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Structure Preserving Pseudo-Runge-Kutta Method

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Abstract: The present paper is intended to propose pseudo-Runge-Kutta method (PRKM) which is quadratically invariant i. e. it preserves structural properties when the PRKM is applied to the Hamiltonian system of equations. We have inserted the area preserving character in the implicit pseudo-Runge-Kutta method and derived the sufficient conditions of symplecticness for the pseudo-Runge-Kutta method and thus developed a qualitative numerical method. These methods are best tuned to solve system of partial differential equations of Hamiltonian type. Though these methods are not self starting but the order of the truncation error is equivalent to its counterpart Runge-Kutta method. These methods can be used to solve numerically the dynamical system of equations of Hamiltonian type such that the Hamiltonian is preserved in the numerical solution. The derivation of sufficient conditions is based on differential forms.

Keywords: Pseudo Runge-Kutta method; Quadratic invariant map; symplectic Runge-Kutta method; Hamiltonian system; Initial value problem.

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1. Introduction

The most important mathematical model for the representation of physical phenomena is the differential equation. Motion of objects, fluid and heat flow, bending and cracking of materials, vibrations, chemical reactions and nuclear reactions are all modelled by systems of differential equations. It is well known that standard Runge-Kutta (RK) methods, partitioned Runge-Kutta (PRK) methods and Runge-Kutta-Nyström (RKN) methods were well developed in the field of numerical solution of ordinary differential equations (ODEs). There is a great number of research papers have been published in the last few decades. An excellent book on almost the whole development of RK method was written by J.C. Butcher[1]. Kalugiratou et al.[2] published a review article on the development of several modified RK methods which can be found in[3] and the references cited therein.

An s-stage classic RK method involves s function evaluations (slopes) per time step. So, an attempt to reduce function evaluation per step termed as the development of pseudo RK method. Pseudo-Runge-Kutta (PRK) method was first introduced by Byrne in his Ph. D. thesis[4] and in later Byrne and Lambert proposed pseudo RK method involving two-points[5]. Several papers in the literature on pseudo RK methods can be seen in Costabile[6] and in Nakashima[7-8] and they developed some other forms of PRK method and implicit PRK method and showed their advantages lying on the fact that they are less expensive than the standard RK methods. Cong et al.[9-10] discovered an explicit pseudo two-step Runge-Kutta method with continuous variable step-size and made compatible these methods for parallel computers. Hoang and Sidje[11] made the functionally-fitting of the explicit pseudo two-step RK method (given in Cong et al.[9]). Currently, Hoang[12] made the functionally-fitting of the Nyström version of PRK method. Recently, Tiwari et al.[13] derived various types of implicit PRK methods and also constructed its exponential-fitting which is used to solve the IVP with oscillatory/periodic solutions efficiently[14].

In order to apply a numerical method to solve a differential equation of order higher than one, the equation should be transformed into a system of first order differential equations. Another category of specially designed methods are symplectic methods which are suitable for the integration of Hamiltonian systems.

It has been widely studied by several authors and established that the symplectic integrators have good advantages for the preservation of qualitative properties of the flow over the standard integrators when they are applied to the Hamiltonian systems. Let U be an open subset of $\mathbb{R}^{2d}$, I is an open subinterval of $\mathbb{R}$ then the Hamiltonian system of differential equations is given by

(1.1 $$\frac{dp}{dt} = -\frac{\partial H(p,q,t)}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial H(p,q,t)}{\partial p},$$

where $(p,q) \in U$, $t \in I$, the integer d is the number of degrees of freedom and $H(p,q,t)$ be a twice continuously differentiable function on $U \times I$. The q variables are generalized coordinates, p variables are the conjugates generalized momenta and $H(p,q,t)$ is the total mechanical energy. The solution operator of a Hamiltonian system is a symplectic transformation. A symplectic numerical method preserves the symplectic structure in the phase space when applied to Hamiltonian problems means it is quadratically invariant and preserves area properties. The theory of these methods can be found in the monographs of Hairer et al.[15] and Sanz Serna and Calvo[16].

Hamiltonian systems often have an oscillatory behavior and have been solved in the literature with exponentially and trigonometrically fitted methods. The idea of combining symplecticity with the exponentially fitting property first appears in the work of Simos and Vigo-Aguiar[17] where, an exponentially-fitted symplectic Runge Kutta method with two stages is presented. Van de Vyer[18] constructed the exponential-fitting of modified Runge-Kutta-Nyström for solving orbital problems.

The development of Symplectic Runge-Kutta type methods that also have other properties is a relatively new area that started in the early 2000s. Moreover as shown in[19-27], numerical methods serving some special purposes including symplecticity-preserving methods for Hamiltonian systems, symmetric methods for time-reversible systems, energy-preserving methods for conservative systems, conjugate-symplectic (upto a finite order) methods for Hamiltonian systems can also be constructed and investigated based on such a new framework.

2. Derivation of the Method

In this section, we give the formulation of pseudo-Runge-Kutta method of 2-stage. This method is not self-starting as it requires the previous two pieces of information to find the current iteration. Initially (at first step) it requires four evaluation functions in which two at the previous node and other two at the very previous node. But from onward steps, it requires only two function evaluations per step.

2.1 Pseudo-Runge-Kutta method (PRKM): In this section, we present the formulation of *s* stage pseudo-Runge-Kutta method. The detailed derivation and development is given in[13]. Consider the initial value problem (IVP) in first-order ordinary differential equation as:

(2.1) $$\frac{du}{dx} = f(u),\ u(x_0) = u_0\,,$$

A general one step method to solve IVP (2.1) can be written as

(2.2) $$u_{n+1} = u_n + h\varphi(u_n, f; h),\quad n = 0,1,2\cdots N-1\,,$$

where $\varphi(u_n, f, h)$ a continuous function of starting is iterate u_n and step size h.
For the general *s*-stage pseudo-Runge-Kutta method, we may choose

(2.3) $$\varphi(\bar{u}_n, f, h) = \sum_{i=1}^{\nu} b_i k_i + \sum_{i=1}^{\nu} \bar{b}_i \bar{k}_i$$

or,

(2.4) $$\varphi(\bar{u}_n, f; h) = \varphi(u_n, f; h) + \varphi(u_{n-1}, f; h)\,,$$

where the slopes (function evaluations) are defined as

(2.5) $$k_i = f\left(u_n + h\sum_{j=1}^{\nu} a_{ij} k_j\right), i = 1,2,\cdots \nu\,,$$

(2.6) $$\bar{k}_i = f\left(u_{n-1} + h\sum_{j=1}^{\nu} \bar{a}_{ij} \bar{k}_j\right), i = 1,2,\cdots \nu\,,$$

with $a_{1j} = \bar{a}_{1j} = 0,\ \forall j = 1,2,\cdots \nu$. In functional form, the above can be rewritten as

(2.7) $$u_{n+1} = u_n + h\left(\sum_{i=1}^{\nu} b_i f(x_n + c_i h, \Gamma_i) + \sum_{i=1}^{\nu} \bar{b}_i f(x_{n-1} + \bar{c}_i h, \Lambda_i)\right), n = 0,1,2,\cdots N-1,$$

where

(2.8) $$\Gamma_i = u_n,\ \ \Lambda_i = u_{n-1}\,,$$

(2.9) $$\Gamma_i = u_n + h\sum_{j=1}^{\nu} a_{ij} f\left(x_n + c_j h, \Gamma_j\right),\ i = 1,2,\cdots \nu\,,$$

(2.10) $$\Lambda_i = u_{n-1} + h\sum_{j=1}^{\nu} \bar{a}_{ij} f\left(x_{n-1} + \bar{c}_j h, \Gamma_j\right), \ i = 1, 2, \cdots \nu$$

The augmented Butcher table representation of s-stage PRKM can be written as

$$\begin{array}{c|c|c|c} c_1 & a_{11} & \bar{c}_1 & \bar{a}_{11} \\ c_2 & a_{21}\ a_{22}\ \ldots & \bar{c}_2 & \bar{a}_{21}\ \bar{a}_{22}\ \ldots \\ \vdots & \vdots \quad \vdots & \vdots & \vdots \quad \vdots \\ c_s & a_{s1}\ a_{s2}\ \ldots\ a_{ss} & \bar{c}_s & \bar{a}_{s1}\ \bar{a}_{s2}\ \ldots\ \bar{a}_{ss} \\ \hline & b_1\ \ b_2\ \ldots\ b_s & & \bar{b}_1\ \ \bar{b}_2\ \ldots\ \bar{b}_s \end{array}$$

Before deriving the symplectic PRKM we give some elementaty definitios and results which are prereqisites for the futher derivation.

Definition[15] 2.1: *A linear mapping* $T : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ *is called symplectic if it satisfies*

$$T^t J T = J$$

or equivantly, it satisfies $\omega(T\xi, T\eta) = \omega(\xi, \eta)$ *for all* $\xi, \eta \in \mathbb{R}^{2d}$ *,*
where, ω *denotes the oriented area of projection onto co-ordinate plane* (p_i, q_i)*,* $'t'$ *satands for transpose and* J *is the skew symmetric matrix which is defined by (* I *is the identity matrix)*

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

Definition[15] 2.2: *A differentiable map* $g : U \to \mathbb{R}^{2d}$ *(where* $U \subset \mathbb{R}^{2d}$ *is an open set) is called symplectic if its Jacobian matrix* $g'(p,q)$ *is everywhere symplectic i. e. if*

$$g'(p,q)^t J\, g'(p,q) = J \ \ or \ \ \omega\big(g'(p,q)\xi, g'(p,q)\eta\big) = \omega(\xi, \eta).$$

Theorem[15,21] 2.1: *If* $\dfrac{dp}{dt} = -\dfrac{\partial H}{\partial q}, \ \dfrac{dq}{dt} = \dfrac{\partial H}{\partial p}$ *be the system of equations with* $H(p,q)$ *as Hamiltonian then a* C^1 *map* $\left(p^*, q^*\right) = \varphi(p,q)$ *is symplectic if*

$dp^* \wedge dq^* = dp \wedge dq$, *where* $\wedge$ *is the Wedge product. In case of symplectic method, Hamiltonian at any step is preserved that is*

$$H\left(p_{n+1}, q_{n+1}\right) = H\left(p_n, q_n\right), \forall n \geq 0.$$

We use the criteria of Theorem 2.1, to establish the sufficient conditions for a PRKM to be symplectic.

Theorem[15,21] 2.2: An s-stage standard Runge-Kutta method, which is represented by Butcher's table representation as

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

is symplectic if its coefficients satisfy $b_i a_{ji} + b_j a_{ji} - b_i b_j = 0$.

Proof: This result was discoved and proved independently by Sanz-Serna[28], Lasagni[29-30].

2.1.1 Structure prserving pseudo-Runge-Kutta method (SPPRKM): Let Ω be a domain in the Euclidean space $\mathbb{R}^{2d}$ with coordinates $(p,q) = (p_1,\ldots,p_d;q_1,\ldots,q_d)$. Let $H(p,q)$ be a sufficiently smooth real function defined on Ω. Consider the following Hamiltonian system of differential equations of d degree of freedom:

(2.11) $$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} =: f_i(p,q), \ \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} =: g_i(p,q), \ i = 1,2,\ldots,d.$$

Consider a pseudo-Runge-Kutta (PRK) method with Butcher table notation

$$\begin{array}{c|c|c} c & A & \bar{A} \\ \hline & b & \bar{b} \end{array}$$

where $A = (a_{ij})$ and $\bar{A} = (\bar{a}_{ij})$ are $s \times s$ matrices, $c = (c_1,\ldots,c_s)^T$, $b = (b_1,\ldots,b_s)^T$ and $\bar{b} = (\bar{b}_1,\ldots\bar{b}_s)^T$.

Applying s-stage PRKM given by (2.2)-(2.6) developed in Section (2.1) to the Hamiltonian system (2.11), we have

$$\Gamma_i = p_n + h\sum_{j=1}^{s} a_{ij} f_i(\Gamma_j, \Lambda_j) + h\sum_{j=1}^{s} \bar{a}_{ij} f_i(\bar{\Gamma}_j, \bar{\Lambda}_j)\,, \tag{2.12}$$

$$\Lambda_i = q_n + h\sum_{j=1}^{s} a_{ij} g_i(\Gamma_j, \Lambda_j) + h\sum_{j=1}^{s} \bar{a}_{ij} g_i(\Gamma_j, \Lambda_j)\,, \tag{2.13}$$

$$\bar{\Gamma}_i = p_{n-1} + h\sum_{j=1}^{s} a_{ij} f_i(\Gamma_j, \Lambda_j) + h\sum_{j=1}^{s} \bar{a}_{ij} f_i(\bar{\Gamma}_j, \bar{\Lambda}_j)\,, \tag{2.14}$$

$$\bar{\Lambda}_i = q_{n-1} + h\sum_{j=1}^{s} a_{ij} g_i(\Gamma_j, \Lambda_j) + h\sum_{j=1}^{s} \bar{a}_{ij} g_i(\bar{\Gamma}_j, \bar{\Lambda}_j)\,, \tag{2.15}$$

$$p_{n+1} = p_n + h\sum_{i=1}^{s} b_i f_i(\Gamma_i, \Lambda_i) + h\sum_{i=1}^{s} \bar{b}_i f_i(\bar{\Gamma}_i, \bar{\Lambda}_i)\,, \tag{2.16}$$

$$q_{n+1} = q_n + h\sum_{i=1}^{s} b_i g_i(\Gamma_i, \Lambda_i) + h\sum_{i=1}^{s} \bar{b}_i g_i(\bar{\Gamma}_i, \bar{\Lambda}_i),\; j = 1, \ldots, s\,. \tag{2.17}$$

The characterization of structure preserving pseudo-Runge-Kutta method is given in the following theorem.

Theorem 2.1.1: *If the coefficient of the Equations (2.12)-(2.17) satisfy the following order conditions:*

$$b_i b_j - b_j a_{ji} - b_i a_{ij} = 0\,, \tag{2.18}$$

$$\bar{b}_i b_j - b_j \bar{a}_{ji} - \bar{b}_i a_{ij} = 0\,, \tag{2.19}$$

$$\bar{b}_i \bar{b}_j - \bar{b}_j \bar{a}_{ji} - \bar{b}_i \bar{a}_{ij} = 0\,. \tag{2.20}$$

then the PRKM method governed by (2.12)-(2.17) is symplectic.

Proof: Rewriting Equations (2.12)-(2.17) in traditional form:

$$p_{n+1} = p_n + h\sum_{i=1}^{s} b_i k_i + h\sum_{i=1}^{s} \bar{b}_i \bar{k}_i\,, \tag{2.21}$$

$$q_{n+1} = q_n + h\sum_{i=1}^{s} b_i l_i + h\sum_{i=1}^{s} \bar{b}_i \bar{l}_i \,, \tag{2.22}$$

where

$$\begin{cases} k_i = f(\Gamma_i, \Lambda_i), \\ \bar{k}_i = f(\bar{\Gamma}_i, \bar{\Lambda}_i), \\ l_i = g(\Gamma_i, \Lambda_i), \\ \bar{l}_i = g(\bar{\Gamma}_i, \bar{\Lambda}_i) \\ \Gamma_i = p_n + h\sum_{j=1}^{s} a_{ij} k_j + h\sum_{j=1}^{s} \bar{a}_{ij} \bar{k}_j, \\ \bar{\Gamma}_i = p_{n-1} + h\sum_{j=1}^{s} a_{ij} k_j + h\sum_{j=1}^{s} \bar{a}_{ij} \bar{k}_j, \\ \Lambda_i = q_n + h\sum_{j=1}^{s} a_{ij} l_j + h\sum_{j=1}^{s} \bar{a}_{ij} \bar{l}_j, \\ \bar{\Lambda}_i = q_{n-1} + h\sum_{j=1}^{s} a_{ij} l_j + h\sum_{j=1}^{s} \bar{a}_{ij} \bar{l}_j, \; i = 1, 2, \ldots, s \end{cases} \tag{2.23}$$

Differentiating the external stages (2.21) and (2.22) and computing dp_{n+1} and dq_{n+1} . Taking the exterior product (wedge product) of these derivatives dp_{n+1} and dq_{n+1} we have

$$\begin{aligned} dp_{n+1} \wedge dq_{n+1} = {} & dp_n \wedge dq_n + h\sum_{j=1}^{s} b_j dp_n \wedge dl_j + h\sum_{j=1}^{s} \bar{b}_j dp_n \wedge d\bar{l}_j \\ & + h\sum_{i=1}^{s} b_i dk_i \wedge dq_n + h\sum_{i=1}^{s} \bar{b}_i d\bar{k}_i \wedge dq_n + h^2 \sum_i \sum_j b_i b_j dk_i \wedge dl_j \\ & + h^2 \sum_i \sum_j b_i \bar{b}_j dk_i \wedge d\bar{l}_j + h^2 \sum_i \sum_j \bar{b}_i b_j d\bar{k}_i \wedge dl_j \\ & + h^2 \sum_i \sum_j \bar{b}_i \bar{b}_j d\bar{k}_i \wedge d\bar{l}_j \quad , \end{aligned} \tag{2.24}$$

$$\begin{aligned} dp_{n+1} \wedge dq_{n+1} - dp_n \wedge dq_n = {} & h^2 \sum_{i=1}^{s} \sum_{j=1}^{s} (b_i b_j - b_j a_{ji} - b_i a_{ij}) dk_i \wedge dl_j \\ & + h^2 \sum_{i=1}^{s} \sum_{j=1}^{s} (\bar{b}_i b_j - b_j \bar{a}_{ji} - \bar{b}_i a_{ij})(d\bar{k}_i \wedge dl_j) \end{aligned} \tag{2.25}$$

$$+h^2\sum_{i=1}^{s}\sum_{j=1}^{s}(\bar{b}_j b_i-\bar{b}_j a_{ji}-b_i\bar{a}_{ij})(dk_j\wedge d\bar{l}_i)$$

$$+h^2\sum_{i=1}^{s}\sum_{j=1}^{s}(\bar{b}_i\bar{b}_j-\bar{b}_i\bar{a}_{ij}-\bar{b}_j\bar{a}_{ji})d\bar{k}_i\wedge d\bar{l}_j\,,$$

Using the following substitutions

$$dp_n\wedge dl_j=d\Gamma_i\wedge dl_j-h\sum_j a_{ij}dk_j\wedge dl_j-h\sum\bar{a}_{ij}d\bar{k}_j\wedge dl_j\,, \tag{2.26}$$

$$dp_n\wedge d\bar{l}_j=d\Gamma_i\wedge d\bar{l}_j-h\sum_j a_{ij}dk_j\wedge d\bar{l}_j-h\sum\bar{a}_{ij}d\bar{k}_j\wedge d\bar{l}_j\,, \tag{2.27}$$

$$dk_i\wedge dq_n=dk_i\wedge d\Lambda_i-h\sum_j a_{ij}dk_i\wedge dl_j-h\sum\bar{a}_{ij}dk_i\wedge d\bar{l}_j\,, \tag{2.28}$$

$$d\bar{k}_i\wedge dq_n=d\bar{k}_i\wedge d\Lambda_i-h\sum_j a_{ij}d\bar{k}_i\wedge dl_j-h\sum\bar{a}_{ij}d\bar{k}_i\wedge d\bar{l}_j\,. \tag{2.29}$$

The simplified form of Equation (2.25) is obtained in view of Equations (2.26)–(2.29). Applying the criteria of the quadratic invariance as $dp_{n+1}\wedge dq_{n+1}=dp_n\wedge dq_n$ (Theorem 2.1). One can get the desired conditions of the theorem. From Equations (2.18)-(2.20), one stage symplectic pseudo-RK method can be obtained in form of Butcher array as

$$a_{11}=\frac{b_1}{2},\quad \bar{a}_{11}=\frac{\bar{b}_1}{2}$$

$$\begin{array}{c|c|c} c_1 & \frac{b_1}{2} & \frac{\bar{b}_1}{2} \\ \hline & b_1 & \bar{b}_1 \end{array}$$

For two stage symplectic pseudo RK method, Butcher array can be written as

$$\begin{array}{c|cc|cc} c_1 & \frac{b_1}{2} & 0 & \frac{\bar{b}_1}{2} & 0 \\ c_2 & b_1 & \frac{b_2}{2} & \bar{b}_1 & \frac{\bar{b}_2}{2} \\ \hline & b_1 & b_2 & \bar{b}_1 & \bar{b}_2 \end{array}$$

An example of 2-satge SPRKM is given by the following Bucher represntation.

$$\begin{array}{c|cc|cc}
\frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{8} & 0 \\
\frac{3}{8} & \frac{1}{4} & \frac{1}{8} & \frac{1}{4} & \frac{1}{8} \\
\hline
 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4}
\end{array}$$

Similarly, for s-stage SPRKM, Butcher array for the coefficient of symplectic pseudo-Runge-Kutta method can be represented as

$$\begin{array}{c|ccccc|ccccc}
 & \frac{b_1}{2} & 0 & 0 & \cdots & 0\ \ c_1\ \ c_2 & \frac{b_1}{2}\ \ c_1 & 0 & 0 & \cdots & 0 \\
c_2 & b_1 & \frac{b_2}{2} & 0 & \cdots & 0 & \bar{b}_1 & \frac{\bar{b}_2}{2} & 0 & \cdots & 0 \\
c_3 & b_1 & b_2 & \frac{b_3}{2} & \cdots & 0 & \bar{b}_1 & \bar{b}_2 & \frac{\bar{b}_3}{2} & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & b_1 & b_2 & b_3 & \cdots & \frac{b_s}{2} & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 & \cdots & \frac{\bar{b}_s}{2} \\
\hline
 & b_1 & b_2 & b_3 & \cdots & b_s & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 & \cdots & \bar{b}_s
\end{array}$$

This is the general s-stage structure-preserving PRKM (symplectic PRKM). It is not self- starting. Initially it requires $s+s=2s$ function evaluations and after the first iteration it requires s evaluations per step as s previous evaluations are already in memory.

2.2 Pseudo Runge-Kutta Nyström method (PRKNM) for second order IVP: In this section, we give a brief formulation of explicit pseudo-Runge-Kutta method of Nyström type to solve the second-order initial value problem

$$\frac{d^2u}{dx^2} = f(x,u), u(x_0) = u_0, u'(x_0) = u'_0 \ . \tag{2.30}$$

Likewise the method in Section (2.2.1), it is aslo not self-starting. For 2-stage method, it requires four slopes in the first step and from the second and onwards steps, it requires only two slopes (evaluation functions) per step. This shows that it incurs less computation cost than classical RKN method of order three as there will half number function evaluations aready in memory. Consider, 2-stage explicit pseudo-RK Nyström formula

(2.31) $$u_{n+1} = u_n + hu'_n + [b_1k_1 + \bar{b}_1\bar{k}_1 + b_2k_2 + \bar{b}_2\bar{k}_2)],$$

(2.32) $$u'_{n+1} = u'_n + \frac{1}{h}[B_1k_1 + \bar{B}_1\bar{k}_1 + B_2k_2 + \bar{B}_2\bar{k}_2],$$

where

$$k_1 = \frac{h^2}{2} f\left(x_n, u_n\right),$$

$$\bar{k}_1 = \frac{h^2}{2} f\left(x_{n-1}, u_{n-1}\right),$$

$$k_2 = \frac{h^2}{2} f\left(x_n + c_2h, u_n + c_2hu'_n + a_{21}k_1\right),$$

$$\bar{k}_2 = \frac{h^2}{2} f\left(x_{n-1} + c_2h, u_{n-1} + c_2hu'_{n-1} + \bar{a}_{21}\bar{k}_1\right).$$

The order conditions governing the coefficients can be found by expressing k_i and $\bar{k}_i$ as Taylor's series. Whose detailed derivation can be found in[13].

2.2.1 Structure prserving pseudo-Runge-Kutta Nyström method (SPRKNM) for second order IVP: Consider the system of differential equation of the special form[31]

(2.33) $$\frac{dp}{dt} = f(q), \frac{dq}{dt} = p = g(p),$$

which equivalently gives the second-order equations as $\frac{d^2q}{dt^2} = f(q)$, to solve this equation directly, PRKNM is aimed to develop. Further for the quadratic invariance of the numerical solution, SPRKNM is constructed. Rewriting the s-stage general PRKNM in functional form, we have

(2.34) $$Q_i = q_n + h\gamma_i p_n + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j) + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(\bar{Q}_j), i = 1, \ldots, s \ ,$$

(2.35) $$\bar{Q}_i = q_{n-1} + h\gamma_i p_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j) + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(\bar{Q}_j), i = 1, \ldots, s \quad ,$$

(2.36) $$p_{n+1} = p_n + h \sum_{j=1}^{s} b_i f(Q_i) + h \sum_{j=1}^{s} \bar{b}_i f(\bar{Q}_i)$$

(2.37) $$q_{n+1} = q_n + hp_n + h^2 \sum_{i=1}^{s} B_i f(Q_i) + h^2 \sum_{i=1}^{s} \bar{B}_i f(\bar{Q}_i), \ n \geq 0 .$$

Theorem 2.2.1: *If the coefficients of Equations (2.34)–(2.34) satisfy following order condidtions then the resulting PRKNM is symplectic*

(2.38) $$b_i - b_i \gamma_i - B_i = 0 ,$$

(2.39) $$\bar{b}_i - \bar{b}_i \gamma_i - \bar{B}_i = 0 ,$$

(2.40) $$b_i (B_j - a_{ij}) = b_j (B_i - a_{ji}) ,$$

(2.41) $$b_i (\bar{B}_j - \bar{a}_{ij}) = \bar{b}_j (B_i - a_{ji}) ,$$

(2.42) $$\bar{b}_i (\bar{B}_j - \bar{a}_{ij}) = \bar{b}_j (\bar{B}_i - \bar{a}_{ji}) .$$

Proof: Rewriting Equations (2.34)–(2.37), we have

(2.43) $$Q_i = q_n + h\gamma_i p_n + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j) + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(\bar{Q}_j), i = 1, \ldots, s ,$$

(2.44) $$\bar{Q}_i = q_{n-1} + h\gamma_i p_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j) + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(\bar{Q}_j), i = 1, \ldots, s ,$$

(2.45) $$p_{n+1} = p_n + h \sum_{j=1}^{s} b_i f(Q_i) + h \sum_{j=1}^{s} \bar{b}_i f(\bar{Q}_i) ,$$

(2.46) $$q_{n+1} = q_n + hp_n + h^2 \sum_{i=1}^{s} B_i f(Q_i) + h^2 \sum_{i=1}^{s} \bar{B}_i f(\bar{Q}_i), \ n \geq 0 .$$

Diffrentiating the external stages (2.45) and (2.46) and taking wedge product, we get
Where we use the notation of slopes as

(2.47) $$\begin{cases} k_i = f(Q_i) \\ \bar{k}_i = f(\bar{Q}_i), \end{cases}$$

(2.48) $$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n + h^2 \sum_{j=1}^{s} \left(B_i - b_i \gamma_i - b_i \right) dp_n \wedge dk_i$$

$$+ h^2 \sum_{j=1}^{s} \left(\bar{B}_i - \bar{b}_i \gamma_i - \bar{b}_i \right) dp_n \wedge d\bar{k}_i + h \sum_{j=1}^{s} b_i dk_i \wedge dQ_i$$

$$- h^3 \sum_{j=1}^{s} \left(a_{ij} b_i - a_{ji} b_j - b_i B_j + b_j B_i \right) dk_i \wedge dk_j$$

$$- h^3 \sum_{j=1}^{s} \left(b_i \bar{a}_{ij} - \bar{b}_i a_{ij} - b_i \bar{B}_j + \bar{b}_j B_i \right) dk_i \wedge d\bar{k}_j + h \sum_{j=1}^{s} \bar{b}_i d\bar{k}_i \wedge dQ_i$$

$$- h^3 \sum_{j=1}^{s} \left(\bar{a}_{ij} \bar{b}_i - \bar{a}_{ji} \bar{b}_j - \bar{b}_i \bar{B}_j + \bar{b}_j \bar{B}_i \right) d\bar{k}_i \wedge d\bar{k}_j .$$

Here, the form of Equation (2.48) is obtained using wedge product of the deriavtives of internal stages (2.43)-(2.44). From Equation (2.48), and using the criteria of syplecticity of Theorem (2.1), we get the desired order conditions (2.38-2.42) of the the theorem.
For 1-satge explicit symplectic pseudo-RKN method can be obtained by solving system of equations (2.38)-(2.42) under the assumpsions $a_{11} = 0$ and $\bar{a}_{11} = 0$, we get

$$B_1 = (1 - \gamma_1) b_1 \ , \ \bar{B}_1 = (1 - \gamma_1) \bar{b}_1 .$$

Butcher array can be written as

$$\begin{array}{c|c|c} & 0 & 0 \\ \gamma_1 & & \\ \hline & B_1 & \bar{B}_1 \\ \hline & b_1 & \bar{b}_1 \end{array}$$

If conditions of Theorem (2.2.1) are satisfied the at any step n Hamiltonian is preserved i. e. $H\left(p_{n+1},q_{n+1}\right)=H\left(p_n,q_n\right)$ at any iteration level *n*. For two stage explicit symplectic pseudo RK method, the system of equations (2.38)-(2.42) gives the valves of some parameters as (under the assumptions $a_{11}=a_{12}=a_{22}=0$ and $\bar{a}_{11}=\bar{a}_{12}=\bar{a}_{22}=0$),

$$B_1=\left(1-\gamma_1\right)b_1,\ B_2=\left(1-\gamma_2\right)b_2\ ,\ \bar{B}_1=\left(1-\gamma_1\right)\bar{b}_1,\ \bar{B}_2=\left(1-\gamma_2\right)\bar{b}_2\,.$$

and

$$a_{21}=\left(\gamma_1-\gamma_1\right)b_1,\ \bar{a}_{21}=\left(\gamma_1-\gamma_1\right)\bar{b}_1\,.$$

Butcher array representation of the method is given:

$$\begin{array}{c|cc|cc}
\gamma_1 & 0 & 0 & 0 & 0 \\
\gamma_2 & \left(\gamma_2-\gamma_1\right)b_1 & 0 & \left(\gamma_2-\gamma_1\right)\bar{b}_1 & 0 \\
\hline
 & B_1 & B_2 & \bar{B}_1 & \bar{B}_2 \\
\hline
 & b_1 & b_2 & \bar{b}_1 & \bar{b}_2
\end{array}$$

3. Conclusion

In this paper, we have proposed two qualitative numerical methods: symplectic pseudo-Runge-Kutta method and symplectic pseudo-Runge-Kutta Nyström method. We have derived the sufficient conditions for symplecticness. These methods preserve the area and preserve the total energy (Hamiltonian) when applied to the Hamiltonian system of equations. The Hamiltonian system of equations frequently occurs in the field of celestial mechanics, physics, chemistry and various branches of engineering. Thus the proposed methods are suitable to solve Hamiltonian systems along with the fact that the total sum of energy at any step (iteration) of the numerical solution is preserved. But, these methods fail to integrate efficiently the Hamiltonian system of equations whose solution is exponential or trigonometric. So the development of pseudo type structure-preserving RK method, which is best tuned to solve the Hamiltonian system of equations having exponential/trigonometric solutions, will be the aim of research in this direction.

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