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Research article

A novel class of Runge-Kutta-Nyström pairs sharing orders 8(6).

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Abstract: We are examining a second-order system of non-stiff Initial Value Problems (IVP), focusing on a scenario where the first derivatives are not present. In the realm of solving IVPs, Runge-Kutta-Nyström (RKN) pairs have proven to be highly effective. In order to achieve a pair with eighth and sixth order accuracy, we need to find a solution to a well-defined set of equations regarding the coefficients. Traditionally, pairs are constructed to go through eight stages per step. However, we propose a novel approach with nine stages per step, which enables the creation of pairs with orders 8 and 6 that have notably smaller truncation errors. Our paper introduces a new pair that, as expected, outperforms existing pairs of the same orders in a range of important problems.

Keywords: initial Value Problem; second order; Runge-Kutta-Nyström
Mathematics Subject Classification: 65L06

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1. Introduction

In this context, we are examining specific Second-order Initial Value Problems (IVP) described by the following equation:

$$\psi'' = \phi(t,\psi), \psi(t_0) = \psi_0, \text{ and } \psi'(t_0) = \psi'_0 \tag{1.1}$$

In this scenario, $\phi : \mathbb{R}\times\mathbb{R}^m \to \mathbb{R}^m$ represents a function that is both continuous and differentiable, and we have $(\psi_0, \psi'_0) \in \mathbb{R}^{2m}$.

Our approach involves approximating the solution to problem (1.1) at a series of distinct points (t_n, ψ_n, ψ'_n) using an explicit Runge-Kutta-Nyström method with an algebraic order denoted as p. Here is an overview of the method's structure:

$$\phi_i = \phi(t_n + \lambda_i\kappa_n, \psi_n + \lambda_i\kappa_n\psi'_n + \kappa_n^2 \sum_{j=1}^{i-1} \theta_{ij}\phi_j), \quad i = 1, 2, \cdots, s$$

$$\psi_{n+1} = \psi_n + \kappa_n\psi'_n + \kappa_n^2 \textstyle\sum_{i=1}^{s} \zeta_i\phi_i,$$
$$\psi'_{n+1} = \psi'_n + \kappa_n \textstyle\sum_{i=1}^{s} \zeta'_i\phi_i,$$

where $\kappa_n = t_{n+1} - t_n$, representing the step size. Throughout the last five decades, there has been a persistent and lasting fascination with these techniques, as illustrated by the contributions of E. Fehlberg [1], Dormand and colleagues [2, 3], El-Mikkawy and Rahmo [4], Papageorgiou and his team [5], Papakostas and collaborators [6], and Simos along with others [7]. Furthermore, there have been introductions of RKN methods boasting unique characteristics. Houven and colleagues delved into RKN methods that minimize phase lags, while Calvo and Sanz-Serna [8], Yoshida [9], and Tsitouras [10] devised RKN algorithms with the symplectic attribute. Numerov type methods may also be selected for addressing such problems [11].

In the upcoming discussion, we establish the value of p as eight and augment this approach with an additional formula of sixth order. As a result, we also compute a fifth-order estimate, utilizing the same values of ϕ_i in the following manner:

$$\hat{\psi}_{n+1} = \psi_n + \kappa_n\psi'_n + \kappa_n^2 \textstyle\sum_{i=1}^{s} \hat{\zeta}_i\phi_i,$$
$$\hat{\psi}'_{n+1} = \psi'_n + \kappa_n \textstyle\sum_{i=1}^{s} \hat{\zeta}'_i\phi_i.$$

In all instances, we utilize the more precise approximations, namely ψ_n and ψ'_n, to progress in time with the solutions.

Consequently, we derive an error estimate as:

$$\mu = ||\psi_{n+1} - \hat{\psi}_{n+1}|| = O(\kappa^7).$$

We then make a comparison between μ and tolerance τ, a small positive value specified by the user. This user-defined value, referred to as the tolerance, enables us to estimate the length of the upcoming step using the following formula:

$$\kappa_{n+1} = 0.9 \cdot \kappa_n \cdot \left(\frac{\tau}{\mu}\right)^{1/7}, \tag{1.2}$$

The procedure for adjusting this step is a widely accepted practice for RKN8(6) pairs [2, 12]. If τ is less than μ, we abstain from advancing the solution. Instead, we essentially reiterate the current step, but this time, we employ κ_{n+1} as the updated, shorter step size, replacing κ_n.

For representing the coefficients, the Butcher tableau serves as a valuable tool [13]. Consequently, the method is structured as:

$$\begin{array}{c|c} \lambda & \Theta \\ \hline & \zeta, \hat{\zeta} \\ & \zeta', \hat{\zeta}' \end{array}$$

In this arrangement, $\Theta \in \mathbb{R}^{s\times s}$, and $\zeta^{\mathrm{T}}, \hat{\zeta}^{\mathrm{T}}, \zeta'^{\mathrm{T}}, \hat{\zeta}'^{\mathrm{T}}, \lambda \in \mathbb{R}^{s}$, with the weights represented as row vectors.

In the following context, we consider a pair involving nine stages ($s = 9$). The Butcher tableau given in Table 1 displays its coefficients.

Table 1. The Butcher tableau associated with the 9 stages RKN pairs sharing orders 8(6).

0									
λ_2	θ_{21}								
λ_3	θ_{31}	θ_{32}							
λ_4	θ_{41}	θ_{42}	θ_{43}						
λ_5	θ_{51}	θ_{52}	θ_{53}	θ_{54}					
λ_6	θ_{61}	θ_{62}	θ_{63}	θ_{64}	θ_{65}				
λ_7	θ_{71}	θ_{72}	θ_{73}	θ_{74}	θ_{75}	θ_{76}			
1	θ_{81}	θ_{82}	θ_{83}	θ_{84}	θ_{85}	θ_{86}	θ_{87}		
1	θ_{91}	θ_{92}	θ_{93}	θ_{94}	θ_{95}	θ_{96}	θ_{97}	0	
8th-order ζ	ζ_1	0	ζ_3	ζ_4	ζ_5	ζ_6	ζ_7	0	0
6th-order $\hat{\zeta}$	$\hat{\zeta}_1$	0	$\hat{\zeta}_3$	$\hat{\zeta}_4$	$\hat{\zeta}_5$	$\hat{\zeta}_6$	$\hat{\zeta}_7$	0	0
8th-order ζ'	ζ'_1	0	ζ'_3	ζ'_4	ζ'_5	ζ'_6	ζ'_7	ζ'_8	ζ'_9
6th-order $\hat{\zeta}'$	$\hat{\zeta}'_1$	0	$\hat{\zeta}'_3$	$\hat{\zeta}'_4$	$\hat{\zeta}'_5$	$\hat{\zeta}'_6$	$\hat{\zeta}'_7$	$\hat{\zeta}'_8$	$\hat{\zeta}'_9$

RKN pairs with orders eight and six, effectively utilizing eight stages per step, were investigated in [3] and [6]. The pairs given there may represented with the same Table 1 but with $\theta_{9j} = \zeta_j$ for $j = 1, 2, \cdots, 8$. By employing such a technique, we only require eight stages per step, as the final stage is recycled as the first stage in the subsequent step. This is commonly referred to as FSAL, which stands for "First Stage As Last".

Eighth-order RKN methods with only seven stages per step have been developed exclusively for the specific case of linear inhomogeneous problems, as mentioned in [14].

2. Runge-Kutta-Nyström methods of eighth order

We utilize an RKN method for (1.1) and make use of the Taylor series expansions for $\psi(t_n+\kappa)-\psi_{n+1}$ and $\psi'(t_n+\kappa)-\psi'_{n+1}$. When aligning expressions up to h^8 for an eighth-order method, the subsequent outcomes are derived:

$$\psi(t_n+\kappa)-\psi_{n+1} = \kappa^2\xi_{2,1}G_{2,1} + \kappa^3\xi_{3,1}G_{3,1} + \cdots + \kappa^8\left(\xi_{8,1}G_{8,1} + \ldots + \xi_{8,20}G_{8,20}\right) + O\left(\kappa^9\right) \tag{2.1}$$

$$\psi'(t_n+\kappa)-\psi'_{n+1}=\kappa\tilde{\xi}_{1,1}G_{1,1}+\kappa^2\tilde{\xi}_{2,1}G_{2,1}+\cdots+\kappa^8\left(\tilde{\xi}_{8,1}G_{8,1}+\ldots+\tilde{\xi}_{8,36}G_{8,36}\right)+O\left(\kappa^9\right) \tag{2.2}$$

The expressions ξ_{ij} depend on ζ, Q, λ, while $\tilde{\xi}_{ij}$ are contingent on ζ', Q, λ. An algorithm for their symbolic derivation is provided in [15]. The expressions Gij involve elementary differentials concerning ψ', ϕ, and their partial derivatives. These elementary differentials are inherent to the problem and are beyond the method's control. However, for an eighth-order RKN method, it becomes necessary to eliminate the coefficients ξ_{ij} and $\tilde{\xi}_{ij}$ in the expressions (2.1-2.2) to achieve the desired level of accuracy. In Table 2, we enumerate the quantity of order conditions, which encompass both ξ_{ij} and $\tilde{\xi}_{ij}$ for each order. For instance, in a third algebraic order method, we need to satisfy $0+1+1=2$ equations for ψ and an additional $1+1+2=4$ order conditions for ψ'.

Table 2. Number of equations of conditions for RKN methods.

		order									
method	$\underbrace{\text{number of}}$ - order→	1	2	3	4	5	6	7	8	9	10
RKN	order conditions for ψ	0	1	1	2	3	6	10	20	36	72
	order conditions for ψ'	1	1	2	3	6	10	20	36	72	137

Upon examination of the Butcher tableau presented above, and in consideration of the available coefficients for a nine-stage method, when compared to the order conditions up to the eighth order as indicated in Table 2, it becomes evident that we have an insufficient number of coefficients. Therefore, we proceed by introducing several simplifying assumptions aimed at significantly reducing the number of order conditions.

First and foremost, we establish the equation:

$$\zeta=\zeta'\cdot(I_s-\lambda), \tag{2.3}$$

Here, $I_s\in\mathbb{R}^{s\times s}$ represents the identity matrix, and $\Lambda=\mathrm{diag}(\lambda)$. With this assumption in place, we automatically satisfy the order conditions for ψ after removing the equations of the same order for ψ'. Our primary objective is to eliminate only $\tilde{\xi}_{ij}$ concerning ζ', Θ, λ.

Once again, when we sum the values in the last row of Table 2, it becomes apparent that we still have an excess of conditions compared to the available coefficients. Hence, we proceed by introducing the following assumptions:

$$\Theta\cdot\mathbb{I}=\frac{1}{2}\lambda^2,\ \Theta\cdot\lambda=\frac{1}{6}\lambda^3,\ \Theta\cdot\lambda^2=\frac{1}{12}\lambda^4, \tag{2.4}$$

Here, λ^i signifies componentwise matrix multiplication (i.e., Hadamard multiplication), while $\lambda^0=\mathbb{I}=[1,1,\cdots,1]^T\in\mathbb{R}^s$. It's important to note that this multiplication operation takes precedence over the dot product.

Additionally, we take into account the row simplification condition for RKN methods.

$$\zeta'\cdot(\Theta+\Lambda-\frac{1}{2}(\lambda\circ\lambda)-\frac{1}{2}I_s)=0_s$$

with $0_s\in\mathbb{R}^{s\times s}$ a matrix with zero entries. Finally we introduce the subsidiary simplifying assumptions

$$(\zeta\cdot\Theta)_2=0,\ (\zeta'\cdot\Theta)_2=0,\ (\zeta'\cdot(\lambda\circ\lambda)\cdot\Theta)_2=0,\ (\hat{\zeta}\cdot\Theta)_2=0.$$

Subsequently, we significantly reduce the quantity of order conditions, allowing us to proceed with the derivation of the coefficients for an eighth-order method (namely, ζ, ζ', Θ and λ) using the following algorithm.

BEGIN ALGORITHM
Select arbitrary values for the coefficients $\zeta_9', \theta_{85}, \theta_{86}, \theta_{87}, \theta_{92}, \lambda_4, \lambda_5, \lambda_6$ and λ_7.
Then compute successively and explicitly

$$\lambda_3 = \frac{\left\{\begin{array}{c} 15 - 20\lambda_4 - 20\lambda_5 + 28\lambda_4\lambda_5 - 20\lambda_6 + 28\lambda_4\lambda_6 + 28\lambda_5\lambda_6 - 42\lambda_4\lambda_5\lambda_6 \\ -20\lambda_7 + 28\lambda_4\lambda_7 + 28\lambda_5\lambda_7 - 42\lambda_4\lambda_5\lambda_7 + 28\lambda_6\lambda_7 \\ -42\lambda_4\lambda_6\lambda_7 - 42\lambda_5\lambda_6\lambda_7 + 70\lambda_4\lambda_5\lambda_6\lambda_7 \end{array}\right\}}{\left\{\begin{array}{c} 2(10 - 14\lambda_4 - 14\lambda_5 + 21\lambda_4\lambda_5 - 14\lambda_6 + 21\lambda_4\lambda_6 + 21\lambda_5\lambda_6 \\ -35\lambda_4\lambda_5\lambda_6 - 14\lambda_7 + 21\lambda_4\lambda_7 + 21\lambda_5\lambda_7 - 35\lambda_4\lambda_5\lambda_7 \\ +21\lambda_6\lambda_7 - 35\lambda_4\lambda_6\lambda_7 - 35\lambda_5\lambda_6\lambda_7 + 70\lambda_4\lambda_5\lambda_6\lambda_7) \end{array}\right\}}$$

$$\lambda_2 = \frac{1}{2}\lambda_3$$

Solve Vandermonde equations

$$\zeta' \cdot e = 1,\ \zeta' \cdot \lambda = \frac{1}{2},\ \zeta' \cdot \lambda^2 = \frac{1}{3},\ \zeta' \cdot \lambda^3 = \frac{1}{4},$$

$$\zeta' \cdot \lambda^4 = \frac{1}{5}, \zeta' \cdot \lambda^5 = \frac{1}{6},\ \zeta' \cdot \lambda^6 = \frac{1}{7},$$

for $\zeta_1', \zeta_3', \zeta_4', \zeta_5', \zeta_6', \zeta_7', \zeta_8'$. The last Vandermonde equation $\zeta' \cdot \lambda^7 = \frac{1}{8}$ since the choice of λ_3 inherently fulfills this condition. Then the vector ζ is found explicitly from (2.3).

Solve $(\Theta \cdot \lambda)_4 = \frac{\lambda_4^2}{2}$, $(\Theta \cdot \lambda^2)_4 = \frac{\lambda_4^3}{6}$, for θ_{42} and θ_{43}.
Solve $(\zeta \cdot \Theta)_2 = 0$, $(\zeta' \cdot \Theta)_2 = 0$, $(\zeta' \cdot (\lambda \circ \lambda) \cdot \Theta)_2 = 0$ and $(\hat{\zeta}' \cdot \Theta)_2 = 0$ for $\theta_{72}, \theta_{62}, \theta_{52}, \theta_{82}$.
Solve the following three integral equations

$$\begin{aligned} &\zeta' \cdot (\lambda - I_s) \cdot (\Lambda - \lambda_7 I_s) \cdot \Theta \cdot (\Lambda - \lambda_3 I_s).(\Lambda - \lambda_4 I_s) \cdot \lambda \\ = &\int_0^1 (x-1)(x-\Lambda_7) \int_0^x \int_0^x (x - x_3)(x - \lambda_4) x dx dx dx, \end{aligned}$$

$$\begin{aligned} &\zeta' \cdot (\Lambda - I_s) \cdot \Theta \cdot (\Lambda - \lambda_3 I_s) \cdot (\Lambda - \lambda_4 I_s).(\Lambda - \lambda_5 I_s) \cdot \lambda \\ = &\int_0^1 (x-1) \int_0^x \int_0^x (x - x_3)(x - \lambda_4)(x - \lambda_5) x dx dx dx, \end{aligned}$$

$$\begin{aligned} &\zeta' \cdot (\Lambda - I_s) \cdot \Theta \cdot (\Lambda - \lambda_3 I_s) \cdot (\Lambda - \lambda_4 I_s).(\Lambda - \lambda_5 I_s) \cdot \lambda \\ = &\int_0^1 (x-1) \int_0^x \int_0^x (x - x_3)(x - \lambda_4)(x - \lambda_5) x dx dx dx, \end{aligned}$$

for $\theta_{65}, \theta_{76}, \theta_{75}$.

Evaluate $\theta_{53}, \theta_{54}, \theta_{63}, \theta_{64}, \theta_{73}, \theta_{74}, \theta_{83}, \theta_{84}$ from $(\Theta \cdot \lambda)_j = \frac{\lambda_j^2}{2}$, $(\Theta \cdot \lambda^2)_j = \frac{\lambda_j^3}{6}$, for $j = 5, 6, 7, 8$.

Evaluate $\theta_{93}, \theta_{94}, \theta_{95}, \theta_{96}, \theta_{97}$ from $\zeta' \cdot (\Theta + \Lambda - \frac{1}{2}(\lambda \circ \lambda) - \frac{1}{2} I_s) = 0_s$ for its respective coordinates.

The first column of Θ is found by

$$\theta_{j1} = \frac{\lambda_j^2}{2} - \sum_{k=2}^{j-1} \theta_{jk}, \; j = 2, 3, \cdots, 9.$$

The vector $\hat{\zeta}'$ comes after solving the corresponding Vandermonde equations along with a remaining integral equation

END OF ALGORITHM

It is worth noting that this streamlined procedure has never been presented before. It proved to be highly advantageous in our process of deriving the pair.

3. Producing a RKN pair of orders 8 and 6

Using the algorithm outlined in the preceding section, we can establish an eighth-order RKN method while adhering to a practical limitation of eight stages per step. This method presents us with six free parameters, which we can leverage to optimize our new approach. Our primary objective is to minimize the terms related to the principal error components, specifically focusing on the Euclidean norm of the ninth-order coefficients $e_{9j},: j = 1, 2, \cdots, 36$ and $\tilde{e}_{9j},: j = 1, 2, \cdots, 72$, as they manifest in the series expansions (2.1-2.2).

In cases where double precision arithmetic is employed, the typical aim is to maintain the coefficients at the smallest feasible magnitude. Coefficients on the order of 10^3, function values at the scale of 10^2, and a tolerance level of $\varepsilon = 10^{-11}$ might strain the available digits. Nevertheless, when employing quadruple precision, we can effectively handle these more substantial coefficients while still preserving tolerances as low as around 10^{-23}. Allowing the coefficients to grow opens up the possibility for initiating a fresh minimization process [16].

Here we focus on double precision computations. In order to address our task, we make use of the Differential Evolution (DE) Algorithm [17, 18]. Differential Evolution represents an iterative process, where at each iteration, known as generation g, we work with a collective of "individuals" $\left(\hat{\zeta}_9'^{(g)}, \theta_{85}^{(g)}, \cdots, \lambda_4^{(g)}, \lambda_5^{(g)}, \lambda_6^{(g)}, \lambda_7^{(g)}\right)_i$, $i = 1, 2, \cdots, P$, with P being the population size. An initial population $\left(\zeta_9'^{(0)}, \theta_{85}^{(0)}, \cdots, \lambda_7^{(0)}\right)_i$, $i = 1, 2, \cdots, P$, is initially created in a random manner during the method's initial step. The fitness function we utilize is defined as follows:

$$s = \sqrt{\xi_{9,1}^2 + \xi_{9,2}^2 + \cdots + \xi_{9,36}^2} + \sqrt{\tilde{\xi}_{9,1}^2 + \tilde{\xi}_{9,2}^2 + \cdots + \tilde{\xi}_{9,72}^2} = \left\|\Xi^{(9)}\right\|_2 + \left\|\tilde{\Xi}'^{(9)}\right\|_2$$

This function quantifies the error associated with a ninth-order method and must be minimized for each individual within the initial population. The optimization process encompasses three phases: Differentiation, Crossover, and Selection. We utilized the DeMat software [19] implemented in MATLAB [20] to execute this technique. Achieving success in a single optimization run is not guaranteed; hence, we ran the procedure multiple times to obtain a solution. Subsequently, the results were further refined to enhance the level of accuracy, employing multi-precision arithmetic and the `NMinimize` function within `Mathematica` [21].

Details regarding the coefficients of the generated method and the integration algorithm utilized in the numerical tests are available in Table 3.

Table 3. Coefficients of the new pair RKNT8(6)9.

0									
$\frac{50636389}{704362245}$	$\frac{3599715}{1393043879}$								
$\frac{101272778}{704362245}$	$\frac{2007339}{582610979}$	$\frac{4014678}{582610979}$							
$\frac{5601632}{13092959}$	$\frac{205315767}{2298909916}$	$-\frac{173142329}{977467009}$	$\frac{138681326}{773264719}$						
$\frac{25660393}{34815795}$	$-\frac{723714874}{549460595}$	$\frac{2439854271}{741682162}$	$-\frac{1702861157}{866963471}$	$\frac{279702247}{1062332866}$					
$\frac{44986679}{52545954}$	$\frac{17756357945}{864039792}$	$-\frac{52998327383}{1059967031}$	$\frac{52493566912}{1639341693}$	$-\frac{3222015486}{1383105619}$	$\frac{134954744}{1084005543}$				
$\frac{14200983}{14248358}$	$-\frac{24139417776}{1745827307}$	$\frac{45957899000}{1361313679}$	$-\frac{13333762455}{626503381}$	$\frac{1619615115}{888431528}$	$\frac{6521545}{391548217}$	$\frac{9620282}{1413707653}$			
1	$-\frac{17114373398}{1072840941}$	$\frac{17619232321}{574444270}$	$-\frac{8358258209}{674963318}$	$-\frac{1686023083}{532011477}$	$-\frac{187948636}{42720231}$	$\frac{361348112}{36989561}$	$-\frac{70523021}{17471878}$		
1	$-\frac{18380168871}{910042447}$	$\frac{163509818}{17684341}$	$\frac{23284410832}{834563425}$	$-\frac{30101365272}{1318750783}$	$-\frac{18886348365}{884006261}$	$\frac{38539543917}{814907704}$	$-\frac{11547380395}{590596501}$	0	0
8th-order ζ	$\frac{34671799}{842260068}$	0	$\frac{144249888}{734327161}$	$\frac{109052807}{596751465}$	$\frac{46947293}{666421313}$	$\frac{3728242}{610500809}$	$\frac{2768777}{893496930}$	0	0
6th-order $\hat{\zeta}$	$\frac{1396355}{33920341}$	0	$\frac{138043832}{702739113}$	$\frac{251710491}{1377376774}$	$\frac{80696586}{1145573765}$	$\frac{4305634}{704519725}$	$\frac{1314393}{424316254}$	0	0
8th-order ζ'	$\frac{34671799}{842260068}$	0	$\frac{283604130}{1236153301}$	$\frac{304520675}{953442212}$	$\frac{1497971628}{5591689039}$	$\frac{47303577}{1114338140}$	$\frac{969222007}{1039950713}$	$-\frac{1290766697}{1230666728}$	$\frac{8502977}{39270418}$
6th-order $\hat{\zeta}'$	$\frac{1396355}{33920341}$	0	$\frac{304714768}{1328178045}$	$\frac{158732101}{496977984}$	$\frac{28494118}{106371239}$	$\frac{33382235}{785800536}$	$\frac{516462388}{554354445}$	$-\frac{1253055931}{1195253697}$	$\frac{171049779}{790529362}$

In

`http://users.uoa.gr/~tsitourasc/rknt869.m`

we included the algorithm of the previous section and the coefficients of the new pair in `Mathematica` format.

Table 4 provides an overview of the fundamental characteristics of the principal eighth-order RKN pairs examined in this context. The norms presented in the table correspond to the Euclidean norm of the ninth-order coefficients (i.e., of κ^9) in expressions (2.1-2.2). It is our expectation that the new method will excel in comparison to others by significantly reducing local truncation errors.

Following the theoretical analysis given in [22] we deduce that the efficiency ratio is

$$\frac{8}{9} \cdot \left(\frac{8.3 \cdot 10^{-7}}{1.5 \cdot 10^{-8}} \right)^{1/8} \approx 1.47,$$

against DEP8(6). i.e. DEP8(6) is theoretically about 47% costlier that our new proposal even if we need a stage more per step. In [6] a pair with smaller principal truncation error was presented, namely PT8(6). Similarly, it can be shown that PT8(6) is about 21% costlier.

Table 4. Basic characteristics of the RKN Pairs considered.

pair	stages	FSAL	$\left\|\Xi^{(9)}\right\|_2$	$\left\|\tilde{\Xi}'^{(9)}\right\|_2$
PT8(6) [6]	8	YES	$1.7 \cdot 10^{-7}$	$1.6 \cdot 10^{-7}$
DEP8(6) [3]	8	YES	$8.3 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$
RKNT8(6)9	9	YES	$1.5 \cdot 10^{-8}$	$1.3 \cdot 10^{-8}$

To explore the linear stability, we employ the methodologies outlined by Horn [23] or Dormand et al. [2]. Consequently, we examine the test problem $\psi'' = \mu^2\psi$ (where μ is a complex number). Taking in account that $\psi' = \mu\psi$, we deduce the recursive relations for ψ and ψ' as follows:

$$
\begin{aligned}
\psi_{n+1} &= \left\{1 + \nu^2\zeta\left(I - \nu^2\Theta\right)^{-1} e + \nu\left(1 + \nu^2\zeta\left(I - \nu^2\Theta\right)^{-1}\lambda\right)\right\} \cdot \psi_n = R(\nu) \cdot \psi_n, \\
\psi'_{n+1} &= \left\{\nu\zeta'\left(I - \nu^2\Theta\right)^{-1} e + \left(1 + \nu^2\zeta'\left(I - \nu^2\Theta\right)^{-1}\lambda\right)\right\} \cdot \psi'_n = R'(\nu) \cdot \psi'_n,
\end{aligned}
$$

with $\nu = \kappa\mu$. Consequently, there exist two absolute stability regions for RKN methods, specifically for ψ and ψ'. These regions are determined by the conditions $|R(\nu)| < 1$ and $|R'(\nu)| < 1$. The corresponding graphical representations are provided in Figure 1, where a comparison is made among the pairs presented in Table 4.

This type of stability analysis is associated with the A-stability property of Runge–Kutta methods. Then we may use higher steplengths and avoid catastrophic consequences. But here, we are interested in using rather short steps and achieve high accuracy. Thus, stability plays a lesser role in our goal.

As an alternative, we can investigate stability concerning the test problem $\psi'' = -\mu^2\psi$ [24], which helps identify intervals of periodicity. Our primary focus in this context is on achieving exceptionally high levels of accuracy. Consequently, the significance of extended stability regions diminishes in our pursuit of such precision.

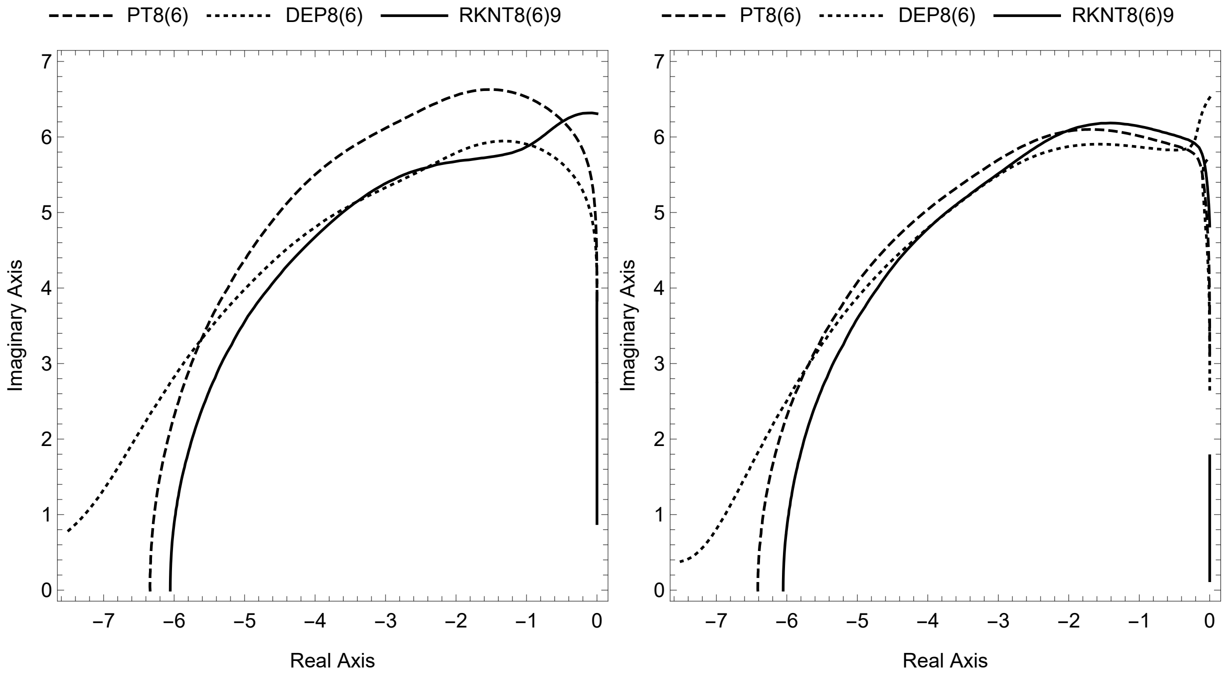

Figure 1. Absolute stability regions for y (left), for y' (right).

4. Numerical results

4.1. The methods

The explicit eighth-order methods chosen for testing include the following:

- PT8(6) : A RKN pair of orders 8(6) given in [6].
- DEP8(6): A RKN pair of orders 8(6) detailed in [3].
- RKNT8(6)9: The RKN pair of orders 8(6) introduced in this study.

These pairs were executed in the standard manner, with an error estimate μ evaluated at each step. Subsequently, we applied formula (1.2) to determine the new step size, considering their error's asymptotic behavior as $O(\kappa^7)$. All simulations were conducted utilizing the framework described in the preceding section. DEP8(6) is so far the most widely known RKN pair of such orders for all-purpose problems. Its outstanding results justify our choice.

4.2. The problems

In our experiments, we opted for several widely recognized problems sourced from existing literature. These problems were tackled with tolerances spanning from $\tau = 10^{-5}, 10^{-6}$ to 10^{-11}. For each of these runs, we meticulously recorded the quantity of steps taken (both accepted and rejected) and the highest global error observed at the grid points. The findings, featuring stage counts in relation to errors, have been visualized in a variety of efficiency plots (in logarithmic scales). All computational tasks were carried out using MATLAB.

4.2.1. Model problem

One of the initial test problems is a Model equation, given by:

$$\psi'' = -\psi(t),\ \psi(0) = 1,\ \psi'(0) = 0,$$

with an established theoretical solution of

$$\psi(t) = \cos(t).$$

We conducted the integration for this problem within the interval $t \in [0, 10\pi]$. The corresponding efficiency plots can be found in the upper left section of Figure 2.

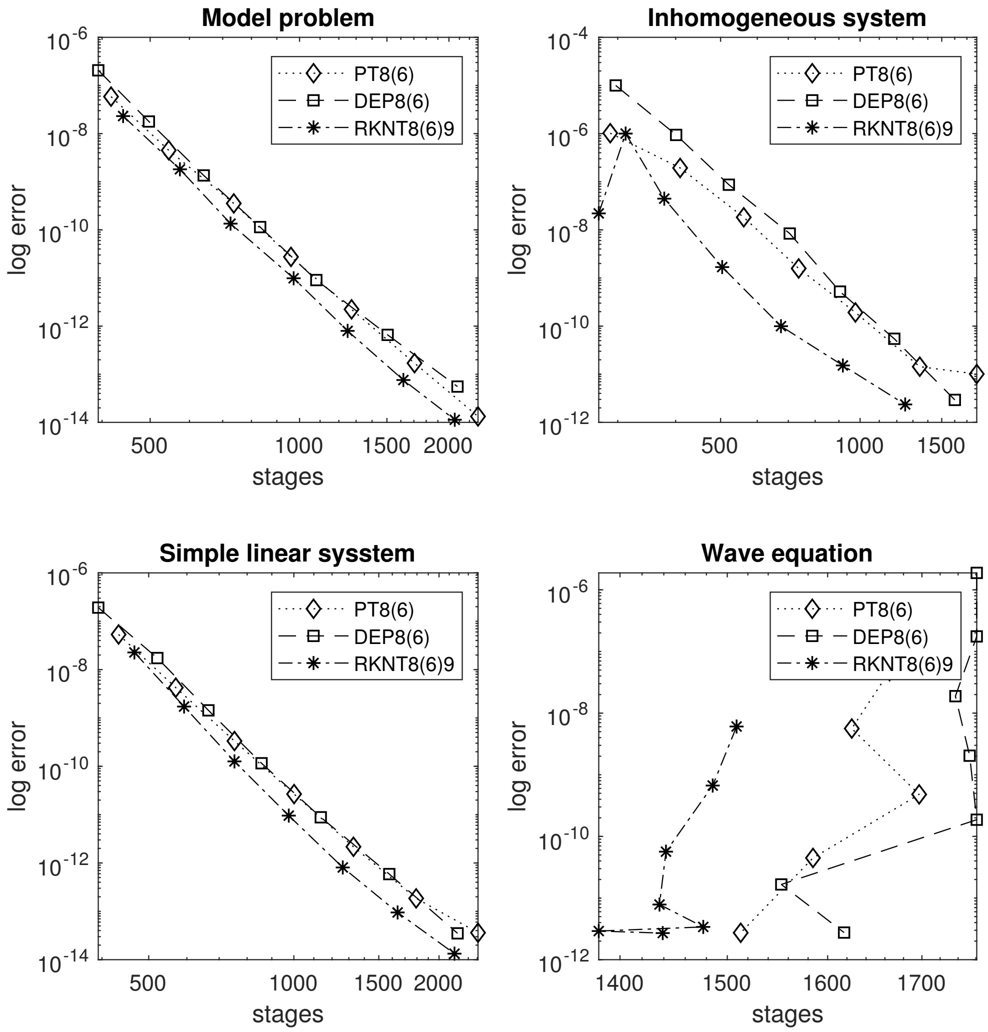

Figure 2. Efficiency plots for the problems under consideration.

4.2.2. Inhomogeneous Linear system: [25]

This differential equation is given as follows:

$$\psi'' = \begin{bmatrix} \frac{1}{100} & -\frac{1}{10} \\ -\frac{1}{10} & \frac{1}{100} \end{bmatrix} \cdot \psi + \begin{bmatrix} 0 \\ \sin t \end{bmatrix},$$

with the theoretical solution being:

$$\psi = \begin{bmatrix} \cos \frac{3}{10}t - \frac{1000}{10101} \sin t \\ \cos \frac{3}{10}t - \frac{10100}{10101} \sin t \end{bmatrix}$$

4.2.3. Simple Linear system

This system of differential equation is described as follows:

$$\psi'' = \begin{bmatrix} -\frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & -\frac{3}{4} \end{bmatrix} \cdot \psi$$

with the theoretical solution being:

$$\psi = \begin{bmatrix} \cos t + \sin t \\ -\cos t - \sin t \end{bmatrix}$$

Integration of this problem was carried out within the interval $t \in [0, 10\pi]$, and the corresponding efficiency plots have been depicted in the lower left section of Figure 2.

4.2.4. Wave equation

We finally consider the Wave equation of the form [26],

$$\begin{aligned} \frac{\partial^2 \psi}{\partial t^2} &= 4\frac{\partial^2 \psi}{\partial r^2} + \sin t \cdot \cos\left(\frac{\pi r}{100}\right), \ 0 \le r \le 100, \ t \in [0, 10\pi], \\ \frac{\partial \psi}{\partial r}(t, 0) &= \frac{\partial \psi}{\partial r}(t, 100) = 0 \\ \psi(0, r) &\equiv 0, \ \frac{\partial \psi}{\partial t}(0, r) = \frac{100^2}{4\pi^2 - 100^2} \cos \frac{\pi r}{100}, \end{aligned}$$

with exact solution

$$\psi(t, r) = \frac{100^2}{4\pi^2 - 100^2} \cdot \sin(t) \cdot \cos \frac{\pi r}{100}.$$

We apply semi-discretization to $\frac{\partial^2 \psi}{\partial r^2}$ using fourth-order symmetric differences at interior points, and employ one-sided differences of the same order at the boundaries. This leads to our resulting system:

$$\begin{bmatrix} \psi_1'' \\ \psi_2'' \\ \\ \\ \psi_{N+1}'' \end{bmatrix} = \frac{4}{(\Delta r)^2} \begin{bmatrix} -\frac{415}{72} & 8 & -3 & \frac{8}{9} & -\frac{1}{8} & 0 & \cdots & & \\ \frac{257}{144} & -\frac{10}{3} & \frac{7}{4} & -\frac{2}{9} & \frac{1}{48} & 0 & \cdots & & \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & & \vdots \\ 0 & & \ddots & \ddots & \ddots & \ddots & \ddots & & 0 \\ \vdots & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & & -\frac{1}{12} \\ & \cdots & 0 & \frac{1}{48} & -\frac{2}{9} & \frac{7}{4} & -\frac{10}{3} & & \frac{257}{144} \\ & \cdots & 0 & -\frac{1}{8} & \frac{8}{9} & -3 & 8 & & -\frac{415}{72} \end{bmatrix} \cdot \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \\ \psi_{N+1} \end{bmatrix}$$

$$+ \sin t \cdot \begin{bmatrix} \cos\left(\frac{0\cdot\Delta r}{r} \cdot \pi\right) \\ \cos\left(\frac{1\cdot\Delta r}{r} \cdot \pi\right) \\ \vdots \\ \\ \cos\left(\frac{N\cdot\Delta r}{r} \cdot \pi\right) \end{bmatrix}.$$

By selecting Δr as $\frac{1}{4}$, we establish a linear system with constant coefficients where $N = 401$. Subsequently, we approximate ψ_1 as $\psi(t, 0)$, ψ_2 as $\psi(t, \Delta r)$, ψ_3 as $\psi(t, 2\Delta r)$, and so forth up to ψ_{401} as $\psi(t, 400\Delta r)$.

We solved the aforementioned equation within the time interval $[0, 10\pi]$, using the same tolerance levels as previously described. The efficiency graph, which records the stages utilized by the four pairs against the maximum global errors observed across the entire grid, is presented in the lower right section of Figure 2.

The results demonstrate that the new pair outperforms the DEP8(6) pair in the examined problems. In most cases, the level of accuracy achieved was approximately one digit. The Wave is a mildly-stiff problem and explicit pairs are not well suited for such type of problems. Even so though, the new pair seems to get some advantage in efficiency. These findings highlight that when it's essential to attain high levels of precision in addressing specific second-order initial value problems (IVPs), the new method significantly excels over previous approaches.

5. Conclusions

In this manuscript, we examined Runge-Kutta-Nyström pairs meticulously tailored for tackling second-order Initial Value Problems in situations where the first derivative is absent. We harnessed the substantial handling capacity of the coefficients available after adding a stage. The primary innovation of our endeavor lies in the remarkably reduced truncation error terms of the suggested method, distinguishing it from the eighth-order pairs previously documented in the literature. Our diligent numerical testing of pertinent problems substantiates the merit of our approach.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

No conflicts of interest are declared by the authors

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