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Numerical algorithms for highly oscillatory dynamic system based on commutator-free method

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Abstract

In the present paper, an efficiently improved modified Magnus integrator algorithm based on commutator-free method is proposed for the second-order dynamic systems with time-dependent high frequencies. Firstly, the second-order dynamic systems are transferred to the frame of reference by introducing new variable so that highly oscillatory behaviour inherited from the entries. Then the modified Magnus integrator method based on local linearization is appropriately designed for solving the above new form. And some optimized strategies for reducing the number of function evaluations and matrix operations are also suggested. Finally, several numerical examples for highly oscillatory dynamic systems, such as Airy equation, Bessel equation, Mathieu equation, are presented to demonstrate the validity and effectiveness of the proposed method.

1. Introduction

In this paper, we consider a second-order differential system with initial-value problems

$$\ddot{y} + g(t)y = 0, \quad t \geqslant 0, \quad y(0) = y_0, \quad y'(0) = y'_0 \tag{1}$$

whose solution oscillates with a timescale much shorter than the fixed integration interval. We will refer to the above dynamic system as highly oscillatory dynamic system, and Petzold stated that such equation is characterized by a fast solution varying regularly about a slow solution [1].

High oscillatory systems often arise in many applications such as vehicle simulations, molecular dynamics, circuit simulations, and flexible body dynamics. Moreover, some applications are folding the antenna of a satellite or the oscillations appearing in the steering of a car. Apart from some direct practical interests, how to find suitable numerical integrators for highly oscillatory problems has been a computational challenge for a long time. To approximate the solution with sufficient accuracy, the step sizes far smaller than the smallest approximate period of the oscillations must be taken with standard integrators. It is well known that classical

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solvers are not very effective for the above problem [1,2]. An early approach to take larger time steps in oscillatory problems was given by Gautschi, who presented trigonometric integrators for differential equations of the form $\ddot{y} + \omega^2 y = g(t, y)$ with a fixed frequency ω [3]. His methods are extended readily to $\ddot{y} + Ay = g(t, y)$ with a constant, symmetric, positive semidefinite matrix A of large norm. For this type of equation, García-Archilla, Sanz-Serna and Skeel proposed and analysed the mollified impulse method [4], and Hochbruck and Lubich analysed Gautschi-type integrators [5]. Recently, based on the Magnus expansion [6,7], Iserles extended the above analytical idea to equations with a time-dependent matrix $A(t)$ and proposed a completely different approach as a suitable numerical method for highly oscillatory linear differential equations. Although some preliminary analyses of Iserles' method are already available, it is clear that much work is still to be done. In particular, the deeper detailed study is needed in order to clarify under which circumstances a particular method is preferable to others, which requires, as a first step, some optimization strategies for reducing the computational cost of the Magnus integrators, in particular by reducing the number of function evaluations and matrix operations (products and/or commutators) involved. Here we will suggest commutator-free method for highly oscillatory dynamic systems, and some numerical examples, such as Airy equation, Bessel equation, Mathieu equation, show that the proposed methods appear to be quite adequate for highly oscillatory dynamic systems.

2. Approximation method for highly oscillatory dynamic systems

2.1. The Magnus methods

The Magnus expansion [8] is a popular perturbative method for preserving the qualitative properties of the exact solution of the linear system. In recent years, Iserles and Nørsett [6] use rooted trees to analyse the Magnus expansion terms, and lead to a recursive procedure to construct practical algorithms for the numerical integration of linear equation. In this section we sketch some basic ideas about approximation methods based on the Magnus expansion for linear dynamic system [5,6]. Firstly, we convert differential equation (1) to the vector equation

$$y' = A(t)y(t), \quad t \geqslant 0, \tag{2}$$

where

$$A(t) = \begin{bmatrix} 0 & 1 \\ -g(t) & 0 \end{bmatrix}, \quad y(0) = \begin{pmatrix} y_0 \\ y_0' \end{pmatrix}.$$

It is known that, from Magnus' idea, the solution of differential equation (2) can be expressed as the form

$$y(t) = \mathrm{e}^{\Omega(t)} y_0, \tag{3}$$

where Ω satisfies the following equation:

$$\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^k A, \quad t \geqslant t_0, \quad \Omega(t_0) = 0,$$

where $\{B_k\}_{k \in Z^+}$ is the Bernoulli number and

$$ad_{\Omega}^0 A = \Omega$$

$$ad_{\Omega}^k A = [A, ad_{\Omega}^{k-1} A] = A ad_{\Omega}^{k-1} A - ad_{\Omega}^{k-1} AA, \quad k > 0.$$

The solution of the previous system is the so-called Magnus expansion of Ω given by

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t), \tag{4}$$

whose terms are linear combinations of integrals and nested commutators involving the matrix A at different times. Thus

$$\Omega_1(t) = \int_{t_0}^{t} A(\xi)\,\mathrm{d}\xi,$$

$$\Omega_2(t) = \tfrac{1}{2}\int_{t_0}^{t}\int_{t_0}^{\xi_1} [A(\xi_2), A(\xi_1)]\,\mathrm{d}\xi_2\,\mathrm{d}\xi_1.$$

In order to discretize solution (3), it is necessary to truncate the infinite Magnus expansion (4) and to replace integrals by quadrature. Therefore, the Magnus numerical scheme consists of advancing the Magnus expansion by step $h>0$ and approximating $y(t_{n+1}) = \mathrm{e}^{\Omega_n(h)}y(t_n)$ by

$$y(t_{n+1}) = \mathrm{e}^{\tilde{\Omega}_n(h)}y(t_n), \tag{5}$$

with $\tilde{\Omega}_n(h)$ truncation of $\Omega_n(h)$, where the integrals are replaced by quadrature.

2.2. Modified Magnus methods

A modified version of the Magnus method for linear dynamic system (2) can be designed explicitly for oscillatory systems as in Refs. [9,10]. The algorithm advances from t_n to $t_n + h$ by setting

$$y(t) = \mathrm{e}^{(t-t_n)A(t_{n+1/2})}x(t), \quad t \geqslant t_n, \tag{6}$$

where $t_{n+1/2} = t_n + \frac{1}{2}h$ and function $x(t)$ satisfies

$$x' = B(t)x, \quad t \geqslant t_n, \quad x(t_n) = y(t_n), \tag{7}$$

with

$$B(t) = \mathrm{e}^{-(t-t_n)A(t_{n+1/2})}[A(t) - A(t_{n+1/2})]\mathrm{e}^{(t-t_n)A(t_{n+1/2})}. \tag{8}$$

The latter equation (7) is discretized by the standard Magnus integrator method so that $x(t) = \mathrm{e}^{\tilde{\Omega}_n(h)}y_n$; therefore, the global approximation is given by

$$y_{n+1} = \mathrm{e}^{hA(t_{n+1/2})}\mathrm{e}^{\tilde{\Omega}_n(h)}y_n, \quad n \in Z_+, \tag{9}$$

when $x(t) = \mathrm{e}^{\tilde{\Omega}_n(h)}y_n$ is discretized by using (5), we can obtain a Modified Magnus scheme.

The idea which is the basis of the above algorithm is that the oscillatory behaviour of (2) is locally well modelled by the linear equation with constant coefficients

$$\tilde{y}' = A(t_{n+1/2})\tilde{y},$$

whose solution is given by a matrix exponential. The first feature of matrix B is according to (8), $B(t) = \mathrm{O}((t - t_{n+1/2}))$; therefore, (9) represents a higher-order correction to the solution. The second is that the vector field $B(t)$ itself is a highly oscillating function. Since the integration process is a smoothing operator opposite of differentiation, forming a Magnus expansion of (9) involves repeated integration of this vector field and lowers the amplitude, hence the highly oscillatory nature of $B(t)$ is likely to render them small.

3. Numerical interator for highly oscillatory dynamic systems

The Magnus expansion (4) has been used as a basis for obtaining efficient numerical integrators [6,7] because the approximate solution is restricted to the same space as the exact flow, giving similar geometric properties of the exact solutions. Provided that $A(t)$ is a bounded matrix, the series is absolutely convergent for a sufficiently small $t-t_0$ [11],

$$\int_{t_0}^{t} ||A(s)||\,\mathrm{d}s < 1.086869, \tag{10}$$

and the accurate approximation can be expected for such interval. In this case the Magnus series is a good candidate for constructing numerical methods. Due to the particular structure, it is possible to e valuate all multidimensional integrals using standard unidimensional quadrature derived from collocation principles [6].

3.1. Fourth-order Magnus scheme

In this section we present the fourth-order Magnus scheme based on the Magnus expansion (4) for linear dynamic system. To take advantage of the time-symmetry property we consider a Taylor expansion of $A(t)$ around $t_{1/2} = t_0 + \frac{h}{2}$,

$$A(t) = \sum_{i=0}^{\infty} a_i (t - t_{1/2})^i, \tag{11}$$

where $a_i = (1/i!)(\mathrm{d}^i A(t)/\mathrm{d}t^i)|_{t=t_{1/2}}$, and then compute the corresponding expression for the terms $\Omega_k(t_0+h, t_0)$ in the Magnus expansion (4).

To get the methods up to order $n = 2s$, it is only necessary to consider $\Omega_1, \ldots, \Omega_{2s-2}$ and the algebra generated by the terms $a_1, \ldots, a_s$ [7,12,13]. Here we are interested in methods up to order $2s = 4$, we have to consider Ω_k, $k = 1, 2$.

$$\Omega = \Omega_1 + \Omega_2 + O(h^5) = b_1 - \tfrac{1}{12}[b_1, b_2], \tag{12}$$

where $b_i = a_{i-1}h^i$, $i = 1, 2$ then b_1, b_2 can be considered as the generators of a graded free Lie algebra with grades 1,2 [12].

We can also consider the following unidimensional integrals [13]:

$$A^{(i)}(h) \equiv \frac{1}{h^i}\int_{t_0}^{t_0+h} (t - t_{1/2})^i A(t)\,\mathrm{d}t = \frac{1}{h^i}\int_{-h/2}^{h/2} t^i A(t + t_{1/2})\,\mathrm{d}t, \quad i = 0, 1, \ldots, s-1, \tag{13}$$

it is clear that $A^{(i)}(-h) = (-1)^{i+1}A^{(i)}(h)$, and

$$A^{(i)} = \sum_{j=1}^{s} \frac{1-(-1)^{i+j}}{(i+j)2^{i+j}} b_j + O(h^{s+1}), \quad i = 0, 1, \ldots s-1. \tag{14}$$

then, we can write the b_j in terms of the $A^{(i)}$ and substitute in the previous expressions for the Ω_k. For example, we can obtain the following fourth-order Magnus method (Magnus4) approximations for $\tilde{\Omega}_n(h)$,

$$\Omega^{[4]} = A^{(0)} + [A^{(1)}, A^{(0)}]. \tag{15}$$

In terms of the fourth-order Gauss–Legendre collocation points, we have $A_i = A(c_i h)$, $\quad i = 1, 2$ with $c_{i,2} = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$, then

$$A^{(0)} = \frac{h}{2}(A_1 + A_2) \approx \int_0^h A(t)\,\mathrm{d}t, \tag{16}$$

$$A^{(1)} = \frac{\sqrt{3}h}{12}(A_2 - A_1) \approx \frac{1}{h}\int_0^h \left(t - \frac{h}{2}\right) A(t)\,\mathrm{d}t. \tag{17}$$

It is important to remark that all integrals can be numerically approximated using the same quadrature points in this paper.

3.2. Fourth-order commutator-free Magnus scheme

We can also choose alternative method, commutator-free method [14], to approximations up to the same order obtained by a product of exponentials of linear combinations of the $A^{(i)}$, while avoiding the presence of commutators.

We can consider

$$\Psi_m^{[4]} \equiv \prod_{i=1}^{m} \exp(\alpha_i^{(0)} A^{(0)} + \alpha_i^{(1)} A^{(1)}) = \exp(\Omega^{[4]}) + O(h^5), \tag{18}$$

where the coefficients $\alpha_k^{(i)}$ have to be determined. Here, notice that using the Lie algebra generated by $A^{(i)}$ is equivalent to use the Lie algebra generated by b_i. Therefore, the number of terms of the Lie algebra is reduced [13,14]. To get fourth-order integrators it suffices to consider the graded free Lie algebra generated by $\{b_1, b_2\}$. Then, the problem is reduced to solve the equations:

$$\Psi_m^{[4]} \equiv \prod_{i=1}^{m} \exp(x_{i,1} b_1 + x_{i,2} b_2) = \exp\left(b_1 - \frac{1}{12}[b_1, b_2]\right) + O(h^5). \tag{19}$$

In the following step, we will apply a time-symmetric method integrator, which means that $\psi_{-h}^{-1} = \psi_h$ and the coefficients has the following symmetry:

$$x_{m+1-i,j} = (-1)^{j+1} x_{i,j}, \quad j = 1, 2, 3, \tag{20}$$

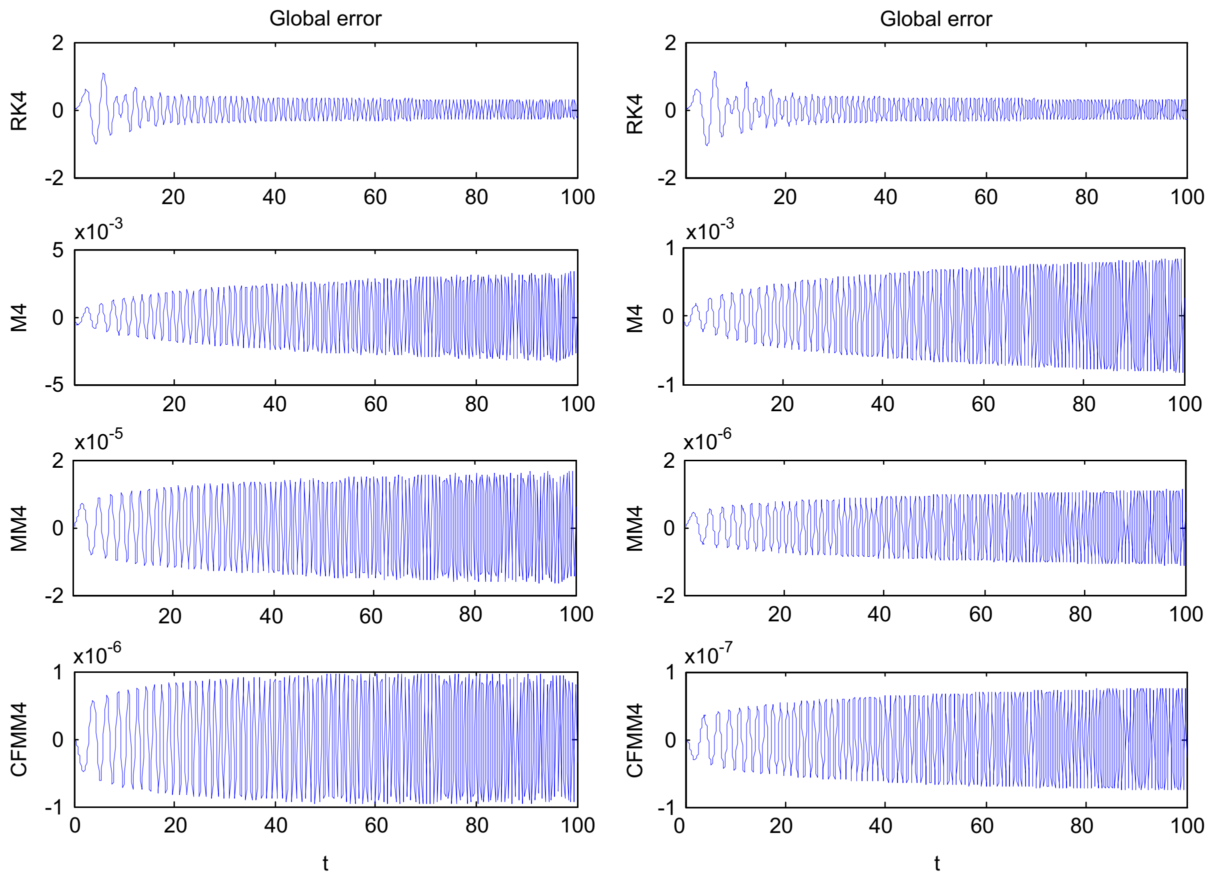

Fig. 1. From top to bottom, the global error in the solution of the Airy equation (27) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

which makes the scheme (19) time-symmetric and all even-order terms are cancelled. In practice, it is usually more convenient to work with (18), i.e., in terms of unidimensional integrals so, any quadrature can be easily used. From (12), and neglecting higher-order terms, we observe that for the fourth-order methods the changes to be done are

$$\begin{cases} A^{(0)} = b_1 \\ A^{(1)} = \frac{1}{12} b_2 \end{cases} \Rightarrow \begin{cases} \alpha_i^{(0)} = x_{i,1} \\ \alpha_i^{(1)} = x_{i,2} \end{cases}. \tag{21}$$

Next we present the order conditions to be satisfied by the coefficients $x_{i,j}$ for time-symmetric fourth-order commutator-free Magnus integrators. Firstly, we illustrate the procedure to obtain the methods (we neglect terms of order $O(h^5)$. The order conditions are obtained from the recurrence given by the following time-symmetric composition:

$$\mathrm{e}^{xb_1+yb_2}\mathrm{e}^{C(\beta^{(k)})}\mathrm{e}^{xb_1-yb_2} = \mathrm{e}^{C(\beta^{(k+1)})}, \tag{22}$$

where $\beta^{(k)} = (\beta_1^{(k)}\beta_2^{(k)}), \quad k = 0, 1, \ldots, N = [m/2]$,

$$C(\beta^{(k)}) = \beta_1^{(k)} b_1 + \beta_2^{(k)}[b_1, b_2]. \tag{23}$$

Then recurrence relations are

$$\begin{aligned} \beta_1^{(k+1)} &= \beta_1^{(k)} + 2x, \\ \beta_2^{(k+1)} &= \beta_2^{(k)} - y(\beta_1^{(k)} + x), \end{aligned} \tag{24}$$

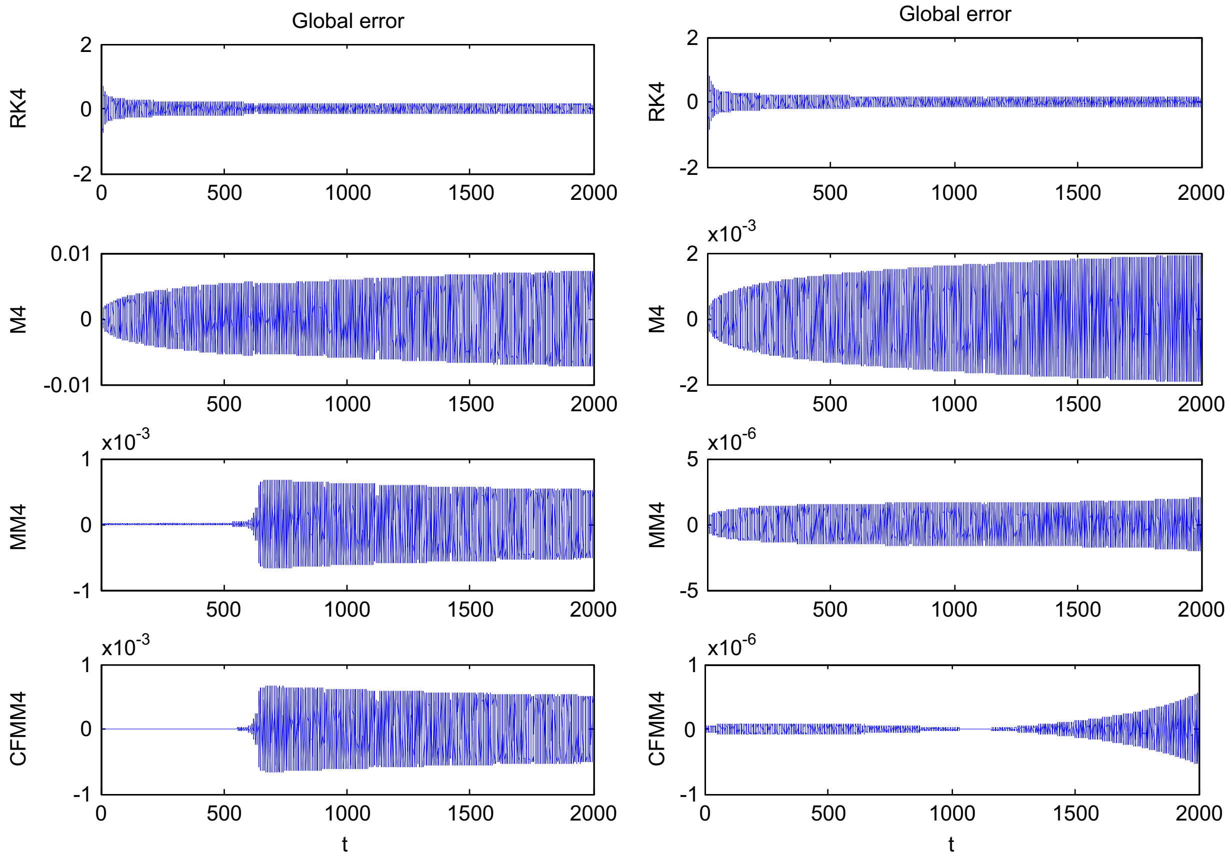

Fig. 2. From top to bottom, the global error in the solution of the Airy equation (27) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

for $k = 1, 2, \ldots, N$. Here we only consider the case of $m = 2$ exponentials and the recurrence has to be started with $\beta^{(0)} = (0, 0)$ and the exponential in the middle is $e^{\beta_1^{(0)} b_1}$. Finally we have to equate to the coefficients given in Eq. (12)

$$(\beta_1^{(N)}, \beta_2^{(N)}) = \left(1, -\frac{1}{12}\right). \tag{25}$$

So we obtain the following order conditions for the coefficients $x_{i,1}, x_{i,2}$

$$\Psi_2^{[4]} \equiv \exp(x_{1,1}b_1 + x_{1,2}b_2)\,\exp(x_{1,1}b_1 - x_{1,2}b_2) \quad \text{with} \quad x_{1,1} = \tfrac{1}{2},\ \ x_{1,2} = \tfrac{1}{6}. \tag{26}$$

Solution (26) is a fourth-order approximation (commutator-free modified Magnus4) for $\tilde{\Omega}_n(h)$ with only two exponentials.

4. Numerical examples

In this section we want to validate the effectiveness of the methods, including the fourth-order classical Runge–Kutta [15], Magnus4, modified Magnus4 and commutator-free modified Magnus4 in the field of oscillatory systems (1). In the following figs, based on different methods, the global errors in the solution of the test examples with fixed time steps $h = \frac{1}{8}$ and $h = \frac{1}{16}$.

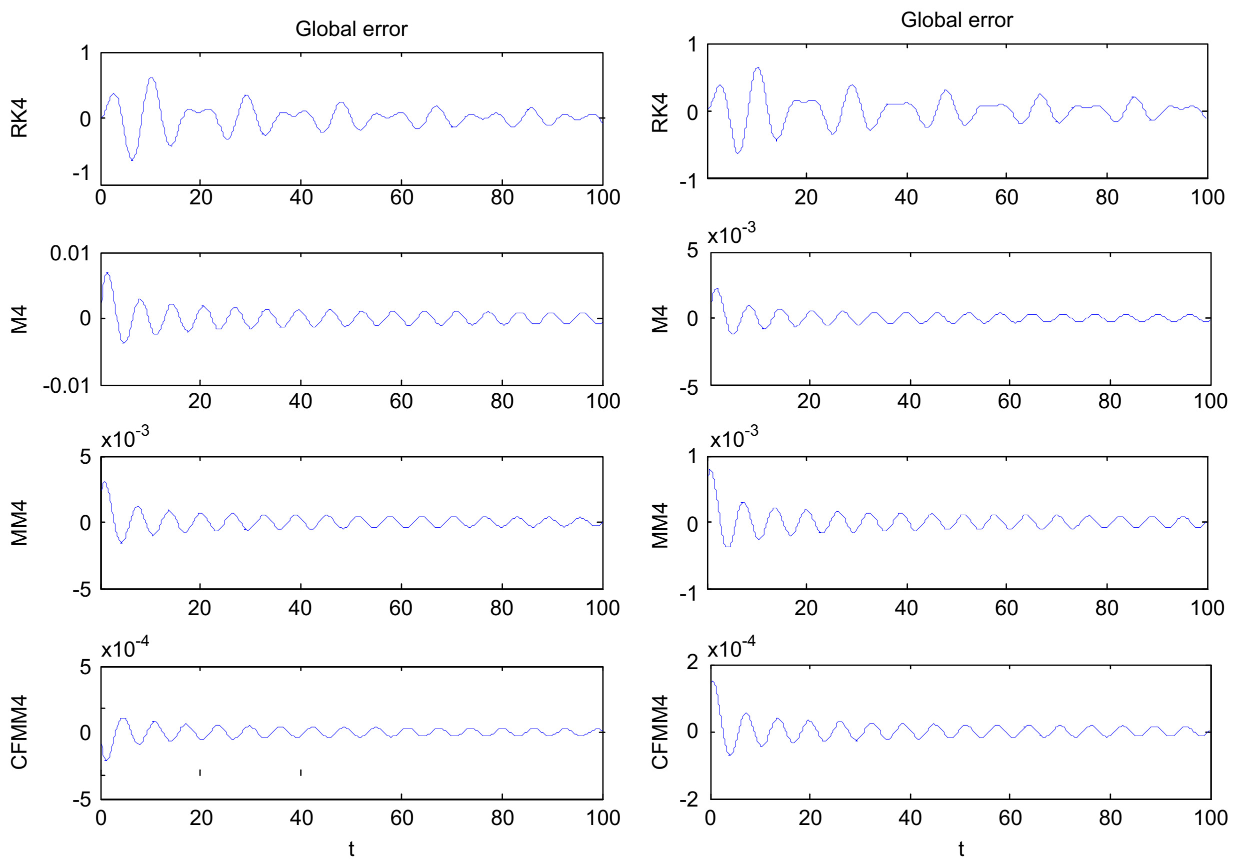

Fig. 3. From top to bottom, the global error in the solution of the Bessel equation (28) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

Example 4.1. The first example to be presented here is Airy equation with the initial-value problem:

$$\ddot{y} + ty = 0, \quad t \geqslant 0, \quad y(0) = 1, \quad y'(0) = 0. \tag{27}$$

The exact solution of (27) is given by $y(t) = \pi[Ai(-t)Bi'(0) - Ai'(0)Bi(-t)]$, where $Ai(z)$ is Airy functions and $Bi(z)$ represents the Airy function of the second kind. It is easy to prove that the trajectory is a bounded function that oscillates like $\sin t^{3/2}$, the frequency increases with time, which indicates that long-time numerical integration is difficult and this can be confirmed by endeavouring to solve (27) with fourth-order classical Runge–Kutta method [15]. Fig. 1 presents the global error in the solution of Airy Eq. (27) by fourth-order classical Runge–Kutta method, Magnus4, modified Magnus4 and commutator-free modified Magnus4 in the time interval [0,100] with different time steps; while Fig. 2 presents the global error in the time interval [0, 2000].

Example 4.2. The second example of a highly oscillatory ODE is Bessel equation with the initial-value problem:

$$t^2y'' + ty' + t^2y = 0, \quad t \geqslant 0, \quad y(0) = 1, \quad y'(0) = 0, \tag{28}$$

whose analyses solution is $y(t) = J_0(t)$, $J_0(t) = \sum_{k=0}^{\infty}((-1)^k/(k!)^2)(t/2)^{2k}$ is a Bessel function of the first kind, whose oscillatory behaviour is well known. Fig. 3 presents the global error in the solution of Bessel equation (28) by fourth-order classical Runge–Kutta method, Magnus4, modified Magnus4 and commutator-free

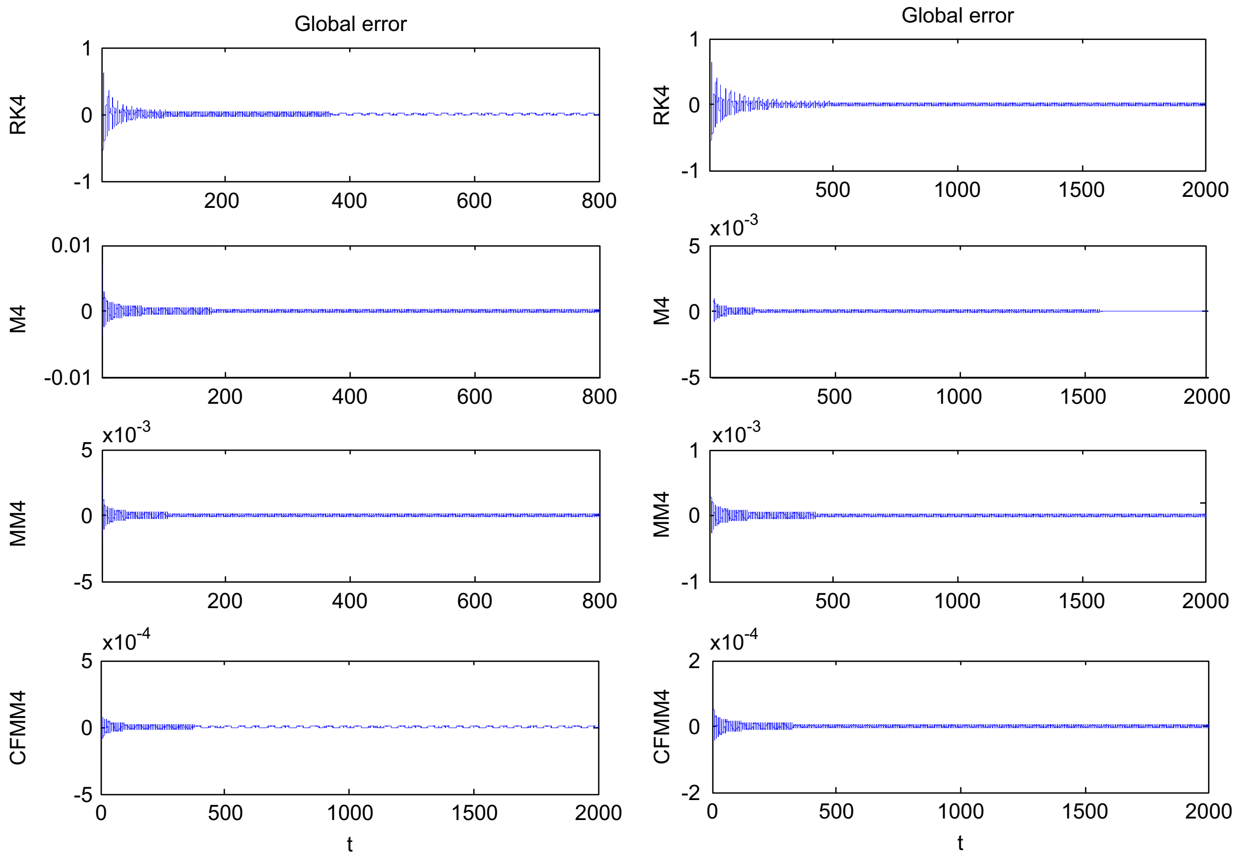

Fig. 4. From top to bottom, the global error in the solution of the Bessel equation (28) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

modified Magnus4 in the time interval [0,100] with different time steps, while Fig. 4 presents the similar error in the time interval [0, 2000].

Example 4.3. The last example we have considered refers to the Mathieu equation:

$$y'' + 2\gamma y' + (\delta + \gamma^2 + \varepsilon\cos(2t))y = 0, \tag{29}$$

which corresponds to an oscillator whose elasticity is a sinusoidal function of time. Doing the transformation $y = e^{\gamma t}z$, this equation becomes $z'' + (\delta + \varepsilon\cos(2t))z = 0$, which is a Hill-type equation. Equations of this type appear in many physical and engineering problems such as stability of a transverse column subjected to a periodic longitudinal load, lunar motion and the excitation of certain electrical systems. There are transition curves separating stable and unstable solutions of this equation, in this example we have chosen different parameters and initial values [16]:

$$\text{Case 1}: \ \delta = 1.000499968748047, \ \ \varepsilon = 0.001, \ \ y(0) = 0, \ \ y'(0) = 1; \tag{30}$$

$$\text{Case 2}: \ \delta = 0.999791843656178, \ \ \varepsilon = 0.001, \ \ y(0) = -1.557212993975872, \ \ y'(0) = 1. \tag{31}$$

The exact solution has been accurately approximated using a sufficiently small time step. Fig. 5 presents the global error in the solution of Mathieu equation (29) by fourth-order classical Runge–Kutta method, Magnus4, modified Magnus4 and commutator-free modified Magnus4 in the time interval $[0, 200\pi]$ using initial value (30) with different time steps, while Fig. 6 presents a similar error using initial value (31).

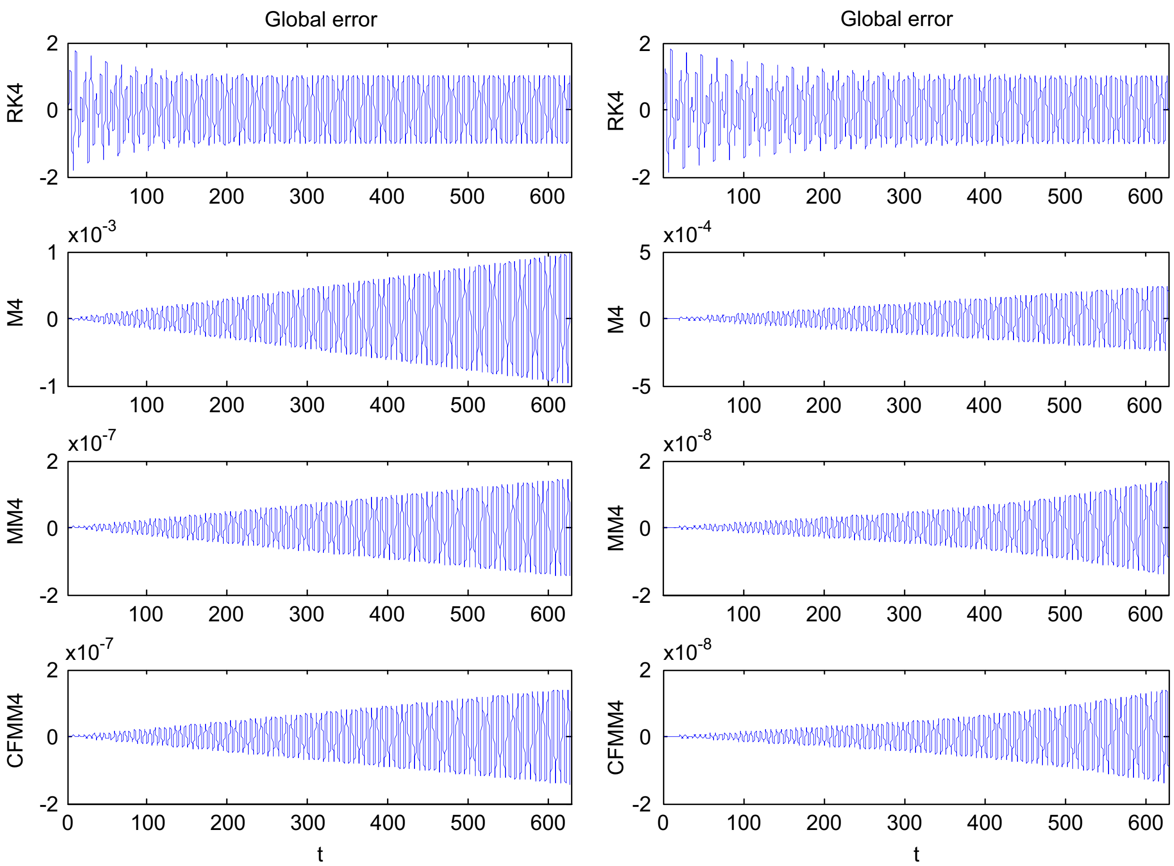

Fig. 5. From top to bottom, the global error in the solution of the Mathieu equation (29) using initial value (30) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

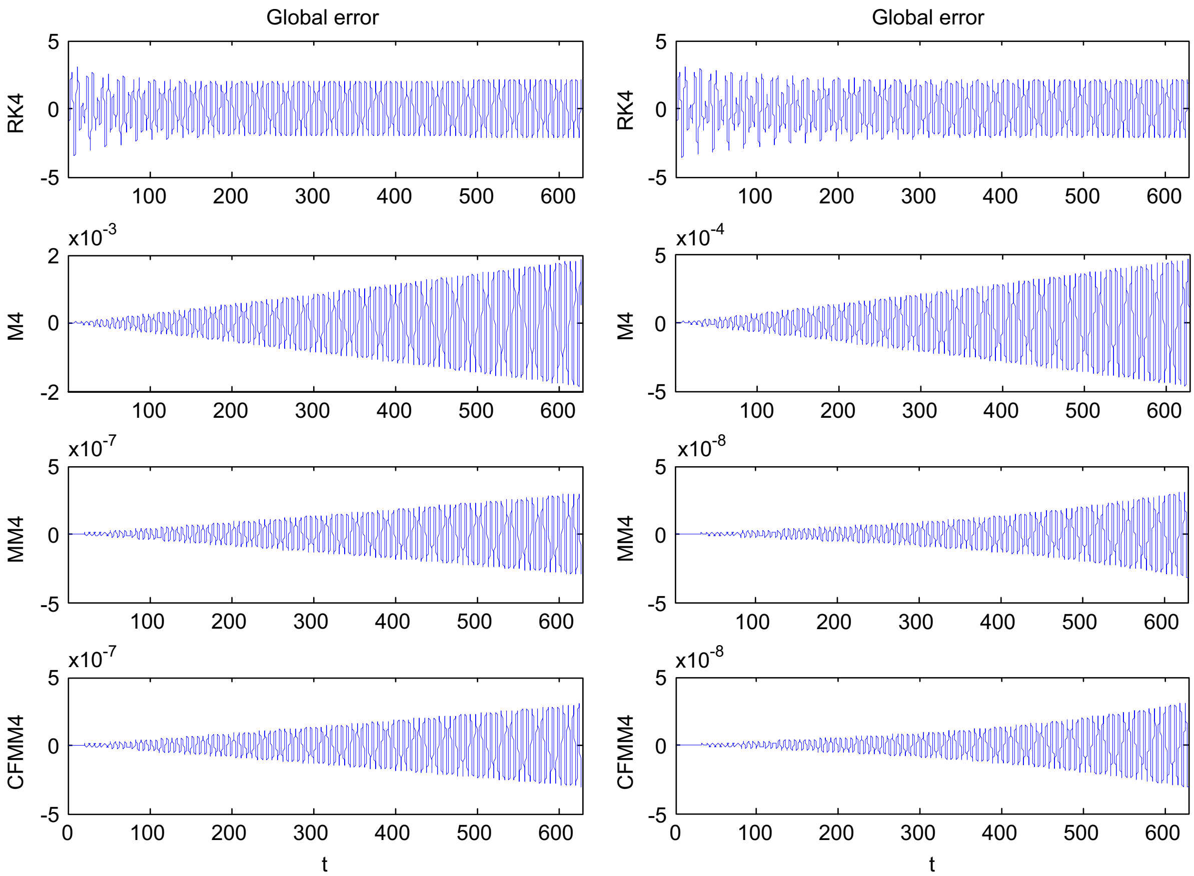

Fig. 6. From top to bottom, the global error in the solution of the Mathieu equation (29) using initial value (31) by using fourth-order Runge–Kutta (RK4), Magnus4 (M4), modified Magnus4 (MM4) and commutator-free modified Magnus4 (CFMM4) with time steps $h = \frac{1}{8}$ (left) and $h = \frac{1}{16}$ (right).

In Figs. 1 and 2, it is evident that the Magnus-type methods perform better than classical Runge–Kutta method on both timescales, when applied to the Airy equation; notice that classical Runge–Kutta method loses accuracy for the longer integration interval, but the Magnus-type methods have a remarkable advantage for numerical integration over long time as shown in Fig. 2; furthermore, concerning the modified Magnus integrator method and commutator-free modified Magnus method, which take a sharp improvement compared to Magnus integrator method; otherwise, the commutator-free modified Magnus method has a more favourable behaviour than the modified Magnus method. We can make similar considerations regarding the performances of the proposed schemes for the solution of the Bessel equation in Figs. 3 and 4, even for the numerical results of Mathieu equation in Figs. 5 and 6.

5. Conclusions

To solve highly oscillatory dynamic systems, we have suggested numerical methods which are based on the solution expression by means of the exponential map, and performed several numerical tests in order to show the effectiveness of those methods with respect to the Magnus method and the classical Runge–Kutta method. Especially a improved modified version of the considered Magnus methods, explicitly designed for oscillatory problems, is taken into account, and we also point out good performance of the improved modified scheme based on commutator-free method. In the further research, we will intend to extend the proposed method to the non-homogeneous case and non-linear case.

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