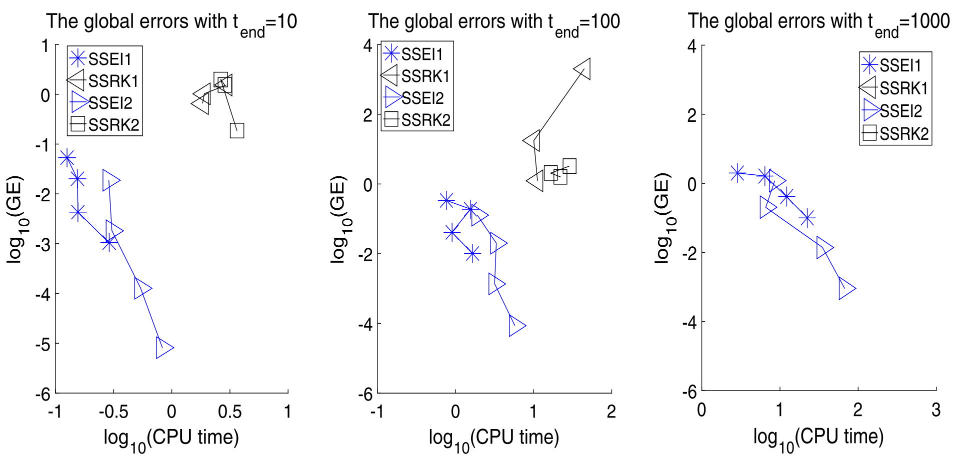

Fig. 11. Problem 5: the relative global errors.

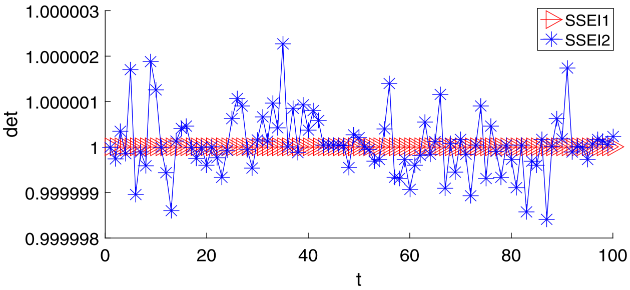

Fig. 12. The determinant of the derivative of the numerical flow as a function of time.

7. Conclusions

This paper studied volume-preserving exponential integrators for dynamical systems. The necessary and sufficient volume-preserving condition for exponential integrators was derived and volume-preserving properties were discussed for four kinds of vector fields. It was shown that symplectic exponential integrators can be volume preserving for a much larger class of vector fields than Hamiltonian systems. It should be noted that some new results on Geometric Integration were presented for second-order highly oscillatory problems and separable partitioned systems. A new result has been proved that a kind of adapted exponential integrators methods is volume preserving for the second-order highly oscillatory systems (22) and (25). Moreover, the volume-preserving property of ERKN/RKN methods was discussed for separable partitioned systems. We also carried out five numerical experiments to demonstrate the remarkable robustness and superiority of volume-preserving exponential integrators in comparison with volume-preserving Runge-Kutta methods.

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