

**ON RUNGE–KUTTA–NYSTROM FORMULAE WITH
CONTRACTIVITY PRESERVING PROPERTIES FOR SECOND
ORDER ODES**

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ABSTRACT. New optimal, explicit, s -stage Runge–Kutta–Nystrom methods of order $p = 3$ to 6, denoted by $\text{CPRKN}(s, p)$, $p = 3, 4, \dots, 6$, that have contractivity-preserving (CP) properties and nonnegative coefficients are constructed for solving the special second-order system of non-stiff ordinary differential equations $y'' = f(t, y)$, $y(t_0) = y_0$, $y'(t_0) = y'_0$, where $y \in \mathbb{R}^N$. Selected $\text{CPRKN}(4, 4)$ and $\text{CPRKN}(6, 6)$ compare well with Dormand–El-Mikkawy–Prince $\text{DEP}(4,3)4\text{FM}$ and $\text{DEP}(6,4)6\text{FM}$, respectively, in solving standard N-body problems over an interval of 1000 periods on the basis of the relative error of energy (EE) as a function of the number of function evaluations (NFE). The existence of these $\text{CPRKN}(s, p)$ would suggest that they can be combined with Taylor series or CP Hermite–Obrechhoff series methods developed earlier to form new higher order, more efficient methods with contractivity-preserving (CP) properties. The coefficients of $\text{CPRKN}(s, p)$, $p = 3, 4, \dots, 6$ are listed in the appendix.

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1. INTRODUCTION

New optimal, explicit, s -stage Runge–Kutta–Nystrom methods of order $p = 3$ to 6, denoted by $\text{CPRKN}(s, p)$, $p = 3, 4, \dots, 6$, that has contractivity-preserving (CP) properties and nonnegative coefficients are constructed for solving the special second-order system of non-stiff ordinary differential equations (ODEs),

$$y'' = f(t, y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \quad \text{where } ' = \frac{d}{dt} \quad \text{and } y \in \mathbb{R}^N. \quad (1)$$

We consider now the following form of the solution y to problem (1):

$$y(t + \Delta t) = y(t) + \Delta t y^{\text{sub}}(t + \Delta t, \Delta t) \quad (2)$$

where the subformula $y^{\text{sub}}(t + \Delta t, \Delta t)$ (which is the slope $[y(t + \Delta t) - y(t)]/\Delta t$) is the series

$$y^{\text{sub}}(t + \Delta t, \Delta t) = y'(t) + \sum_{m=2}^{\infty} \frac{(\Delta t)^{m-1}}{m!} y^{(m)}(t).$$

In our construction of formulae for y^{sub} defined in (2) and y' of CPRKN(s, p), $p = 3, 4, \dots, 6$, we rewrite formulae for y^{sub} and y' as a convex combination of forward Euler (FE) method (approximating $y'(t + \Delta t)$),

$$y'_{n+1} = y'_n + \Delta t y''_n. \quad (3)$$

If FE is contractive in a given norm, then formulae for y^{sub} and y' of CPRKN(s, p) will be contractive as a convex combination of FE with modified step sizes.

The regions of absolute stability of CPRKN(s, p), $p = 3, 4, \dots, 6$, are derived under the assumption that two solution derivatives, y' and \tilde{y}' , to problem (1) are *contractive*:

$$\|y'(t + \Delta t) - \tilde{y}'(t + \Delta t)\| \leq \|y'(t) - \tilde{y}'(t)\|, \quad \forall \Delta t \geq 0, \quad (4)$$

and the two subformulae $y^{\text{sub}}(t, \Delta t)$ and $\tilde{y}^{\text{sub}}(t, \Delta t)$ defined in (2) are contractive:

$$\|y^{\text{sub}}(t + \Delta t, \Delta t) - \tilde{y}^{\text{sub}}(t + \Delta t, \Delta t)\| \leq \|y^{\text{sub}}(t, \Delta t) - \tilde{y}^{\text{sub}}(t, \Delta t)\|, \quad \forall \Delta t \geq 0, \quad (5)$$

and

$$\begin{aligned} \|y'(t + \Delta t) - \tilde{y}'(t + \Delta t)\| &\leq \|y^{\text{sub}}(t + \Delta t, \Delta t) - \tilde{y}^{\text{sub}}(t + \Delta t, \Delta t)\| \\ &\leq \|y'(t) - \tilde{y}'(t)\| \quad \forall \Delta t \geq 0. \end{aligned} \quad (6)$$

We assume that there exists a maximum stepsize Δt_{FE} such that, when FE is employed with $\Delta t \leq \Delta t_{\text{FE}}$, f satisfies a discrete analog of (4):

$$\|y'_{n+1} - \tilde{y}'_{n+1}\| \equiv \left\| y'_n + \Delta t f(t_n, y_n) - \left(\tilde{y}'_n + \Delta t f(t_n, \tilde{y}_n) \right) \right\| \leq \|y'_n - \tilde{y}'_n\|, \quad (7)$$

with

$$\left\| y_n^{\text{sub}} + \Delta t f(t_n, y_n) - \left(\tilde{y}_n^{\text{sub}} + \Delta t f(t_n, \tilde{y}_n) \right) \right\| \leq \|y'_n - \tilde{y}'_n\|, \quad (8)$$

when y'_n and \tilde{y}'_n are replaced by y_n^{sub} and \tilde{y}_n^{sub} , respectively, in the two FE formulae in (7), and, when FE is employed with $\Delta t \leq \Delta t_{\text{FE}}$, f satisfies a discrete analog of (6):

$$\|y'_{n+1} - \tilde{y}'_{n+1}\| \leq \|y_{n+1}^{\text{sub}} - \tilde{y}_{n+1}^{\text{sub}}\| \leq \|y'_n - \tilde{y}'_n\|. \quad (9)$$

Here y'_n and \tilde{y}'_n are two derivatives of the numerical solutions generated by FE with different *neighbouring* starting (or previous) values $y'_0 = y'(t_0)$ and $\tilde{y}'_0 = \tilde{y}'(t_0)$.

By interpreting \tilde{y}'_0 as a perturbation of y'_0 due to numerical error, we see that contractivity implies that these errors do not grow as they are propagated.

We are interested in a higher-order formula for y^{sub} of CPRKN(s, p), $p = 3, 4, \dots, 6$, that maintains the *contractivity-preserving property*

$$\|y_{n+1}^{\text{sub}} - \tilde{y}_{n+1}^{\text{sub}}\| (\leq \|y'_n - \tilde{y}'_n\|) \leq \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|, \quad (10)$$

together with a higher-order formula for y' that maintains the contractivity-preserving property,

$$\|y'_{n+1} - \tilde{y}'_{n+1}\| \leq \|y'_n - \tilde{y}'_n\|, \quad (11)$$

for $0 \leq \Delta t \leq \Delta t_{\text{max}} = c\Delta t_{\text{FE}}$ whenever inequality (7) holds. Here c , called the contractivity-preserving coefficient (CP coefficient), depends only on the numerical integration method but not on f . This definition of the CP coefficient of CPRKN(s, p), $p = 3, 4, \dots, 6$, follows closely the definition of the strong stability preserving (SSP) coefficient of RK (see [3]).

In [8], similar CP RK methods have been constructed and tested on DETEST problems [7].

The aim of CPRKN(s, p), $p = 3, 4, \dots, 6$, is to maintain simultaneously the CP properties (10) and (11) while achieving higher-order accuracy, perhaps with a modified time-step restriction, measured here with the CP coefficient $c(\text{CPRKN}(s, p))$:

$$\Delta t \leq c(\text{CPRKN}(s, p))\Delta t_{\text{FE}}. \quad (12)$$

This coefficient describes the ratio of the maximal CPRKN(s, p) time step to the time step Δt_{FE} , for which conditions (7), (8) and (9) hold.

Similar to Huang and Innanen [6], we compare the numerical performance of selected CPRKN(4, 4), CPRKN(6, 6), Dormand–El-Mikkawy–Prince DEP(4,3)4FM and DEP(6,4)6FM [1] on Kepler orbit with eccentricities $e = 0.3, 0.5, 0.7$ over an interval of 1000 periods on the basis of the relative energy error (EE) as a function of the number of function evaluations (NFE). It is seen that CPRKN(4,4) and CPRKN(6,6) compare well with DEP(4,3)4FM and DEP(6,4)6FM.

The existence of the new methods CPRKN(s, p) and the above results would suggest that these CPRKN(s, p) can be combined with Taylor series or HO series methods developed earlier [10] to form new higher order methods with contractivity-preserving (CP) properties and nonnegative coefficients for solving efficiently equations (1).

Section 2 introduces new CPRKN(s, p), $p = 3, 4, \dots, 6$ and the necessary order conditions are listed in Section 3. Section 4 derives Y_i^{sub} , $i = 2, 3, \dots, s + 1$, of

CPRKN(s, p) in contractivity-preserving form (CP form). Section 5 presents y'_{n+1} of CPRKN(s, p) in CP form for deriving contractivity-preserving (CP) property. Optimizing CP coefficient c of CPRKN(s, p) is considered in Section 6. Section 7 describes the intervals of absolute stability of CPRKN(4,4) and CPRKN(6,6). In Section 8, numerical results are used to compare CPRKN(4,4) and CPRKN(6,6) with Dormand–El-Mikkawy–Prince DEP(4,3)4FM and DEP(6,4)6FM. Coefficients of CPRKN(s, p), $p = 3, 4, \dots, 6$, are listed in Appendix A.

2. NEW CPRKN(s, p) WITH CONTRACTIVITY-PRESERVING PROPERTIES

New CPRKN(s, p) are constructed by the following $(s + 1)$ formulae which perform integration from t_n to t_{n+1} .

Let Δt denote the step size. The abscissa vector $[c_1, c_2, \dots, c_s]^T$ defines the s off-step points $t_n + c_j \Delta t$, $j = 1, 2, \dots, s$ and $c_{s+1} = 1$. In all cases $c_1 = 0$ and, by convention, $c_1^0 = 1$. Let $Y_1'' = y_n''$.

A Hermite–Birkhoff (HB) polynomial is used as stage formula P_i to obtain the stage value Y_i ,

$$Y_i = y_n + c_i \Delta t y_n' + \Delta t^2 \left(\sum_{j=1}^{i-1} \bar{a}_{ij} Y_j'' \right), \quad i = 2, 3, \dots, s. \quad (13)$$

HB polynomials are used as the integration formula IF for y and IF' for y' to obtain $y_{n+1} = Y_3$ and y'_{n+1} , respectively, to order p ,

$$y_{n+1} = Y_{s+1} = y_n + \Delta t y_n' + \Delta t^2 \left(\sum_{j=1}^s \bar{b}_j Y_j'' \right), \quad (14)$$

$$y'_{n+1} = y_n' + \Delta t \left(\sum_{j=1}^s b_j Y_j'' \right), \quad (15)$$

where $Y_i'' := f(t_n + c_i \Delta t, Y_i)$, $i = 2, 3, \dots, s$ denotes the stage second derivatives.

Formulae (13)–(15) are the usual form of CPRKN(s, p).

The defining formulae of CPRKN(s, p) involve the usual Runge–Kutta–Nystrom (RKN) parameters c_i , $\bar{a}_{i,j}$, \bar{b}_j and b_j .

Thus we can represent CPRKN(s, p) by its *coefficient scheme* (A, \bar{b}, b) , where $A = (\bar{a}_{i,j})$ is a $s \times s$ matrix, $\bar{b} = (\bar{b}_1, \bar{b}_2, \dots, \bar{b}_s)^T$, $b = (b_1, b_2, \dots, b_s)^T$ are two s -vector. One can display the coefficient scheme (A, \bar{b}, b) , and the c_i in the Butcher tableau

$$\begin{array}{c|cccccc}
 c_1 & & & & & & \\
 c_2 & \bar{a}_{21} & & & & & \\
 c_3 & \bar{a}_{31} & \bar{a}_{32} & & & & \\
 c_4 & \bar{a}_{41} & \bar{a}_{42} & \bar{a}_{43} & & & \\
 \vdots & \vdots & & \ddots & \ddots & & \\
 c_s & \bar{a}_{s1} & \bar{a}_{s2} & \bar{a}_{s3} & \cdots & \bar{a}_{s,s-1} & \\
 & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 & \cdots & \bar{b}_{s-1} & \bar{b}_s \\
 \hline
 & b_1 & b_2 & b_3 & \cdots & b_{s-1} & b_s
 \end{array}$$

2.1. Subformulae of Y_i , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p)

We consider now the following form of Y_i , $i = 2, 3, \dots, s + 1$ with $Y_{s+1} = y_{n+1}$ defined in (13) and (14) respectively,

$$Y_i = y_n + \Delta t \left(Y_i^{\text{sub}} \right), \quad i = 2, 3, \dots, s, \quad (16)$$

$$y_{n+1} = Y_{s+1} = y_n + \Delta t \left(y_{n+1}^{\text{sub}} \right), \quad (17)$$

where subformulae Y_i^{sub} , $i = 2, 3, \dots, s + 1$ are

$$Y_i^{\text{sub}} = c_i y'_n + \Delta t \left(\sum_{j=1}^{i-1} \bar{a}_{ij} Y_j'' \right), \quad i = 2, 3, \dots, s, \quad (18)$$

$$y_{n+1}^{\text{sub}} = Y_{s+1}^{\text{sub}} = y'_n + \Delta t \left(\sum_{j=1}^s \bar{b}_j Y_j'' \right). \quad (19)$$

Subformulae (18) and (19) are called the *usual form* of Y_i^{sub} , $i = 2, 3, \dots, s + 1$.

3. ORDER CONDITIONS FOR CPRKN(s, p)

As in similar search for solvers of (1), we impose the following simplifying assumptions for Y_i :

$$\sum_{j=1}^{i-1} \bar{a}_{i,j} = \frac{c_i^2}{2}, \quad i = 2, 3, \dots, s. \quad (20)$$

Under the assumption $\bar{b}_i = b_i(1 - c_i)$, $i = 1, 2, \dots, s$, there remains the following 11 sets of equations for y'_{n+1} to be solved:

$$\sum_{i=1}^s b_i \frac{c_i^k}{k!} = \frac{1}{(k+1)!}, \quad k = 0, 1, \dots, p-1, \quad (21)$$

$$\sum_{i=2}^s b_i \left[\sum_{j=1}^{i-1} \bar{a}_{ij} c_j \right] = \frac{1}{4!}, \quad (22)$$

$$\sum_{i=2}^s b_i \frac{c_i}{4} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} c_j \right] = \frac{1}{5!}, \quad (23)$$

$$\sum_{i=2}^s b_i \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \frac{c_j^2}{2!} \right] = \frac{1}{5!}, \quad (24)$$

$$\sum_{i=2}^s b_i \frac{c_i^2}{4 \times 5} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} c_j \right] = \frac{1}{6!}, \quad (25)$$

$$\sum_{i=2}^s b_i \frac{c_i}{5} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \frac{c_j^2}{2!} \right] = \frac{1}{6!}, \quad (26)$$

$$\sum_{i=2}^s b_i \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \frac{c_j^3}{3!} \right] = \frac{1}{6!}, \quad (27)$$

$$\sum_{i=2}^s b_i \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \left[\sum_{k=1}^{j-1} \bar{a}_{jk} c_k \right] \right] = \frac{1}{6!}, \quad (28)$$

$$\sum_{i=2}^s b_i \frac{c_i}{6} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \left[\sum_{k=1}^{j-1} \bar{a}_{jk} c_k \right] \right] = \frac{1}{7!}, \quad (29)$$

$$\sum_{i=2}^s b_i \frac{c_i^2}{5 \times 6} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \frac{c_j^2}{2!} \right] = \frac{1}{7!}, \quad (30)$$

$$\sum_{i=2}^s b_i \frac{c_i}{6} \left[\sum_{j=1}^{i-1} \bar{a}_{ij} \frac{c_j^3}{3!} \right] = \frac{1}{7!}. \quad (31)$$

Besides conditions (20),

- CPRKN(2, 3) satisfies (21) with $k = 0, 1, 2$,
- CPRKN(3, 4) satisfies (21) with $k = 0, 1, \dots, 4$ and (22),
- CPRKN(4, 4) satisfies (21) with $k = 0, 1, \dots, 4$, (22) and (23), (32)
- CPRKN(5, 5) satisfies (21) with $k = 0, 1, \dots, 5$, (22) to (27),
- CPRKN(6, 6) satisfies (21) with $k = 0, 1, \dots, 6$, (22) to (31).

It is to be noted that, in (32), to reduce the norm of the principal local truncation error coefficients, some additional order conditions associated with $(\Delta t)^{p+1}$ are

satisfied.

4. FROM MODIFIED CONTRACTIVITY-PRESERVING (CP) FORM TO CANONICAL CP FORM OF Y_i^{SUB} , $i = 2, 3, \dots, s + 1$ OF CPRKN(s, p)

Gottlieb, Ketcheson and Shu presented canonical Shu–Osher forms in compact vector notation for RK methods (see [4, Section 3.1–3.4] for details).

Our construction of the canonical CP form (similar to the canonical Shu–Osher form for RK methods) of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p) proceeds in three steps in Subsections 4.1–4.3.

4.1. Contractivity preserving of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p)

Similar to the Shu–Osher form of RK methods [12], equations (18)–(19) of Y_i^{sub} , $i = 2, 3, \dots, s$ and $Y_{s+1}^{\text{sub}} = y_{n+1}^{\text{sub}}$, respectively, can be written in the form,

$$Y_i^{\text{sub}} = \bar{\alpha}_{i1}y'_n + \Delta t \bar{\beta}_{i1}y''_n + \left[\sum_{j=1}^{i-1} \bar{\alpha}_{ij}Y_j^{\text{sub}} + \Delta t \bar{\beta}_{ij}Y_j'' \right], \quad i = 2, 3, \dots, s + 1, \quad (33)$$

$$y_{n+1}^{\text{sub}} = Y_{s+1}^{\text{sub}},$$

with consistency conditions:

$$\bar{\alpha}_{i1} + \sum_{j=2}^{i-1} \bar{\alpha}_{ij}c_j = c_i, \quad i = 2, 3, \dots, s + 1. \quad (34)$$

Form (33) is called the *contractivity preserving form* (CP form) (similar to Shu–Osher form for RK methods [4]) of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p).

By setting $\bar{v}_i = \bar{\alpha}_{i1}$ and $\bar{w}_i = \bar{\beta}_{i1}$, $i = 2, 3, \dots, s + 1$, in (33), we have the *modified CP form* of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p):

$$Y_i^{\text{sub}} = \bar{v}_iy'_n + \Delta t \bar{w}_iy''_n + \left[\sum_{j=2}^{i-1} \bar{\alpha}_{ij}Y_j^{\text{sub}} + \Delta t \bar{\beta}_{ij}Y_j'' \right], \quad i = 2, 3, \dots, s + 1, \quad (35)$$

$$y_{n+1}^{\text{sub}} = Y_{s+1}^{\text{sub}}.$$

We can rearrange the stage values Y_i^{sub} , $i = 2, 3, \dots, s + 1$, in (35) as follows:

$$Y_i^{\text{sub}} = \bar{v}_i \left[y'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} y''_n \right] + \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \left(Y_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} Y_j'' \right), \quad i = 2, 3, \dots, s + 1, \quad (36)$$

with consistency conditions:

$$\bar{v}_i + \sum_{j=2}^{i-1} \bar{\alpha}_{ij} c_j = c_i, \quad i = 2, 3, \dots, s+1. \quad (37)$$

Thus we obtain the difference $Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}$, $i = 2, 3, \dots, s+1$, from (36) as follows:

$$\begin{aligned} Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}} &= \bar{v}_i \left[\left(y'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} y''_n \right) - \left(\tilde{y}'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} \tilde{y}''_n \right) \right] \\ &+ \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \left[\left(Y_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} Y_j'' \right) - \left(\tilde{Y}_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} \tilde{Y}_j'' \right) \right], \quad i = 2, 3, \dots, s+1. \end{aligned} \quad (38)$$

Provided all the coefficients of (36) are nonnegative, the following straightforward extension of a result presented in [2, 5] holds.

Theorem 1. *If f satisfies conditions (7), (8) and (9) of the FE method, then $y_{n+1}^{\text{sub}} = Y_{s+1}^{\text{sub}}$ of the CPRKN(s, p) method (36) satisfies the CP property*

$$\|y_{n+1}^{\text{sub}} - \tilde{y}_{n+1}^{\text{sub}}\| \leq \|y'_n - \tilde{y}'_n\| \leq \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|$$

provided

$$\Delta t \leq c_{\text{feasible}} \Delta t_{\text{FE}},$$

where the *feasible CP coefficient*, c_{feasible} , is the minimum of the following numbers:

$$\frac{\bar{\alpha}_{ij}}{\bar{\beta}_{ij}}, \quad j = 2, 3, \dots, i-1, \quad \text{and} \quad \frac{\bar{v}_i}{\bar{w}_i}, \quad i = 2, 3, \dots, s+1, \quad (39)$$

under the assumption that all coefficients of (36) are nonnegative, with the convention that the ratios $a/0 = +\infty$, and the ratios $0/0$ are ignored.

Proof. The difference $Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}$ of CPRKN(s, p) can be rewritten as a convex combination of the two terms on the right-hand side of (38). Thus, by the convexity of the norm $\|\cdot\|$, we have

$$\begin{aligned} \|Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}\| &\leq \bar{v}_i \left\| \left(y'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} y''_n \right) - \left(\tilde{y}'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} \tilde{y}''_n \right) \right\| \\ &+ \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \left\| \left(Y_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} Y_j'' \right) - \left(\tilde{Y}_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} \tilde{Y}_j'' \right) \right\|, \quad i = 2, 3, \dots, s+1. \end{aligned} \quad (40)$$

We present a proof by induction on i . When $i = 2$, the right-hand side of (40) has the following upper bound, since $\frac{\bar{w}_2}{\bar{v}_2} \Delta t \leq \frac{\Delta t}{c_{\text{feasible}}} \leq \Delta t_{\text{FE}}$,

$$\begin{aligned} & \bar{v}_2 \left\| \left(y'_n + \Delta t \frac{\bar{w}_2}{\bar{v}_2} y''_n \right) - \left(\tilde{y}'_n + \Delta t \frac{\bar{w}_2}{\bar{v}_2} \tilde{y}''_n \right) \right\| \\ & \leq \bar{v}_2 \|y'_n - \tilde{y}'_n\| \quad \text{by (7),} \\ & \leq c_2 \|y'_n - \tilde{y}'_n\| \quad \text{by (37) with } i = 2, \\ & \leq c_2 \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\| \quad \text{by (9).} \end{aligned} \tag{41}$$

Suppose now that, for $k = 2, 3, \dots, i-1$, $\|Y_k^{\text{sub}} - \tilde{Y}_k^{\text{sub}}\|$ of (40) has the following upper bound,

$$\|Y_k^{\text{sub}} - \tilde{Y}_k^{\text{sub}}\| \leq c_k \|y'_n - \tilde{y}'_n\| \leq c_k \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|. \tag{42}$$

Then, for $k = i$, $\|Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}\|$ of (40) has the following upper bound, since $\frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} \Delta t \leq \frac{\Delta t}{c_{\text{feasible}}} \leq \Delta t_{\text{FE}}$,

$$\begin{aligned} \|Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}\| & \leq \bar{v}_i \left\| \left(y'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} y''_n \right) - \left(\tilde{y}'_n + \Delta t \frac{\bar{w}_i}{\bar{v}_i} \tilde{y}''_n \right) \right\| \\ & \quad \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \left\| \left(Y_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} Y_j'' \right) - \left(\tilde{Y}_j^{\text{sub}} + \Delta t \frac{\bar{\beta}_{ij}}{\bar{\alpha}_{ij}} \tilde{Y}_j'' \right) \right\| \\ & \leq \bar{v}_i \|y'_n - \tilde{y}'_n\| + \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \left\| \left(Y_j^{\text{sub}} + \frac{\Delta t}{c_{\text{feasible}}} Y_j'' \right) - \left(\tilde{Y}_j^{\text{sub}} + \frac{\Delta t}{c_{\text{feasible}}} \tilde{Y}_j'' \right) \right\| \\ & \leq \bar{v}_i \|y'_n - \tilde{y}'_n\| + \sum_{j=2}^{i-1} \bar{\alpha}_{ij} \|Y_j^{\text{sub}} - \tilde{Y}_j^{\text{sub}}\| \quad \text{by (8) and (9),} \\ & \leq \bar{v}_i \|y'_n - \tilde{y}'_n\| + \sum_{j=2}^{i-1} \bar{\alpha}_{ij} c_j \|y'_n - \tilde{y}'_n\| \quad \text{by (42),} \\ & \leq c_i \|y'_n - \tilde{y}'_n\| \quad \text{by (37),} \\ & \leq c_i \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\| \quad \text{by (9).} \end{aligned} \tag{43}$$

$$\leq c_i \|y'_n - \tilde{y}'_n\| \quad \text{by (37),} \tag{44}$$

$$\leq c_i \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\| \quad \text{by (9).} \tag{45}$$

Thus, we have, from (44) and (45), the following upper bound of $\|Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}\|$,

$$\|Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}}\| \leq c_i \|y'_n - \tilde{y}'_n\|, \tag{46}$$

$$\leq c_i \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|, \quad i = 2, 3, \dots, s+1, \tag{47}$$

and, naturally,

$$\left\| Y_i^{\text{sub}} - \tilde{Y}_i^{\text{sub}} \right\| \leq \|y'_n - \tilde{y}'_n\|, \quad (48)$$

$$\leq \left\| y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}} \right\|, \quad i = 2, 3, \dots, s+1. \quad (49)$$

In particular, this yields $\|y_{n+1}^{\text{sub}} - \tilde{y}_{n+1}^{\text{sub}}\| \leq \|y'_n - \tilde{y}'_n\| \leq \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|$.

It is to be noted here that each representation (36) of Y_i^{sub} , $i = 2, 3, \dots, s+1$ (to obtain $Y_{s+1} = y_{n+1}$ to order p) with coefficients \bar{v}_i , \bar{w}_i , $\bar{\alpha}_{ij}$ and $\bar{\beta}_{ij}$, will produce a feasible CP coefficient, c_{feasible} , defined in Theorem 1 and *feasible* Y_i^{sub} , $i = 2, 3, \dots, s+1$ of CPRKN(s, p) in modified CP form (36). What we really want is not merely feasible Y_i^{sub} , $i = 2, 3, \dots, s+1$ of method CPRKN(s, p) in CP form but best Y_i^{sub} , $i = 2, 3, \dots, s+1$. This question will be considered in Section 6.

Transforming the usual form (18)–(19) into the modified CP form (35) of Y_i^{sub} , $i = 2, 3, \dots, s+1$ of CPRKN(s, p) and vice versa will be considered in Subsection 4.2.

4.2. Vector notation of Y_i^{sub} , $i = 2, 3, \dots, s+1$ of CPRKN(s, p)

Vector and matrix notation will help represent Y_i^{sub} , $i = 2, 3, \dots, s+1$ of CPRKN(s, p) in canonical CP form.

We define $(s+1)$ -vectors

$$\bar{\mathbf{v}} = [0, \bar{v}_2, \bar{v}_3, \dots, \bar{v}_{s+1}]^T, \quad \bar{\mathbf{w}} = [0, \bar{w}_2, \bar{w}_3, \dots, \bar{w}_{s+1}]^T,$$

strictly lower triangular real matrices $\bar{\boldsymbol{\alpha}}, \bar{\boldsymbol{\beta}} \in \mathbb{R}^{(s+1) \times (s+1)}$,

$$\bar{\boldsymbol{\alpha}} = \{\bar{\alpha}_{ij}\}, \quad \bar{\boldsymbol{\beta}} = \{\bar{\beta}_{ij}\}.$$

The components \bar{v}_i , \bar{w}_i , $\bar{\alpha}_{ij}$, $\bar{\beta}_{ij}$ come from the modified CP form (35) of Y_i^{sub} , $i = 2, 3, \dots, s+1$ of CPRKN(s, p).

Moreover,

$$\mathbf{Y}^{\text{sub}} = [0, Y_2^{\text{sub}}, Y_3^{\text{sub}}, \dots, Y_{s+1}^{\text{sub}}]^T, \quad \mathbf{F} = [0, Y_2'', Y_3'', \dots, Y_{s+1}'']^T, \quad (50)$$

with the following N -vectors: $Y_j^{\text{sub}}, Y_j, Y_j''$ for $j = 1, 2, 3, \dots, s+1$, $Y_1 = y_n$, $Y_1'' = y_n'' = f_n$, $Y_{s+1}^{\text{sub}} = y_{n+1}^{\text{sub}}$ and $Y_{s+1}'' = y_{n+1}'' = f_{n+1}$.

4.2.1. Modified CP form of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ in vector notation

Using the above notation, we rewrite the modified CP form (35) of Y_j^{sub} , $i = 2, 3, \dots, s + 1$ of CPRKN(s, p) in vector notation:

$$\begin{aligned} \mathbf{Y}^{\text{sub}} &= \bar{\mathbf{v}}(y'_n)^T + \Delta t \bar{\mathbf{w}}(y''_n)^T + \bar{\boldsymbol{\alpha}} \mathbf{Y}^{\text{sub}} + \Delta t \bar{\boldsymbol{\beta}} \mathbf{F}, \\ y_{n+1}^{\text{sub}} &= Y_{s+1}^{\text{sub}}, \end{aligned} \quad (51)$$

with consistency conditions (37) written in vector form,

$$\bar{\mathbf{v}} + \bar{\boldsymbol{\alpha}} \mathbf{e}_{s+1} = \mathbf{e}_{s+1}, \quad (52)$$

where

$$\mathbf{e}_{s+1} = [0, c_2, c_3, \dots, c_{s+1}]^T \in \mathbb{R}^{s+1}. \quad (53)$$

It is to be noted that, by setting the first row of matrices \mathbf{Y}^{sub} , \mathbf{F} equal to zero, $\bar{\alpha}_{i1}$ and $\bar{\beta}_{i1}$, $i = 2, 3, \dots, s + 1$ are not used in formulae (51) and are replaced by \bar{v}_i and \bar{w}_i , $i = 2, 3, \dots, s + 1$, respectively.

4.2.2. Usual form of Y_i^{sub} , $i = 2, 3, \dots, s + 1$ in vector notation

If $\bar{\boldsymbol{\alpha}} = \mathbf{0}$, then the modified CP form (51) becomes

$$\begin{aligned} \mathbf{Y}^{\text{sub}} &= \bar{\mathbf{v}}(y'_n)^T + \Delta t \bar{\mathbf{w}}(y''_n)^T + \Delta t \bar{\boldsymbol{\beta}} \mathbf{F}, \\ y_{n+1}^{\text{sub}} &= Y_{s+1}^{\text{sub}}, \end{aligned} \quad (54)$$

which is the usual form. The elements $\bar{\mathbf{v}}$, $\bar{\mathbf{w}}$, $\bar{\boldsymbol{\beta}}$ of (54) are then denoted as $\bar{\mathbf{v}}_0$, $\bar{\mathbf{w}}_0$, $\bar{\boldsymbol{\beta}}_0$ respectively, and hence the usual form (54) can be rewritten as

$$\begin{aligned} \mathbf{Y}^{\text{sub}} &= \bar{\mathbf{v}}_0(y'_n)^T + \Delta t \bar{\mathbf{w}}_0(y''_n)^T + \Delta t \bar{\boldsymbol{\beta}}_0 \mathbf{F}, \\ y_{n+1}^{\text{sub}} &= Y_{s+1}^{\text{sub}}, \end{aligned} \quad (55)$$

with the consistency condition,

$$\bar{\mathbf{v}}_0 = \mathbf{e}_{s+1}, \quad (56)$$

where \mathbf{e}_{s+1} is defined in (53).

To find the relation between the CP form coefficients and the usual form coefficients, we can solve (51) for \mathbf{Y}^{sub} since $\mathbf{I} - \bar{\boldsymbol{\alpha}}$ is invertible because the matrix $\bar{\boldsymbol{\alpha}}$ is strictly lower triangular,

$$\mathbf{Y}^{\text{sub}} = (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\mathbf{v}}(y'_n)^T + \Delta t (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\mathbf{w}}(y''_n)^T + \Delta t (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\boldsymbol{\beta}} \mathbf{F}. \quad (57)$$

Comparing (57) with (55), we have the following relations between the generalized CP form coefficients and the usual form coefficients,

$$\bar{\mathbf{v}}_0 = (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\mathbf{v}}, \quad \bar{\mathbf{w}}_0 = (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\mathbf{w}}, \quad \bar{\boldsymbol{\beta}}_0 = (\mathbf{I} - \bar{\boldsymbol{\alpha}})^{-1} \bar{\boldsymbol{\beta}}. \quad (58)$$

These relations allow a simple transformation of the vectors and matrices $\bar{\mathbf{v}}, \bar{\mathbf{w}}, \bar{\boldsymbol{\beta}}$ of a CP form into $\bar{\mathbf{v}}_0, \bar{\mathbf{w}}_0, \bar{\boldsymbol{\beta}}_0$ of a usual form and vice versa.

In fact, the form (55) is the usual form (18) and (19) with

$$\bar{\mathbf{v}}_0 = [0, c_2, c_3, \dots, c_{s+1}]^T, \quad \bar{\mathbf{w}}_0 = [0, \bar{a}_{21}, \bar{a}_{31}, \dots, \bar{b}_1]^T, \quad (59)$$

$$\bar{\boldsymbol{\beta}}_0 = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \bar{a}_{21} & 0 & 0 & 0 & \cdots & 0 & 0 \\ \bar{a}_{31} & \bar{a}_{32} & 0 & 0 & \cdots & 0 & 0 \\ \bar{a}_{41} & \bar{a}_{42} & \bar{a}_{43} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \ddots & \ddots & & \vdots \\ \bar{a}_{s1} & \bar{a}_{s2} & \bar{a}_{s3} & \cdots & \bar{a}_{s,s-1} & 0 & 0 \\ \bar{b}_1 & \bar{b}_2 & \bar{b}_3 & \cdots & \bar{b}_{s-1} & \bar{b}_s & 0 \end{bmatrix}. \quad (60)$$

4.3. Canonical CP form of \mathbf{Y}^{sub} of CPRKN(s, p) in vector notation

To find the CP coefficient of CPRKN(s, p), it is useful to consider a particular modified CP form (51) where the elements of the matrices $\bar{\boldsymbol{\alpha}}$ and $\bar{\boldsymbol{\beta}}$ satisfy the same ratio $r = \frac{\bar{\alpha}_{ij}}{\bar{\beta}_{ij}}$ for every i, j , $i = 3, 4, \dots, s+1$ and $j = 2, 3, \dots, i-1$, such that $\bar{\beta}_{ij} \neq 0$, or, in vector notation,

$$\bar{\boldsymbol{\alpha}}_r = r \bar{\boldsymbol{\beta}}_r. \quad (61)$$

Substituting this relation into (58), we can solve for $\bar{\boldsymbol{\beta}}_r$ in terms of $\bar{\boldsymbol{\beta}}_0$ and r .

First, we have

$$(\mathbf{I} - r \bar{\boldsymbol{\beta}}_r)^{-1} \bar{\boldsymbol{\beta}}_r = \bar{\boldsymbol{\beta}}_0 \quad \Leftrightarrow \quad \bar{\boldsymbol{\beta}}_r = \bar{\boldsymbol{\beta}}_0 - r \bar{\boldsymbol{\beta}}_r \bar{\boldsymbol{\beta}}_0 \quad \Leftrightarrow \quad \bar{\boldsymbol{\beta}}_r (\mathbf{I} + r \bar{\boldsymbol{\beta}}_0) = \bar{\boldsymbol{\beta}}_0.$$

Then, since $\mathbf{I} + r \bar{\boldsymbol{\beta}}_0$ is invertible, the coefficients of the CP form (51) are given in terms of the coefficients of the usual form (55) by the expressions

$$\bar{\mathbf{v}}_r = (\mathbf{I} + r \bar{\boldsymbol{\beta}}_0)^{-1} \bar{\mathbf{v}}_0 = (\mathbf{I} - \bar{\boldsymbol{\alpha}}_r) \bar{\mathbf{v}}_0, \quad (62)$$

$$\bar{\mathbf{w}}_r = (\mathbf{I} + r \bar{\boldsymbol{\beta}}_0)^{-1} \bar{\mathbf{w}}_0 = (\mathbf{I} - \bar{\boldsymbol{\alpha}}_r) \bar{\mathbf{w}}_0, \quad (63)$$

$$\bar{\boldsymbol{\alpha}}_r = r \bar{\boldsymbol{\beta}}_r = r \bar{\boldsymbol{\beta}}_0 (\mathbf{I} + r \bar{\boldsymbol{\beta}}_0)^{-1} = r \bar{\boldsymbol{\beta}}_0 (\mathbf{I} - \bar{\boldsymbol{\alpha}}_r), \quad (64)$$

$$\bar{\boldsymbol{\beta}}_r = \bar{\boldsymbol{\beta}}_0 (\mathbf{I} + r \bar{\boldsymbol{\beta}}_0)^{-1} = \bar{\boldsymbol{\beta}}_0 (\mathbf{I} - \bar{\boldsymbol{\alpha}}_r), \quad (65)$$

where the identity $(\mathbf{I} - \bar{\alpha}_r) = (\mathbf{I} + r\bar{\beta}_0)^{-1}$ follows from

$$(\mathbf{I} - \bar{\alpha}_r)(\mathbf{I} + r\bar{\beta}_0) = (\mathbf{I} - r\bar{\beta}_r)(\mathbf{I} + r\bar{\beta}_0) = \mathbf{I} + r\bar{\beta}_0 - r\bar{\beta}_r - r^2\bar{\beta}_r\bar{\beta}_0 = \mathbf{I},$$

since $r\bar{\beta}_r = r\bar{\beta}_0 - r^2\bar{\beta}_r\bar{\beta}_0$.

It is to be noted that using (58) and (65), $\bar{\beta}_r$ can then be written as

$$\bar{\beta}_r = \bar{\beta}_0(\mathbf{I} + r\bar{\beta}_0)^{-1} = \bar{\beta}_0(\mathbf{I} - \bar{\alpha}_r) = (\mathbf{I} - \bar{\alpha}_r)\bar{\beta}_0 = (\mathbf{I} + r\bar{\beta}_0)^{-1}\bar{\beta}_0. \quad (66)$$

As in [4], we shall refer to the form given by the coefficients (62)–(65), as the *canonical CP form* of CPRKN(s, p):

$$\mathbf{Y}^{\text{sub}} = \bar{\mathbf{v}}_r(y'_n)^T + \Delta t \bar{\mathbf{w}}_r(y''_n)^T + \bar{\alpha}_r \mathbf{Y}^{\text{sub}} + \Delta t \bar{\beta}_r \mathbf{F}, \quad (67)$$

which can be written solely in terms of the vectors and matrices $\bar{\mathbf{v}}_0$, $\bar{\mathbf{w}}_0$, $\bar{\beta}_0$ of the usual form (55),

$$\begin{aligned} \mathbf{Y}^{\text{sub}} &= (\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{\mathbf{v}}_0(y'_n)^T + \Delta t (\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{\mathbf{w}}_0(y''_n)^T \\ &\quad + r\bar{\beta}_0 (\mathbf{I} + r\bar{\beta}_0)^{-1} \mathbf{Y}^{\text{sub}} + \Delta t \bar{\beta}_0 (\mathbf{I} + r\bar{\beta}_0)^{-1} \mathbf{F}. \end{aligned} \quad (68)$$

The canonical CP form (67) and the form (68) will allow us to formulate simply the optimization problem considered in Section 6.

Using (66) and (68), we obtain

$$\mathbf{Y}^{\text{sub}} = (\mathbf{I} + r\bar{\beta}_0)^{-1} \left[\bar{\mathbf{v}}_0(y'_n)^T + \Delta t \bar{\mathbf{w}}_0(y''_n)^T + \bar{\beta}_0 (r\mathbf{Y}^{\text{sub}} + \Delta t \mathbf{F}) \right]. \quad (69)$$

Here consistency requires that

$$(\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{\mathbf{v}}_0 + r (\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{\beta}_0 \mathbf{e}_{s+1} = \mathbf{e}_{s+1}, \quad (70)$$

where \mathbf{e}_{s+1} is defined in (53). Condition (70) is equivalent to the consistency condition (52).

Note that the vectorial usual form (55), with $\bar{\mathbf{v}}_0$, $\bar{\mathbf{w}}_0$, $\bar{\beta}_0$, corresponds to the canonical CP form (67) or (69) with $r = 0$.

Relations (62)–(65) will enable us to obtain simply the vectors and matrices of a canonical CP form (67) from those of a usual form (55) and vice versa.

To simplify notation, in the following theorem, the ratio $r = \frac{\bar{\alpha}_{ij}}{\bar{\beta}_{ij}}$ which is the same for every i, j , $i = 3, 4, \dots, s+1$ and $j = 2, 3, \dots, i-1$, becomes a feasible CP coefficient of CPRKN(s, p). Hence, r must satisfy the conditions:

$$r \leq \frac{\bar{v}_i}{\bar{w}_i}, \quad i = 2, 3, \dots, s+1. \quad (71)$$

Therefore, the following slight modification of Theorem 1 holds.

Theorem 2. *If f satisfies conditions (7), (8) and (9) of the FE method, then y_{n+1}^{sub} of CPRKN(s, p) method (36) satisfies the CP property*

$$\|y_{n+1}^{\text{sub}} - \tilde{y}_{n+1}^{\text{sub}}\| \leq \|y'_n - \tilde{y}'_n\| \leq \|y_n^{\text{sub}} - \tilde{y}_n^{\text{sub}}\|$$

provided

$$\Delta t \leq c(\bar{\mathbf{v}}_r, \bar{\mathbf{w}}_r, \bar{\boldsymbol{\alpha}}_r, \bar{\boldsymbol{\beta}}_r) \Delta t_{\text{FE}},$$

where

- $c(\bar{\mathbf{v}}_r, \bar{\mathbf{w}}_r, \bar{\boldsymbol{\alpha}}_r, \bar{\boldsymbol{\beta}}_r)$ is equal to

$$r = \frac{\bar{\alpha}_{ij}}{\bar{\beta}_{ij}}, \quad \begin{cases} i = 3, 4, \dots, s+1, \\ j = 2, 3, \dots, i-1, \end{cases} \quad (72)$$

and satisfies conditions (71),

under the assumption that all coefficients of (36) are nonnegative, with the convention that ratios $a/0 = +\infty$, and ratios $0/0$ are ignored.

5. CONTRACTIVITY PRESERVING (CP) FORM OF y'_{n+1} OF CPRKN(s, p) FOR DERIVING CP PROPERTY

Similar to the Shu–Osher form of RK methods [12], equation (15) of y'_{n+1} can be written in the following CP form,

$$y'_{n+1} = \alpha_{s+1,1} y'_n + \Delta t \beta_{s+1,1} y''_n + \sum_{j=2}^s \left[\alpha_{s+1,j} Y_j^{\text{sub}} + \Delta t \beta_{s+1,j} Y_j'' \right], \quad (73)$$

with consistency condition:

$$\alpha_{s+1,1} + \sum_{j=2}^s \alpha_{s+1,j} c_j = 1. \quad (74)$$

To find the relation between the CP form and the usual form coefficients, comparing (73) with (15), we have the following relations between the CP form coefficients and the usual form coefficients (here Y_j^{sub} , $j = 2, 3, \dots, s$ in (73) are replaced by the formula (36) for $j = 2, 3, \dots, s$, respectively),

$$\left. \begin{aligned} \beta_{s+1,j} &= b_j - \left(\sum_{k=j+1}^s \alpha_{s+1,k} \bar{a}_{kj} \right) \\ \alpha_{s+1,j} &= r \beta_{s+1,j} \end{aligned} \right\} j = s, s-1, \dots, 2, \quad (75)$$

$$\left. \begin{aligned} \beta_{s+1,1} &= b_1 - \left(\sum_{k=2}^s \alpha_{s+1,k} \bar{a}_{k1} \right) \\ \alpha_{s+1,1} &= 1 - \left(\sum_{k=2}^s \alpha_{s+1,k} c_k \right) \end{aligned} \right\} j = 1. \quad (76)$$

Using the order mentioned above of substitution operations, relations (75) and (76) allow a simple transformation of the usual coefficients of (15) to convenient CP coefficients of (73) for deriving CP property.

It is to be noted that one can also obtain relations (75) and (76) by using naturally the canonical CP form (67) and the form (68) with \bar{b}_i (in $\bar{\beta}_0$ and \bar{w}_0) replaced by b_i , $i = 1, 2, \dots, s$.

Form (73) is called the CP form of y'_{n+1} . We can rearrange y'_{n+1} in (73) as follows:

$$y'_{n+1} = \alpha_{s+1,1} \left[y'_n + \Delta t \frac{\beta_{s+1,1}}{\alpha_{s+1,1}} y''_n \right] + \sum_{j=2}^s \alpha_{s+1,j} \left[Y_j^{\text{sub}} + \Delta t \frac{\beta_{s+1,j}}{\alpha_{s+1,j}} Y_j'' \right], \quad (77)$$

with consistency condition (74).

Thus we obtain the difference $y'_{n+1} - \tilde{y}'_{n+1}$ from (77) as follows:

$$\begin{aligned} y'_{n+1} - \tilde{y}'_{n+1} &= \alpha_{s+1,1} \left[\left(y'_n + \Delta t \frac{\beta_{s+1,1}}{\alpha_{s+1,1}} y''_n \right) - \left(\tilde{y}'_n + \Delta t \frac{\beta_{s+1,1}}{\alpha_{s+1,1}} \tilde{y}''_n \right) \right] \\ &+ \sum_{j=2}^s \alpha_{s+1,j} \left[\left(Y_j^{\text{sub}} + \Delta t \frac{\beta_{s+1,j}}{\alpha_{s+1,j}} Y_j'' \right) - \left(\tilde{Y}_j^{\text{sub}} + \Delta t \frac{\beta_{s+1,j}}{\alpha_{s+1,j}} \tilde{Y}_j'' \right) \right]. \end{aligned} \quad (78)$$

To find the CP coefficient of y'_{n+1} of CPRKN(s, p), it is natural and useful to consider a particular CP form (77) where $(\alpha_{s+1,j}, \beta_{s+1,j})$, $j = 2, 3, \dots, s$ satisfy the same ratio r defined in (61) for \mathbf{Y}^{sub} ,

$$r = \frac{\alpha_{s+1,j}}{\beta_{s+1,j}}, \quad j = 2, 3, \dots, s \quad \text{and} \quad r \leq \frac{\alpha_{s+1,1}}{\beta_{s+1,1}}. \quad (79)$$

Provided all the coefficients of (77) are nonnegative, the following straightforward extension of a result presented in [2, 5] holds.

Theorem 3. *If f satisfies conditions (7), (8) and (9) of the FE method, then y'_{n+1} of (77) of CPRKN(s, p) method satisfies the CP property*

$$\|y'_{n+1} - \tilde{y}'_{n+1}\| \leq \|y'_n - \tilde{y}'_n\|$$

provided

$$\Delta t \leq c'_{\text{feasible}} \Delta t_{\text{FE}},$$

where the *feasible CP coefficient* c'_{feasible} is equal to r of (79) under the assumption that all coefficients of (77) are nonnegative, with the convention that the ratios $a/0 = +\infty$, and the ratios $0/0$ are ignored.

Proof. The proof of this theorem is similar to the proof of theorem 1.

It is to be noted here that each representation (77) of y'_{n+1} (to obtain y'_{n+1} to order p) with coefficients $\alpha_{s+1,j}, \beta_{s+1,j}$ will produce a feasible CP coefficient, c'_{feasible} , defined in Theorem 3 and a *feasible* y'_{n+1} of CPRKN(s, p) in CP form (77). What we really want is not merely a feasible y'_{n+1} of method CPRKN(s, p) in CP form but a best y'_{n+1} . This question will be considered in Section 6.

6. OPTIMIZING CP COEFFICIENT $c(\text{CPRKN}(s, p))$ OF CPRKN(s, p)

We can now formulate the problem to optimize simultaneously

- formulae for $Y_i^{\text{sub}}, i = 2, 3, \dots, s + 1$ using the CP form (68) which is written solely in terms of the vectors and matrices of the usual form,
- formula for y'_{n+1} , using the usual form (15) and the CP form (77),

and obtain the CP coefficient $c(\text{CPRKN}(s, p))$.

Hence, the problem of optimizing CPRKN(s, p) can be formulated as

$$\text{maximize } r, \tag{80}$$

subject to

- the componentwise inequalities for Y_i^{sub} ,

$$\bar{v}_r = (\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{v}_0 \geq 0, \tag{81}$$

$$\bar{w}_r = (\mathbf{I} + r\bar{\beta}_0)^{-1} \bar{w}_0 \geq 0, \tag{82}$$

$$\bar{\beta}_r = \bar{\beta}_0 (\mathbf{I} + r\bar{\beta}_0)^{-1} \geq 0, \tag{83}$$

together with conditions (71) and order conditions mentioned in (32) for RKN(s, p) to obtain $Y_{s+1} = y_{n+1}$ to order p ,

- the following inequalities for y'_{n+1} ,

$$b_i \geq 0, \quad i = 1, 2, \dots, s, \quad (84)$$

$$\alpha_{s+1,j} \geq 0, \quad j = 1, 2, \dots, s, \quad (85)$$

$$\beta_{s+1,j} \geq 0, \quad j = 1, 2, \dots, s, \quad (86)$$

together with conditions (79) and order conditions mentioned in (32) for RKN(s, p) to obtain y'_{n+1} to order p .

Here a maximized r is the CP coefficient $c(\text{CPRKN}(s, p))$.

Since the consistency condition (70) is satisfied, condition (81) is equivalent to the following condition, in vector notation,

$$r\bar{\beta}_0 (\mathbf{I} + r\bar{\beta}_0)^{-1} \mathbf{e}_{s+1} \leq \mathbf{e}_{s+1}.$$

It is to be noted here that

- each representation of the canonical CP form (67) of \mathbf{Y}^{sub} with coefficients $(\bar{\mathbf{v}}_r, \bar{\mathbf{w}}_r, \bar{\boldsymbol{\alpha}}_r, \bar{\boldsymbol{\beta}}_r)$, which satisfy conditions (81)–(83) together with conditions (71) and order conditions mentioned in (32) for RKN(s, p) to obtain y_{n+1} to order p , will produce a feasible CP coefficient $r = c(\bar{\mathbf{v}}_r, \bar{\mathbf{w}}_r, \bar{\boldsymbol{\alpha}}_r, \bar{\boldsymbol{\beta}}_r)$ and a feasible Y_i^{sub} , $i = 2, 3, \dots, s + 1$, in CP form (36),
- each representation of the CP form (77) of y'_{n+1} with coefficients $b_i, \alpha_{s+1,j}, \beta_{s+1,j}$ which satisfy conditions (84)–(86) together with conditions (79) and order conditions mentioned in (32) for RKN(s, p) to obtain y'_{n+1} to order p , will produce a feasible CP coefficient r and a feasible y'_{n+1} , in CP form (77).

7. INTERVALS OF ABSOLUTE STABILITY OF CPRKN(4, 4) AND CPRKN(6, 6)

To obtain the numerical stability of the new methods, we consider the linear test equation

$$y' = \lambda y, \quad y_0 = 1, \quad (87)$$

similar to Huang and Innanen [6].

For given numbers s and p of CPRKN(s, p), we have the following equations:

1. the difference equation and corresponding characteristic equation

$$\eta_0(z) y_n + \eta_1(z) y_{n+1} = 0, \quad \eta_0(z) y_n + \eta_1(z) r = 0, \quad (88)$$

(for y of CPRKN(s, p)) obtained by applying the predictors P_2, P_3, \dots, P_s (13) and the integration formula IF (14) with constant step size h to the test equation (87). Here $z = \lambda h$.

Table 1: Intervals of absolute stability for y and y' of CPRKN(4,4) and of CPRKN(6,6) respectively.

Method	Interval of absolute stability for	
	y	y'
CPRKN(4,4)	$(-3.92, 0)$	$(-4.00, 0)$
CPRKN(6,6)	$(-4.96, 0)$	$(-4.96, 0)$

2. the difference equation and corresponding characteristic equation

$$\eta'_0(z) y_n + \eta'_1(z) y_{n+1} = 0, \quad \eta'_0(z) y_n + \eta'_1(z) r = 0, \quad (89)$$

(for y') obtained by applying the predictors P_2, P_3, \dots, P_s and the integration formula IF' (15).

Similar to Dormand *et al.* [1], we have two regions of absolute stability \mathcal{R} and \mathcal{R}' : a complex number z is in \mathcal{R} for y and \mathcal{R}' for y' if the root of the characteristic equation in (88) and (89), respectively, satisfies the root condition (see [9, pp. 70]).

The scanning method used to find the regions of absolute stability is similar to the one used for Runge–Kutta methods (see [9]).

The intervals of absolute stability for y and y' of CPRKN(4,4) and of CPRKN(6,6), respectively, are shown in Table 1.

8. NUMERICAL RESULTS

The relative energy error (EE(t)) at time t is defined as

$$EE(t) = \left| \frac{E(t) - E(0)}{E(0)} \right|, \quad (90)$$

where $E(t)$ is the energy at time t .

We compare the relative energy error (EE(t)) as a function of number of function evaluations (NFE) of CPRKN(4,4), CPRKN(6,6), Dormand–El-Mikkawy–Prince DEP(4,3)4FM and DEP(6,4)6FM [1] after a 1000 periods integration of a Hamiltonian system (Huang and Innanen [6]) using fixed step sizes.

Tables 2, 3 and 4 list relative energy errors (EE) at $t = 2000\pi$ as a function of number of function evaluations (NFE) for CPRKN(4,4), CPRKN(6,6), DEP(4,3)4FM and DEP(6,4)6FM after a 1000 periods integration of Kepler's two-body problem with eccentricities $e = 0.3, 0.5, 0.7$ respectively. It is seen, from Tables 2, 3 and

Table 2: Relative energy error (EE) at $t = 2000\pi$ as a function of number of function evaluations (NFE) after a 1000 periods integration of Kepler’s two-body problem with eccentricity $e = 0.3$.

NFE	Relative energy error in		NFE	Relative energy error in	
	CPRKN(4, 4)	DEP(4,3)4FM		CPRKN(6, 6)	DEP(6,4)6FM
2.24e+05	3.55e-04	2.82e-03	1.50e+05	4.48e-04	5.75e-04
7.44e+05	8.99e-07	7.00e-06	2.64e+05	9.30e-06	1.11e-05
1.26e+06	6.36e-08	4.95e-07	3.78e+05	7.70e-07	9.04e-07
1.78e+06	1.14e-08	8.85e-08	4.92e+05	1.23e-07	1.43e-07
2.30e+06	3.16e-09	2.47e-08	6.06e+05	2.86e-08	3.35e-08
2.82e+06	1.14e-09	8.92e-09	7.20e+05	8.59e-09	1.00e-08
3.34e+06	4.91e-10	3.83e-09	8.34e+05	3.07e-09	3.60e-09
3.86e+06	2.38e-10	1.86e-09	9.48e+05	1.25e-09	1.47e-09
4.38e+06	1.27e-10	9.90e-10	1.06e+06	5.67e-10	6.65e-10
4.90e+06	7.22e-11	5.65e-10	1.18e+06	2.78e-10	3.26e-10
5.42e+06	4.38e-11	3.42e-10	1.29e+06	1.45e-10	1.71e-10

4, that CPRKN(4,4) and CPRKN(6,6) compare favorably with DEP(4,3)4FM and DEP(6,4)6FM.

The *NFE percentage efficiency gain* (NFE PEG) is defined by the formula (cf. Sharp [11]),

$$(\text{NFE PEG}) = 100 \sum_j \left[\frac{\text{NFE}_{1,j}}{\text{NFE}_{2,j}} - 1 \right], \quad (91)$$

where $\text{NFE}_{1,j}$ and $\text{NFE}_{2,j}$ are the NFE of methods 1 and 2, respectively, associated with a given problem P, and $j = -\log_{10}(\text{EE})$. The NFE was obtained from the curves which fit, in a least-squares sense, the data $(\log_{10}(\text{EE}), \log_{10}(\text{NFE}))$ by means of MATLAB’s `polyfit`.

Table 5 lists the NFE PEGs of CPRKN(4,4) and CPRKN(6,6) over DEP(4,3)4FM and DEP(6,4)6FM after a 1000 periods integration of Kepler’s two-body problem with $e = 0.3, 0.5, 0.7$ respectively. It is seen that CPRKN(4, 4) wins over DEP(4,3)4FM and CPRKN(6, 6) is similar to DEP(6,4)6FM.

Table 3: Relative energy error (EE) at $t = 2000\pi$ as a function of number of function evaluations (NFE) after a 1000 periods integration of Kepler's two-body problem with eccentricity $e = 0.5$.

NFE	Relative energy error in		NFE	Relative energy error in	
	CPRKN(4, 4)	DEP(4,3)4FM		CPRKN(6, 6)	DEP(6,4)6FM
7.20e+05	2.65e-05	2.03e-04	4.80e+05	1.34e-05	1.70e-05
1.55e+06	5.81e-07	4.43e-06	7.20e+05	8.05e-07	9.98e-07
2.38e+06	6.84e-08	5.21e-07	9.60e+05	1.08e-07	1.33e-07
3.20e+06	1.53e-08	1.17e-07	1.20e+06	2.28e-08	2.80e-08
4.03e+06	4.86e-09	3.70e-08	1.44e+06	6.38e-09	7.83e-09
4.86e+06	1.91e-09	1.46e-08	1.68e+06	2.17e-09	2.67e-09
5.69e+06	8.70e-10	6.63e-09	1.92e+06	8.54e-10	1.05e-09
6.52e+06	4.41e-10	3.36e-09	2.16e+06	3.75e-10	4.60e-10
7.34e+06	2.43e-10	1.85e-09	2.40e+06	1.79e-10	2.20e-10
8.17e+06	1.42e-10	1.08e-09	2.64e+06	9.20e-11	1.13e-10
9.00e+06	8.79e-11	6.69e-10	2.88e+06	5.02e-11	6.15e-11

Table 4: Relative energy error (EE) at $t = 2000\pi$ as a function of number of function evaluations (NFE) after a 1000 periods integration of Kepler's two-body problem with eccentricity $e = 0.7$.

NFE	Relative energy error in		NFE	Relative energy error in	
	CPRKN(4, 4)	DEP(4,3)4FM		CPRKN(6, 6)	DEP(6,4)6FM
1.04e+06	4.23e-04	3.29e-03	1.08e+06	2.77e-05	3.59e-05
2.74e+06	3.45e-06	2.61e-05	1.50e+06	2.85e-06	3.61e-06
4.43e+06	3.11e-07	2.35e-06	1.92e+06	5.11e-07	6.43e-07
6.13e+06	6.15e-08	4.65e-07	2.34e+06	1.29e-07	1.61e-07
7.82e+06	1.81e-08	1.37e-07	2.76e+06	4.06e-08	5.09e-08
9.52e+06	6.80e-09	5.14e-08	3.18e+06	1.51e-08	1.89e-08
1.12e+07	3.00e-09	2.26e-08	3.60e+06	6.34e-09	7.94e-09
1.29e+07	1.48e-09	1.12e-08	4.02e+06	2.93e-09	3.67e-09
1.46e+07	8.00e-10	6.05e-09	4.44e+06	1.46e-09	1.83e-09
1.63e+07	4.62e-10	3.49e-09	4.86e+06	7.78e-10	9.75e-10
1.80e+07	2.81e-10	2.13e-09	5.28e+06	4.35e-10	5.46e-10

Table 5: NFE PEG of CPRKN(4,4) over DEP(4,3)4FM and CPRKN(6,6) over DEP(6,4)6FM after a 1000 periods integration of Kepler’s two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$, respectively.

NFE PEG over DEP(4,3)4FM for two-body problem with:			
method	$e = 0.3$	$e = 0.5$	$e = 0.7$
CPRKN(4,4)	51 %	50 %	50 %
NFE PEG over DEP(6,4)6FM for two-body problem with:			
method	$e = 0.3$	$e = 0.5$	$e = 0.7$
CPRKN(6,6)	2 %	3 %	3 %

9. CONCLUSION

We constructed new optimal, explicit, s -stage Runge–Kutta–Nystrom method of order p , $p = 3, 4, \dots, 6$ (CPRKN(s, p)), that have contractivity-preserving properties and nonnegative coefficients.

On the basis of NFE versus the relative energy error, selected CPRKN(4,4) and CPRKN(6,6) compare favorably with Dormand–El-Mikkawy–Prince DEP(4,3)4FM and DEP(6,4)6FM, respectively, in solving Kepler’s problem with varying eccentricity over an interval of 1000 periods.

In the light of the results obtained in this paper, these new CPRKN(s, p), $p = 3, 4, \dots, 6$ appear to be promising solvers which can be combined with Taylor series or CP HO series methods developed earlier [10] to form new higher order methods with contractivity-preserving (CP) properties and nonnegative coefficients for solving efficiently the second-order system of non-stiff ordinary differential equations.

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A. COEFFICIENTS OF CPRKN(s, p), $p = 3, 4, \dots, 6$

The appendix lists the usual form of five new CPRKN(s, p) methods with their CP coefficient $c(\text{CPRKN}(s, p))$.

CPRKN(2,3). $c(\text{CPRKN}(2,3)) = 1.5$.

0	\bar{a}_{ij}	
$\frac{2}{3}$	$\frac{2}{9}$	
\bar{b}_i	$\frac{1}{4}$	$\frac{1}{4}$
b_i	$\frac{1}{4}$	$\frac{3}{4}$

CPRKN(3,4). $c(\text{CPRKN}(3,4)) = 2.2542293787479135$.

0	\bar{a}_{ij}		
$\frac{5703594}{16064153}$	$\frac{547322}{8683431}$		
$\frac{10360559}{12261757}$	$\frac{112823}{2496535}$	$\frac{4709345}{15104824}$	
\bar{b}_i	$\frac{1}{9}$	$\frac{1885193}{5703594}$	$\frac{499307}{8555391}$
b_i	$\frac{1}{9}$	$\frac{20603748}{40203547}$	$\frac{2862467}{7604792}$

CPRKN(4,4). $c(\text{CPRKN}(4,4)) = 2.4743852177875874$.

0	\bar{a}_{ij}			
$\frac{26971918}{107581049}$	$\frac{11868682}{377642077}$			
$\frac{58977037}{101250069}$	$\frac{972878}{65595991}$	$\frac{41074969}{265316004}$		
$\frac{23277231}{26105459}$	$\frac{83526627}{846839644}$	$\frac{44674505}{248163904}$	$\frac{15185060}{127738057}$	
\bar{b}_i	$\frac{26994554}{328987169}$	$\frac{53393375}{207511886}$	$\frac{208549974}{1569486133}$	$\frac{25168925}{906469463}$
b_i	$\frac{17891713}{218049315}$	$\frac{14894263}{43373362}$	$\frac{40778691}{128129371}$	$\frac{27846884}{108654621}$

CPRKN(5,5). $c(\text{CPRKN}(5,5)) = 2.4307903085928104.$

0					
$\frac{68909267}{178744101}$	$\frac{31624111}{425555783}$				\bar{a}_{ij}
$\frac{13013228}{65692391}$	$\frac{2299759}{274780277}$	$\frac{5514383}{490121757}$			
$\frac{119047355}{176052511}$	$\frac{1570365}{104029019}$	$\frac{20347847}{284778633}$	$\frac{12591039}{88620110}$		
$\frac{69512934}{74012023}$	$\frac{12808156}{182165325}$	$\frac{4231711}{164606135}$	$\frac{58976315}{260757231}$	$\frac{182143463}{1532329653}$	
\bar{b}_i	$\frac{14520741}{223581817}$	$\frac{11229819}{101906302}$	$\frac{46531259}{226905735}$	$\frac{31617786}{287289619}$	$\frac{10588203}{1087932953}$
b_i	$\frac{14520741}{223581817}$	$\frac{16327696}{91046147}$	$\frac{69883863}{273275923}$	$\frac{19674557}{57884909}$	$\frac{15571109}{97257192}$

CPRKN(6,6) with $c(\text{CPRKN}(6,6)) = 2.4672918884438562.$

0						
$\frac{6648706}{39027077}$	$\frac{3999571}{275613952}$				\bar{a}_{ij}	
$\frac{30648937}{79250275}$	$\frac{1350862}{522581577}$	$\frac{9232128}{127873411}$				
$\frac{75321914}{105966849}$	$\frac{20814370}{224800513}$	$\frac{10697606}{442107819}$	$\frac{47016859}{346130514}$			
$\frac{6255665}{10780901}$	$\frac{2905627}{204565870}$	$\frac{18175723}{134876122}$	$\frac{3672823}{307407819}$	$\frac{1030929}{138615316}$		
$\frac{469000023}{506551154}$	$\frac{16231130}{578987087}$	$\frac{3336798}{14855867}$	$\frac{43589951}{610836173}$	$\frac{8006719}{151269626}$	$\frac{8085943}{156460637}$	
\bar{b}_i	$\frac{10892061}{206668234}$	$\frac{252458291}{1241932224}$	$\frac{14535418}{137797841}$	$\frac{55242801}{1159422986}$	$\frac{10863867}{140225018}$	$\frac{4041093}{301275815}$
b_i	$\frac{10892061}{206668234}$	$\frac{139166744}{567979543}$	$\frac{24185509}{140610440}$	$\frac{40325482}{244756631}$	$\frac{30769025}{166702063}$	$\frac{106285627}{587407756}$

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