Trigonometrically Fitted Symplectic Integration Methods of Two-Stage, Second-Order and Three-Stage, Third-Order

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Recently, a new set of coefficients are found for the third-order Yoshida-Ruth type symplectic integration algorithm (SIA). This method has larger stability limit and less phase error than the Ruth’s coefficients. We consider trigonometric fitting (TF) method based on this new set of coefficients. This new TF-SIA is compared with the TF methods by Simons for the harmonic oscillator problem.

1 INTRODUCTION

The symplectic integration algorithm (SIA) has been proven to be an accurate and robust tool for problems occurring in the motion of particles, pendulums and celestial orbits. Among these symplectic methods, the three-stage, third-order methods appear to be attractive candidates for problems in which the function evaluation requires a lot of computing time. For this class of methods, a method with larger stability limit and smaller phase error than the Ruth’s method was found recently.

On the other hand, Simons et al. proposed trigonometric fitting (TF) methods, which are very accurate for the problems whose system frequency is known. They demonstrated that trigonometrically fitted symplectic methods based on the Ruth’s coefficients integrate equations of motion with extreme high accuracy.

In the present study, we apply the trigonometric fitting method to the newly found three-stage, third-order symplectic integration method mentioned above. Comparison is made of the stability and accuracy of the new TF-SIA and the TF-SIAs by Simons et al.

2 SYMPLECTIC INTEGRATION METHOD

2.1 SYMPLECTIC RUNGE-KUTTA METHOD

In this study, explicit partitioned Runge-Kutta methods of s-stage is considered:

\[ p^{i+1} = a_i p^i - c_i h H_q(q^i) \]  \hspace{1cm} (1)

\[ q^{i+1} = b_i q^i + d_i h H_p(p^{i+1}) \]  \hspace{1cm} (2)

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where \( a_i = b_i = 1, \ i = 1, \cdots, s, \ y = (q, p), \ y^t = y(t), \ y^{t+1} = y(t+h) \) and \( H(q, p) = V(q) + A(p) \).

The coefficients that satisfy the third-order symplecticity conditions

\[
\begin{align*}
c_1 + c_2 + c_3 &= 1, \\
d_1 + d_2 + d_3 &= 1, \\
c_2 d_1 + c_3 (d_1 + d_2) &= \frac{1}{2}, \\
c_2 d_1^2 + c_3 (d_1 + d_2)^2 &= \frac{1}{3}, \\
d_3 + d_2 (c_1 + c_2)^2 + d_1 c_1^2 &= \frac{1}{3}.
\end{align*}
\]

are obtained by Ruth \(^2\):

\[
c_1 = \frac{7}{24}, \quad c_2 = \frac{3}{4}, \quad c_3 = -\frac{1}{24}, \quad d_1 = \frac{2}{3}, \quad d_2 = -\frac{2}{3}, \quad d_3 = 1.
\]

Recently reported coefficients with better dispersion property \(^7\) are:

\[
\begin{align*}
c_1 &= \frac{1}{12} \left( -7 + \sqrt{\frac{209}{2}} \right), \quad c_2 = \frac{11}{12}, \quad c_3 = \frac{1}{12} \left( 8 - \sqrt{\frac{209}{2}} \right), \\
d_1 &= \frac{2}{9} \left( 1 + \sqrt{\frac{38}{11}} \right), \quad d_2 = \frac{2}{9} \left( 1 - \sqrt{\frac{38}{11}} \right), \quad d_3 = \frac{5}{9}.
\end{align*}
\]

For the sake of convenience, let us call this set of coefficients, the solution \( A \).

### 2.2 STABILITY AND ACCURACY LIMITS

The equations of motion of one-dimensional oscillator is taken as test equations \(^{10}\):

\[
\begin{align*}
p_i &= -\omega^2 q_i, \\
q_i &= p
\end{align*}
\]

where, \( H(p, q) = \frac{1}{2} (p^2 + \omega^2 q^2) \). Let us denote one-stage of the Runge-Kutta integration in a matrix form as

\[
\begin{pmatrix}
p_{i+1} \\
q_{i+1}
\end{pmatrix} = \begin{pmatrix}
1 & -c_i \omega \nu \\
d_i h & 1 - c_i d_i \nu^2
\end{pmatrix} \begin{pmatrix}
p_i \\
q_i
\end{pmatrix}
\]

where \( i = 1, \cdots, s \) and \( \nu = \omega h \). Noting that the three-stage method is \( M = M_3 M_2 M_1 \) and requiring the asymptotic stability condition \( |\lambda| \leq 1 \), where \( \lambda \) is the eigenvalues of \( M \), stability limits are obtained as \( \nu \leq 2.507 \) and \( \nu \leq 2.666 \) for the Ruth’s method and the solution \( A \). \(^7\)

The phase of the SIAs, \( \omega^* h = \nu^* \) is given by

\[
\cos (\nu^*) = \frac{1}{2} \frac{\text{tr}(M)}{\sqrt{\det(M)}} = 1 - \frac{1}{2} \nu^2 + \frac{1}{24} \nu^4 - C_3 \nu^6
\]

where the value of \( C_3 \) is \( \frac{7}{5456} \approx 2.03 \cdot 10^{-3} \) and \( \frac{5}{776} \left( \frac{107}{2} - 5 \sqrt{\frac{209}{2}} \right) \approx 1.54 \cdot 10^{-3} \) for the Ruth’s method and the solution \( A \) respectively, while the exact value is \( \frac{1}{6} \approx 1.39 \cdot 10^{-3} \).

Thus, it is shown that the solution \( A \) has larger stability limit and smaller phase error than the Ruth’s method.
3 TF SYMPLECTIC INTEGRATION METHOD

Trigonometrically fitted (TF) methods \(^9\) integrate the solution very accurately if the frequency of the system is known beforehand. Let us denote the solution at time \(t\) as \(y_0\), then the exact solution at time \(t+h\) is, \(y(t+h) = y_0 e^{th}\). Thus, conditions on the coefficients such that the matrix of the time integration method mimics the exact solution is

\[
M = \begin{pmatrix}
\cos \nu & -\omega \sin \nu \\
\sin \nu \omega & \cos \nu
\end{pmatrix}.
\]

Since the number of conditions are less than the number of coefficients, additional conditions are imposed that some of the coefficients coincide with the coefficients of symplectic method \(^9\). TF methods of two-stage, second-order and three-stage, third-order are derived in the following. The previously obtained TF methods \(^9\) have coefficients \(a_i \neq 1, b_i \neq 1\), however, coefficients of the present TF methods are \(a_i = b_i = 1\).

3.1 TWO-STAGE, SECOND-ORDER TF METHOD

The coefficients obtained in the present study are

\[
c_1 = \frac{1}{\cos \nu} \left( \frac{1}{2d_1} \sin^2 \left( \frac{\nu}{2} \right) \right),
\]

\[
c_2 = \frac{1}{2d_1} \sin^2 \left( \frac{\nu}{2} \right),
\]

\[
d_2 = \frac{1}{\cos \nu} \left( \frac{1}{d_1} \left( \sin \nu - d_1 \right) \right)
\]

where \(\sin \nu = \sin(\nu)/\nu\) and \(d_1\) is a parameter that we can choose its value freely. If we choose \(d_1 = \frac{1}{4}\), then \(c_1 \rightarrow 0, c_2 \rightarrow 1, d_2 \rightarrow \frac{1}{2}\) (coefficients by Yoshida) as \(\nu \rightarrow 0\). In case we choose \(d_1 = \frac{1}{\sqrt{2}}\), then \(c_1 \rightarrow 1 - \frac{1}{\sqrt{2}}, c_2 \rightarrow \frac{1}{\sqrt{2}}, d_2 \rightarrow 1 - \frac{1}{\sqrt{2}}\) (coefficients by McLachlan) as \(\nu \rightarrow 0\). If \(d_1\) is chosen as to satisfy

\[
\frac{1}{2} \left( \frac{\sin^2 \left( \frac{\nu}{2} \right)}{\sin \nu} \right) \leq d_1 \leq \sin \nu,
\]

all the coefficients are positive. This suggests us to take \(d_1\) as an average of the left hand side and the right hand side of the inequality. Hence, the present method covers wider range of groups than the methods proposed by Monovasilis and Simos \(^9\).

3.2 THREE-STAGE, THIRD-ORDER TF METHODS

In the present study, a total of seven different sets of coefficients are obtained for the tree-stage, third-order method. Five sets of coefficients with relatively simple function expressions have been coded in the computer programs and their numerical performances were tested. Two sets of coefficients, denoted as TF3B and TF3E, are reported in the following. The method TF3B has the following coefficients:

\[
c_1 = \frac{7}{24}, \quad d_1 = \frac{2}{3}, \quad d_2 = -\frac{2}{3},
\]

\[
c_2 = -\frac{54(\cos \nu - 1)}{\nu^2 (24 \nu \sin \nu - (7 \nu^2 - 36) \cos \nu)}
\]
Figure 1: Error in $H$

$$c_3 = \frac{-7 \nu^2 \cos(\nu) + 36(\cos(\nu) - 1) + 24 \nu \sin(\nu)}{24 \nu^2},$$
$$d_3 = \frac{24 \nu (1 - \cos(\nu)) + (36 - 7 \nu^2) \sin(\nu)}{\nu (24 \nu \sin(\nu) - (7 \nu^2 - 36) \cos(\nu))}.$$  

TF-3B approaches the Ruth’s coefficients when $\nu \to 0$. We found one set of coefficients that approaches the solution A in the limit $\nu \to 0$ and denote it, the method TF3E:

$$c_2 = \frac{11}{12}, \quad c_3 = \frac{1}{12} \left( 8 - \sqrt{\frac{209}{2}} \right), \quad d_3 = \frac{5}{9},$$

$$c_1 = \frac{c_3 (36 \cos(\nu) + 20 \nu \sin(\nu)) - 36 \sin(\nu)}{4 (c_3 \nu (5 \nu \cos(\nu) - 9 \sin(\nu)) - 9 \cos(\nu))},$$
$$d_1 = \frac{4c_3 \nu (5 \nu \cos(\nu) - 9 \sin(\nu)) + 9(1 - \cos(\nu))}{33 \nu^2},$$
$$d_2 = \frac{(12 c_3 + 11) \nu (5 \nu \cos(\nu) - 9 \sin(\nu)) + 108(1 - \cos(\nu))}{11 \nu^2 (c_3 \nu (5 \nu \cos(\nu) - 9 \sin(\nu)) - 9 \cos(\nu))}.$$

4 NUMERICAL RESULTS

One-dimensional harmonic oscillator with $\omega = 1$ and the initial condition $(q, p) = (1, 0)$ at $t = 0$ is chosen as a model problem. Error in $H$ and $(q, p)$ at time $t = 1000$ is shown in figures 1 and 2 for various symplectic methods. Signs indicate that Y2: Yoshida’s second-order method\(^{11}\), M2: McLachlan’s second-order method, MS2: second-order TF method
by Monovasilis and Simos that approaches to Y2 when \(\nu \to 0\), TF2: present second-order TF method, R3: Ruth’s method (third-order), A3: solution A (third-order), MS3: third-order TF method by Monovasilis and Simos, TF3B: present third-order TF method that approaches to the Ruth’s method when \(\nu \to 0\), TF3E: present third-order TF method that approaches to the solution A when \(\nu \to 0\), and Y4: Yoshida’s fourth-order method.

It is observed in the errors plotted in figures 1 and 2 that while the conventional symplectic methods, Y2, M2, R3, A3 and Y4 all show the scaling low between the error \(\epsilon\) and the order of accuracy \(p\), i.e., \(\epsilon \propto h^p\), the TF methods are accurate to the machine accuracy of 64-bits floating point operation of real numbers for most of the values of \(h\) tested.

5 CONCLUSION

The three-stage, third-order symplectic integration method ‘solution A’ is more stable (in terms of \(\nu\) or CFL number, 7 ~ 8% larger) and less dispersive than the Ruth’s method \(^{7}\). TF methods that approaches to the solution A in the limit \(\nu \to 0\), together with the second-order TF method with positive coefficients and the third-order TF method based on the Ruth’s method are derived and tested for the one-dimensional oscillator. The outcome of the numerical test shows that all the TF methods exhibit practically similar degree of high accuracy. However, close examination reveals that the error in \(H\) and \((q, p)\) of TF2, TF3B and TF3E is one to two order of magnitude smaller than MS2 and MS3. The error in \((q, p)\) for \(h < \frac{1}{3}\) of TF3E is one order of magnitude smaller than TF3B. This result is indicative of effectiveness of adopting the coefficients with smaller phase error for
TF method.

On the one hand, superiority of the TF methods is obvious. On the other hand, the frequency $\omega$ of the system should be known beforehand. Otherwise, very high accuracy of the TF methods is lost and usual algebraic order of accuracy is retrieved. Similarly, for the nonlinear problems that are characterized with a spectrum of frequencies, the advantage of the TF methods will not be fully appreciated. Therefore, the proposed methods are suitable for problems in which the system is expected to be dominated by a single frequency.

References


