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EXPLICIT CANONICAL METHODS FOR HAMILTONIAN SYSTEMS

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ABSTRACT. We consider canonical partitioned Runge-Kutta methods for separable Hamiltonians $H = T(p) + V(q)$ and canonical Runge-Kutta-Nyström methods for Hamiltonians of the form $H = \frac{1}{2}p^T M^{-1} p + V(q)$ with M a diagonal matrix. We show that for explicit methods there is great simplification in their structure. Canonical methods of orders one through four are constructed. Numerical experiments indicate the suitability of canonical numerical schemes for long-time integrations.

1. INTRODUCTION

Time-independent Hamiltonian systems are of the form

$$\frac{d}{dt}q_i = \frac{\partial H}{\partial p_i}(q, p), \qquad \frac{d}{dt}p_i = -\frac{\partial H}{\partial q_i}(q, p), \tag{1}$$

where $p, q \in \mathbf{R}^N$ and the Hamiltonian function H is a continuously differentiable function of the generalized coordinates q and the generalized momenta p. The $2N$-dimensional space with coordinates $q_1, q_2, \dots, q_N, p_1, p_2, \dots, p_N$ is the phase space of the system. Let $z = \binom{q}{p}$. A transformation $z \to \bar{z}$ is said to be canonical if $(\frac{\partial \bar{z}}{\partial z})^T J (\frac{\partial \bar{z}}{\partial z}) = J$, where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.

The phase flow of (1),

$$G_t : \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} \mapsto \begin{pmatrix} q(t) \\ p(t) \end{pmatrix},$$

is a one-parameter group of transformations of phase space. The transformation G_t is canonical and by Liouville's theorem preserves volume in phase space, an important property of (1). The same is true of all canonical transformations. In terms of differential forms, the flow preserves the differential 2-form $\omega = \sum dq^i \wedge dp^i$ (that is, the sum of areas of projections of any two-dimensional surface S in phase space onto the q_i-p_i planes), and all powers of ω, whose integrals are the Poincaré invariants [1, 6]. In numerically solving (1), it may be important for the numerical integrators to be canonical so that, in particular,

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volume in phase space is preserved. This requirement was first considered by DeVogelaere (cf. [3]) and in a published paper by Ruth [11]. For information about the history of canonical numerical integrators, see [3] and its references.

A separable Hamiltonian has the form $H(q, p) = T(p) + V(q)$, where $T(p)$ and $V(q)$ are kinetic and potential energies, respectively. In this paper, we consider the case where $T(p) = \frac{1}{2}p^{\mathrm{T}}M^{-1}p$ with M a diagonal matrix, and the resulting Hamiltonian system

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -\frac{\partial V}{\partial q} \tag{2}$$

is one describing the motion of $\frac{N}{3}$ particles. Examples of (2) abound in molecular dynamics, astronomy, etc.

The system (2) can be written as a second-order system thus:

$$\ddot{q} = -M^{-1}\frac{\partial V}{\partial q} = f(q). \tag{3}$$

Suris [14] examined Runge-Kutta-Nyström (RKN) methods for (3) and obtained, using matrix algebra, the conditions for it to be canonical.

In our earlier paper [9], we obtained the same conditions using exterior forms. Furthermore, we showed that an explicit RKN method is canonical if and only if its adjoint is explicit. This paper builds on that work by using it to construct explicit schemes for (2). Section 2 gives a brief description of existing results for canonical Runge-Kutta-Nyström methods and shows that for explicit methods there is great simplification in their structure. Section 3 details the construction of methods of orders one through four. Section 4 reviews partitioned Runge-Kutta (pRK) methods for separable Hamiltonians proposed by Sanz-Serna [12] and shows again the simplification that occurs for explicit methods. Section 5 considers numerical illustrations.

2. Canonical Runge-Kutta-Nyström methods

We associate with any given (one-step) method a mapping

$$\Phi\colon z_n, h, H(p, q) \mapsto z_{n+1}, \tag{4}$$

where h is the time step. This gives a transformation of z from time t_n to t_{n+1}. A method is said to be canonical if $\Phi = \Phi_h$ is a canonical mapping for any Hamiltonian H and stepsize h. The method is of order p if Φ_h differs from the phase flow G_h by $O(h^{p+1})$. It is becoming increasingly evident through numerical experiments [3, 12] that the dynamics of canonical Φ_h and G_h are closely related in long-time integrations. For details of the advantages of canonical Φ_h over classical (noncanonical) methods, see [12]. In writing a method in the form (4), different methods may yield the same mapping Φ_h. We shall identify a method with its Φ_h *and* the details of its internal stages. Since different methods may give the same mapping Φ_h, it is essential to introduce the concepts of equivalence and redundancy. Two methods are said to be *equivalent* if their corresponding mappings Φ_h are identical. A method may be equivalent to a method of a lesser stage number. In this case, the method is regarded as *redundant*.

An s-stage Runge-Kutta-Nyström method for (3) is given by

$$
\begin{aligned}
y_i &= q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{s} a_{ij} f(y_j), \qquad i = 1, 2, \ldots, s,\\
q_{n+1} &= q_n + h\dot{q}_n + h^2 \sum_{i=1}^{s} b_i f(y_i), \qquad (5)\\
\dot{q}_{n+1} &= \dot{q}_n + h \sum_{i=1}^{s} B_i f(y_i).
\end{aligned}
$$

Naturally, we define $z_n = \binom{q_n}{M\dot{q}_n}$. The corresponding tableau [2, 8] is:

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s}\\
c_2 & a_{21} & a_{22} & \cdots & a_{2s}\\
\vdots & \vdots & \vdots & & \vdots\\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss}\\
\hline
 & b_1 & b_2 & \cdots & b_s\\
 & B_1 & B_2 & \cdots & B_s
\end{array}
$$

If we interchange z_n and h with z_{n+1} and $-h$, respectively, in (4), we get the adjoint method [8]. Following are the coefficients of the adjoint method of (5):

$$
\begin{aligned}
\tilde{c}_i &= 1 - c_{s+1-i},\\
\tilde{a}_{ij} &= B_{s+1-j} - b_{s+1-j} - c_{s+1-i}B_{s+1-j} + a_{s+1-i,s+1-j}, \qquad (6)\\
\tilde{b}_j &= B_{s+1-j} - b_{s+1-j}, \qquad i \le i, j \le s,\\
\widetilde{B}_j &= B_{s+1-j}.
\end{aligned}
$$

A method is time-reversible if $\tilde{c}_i = c_i$, $\tilde{a}_{ij} = a_{ij}$, $\tilde{b}_i = b_i$, and $\widetilde{B}_i = B_i$. We now give the conditions for an RKN method to be canonical, which are found in [9, 14].

Theorem 1 (Suris [14]). *An s-stage RKN is canonical if and only if*

$$b_i - B_i + c_i B_i = 0, \qquad 1 \le i \le s, \tag{7a}$$

$$-B_j a_{ji} + B_i a_{ij} + B_j b_i - B_i b_j = 0, \qquad 1 \le i < j \le s. \tag{7b}$$

An RKN method is explicit if $a_{ij} = 0$ for $j \ge i$. For an explicit RKN method, equation (7b) reduces to

$$B_i a_{ij} + B_j b_i - B_i b_j = 0, \qquad j < i. \tag{8}$$

From equations (7a) and (8), we get

(9a) $$b_i = B_i(1-c_i),$$

(9b) $$B_i a_{ij} = B_i B_j(c_i - c_j), \qquad j < i.$$

We would like to conclude from the second of these two that $a_{ij} = B_j(c_i - c_j)$, but that would not be quite correct. What can be proved is that the method is *equivalent* to one with this choice for a_{ij}.

Lemma 1. *An explicit canonical* $(r+1)$*-stage RKN method* (5) *is equivalent to*

(10)
$$\begin{aligned}
y_i &= q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{i-1} a_{ij} f(y_j), \qquad i = 1, 2, \ldots, r, \\
y_{r+1} &= q_n + c_{r+1} h\dot{q}_n + h^2 \sum_{j=1}^{r} B_j(c_{r+1} - c_j) f(y_j), \\
q_{n+1} &= q_n + h\dot{q}_n + h^2 \sum_{i=1}^{r+1} B_i(1-c_i) f(y_i), \\
\dot{q}_{n+1} &= \dot{q}_n + h \sum_{i=1}^{r+1} B_i f(y_i).
\end{aligned}$$

Proof. It is enough to show that

$$\begin{aligned}
&B_{r+1} f\left(q_n + c_{r+1} h\dot{q}_n + h^2 \sum_{j=1}^{r} B_j(c_{r+1} - c_j) f(y_j)\right) \\
&\qquad = B_{r+1} f\left(q_n + c_{r+1} h\dot{q}_n + h^2 \sum_{j=1}^{r} a_{r+1,j} f(y_j)\right).
\end{aligned}$$

From (9b),

$$\text{either} \quad B_{r+1} = 0 \quad \text{or} \quad a_{r+1,j} = B_j(c_{r+1} - c_j), \qquad j < r+1,$$

and the result follows. □

Theorem 2. *An explicit canonical RKN method is equivalent to*

(11)
$$\begin{aligned}
y_i &= q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{i-1} B_j(c_i - c_j) f(y_j), \qquad i = 1, 2, \ldots, s, \\
q_{n+1} &= q_n + h\dot{q}_n + h^2 \sum_{i=1}^{s} B_i(1-c_i) f(y_i), \\
\dot{q}_{n+1} &= \dot{q}_n + h \sum_{i=1}^{s} B_i f(y_i).
\end{aligned}$$

Proof. Repeatedly apply Lemma 1 and use the fact that each embedded method, namely

$$
\begin{array}{c|ccccc}
c_1 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_r & a_{r1} & a_{r2} & \cdots & a_{r,r-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{r-1} & b_r \\
 & B_1 & B_2 & \cdots & B_{r-1} & B_r
\end{array}
$$

is itself canonical. □

The only free parameters for a canonical explicit RKN method are therefore B_i and c_i. The form (11) of writing an explicit canonical RKN method enables us to prove the following propositions. The first proposition shows that a canonical explicit RKN method requires minimal possible storage of any method.

Proposition 1. *The explicit canonical RKN method* (11) *can be expressed as*

$$
\begin{aligned}
&y_0 = q_n, \\
&\dot{y}_n = \dot{q}_n, \\
&\textit{for } i = 1, 2, \ldots, s \\
&\qquad y_i = y_{i-1} + h(c_i - c_{i-1})\dot{y}_{i-1}, \qquad \textit{where } c_0 = 0, \\
&\qquad \dot{y}_i = \dot{y}_{i-1} + hB_i f(y_i), \\
&q_{n+1} = y_s + h(1 - c_s)\dot{y}_s, \\
&\dot{q}_{n+1} = \dot{y}_s.
\end{aligned}
$$

Proof. We can always write down the above method. We need to show that it computes the same $(q_{n+1}, \dot{q}_{n+1})$ as (5):

$$
\begin{aligned}
\dot{y}_i &= \dot{q}_n + h\sum_{j=1}^{i} B_j f(y_j), \\
y_i &= q_n + h\sum_{k=1}^{i}(c_k - c_{k-1})\dot{y}_{k-1} \\
&= q_n + h(c_i - c_0)\dot{q}_n + h^2\sum_{k=1}^{i}(c_k - c_{k-1})\sum_{j=1}^{k-1} B_j f(y_j) \\
&= q_n + hc_i\dot{q}_n + h^2\sum_{j=1}^{i-1}(c_i - c_j)B_j f(y_j) \\
&= q_n + hc_i\dot{q}_n + h^2\sum_{j=1}^{i-1} a_{ij} f(y_j),
\end{aligned}
$$

$$\dot{q}_{n+1} = \dot{q}_n + h \sum_{j=1}^{s} B_j f(y_j),$$

$$\begin{aligned} q_{n+1} &= q_n + hc_s\dot{q}_n + h^2 \sum_{j=1}^{s-1} a_{sj} f(y_j) + h(1-c_s) \\ &\quad \times \left(\dot{q}_n + h \sum_{j=1}^{i} B_j f(y_j) \right) \\ &= q_n + h\dot{q}_n + h^2 \sum_{j=1}^{s} (B_j c_s - B_j c_j + (1-c_s)B_j) \\ &= q_n + h\dot{q}_n + h^2 \sum_{j=1}^{s} b_j f(y_j). \quad \square \end{aligned}$$

From Proposition 1, if either $c_i = c_{i-1}$ or $B_i = 0$, then the ith stage is redundant, and hence the following assertion.

Proposition 2. *A nonredundant explicit canonical RKN method has* $B_i \neq 0$, $i = 1, 2, \ldots, s$, *and* $c_i \neq c_{i-1}$, $i = 2, 3, \ldots, s$.

Suris, in his paper [13], showed that an explicit RKN method is Liouville (i.e., volume preserving) if and only if its adjoint is *equivalent to* an explicit method. Canonical RKN methods form a subset of Liouville RKN methods. For example, explicit 2-stage RKN methods require $c_1 = c_2$ or $B_2 a_{21} + B_2 b_1 - B_1 b_2$ to be Liouville. What this means is that if we choose c_1 so that it is equal to c_2, then the method is Liouville but may or may not be canonical. The method

$$\begin{array}{c|cc} \frac{1}{2} & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & \frac{1}{4} & \frac{1}{4} \\ & \frac{1}{2} & \frac{1}{2} \end{array}$$

is Liouville but not canonical. The following results are found in [9].

Theorem 3. *If a method is canonical, then its adjoint is canonical.*

Theorem 4. *An explicit RKN method is canonical if and only if its adjoint is explicit.*

A corollary of Theorem 4 is

Corollary 1. *If an explicit RKN method is equal to its adjoint (symmetric), then it is canonical.*

Because the adjoint of an explicit canonical RKN method is explicit, it can be expressed entirely in terms of its coefficients $\widetilde{B}_i$ and $\tilde{c}_i$. These are given by (6) as

$$\tilde{c}_i = 1 - c_{s+1-i}, \qquad \widetilde{B}_j = B_{s+1-j}. \tag{12}$$

3. Construction of canonical RKN methods

Order conditions for RKN methods are specified in [8] for q and $\dot{q}$ involving b_i and B_i. To construct explicit canonical RKN methods, we need only satisfy the conditions involving B_i. This is because $b_i = B_i(1 - c_i)$ for canonical methods, and according to [8, p. 268] the other order conditions, involving b_i, are automatically satisfied. For an s-stage canonical RKN method we are left with the following conditions. The first-order condition is

$$\sum B_i = 1. \tag{13}$$

In addition to the first-order condition, the second-order conditions are

$$\sum B_i c_i = \tfrac{1}{2}. \tag{14}$$

The third-order conditions, in addition to the first- and second-order conditions, are

$$\sum B_i c_i^2 = \tfrac{1}{3}, \tag{15a}$$

$$\sum\sum B_i a_{ij} = \sum\sum_{j<i} B_i B_j (c_i - c_i) = \tfrac{1}{6}. \tag{15b}$$

Finally, the fourth-order conditions, in addition to first-, second-, and third-order conditions, are

$$\sum B_i c_i^3 = \tfrac{1}{4}, \tag{16a}$$

$$\sum\sum B_i c_i a_{ij} = \sum\sum_{j<i} B_i B_j c_i (c_i - c_j) = \tfrac{1}{8}, \tag{16b}$$

$$\sum\sum B_i a_{ij} c_j = \sum\sum_{j<i} B_i B_j (c_i - c_j) c_j = \tfrac{1}{24}. \tag{16c}$$

The last of these turns out to be superfluous because we have

$$\begin{aligned}\sum\sum_{j<i} B_i B_j (c_i - c_j) c_j &= -\sum\sum_{j<i} B_i B_j c_i (c_i - c_j) \\ &= \sum\sum_{j<i} B_i B_j c_i (c_i - c_j) - \sum\sum B_i B_j c_i (c_i - c_j) \\ &= \tfrac{1}{8} - (\tfrac{1}{3} \cdot 1 - \tfrac{1}{2} \cdot \tfrac{1}{2}) = \tfrac{1}{24},\end{aligned}$$

if all the others are satisfied.

There is no limit to the order attainable by a canonical explicit RKN method. By means of a Lie group analysis, Yoshida [15] gives a construction of a 3^n-stage method of order $2n + 2$ for any n. See also Forest and Ruth [4].

3.1. **One-stage methods.** There is a one-parameter family of canonical explicit 1-stage RKN methods of order 1: c_1 is the free parameter, $B_1 = 1$. Imposing the second-order condition gives a canonical 1-stage RKN method of order 2 with $c_1 = \frac{1}{2}$. This is equivalent to the Störmer, "leapfrog," or Verlet method commonly used for solving Newton's equations of motion occurring in molecular dynamics.

3.2. **Two-stage methods.** We have a two-parameter family of canonical explicit 2-stage RKN methods of order 2, namely,

$$c_1 = \tfrac{1}{2} + \alpha, \quad c_2 = \tfrac{1}{2} + \beta, \quad B_1 = \frac{\beta}{\beta - \alpha}, \quad B_2 = \frac{-\alpha}{\beta - \alpha}, \qquad \alpha \neq \beta.$$

A simple choice for α and β results in the method

$$\begin{array}{c|cc} 0 & & \\ 1 & \tfrac{1}{2} & \\ \hline & \tfrac{1}{2} & 0 \\ & \tfrac{1}{2} & \tfrac{1}{2} \end{array}$$

This is another form of the Störmer-Verlet method. The only explicit 2-stage RKN of order 3 that is canonical has imaginary coefficients, which are difficult to work with.

3.3. **Three-stage methods.** Imposing third-order conditions, except for (16b) and canonical conditions, we obtain a three-parameter family of explicit 3-stage Runge-Kutta-Nyström methods with the coefficients

$$c_1 = \frac{1}{2} + \alpha, \quad c_2 = \frac{1}{2} + \beta, \quad c_3 = \frac{1}{2} + \gamma,$$
$$B_1 = \frac{\frac{1}{2} + \beta\gamma}{(\beta - \alpha)(\gamma - \alpha)}, \quad B_2 = -\frac{\frac{1}{12} + \alpha\gamma}{(\beta - \alpha)(\gamma - \beta)}, \quad B_3 = \frac{\frac{1}{12} + \alpha\beta}{(\gamma - \alpha)(\gamma - \beta)},$$

where α, β, and γ are all distinct. Through (16b), the parameters α, β, and γ are constrained by the following nonlinear equation:

$$1 + 24\alpha\gamma + 24(\beta - \alpha)(\gamma - \alpha)(\gamma - \beta) + 144\alpha\beta\gamma(\alpha + \gamma - \beta) = 0. \tag{17}$$

If $\gamma = \alpha$, that is, $c_1 = c_3$, then from equations (14) and (15) we get

$$B_1 + B_3 = \frac{c_2 - \frac{1}{2}}{c_2 - c_1}, \qquad B_2 = \frac{\frac{1}{2} - c_1}{c_2 - c_1}. \tag{18}$$

With this, the order condition (16b) reduces to

$$(\tfrac{1}{2} - c_1)(B_1 - B_3) = \tfrac{1}{6}. \tag{19}$$

Combining (18) and (19), we solve for the coefficients to obtain a two-parameter family of 3-stage RKN methods. The coefficients are

$$c_1 = \frac{1}{2} + \alpha, \quad c_2 = \frac{1}{2} + \beta, \quad c_3 = \frac{1}{2} + \alpha,$$
$$B_1 = \frac{\beta}{2(\beta - \alpha)} - \frac{1}{12\alpha}, \quad B_2 = -\frac{\alpha}{(\beta - \alpha)}, \quad B_3 = \frac{\beta}{2(\beta - \alpha)} + \frac{1}{12\alpha},$$

where $\alpha \neq \beta$ and $\alpha \neq 0$. Condition (16a) constrains the parameters α and β by $\frac{1}{12} + \alpha\beta = 0$ and makes the method of order 3.

For a symmetric canonical explicit 3-stage RKN method (that is, an RKN method which is equal to its adjoint), it is sufficient to impose in addition to (17) only two conditions, namely, $\alpha = -\gamma$ and $\beta = 0$. Solving for the coefficients, we have

$$c_1 = \frac{1}{2} - \gamma, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{1}{2} + \gamma,$$
$$B_1 = \frac{1}{24\gamma^2}, \quad B_2 = 1 - \frac{1}{12\gamma^2}, \quad B_3 = \frac{1}{24\gamma^2},$$

where γ is a zero of $p(x) = 48x^3 - 24x^2 + 1$. The only real zero of this polynomial is $\frac{1}{12}(2 - \sqrt[3]{4} - \sqrt[3]{16}) \approx -0.1756035959798288$. It is easily verified from (16a), (16b), and (16c) that this is a symmetric canonical 3-stage RKN method of order four (we use the acronym SYRKN for this method). This 3-stage fourth-order method was apparently [15] first discovered by E. Forest and first published by Forest and Ruth [4].

4. Partitioned RK methods

Consider a separable Hamiltonian system

$$\dot{q} = \frac{\partial T}{\partial p} = G(p), \quad \dot{p} = -\frac{\partial V}{\partial q} = F(q). \tag{20}$$

In what follows, we give an overview of partitioned Runge-Kutta (pRK) methods for (20), proposed by Sanz-Serna [12], an approach which is actually a generalization of a 3-stage RK method obtained by Ruth [11] using generating functions via Hamilton-Jacobi equations. Sanz-Serna [12] considered 3-stage, and Qin and Zhang [10] considered 4-stage, pRK methods of order four. Here, we provide results concerning this class of methods.

Definition 1 (Sanz-Serna [12]). An s-stage partitioned RK method is

$$\begin{aligned} Y_i &= q_n + h\sum_j a_{ij}G(Z_j), & Z_i &= p_n + h\sum_j A_{ij}F(Y_j), \\ q_{n+1} &= q_n + h\sum_i b_iG(Z_i), & p_{n+1} &= p_n + h\sum_i B_iF(Y_i). \end{aligned} \tag{21}$$

Note that this formalism includes those pRK methods that use an unequal number of G and F evaluations to take one step; it is only necessary to insert appropriate dummy stages. A pRK method is said to be explicit if $a_{ij} = 0$ for $j > i$ and $A_{ij} = 0$ for $j \geq i$. It is true that there are methods equivalent to explicit methods which do not satisfy this. However, for simplicity we shall restrict the term "explicit" to methods of this form. The Butcher array for a partitioned RK method is

$$\begin{array}{c|c} & a \\ \hline & b \end{array} \qquad \begin{array}{c|c} & A \\ \hline & B \end{array}$$

Sanz-Serna in his paper [12] showed that method (21) is canonical if

$$B_j a_{ji} + b_i A_{ij} - B_j b_i = 0, \qquad 1 \leq i, j \leq s. \tag{22}$$

As pointed out in [12], if we define $\overline{q}(\overline{t}) = p(-\overline{t})$ and $\overline{p}(\overline{t}) = q(-\overline{t})$, these satisfy a Hamiltonian system with Hamiltonian $\overline{H}(\overline{q}, \overline{p}) = H(\overline{p}, \overline{q})$. If we apply a one-step method to this transformed system, we get equations for $\overline{q}_{n+1}$ and $\overline{p}_{n+1}$ in terms of $\overline{q}_n$ and $\overline{p}_n$. For these numerically determined values we could then undo the transformation by the substitutions $\overline{q}_{n+1} \to p_n$, $\overline{p}_{n+1} \to q_n$, $\overline{q}_n \to p_{n+1}$, $\overline{p}_n \to q_{n+1}$, and $\overline{H}(\overline{q}, \overline{p}) \to H(\overline{p}, \overline{q})$. It turns out that q_{n+1} and p_{n+1} are given in terms of q_n and p_n by a pRK method with coefficients

$$\begin{aligned} \tilde{a}_{ij} &= B_{s+1-j} - A_{s+1-i,s+1-j}, & \tilde{b}_j &= B_{s+1-j}, \\ \widetilde{A}_{ij} &= b_{s+1-j} - a_{s+1-i,s+1-j}, & \widetilde{B}_j &= b_{s+1-j}. \end{aligned}$$

We call this the *G-adjoint* method. A *G*-symmetric method is one which is equal to its G-adjoint. It satisfies conditions which reduce to

$$\left.\begin{aligned} a_{ij} &= b_j - A_{s+1-i,s+1-j}, \\ A_{ij} &= B_j - a_{s+1-i,s+1-j}, \end{aligned}\right. \qquad 1 \le i, j \le s.$$

The justification for a G-symmetric method is that if a problem has two equivalent formulations, then it seems desirable that a method applied to both formulations should yield equivalent solutions.

If we impose canonical conditions (22) on an explicit pRK method, we have

$$(23) \qquad B_i a_{ij} = B_i b_j \quad \text{for } j \le i, \qquad b_i A_{ij} = b_i B_j \quad \text{for } j < i, \qquad 1 \le i \le s.$$

As with RKN methods, we cannot conclude that $a_{ij} = b_j$, nor that $A_{ij} = B_j$, but we can prove that the method is equivalent to one with this choice of coefficients. Such a choice is mentioned in [12].

Lemma 2. *Let*

$$\begin{array}{c|c} & a \\ \hline & b \end{array} \qquad \begin{array}{c|c} & A \\ \hline & B \end{array}$$

be an explicit canonical $(r+1)$*-stage pRK method. This is equivalent to*

$$\begin{array}{c|ccc|c} & a_{11} & \cdots & a_{1r} & 0 \\ & \vdots & & \vdots & \vdots \\ & a_{r1} & \cdots & a_{rr} & 0 \\ \hline & b_1 & \cdots & b_r & b_{r+1} \\ \hline & b_1 & \cdots & b_r & b_{r+1} \end{array} \qquad \begin{array}{c|ccc|c} & A_{11} & \cdots & A_{1r} & 0 \\ & \vdots & & \vdots & \vdots \\ & A_{r1} & \cdots & A_{rr} & 0 \\ \hline & B_1 & \cdots & B_r & 0 \\ \hline & B_1 & \cdots & B_r & B_{r+1} \end{array}$$

Proof. It is enough to show that

$$b_{r+1} G\left(p_n + h \sum_{j=1}^{r} A_{r+1,j} F_j\right) = b_{r+1} G\left(p_n + h \sum_{j=1}^{r} B_j F_j\right),$$

and

$$B_{r+1}F\left(q_n + h\sum_{j=1}^{r+1} a_{r+1,j}G_j\right) = B_{r+1}F\left(q_n + h\sum_{j=1}^{r+1} b_jG_j\right).$$

From (23) we know that

$$\text{either} \quad b_{r+1} = 0 \quad \text{or} \quad A_{r+1,j} = B_j, \qquad j < r+1,$$

and

$$\text{either} \quad B_{r+1} = 0 \quad \text{or} \quad a_{r+1,j} = b_j, \qquad j \le r+1. \quad \square$$

Theorem 5. *An explicit canonical pRK method*

$$\begin{array}{c|c} & a \\ \hline & b \end{array} \qquad \begin{array}{c|c} & A \\ \hline & B \end{array}$$

is equivalent to

$$\begin{array}{c|ccccc} & b_1 & & & & \\ & b_1 & b_2 & & & \\ & b_1 & b_2 & b_3 & & \\ & \vdots & \vdots & \ddots & \ddots & \\ & b_1 & b_2 & \cdots & b_{s-1} & b_s \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array} \qquad \begin{array}{c|ccccc} & 0 & & & & \\ & B_1 & 0 & & & \\ & B_1 & B_2 & 0 & & \\ & \vdots & \vdots & \ddots & \ddots & \\ & B_1 & B_2 & \cdots & B_{s-1} & 0 \\ \hline & B_1 & B_2 & \cdots & B_{s-1} & B_s \end{array}$$

Proof. Repeatedly apply Lemma 2. □

Without loss of generality, the algorithm for an explicit canonical pRK method can be written as

$$\begin{aligned} &Y_0 = q_n, \\ &Z_1 = p_n, \\ &\text{for } i = 1, 2, \dots, s \\ &\qquad Y_i = Y_{i-1} + hb_iG(Z_i), \\ &\qquad Z_{i+1} = Z_i + hB_iF(Y_i), \\ &q_{n+1} = Y_s, \\ &p_{n+1} = Z_{s+1}. \end{aligned}$$

Note that this algorithm requires minimal possible storage.

There is an obvious correspondence between this and the algorithm of Proposition 1. Every explicit canonical r-stage RKN method comes from an explicit canonical $(r+1)$-stage pRK method with B_i the same for $i = 1, 2, \dots, r$ and $B_{r+1} = 0$, and with $b_i = c_i - c_{i-1}$ for $i = 1, 2, \dots, r, r+1$, where $c_0 = 0$ and $c_{r+1} = 1$. (If $c_r = 1$, then the $(r+1)$st stage is not needed.) We can characterize either an explicit RKN or an explicit pRK method in terms of parameters

$$\begin{array}{lllll} b: & b_1 & b_2 & \cdots & b_s \\ B: & B_1 & B_2 & \cdots & B_s \end{array}$$

rather than the Butcher tableau. The G-adjoint of the explicit pRK method above has parameters

$$\begin{array}{lllll} \tilde{b}: & B_s & B_{s-1} & \cdots & B_1 \\ \widetilde{B}: & b_s & b_{s-1} & \cdots & b_1 . \end{array}$$

The adjoint has parameters

$$\begin{array}{llllll} \tilde{b}: & 0 & b_s & b_{s-1} & \cdots & b_1 \\ \widetilde{B}: & B_s & B_{s-1} & \cdots & B_1 & 0 . \end{array}$$

For the special case $T(p) = \frac{1}{2}p^{\mathrm{T}}M^{-1}p$ we have available the explicit RKN order conditions in terms of c_i and B_i, where $c_i = \sum_{j=1}^{i} b_i$ *if* we assume that $\sum_{j=1}^{s} b_j = 1$ (which is needed for consistency).

Sanz-Serna [12] has suggested a concatenation of a G-symmetric 3-stage pRK method of order 3,

$$\begin{array}{llll} b: & 0.268330 & -0.187992 & 0.919662 \\ B: & 0.919662 & -0.187992 & 0.268330, \end{array}$$

with its adjoint method to get a method of order 4 (we give it the acronym SYPRK1):

$$\begin{array}{lllllll} b: & 0.134165 & -0.093996 & 0.459831 & 0.459831 & -0.093996 & 0.134165 \\ B: & 0.459831 & -0.093996 & 0.268330 & -0.093996 & 0.459831 & 0. \end{array}$$

(These coefficients are approximate.) We suggest another method which is a concatenation of a method obtained by Ruth [11], namely,

$$\begin{array}{llll} b: & \frac{7}{24} & \frac{3}{4} & -\frac{1}{24} \\ B: & \frac{2}{3} & -\frac{2}{3} & 1, \end{array}$$

and its adjoint. The result of this concatenation is a method of order 4 (acronym: SYPRK2):

$$\begin{array}{lllllll} b: & \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & \frac{7}{48} \\ B: & \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0 \end{array}$$

5. Numerical experiments

For illustrative purposes, we consider two well-known Hamiltonians, the Hénon-Heiles and a Kepler Hamiltonian. The experiments considered are not exhaustive and do not erase all doubts about the advantages of canonical over noncanonical schemes. More work needs to be done. For these experiments we consider also a noncanonical RKN of order four (acronym: NCRKN) obtained from [8, p. 262].

5.1. **Hénon-Heiles Hamiltonian.** In the process of investigating the existence of a third isolating integral of galactic motion in celestial mechanics, Hénon and Heiles [7] approximated the Hamiltonian, and hence the total energy, by

$$H = \tfrac{1}{2}(p_1^2 + p_2^2) + \tfrac{1}{2}(q_1^2 + q_2^2 + 2q_1^2 q_2 - \tfrac{2}{3}q_2^3).$$

Hénon and Heiles found that a third integral exists only at low energy. For energies higher than $\frac{1}{8}$, the system exhibits a chaotic behavior. The reason for considering it here is numerical and has nothing to do with theoretical questions. Hénon and Heiles [7] in their experiments considered the intersections of the trajectory with the plane $q_1 = 0$. They plotted the values of q_2 and p_2 at these intersections in the (q_2, p_2)-plane. We shall do likewise, in addition to the quantities computed by Sanz-Serna [12].

Similar to [3], we choose $(q_1, q_2, p_1, p_2) = (0.12, 0.12, 0.12, 0.12)$, giving an energy of 0.029952. The solution is computed for $1{,}200{,}000$ time steps, with the time step being $\frac{1}{6}$. Figure 1 depicts the Poincaré sections of the

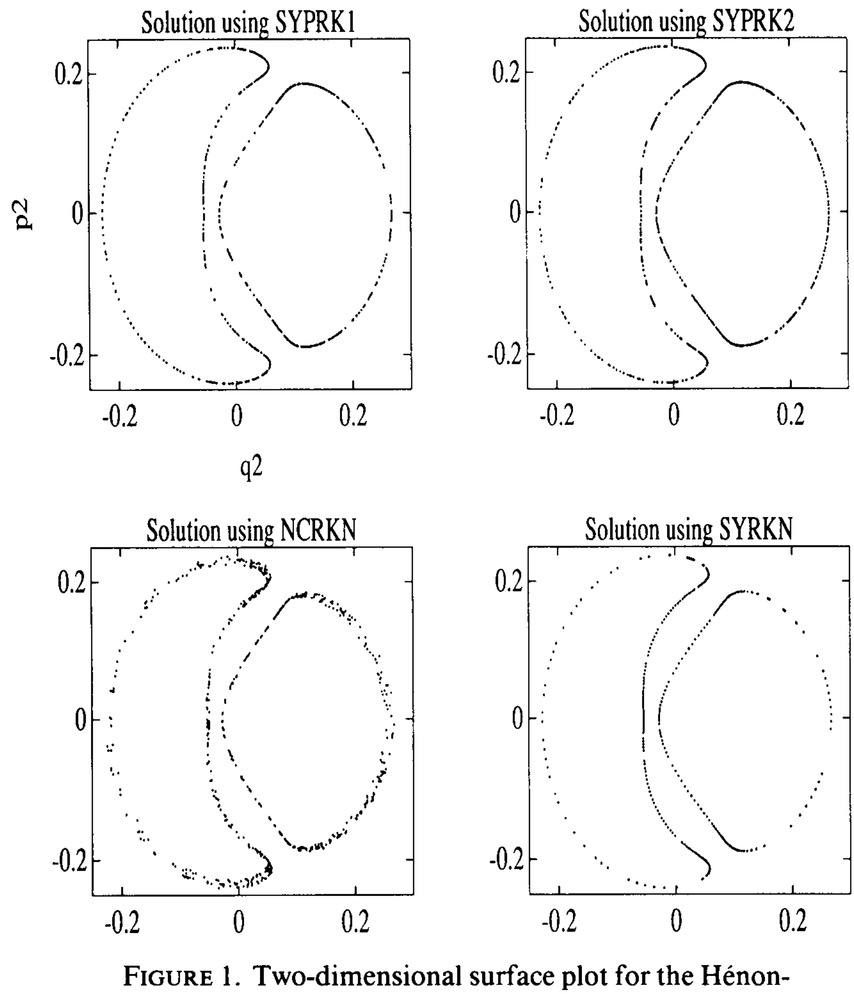

FIGURE 1. Two-dimensional surface plot for the Hénon-Heiles problem using canonical and noncanonical methods $(H = 0.029952)$

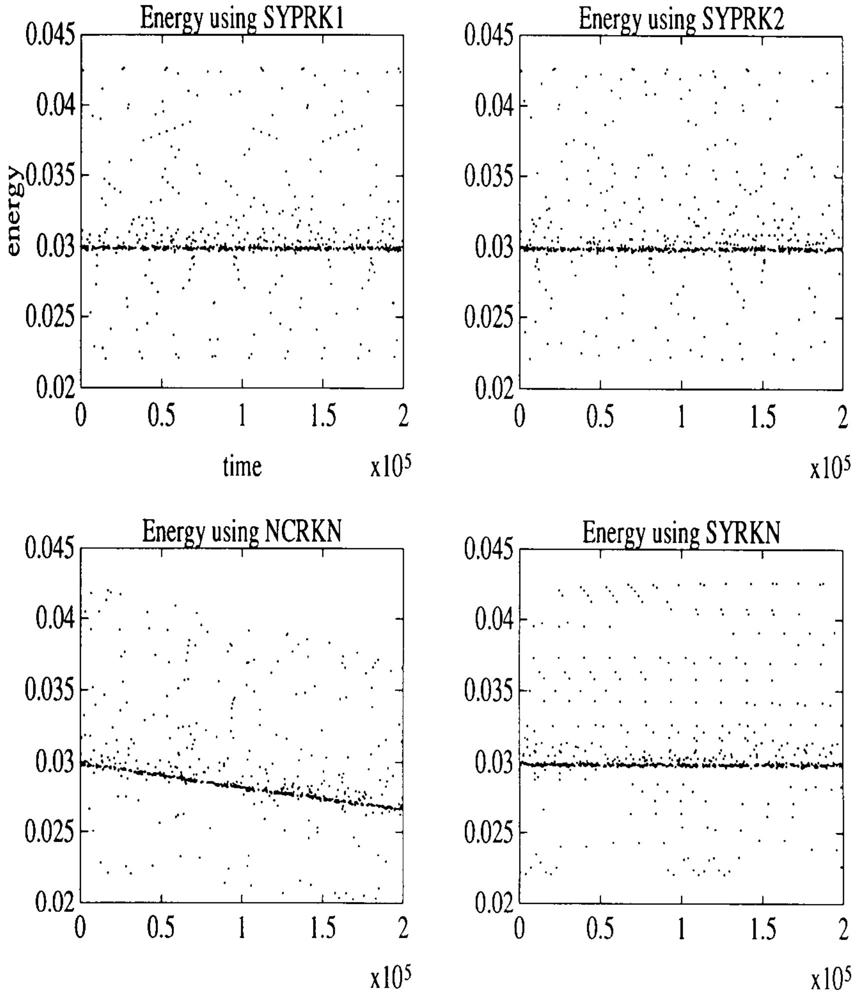

FIGURE 2. Energy plots for the Hénon-Heiles problem using canonical and noncanonical methods ($H = 0.029952$)

(q_2, p_2)-plane, using SYPRK1, SYPRK2, SYRKN, and NCRKN. As expected, the noncanonical scheme gives solution points which lie on the curves for some time and gradually drift away from the two submanifolds, displaying, perhaps, the noncanonical effects, a phenomenon common with such methods [11]. On the other hand, the solution points computed by all the canonical schemes lie on the two submanifolds. It is hoped that this feature would remain so for an infinite number of time steps. Figure 2 represents the energy behavior of all the schemes. This clearly shows the significance of canonical schemes for long-time computations.

We also solve the problem choosing

$$(q_1, q_2, p_1, p_2) = (0, 0.2, 0.4483395, 0),$$

where p_1 was computed so that $H = 0.117835$. The number of time steps is 5,000 with $h = 0.5$. Figure 3 shows the trajectories on the (q_1, q_2)-plane using all the methods.

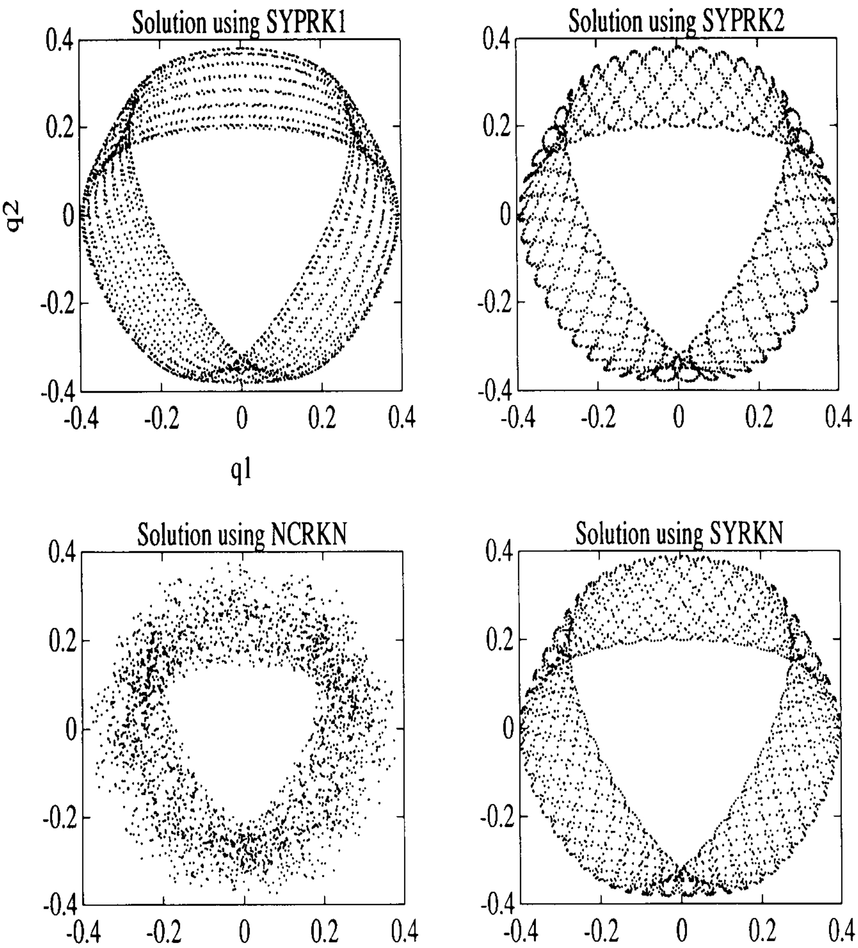

FIGURE 3. Trajectories for the Hénon-Heiles problem using canonical and noncanonical methods ($H = 0.117835$)

5.3. **Kepler's problem.** The motion of two bodies under mutual gravitational attraction is governed by the Hamiltonian

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

where α is a constant involving the gravitational constant [5, pp. 132, 133], the masses of the bodies, and units of measurement. Different choices of initial conditions lead to different solution orbits. For this problem, we use $(q_1, q_2, p_1, p_2) = (0.75, 0, 0, \alpha\sqrt{\frac{5}{3}})$ as initial conditions and $\frac{\pi}{4}$ for α. The solution orbit is an ellipse with low eccentricity of 0.25 and a focus at the origin. The solution is periodic with period $T = 8$. The plots of the global error (i.e., $\|\mathbf{q}(t_n) - \mathbf{q}_n\|/\|\mathbf{q}(t_n)\|$) versus time, using SYPRK1, SYPRK2, NCRKN, and SYRKN with scaled stepsize (i.e., the actual stepsize divided by the number of stages of a method) of $\frac{T}{450}$ are shown in Figure 4 (see next page). The solution was computed for 100 time periods. It is remarkable to see from the

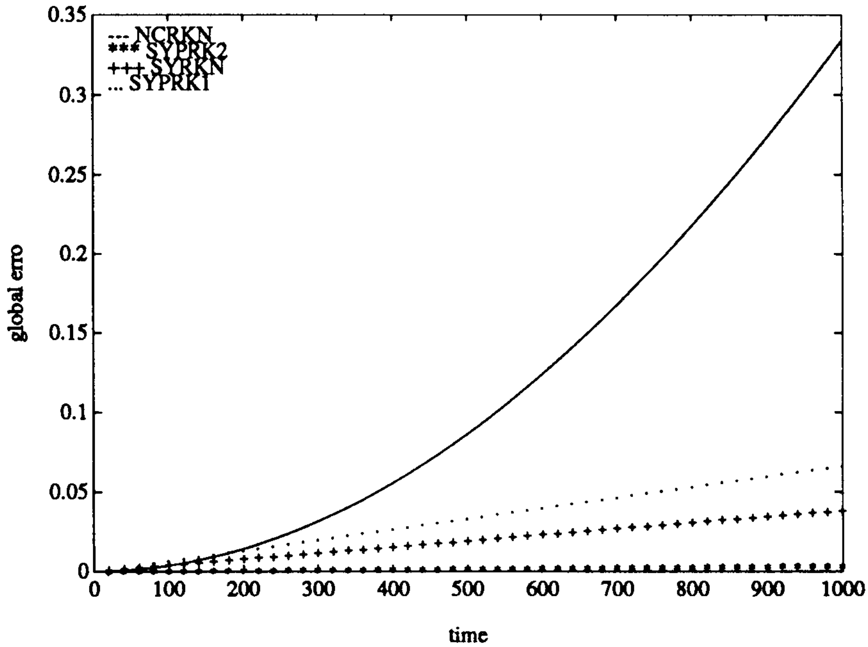

FIGURE 4. Error analysis of canonical and noncanonical schemes (Kepler's problem)

figure that, while canonical methods exhibit linear growth in global error, the noncanonical method gave an exponential growth. This again shows the advantage of canonical numerical mappings over noncanonical ones for long-time computation.

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