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Phase-fitted partitioned Runge-Kutta methods for separable oscillatory Hamiltonian systems and related problems

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Abstract

We present an approach for deriving some phase-fitted Partitioned Runge-Kutta (PRK) methods for numerical integration of separable Hamiltonian and related systems. The approach constitute the modification of the existing PRK such that some parameters are modified to eliminate the phase-lag and the amplification error using the analysis of phase properties. The new coefficients are derived such that an estimate of the frequency of the problem is adapted to the new coefficient such that oscillatory properties of the system is effectively handled by the modified schemes. Numerical results obtained for well-known test problems show the efficiency of the new method.

1. Introduction

Consider the general autonomous separable Hamiltonian equation given by

$$H(p,q) = T(p) + V(q) \tag{1}$$

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where T is the energy and V is the potential energy. The Hamiltonian system is

$$p' = f(q), \qquad q' = g(p) \tag{2}$$

where

$$f(q) = -\frac{\partial H}{\partial q}(p,q) = -\frac{\partial V}{\partial q}(q)$$
$$g(p) = -\frac{\partial H}{\partial p}(p,q) = -\frac{\partial T}{\partial p}(p)$$

The partitioned Runge-Kutta method for the numerical integration of the system (2) is given by

$$\begin{aligned} P_i &= p^n + h\sum_{j=1}^{s} a_{ij} f(Q_j), \\ Q_i &= q^n + h\sum_{j=1}^{s} A_{ij} g(P_j), \qquad j = 1, 2, \ldots, s \\ p^{n+1} &= p^n + h\sum_{i=1}^{s} b_i f(Q_i), \\ q^{n+1} &= q^n + h\sum_{i=1}^{s} B_i f(P_i), \end{aligned} \tag{3}$$

which can be presented in the Butcher's tableau given by

$$\begin{array}{c|c} c & a \\ \hline & b \end{array}, \quad \begin{array}{c|c} C & A \\ \hline & B \end{array} ,$$

where a, A are $s \times s$ matrices and c, C, b, B are s dimensional vectors. Let $e = (1, 1, \ldots, 1)$, then $c = a \cdot e$ and $C = A \cdot e$.

The partitioned Runge-Kutta methods can be seen as an additive Runge-Kutta (RK) methods which has corresponding order conditions which conforms with the P-series which are expressed in terms of bicoloured trees as given in Hairer *et al.* (1993) or the set of order conditions given in Kennedy and Carpenter (2001). Also, Abia and Sanz-Serna (1993) considered the symplectic conditions and equally gave the order condition in their celebrated paper.

In recent times, various methods have been proposed for the numerical integration of separable systems. Some of these methods are structure preserving, such that the qualitative properties of the systems is preserved. Special attention has been focused on systems whose vector field is separable. The separability of these systems often create options for special approaches to solving the system. On one part, are separable systems having a number of exactly solvable parts. A class of numerical methods known as splitting methods have been explored for these class of problems and the experiments were practicable, (for example see Blanes and Moan (2000), Blanes and Moan (2002), Blanes (2013)). On the other hand, are systems in which different class of numerical methods are used for the separated vector fields or the exact solution and a numerical method are combined

to advance the solution of the system have also been explored in the literature Ascher *et al.* (1985).

Hamiltonian systems appear in many areas of science and engineering and are mostly tackled by symplectic methods. The symplectic conditions for Runge-Kutta (partitioned) methods were discovered by Sanz-Serna (1988). Among pioneers in these areas are Forest and Ruth (1990), Yoshida (1990), Feng and Qing (1991), McLachlan and Atleta (1992), Gan *et al.* (2013) to mention a few. Due to the fact that these Hamiltonian systems are separable, the partitioned Runge-Kutta methods are very efficient for separable system. In real applications, the solution to these separable Hamiltonian systems are oscillatory in nature and this cases motivates the combination of exponentially fitting on some Runge-Kutta methods for Hamiltonian systems, for example see Berghe and Van Daele (2010), Franco (2014), Calvo *et al.* (2008), Ehigie *et al.* (2017) and the monograph of Wu *et al.* (2013), for exponentially-fitted partitioned Runge-Kutta methods, see Monovalis *et al.* (2009). This motivates us to investigate some phase-fitted partitioned Runge-Kutta methods for the numerical integration of (2). Vyver (2007) noted that standard integration methods require a very high computational effort for the simulation of highly oscillatory problems. Recently, Monovasilis and coworkers derived some new methods based on the phase properties in Monovasilis and Simos (2007), Monovasilis (2010), Monovasilis (2012a), Monovasilis (2012b). In this paper, we adapt the phase-lag and the dissipation property initially proposed by Brusa and Nigro (1980) and discussed in Vyver (2005), Raptis and Simos (1991) to some standard partitioned Runge-Kutta methods in the literature and experiment their performance on separable oscillatory Hamiltonian systems. The rest of the paper is organized as follows: In section 2, some PRK methods in the literature were discussed and presented. In section 3, we discussed the phase analysis and phase properties of PRK methods. A note on order conditions are discussed in section 4. Section 5, focuses on the construction of the new phase-fitted methods and some practical methods based on the phase-fitted properties are presented. In section 6, numerical results to show the accuracy of the new phase-fitted PRK methods are reported. Finally, we give some concluding remarks.

2. Partitioned Runge-Kutta methods

In this section, we present a class of partitioned Runge-Kutta methods that have appeared in the literature. A special form of (3) is of the form

$$\begin{aligned} Q_0 &= q^n, \\ P_1 &= p^n, \qquad i = 1, 2, \ldots, s \\ Q_i &= Q_{i-1} + hb_i g(Q_i), \\ P_{i+1} &= P_i + hB_i f(P_i), \\ q^{n+1} &= Q_s, \\ p^{n+1} &= P_{s+1}. \end{aligned} \tag{4}$$

with Butcher tableau

$$\begin{array}{c|ccccc} c_1 & b_1 & 0 & 0 & \ldots & 0 \\ c_2 & b_1 & b_2 & 0 & \ldots & 0 \\ c_3 & b_1 & b_2 & b_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ c_s & b_1 & b_2 & b_3 & \ldots & b_s \\ \hline & b_1 & b_2 & b_3 & \ldots & b_s \end{array} \quad , \quad \begin{array}{c|ccccc} C_1 & B_1 & 0 & 0 & \ldots & 0 \\ C_2 & B_1 & B_2 & 0 & \ldots & 0 \\ C_3 & B_1 & B_2 & B_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ C_s & B_1 & B_2 & B_3 & \ldots & B_s \\ \hline & B_1 & B_2 & B_3 & \ldots & B_s \end{array}$$

Specifically, Yoshida (1990) derived a two-stage second order method with coefficients

$$b_1 = 0, \qquad b_2 = 1, \qquad B_1 = \frac{1}{2}, \qquad B_2 = \frac{1}{2}, \tag{5}$$

and a four-stage third order method were derived independently by Yoshida (1990) and Forest and Ruth (1990) with coefficients

$$\begin{aligned} &x_0 = 2^{\frac{1}{3}}, \qquad x_1 = -\frac{x_0}{2 - x_0}, \qquad x_2 = \frac{1}{2 - x_0}, \qquad b_1 = b_4 = \frac{x_2}{2} \\ &b_2 = b_3 = \frac{x_1 + x_2}{2}, \qquad B_1 = B_3 = x_2, \qquad B_2 = x_1, \qquad B_4 = 0. \end{aligned} \tag{6}$$

Ruth (1983) derived a three-stage third order method with coefficients

$$b_1 = \frac{7}{24}, \qquad b_2 = \frac{3}{4} \qquad b_3 = -\frac{1}{24}, \qquad B_1 = \frac{2}{3}, \qquad B_2 = -\frac{2}{3}, \qquad B_3 = 1. \tag{7}$$

Monovasilis and Simos (2007) constructed a three-stage third order method with coefficients

$$(8)\qquad \begin{array}{lll} b_1=\dfrac{9+3\cdot 3^{\frac{1}{3}}+3^{\frac{2}{3}}}{24}, & b_2=\dfrac{3-3\cdot 3^{\frac{1}{3}}-3^{\frac{2}{3}}}{12}, & b_3=b_1 \\ B_1=\dfrac{9-3\cdot 3^{\frac{1}{3}}-4\cdot 3^{\frac{2}{3}}}{30}, & B_2=\dfrac{3+3^{\frac{2}{3}}}{6}, & B_3=\dfrac{6+3\cdot 3^{\frac{1}{3}}-3^{\frac{2}{3}}}{30} \end{array},$$

while McLachlan and Atela (1992) also presented a two-stage second order method with coefficients

$$(9)\qquad b_1=\frac{2-\sqrt{2}}{2}, \qquad b_2=\frac{\sqrt{2}}{2}, \qquad B1=b2, \qquad B2=b1$$

and a four-stage fourth order methods with coefficients

(10)

$$b_1=0.1344962, \qquad b_2=-0.2248198, \qquad b_3=0.75632, \qquad b_4=0.3340036$$

$$B_1=0.515353, \qquad B_2=-0.085782, \qquad B_3=0.441583, \qquad B_4=0.128846.$$

3. Phase-lag properties of PRK methods

To study the phase analysis, we follow the method of Koto and Song (2014). We consider the test harmonic oscillator

$$(11)\qquad \frac{dq}{dt}=\omega p, \qquad \frac{dp}{dt}=-\omega q, \qquad \omega\geq 0,$$

which has a Hamiltonian $H(p,q)=(\omega/2)(p^2+q^2)$, $\omega\geq 0$. For $\nu=\omega h$, it should be noted that the exact solution to (11) is given by

$$(12)\qquad \begin{bmatrix} q(t_{n+1}) \\ p(t_{n+1}) \end{bmatrix} = M(\nu) \begin{bmatrix} q(t_n) \\ p(t_n) \end{bmatrix},$$

where

$$(13)\qquad M(\nu)=\begin{bmatrix} \cos\nu & \sin\nu \\ -\sin\nu & \cos\nu \end{bmatrix}$$

is known as the amplification matrix. Applying the method (4) to the test equation (11), we obtain a difference equation of the form

$$(14)\qquad \begin{bmatrix} q_{n+1} \\ hp_{n+} \end{bmatrix} = \mathcal{M}_n \begin{bmatrix} q_n \\ hp_n \end{bmatrix}, \qquad \mathcal{M}_n=\begin{bmatrix} \mathcal{M}_{11}(\nu^2) & \mathcal{M}_{12}(\nu^2) \\ \mathcal{M}_{21}(\nu^2) & \mathcal{M}_{22}(\nu^2) \end{bmatrix}.$$

The eigenvalues of the matrix $\mathcal{M}_n$ are the roots of the characteristic equation

$$\xi^2-\mathrm{tr}(\mathcal{M}(\nu^2))\xi+\det(\mathcal{M}(\nu^2))=0$$

The quantities

$$disp(\nu) = \nu - \arccos\left(\frac{\mathrm{tr}(\mathcal{M}(\nu^2))}{2\sqrt{\det(\mathcal{M}(\nu))}}\right), \quad dis(\nu) = 1 - \sqrt{\det(\mathcal{M}(\nu))} \tag{15}$$

are called the *phase-lag* and *dissipation* of the method, respectively. If

$$disp(\nu) = C_{q+1}(r)\zeta^{q+1} + \mathcal{O}(\zeta^{q+3}), \qquad dis(\nu) = D_{p+1}(r)\zeta^{p+1} + \mathcal{O}(\zeta^{p+3}),$$

then the method is called *dispersive* of order q and *dissipative* of order p, respectively. The method is called *phase-fitted (zero-dispersive)* if $disp(\zeta) = 0$ and *zero-dissipative* if $dis(\zeta) = 0$.
Our main goal of this research is to make some existing methods in the literature phase-fitted by eliminating the phase-lag and amplification errors and to investigate their effectiveness on separable oscillatory Hamiltonian systems.

4. A note on Order-Conditions for the Phase-Fitted PRK methods

The class of methods are modifications to the well known Runge-Kutta methods which combines the explicit and implicit schemes for the effective integration of Hamiltonian systems. The order conditions for the PRK methods can be derived from the p-series rooted tree formulation by Hairer and Wanner (1993) or from the additive PRK methods developed by Kennedy and Carpenter (2001) for additive Runge-Kutta methods. The idea is to recover the results by substitution of the new coefficients in the PRK methods. These new conditions consist of Order conditions of the Implicit RK method, Explicit RK method together with some coupling conditions, see Monovalis and Simos (2007) and Monovalis *et al.* (2010) for a three-stage third order condition.
A modified PRK method (3) has order p if for any sufficient problem (2), the local truncation error of the solution satisfies

$$q(t_n + h) - q_n = \mathcal{O}(h^p) \qquad p(t_n + h) - p_n = \mathcal{O}(h^p), ash \to 0.$$

The coefficients of the proposed phase-fitted PRK methods given in its series form of the stepsize h may be written as

$$b_i = b_i^{(0)} + b_i^{(2)}h^2 + b_i^{(4)}h^4 + \dots$$

$$B_i = B_i^{(0)} + B_i^{(2)}h^2 + B_i^{(4)}h^4 + \dots, \qquad 1 \le i \le s.$$

Specifically, the modified order conditions for the three-stage third order conditions in Monovalis *et al.* 2010 is given by

$$b_1^{(0)} + b_2^{(0)} + b_3^{(0)} = 1 + \mathcal{O}(h^3)$$

$$B_1^{(0)} + B_2^{(0)} + B_3^{(0)} = 1 + \mathcal{O}(h^3)$$

$$B_1^{(0)} b_1^{(0)} + B_2^{(0)} \big(b_1^{(0)} + b_2^{(0)}\big) + B_3^{(0)} \big(b_1^{(0)} + b_2^{(0)} + b_3^{(0)}\big) = \frac{1}{2} + \mathcal{O}(h^2)$$

$$b_2^{(0)} B_1^{(0)} + b_3^{(0)} \big(B_1^{(0)} + B_2^{(0)}\big) = \frac{1}{2} + \mathcal{O}(h^2)$$

$$b_2^{(0)} B_1^{(0)2} + b_3^{(0)} \big(B_1^{(0)} + B_2^{(0)}\big)^2 = \frac{1}{3} + \mathcal{O}(h)$$

$$B_1^{(0)} b_1^{(0)2} + B_2^{(0)} \big(b_1^{(0)} + b_2^{(0)}\big)^2 + B_3^{(0)} \big(b_1^{(0)} + b_2^{(0)} + b_3^{(0)}\big)^2 = \frac{1}{3} + \mathcal{O}(h)$$

$$b_2^{(0)} B_1^{(0)} b_1^{(0)} + b_3^{(0)} \big(B_1^{(0)} b_1^{(0)} + B_2^{(0)} \big(b_1^{(0)} + b_2^{(0)}\big)\big) = \frac{1}{3} + \mathcal{O}(h)$$

$$b_2^{(0)} B_1^{(0)} \big(B_2^{(0)} + B_3^{(0)}\big) + B_3^{(0)} b_3^{(0)} \big(B_1^{(0)} + B_2^{(0)}\big) = \frac{1}{3} + \mathcal{O}(h)$$

$$b_1^{(2)} + b_2^{(2)} + b_3^{(2)} = \mathcal{O}(h)$$

$$B_1^{(2)} + B_2^{(2)} + B_3^{(2)} = \mathcal{O}(h)$$

5. Construction of some phase-fitted PRK methods

5.1. **one-stage phase-fitted PRK.** Let us consider the one-stage PRK which corresponds to the symplectic Euler method given by

$$\begin{aligned} p_{n+1} &= p_n + h b_1 f(q_n) \\ q_{n+1} &= q_n + h B_1 f(p_{n+1}), \end{aligned} \tag{16}$$

we obtain a difference equation in the form (14) given by

$$\begin{bmatrix} q_{n+1} \\ h p_{n+1} \end{bmatrix} = \begin{bmatrix} 1 - \nu^2 b_1 B_1 & -\nu B_1 \\ -\nu b_1 & 1 \end{bmatrix} \begin{bmatrix} q_n \\ h p_n \end{bmatrix} \tag{17}$$

The coefficients of the new phase-fitted methods are obtain by solving the following equations:

$$2 - \nu^2 b_1 B_1 = 2\cos(\nu)$$

$$\nu b_1 = \sin(\nu)$$

which yields

$$
\begin{aligned}
b_1 &= \frac{\sin(\nu)}{\nu} = 1 - \frac{1}{6}\,\nu^2 + \frac{1}{120}\,\nu^4 - \frac{1}{5040}\,\nu^6 + \mathcal{O}(h^8) \\
B_1 &= \frac{2\tan\left(\frac{\nu}{2}\right)}{\nu} = 1 + \frac{1}{12}\,\nu^2 + \frac{1}{120}\,\nu^4 + \frac{17}{20160}\,\nu^6 + \mathcal{O}(h^8)
\end{aligned} \tag{18}
$$

For small values of ν, the coefficients are subject to heavy cancellations and then in practical computation, it is preferable to use the truncated Taylor series. It is noted that as $\nu \to 0$ our new explicit methods reduce to the symplectic Euler method.

5.2. **two-stage phase-fitted PRK.** Similarly, we repeat the same process as in the previous subsection for two known two-stage second order method presented by Yoshida (1990) and McLachlan and Atela (1992). The difference equation obtained on applying a two-stage PRK (4) is given by

$$
\begin{bmatrix} q_{n+1} \\ hp_{n+1} \end{bmatrix} = \begin{bmatrix} 1 - \nu^2 b_2 B_1 & \nu(b_1 + b_2) - \nu^3 B_1 b_1 b_2 \\ -\nu(b_1 + b_2) + \nu^3 B_1 b_1 b_2 & 1 - \nu^2(B_1 b_1 + B_2 b_1 + B_2 b_2) + \nu^4 B_1 B_2 b_1 b_2 \end{bmatrix} \begin{bmatrix} q_n \\ hp_n \end{bmatrix}. \tag{19}
$$

With a free parameter b_1, the phase-fitted coefficients of the method of Yoshida (1990) given in Taylors series are

$$
\begin{aligned}
b_1 &= 0, \qquad b_2 = 1 - \frac{1}{6}\nu^2 + \frac{1}{120}\nu^4 - \frac{1}{5040}\nu^6 + \mathcal{O}(\nu^8) \\
B_1 &= B_2 = \frac{1}{2} + \frac{1}{24}\nu^2 + \frac{1}{240}\nu^4 + \frac{17}{40320}\nu^6 + \mathcal{O}(\nu^8)
\end{aligned} \tag{20}
$$

while the phase-fitted coefficients of McLachlan and Atela (1992) is given by

$$
\begin{aligned}
b_1 &= 1 - \frac{1}{\sqrt{2}}, \\
b_2 &= \frac{1}{\sqrt{2}} + \frac{\left(4 - 3\sqrt{2}\right)}{12}\nu^2 + \frac{\left(5\sqrt{2} - 8\right)}{240}\nu^4 + \frac{\left(12 - 7\sqrt{2}\right)}{10080}\nu^6 + \mathcal{O}(\nu^8) \\
B_1 &= \frac{1}{\sqrt{2}} + \frac{\left(5\sqrt{2} - 8\right)}{24}\nu^2 + \frac{\left(141\sqrt{2} - 196\right)}{720}\nu^4 + \frac{\left(20507\sqrt{2} - 29040\right)}{120960}\nu^6 + \mathcal{O}(\nu^8) \\
B_2 &= \left(1 - \frac{1}{\sqrt{2}}\right) + \frac{\left(16 - 11\sqrt{2}\right)}{24}\nu^2 + \frac{\left(412 - 291\sqrt{2}\right)}{720}\nu^4 + \frac{\left(60432 - 42725\sqrt{2}\right)}{120960}\nu^6 + \mathcal{O}(\nu^8)
\end{aligned} \tag{21}
$$

we also observe that these methods reduce to their prototype methods with constant coefficients as derived by Yoshida (1990) and McLachlan and Atela (1992).

5.3. **three-stage phase-fitted PRK.** We equally repeat the approach for the three-stage PRK method and obtain the difference equation

$$\begin{bmatrix} q_{n+1} \\ hp_{n+1} \end{bmatrix} = \begin{bmatrix} \mathcal{M}_{11}(\nu^2) & \mathcal{M}_{12}(\nu^2) \\ \mathcal{M}_{21}(\nu^2) & \mathcal{M}_{22}(\nu^2) \end{bmatrix} \begin{bmatrix} q_n \\ hp_n \end{bmatrix}, \tag{22}$$

with

$$\mathcal{M}_{11}(\nu^2) = 1 + \nu^2(B_1b_2 - B_1b_3 - B_2b_3) + \nu^4(B_1B_2b_2b_3),$$

$$\mathcal{M}_{12}(\nu^2) = \nu(b_1 + b_2 + b_2) - \nu^3(B_1b_1b_2 + B_1b_1b_3 + B_2b_1b_3 + B_2b_2b_3) + \nu^5(B_1B_2b_1b_2b_3),$$

$$\mathcal{M}_{21}(\nu^2) = -\nu(b_1 + b_2 + b_2) + \nu^3(B_1b_1b_2 + B_1b_1b_3 + B_2b_1b_3 + B_2b_2b_3) - \nu^5(B_1B_2b_1b_2b_3),$$

$$\mathcal{M}_{22}(\nu^2) = \begin{array}{l} 1 - \nu^2(B_1b_1 + B_2(b_1 + b_2) + B_3(b_1 + b_2 + B_3) \\ +\nu^4(B_1B_2b_1b_2 + B_1B_3b_1b_2 + B_1B_3b_1b_3 + B_2B_3b_1b_3) - \nu^6B_1B_2B_3b_1b_2b_3, \end{array}$$

Using free parameter $b_1 = \dfrac{7}{24}$, $b_3 = -\dfrac{1}{24}$ and $B_1 = \dfrac{2}{3}$ obtained from the coefficients of Ruth [25] and imposing the phase-fitted conditions, we obtain a new set of phase-fitted coefficients for the method of Ruth [25] given by

$$\begin{aligned} b_1 &= \frac{7}{24}, \qquad b_3 = -\frac{1}{24}, \qquad B_1 = \frac{2}{3} \\ b_2 &= \frac{3}{4} - \frac{71}{2880}\nu^4 + \frac{359}{145152}\nu^6 + \mathcal{O}(\nu^8) \\ B_2 &= -\frac{2}{3} + \frac{2}{3}\nu^2 - \frac{17}{180}\nu^4 + \frac{59}{15120}\nu^6 + \mathcal{O}(\nu^8) \\ B_3 &= 1 - \frac{2}{3}\nu^2 + \frac{11}{180}\nu^4 + \frac{439}{22680}\nu^6 + \mathcal{O}(\nu^8) \end{aligned} \tag{23}$$

The method reduces to their prototype methods with constant coefficients as derived by Ruth (1983).

6. Numerical Experiments

In this section, we investigate the performance of the new phase-fitted PRK methods to four practical Hamiltonian problems arising from mechanics. The criterion for effectiveness used in the numerical integration of the model problems is the test based on computing the maximum global error ($\log_{10}(MGE)$) versus respective stepsizes. We also verify the preservation of the Hamiltonian by the numerical methods with some fixed time step by verifying the global error ($max|(H_n - H_0)|$) over a large time interval. The methods for comparison are listed below:

- Heun: two-stage second order Heun's method.
- RK4: four-stage fourth-order Runge-Kutta method.

- PRK1s1: one-stage symplectic Euler.
- PRK2s2a: two-stage second order method derived in Yoshida (1990).
- PRK2s2b: two-stage second order method derived in McLachlan and Atela (1992).
- PRK3s3a: three-stage third order method derived by Ruth [25].
- PRK3s3b: three-stage third order method derived by Monovasilis and Simos (2007).
- Ph-PRK1s1: one-stage phase-fitted symplectic Euler derived in this paper.
- Ph-PRK2s2a: two-stage phase-fitted second order method derived in this paper.
- Ph-PRK2s2b: two-stage phase-fitted second order method derived in this paper.
- Ph-PRK3s3a: three-stage phase-fitted third order method derived in this paper.
- Ph-PRK3s3b: three-stage phase-fitted third order method derived in this paper.

Problem 5.1: The standard pendulum

Consider the differential equation describing the standard pendulum given by

$$q' = p, \quad p' = -\sin(q), \quad q(0) = 0, \quad p(0) = 1.5.$$

We integrate the problem in the interval $[0, 1000]$ with stepsizes $h = 1/2^j,\ i = 3, 4, 5, 6$. Numerical results obtained are presented in Figure 1.

Problem 5.2: An orbit problem of Stiefel and Bettis

Next, we consider the following almost periodic orbit problem studied by Stiefel and Bettis given by

$$q_1' = p_1, \qquad q_2' = p_2 \qquad p_1' = -q_1 + 0.001\cos x, \qquad p_2' = -q_2 + 0.001\sin x$$

with initial conditions

$$q_1(0) = 1, \qquad q_2(0) = 0, \qquad p_1(0) = 0 \qquad p_2(0) = 0.9995.$$

The analytical solution is given by

$$q_1(x) = \cos x + 0.005x\sin x, \qquad q_2(x) = \sin x - 0.005x\cos x.$$

The numerical evidence for this problem with several stepsizes $h = \frac{1}{2^j},\ j = 2, 3, 4, 6$ is given in Figure 2. The integration interval is $[0, 1000]$.

The next two experiments are devoted to investigation of the Hamiltonian error of the numerical methods used for comparison. The Hamiltonian error is calculated as $\max_{i \le n \le N} |H_0 - H_N|$ for several long time intervals.

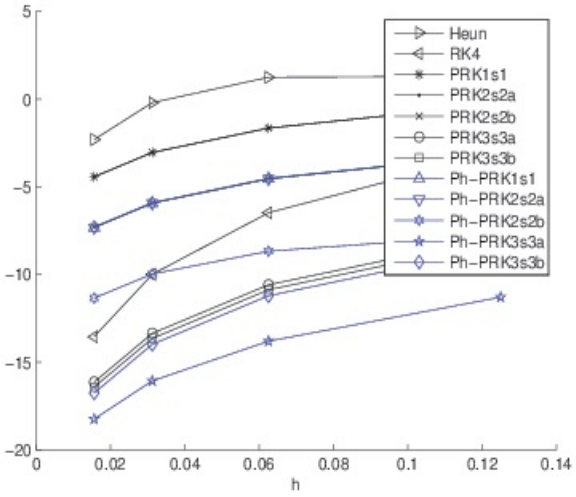

Figure 1: Problem 5.1. Accuracy comparison

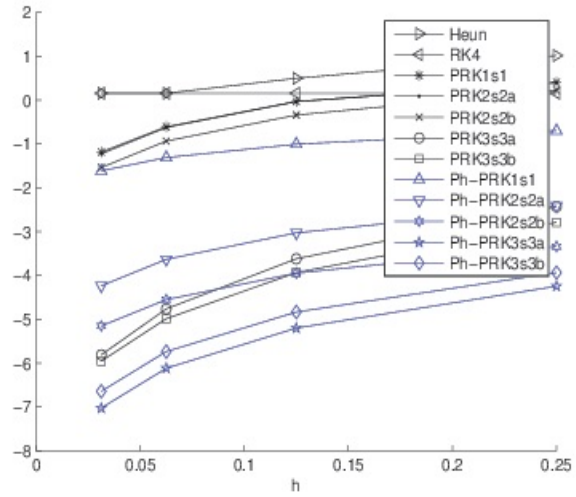

Figure 2: Problem 5.2. Accuracy comparison

Problem 5.3: The 2D harmonic oscillator with an integer frequency ratio

The two dimensional harmonic oscillator is described by the Hamiltonian

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2).$$

The equations of motion are

$$q_1' = p_1, \qquad p_1' = -q_1, \qquad q_2' = p_2, \qquad p_2' = -q_2, \tag{24}$$

with initial conditions

$$q_1(0) = 1, \qquad q_2(0) = 0, \qquad p_1(0) = 0 \qquad p_2(0) = 1.$$

The exact solution of this problem is $q_1(x) = \cos x$ and $q_2(x) = \sin x$. For this problem, we take the fitting frequency $\omega = 1$ and integrate in the interval $[0, 1000]$ with stepsizes $h = 1/2^j,\ i = 2, 3, 4, 5$. Then the problem is integrated on the interval $[0, 10000]$ with the stepsize $h = 1/8$ to investigate the Hamiltonian error for different time intervals. Numerical results obtained are presented in Figures 3 and 4.

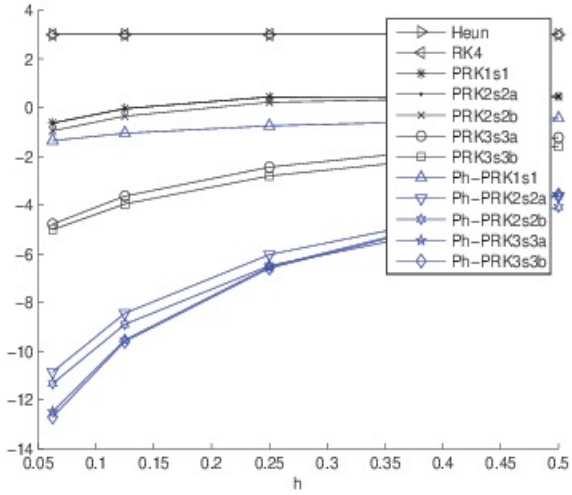

Figure 3: Problem 5.3. Accuracy comparison

Problem 5.4: Perturbed Kepler's Problem

Lastly, we consider the Hamiltonian system studied by Franco [13]

$$H(p, q) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{\omega^2}{2}(q_1^2 + q_2^2) + \frac{\alpha}{6}(q_1^2 + q_2^2)^3, \tag{25}$$

with the initial data

$$q_1(0) = 1, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \omega + \epsilon,$$

where $\alpha = \epsilon(2\omega + \epsilon)$. The analytic solution is given by

$q_1(t) = \cos((\omega+\epsilon)t)$, $q_2(t) = \sin((\omega+\epsilon)t)$, $p_1(t) = -(\omega+\epsilon)\sin((\omega+\epsilon)t)$, $p_2(t) = (\omega+\epsilon)\cos((\omega+\epsilon)t)$,

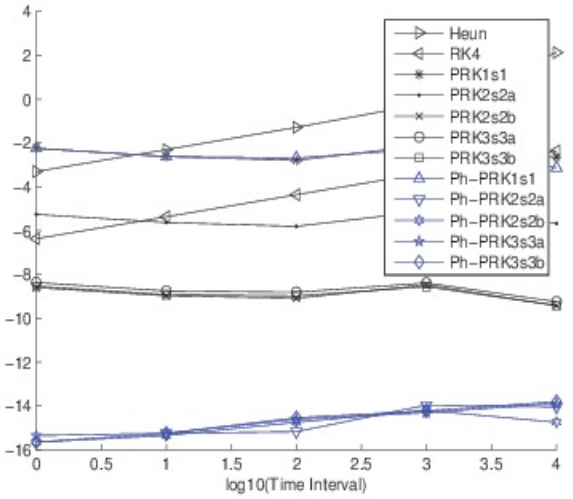

Figure 4: Problem 5.3. Hamiltonian error

representing a periodic motion. In this experiment, we have chosen the parameter values $\epsilon = 10^{-2}$, $\omega = 5$, and the integration carried out on the interval $[0, 1000]$ with stepsizes $h = \frac{1}{2^j}$, $j = 4, 5, 6, 7$, while the Hamiltonian error is obtained on the interval $[0, 10000]$. The numerical results are presented in Figures 5 and 6.

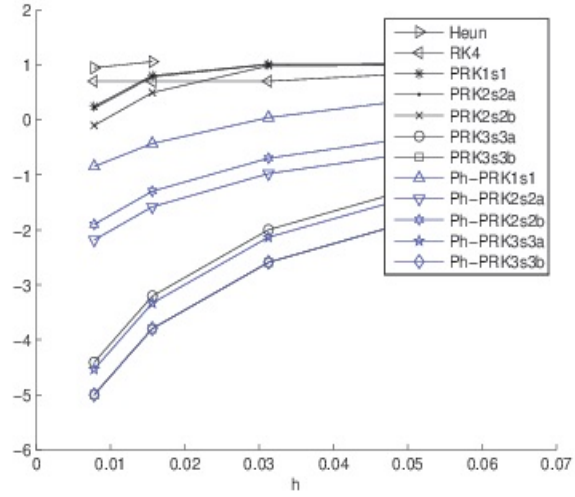

Figure 5: Problem 5.4. Accuracy comparison

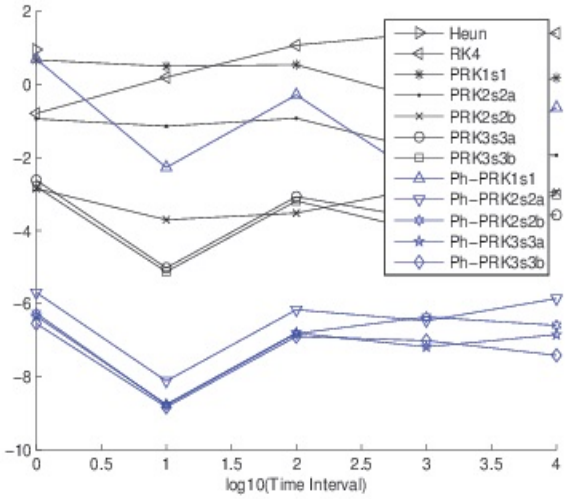

Figure 6: Problem 5.4. Hamiltonian error

In view of numerical results obtained from Problem 5.1-5.4, the new phase-fitted PRK methods derived in Section 5 are superior to the other methods for comparison. In Problem 5.1 and 5.2 respectively, Figures 1 and 2 show that the method Ph-PRK3s3b performs best, while it is observed that the phase-fitted methods are more accurate than the prototype methods. For Problem 5.3 and 5.4, where the Hamiltonian error are also presented, Figures 3 and 5, show the superiority of the phase-fitted numerical results derived in this paper, while the Hamiltonian error shown in Figures 4 and 6 evidently shows the superiority of the new method for the preservation of the Hamiltonian.

Conclusion

We have developed a class of phase-fitted PRK methods for the numerical integration of separable oscillatory Hamiltonian problems. The new methods reduce to their classical counterpart which have appeared in the literatures, when the frequency used in the fitting process is set to zero. Numerical experiments are carried out to show the effectiveness of the methods over existing methods.

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