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Two new solutions to the third-order symplectic integration method

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ABSTRACT

Two new solutions are obtained for the symplecticity conditions of explicit third-order partitioned Runge–Kutta time integration method. One of them has larger stability limit and better dispersion property than the Ruth's method.

1. Introduction

The notion of symplectic integrator [1,2] has proven to be an attractive tool for numerical simulation of Hamiltonian dynamical systems. Among symplectic integrators, the explicit methods studied by Ruth [3] are particularly interesting because they use minimal number of stages and they are low-storage. For even order integrators, a general construction method using a formula of Lie groups is developed [4–6,8,9]. However, for the third-order method, one particular solution according to Ruth [3,4] appeared to be the only solution available in the literatures. The purpose of this report is to show that another solution exists that is more stable and less dispersive than the Ruth's method.

2. Coefficients of third-order symplectic time integration method

Consider partitioned Runge–Kutta methods of order s for the equation of motion of the form

$$u^{(i+1)} = u^{(i)} - c_i \Delta t V_p\big(p^{(i)}\big), \tag{1}$$

$$p^{(i+1)} = p^{(i)} + d_i \Delta t A_u\big(u^{(i+1)}\big) \tag{2}$$

where $i = 1, \dots, s$ and Δt is the discrete time interval. The symplecticity conditions for $s = 3$ are [3,4,7]

$$c_1 + c_2 + c_3 = 1, \tag{3}$$

$$d_1 + d_2 + d_3 = 1, \tag{4}$$

$$c_2 d_1 + c_3(d_1 + d_2) = \frac{1}{2}, \tag{5}$$

$$c_2 d_1^2 + c_3(d_1 + d_2)^2 = \frac{1}{3}, \tag{6}$$

$$d_3 + d_2(c_1 + c_2)^2 + d_1 c_1^2 = \frac{1}{3}. \tag{7}$$

According to Ruth [3], the above system of coefficient equations has a solution $c_1 = \frac{7}{24}$, $c_2 = \frac{3}{4}$, $c_3 = -\frac{1}{24}$, $d_1 = \frac{2}{3}$, $d_2 = -\frac{2}{3}$, $d_3 = 1$. As far as the author is aware of, no other solution has been utilized for practical problems.

First of all, it is noted that the system of equations has symmetry, i.e., if c_i, d_i $(i = 1, \dots, 3)$ are the Ruth's solution, then $c_i' = d_{4-i}$, $d_i' = c_{4-i}$ $(i = 1, \dots, 3)$ satisfy the equations.

Let us start by defining $d = d_1 + d_2$, then

$$d_3 = 1 - d. \tag{8}$$

If we assume here $d = 0$, then it is a straightforward task to show that the set of coefficients obtained by Ruth is the only solution of Eqs. (3) to (7).

In case $d \neq 0$, after some manipulations, given system is transformed into the following equations

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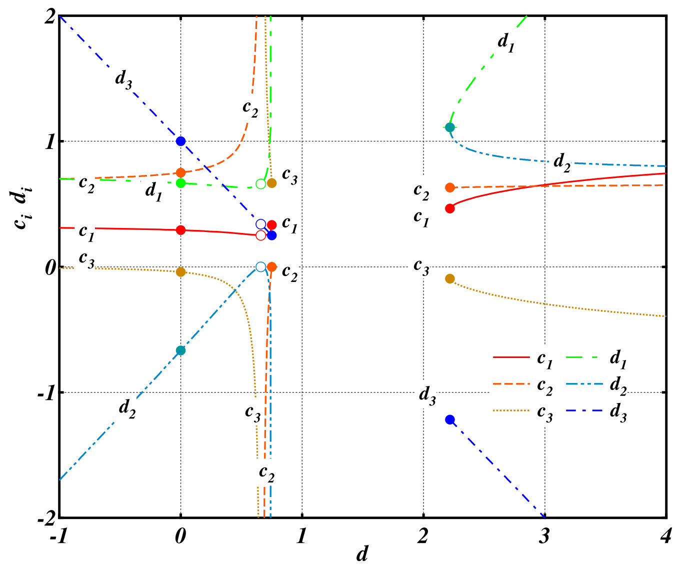

Fig. 1. c_1, c_2, c_3, d_1, d_2 and d_3 as a function of d.

$$c_1 = 1 + \frac{1}{d_1 d}\left(\frac{1}{3} - \frac{d_1 + d}{2}\right), \tag{9}$$

$$c_2 = \frac{1}{d_1 d_2}\left(\frac{d}{2} - \frac{1}{3}\right), \tag{10}$$

$$c_3 = -\frac{1}{d d_2}\left(\frac{d_1}{2} - \frac{1}{3}\right), \tag{11}$$

$$\left(\frac{d}{2} - \frac{1}{3}\right)^2 = \frac{d_1 d_2}{3}\left(d - \frac{3}{4}\right) \tag{12}$$

with accompanying constraints

$$d_1 \neq 0, \qquad d_2 \neq 0, \qquad d \neq \frac{3}{4}.$$

Under these conditions, we define $e = d_1 d_2$. Then, if the quadratic equation

$$z^2 - dz + e = 0 \tag{13}$$

has real root(s) that satisfy Eq. (12), these roots present the solution (d_1, d_2) that we are seeking for. In order the quadratic equation has real root(s), the determinant $\mathcal{D} = d^2 - 4e$ of Eq. (13) should be non-negative. Above inequality gives further conditions on d,

$$d < \frac{3}{4} \quad \text{or} \quad d \geqslant d_0,$$

where d_0 is the real root of $d^3 - \frac{15}{4}d^2 + 4d - \frac{4}{3} = 0$. We are now able to explicitly write down the formal solution to the given system of equations.

$$(d_1, d_2) = \frac{1}{2}\left(d \pm \sqrt{d^2 - 4e}\right) \quad \text{or} \tag{14}$$

$$(d_1, d_2) = \frac{1}{2}\left(d \mp \sqrt{d^2 - 4e}\right). \tag{15}$$

For the sake of convenience, let us call the former and latter expressions, the solution branches A and B, respectively.

In order to obtain a clear image on the behavior of the coefficients, all the coefficients for the solution branch A are plotted in Fig. 1 as a function of d. When d_1 and d_2 are exchanged in this figure and c_i $(i = 1, \ldots, 3)$ are recalculated, the solution branch B is obtained.

Table 1
Coefficients of third-order symplectic time integration method.

	c_1	c_2	c_3	d_1	d_2	d_3
Ruth	$\frac{7}{24}$	$\frac{3}{4}$	$-\frac{1}{24}$	$\frac{2}{3}$	$-\frac{2}{3}$	1
solution A	$\frac{1}{12}(-7 + \sqrt{\frac{209}{2}})$	$\frac{11}{12}$	$\frac{1}{12}(8 - \sqrt{\frac{209}{2}})$	$\frac{2}{9}(1 + \sqrt{\frac{38}{11}})$	$\frac{2}{9}(1 - \sqrt{\frac{38}{11}})$	$\frac{5}{9}$
solution B	$-\frac{1}{12}(7 + \sqrt{\frac{209}{2}})$	$\frac{11}{12}$	$\frac{1}{12}(8 + \sqrt{\frac{209}{2}})$	$\frac{2}{9}(1 - \sqrt{\frac{38}{11}})$	$\frac{2}{9}(1 + \sqrt{\frac{38}{11}})$	$\frac{5}{9}$

Table 2
Stability and dispersion limits of the symplectic methods in ν (and points per period $T = 2\pi/\nu$).

	Stability $\lvert G(\nu)\rvert \leqslant 1$	Dispersion $\lvert \nu^* - \nu\rvert < 5 \times 10^{-4}$
Ruth	2.51 (2.51)	0.92 (6.83)
solution A	2.67 (2.36)	1.17 (5.37)
solution B	1.57 (3.99)	0.38 (16.5)

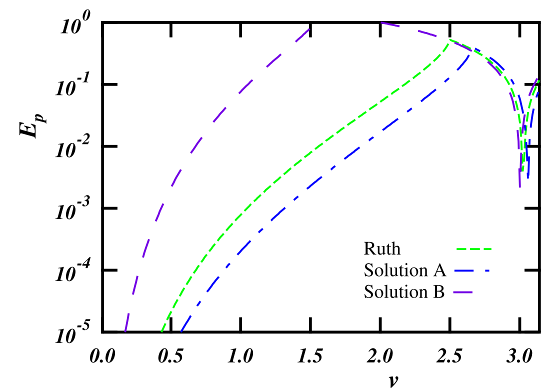

Fig. 2. Phase error E_p as a function of ν.

Some of the values of c_i, d_i $(i = 1, \ldots, 3)$ in the vicinity of $d = 0$, $\frac{2}{9}$ and $d \to \frac{3}{4} - 0$ are not bounded and they are inappropriate as coefficients.

$d = 0$ corresponds to the already known Ruth's solution.

$d = \frac{4}{9}$ represents two new solutions that has not been reported in the previous literatures. Let us call these new solutions as solution A and solution B. Precise values of their coefficients are listed in Table 1. In the following, it will be shown that the solution A has larger stability limit and less phase error than the Ruth's solution.

3. Stability and accuracy limits

Stability and accuracy of three integration methods are analyzed for the equation of motion of one-dimensional harmonic oscillator as the test equation [15]. By noting that one stage of partitioned Runge–Kutta method for the test equation is written in matrix form as

$$\begin{pmatrix} u^{(i+1)} \\ p^{(i+1)} \end{pmatrix} = \overbrace{\begin{pmatrix} 1 & -c_i \omega \nu \\ d_i \Delta t & 1 - c_i d_i \nu^2 \end{pmatrix}}^{M_i} \begin{pmatrix} u^{(i)} \\ p^{(i)} \end{pmatrix},$$
$$i = 1, \ldots, s, \tag{16}$$

where $\omega \Delta t = \nu$, and the transformation of one time step M is expressed as $M = M_3 M_2 M_1$, the amplification factor [16] of the algorithm $G(\nu)$ is given by the eigenvalue λ of M:

$$\lambda^2 - \operatorname{tr}(M)\lambda + \det(M) = 0. \tag{17}$$

The stability limit of the integration method is obtained by requiring $|\lambda| \leqslant 1$. As shown in Table 2, stability limit of solution A is larger than the Ruth's method.

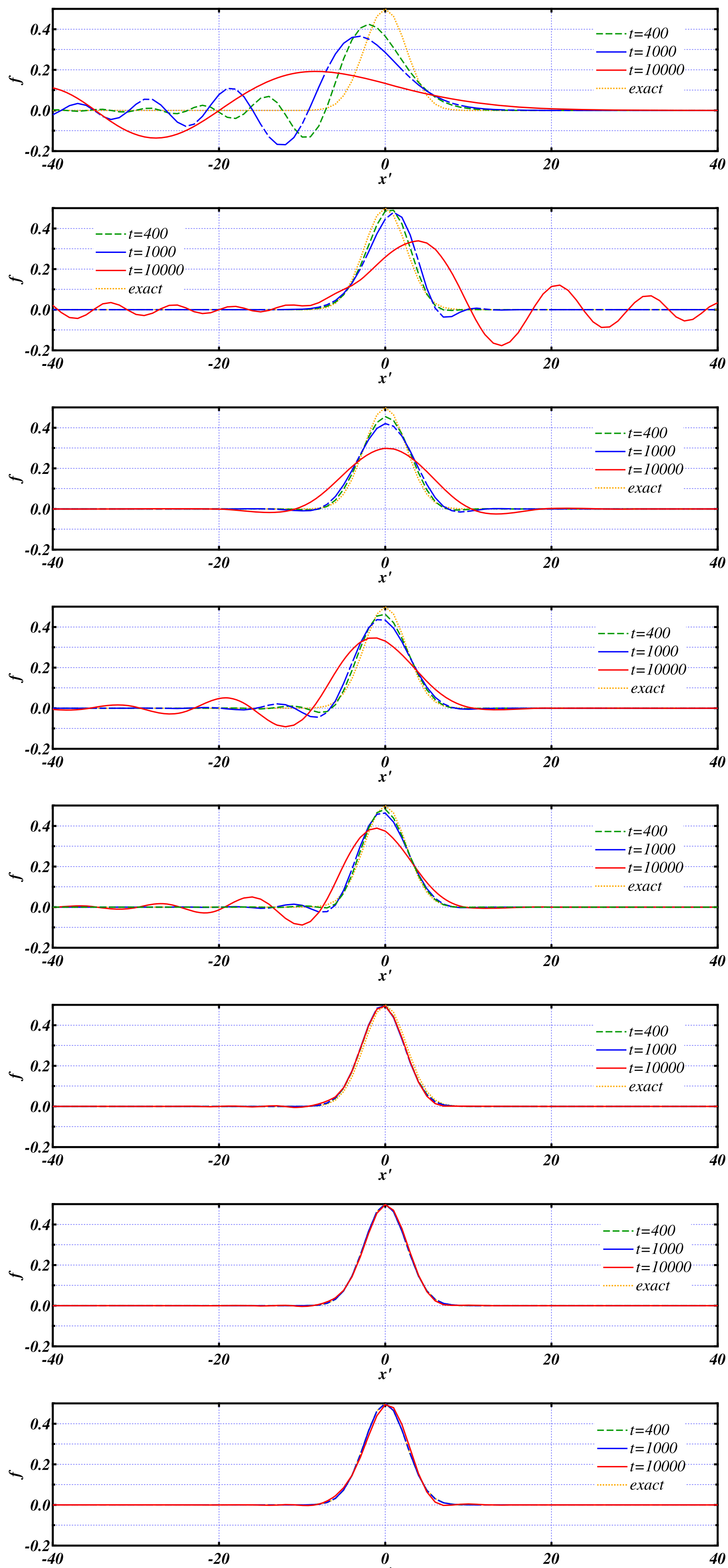

Fig. 3. Comparison of various methods, $x' = x - ct$: from top to bottom, FDTD ($\sigma = 0.7$), LF-CD6 ($\sigma = 0.25$), RK3W ($\sigma = 0.5$), RK3CK ($\sigma = 1.0$), RK4CK ($\sigma = 1.0$), Ruth's method ($\sigma = 0.7$), solution A ($\sigma = 1.0$) and solution B ($\sigma = 0.25$).

The stability condition is satisfied only if eigenvalues are complex numbers. When λ are conjugate complex numbers, it follows from $\det(M) = 1$ that $|\lambda| = 1$. Therefore, the amplification error [16] of the symplectic algorithm is exactly zero up to the stability limit:

$$1 - \left|G(\nu)\right| \equiv 0.$$

This implies that in terms of the dissipation error, all the symplectic methods are expected to perform equally accurately.

The phase of the time integration method $\omega^* \Delta t = \nu^*$ is

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

where the value of C_3 is $\frac{7}{3456} \simeq 2.03 \times 10^{-3}$, $\frac{5}{7776}(\frac{107}{2} - 5\sqrt{\frac{209}{2}}) \simeq 1.54 \times 10^{-3}$ and $\frac{5}{7776}(\frac{107}{2} + 5\sqrt{\frac{209}{2}}) \simeq 6.73 \times 10^{-2}$ for the Ruth's method, solution A and solution B, respectively, while the exact value is $\frac{1}{6!} \simeq 1.39 \times 10^{-3}$. The dispersion error $E_p = |\nu^* - \nu|$ for three methods is plotted in Fig. 2 as a function of ν. The error limit of phase lag defined as in [16] is presented in Table 2. Inspection of the coefficient C_3, E_p and the phase error limit all disclose that the solution A has smaller phase lag than the Ruth's solution.

4. One-dimensional wave propagation

Numerical solution of an initial value problem

$$f_t + f_x = 0,$$
$$f(x, 0) = \frac{1}{2} \exp\left(-\ln(2)\left(\frac{x}{3}\right)^2\right),$$
$$-40 \leqslant x \leqslant t + 60, \qquad \Delta x = 1.0$$

is obtained at time $t = 400$, 1000 and 10 000. This is an extension of the benchmark problem posed in [10] where numerical solution was required at $t = 400$. Above convection equation is recast into a form of linear sound wave equations

$$u_t = -V_p(p) \equiv -\frac{1}{\rho_0} p_x,$$
$$p_t = A_u(u) \equiv -\rho_0 c^2 u_x$$

where u is the velocity, p the pressure disturbance, ρ_0 the density, $c(= 1)$ the sound speed, with initial value condition $p(x, 0) = f(x, 0)$ and $u(x, 0) = p(x, 0)/\rho_0 c$. For the spatial discretization, sixth-order compact staggered finite difference scheme [11] is used with the third and fourth order closure at the boundaries (hereafter referred to as CD6).

Integration methods compared with the solutions A, B are the conventional finite difference time domain (FDTD) method [12], the Leap-Frog method (LF), Williamson's 2N-storage third-order Runge–Kutta method (RK3W) [13], 2N-storage Runge–Kutta method by Carpenter and Kennedy (RK3CK) [14] which is fourth-order for linear problems, optimized 2N-storage five-stage fourth-order Runge–Kutta method by Carpenter and Kennedy (RK4CK) [14] and Ruth's method. CD6 is combined with these integration methods except for the FDTD.

The results of long-time integration are now shown in Fig. 3. Because the stability limit differs among methods, we have to compare the results at different Courant numbers, where the Courant (CFL) number is $\sigma = c\frac{\Delta t}{\Delta x}$. Numerical error defined as $E_n = \frac{1}{n-2}\sum_{j=2}^{n-1} |f_j - f(x_j)|$ at times $t = 400$ and 10 000 is plotted in Fig. 4 as a function of σ.

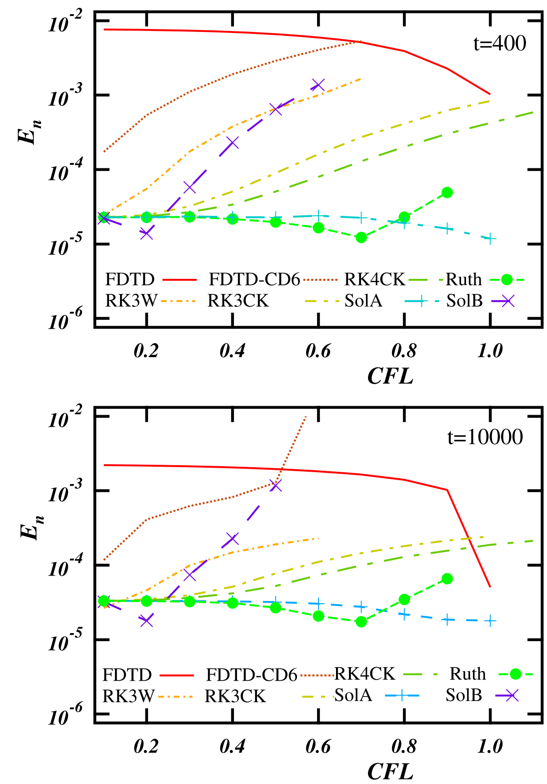

Fig. 4. Numerical error E_n as a function of σ.

It is observed that (1) replacement of the explicit second-order finite difference scheme (ED2) in FDTD to CD6 greatly improves the results for $\sigma < 0.5$, but refinement of the spatial resolution alone is not sufficient for accurate integration over a long-time period. (2) Low-storage Runge–Kutta methods perform nicely for short time integration, but they are dissipative for long-time integration, if used at $\sigma > 0.5$. (3) Three symplectic methods perform excellently good, illustrating the effectiveness of the wave energy preserving properties of the methods. The most stable method among them is the solution A that runs at $\sigma = 1.0$ for this problem. (4) In order to obtain numerical solutions of comparable accuracy to the solution A, we have to chose $\sigma \leqslant 0.75$ for Ruth's method and $\sigma \leqslant 0.25$ for solution B. While the numerical error E_n of both methods exhibits gradual increase when σ exceeds a certain value, E_n of the solution A is almost flat over the whole stability interval.

5. Concluding remarks

Our motivation is to simulate low frequency ($\nu \sim O(10^1)$ Hz) sound noise propagation which requires very long-time integrations. Computing cost is another important factor because evaluation of the compact schemes consumes large computing time. Therefore, three-stage third-order methods appear to be a good compromise between small computing cost and reasonably good integration accuracy. It is stressed that the newly found solution A is more stable and less dispersive than the previously known Ruth's method. Preference for the rational numbers should not be a problem once coefficients are coded in the computer programs.

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