Two new classes of exponential Runge–Kutta integrators for efficiently solving stiff systems or highly oscillatory problems

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Abstract

We note a fact that stiff systems or differential equations that have highly oscillatory solutions cannot be solved efficiently using conventional methods. In this paper, we study two new classes of exponential Runge–Kutta (ERK) integrators for efficiently solving stiff systems or highly oscillatory problems. We first present a novel class of explicit modified version of exponential Runge–Kutta (MVERK) methods based on the order conditions. Furthermore, we consider a class of explicit simplified version of exponential Runge–Kutta (SVERK) methods. Numerical results demonstrate the high efficiency of the explicit MVERK integrators and SVERK methods derived in this paper compared with the well-known explicit ERK integrators for stiff systems or highly oscillatory problems in the literature.

Keywords: Exponential integrators, stiff systems, highly oscillatory problems, Explicit methods, Runge–Kutta-type methods

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1. Introduction

The advantages of exponential methods have been clarified in the literature (see, e.g. \cite{13, 19}), and there is a MATLAB package for exponential integrators named EXPINT which is described in \cite{2}. Generally speaking, exponential methods permit larger stepsize and achieve higher accuracy than non-exponential ones. There is no doubt that the idea to make use of matrix exponentials in a Runge–Kutta-type integrator by no means new. However, most of them appeared in the literature are expensive since the coefficients of these integrators are heavily dependent on the evaluations of matrix exponentials, even though an explicit exponential Runge–Kutta-type integrator of them is also expensive when applied to the underlying systems in practice. Therefore, we try to design two novel classes of exponential Runge–Kutta methods, which can reduce the computational cost to some extent. To this end, we first pay our attention to a modified version of exponential Runge–Kutta (MVERK) integrators in this study. We then consider a simplified version of exponential Runge–Kutta (SVERK) methods, and this motivates the present paper.
We now consider initial value problems expressed in the autonomous form of first-order differential equations
\[
\begin{align*}
\frac{dy}{dt} &= My(t) + f(y(t)), \quad t \in [t_0, T_{\text{end}}], \\
y(t_0) &= y_0,
\end{align*}
\] (1)
where \( y : \mathbb{R} \rightarrow \mathbb{R}^d, f : \mathbb{R}^d \rightarrow \mathbb{R}^d, \) and the matrix \((-M)\) is a \(d \times d\) symmetric positive definite or skew-Hermitian with eigenvalues of large modulus. Problems of the form (1) arise in a variety of fields in science and engineering, such as quantum mechanics, fluid mechanics, flexible mechanics, and electrodynamics. This system is frequently yielded from linearising the integration of large stiff systems of nonlinear initial value problems
\[
\begin{align*}
\frac{dz}{dt} &= g(z(t)), \\
z(t_0) &= z_0.
\end{align*}
\]

Semidiscretised mixed initial-boundary value problems of evolution PDEs, such as advection-diffusion equations and the rewritten Navier-Stokes equations (see, e.g. [3]), also provide examples of this type, which can be formulated as an abstract form:
\[
\begin{align*}
\frac{\partial u(x,t)}{\partial t} &= Lu + Nu, \quad x \in D, \ t \in [t_0, T_{\text{end}}], \\
B(x)u(x,t) &= 0, \quad x \in \partial D, \ t \geq t_0, \\
u(x,t_0) &= g(x), \quad x \in D,
\end{align*}
\] (2)
where \( D \) is a spatial domain with boundary \( \partial D \) in \( \mathbb{R}^d, L \) and \( N \) represent respectively linear and nonlinear operators, and \( B(x) \) denotes a boundary operator.

The standard Runge–Kutta (RK) methods have been deeply rooted in researches and engineers who are interested in scientific computing due to their simplicity and their ease of implementation. Unfortunately, however, it is known that stiff systems or highly oscillatory problems cannot be solved efficiently using standard explicit methods since standard explicit methods need a very small stepsize and hence a long runtime to reach an acceptable accuracy. Therefore, in the development and design of numerical algorithms, established methods are constantly improved with the development of computing technology. It is true that exponential integrators (see, e.g. [1, 4, 6, 8, 10, 11, 12, 13, 14, 15, 16, 17, 18, 23, 28]):
\[
\begin{align*}
Y_i &= e^{i\beta_M}Y_0 + h \sum_{j=1}^{s} \tilde{a}_{ij}(\beta_M)f(Y_j), \quad i = 1, \ldots, s, \\
y_1 &= e^{i\beta_M}y_0 + h \sum_{i=1}^{s} \tilde{b}_i(\beta_M)f(Y_i),
\end{align*}
\] (3)
that can exactly integrate the linear equation \( y'(t) = My(t) \) are more favorable than non-exponential integrators in solving the problem (1), which exhibits remarkable ‘stiffness’ properties. In (3), \( c_i \) for \( i = 1, \ldots, s \) are constants, \( \tilde{a}_{ij}(\beta_M) \) and \( \tilde{b}_i(\beta_M) \) are matrix-valued functions of \( \beta_M \). It is worth noting that an ERK method reduces to a classical RK method if \( M \rightarrow 0 \). With regard to semilinear Hamiltonian systems, symplectic exponential methods and energy-preserving exponential methods are important in the sense of geometric integration (see, e.g. [12, 21, 22, 23, 26]), but all of them are implicit (normally depending on a Newton–Raphson procedure due to the stiffness), and hence they are not the subject of this paper.
The main theme of this paper is two new classes of exponential Runge–Kutta (ERK) integrators and we will focus on explicit methods. Hence, the main contribution of this study is to present new explicit ERK methods for solving the system (1) with lower computational cost. Moreover, these ERK methods will reduce the computation of matrix exponentials as far as possible, and be more closer to the distinguishing feature of standard Runge–Kutta methods: simplicity and ease of implementation.

The remainder of this paper is organised as follows. In Section 2 we first formulate a modified version of explicit exponential Runge–Kutta (MVERK) methods. We then present a simplified version of explicit exponential Runge–Kutta (SVERK) integrators in Section 3. We are concerned with the analytical aspect for our new explicit ERK methods in Section 4. Numerical experiments including Allen–Cahn equation, the averaged system in wind-induced oscillation and the nonlinear Schrödinger equation are implemented in Section 5, and the numerical results show the comparable accuracy and efficiency of our new explicit ERK integrators. We draw our conclusions in the last section.

2. A modified version of ERK methods

The idea of the underlying modified version of ERK methods is based on inheriting the internal stages and modifying the update of standard RK methods.

**Definition 2.1.** An s-stage modified version of ERK (MVERK) methods applied with stepsize $h > 0$ for solving (1) is defined by

$$
\begin{align*}
Y_i &= y_0 + h \sum_{j=1}^{s} \bar{a}_{ij}(MY_j + f(Y_j)), \quad i = 1, \ldots, s, \\
y_1 &= e^{hM}y_0 + h \sum_{i=1}^{s} \bar{b}_i f(Y_i) + w_s(hM),
\end{align*}
$$

where $\bar{a}_{ij}$ and $\bar{b}_i$ are real constants, $w_s(hM)$ is a suitable matrix-valued function of $hM$ (or zero), and in particular, $w_s(hM) = 0$ when $M \rightarrow 0$.

**Remark 2.2.** Differently from the standard ERK methods, MVERK methods are dependent on a matrix-valued function $w_s(hM)$.

**Remark 2.3.** It is important to note that $w_s(hM)$ appearing in (4) is independent of matrix-valued exponentials and will change with the order $p$ of the underlying MVERK method. However, the MVERK methods with same order $p$ share the same $w_s(hM)$. The choice of $w_s(hM)$ relies heavily on the order conditions, which must coincide with the order conditions for the standard RK methods.

It is clear that our MVERK methods exactly integrate the following homogeneous linear system

$$
y'(t) = My(t), \quad y(0) = y_0,
$$

which has exact solution

$$
y(t) = e^{tM}y_0.
$$
This is an essential property of an exponential integrator. Since \((-M)\) appearing in (1) is symmetric positive definite or skew-Hermitian with eigenvalues of large modulus, the exponential $e^{tM}$ possesses many nice features such as uniform boundedness. In particular, the exponential contains the full information on linear oscillations when (1) is a highly oscillatory problem.

The MVERK method (4) can be represented briefly in Butcher’s notation by the following block tableau of coefficients:

\[
\begin{bmatrix} \bar{c} \\ e^{hM} \end{bmatrix}_{w_j(hM)} \begin{bmatrix} I \\ \bar{A} \end{bmatrix} = \begin{bmatrix} \bar{c}_1 \\ \vdots \\ \bar{c}_s \\ e^{hM} \end{bmatrix}_{w_j(hM)} \begin{bmatrix} I \\ \bar{a}_{i1} \\ \vdots \\ \bar{a}_{is} \end{bmatrix}_{\bar{b}_1} \cdots \bar{b}_s
\]

with $\bar{c}_i = \sum_{j=1}^s \bar{a}_{ij}$. Explicitly, the method (4) utilises the matrix exponential of $M$ and a related function, and hence its name “exponential integrators”. Moreover, since the computational cost of the product of a matrix exponential function with a vector is expensive, the internal stages of the method (4) avoid matrix exponentials, namely, the update makes use of the matrix exponential of $M$ only once at each step, and hence its name “modified version of exponential integrators”.

According to the definition of MVERK methods, it is clear that MVERK methods can be thought of as a generalization of standard RK methods, but the most important aspect is that MVERK methods are specially designed for efficiently solving (1). In fact, when $M \to 0$, $w_j(hM) = 0$, and then the MVERK method (4) reduces to the standard RK method:

\[
\begin{cases}
Y_i = y_0 + h \sum_{j=1}^s \bar{a}_{ij}f(Y_j), & i = 1, \ldots, s, \\
y_1 = y_0 + h \sum_{j=1}^s \bar{b}_1 f(Y_j).
\end{cases}
\]

In what follows, we will present some examples of explicit MVERK methods. As the first example of explicit MVERK methods, we consider the special case of the one-stage explicit MVERK method with $w_j(hM) = 0$:

\[
\begin{cases}
Y_1 = y_0, \\
y_1 = e^{hM}y_0 + h\bar{b}_1 f(Y_1).
\end{cases}
\]

We will compare the Taylor series of the numerical solution $y_1$ with the Taylor series of the exact solution $y(h)$ under the assumption $y(0) = y_0$. An MVERK method whose series when expanded about $y_0$ agrees with that of the exact solution up to the term in $h^p$ is said to be of order $p$. The series for the numerical solution involve the same derivatives as for the exact solution but have coefficients that depend on the method. The resulting conditions on these coefficients are called the order conditions.
The Taylor series for the exact solution is given by

\[ y(h) = y(0) + hy'(0) + \frac{h^2}{2!}y''(0) + \frac{h^3}{3!}y'''(0) + \frac{h^4}{4!}y^{(4)}(0) + \cdots \]

\[ = y(0) + h(My(0) + f(y(0))) \]

\[ + \frac{h^2}{2} (My'(0) + f'(y(0))y'(0)) \]

\[ + \frac{h^3}{3!} y''''(0) + \frac{h^4}{4!} y^{(5)}(0) + \cdots \]

The Taylor series for the exact solution is to be compared with the Taylor series for the numerical solution. First, we regard the internal stage vector \( Y(h) \) as a function of \( h \) and compute derivatives with respect to \( h \), getting

\[ Y_1 = y_0, \]

\[ y_1 = e^{hM}y_0 + h\tilde{b}_1f(Y_1) \]

\[ = e^{hM}y_0 + h\tilde{b}_1f(y_0) \]

\[ = (I + hM)y_0 + h\tilde{b}_1f(y_0) + O(h^2), \]

\[ y(h) = y_0 + hy'(0) + O(h^2) = y_0 + h(My_0 + f(y_0)) + O(h^2) \]

If we consider the underlying one-stage MVERK method is of order one, we then obtain \( \tilde{b}_1 = 1 \). This gives the following first-order explicit MVERK method with one stage

\[ y_1 = e^{hM}y_0 + hf(y_0), \]

which can be expressed in the Butcher tableau

\[
\begin{array}{c|cc}
0 & I & 0 \\
e^{hM} & 0 & 1 \\
\end{array}
\]

The first-order explicit MVERK method with one stage is also termed the modified exponential Euler method, which is different from the exponential Euler method as it stands (see, e.g. Acta Numer. (2010) by Hochbruck et al.)

\[ y_1 = e^{hM}y_0 + h\varphi_1(hM)f(y_0), \]

where

\[ \varphi_1(z) = \frac{e^z - 1}{z}. \]

They would be same if \( \varphi_1(z) \) were replaced by 1. Here, it is worth mentioning that the exponential Euler method \( (10) \) is very popular, which is the prototype exponential method appeared repeatedly in the literature.

It is noted that when \( M \to 0 \), the modified exponential Euler method \( (8) \) reduces to the well-known explicit Euler method for \( y' = f(y) \).
As the second example of MVERK methods, we then consider two-stage explicit MVERK methods with
\[ w_2(hM) = \frac{h^2}{2} M f(y_0) \]

\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= y_0 + h\bar{a}_{21}(M y_0 + f(y_0)), \\
y_1 &= e^{hM} y_0 + h(\bar{b}_1 f(Y_1) + \bar{b}_2 f(Y_2)) + \frac{h^2}{2} M f(y_0).
\end{align*}
\]

(12)

Considering the second-order explicit MVERK method with two stages yields
\[
\begin{align*}
\bar{b}_1 + \bar{b}_2 &= 1, \\
2\bar{a}_{21}\bar{b}_2 &= 1.
\end{align*}
\]

(13)

Let \( \bar{a}_{21} \neq 0 \) be real parameter. We obtain a one-parameter family of second-order explicit
MVERK method:
\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= y_0 + h\bar{a}_{21}(M y_0 + f(y_0)), \\
y_1 &= e^{hM} y_0 + h(\bar{b}_1 f(Y_1) + \bar{b}_2 f(Y_2)) + \frac{h^2}{2} M f(y_0),
\end{align*}
\]

(14)

which can be denoted by the Butcher tableau

\[
\begin{bmatrix}
0 & I & 0 & 0 \\
1 & I & 1 & 0
\end{bmatrix}
\]

(15)

The choice of \( \bar{a}_{21} = 1 \) gives \( \bar{b}_1 = \bar{b}_2 = \frac{1}{2} \). This suggests the following second-order explicit
MVERK method with two stages
\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= y_0 + h(M y_0 + f(y_0)), \\
y_1 &= e^{hM} y_0 + h(\bar{b}_1 f(Y_1) + \bar{b}_2 f(Y_2)),
\end{align*}
\]

(16)

which can be presented by the Butcher tableau

\[
\begin{bmatrix}
0 & I & 0 & 0 \\
\frac{1}{2} & 0 & 0 & 0
\end{bmatrix}
\]

(17)
It is noted that when $M \to 0$, the second-order explicit MVERK methods \cite{14} and \cite{16} with two stages reduce to the second-order RK method by Heun, and the so-called modified Euler method by Runge, respectively.

In what follows we consider three-stage explicit MVERK methods of order three with $w_3(hM) = \frac{1}{6}h^2M(3f(y_0) + h(Mf(y_0) + f'(y_0)(My_0 + f(y_0))))$:

\[
\begin{aligned}
Y_1 &= y_0, \\
Y_2 &= y_0 + h\tilde{a}_{21}(My_0 + f(y_0)), \\
Y_3 &= y_0 + h(\tilde{a}_{31}(MY_1 + f(Y_1)) + \tilde{a}_{32}(MY_2 + f(Y_2))) \\
y_1 &= e^{hM}y_0 + h(\tilde{b}_1f(Y_1) + \tilde{b}_2f(Y_2) + \tilde{b}_3f(Y_3)) \\
&+ \frac{1}{6}h^2M(3f(y_0) + h(Mf(y_0) + f'(y_0)(My_0 + f(y_0))))).
\end{aligned}
\]

The order conditions for the three-order explicit MVERK methods with three stages are given by

\[
\begin{align*}
\bar{b}_1 + \bar{b}_2 + \bar{b}_3 &= 1, \\
\bar{b}_2\bar{a}_{21} + \bar{b}_3(\bar{a}_{31} + \bar{a}_{32}) &= \frac{1}{2}, \\
\bar{b}_2^2\bar{a}_{21}^2 + \bar{b}_3(\bar{a}_{31} + \bar{a}_{32})^2 &= \frac{1}{3}, \\
\bar{b}_3\bar{a}_{32}\bar{a}_{21} &= \frac{1}{6}.
\end{align*}
\]

The system (19) has infinitely many solutions, and we refer the reader to Chap. 3 in \cite{5} for details. It can be verified that $\tilde{b}_2 = \tilde{a}_{31} = 0$, $\tilde{a}_{21} = \frac{1}{4}$, $\tilde{a}_{32} = \frac{2}{5}$, $\tilde{b}_1 = \frac{1}{4}$, and $\tilde{b}_3 = \frac{3}{10}$ satisfy the order conditions stated above. Accordingly, we obtain the three-order explicit MVERK method with three stages as follows:

\[
\begin{aligned}
Y_1 &= y_0, \\
Y_2 &= y_0 + \frac{1}{3}hg_0, \\
Y_3 &= y_0 + \frac{2}{3}h(MY_2 + f(Y_2)) \\
y_1 &= e^{hM}y_0 + \frac{1}{4}h(f(Y_1) + 3f(Y3)) \\
&+ \frac{1}{6}h^2M(3f(y_0) + h(Mf(y_0) + f'(y_0)(My_0 + f(y_0))))),
\end{aligned}
\]

where $g_0 = My_0 + f(y_0)$.

The MVERK method (20) can be expressed in the Butcher tableau

\[
\begin{array}{ccc}
0 & I & 0 \\
\frac{1}{3} & I & \frac{1}{3} \\
\frac{2}{3} & I & 0 \\
\frac{1}{2} & w_3(hM) & \frac{1}{4} & 0 & \frac{1}{4}
\end{array}
\]
When $M \to 0$, the MVERK method (20) reduces to Heun’s three-order RK method. It is true that (20) uses the Jacobian matrix of $f(y)$ with respect to $y$ at each step. However, as is known, an A-stable RK method is implicit, and the Newton–Raphson iteration is required when applied to stiff systems. This implies that an A-stable RK method when applied to stiff systems depends on the evaluation of Jacobian matrix of $f(y)$ with respect to $y$ at each step as well. As we have emphasised in Introduction that implicit exponential integrators need to use the evaluation of Jacobian matrix of $f(y)$ with respect to $y$, depending on an iterative procedure due to the stiffness of (1). On the other hand, the computational cost of explicit exponential integrators appeared in the literature depends on evaluations of matrix exponentials heavily. If the cost of computing the Jacobian matrix of $f(y)$ with respect to $y$ for the underlying system (1) is cheaper than that of the evaluations of matrix exponentials for the explicit exponential integrators appeared in the literature, we are also hopeful of obtaining the high efficiency of our three-order explicit exponential integrators with three stages.

Also, it can be verified that $\bar{a}_{21} = \frac{1}{2}$, $\bar{a}_{31} = 0$, $\bar{a}_{32} = \frac{3}{4}$, $\bar{b}_1 = \frac{2}{9}$, $\bar{b}_2 = \frac{1}{9}$, and $\bar{b}_3 = \frac{1}{9}$ satisfy the order conditions. Consequently, we obtain another three-order explicit MVERK method with three stages as follows:

\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= y_0 + \frac{1}{2}hg_0, \\
Y_3 &= y_0 + \frac{3}{4}h(MY_2 + f(Y_2)) \\
y_1 &= e^{hM}y_0 + \frac{1}{9}h(2f(Y_1) + 3f(Y_2) + 4f(Y_3)) \\
&\quad + \frac{1}{6}h^2M(3f(y_0) + h(Mf(y_0) + f'(y_0)g_0)),
\end{align*}
\]

where

\[g_0 = My_0 + f(y_0).\]

The MVERK method (22) can be denoted by the Butcher tableau

\[
\begin{array}{c|cc}
0 & I & 0 \\
\frac{1}{2} & I & \frac{1}{2} \\
\frac{1}{4} & I & 0 \\
\hline
& & \hfill w_3(hM) \\
\end{array}
\]

When $M \to 0$, the MVERK method (22) reduces to the classical third-order RK method with three stages.

3. A simplified version of ERK methods

Following the idea stated in the previous section, in this section we will consider a simplified version of ERK methods, which also allows internal stages to use matrix exponentials of $hM$ to some extent.

Differently from MVERK methods, here the internal stages make use of matrix exponentials of $hM$, but all the coefficients of the simplified version are independent of matrix exponentials.
Definition 3.1. An $s$-stage simplified version of ERK (SVERK) method applied with stepsize $h > 0$ for solving (1) is defined by

$$\begin{align*}
Y_i & = e^{hM}y_0 + h \sum_{j=1}^{s} \bar{a}_{ij} f(Y_j), \quad i = 1, \ldots, s, \\
y_1 & = e^{hM}y_0 + h \sum_{j=1}^{s} \bar{b}_{ij} f(Y_j) + \bar{w}_i(hM),
\end{align*}$$

(24)

where $\bar{a}_{ij}$ and $\bar{b}_i$ are real constants, $\bar{c}_i = \sum_{j=1}^{s} \bar{a}_{ij}$, $\bar{w}_i(hM)$ is a suitable matrix-valued function of $hM$ (or zero), and in particular, $\bar{w}_i(hM) = 0$ when $M \rightarrow 0$.

Likewise, differently from the standard ERK methods, SVERK methods are dependent on a matrix-valued function $\bar{w}_i(hM)$. Here $\bar{w}_i(hM)$ appearing in (24) is independent of matrix-valued exponentials, and will change with the order $p$ of the underlying SVERK method. However, the SVERK methods with same order $p$ share the same $\bar{w}_i(hM)$. The choice of $\bar{w}_i(hM)$ relies heavily on the order conditions, which must coincide with the order conditions for the standard RK methods. Obviously, our SVERK methods exactly integrate (5) as well.

The method (24) can be represented briefly in Butcher’s notation by the following block tableau of coefficients:

$$\begin{bmatrix}
\bar{c} \\
e^{hM} \\
\bar{w}_1(hM) \\
e^{hM} \\
\bar{w}_s(hM)
\end{bmatrix}
\begin{bmatrix}
e^{hM} & \bar{a}_{11} & \cdots & \bar{a}_{1s} \\
\vdots & \vdots & \ddots & \vdots \\
e^{hM} & \bar{a}_{s1} & \cdots & \bar{a}_{ss} \\
\bar{b}_1 & \cdots & \bar{b}_s
\end{bmatrix}
\begin{bmatrix}
y_0 \\
y_1 \\
y_2 \\
y_s
\end{bmatrix}$$

(25)

We first consider the explicit one-stage SVERK method of order one with $\bar{w}_1(hM) = 0$. It is easy to see that $\bar{b}_1 = 1$. This implies the following first-order explicit SVERK method with one stage:

$$y_1 = e^{hM}y_0 + hf(y_0),$$

(26)

which is identical to (3).

We next consider second-order explicit SVERK methods with $\bar{w}_2(hM) = \frac{h^2}{2} Mf(y_0)$:

$$\begin{align*}
Y_1 &= y_0, \\
Y_2 &= e^{hM}y_0 + h\bar{a}_{21} f(y_0), \\
y_1 &= e^{hM}y_0 + h(\bar{b}_1 f(Y_1) + \bar{b}_2 f(Y_2)) + \frac{h^2}{2} Mf(y_0).
\end{align*}$$

(27)

Considering the second-order SVERK method with two stages yields

$$\bar{c}_2 = \bar{a}_{21}, \quad \bar{b}_1 + \bar{b}_2 = 1, \quad 2\bar{a}_{21}\bar{b}_2 = 1.$$  

This is the same as (13) of the order conditions for MVERK methods. Let $\bar{a}_{21} \neq 0$ be real parameter. We obtain a one-parameter family of second-order explicit SVERK method:

$$\bar{b}_2 = \frac{1}{2\bar{a}_{21}}, \quad \bar{b}_1 = 1 - \frac{1}{2\bar{a}_{21}}, \quad \bar{a}_{21} \neq 0.$$
The choice of \( \bar{a}_{21} = 1 \) gets \( \bar{b}_1 = \frac{1}{2} \). This results in the following second-order SVERK method with two stages:

\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= e^{M}y_0 + hf(y_0), \\
y_1 &= e^{M}y_0 + \frac{h}{2}(f(Y_1) + f(Y_2)) + \frac{h^2}{2}Mf(y_0),
\end{align*}
\]

which can be denoted by the Butcher tableau

\[
\begin{array}{ccc}
0 & I & 0 \\
1 & e^{M} & 1 \\
\end{array}
\]

The choice of \( \bar{a}_{21} = \frac{1}{2} \) yields \( \bar{b}_1 = 0 \) and \( \bar{b}_2 = 1 \). This arrives at another second-order explicit SVERK method with two stages

\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= e^{\frac{2}{3}M}y_0 + \frac{h}{2}f(y_0), \\
y_1 &= e^{M}y_0 + hf(Y_2) + \frac{h^2}{2}Mf(y_0),
\end{align*}
\]

which can be expressed in the Butcher tableau

\[
\begin{array}{ccc}
0 & I & 0 \\
\frac{1}{\sqrt{3}} & e^{\frac{2}{3}M} & \frac{1}{\sqrt{3}} \\
\end{array}
\]

It is noted that when \( M \to 0 \) and \( hM \to 0 \), the 2-stage SVERK methods (28) and (30) of order two reduce to the well-known explicit RK method of order two by Heun and the so-called modified Euler method, respectively.

Likewise, we derive three-stage explicit SVERK methods with \( \bar{w}_3(hM) = \frac{h^3}{2}Mf(y_0) + \frac{1}{2}h^3((M + f'(y_0))Mf(y_0) + Mf'(y_0)(My_0 + f(y_0))) \):

\[
\begin{align*}
Y_1 &= y_0, \\
Y_2 &= e^{2hM}y_0 + h\bar{a}_{21}f(Y_1), \\
Y_3 &= e^{3hM}y_0 + h(\bar{a}_{31}f(Y_1) + \bar{a}_{32}f(Y_2)), \\
y_1 &= e^{M}y_0 + h(\bar{b}_1f(Y_1) + \bar{b}_2f(Y_2) + \bar{b}_3f(Y_3)) + \frac{h^2}{2}Mf(y_0) \\
&+ \frac{1}{6}h^3((M + f'(y_0))Mf(y_0) + Mf'(y_0)(My_0 + f(y_0))).
\end{align*}
\]

The order conditions for 3-stage SVERK methods of order three are the same as (19).

We choose \( \bar{a}_{21} = \frac{1}{3}, \bar{a}_{31} = 0, \bar{a}_{32} = \frac{3}{4}, \bar{b}_1 = \frac{2}{3}, \bar{b}_2 = \frac{7}{7} \) and \( \bar{b}_3 = \frac{4}{7} \). It can be verified that this choice satisfies the order conditions (19). Hence, we have following third-order explicit SVERK methods with three stages:
\[
\begin{aligned}
Y_1 &= y_0, \\
Y_2 &= e^{\frac{h}{2}\Delta M}y_0 + \frac{h}{2}f(y_0), \\
Y_3 &= e^{\frac{3}{4}h\Delta M}y_0 + \frac{3}{4}hf(Y_2), \\
y_1 &= e^{\Delta M}y_0 + \frac{h}{3}(2f(Y_1) + 3f(Y_2) + 4f(Y_3)) + \frac{h^2}{2}Mf(y_0) \\
&\quad + \frac{1}{6}h^3((M + f'_y(y_0))Mf(y_0) + Mf'_y(y_0)(My_0 + f(y_0))).
\end{aligned}
\] (33)

The SVERK method (33) can be expressed in the Butcher tableau

\[
\begin{array}{c|ccc}
0 & I & 0 \\
\frac{1}{3} & e^{h\Delta M} & \frac{1}{3} & 0 \\
\frac{1}{2} & e^{\frac{3}{4}h\Delta M} & 0 & \frac{1}{3} & 0 \\
\frac{1}{3} & e^{\frac{1}{3}h\Delta M} & \frac{1}{3} & 0 & \frac{4}{15} & \frac{4}{15} & \frac{1}{15}
\end{array}
\] (34)

Another option is that \(a_{31} = \frac{1}{3}, a_{31} = 0, a_{32} = \frac{1}{3}, b_1 = \frac{1}{4}, b_2 = 0\) and \(b_3 = \frac{3}{4}\). It is easy to see that this choice satisfies the order conditions (19). Thus, we obtain the third-order explicit SVERK methods with three stages as follows:

\[
\begin{aligned}
Y_1 &= y_0, \\
Y_2 &= e^{\frac{1}{3}h\Delta M}y_0 + \frac{1}{3}hf(y_0), \\
Y_3 &= e^{\frac{2}{3}h\Delta M}y_0 + \frac{2}{3}hf(Y_2), \\
y_1 &= e^{\Delta M}y_0 + \frac{h}{4}(f(Y_1) + 3f(Y_2)) + \frac{h^2}{2}Mf(y_0) \\
&\quad + \frac{1}{6}h^3((M + f'_y(y_0))Mf(y_0) + Mf'_y(y_0)(My_0 + f(y_0))),
\end{aligned}
\] (35)

which can be denoted by the Butcher tableau

\[
\begin{array}{c|ccc}
0 & I & 0 \\
\frac{1}{4} & e^{h\Delta M} & \frac{1}{4} & 0 \\
\frac{1}{3} & e^{\frac{2}{3}h\Delta M} & 0 & \frac{1}{4} & 0 \\
\frac{1}{3} & e^{\frac{1}{3}h\Delta M} & \frac{1}{3} & 0 & \frac{1}{12} & \frac{1}{12} & \frac{1}{12}
\end{array}
\] (36)

When \(M \to 0\), the third-order explicit SVERK methods (33) and (35) with three stages reduce to the classical explicit third-order RK method and the well-known Heun’s method of order three, respectively.

4. Analysis issues

In this section, we aim at some analytical aspects associated with our new explicit ERK methods.
Theorem 4.1. All the new exponential integrators presented in this paper are A-stable in the sense of Dahlquist (see [8]).

Proof. It is easy to see that when applied to the initial value problem \( y' = \lambda y, \quad y(0) = y_0 \), these new exponential integrators with stepsize \( h \) generate the approximate solution \( y_n = (e^{h \lambda})^n y_0 \). If \( \lambda \) is a complex scalar with negative real part, then \( \lim_{n \to \infty} y_n = 0 \), establishing A-stability in the sense of Dahlquist.

Theorem 4.2. If \( \bar{c} = (\bar{c}_1, \ldots, \bar{c}_q), \bar{b} = (\bar{b}_1, \ldots, \bar{b}_s) \) and \( \bar{\Lambda} = (\bar{\alpha}_{ij}) \) for \( s = 1, 2, 3 \) are coefficients of a standard explicit RK method of order \( s \), then the explicit MVERK and SVERKN methods with the same nodes \( \bar{c} \), weights \( \bar{b} \) and coefficients \( \bar{\Lambda} \) are also of order \( s \) when applied to (1). Moreover, all of them are A-stable in the sense of Dahlquist.

Proof. The conclusion of this theorem follows from Theorem 4.1 and the derivation for explicit MVERK and SVERKN methods in Section 2 and Section 3.

We next analyse the convergence of the first-order explicit MVERK method (5) and the following theorem states the corresponding result. Our analysis below will be based on an abstract formulation of (1) as an evolution equation in a Banach space \((X, \| \cdot \|)\). We choose

\[
0 \leq \alpha < 1
\]

and define \( V = D(\tilde{M}^\alpha) \subset X \), where \( \tilde{M} \) denotes the shifted operator \( \tilde{M} = M + \omega I \) with \( \omega > -\alpha \) and \( D(\tilde{M}^\alpha) \) stands for the domain of \( \tilde{M}^\alpha \) in \( X \). The linear space \( V \) is a Banach space with norm \( \| \cdot \|_V = \| \tilde{M}^\alpha \cdot \| \). Then the convergence of the method (5) is given by

\[
\| e_n \|_V \leq C h,
\]

where \( e_n = y_n - y(t_n) \), and the constant \( C \) is dependent on \( T \), but independent of \( n \) and \( h \).

Proof. Inserting the exact solution into the method (5), we obtain

\[
y(t_{n+1}) = e^{hM} y(t_n) + h \bar{f}(t_n) + \delta_{n+1},
\]

where \( \delta_{n+1} \) presents the discrepancies of the method (5), and \( \bar{f}(t) = f(y(t)) \). It follows from the variation-of-constants formula and Taylor series that

\[
y(t_n + h) = e^{hM} y(t_n) + \int_0^h e^{hM} \bar{f}(t_n + \tau) d\tau
\]
\[
= e^{hM} y(t_n) + \int_0^h e^{(h\tau - t_n)} M \bar{f}(t_n) d\tau + \int_0^h e^{(h\tau - t_n)} \int_0^\sigma \bar{f}'(t_n + \sigma) d\sigma d\tau
\]
\[
= e^{hM} y(t_n) + h \bar{f}(hM) \bar{f}(t_n) + \int_0^h e^{(h\tau - t_n)} \int_0^\sigma \bar{f}'(t_n + \sigma) d\sigma d\tau.
\]

It is noted that for this \( \bar{\gamma} \) and the \( \alpha \) introduced in [37], this is no relation between them.
We estimate the global error using recursion formula, one has

\[ \delta_{n+1} = h(\varphi_1(hM) - I)\hat{f}(t_n) + \int_0^h e^{(h-\tau)M} \int_0^\tau \hat{f}(t_n + \sigma)d\sigma d\tau. \]

(40)

Let \( e_n = y_n - y(t_n) \), and from (38) and (39), it follows that

\[ e_{n+1} = e^{hM}e_n + h(f(y_n) - \hat{f}(t_n)) - \delta_{n+1}. \]

Using recursion formula, one has

\[ \sum_{j=0}^{n-1} (e^{(n-j)hM}e_j - e^{(n-j)hM}M_j) = h \sum_{j=0}^{n-1} e^{(n-j)hM}(f(y_j) - \hat{f}(t_j)) - \sum_{j=0}^{n-1} e^{(n-j)hM}\delta_{j+1}. \]

Then, we have

\[ e_n = h \sum_{j=0}^{n-1} e^{(n-j)hM}(f(y_j) - \hat{f}(t_j)) - \sum_{j=0}^{n-1} e^{hM}\delta_{n-j}. \]

We estimate the global error \( e_n \) in the norm \( \| \cdot \|_V \) by

\[ \| e_n \|_V \leq h \left\| \sum_{j=0}^{n-1} e^{(n-j)hM}(f(y_j) - \hat{f}(t_j)) \right\|_V + h \left\| \sum_{j=0}^{n-1} e^{hM}\delta_{n-j} \right\|_V. \]

(41)

It is easily deduced from \( \| \cdot \|_V = \| M^\alpha \| \) and the Lemma 3.1 of [14] that

\[ h \left\| \sum_{j=0}^{n-1} e^{(n-j)hM}(f(y_j) - \hat{f}(t_j)) \right\|_V \leq h \sum_{j=0}^{n-1} \| e^{(n-j)hM} \| \| f(y_j) - \hat{f}(t_j) \| \leq C L h \sum_{j=0}^{n-1} \| e_j \|_V. \]

Inserting the formula (40) into the second term on the right-hand side of (41) gives

\[ \left\| \sum_{j=0}^{n-1} e^{hM}\delta_{n-j} \right\|_V \leq \left\| \sum_{j=0}^{n-1} \tilde{M}^\alpha e^{hM}\delta_{n-j} \right\| \leq C L h \sum_{j=0}^{n-1} \| e_j \|_V. \]

(42)

We note that there exists a bounded operator \( \bar{\varphi}(hM) \) with

\[ \varphi_1(hM) - I = \varphi_1(hM) - \varphi_1(0) = hM\bar{\varphi}(hM). \]

Then combining with the Lemma 2 of [15] yields

\[ \left\| \sum_{j=0}^{n-1} \tilde{M}^\alpha e^{hM}\delta_{n-j} \right\|_V \leq h \sum_{j=0}^{n-2} \| W_\alpha \| \| v_{n-j} - v_{n-j} \|. \]
Finally, using the Gronwall’s inequality, we arrive at the final conclusion as follows

$$\|e_n\|_V \leq CLh \sum_{j=0}^{n-1} \|e_j\|_V + Ch.$$
5. Numerical experiments

Since it is well known that explicit exponential integrators outperform standard integrators, we do not consider standard integrators in our numerical experiments. Differently from multistep methods, a significant advantage of one-step methods is conceptually simple and easy to change stepsize. Therefore, it seems plausible that our numerical experiments are implemented under the assumption that the variable stepsize is allowed at each time step.

In this section, we carry out numerical experiments to show the high efficiency of our methods. We select the following methods to make comparisons:

- First-order methods:
  - E-Euler: the explicit exponential Euler method \(10\) of order one proposed in \(16\);
  - MVERK1: the 1-stage explicit MVERK/SVERK \(8\) of order one presented in this paper.

- Second-order methods:
  - ERK2: the explicit exponential Runge-Kutta method of order two proposed in \(16\);
  - MVERK2-1: the 2-stage explicit MVERK \(14\) of order two presented in this paper;
  - MVERK2-2: the 2-stage explicit MVERK \(16\) of order two presented in this paper;
  - SVERK2-1: the 2-stage explicit SVERK \(28\) of order two presented in this paper;
  - SVERK2-2: the 2-stage explicit SVERK \(30\) of order two presented in this paper.

- Third-order methods:
  - ERK3: the explicit exponential Runge-Kutta method of order three proposed in \(16\);
  - MVERK3-1: the 3-stage explicit MVERK \(20\) of order three presented in this paper;
  - MVERK3-2: the 3-stage explicit MVERK \(22\) of order three presented in this paper;
  - SVERK3-1: the 3-stage explicit SVERK \(33\) of order three presented in this paper;
  - SVERK3-2: the 3-stage explicit SVERK \(35\) of order three presented in this paper.

Problem 1. We first consider a stiff partial differential equation: Allen–Cahn equation. Allen–Cahn equation (see, e.g. \([8, 17]\)) is a reaction-diffusion equation of mathematical physics, given by

\[
  u_t - \varepsilon u_{xx} = u - u^3, \quad x \in [-1, 1],
\]

with \(\varepsilon = 0.01\) and initial conditions

\[
  u(x, 0) = 0.53x + 0.47 \sin(-1.5\pi x), \quad u(-1, t) = -1, \quad u(1, t) = 1.
\]

We use a 32-point Chebyshev spectral method which yields a system of ordinary differential equations

\[
  U_t - AU = U - U^3.
\]

We apply the MATLAB function \textit{cheb} from \([24]\) for the grid generation and obtain the differentiation matrix \(M\). The form of this Chebyshev differentiation matrix is referred to Theorem 7 of Chapter 6 in \([24]\). It is noted that the differentiation matrix \(M\) in this example is full. This
The accuracy of first order methods

\[ \text{EEuler} \]
\[ \text{MVERK1} \]

slope 1

(a)

The accuracy of second order methods

\[ \text{ERK2} \]
\[ \text{MVERK2-1} \]
\[ \text{MVERK2-2} \]
\[ \text{SVERK2-1} \]
\[ \text{SVERK2-2} \]

slope 2

(b)

The accuracy of third order methods

\[ \text{ERK3} \]
\[ \text{MVERK3-1} \]
\[ \text{MVERK3-2} \]
\[ \text{SVERK3-1} \]
\[ \text{SVERK3-2} \]

slope 3

(c)

Figure 1: Results for accuracy of Problem 1: The log-log plots of global errors against \( h \).

The efficiency of first order methods

\[ \text{EEuler} \]
\[ \text{MVERK1} \]

(a)

The efficiency of second order methods

\[ \text{ERK2} \]
\[ \text{MVERK2-1} \]
\[ \text{MVERK2-2} \]
\[ \text{SVERK2-1} \]
\[ \text{SVERK2-2} \]

(b)

The efficiency of third order methods

\[ \text{ERK3} \]
\[ \text{MVERK3-1} \]
\[ \text{MVERK3-2} \]
\[ \text{SVERK3-1} \]
\[ \text{SVERK3-2} \]

(c)

Figure 2: Results for efficiency of Problem 1: The log-log plots of global errors against the CPU time.

The system is integrated on \([0,1]\) with different stepizes \( h = 1/2^k \) for \( k = 8, 9, \ldots, 13 \). The global errors \( GE := \| U_n - U(t_n) \| \) against the stepizes and the CPU time are given in Figs. 1 and 2, respectively.

**Problem 2.** Consider the following averaged system in wind-induced oscillation (see [20])

\[
\begin{pmatrix}
  x_1 \\
  x_2
\end{pmatrix}' = \begin{pmatrix}
  -\zeta & -\lambda \\
  \lambda & -\zeta
\end{pmatrix} \begin{pmatrix}
  x_1 \\
  x_2
\end{pmatrix} + \begin{pmatrix}
  1/2 (x_1^2 - x_2^2)
\end{pmatrix},
\]

where \( \zeta \geq 0 \) is a damping factor and \( \lambda \) is a detuning parameter. We solve this system on \([0,10]\) with \( h = 1/2^k \) for \( k = 3, 4, \ldots, 8 \). Figs. 3 and 4 display the global errors \( GE \) against the stepizes and the CPU time, respectively.

**Problem 3.** Consider the nonlinear Schrödinger equation (see [7])

\[ i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \quad \psi(x,0) = 0.5 + 0.025 \cos(\mu x), \]

with the periodic boundary condition \( \psi(0,t) = \psi(L,t) \). Following [7], we choose \( L = 4 \sqrt{2} \pi \) and \( \mu = 2\pi/L \). The initial condition chosen here is in the vicinity of the homoclinic orbit.
Using $\psi = p + i q$, this equation can be rewritten as a pair of real-valued equations

\begin{align*}
 p_t + q_{xx} + 2(p^2 + q^2)q &= 0, \\
 q_t - p_{xx} - 2(p^2 + q^2)p &= 0.
\end{align*}

Discretising the spatial derivative $\partial_{xx}$ by the pseudospectral method given in [7], this problem is converted into the following system:

\begin{equation}
\begin{pmatrix}
 p \\
 q
\end{pmatrix}' = \begin{pmatrix}
 0 & -D_2 \\
 D_2 & 0
\end{pmatrix}
\begin{pmatrix}
 p \\
 q
\end{pmatrix} + \begin{pmatrix}
 -2(p^2 + q^2) \cdot q \\
 2(p^2 + q^2) \cdot p
\end{pmatrix}
\end{equation}

(45)

where $\mathbf{p} = (p_0, p_1, \ldots, p_{N-1})^T$, $\mathbf{q} = (q_0, q_1, \ldots, q_{N-1})^T$ and $D_2 = (D_2)_{0 \leq j,k \leq N-1}$ is the pseudospectral differential matrix defined by:

\begin{equation}
(D_2)_{jk} = \begin{cases}
 \frac{1}{2} \mu^2 (-1)^{j+k+1} \frac{1}{\sin^2(\mu(x_j - x_k)/2)} & j \neq k, \\
 -\mu^2 \frac{2(N/2)^2 + 1}{6} & j = k.
\end{cases}
\end{equation}
In this test, we choose $N = 64$ and integrate the system on $[0, 1]$ with $h = 1/2^k$ for $k = 2, 3, \ldots, 7$. The global errors $GE$ against the stepsizes and the CPU time are respectively presented in Figs. 5 and 6.

From the results of these three numerical experiments, we have the following observations. Although the MVERK and SVERK methods derived in this paper have comparable accuracy in comparison with standard exponential integrators, our exponential methods demonstrate lower computational cost and more competitive efficiency.

![Figure 5: Results for accuracy of Problem 3: The log-log plots of global errors against $h$.](image)

![Figure 6: Results for efficiency of Problem 3: The log-log plots of global errors against the CPU time.](image)

6. Conclusions and further research

As we have known, exponential integrators are very promising for solving semi-linear systems whose linear part generates the dominant stiffness or high oscillation of the underlying problem. In this work, we have presented two new classes of exponential integrators to solve stiff systems or highly oscillatory problems. A distinctive feature of these new integrators is the exact evaluation of the contribution brought by the linear term appearing in (1). We mainly focus on explicit modified and simplified exponential integrators in this paper.
A key feature of our approach is that, unlike standard exponential integrators, our new exponential integrators reduce computational cost brought by evaluations of matrix exponentials, whereas the computational cost of exponential integrators appeared in the literature is heavily dependent on the evaluations of matrix exponentials. For instance, the numerical results of both first-order explicit exponential methods (8) and (10) show almost the same accuracy. However, a closer look at the CPU time reveals that our first-order explicit exponential method (8) is better than the well-known prototype exponential method (10). The main reason is that the coefficient of our method (8) is independent of the evaluation of exponential matrix. On the contrary, the prototype exponential method (10) is dependent on the evaluation of exponential matrix determined by (11). For comparable accuracy, our explicit exponential methods require in general less work than the standard explicit exponential method in the literature. Moreover, the larger the dimension $d$ of matrix $M$ is, the higher computational cost will be.

We analysed the convergence of the explicit MVERK method (8). An interesting conclusion from Theorem 4.2 is that the explicit MVERK and SVERKN methods yielded from order conditions of standard $p$th-order RK methods are of order $p$ for $p = 1, 2, 3$, when applied to (1). Moreover, all of them are $A$-stable in the sense of Dahlquist.

Finally, we presented numerical examples based on Allen–Cahn equation, the averaged system in wind-induced oscillation and the nonlinear Schrödinger equation, which are very relevant in applications. It follows from the numerical results that our new explicit ERK integrators have higher efficiency than the standard ERK methods.

The implicit MVERK integrators and SVERK integrators can be further investigated.

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