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NOTE ON THE PERFORMANCE OF DIRECT AND INDIRECT RUNGE-KUTTA-NYSTRÖM METHODS

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Abstract: This paper deals with predictor-corrector iteration of Runge-Kutta-Nyström (RKN) methods for integrating initial-value problems for special second-order, ordinary differential equations. We consider RKN correctors based on both direct and indirect collocation techniques. The paper focusses on the convergence factors and stability regions of the iterated RKN correctors. It turns out that the methods based on direct collocation RKN correctors possess smaller convergence than those based on indirect collocation RKN correctors. Both families of methods have sufficiently large stability boundaries for nonstiff problems.

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1. Introduction

We will investigate a class of (explicit) predictor-corrector (PC) methods obtained by predictor-corrector iteration (or: fixed point iteration) of Runge-Kutta-Nyström correctors for solving the initial-value problem (IVP) for nonstiff, special second-order, ordinary differential equations (ODEs)

$$\frac{d^2y(t)}{dt^2} = f(y(t)). \tag{1.1}$$

The methods described in this note have the same nature as the PIRKN methods (parallel, iterated RKN methods) proposed in [13]. The present note is concerned with a comparison of the convergence factors and stability regions of PIRKN methods based on *direct* and *indirect* RKN methods. Indirect RKN methods are derived from RK methods for first-order ODEs (as have also been used in [13]), whereas direct RKN methods are directly constructed for second-order ODEs (see [9]). The iterated methods will be referred to as *indirect* and *direct* PIRKN methods. It turned out that for direct PIRKN methods the convergence factors and error constants are smaller than those of indirect PIRKN methods, resulting in a better performance of the *direct* PIRKN methods. The stability of the two types of methods is comparable, in spite of the fact that the direct RKN correctors used are only conditionally stable, while the indirect RKN methods are unconditionally stable (see [9]). In two numerical experiments the superiority of direct PIRKN methods over indirect PIRKN methods is demonstrated.

For notational convenience, we assume that the equation (1.1) is a scalar equation. However, all considerations below can be straightforwardly extended to a system of ODEs, and therefore, also to nonautonomous equations.

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2. Direct PIRKN and Indirect PIRKN methods

The starting point is a fully implicit s-stage RKN method. For a scalar equation, this method assumes the form

(2.1) $$Y = y_n e + hcy'_n + h^2 Af(Y),\ \ y_{n+1} = y_n + hy'_n + h^2 b^T f(Y),\ \ y'_{n+1} = y'_n + hd^T f(Y),$$

where A is an s-by-s matrix, **b**, **d**, **c** are s-dimensional vectors, and **e** is the unit vector. Furthermore, we use the convention that for any given vector $v = (v_j)$, $f(v)$ denotes the vector with entries $f(v_j)$.

Consider the following fixed point iteration scheme (cf. [13]):

(2.2a) $$Y^{(0)} = y_n e + hcy'_n,$$

(2.2b) $$Y^{(j)} = y_n e + hcy'_n + h^2 Af(Y^{(j-1)}),\ \ j = 1, ..., m.$$

(2.2c) $$y_{n+1} = y_n + hy'_n + h^2 b^T f(Y^{(m)}),\ \ y'_{n+1} = y'_n + hd^T f(Y^{(m)}),$$

Notice that the s components of the vectors $Y^{(j)}$ can be computed in parallel, provided that s processors are available, so that the computational time needed for one iteration of (2.2b) is equivalent to the time required to evaluate one right-hand side function on a sequential computer. Therefore, the method (2.2) was called a PIRKN method (parallel, iterated RKN methods).

Regarding the prediction formula (2.2a) as the predictor method and (2.1) as the corrector method, (2.2) may be considered as a conventional PC method (in $P(CE)^m E$ mode). Assuming that the function f(y) is Lipschitz continuous and observing that (2.2a) defines a first-order predictor formula (i.e., $Y^{(0)} - Y = O(h^2)$), the following theorem easily follows (see also [10], [13]):

Theorem 2.1. Let p be the order of the corrector method (2.1). Then on s-processor computers the PIRKN method (2.2) represents an explicit RKN method of order $p^* = \min\{p, 2m+2\}$ requiring m+1 sequential right-hand side evaluations per step. []

Remark. From Theorem 2.1, we see that by setting $m = [(p-1)/2]$, [.] denoting the integer function, we have a PIRKN method of maximum order $p^* = p$ (order of the corrector) with only $[(p+1)/2]$ sequential right-hand side evaluations per step. []

In the following subsections, we concentrate on the convergence factors and stability regions of direct and indirect PIRKN methods. Specification of the parameters (A, **b**, **d**, **c**) of the direct collocation corrector methods can be found in the Appendix to this paper.

2.1. Convergence

In actual integration, the number of iterations m is determined by some iteration strategy, rather than by order considerations. Therefore, it is of interest to know how the integration step affects the rate of convergence. The step size should be such that a reasonable convergence speed is achieved.

We shall determine the rate of convergence by using the test equation $y'' = \lambda y$, where λ runs through the eigenvalues of the Jacobian matrix $\partial f/\partial y$. For this equation, we obtain the iteration error equation

$$Y^{(j)} - Y = zA\,[Y^{(j-1)} - Y],\ \ z := \lambda h^2,\ \ j = 1, \dots, m.$$

Hence, with respect to the test equation, the rate of convergence is determined by the spectral radius $\rho(A)$ of the matrix A. We shall call $\rho(A)$ the *convergence factor* of the PIRKN method. Requiring that $\rho(zA) < 1$, leads us to the convergence condition

(2.3) $$|z| < \frac{1}{\rho(A)} \ \text{ or } \ h^2 \le \frac{1}{\rho(A)\,\rho(\partial f/\partial y)}.$$

This convergence condition is of the same form as the stability condition associated with RKN methods. In analogy with the notion of the *stability boundary*, we shall call $1/\rho(A)$ the *convergence boundary*.

Let the RKN matrices generating the direct PIRKN methods and indirect PIRKN methods be denoted by A_{direct} and $A_{indirect}$, respectively. Table 2.1 lists the convergence boundaries $1/\rho(A_{direct})$ and $1/\rho(A_{indirect})$, and the reduction factors $\varepsilon = \rho(A_{direct}) / \rho(A_{indirect})$ of a number of indirect PIRKN methods and their direct analogues. These figures show that the direct PIRKN methods have much larger convergence boundaries, and hence much smaller convergence factors, than indirect PIRKN methods of the same order.

Table 2.1. Convergence boundaries $1/\rho(A)$ and reduction factors ε

P-order correctors	p = 3	p = 4	p = 5	p = 6	p = 7	p = 8	p = 9	p = 10
Indirect Gauss-Legendre		12.04		21.73		37.03		52.63
Direct Gauss-Legendre		20.83		34.48		55.54		76.92
Indirect Radau IIA	5.98		13.15		25.64		40.00	
Direct Radau IIA	10.41		20.40		37.03		55.55	
Reduction factors ε	0.57	0.58	0.64	0.63	0.69	0.66	0.72	0.68

2.2. Stability boundaries

The linear stability of the PIRKN method (2.2) is investigated by again using the model equation $y'' = \lambda y$, where λ runs through the eigenvalues of $\partial f/\partial y$. Applying (2.2) to the model equation, we obtain the recursion

$$V_{n+1} = M_m(z)V_n, \quad V_{n+1} = \begin{pmatrix} y_{n+1} \\ hy'_{n+1} \end{pmatrix}, \text{ with}$$

$$\text{(2.4)} \qquad M_m(z) := \begin{pmatrix} 1+zb^T(I-zA)^{-1}(I-(zA)^{m+1})e & 1+zb^T(I-zA)^{-1}(I-(zA)^{m+1})c \\ zd^T(I-zA)^{-1}(I-(zA)^{m+1})e & 1+zd^T(I-zA)^{-1}(I-(zA)^{m+1})c \end{pmatrix}.$$

From (2.4) we see that if z satisfies (2.3), then $M_m(z)$ converges to the amplification matrix M(z) of the corrector as $m \to \infty$ (see [9]). Hence, the *asymptotic* stability interval for $m \to \infty$ is the intersection on the negative z-axis of the stability interval $(-\beta_{corr},0)$ of the generating corrector and the region of convergence in the complex z-plane defined by (2.3). For indirect PIRKN methods, where the corrector method is A-stable, the asymptotic stability region is completely determined by its region of convergence. For direct PIRKN methods, where the corrector method is conditionally stable with stability boundaries less than the convergence boundaries, the asymptotic stability region coincides with the stability region of the corrector method (see Table 2.1 for convergence boundaries and Appendix for stability boundaries of direct collocation RKN correctors).

Table 2.2. Stability boundaries β_{direct} and $\beta_{indirect}$ for direct and indirect PIRKN methods

Generating corrector methods	p	m=1	m=2	m=3	m=4	m=5	m=6	... m=∞	α_{crit}
Indirect Radau IIA	3	4.94	4.99	3.52	5.03	5.44	4.90	... 5.98	1.00
Direct Radau IIA	3	6.00	7.84	4.44	7.04	8.62	6.96	... 8.61	0.57
Indirect Gauss-Legendre	4	12.00	12.00	0.00	12.00	12.00	0.00	... 12.04	0.75
Direct Gauss-Legendre	4	6.83	0.00	0.00	8.57	0.00	0.00	... 9.00	0.43
Indirect Radau IIA	5	7.06	**2.19**	10.46	4.76	11.70	7.81	... 13.15	0.73
Direct Radau IIA	5	7.06	**0.49**	14.33	5.33	9.51	9.55	... 9.55	0.47
Indirect Gauss-Legendre	6	7.06	**0.00**	9.81	0.00	9.75	0.00	... 21.73	0.45
Direct Gauss-Legendre	6	7.06	**0.00**	18.77	0.00	9.80	0.00	... 9.77	0.28
Indirect Radau IIA	7	7.06	0.00	9.50	18.21	5.40	18.57	... 25.64	0.38
Direct Radau IIA	7	7.06	0.00	**9.51**	26.9	6.06	9.84	... 9.84	0.27
Indirect Gauss-Legendre	8	7.06	0.00	9.51	0.00	0.00	9.86	... 37.03	0.27
Direct Gauss-Legendre	8	7.06	0.00	9.51	0.00	0.37	9.86	... 9.86	0.18
Indirect Radau IIA	9	7.06	0.00	9.51	**0.21**	26.35	5.80	... 40.00	0.25
Direct Radau IIA	9	7.06	0.00	9.51	**0.03**	9.86	6.13	... 9.86	0.18
Indirect Gauss-Legendre	10	7.06	0.00	9.51	**0.00**	9.86	0.00	... 52.63	0.70
Direct Gauss-Legendre	10	7.06	0.00	9.51	**0.00**	9.86	0.01	... 36.65	0.48

For finite m, the stability intervals are given by

$$(-\beta(m),0) := \{z: \rho(M_m(z)) < 1, \; z \le 0\}.$$

Table 2.2. lists the stability boundaries $\beta_{direct}(m)$ and $\beta_{indirect}(m)$ of direct PIRKN and indirect PIRKN, respectively. The stability boundaries corresponding to the minimal value of m needed to reach the order of the correctors are indicated

in bold face. In actual computation, the stepsize h should of course be substantially smaller than allowed by condition (2.3), that is, we want $|z| < \alpha / \rho(A)$, where α is significantly smaller than 1. In Table 2.2, we added the value of α for which $0 \geq z \geq -\min\{\beta_{direct}(\infty), \beta_{indirect}(\infty)\}$. This value is denoted by α_{crit}. Table 2.2 shows that usually the stability boundaries of the indirect PIRKN methods are larger than those of the direct PIRKN methods. However, in actual computation, we also need fast convergence, so that the integration step may be much smaller than allowed by stability. The values of α_{crit} in the last column indicate that, as far as convergence is concerned, the direct methods are superior. By means of Table 2.2 we can select the number of iterations needed to achieve an acceptable stability boundary (the corresponding boundaries are underlined). In this selection, the 5-, 6-, 9- and 10-order methods require one iteration more than the number of iterations needed to reach the order of the corrector (see Theorem 2.1).

2.3. The truncation error

Let us denote the step values associated with the corrector by u_{n+1} and u'_{n+1}, and define

$$E_m(z) := \begin{pmatrix} zb^T(zA)^{m+1}(I-zA)^{-1}e & zb^T(zA)^{m+1}(I-zA)^{-1}c \\ zd^T(zA)^{m+1}(I-zA)^{-1}e & zd^T(zA)^{m+1}(I-zA)^{-1}c \end{pmatrix}, \quad w_{n+1} = \begin{pmatrix} u_{n+1} \\ hu'_{n+1} \end{pmatrix}, \quad v_{n+1} = \begin{pmatrix} y_{n+1} \\ y'_{n+1} \end{pmatrix}.$$

It can be shown that $w_{n+1} - v_{n+1} = E_m v_n$ (see [10], [11]), so that the local truncation error of PIRKN methods can be written as the sum of the truncation error of the corrector and the iteration error of the PIRKN method:

$$\begin{pmatrix} y(t_{n+1}) \\ hy'(t_{n+1}) \end{pmatrix} - v_{n+1} = \begin{pmatrix} y(t_{n+1}) \\ hy'(t_{n+1}) \end{pmatrix} - w_{n+1} + E_m v_n.$$

Our numerical experiments have shown that the truncation error of direct RKN correctors is smaller than that of indirect RKN correctors. Since the convergence factors of the direct PIRKN methods are also smaller than those of indirect PIRKN methods, there are two potential effects to expect that the truncation error of direct PIRKN methods is smaller than that of indirect PIRKN methods.

3. Numerical experiments

In this section we report numerical results obtained by direct and indirect PIRKN methods. The absolute error obtained at the end of integration interval is presented in the form 10^{-d} (d may be interpreted as the number of correct decimal digits (NCD)). In order to see the efficiency of the direct PIRKN methods, we follow a dynamical strategy for determining the number of iterations in the successive steps. It seems natural to require that the iteration error is of the same order in h as the local error of the corrector. This leads us to the stopping criterion

$$\text{(3.1)} \qquad \| Y^{(m)} - Y^{(m-1)} \|_\infty \leq C\, h^{p+1},$$

where C is a problem and method dependent parameter. Furthermore, in the tables of results, N_{seq} denotes the total number of sequential right hand side evaluations, and N_{steps} denotes the total number of integration steps. The following two problems possess exact solutions in closed form. Initial conditions are taken from the exact solutions.

3.1. Linear nonautonomous problem

As a first numerical test, we apply the various PIRKN methods to the linear problem (cf. [11, problem 5.1])

$$\text{(3.2)} \qquad \frac{d^2y(t)}{dt^2} = \begin{pmatrix} -2\,\alpha(t)+1 & -\alpha(t)+1 \\ 2(\alpha(t)-1) & \alpha(t)-2 \end{pmatrix} y(t), \quad \alpha(t) = \max\,(2\cos^2(t), \sin^2(t)), \quad 0 \leq t \leq 20,$$

with exact solution $y(t) = (-\sin(t), 2\sin(t))^T$. Table 3.1 clearly shows the improved accuracy of the direct PIRKN methods. In all experiments, the (averaged) number of iterations m needed to satisfy the stopping criterion (approximately) varies between [p/2] and [(p+1)/2].

Table 3.1. Values of NCD / N_{seq} for problem (3.2) obtained by PIRKN methods.

Generating corrector methods	p	N_{steps}=80	N_{steps}=160	N_{steps}=320	N_{steps}=640	N_{steps}=1280	C
Indirect Radau IIA	3	2.1 / 160	3.0 / 320	3.9 / 640	4.8 / 1280	5.7 / 2560	10^4
Direct Radau IIA	3	2.5 / 160	3.5 / 320	4.4 / 640	5.3 / 1280	6.2 / 2560	10^4
Indirect Gauss-Legendre	4	4.0 / 227	5.3 / 476	6.5 / 958	7.7 / 1920	8.9 / 3840	10^1
Direct Gauss-Legendre	4	5.0 / 226	6.4 / 477	7.6 / 959	8.8 / 1920	10.0 / 3840	10^1
Indirect Radau IIA	5	5.3 / 238	6.8 / 480	8.3 / 1179	9.8 / 2511	11.3 / 5098	10^1
Direct Radau IIA	5	5.8 / 238	7.5 / 480	8.9 / 1179	10.4 / 2511	11.9 / 5098	10^1
Indirect Gauss-Legendre	6	7.4 / 318	9.2 / 640	11.0 / 1280	12.8 / 2560	14.6 / 5120	10^{-1}
Direct Gauss-Legendre	6	8.1 / 318	9.9 / 640	11.7 / 1280	13.5 / 2560	15.3 / 5120	10^{-1}
Indirect Radau IIA	7	8.7 / 320	10.9 / 737	13.0 / 1570	15.1 / 3184	17.2 / 6393	10^{-1}
Direct Radau IIA	7	9.1 / 320	11.6 / 737	13.7 / 1570	15.8 / 3184	17.9 / 6393	10^{-1}
Indirect Gauss-Legendre	8	11.0 / 395	13.4 / 799	15.8 / 1600	18.2 / 3200	20.6 / 6400	10^{-2}
Direct Gauss-Legendre	8	12.4 / 395	16.1 / 799	18.6 / 1600	21.3 / 3200	23.8 / 6400	10^{-2}
Indirect Radau IIA	9	13.5 / 400	15.2 / 926	17.9 / 1903	20.6 / 3830	23.4 / 7673	10^{-3}
Direct Radau IIA	9	12.7 / 400	16.0 / 926	18.7 / 1903	21.4 / 3830	24.2 / 7673	10^{-2}
Indirect Gauss-Legendre	10	14.9 / 477	17.8 / 959	20.8 / 1920	23.8 / 3840		10^{-3}
Direct Gauss-Legendre	10	16.6 / 477	18.6 / 959	21.6 / 1920	24.6 / 3840		10^{-3}

Table 3.1 also shows that the number of iterations are for both the indirect and direct method the same, so that the smaller convergence factor of the direct methods does not seem to play a role. For problems which are locally of the form $y' = \lambda y$ (such as problem (3.2)), this can be explained by considering the stopping criterion (3.1) more closely. Let us denote the step point values and the iterates corresponding to the direct and indirect PIRKN method by y_n, y'_n, $Y^{(j)}$ and x_n, x'_n, $X^{(j)}$, respectively, and define

$$\delta_m := [Y^{(m)} - Y^{(m-1)}] - [X^{(m)} - X^{(m-1)}],$$

where m is the actual number of iterations performed per step. If it turns out that the magnitude of δ_m is much smaller than that of the tolerance C h^{p+1}, then this would explain that the direct and indirect PIRKN methods use the same number of iterations. Writing the recursion (2.2b) in the form

$$\text{(2.2b)} \qquad Y^{(j)} = \left[I + zA + z^2A^2 + ... + z^jA^j\right] (y_n e + hy'_n c),$$

and a similar expression for $X^{(j)}$, we obtain

$$\delta_m = z^m(A_{direct})^m (y_n e + hy'_n c) - z^m(A_{indirect})^m (x_n e + hx'_n c).$$

Hence, defining the defect

$$D_j(v) := \| (A_{direct})^j v - (A_{indirect})^j v \|_\infty,$$

the quantity δ_m is bounded by

$$\| \delta_m \|_\infty \le | z^m | \left[|y_n| D_m(e) + h |y'_n| D_m(c)\right] + | z^m | \, \| (A_{indirect})^m [(x_n - y_n)e + h(x'_n - y'_n)c] \|$$

$$\le h^{2m} | \lambda^m | (|y_n| + h |y'_n|) D_m + O(h^{p+2m}), \quad D_m := \max \{D_m(e), D_m(c)\},$$

where λ runs through the spectrum of the Jacobian of the ODE. Ignoring the $O(h^{p+2m})$ term, we conclude that the iteration processes in the direct and indirect methods are expected to satisfy the stopping criterion (3.1) after equal numbers of iteration if $h^{2m} | \lambda^m | (|y_n| + h |y'_n|) D_m << C h^{p+1}$. For nonstiff problems (i.e., $| \lambda | \le 1$), this condition takes the form

$$(3.3)\qquad D_m << \frac{C\, h^{p+1-2m}}{|y_n| + h\,|y'_n|} .$$

Table 3.2 lists the values of D_m for the correctors of Table 3.1 (notice that D_m vanishes for m = 1, and, if p = 9 or 10, also for m = 2; this is a direct consequence of the order condition $(q+1)(q+2)Ac^q = c^{q+2}$ satisfied by RKN correctors derived from collocation, see [6, p.270]). By means of Table 3.2 it can be verified that the values of m, C and h used in Table 3.1 satisfy (3.3), explainig the identiacla performance of the iteration processes.

Table 3.2. Values of $D_m := \max\{D_m(e), D_m(c)\}$ for RKN correctors.

Correctors	p	m=1	m=2	m=3	m=4	m=5	m=6	m=7	m=8
Radau IIA	3	2.5E-02	1.7E-02	8.2E-03	1.5E-03	1.2E-04	6.0E-05	4.5E-06	1.2E-06
Gauss-Legendre	4	8.0E-03	4.0E-03	6.9E-04	1.5E-04	9.1E-06	3.7E-07	1.0E-07	6.2E-09
Radauu IIA	5	0	1.1E-03	2.6E-04	8.4E-05	1.2E-05	8.5E-07	5.1E-08	4.9E-09
Gauss-Legendre	6	0	5.2E-04	6.8E-05	9.9E-06	1.3E-06	8.4E-08	3.1E-09	1.2E-10
Radauu IIA	7	0	4.8E-05	2.8E-05	2.2E-06	3.7E-07	5.2E-08	3.1E-09	1.1E-10
Gauss-Legendre	8	0	2.5E-05	1.2E-05	5.9E-07	3.2E-08	5.6E-09	3.5E-10	1.2E-11
Radauu IIA	9	0	0	2.0E-06	3.0E-07	1.2E-08	1.2E-09	1.5E-10	7.9E-12
Gauss-Legendre	10	0	0	1.0E-06	1.3E-07	3.3E-09	1.4E-10	1.6E-11	9.3E-13

3.2. Nonlinear Fehlberg problem

For the second numerical example, we consider the orbit equation (see [2])

$$(3.4)\qquad \frac{d^2y(t)}{dt^2} = \begin{pmatrix} -4t^2 & -2/r(t) \\ 2/r(t) & -4t^2 \end{pmatrix} y(t),\quad r(t) = \sqrt{y_1{}^2(t) + y_2{}^2(t)}\,,\quad \sqrt{\pi/2} \le t \le 3\pi,$$

with exact solution $y(t) = (\cos(t^2), \sin(t^2))^T$. The results are reported in Table 3.3. In this nonlinear problem, the superiority of direct PIRKN methods is once again demonstrated.

Table 3.3. Values of NCD / N_{seq} for problem (3.4) obtained by PIRKN methods.

Generating corrector methods	p	N_{steps}=200	N_{steps}=400	N_{steps}=800	N_{steps}=1600	N_{steps}=3200	C
Indirect Radau IIA	3	0.8 / 556	1.7 / 1182	2.6 / 2400	3.5 / 4800	4.4 / 9600	10^4
Direct Radau IIA	3	1.3 / 556	2.2 / 1182	3.1 / 2400	4.0 / 4800	4.9 / 9600	10^4
Indirect Gauss-Legendre	4	1.9 / 570	3.2 / 1208	4.4 / 2554	5.6 / 5353	6.8 / 11122	10^5
Direct Gauss-Legendre	4	2.7 / 570	3.9 / 1200	5.1 / 2510	6.3 / 5276	7.5 / 10991	10^5
Indirect Radau IIA	5	3.2 / 652	4.7 / 1411	6.2 / 2967	7.7 / 6147	9.2 / 12594	10^6
Direct Radau IIA	5	3.8 / 652	5.3 / 1411	6.8 / 2967	8.3 / 6147	9.8 / 12594	10^6
Indirect Gauss-Legendre	6	4.5 / 845	6.3 / 1765	8.1 / 3596	9.9 / 7301	11.7 / 14809	10^5
Direct Gauss-Legendre	6	5.3 / 841	7.2 / 1760	9.0 / 3585	10.8 / 7291	12.6 / 14790	10^5
Indirect Radau IIA	7	5.7 / 808	7.9 / 1760	10.0 / 3648	12.1 / 7482	14.2 / 15304	10^7
Direct Radau IIA	7	6.2 / 808	8.6 / 1760	10.7 / 3648	12.8 / 7482	14.9 / 15304	10^7
Indirect Gauss-Legendre	8	7.2 / 992	9.6 / 2060	12.0 / 4246	14.4 / 8684	16.8 / 17556	10^6
Direct Gauss-Legendre	8	8.1 / 991	10.5 / 2057	12.9 / 4244	15.3 / 8672	17.7 / 17549	10^6
Indirect Radau IIA	9	8.6 / 1036	11.3 / 2174	14.0 / 4479	16.8 / 9094	19.5 / 18422	10^7
Direct Radau IIA	9	9.4 / 1036	12.1 / 2174	14.8 / 4479	17.5 / 9094	20.2 / 18422	10^7
Indirect Gauss-Legendre	10	10.1 / 1207	13.1 / 2473	16.1 / 5054	19.1 / 10273	22.2 / 20826	10^6
Direct Gauss-Legendre	10	11.1 / 1207	14.1 / 2473	17.1 / 5052	20.1 / 10270	23.3 / 20825	10^6

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APPENDIX

A.1. Additional numerical experiments

In addition to the experiments reported in Section 3., we present further experiments. As in the preceding examples, the superiority of direct PIRKN methods over indirect PIRKN methods is demonstrated. The integration strategy is identical with (3.1).

A.1.1. Duffing equation

As a first additional example we consider the Duffing equation forced by a harmonic function (cf. [1])

$$\frac{d^2y(t)}{dt^2} = -y^3(t) - y(t) + \cos(1.01t), \;\; 0 \le t \le 24\pi, \;\; y(0) = y_G(0), \;\; y'(0) = 0, \tag{A.1}$$

where $y_G(t)$ is Galerkins's approximation of order nine to a periodic solution computed by Van Dooren (see also [1]):

$$y_G(t) = \sum_{i=0}^{4} a_{2i+1} \cos((2i+1)1.01t),$$

where $a_1 = 0.200179477536$, $a_3 = 0.246946143E\text{-}3$, $a_5 = 0.304014E\text{-}6$, $a_7 = 0.374E\text{-}9$ and $a_9 = 0.0$.

Table A.1a. Value of NCD / N_{seq} for problem (A.1) obtained by 3-, 4-, 5-, 6-order PIRKN methods.

Correctors of PIRKN methods	p	N_{steps}=100	N_{steps}=200	N_{steps}=400	N_{steps}=800	N_{steps}=1600	C
Indirect Radau IIA	3	1.9 / 252	2.6 / 581	3.5 / 1188	4.4 / 2400	5.3 / 4800	10^{-1}
Direct Radau IIA	3	2.6 / 259	3.1 / 581	4.0 / 1188	4.9 / 2400	5.8 / 4800	10^{-1}
Indirect Gauss-Legendre	4	2.2 / 295	3.5 / 662	4.7 / 1470	5.9 / 3056	7.1 / 6280	10^{-2}
Direct Gauss-Legendre	4	3.0 / 294	4.2 / 600	5.4 / 1444	6.6 / 3043	7.8 / 6232	10^{-2}
Indirect Radau IIA	5	3.8 / 357	5.3 / 776	6.9 / 1588	8.4 / 3200	9.9 / 6398	10^{-2}
Direct Radau IIA	5	4.3 / 357	5.9 / 776	7.5 / 1588	9.0 / 3200	10.4 / 6398	10^{-2}
Indirect Gauss-Legendre	6	4.5 / 397	6.4 / 800	8.2 / 1600	10.0 / 3664	11.4 / 7688	10^{-3}
Direct Gauss-Legendre	6	5.3 / 396	7.3 / 800	9.2 / 1600	10.9 / 3642		10^{-3}

Table A.1b. Value of NCD / N_{seq} for problem (A.1) obtained by 7-, 8-, 9-, 10-order PIRKN methods.

Correctors of PIRKN methods	p	N_{steps}=25	N_{steps}=50	N_{steps}=100	N_{steps}=200	N_{steps}=400	C
Indirect Radau IIA	7	1.2 / 104	4.0 / 247	6.2 / 500	8.5 / 996	10.6 / 2000	10^{-5}
Direct Radau IIA	7	2.6 / 118	4.3 / 247	7.3 / 500	9.4 / 996	11.2 / 2000	10^{-5}
Indirect Gauss-Legendre	8	2.0 / 157	4.8 / 298	7.2 / 599	9.6 / 1196	11.4 / 2400	10^{-7}
Direct Gauss-Legendre	8	4.2 / 148	5.3 / 298	8.1 / 600	10.5 / 1195		10^{-7}
Indirect Radau IIA	9	2.9 / 155	5.5 / 298	8.7 / 600	11.2 / 1200		10^{-7}
Direct Radau IIA	9	3.4 / 147	5.6 / 298	9.3 / 600	11.4 / 1200		10^{-7}
Indirect Gauss-Legendre	10	4.0 / 162	7.0 / 336	9.6 / 688	11.5 / 1387		10^{-8}
Direct Gauss-Legendre	10	4.6 / 161	7.1 / 336	10.9 / 688			10^{-8}

A.1.2. Newton's equations of motion

The second example is the two-body gravitational problem for Newton's equation of motion (see [12, p. 245]):

$$\frac{d^2y_1(t)}{dt^2} = -\frac{y_1(t)}{r^3(t)}$$

(A.2) $$0 \le t \le 20,\ y_1(0) = 1 - \varepsilon,\ y_2(0) = 0,\ y'_1(0) = 0,\ y'_2(0) = \sqrt{(1+\varepsilon)/(1-\varepsilon)}\ ,$$

$$\frac{d^2y_2(t)}{dt^2} = -\frac{y_2(t)}{r^3(t)}$$

where $r(t) = \sqrt{y_1^2(t) + y_2^2(t)}$. The solution components are $y_1(t) = \cos(u) - \varepsilon$, $y_2(t) = \sqrt{(1+\varepsilon)(1-\varepsilon)}\ \sin(u)$, where u is the solution of Kepler's equation $t = u - \varepsilon \sin(u)$ and ε denotes the eccentricity of the orbit. In this experiment we set $\varepsilon = 0.3$.

Table A.2a. Value of NCD / N_{seq} for problem (A.2) obtained by 3-, 4-, 5-, 6-order PIRKN methods.

Correctors of PIRKN methods	p	N_{steps}=200	N_{steps}=400	N_{steps}=800	N_{steps}=1600	N_{steps}=3200	C
Indirect Radau IIA	3	1.3 / 406	2.2 / 1200	3.1 / 2400	4.0 / 4800	4.9 / 9600	10^2
Direct Radau IIA	3	1.8 / 406	2.7 / 1200	3.6 / 2400	4.5 / 4800	5.4 / 9600	10^2
Indirect Gauss-Legendre	4	3.7 / 600	4.9 / 1200	6.1 / 2400	7.3 / 4800	8.5 / 9600	10^2
Direct Gauss-Legendre	4	4.9 / 600	6.2 / 1200	7.4 / 2400	8.6 / 4800	9.8 / 9600	10^2
Indirect Radau IIA	5	4.5 / 680	6.0 / 1504	7.5 / 3200	9.0 / 6400	10.6 / 12800	10^1
Direct Radau IIA	5	5.1 / 680	6.6 / 1504	8.1 / 3200	9.7 / 6400	11.2 / 12800	10^1
Indirect Gauss-Legendre	6	7.0 / 662	8.6 / 1600	10.4 / 3200	12.2 / 6400	14.0 / 12800	10^2
Direct Gauss-Legendre	6	7.8 / 661	9.3 / 1600	11.1 / 3200	12.9 / 6400	14.8 / 12800	10^2

Table A.2b. Value of NCD / N_{seq} for problem (A.2) obtained by 7-, 8-, 9-, 10-order PIRKN methods.

Correctors of PIRKN methods	p	N_{steps}=50	N_{steps}=100	N_{steps}=200	N_{steps}=400	N_{steps}=800	C
Indirect Radau IIA	7	3.6 / 215	5.6 / 447	7.7 / 939	9.8 / 2000	12.0 / 4000	10^{-1}
Direct Radau IIA	7	4.3 / 215	6.3 / 447	8.4 / 939	10.5 / 2000	12.6 / 4000	10^{-1}
Indirect Gauss-Legendre	8	5.4 / 238	7.7 / 516	10.1 / 1047	12.5 / 2121	14.9 / 4294	10^{-2}
Direct Gauss-Legendre	8	6.2 / 237	9.0 / 515	11.4 / 1047	13.8 / 2119	16.2 / 4291	10^{-2}
Indirect Radau IIA	9	5.6 / 261	8.2 / 537	10.9 / 1099	13.6 / 2258	16.3 / 4800	10^{-2}
Direct Radau IIA	9	6.4 / 261	9.0 / 537	11.7 / 1099	14.4 / 2258	17.1 / 4800	10^{-2}
Indirect Gauss-Legendre	10	7.3 / 265	10.2 / 548	13.2 / 1160	16.2 / 2400	19.2 / 4870	10^{-2}
Direct Gauss-Legendre	10	8.5 / 265	10.9 / 548	14.0 / 1158	17.0 / 2400	20.0 / 4869	10^{-2}

A.2. Butcher arrays of direct collocation-based Runge-Kutta-Nyström methods

Here we give the Butcher arrays together with the stability boundaries β_{corr} for a few high-order direct collocation Runge-Kutta-Nyström methods based on Gauss-Legendre and Radau IIA collocation points. These methods have been used as corrector methods in this paper. For full details about direct collocation-based Runge-Kutta-Nyström methods we refer to [9] and also to Report NM-R9016, September 1990, Centre for Mathematics and Computer Science, Amsterdam.

A.2.1. The 2-stage direct collocation-based Radau IIA Runge-Kutta-Nyström corrector method

.33333333333333	.07407407407407	-.01850185018501
1.0000000000000	.50000000000000	.00000000000000
	.50000000000000	.00000000000000
	.75000000000000	.25000000000000

with stability boundary $\beta_{corr} = 8.61$

A.2.2. The 2-stage direct collocation-based Gauss-Legendre Runge-Kutta-Nyström corrector method

.21132486540519	.02777777777778	-.00544867840852
.78867513459481	.28322645618630	.02777777777778
	.39433756729741	.10566243270259
	.50000000000000	.50000000000000

with stability boundary $\beta_{corr} = 9.00$

A.2.3. The 3-stage direct collocation-based Radau IIA Runge-Kutta-Nyström corrector method

.15505102572168	.01637627564304	-.00686652290351	.00251065754914
.64494897427832	.18119985623684	.02862372435696	-.00184399088247
1.0000000000000	.31804138174398	.18195861825602	.00000000000000
	.31804138174398	.18195861825602	.00000000000000
	.37640306270047	.51248582618842	.11111111111111

with stability boundary $\beta_{corr} = 9.55$

A.2.4. The 3-stage direct collocation-based Gauss-Legendre Runge-Kutta-Nyström corrector method

.11270166537926	.00833333333333	-.00273296324905	.00075046260535
.50000000000000	.10587476869733	.02083333333333	-.00170810203066
.88729833462074	.21591620406132	.16939962991572	.00833333333333
	.24647175961687	.22222222222222	.03130601816091
	.27777777777778	.44444444444444	.27777777777778

with stability boundary $\beta_{corr} = 9.77$

A.2.5. The 4-stage direct collocation-based Radau IIA Runge-Kutta-Nyström corrector method

.08858795951270	.00538267552947	-.00242159178326	.00156464563415	-.00060181609506
.40946686444073	.06955830402056	.01612025009105	-.00247876656799	.00063176899384
.78765946176085	.15453781373038	.14485808726103	.01115013560396	-.00034232274468
1.0000000000000	.20093191373896	.22924110635959	.06982697990145	.00000000000000
	.20093191373896	.22924110635959	.06982697990145	.00000000000000
	.22046221117677	.38819346884317	.32884431998006	.06250000000000

with stability boundary $\beta_{corr} = 9.84$

A.2.6. The 4-stage direct collocation-based Gauss-Legendre Runge-Kutta-Nyström corrector method

.06943184420297	.00323055316068	-.00125019789572	.00059911990284	-.00016908467309
.33000947820757	.04465473951622	.01105516112504	-.00157634391318	.00031957112534
.66999052179243	.10477319401975	.10928215124631	.01105516112504	-.00066685674526
.93056815579703	.14960613448281	.19642483580315	.08371702284510	.00323055316068
	.16185132086231	.21846553629538	.10760704113589	.01207610170642
	.17392742256873	.32607257743127	.32607257743127	.17392742256873

with stability boundary $\beta_{corr} = 9.86$

A.2.7. The 5-stage direct collocation-based Radau IIA Runge-Kutta-Nyström corrector method

.05710419611452	.00224347112086	-.00103687182778	.00073133548477	-.00050560983563	.00019811966472
.27684301363812	.03108273511543	.00834170664325	-.00157102933696	.00070672593038	-.00023911125198
.58359043236892	.07589152043041	.08508291363323	.01012552665068	-.00100095211071	.00018988777267
.86024013565622	.11533394404710	.16450067926681	.08525394016214	.00500946019427	-.00009147817341
1.0000000000000	.13550691343149	.20346456801027	.12984754760823	.03118097095001	.00000000000000
	.13550691343149	.20346456801027	.12984754760823	.03118097095001	.00000000000000
	.14371356079122	.28135601514946	.31182652297574	.22310390108357	.04000000000000

with stability boundary $\beta_{corr} = 9.86$

A.2.8 The 5-stage direct collocation-based Gauss-Legendre Runge-Kutta-Nyström corrector method

.04691007703067	.00149031739012	-.00062259679760	.00036153237990	-.00018017673448	.00005120142557
.23076534494716	.02147193514388	.00591709001729	-.00103452586322	.00036101254307	-.00008918962672
.50000000000000	.05382516053910	.06356132506917	.00833333333333	-.00087038743098	.00015056848937
.76923465505284	.08547986650844	.12922443754336	.07554777601848	.00591709001729	-.00030819282043
.95308992296933	.10740038552504	.17268244948941	.12924044380229	.04337660442598	.00149031739012
	.11290631331378	.18408888012499	.14222222222222	.05522545512469	.00555712921431
	.11846344252809	.23931433524968	.28444444444444	.23931433524968	.11846344252809

with stability boundary $\beta_{corr} = 36.65$