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We analyse the attainable order and the stability of Runge-Kutta-Nyström (RKN) methods for special second-order initial-value problems derived by collocation techniques. Like collocation methods for first-order equations the step point order of s-stage methods can be raised to 2s if s is even and to 2s-1 if s is odd. The attainable stage order is one higher and equals s+1. However, the stability results derived in this paper show that we have to pay a high price for the increased stage order.

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1. Introduction

In this paper we shall be concerned with the analysis of implicit Runge-Kutta-Nyström methods (RKN methods) based on collocation for integrating the initial-value problem for systems of special second-order, ordinary differential equations (ODEs) of dimension d, i.e. the problem,

$$(1.1)\qquad y''(t) = f(t, y(t)),\quad y(t_0) = y_0,\ y'(t_0) = u_0,\quad y : \mathbb{R} \to \mathbb{R}^d,\quad f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d,\quad t_0 \le t \le T.$$

Our motivation for studying implicit RKN methods is the arrival of parallel computers which enables us to solve the implicit relations occurring in the stage vector equation quite efficiently, so that, what is so far considered as the main disadvantage of fully implicit RKN methods, is reduced a great deal. In a forthcoming paper, the results obtained here will be used in the design of parallel RKN-based predictor-corrector methods.

We consider two types of collocation methods for second-order equations: methods based on *direct* collocation and on *indirect* collocation (that is, methods obtained by writing the special second-order equation in first-order form and by applying collocation methods for first-order equations [6]). The theory of *indirect* collocation methods for problem (1.1) completely parallels the well-known theory of collocation methods for first-order equations (cf. [3], [7]). The attainable step point and stage order using s stages equals 2s and s. By a suitable choice of the collocation parameters, these methods can be made A-stable for all even s (generated by Gauss methods) or L-stable for all odd s (Radau IIA methods). There even exist indirect collocation methods with stage order s using only s-1 implicit stages (and one explicit stage) which are known to be A-stable for s≤9 (Newton-Cotes methods [17]) or strongly A-stable for s≤5 (Lagrange methods [9]). In the following, k will denote the number of implicit stages of the method. Since in actual computation, it is the number of *implicit* stages that determines the computational complexity of the method, we shall often characterize RKN methods by k rather than by s.

The stability of direct collocation was investigated in Kramarz [12]. The main object of this paper is to extend the work of Kramarz and to derive order and stability results for direct collocation methods. It will be shown that the attainable step point order is similar to that of indirect collocation methods, but the stage order can be raised to s+1 leaving all but one collocation parameters free. High stage orders are attractive in the case of stiff problems, provided that the method is A or P-stable. However, it seems that the increased-stage-order methods all have *finite* stability boundaries (i.e., no A-stability). If the stage order is decreased to s, then infinite stability boundaries (i.e., strong A-stability) can be obtained. We found A-stable methods with k=s=2, k=s=3 and with k=s-1=4 implicit stages.

We also investigated two stabilizing techniques for achieving A-stability. The first stabilizing technique is based on the *preconditioning* of the righthand side in (1.1), that is, stiff components in the righthand side are damped. In this way, it is possible to transform conditionally stable RKN methods into unconditionally stable preconditioned RKN methods (*PRKN methods*) at the cost of a slightly more complicated implicit relation for the stage vector. For autonomous systems, the preconditioner hardly decreases the accuracy. However, for nonautonomous systems the accuracy may drop considerably.

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The second stabilizing technique is based on the application of different, conditionally stable RKN methods. We will give examples of A-stable, composite methods (*CRKN methods*) with stage order s and k=s-1 implicit stages for $k \le 4$.

Summarizing, this paper presents order and stability results for three families of methods based on direct collocation. Assuming that these methods all have k implicit stages (including those the CRKN methods are composed of), we get the following survey of main characteristics (p and r denote the step point and stage order of the methods):

Table 1.1. Survey of characteristics of methods based on direct collocation

Family		s	p	r	Stability	With preconditioning	Subsections
A. single:	Gauss	k	2k	k+1	Finite stability boundary	Weakly A-stable	4.2.1, 4.3
	Radau	k	2k-1	k+1	Finite stability boundary	Weakly A-stable	4.2.1, 4.3
	Lobatto	k+1	2k	k+2	Finite stability boundary	Weakly A-stable	4.2.1, 4.3
B. single:	k=2,3	k	k	k	Strongly A-stable	-	4.2.2
	k=4	k+1	k+1	k+1	Strongly A-stable	-	4.2.2
C. composite:	$k \le 4$		k+1	k+1	Strongly A-stable	-	4.2.3

2. RKN Methods

For the sake of simplicity of notation, we assume that (1.1) is a scalar initial-value problem (IVP). However, all considerations can be trivially extended to systems of equations. For scalar ODEs, the general s-stage RKN method is defined by

$$
\begin{aligned}
y_{n+1} &= y_n + hy'_n + h^2\mathbf{b}^T f(\mathbf{e}t_n + \mathbf{c}h, \mathbf{Y}),\\
y'_{n+1} &= y'_n + h\mathbf{d}^T f(\mathbf{e}t_n + \mathbf{c}h, \mathbf{Y}),\\
\mathbf{Y} &= \mathbf{e}y_n + \mathbf{c}hy'_n + h^2 A f(\mathbf{e}t_n + \mathbf{c}h, \mathbf{Y}),
\end{aligned}
\tag{2.1}
$$

where h is the stepsize, $\{t_n\}$ is the set of step points and y_{n+1}, y'_{n+1} denote the numerical approximations to $y(t_{n+1})$, $y'(t_{n+1})$. Furthermore, **b**, **c** and **d** are s-dimensional vectors, **e** is the s-dimensional vector with unit entries, A is an s-by-s matrix, and, for any pair of vectors $\mathbf{v}=(v_i)$, $\mathbf{w}=(w_i)$, $f(\mathbf{v},\mathbf{w})$ denotes the vector with entries $f(v_i,w_i)$. In presenting RKN methods, we shall mostly use the Butcher array notation, i.e., (2.1) is presented by

$$
\begin{array}{c|c}
\mathbf{c} & A \\
\hline
 & \mathbf{b}^T \\
 & \mathbf{d}^T
\end{array}\ .
\tag{2.1'}
$$

If the last row of A equals the row vector $\mathbf{b}^T$, i.e., $\mathbf{b}^T = \mathbf{e}_s^T A$, then, as in the case of RK methods for first-order IVPs, such methods are said to be *stiffly accurate*, and *nonstiffly accurate* otherwise. In general, stiffly accurate methods perform better on stiff problems than nonstiffly accurate methods.

In the following subsections, we discuss the order of accuracy p, the stage order r, the stability boundary β_{stab}, and the periodicity boundary β_{per} of RKN methods. The number of stages will always be denoted by s and the number of *implicit* stages by k (the computational effort to solve for the stage vector **Y** is essentially determined by k).

2.1. Order of accuracy

Let $\mathbf{Y}(t_{n+1})$ denote the vector with components $y(t_n+c_ih)$ with y the locally exact solution of (1.1) satisfying $y(t_n)=y_n$ and $y'(t_n)=y'_n$, and suppose that the local errors are given by

$$
\begin{aligned}
&y(t_{n+1}) - y_{n+1} = O(h^{p_1+1}), \quad y'(t_{n+1}) - y'_{n+1} = O(h^{p_2+1}),\\
&\mathbf{Y}(t_{n+1}) - \mathbf{e}y_n - \mathbf{c}hy'_n - h^2 A f(\mathbf{e}t_n + \mathbf{c}h, \mathbf{Y}(t_{n+1})) = O(h^{p_3+1}),
\end{aligned}
\tag{2.2}
$$

then the order of accuracy p and the stage order r are respectively defined by

$$
p=\min\{p_1,p_2\}, \quad r=\min\{p_1,p_2,p_3\}.
\tag{2.3}
$$

For stiff *first-order* ODEs the accuracy reducing effect of order reduction for methods with low stage orders is well known [4], and therefore collocation methods (which automatically possess high stage orders) are rather accurate integration methods for stiff problems. The following example reveals that a similar phenomenon occurs in the case of stiff *second-order* equations.

Example 2.1. Consider the system of (uncoupled) second-order Prothero-Robinson-type equations (cf. [15]):

(2.4) $$y''(t) = J\,[y(t) - g(t)] + g''(t),\quad J := \mathrm{diag}\big(-100^{i-1}\big),\quad g(t) = \big(\cos(it)\big),\quad i = 1, \ldots, 6;\quad 0 \le t \le t_{end} = 10\pi,$$

with initial values $y(0)=g(0)$, $y'(0)=g'(0)$, so that its exact solution is given by $y(t)=g(t)$. The spectrum of the Jacobian matrix of the righthand side is given by $\{-100^0, \ldots, -100^5\}$. The RKN methods tested are the indirect versions of the Gauss, Radau IIA, and Lagrange methods (cf. Subsection 3.1 for indirect collocation, and [9] for specification of the Lagrange methods). Table 2.1 below lists the number of correct digits (NCD) obtained at the end of the integration interval, together with the observed order of convergence p* and, in brackets, the component that is most inaccurate. Here, the NCD-value and p* are defined by

$$\mathrm{NCD}(h) := -\log(\|y(t_{end}) - y(t_{end},h)\|_\infty),\quad p^*(h) := \frac{\mathrm{NCD}(h) - \mathrm{NCD}(2h)}{\log(2)},$$

where $y(t_{end},h)$ denotes the numerical approximation at $t=t_{end}$ obtained for stepsize h.

Table 2.1. NCD and p* values produced by the (indirect) Gauss, Radau IIA and Lagrange methods for problem (2.4).

	Method	s	p	r	h=2π/3	h=π/3	h=π/6	h=π/12	h=π/24	h=π/48	p*(π/48)
k=2	Gauss	2	4	2	-0.2 (3)	0.2 (3)	1.0 (4)	1.6 (3)	1.7 (5)	2.3 (5)	2.0
	Radau IIA	2	3	2	0.0 (1)	0.4 (1)	1.2 (1)	2.1 (1)	3.0 (1)	3.9 (1)	3.0
	Lagrange	3	3	3	0.1 (1)	0.7 (1)	1.5 (1)	2.4 (1)	3.3 (1)	4.2 (1)	3.0
k=3	Gauss	3	6	3	-0.9 (5)	0.9 (4)	1.1 (4)	2.7 (5)	3.6 (5)	4.5 (6)	3.0
	Radau IIA	3	5	3	0.9 (1)	2.2 (2)	2.7 (2)	4.3 (3)	4.8 (3)	5.6 (3)	2.7
	Lagrange	4	4	4	0.7 (1)	2.1 (1)	3.6 (1)	5.1 (1)	6.6 (1)	8.1 (1)	5.0
k=4	Gauss	4	8	4	0.1 (2)	1.4 (4)	2.5 (4)	3.3 (5)	4.7 (4)	5.3 (6)	2.0
	Radau IIA	4	7	4	1.5 (2)	2.5 (2)	3.6 (2)	5.8 (3)	7.6 (3)	9.1 (4)	5.0
	Lagrange	5	5	5	2.1 (2)	3.5 (2)	4.3 (2)	6.4 (3)	8.0 (3)	8.9 (3)	3.0

The results in Table 2.1 show an irregular order behaviour for all methods. The better performance of the Radau IIA and Lagrange methods can be explained by observing that these methods are stiffly accurate (that is, they are highly accurate for the stiff components), so that the overall accuracy is largely determined by the nonstiff components. □

2.2. Linear stability

The linear stability of RKN methods is investigated by applying them to the test equation $y''=\lambda y$, where λ runs through the eigenvalues of $\partial f/\partial y$. This leads to recursions of the form

(2.5a) $$v_{n+1} = M(z)v_n,\quad v_n := (y_n, hy'_n)^T,\quad z := \lambda h^2,$$

where the so-called amplification matrix M(z) is defined by

(2.5b) $$M(z) := \begin{pmatrix} 1 + z\mathbf{b}^T(I - Az)^{-1}\mathbf{e} & 1 + z\mathbf{b}^T(I - Az)^{-1}\mathbf{c} \\ z\mathbf{d}^T(I - Az)^{-1}\mathbf{e} & 1 + z\mathbf{d}^T(I - Az)^{-1}\mathbf{c} \end{pmatrix}.$$

The eigenvalues $\mu(z)$ of the amplification matrix M(z) are the roots of the equation

$$\mu^2 - S(z)\mu + P(z) = 0,\quad S(z) := \mathrm{trace}\, M(z),\quad P(z) := \det M(z).$$

The damping effect of the matrix M(z) can be characterized by the *stability function* R(z) of the RKN method defined by the spectral radius of M(z):

(2.6) $$R(z) := \rho(M(z)).$$

Definition 2.1. The region on the negative real z-axis is called the region of

(strong) stability if $R(z) < 1$
weak stability if $|\mu(z)| = 1$
periodicity if $|\mu(z)| = 1$ and $[S(z)]^2 - 4P(z) < 0$

in that region. If the strong stability region contains an interval $(-\beta_{stab}, 0)$, then β_{stab} is called the *stability boundary*, and if the periodicity region contains an interval $(-\beta_{per}, 0)$, then β_{per} is called the *periodicity boundary*. If $\beta_{stab}=\infty$, then the RKN method is called *A-stable* and if $\beta_{per}=\infty$, then it is called *P-stable*. An A-stable RKN method is called *L-stable* if $R(-\infty)=0$ and *strongly A-stable* if $R(-\infty)<1$. □

The definition of the periodicity boundary is a direct extension of the definition given in [13] for linear multistep methods. In this paper, stability regions will always be understood to be regions of *strong* stability. As a consequence, we have that for methods with nonempty periodicity regions the stability region is empty. Hence, such methods have no damping, and in particular, they do not damp stiff components. Thus, in problems where such dissipation-free methods are required, RKN methods with nonempty periodicity regions are desirable integration methods.

As we shall see in Section 3, the RKN parameters in collocation-based methods can explicitly be expressed in terms of the collocation vector **c**. By means of these expressions, the search for A-stable and P-stable methods is relatively easy but may be rather time-consuming if the number of free collocation parameters in **c** increases. Therefore, it is helpful to derive conditions on the collocation parameters which lower the dimension of the space of free parameters. Below, necessary conditions for A-stability, L-stability or P-stability are derived by considering the amplification matrix $M(z)$ at infinity. These conditions can be used in a numerical search for stable methods because they limit the dimension of the parameter space. We shall distinguish stiffly and nonstiffly accurate methods. Furthermore, we distinguish the cases $c_1=0$ and $c_1\neq0$. If $c_1=0$, then the first row of A vanishes, so that the RKN method has only $k=s-1$ implicit stages (and one explicit stage).

For methods with $c_1=0$, the matrix A in (2.5b) becomes singular, so that we cannot use this representation at infinity. An alternative representation for the nonstiffly accurate case is obtained by writing (2.1') in the form

$$\begin{array}{c|cc} 0 & 0 & \mathbf{0}^T \\ \mathbf{c}^* & \mathbf{a} & A^* \\ \hline & b_1 & \mathbf{b}^{*T} \\ & d_1 & \mathbf{d}^{*T} \end{array}\;,$$

and by considering the corresponding recursions

$$(2.7)\qquad \begin{aligned} &y_{n+1} = y_n + hy'_n + zb_1y_n + z\mathbf{b}^{*T}\mathbf{Y}^*, \quad hy'_{n+1} = hy'_n + zd_1y_n + z\mathbf{d}^{*T}\mathbf{Y}^*, \\ &\mathbf{Y}^* = [I - zA^*]^{-1}[\mathbf{e}^*y_n + \mathbf{c}^*hy'_n + z\mathbf{a}y_n]. \end{aligned}$$

Thus,

$$M(z) := \begin{pmatrix} 1 + zb_1 + z\mathbf{b}^{*T}(I - A^*z)^{-1}[\mathbf{e}^* + z\mathbf{a}] & 1 + z\mathbf{b}^{*T}(I - A^*z)^{-1}\mathbf{c}^* \\ zd_1 + z\mathbf{d}^{*T}(I - A^*z)^{-1}[\mathbf{e}^* + z\mathbf{a}] & 1 + z\mathbf{d}^{*T}(I - A^*z)^{-1}\mathbf{c}^* \end{pmatrix}.$$

This representation shows that the entries of $M(z)$ are bounded as z tends to infinity, provided that $b_1=\mathbf{b}^{*T}A^{*-1}\mathbf{a}$ and $d_1=\mathbf{d}^{*T}A^{*-1}\mathbf{a}$. Clearly, in the case of A-stable or P-stable methods, the entries of the amplification matrix $M(z)$ should be bounded as z tends to infinity, so that these conditions are necessary conditions.

For stiffly accurate methods with $c_1=0$, we have $\mathbf{b}^T=\mathbf{e}_s{}^TA$ which implies that $y_{n+1}=\mathbf{e}_s{}^T\mathbf{Y}=\mathbf{e}_{s-1}{}^T\mathbf{Y}^*$, so that inserting this relation into (2.7) yields

$$M(z) := \begin{pmatrix} \mathbf{e}_{s-1}{}^T(I - A^*z)^{-1}[\mathbf{e}^* + z\mathbf{a}] & \mathbf{e}_{s-1}{}^T(I - A^*z)^{-1}\mathbf{c}^* \\ zd_1 + z\mathbf{d}^{*T}(I - A^*z)^{-1}[\mathbf{e}^* + z\mathbf{a}] & 1 + z\mathbf{d}^{*T}(I - A^*z)^{-1}\mathbf{c}^* \end{pmatrix}.$$

Again, in the case of A-stable or P-stable methods, the entries of the amplification matrix $M(z)$ should be bounded as z tends to infinity, which leads to the necessary condition $d_1=\mathbf{d}^{*T}A^{*-1}\mathbf{a}$.

Finally, we consider stiffly accurate methods with $c_1\neq0$. Again we have $y_{n+1}=\mathbf{e}_s{}^T\mathbf{Y}$, and similar to the derivation above, we obtain

$$M(z) := \begin{pmatrix} \mathbf{e}_s{}^T(I - Az)^{-1}\mathbf{e} & \mathbf{e}_s{}^T(I - Az)^{-1}\mathbf{c} \\ z\mathbf{d}^T(I - Az)^{-1}\mathbf{e} & 1 + z\mathbf{d}^T(I - Az)^{-1}\mathbf{c} \end{pmatrix}.$$

Here, we have bounded entries for all values of z. In this particular case, we can derive a simple expression for the stability function $R(z)$ at infinity (cf. (2.6)). From the above representation for $M(z)$ it follows that $P(z)=\det M(z)$ vanishes at infinity, so that $M(z)$ has eigenvalues 0 and $S(-\infty)=\mathrm{trace}\, M(-\infty)=1-\mathbf{d}^TA^{-1}\mathbf{c}$ at infinity. Hence, assuming that A is nonsingular

$$(2.8)\qquad R(z) \approx 1 - \mathbf{d}^TA^{-1}\mathbf{c} \quad \text{as } z \to \infty.$$

From this relation necessary conditions for stiffly accurate RKN methods with $c_1\neq0$ to be strongly A-stable or L-stable are immediate.

3. RKN Methods Based on Collocation

We shall describe the construction of collocation methods and we derive order results for direct collocation methods. We distinguish *direct* and *indirect* collocation methods.

3.1. Indirect collocation methods

Indirect collocation methods are generated by applying an RK collocation method to the first-order representation of (1.1). Thus, writing (1.1) in the form

(1.1') $\quad y'(t) = u(t),\quad u'(t) = f(t, y(t)),\quad y(t_0) = y_0,\quad u(t_0) = u_0,$

and applying an RK method for first-order equations defined by the Butcher array

$$\begin{array}{c|c} \mathbf{c} & \mathring{A} \\ \hline & \mathbf{d}^T \end{array},$$

we obtain the RKN method (cf. [6])

$$\text{(3.1)}\qquad \begin{array}{c|c} \mathbf{c} & \mathring{A}^2 \\ \hline & \mathbf{d}^T\mathring{A} \\ & \mathbf{d}^T \end{array}.$$

Notice that when the generating RK method has order p and k implicit stages, then the RKN method (3.1) also does. Now, let the generating RK method be a collocation method based on the s distinct collocation points

$$\{t_{nj}: t_{nj} := t_n + c_jh,\ j = 1, \dots, s\},$$

then (cf., e.g., [7])

$$\text{(3.2)}\qquad \mathring{A} = (\mathring{a}_{ij}) := \big(\alpha_j(c_i)\big),\ \mathbf{d} = (d_i) := \big(\alpha_i(1)\big),\ \alpha_j(x) := \int_0^x L_j(\xi)\, d\xi,\ L_j(x) := \prod_{i=1,i\neq j}^{s} \frac{x - c_i}{c_j - c_i},\qquad i, j = 1, \dots, s.$$

Here, $L_j(x)$ is the jth Lagrange polynomial associated with the s collocation parameters $\{c_i\}$. The family of indirect collocation methods defined by (3.1) and (3.2) has order p=r=s for all collocation vectors **c** (cf., e.g., [4]). The RKN method will be called *symmetric* if the location of the collocation points t_{nj} is symmetric with repect to t_n+h/2.

By a special choice of the collocation points, it is possible to increase the step point order p beyond s (superconvergence at the step points). This is easily seen by applying the generating RK method to the equation y'=g(t,y(t)) and by writing the relation for the local error in the form

$$\text{(3.3)}\qquad \int_{t_n}^{t_{n+1}} g(t,y(t))\, dt = y(t_{n+1}) - y_n = h\mathbf{d}^T g(\mathbf{e}t_n + \mathbf{c}h, Y) + O\big(h^{p+1}\big).$$

This relation shows that $h\mathbf{d}^T g(\mathbf{e}t_n + \mathbf{c}h, Y)$ can be interpreted as a quadrature formula for the integral term. We now use the following result for interpolatory quadrature formulas: Let **d** be defined as in (3.2) and let $\mathbf{c}=(c_i)$ be such that

$$\text{(3.4)}\qquad P_j(1) = 0,\quad P_j(x) := \int_0^x \xi^{j-1} \prod_{i=1}^{s} (\xi - c_i)\, d\xi,\quad j = 1, 2, \dots, q,$$

then for sufficiently differentiable functions G we have that

$$\text{(3.5)}\qquad \int_{t_n}^{t_{n+1}} G(t)\, dt \;=\; h\mathbf{d}^T G(\mathbf{e}t_n + \mathbf{c}h) + O\big(h^{s+q+1}\big).$$

It can be proved that if **c** is such that (3.5) is satisfied, then (3.3) is also satisfied with p=s+q (cf., e.g. [7, p.207]). We summarize the preceding considerations in the following theorem:

Theorem 3.1. The indirect RKN method defined by {(3.1),(3.2)} has global step point order and global stage order $p=r=s$ for all sets of distinct collocation parameters c_i. If, in addition, (3.4) is satisfied, then $p=s+q$. □

3.2. Direct collocation methods

Direct collocation methods for second-order equations (1.1) were studied in e.g. [1] and [12]. In these papers, the exact solution of (1.1) is approximated by polynomials which satisfy, at the collocation points defined above, the equation (1.1) and possibly the (repeatedly) differentiated form of (1.1). In this paper, we consider collocation methods that only satisfy the (nondifferentiated) equation (1.1).

3.2.1. Methods of order p=r=s. Following [2, p.241], let S be the space of real, piecewise continuously differentiable polynomials of degree not exceeding s+1 associated with the set of intervals $[t_n,t_{n+1}]$. Thus, if u is in S, then u(t) is a polynomial of degree $\le s+1$ on each interval $[t_n,t_{n+1}]$, $n = 0, \dots, N-1$. For such functions u, the second derivative u" is a polynomial of degree not exceeding s-1 on each of the intervals $[t_n,t_{n+1}]$, so that we may write

$$\text{(3.6a)}\qquad u''(t_n + xh) = \sum_{j=1}^{s} L_j(x)u''(t_{nj}),$$

where $L_j(x)$ is again the jth Lagrange polynomial associated with the s distinct collocation parameters $\{c_j\}$. By integrating (3.6a) we derive

$$\text{(3.6b)}\qquad u'(t_n + xh) = u'(t_n) + h\sum_{j=1}^{s} \alpha_j(x)u''(t_{nj}),\quad u(t_n + xh) = u(t_n) + xhu'(t_n) + h^2\sum_{j=1}^{s} \beta_j(x)u''(t_{nj}),$$

where $\alpha_j(x)$ is defined in (3.2) and

$$\text{(3.7)}\qquad \beta_j(x) := \int_0^x \int_0^\eta L_j(\xi)\, d\xi d\eta.$$

In passing, we observe that the derivation of $\beta_j(x)$ can be simplified by using Dirichlet's integral formula which yields

$$\text{(3.7')}\qquad \beta_j(x) := \int_0^x \int_0^\eta L_j(\xi)\, d\xi d\eta = \int_0^x \int_\xi^x L_j(\xi)\, d\eta d\xi = \int_0^x (x - \xi)\, L_j(\xi)\, d\xi = x\alpha_j(x) - \int_0^x \xi L_j(\xi)\, d\xi.$$

Next, we require that the function u satisfies the ODE (1.1) at the collocation points, i.e.,

$$\text{(3.8)}\qquad u''(t_{nj}) = f(t_{nj},u(t_{nj})),\quad j = 1, \dots, s,$$

then (3.6b) leads to :

$$\text{(3.9a)}\qquad u(t_{ni}) = u(t_n) + c_ihu'(t_n) + h^2\sum_{j=1}^{s} \beta_j(c_i)\, f(t_{nj},u(t_{nj})),\quad u'(t_{ni}) = u'(t_n) + h\sum_{j=1}^{s} \alpha_j(c_i)f(t_{nj},u(t_{nj})),\ i = 1, \dots, s.$$

Furthermore, we derive from (3.6b)

$$\text{(3.9b)}\qquad u(t_{n+1}) = u(t_n) + hu'(t_n) + h^2\sum_{j=1}^{s} \beta_j(1)f(t_{nj},u(t_{nj})),\quad u'(t_{n+1}) = u'(t_n) + h\sum_{j=1}^{s} \alpha_j(1)f(t_{nj},u(t_{nj})).$$

The method (3.9) is recognized as the s-stage RKN method (2.1) by introducing the quantities

$$\text{(3.10)}\qquad \begin{aligned} &y_n := u(t_n),\quad y'_n := u'(t_n),\quad \mathbf{Y} := (u(t_{ni})),\\ &\mathbf{b} := (b_i),\quad \mathbf{d} := (d_i),\quad A = (a_{ij}),\quad b_i := \beta_i(1),\quad d_i := \alpha_i(1),\quad a_{ij} := \beta_j(c_i). \end{aligned}$$

As in the case of indirect collocation methods, the RKN method (3.6) will be called *symmetric* if the location of the collocation points t_{nj} is symmetric with repect to $t_n+h/2$.

Since in the interval $[t_n,t_{n+1}]$ the function u is a polynomial of degree $\le s+1$ and satisfies the collocation equations (3.8), it follows form (2.3) that $p_1=s+1$, $p_2=s$ and $p_3=s+1$, so that $p=r=s$.

Theorem 3.2. The direct RKN method defined by (3.10) has global step point order and global stage order $p=r=s$ for all sets of distinct collocation parameters c_i. □

3.2.2. Superconvergence. As in the case of indirect collocation, it is possible to increase the orders p_1 and p_2 beyond s+1 and s by a special choice of the collocation points (superconvergence at the step points). We first consider the local order of y'_{n+1}. In analogy with (3.3), we write the local error of y'_{n+1} in the form

$$\int_{t_n}^{t_{n+1}} f(t,y(t))\,dt = y'(t_{n+1}) - y'_n = hd^T f(et_n + ch, Y) + O(h^{p_2+1}). \tag{3.11}$$

A comparison with (3.5) reveals that $p_2=s+q$ if the collocation points satisfy the relations (3.4). Thus, setting q=1, we have the theorem:

Theorem 3.3. If (3.4) is satisfied for q=1, then the direct RKN method defined by (3.10) has global step point order and global stage order $p=r=s+1$. □

Example 3.1. For s=2 and q=1 condition (3.4) yields $c_2=(2-3c_1)/(3-6c_1)$. Choosing $c_1=0$, we find that $c_2=2/3$. Thus, the direct collocation method with $c=(0,2/3)^T$ has order $p=r=3$ and requires only one implicit stage. Furthermore, we have for $c=(1/3,1)^T$ a stiffly accurate method with order $p=r=3$. □

Theorem 3.4. For all symmetric methods with an odd number of stages, condition (3.4) is satisfied for q=1.

Proof. Let s=2m+1, then the symmetry condition implies $c_{m+1}=1/2$ and $c_i=1-c_{2m+2-i}$ for i=1,...,m. Hence, setting $\xi=\eta+1/2$, the polynomial $P_1(x)$ in (3.4) reads

$$P_1(x) := \int_{-1/2}^{x-1/2} \eta \prod_{i=1}^{m} (\eta + 1/2 - c_i)(\eta - 1/2 + c_i)\,d\eta .$$

It is easily seen that $P_1(1)$ vanishes for all values of the m free parameters c_i. □

Theorem 3.5. If condition (3.4) is satisfied, then the direct RKN method (3.10) has global step point order p=s+q.

Proof. From the condition (3.4) it follows that $p_2=s+q$ (cf. (3.11)). Furthermore, the condition $P_1(1)=0$ implies

$$\int_0^1 \prod_{i=1}^{s} (\xi-c_i)\,d\xi = \int_0^1 (\xi - c_j) \prod_{i=1,i\ne j}^{s} (\xi-c_i)\,d\xi = 0.$$

Hence, from the definition of the Lagrange polynomials L_j in (3.2) it follows that

$$\int_0^1 \xi L_j(\xi)\,d\xi - \int_0^1 c_j L_j(\xi)\,d\xi = 0. \tag{3.12}$$

By observing that (cf. (3.10)) $b_i = \beta_i(1) = \alpha_i(1) - \int_0^1 \xi L_i(\xi)\,d\xi$ and $d_i = \alpha_i(1) = \int_0^1 L_i(\xi)\,d\xi$, we derive from (3.12)

$$b_i = d_i - d_i c_i, \quad i = 1, \dots, s. \tag{3.13}$$

There remains to show that condition (3.4) together with (3.13) implies that $p_1=s+q$. Condition (3.13) is recognized as a well-known simplifying condition for RKN methods (see, e.g. [7, p.268]). According to a lemma of Hairer [5], this simplifying condition implies that the order conditions for the y-component are a subset of the order conditions for the y'-component. Thus, if $p_2=s+q$, then $p_1=s+q$, so that the assertion of the theorem is proved. □

Corollary 3.1. Direct and indirect collocation methods with the same collocation points have the same step point order. For methods satisfying $P_1(1)=0$, the stage order of direct collocation methods is one higher. □

Example 3.2. We illustrate Corollary 3.1 by applying indirect and direct collocation methods based on the 3-point Radau vector

$$c^T = \left(\frac{4-\sqrt{6}}{10}, \frac{4+\sqrt{6}}{10}, 1 \right)$$

to the initial-value problem for

$$(3.14) \qquad u'' = -4t^2u - \frac{2v}{\sqrt{u^2+v^2}}, \quad v'' = -4t^2v + \frac{2u}{\sqrt{u^2+v^2}}, \quad \sqrt{\pi/2} \le t \le 3\pi,$$

where the initial values are chosen such that the exact solution is given by $u(t)=\cos(t^2)$ and $v(t)=\sin(t^2)$.

Table 3.2. NCD and p* values produced by indirect and direct Radau for problem (3.14) for $h=(3\pi-\sqrt{\pi/2})/N$.

Method	s	p	r	N=80	N=160	N=320	N=640	N=1280	p*
Indirect Radau	3	5	3	1.2	2.7	4.2	5.7	7.2	5.0
Direct Radau	3	5	4	1.8	3.3	4.8	6.3	7.8	5.0

The results in Table 3.1 show that both methods behave as fifth-order methods and that direct collocation is slightly more accurate than indirect collocation. □

4. Stability of Collocation Methods

In this section, we discuss the linear stability of RKN methods based on collocation. For the sake of completeness, we also briefly summarize known results for indirect collocation.

4.1. Indirect collocation

In the case of the indirect collocation methods, we can resort to the theory of collocation methods for first-order equations and the derivation of suitable methods is straightforward. For indirect methods of the form (3.1) it can be derived that the amplification matrix M(z) defined in (2.5b) is given by

$$(4.1) \qquad M(z) = R^*(Z), \quad Z := \begin{pmatrix} 0 & 1 \\ z & 0 \end{pmatrix}, \quad R^*(w) := 1 + wb^T(I - Aw)^{-1}e, \quad z := \lambda h^2,$$

where $R^*(w)$ denotes the stability function of the generating RK method. Hence, the stability function of the generated RKN method is given by

$$(4.2) \qquad R(z) := \rho(M(z)) = \text{Max}\ \{R^*(\pm\sqrt{z})\}.$$

From this formula, we conclude that if, and only if, (2.1) possesses the stability interval $(-\beta_{stab},0)$, then the generating RK method possesses the imaginary stability boundary $(\beta_{stab})^{1/2}$. Hence, A-stable RK methods (i.e., $(\beta_{stab})^{1/2}=\infty$) generate A-stable RKN methods. In particular, the s-stage Radau IIA methods generate L-stable RKN methods with step point order 2s-1 and stage order equal to the number of implicit stages s. However, the Lagrange methods derived in [9] generate (strongly) A-stable RKN methods where the stage order equals the number of implicit stages plus one.

If one wants RKN methods with a nonempty periodicity interval, we have to choose generating RK methods with stability functions that have modulus 1 along the imaginary axis. This means that $R^*(w)$ should satisfy the (necessary and sufficient) condition $R^*(w)R^*(-w)=1$. For example, the diagonal elements of the Padé table associated with exp(w) satisfy this condition, and hence, the s-stage Gauss-Legendre methods generate s-stage, P-stable RKN methods with stage order s and step point order 2s (cf. [6]).

4.2. Direct collocation

For the direct collocation methods defined in (3.10), the stability analysis is more complicated than for indirect methods, because the stability function which determines the stability region is much more complicated than (4.2). The stability of a general class of direct collocation methods, including the RKN methods (3.10), was studied by Kramarz [12]. The following theorem summarizes the stability results derived in [12] as far as they apply to the RKN methods of the form (3.10).

Theorem 4.1. Let the RKN method be defined by (3.10), and let the collocation parameters be restricted to the interval [0,1], then the following assertions hold:

(a) Symmetric methods possess a nonempty interval $(-\beta,0)$ of weak stability.
(b) If $c_1=0$, $c_s\neq1$ or if $c_1\neq0$, $c_s=1$, then there is no interval of weak stability of the form $(-\beta,0)$.

(c) Symmetric two-stage methods have the largest interval of weak stability of the form $(-\beta,0)$ if $c_1=0$; this maximal interval is given by (-12,0).
(d) Two-stage, stiffly accurate ($c_2=1$) methods are A-stable if $7/10\le c_1\le 1$.
(e) Symmetric three-stage methods are weakly stable at least in (-8,0).
(f) Symmetric three-stage methods have the largest interval of weak stability of the form $(-\beta,0)$ if $c_1\approx 0.129$; this maximal interval is approximately given by (-33,0). □

It can be easily verified that the weak stability results of this theorem are in fact periodicity results.

The derivation of A-stable or P-stable methods becomes increasingly difficult for three-stage and higher-stage methods, and for these methods it is not feasible to analyse the stability function by analytical methods, so that we have to apply numerical techniques. By expressing the RKN parameters explicitly in terms of the collocation vector **c**, the search for A-stable and P-stable methods is relatively easy (see the Appendix to the institute report version [10] of this paper where full details on the derivation of the RKN parameters can be found). It turns out that the situation for direct collocation methods is less favourable than for indirect methods in the sense that the construction of direct collocation methods which are A-stable or P-stable and have RKN parameters of acceptable magnitude (say, not greater than 10 in magnitude) is quite cumbersome. For instance, we did not find stiffly accurate methods in the family A of Table 1.1 that are A-stable or P-stable. For two-stage methods this immediately follows from the above results of Kramarz, viz., according to Example 3.1, the two-stage, stiffly accurate method with stage order r=3 is generated by $c=(1/3,1)^T$ and from part (d) of Theorem 4.1 it then follows that this method cannot be A-stable.

In the following subsections, we present stability results for a number of methods belonging to the families A, B and C of Table 1.1.

4.2.1. Conditionally stable RKN methods. In Table 4.1 order and stability characteristics of methods generated by conventional sets of collocation points are listed (these methods belong to family A of Table 1.1). In general, these methods have a stability region consisting of a number of intervals of instability of which the first two are listed. They are indicated by U_1 and U_2, and the corresponding maximum values of the stability function R are denoted by $R_{max}(U_i)$.

Table 4.1. Order and stability characteristics of direct Gauss, Radau and Lobatto collocation methods.

	Method	c^T	p	r	U_1	$R_{max}(U_1)$	U_2	$R_{max}(U_2)$	$R(\infty)$
k=2	Gauss	$(3-\sqrt{3}, 3+\sqrt{3})/6$	4	3	(-12, -9)	1.23	$(-\infty, -35.9)$	13.9	13.9
	Radau	(1/3, 1)	3	3	(-16.73, -8.61)	1.25	$(-\infty, -108)$	2.0	2.0
	Lobatto	(0, 1/2, 1)	4	4	(-12.0, -9.6)	1.17	$(-\infty, -48)$	7.9	7.9
k=3	Gauss	$(5-\sqrt{15}, 5, 5+\sqrt{15})/10$	6	4	(-10.01, -9.77)	1.01	(-60.1, -34.2)	2.1	26.0
	Radau	$(4-\sqrt{6}, 4+\sqrt{6}, 10)/10$	5	4	(-10.32, -9.55)	1.04	(-103.1, -34.9)	1.97	3.0
	Lobatto	$(0, 5-\sqrt{5}, 5+\sqrt{5}, 10)/10$	6	5	(-10, -9.82)	1.01	$(-\infty, -37.5)$	13.9	13.9
k=4	Gauss	cf. [7]	8	5	(-9.876, -9.865)	1.0007	(-42.1, -37.8)	1.17	42.0
	Radau	cf. [9]	7	5	(-9.90, -9.84)	1.002	(-45.8, -36.5)	1.29	4.0
	Lobatto	cf. [9]	8	6	(-9.876, -9.866)	1.0006	(-42, -38.5)	1.13	21.9

These stability results indicate that, from a practical point of view, direct collocation methods based on Gauss, Radau and Lobatto collocation points are of limited value, because the rather small stability or periodicity boundaries make them unsuitable for stiff problems (which is the main class of problems where implicit RKN methods are used). The A-stable, indirect analogues are clearly more suitable for integrating stiff problems.

However, in Section 4.4, we shall describe a stabilizing technique based on preconditioning matrices that removes stiff components from the righthand side function and transforms conditionally stable methods into A-stable or P-stable methods. By means of this technique the above methods can be made A-stable or P-stable.

4.2.2. A-stable RKN methods with p=r=s. If we drop the additional order condition (3.4), then the orders are given by $p_1=p_3=s+1$ and $p_2=s$ (see Section 2.1), so that p=r=s (family B of Table 1.1). We found A-stable methods with k=s implicit stages for k=2 and k=3, and an A-stable method with k=s-1 implicit stages for k=4:

(4.3) $\quad c^T = (3/4, 1), \quad c^T = (-1/5, 9/10, 1), \quad c^T = (-1/4, 0, 9/10, 19/20, 1).$

In the following subsection these methods will be compared with A-stable methods based on composition of RKN methods. The Butcher arrays of these methods are given in the Appendix to [10].

4.2.3. A-stable composite methods with p=r=k+1. It is sometimes possible to construct methods with improved stability properties by composing a new method from a sequence of given RKN methods (preferrably with equal numbers of implicit stages). In order to define these *composite* RKN methods (CRKN methods), we write the RKN method (2.1) in the form

$$w_{n+1} = L(h, w_n), \quad w_n := (y_n, y'_n)^T,$$

where L is a (nonlinear) operator defined by the RKN method. Suppose that we are given ν RKN methods (not necessarily with the same number of stages) characterized by operators L_i and all of order p. Then we may define the methods

$$w_{n+i} = L_i(h, w_{n+i-1}), \quad n = 0, \nu, 2\nu, \dots, \quad i = 1, \dots, \nu.$$

Evidently, these CRKN methods are again of order p. Applying the CRKN method to the equation $y''=\lambda y$, we may write

$$w_{n+i} = M_i(z)w_n, \quad z := \lambda h^2,$$

where the $M_i(z)$ denote the amplification matrices of the individual methods. The stability function becomes

$$R_C(z) := \rho\Big(\prod_{i=\nu}^{1} M_i(z)\Big).$$

Presenting CRKN methods by the formula Πc_i^T, where the c_i correspond to the individual RKN methods, we have the following three examples of A-stable CRKN methods with p=r=k+1 (family C of Table 1.1):

(4.4) $\quad (1/3,1) * (0,19/20,1)^2, \; (0,1/2,19/20,1) * (0,9/10,19/20,1)^2, \; (1/10,26/53,19/20,1) * (0,1/4,9/10,19/20,1)^2.$

The first two methods improve on the k=2 and k=3 methods of family B. We remark that the collocation vector (1/10,26/53,19/20,1) occurring in the third method satisfies condition (3.4) for q=1. The Butcher arrays for these methods are given in the Appendix to [10].

Example 4.1. The A-stable methods of the families B and C are applied to the semidiscretization of the partial differential equation

$$(4.5) \qquad \frac{\partial^2 u}{\partial t^2} = \frac{u^2}{1+2x-2x^2}\frac{\partial^2 u}{\partial x^2} + u(4\cos^2(t) - 1), \quad 0 \le t \le 2\pi, \quad 0 \le x \le 1,$$

with initial and Dirichlet boundary conditions such that its exact solution is given by $u=(1+2x-2x^2)\cos(t)$. By using standard symmetric spatial discretization on a uniform grid with mesh $\Delta x=1/20$, we obtain a set of 19 ODEs.

Table 4.2. NCD and p* values produced by A-stable methods from the families B and C for problem (4.5).

	Method	p	r	h=π/15	h=π/30	h=π/60	p*(π/60)
k=2	(3/4,1)	2	2	*	3.6	4.1	1.7
	$(1/3,1) * (0,19/20,1)^2$	3	3	3.7	4.6	5.5	3.0
k=3	(-1/5,9/10,1)	3	3	*	4.4	5.3	3.0
	$(0,1/2,19/20,1) * (0,9/10,19/20,1)^2$	4	4	6.3	7.3	8.5	4.0
k=4	(-1/4,0,9/10,19/20,1)	5	5	6.9	8.4	9.9	5.0
	$(1/10,26/53,19/20,1) * (0,1/4,9/10,19/20,1)^2$	5	5	7.8	9.2	10.8	5.3

Table 4.2 lists results for a sequence of time steps $\Delta t=h$. The composite methods perform rather well, in particular in the cases k=2 and k=3. □

4.3. A-stable preconditioned methods

As observed above RKN methods based on direct collocation methods often have finite stability boundaries. A simple technique for constructing methods with large stability boundaries replaces the scalar parameters in an RKN method by matrix operators, usually functions of h and of the Jacobian matrix of the system of ODEs. In [8] such methods were called *generalized RK(N) methods*. Special cases are the celebrated Rosenbrock methods [16] and the Liniger-Willoughby methods [14]. In this paper, we consider generalized RKN methods obtained by replacing in the RKN method all righthand side evaluations **f** by S**f**. The preconditioning matrix S is required to be such that S**f** converges to **f** as h tends to 0. The technique of premultiplying the righthand side function by a preconditioning matrix is related to righthand side smoothing (cf. [11]).

Let us consider righthand side preconditioning by introducing the preconditioning matrix

(4.6) $S = \left[T(h^2J_n)\right]^{-1}, \quad T(z) := 1 + \varepsilon\,(-z)^{\sigma}, \quad J_n := \frac{\partial f(t_n,y_n)}{\partial y},$

where σ is a positive integer, and ε is nonnegative. S may be considered as a perturbed identity matrix which is closer to I as ε and σ are smaller. The resulting method will be called a *preconditioned* RKN method (PRKN method). The following theorem presents a condition for A and P-stability.

Theorem 4.2. Given an RKN method with step point and stage order p, with stability boundary β_{stab}, and with periodicity boundary β_{per}. The PRKN method generated by (4.6) has step point and stage order p if $2\sigma \geq p$, and it is A-stable if ε satisfies the stability condition

(4.7) $\varepsilon \geq \frac{(\sigma-1)^{\sigma-1}}{(\sigma\beta_{stab})^{\sigma}}$.

The method is P-stable if in (4.7) β_{stab} is replaced by β_{per}, provided that $\beta_{per} \neq 0$.

Proof. Evidently, by replacing **f** by S**f**, we introduce local perturbations at worst of $O(h^{p+1})$, so that the global step point and stage order of the PRKN method is still p. Furthermore, if the PRKN method is applied to the test equation $y''=\lambda y$, then the recursion (2.5a) assumes the form

$$v_{n+1} = M(\zeta(z))v_n, \quad v_n := (y_n, hy'_n)^T, \quad z := \lambda h^2, \quad \zeta(z) := \frac{z}{1 + \varepsilon(-z)^{\sigma}} .$$

The corresponding stability function takes the form

(4.8) $R^*(z) := \rho\big(M(\zeta(z))\big) = R(\zeta(z))$.

where R(z) denotes the stability function of the original RKN method. The stabilized RKN method is A-stable if the function $\zeta(z)$ satisfies the inequality $-\beta_{stab} \leq \zeta(z) \leq 0$, where β_{stab} denotes the stability boundary of the original RKN method. It is easily verified that this leads to the stability condition (4.7).

If (4.7) is satisfied with β_{stab} replaced by β_{per}, and by observing that the values of R^* on the negative z-axis are composed of the values of R on the interval $(-\beta_{per},0)$ which equal 1, it is immediate that we achieve P-stability. □

Preconditioning requires the computation of the matrix $T(h^2J_n)$. However, since this matrix is only used for stabilizing the RKN method, we can use the same matrix for a number of steps, and only have to update $T(h^2J_n)$ if the Jacobian matrix J_n has changed too much. Furthermore, we have to solve a slightly more complicated stage vector equation than in the case $T(h^2J_n)=S^{-1}=I$ (see the Appendix to [10]). In a forthcoming paper, we shall study the solution of this equation by iteration methods that are suitable for use on multi-processor computers.

Example 4.2. In order to see the effect of the preconditioning technique on the accuracy we choose a conditionally stable method from family A (see Table 1.1), and we perform computations with and without preconditioning. The sequence of stepsizes is chosen such that for certain values of h (in the tables of results indicated in bold face) the eigenvalues of h^2J_n enter the region of instability U of the method. By choosing large integration intervals, we achieve that there are sufficiently many steps to develop instabilities when the region U is entered. Hence, we expect a sudden drop of accuracy when this happens. If preconditioning is applied, then such a drop of accuracy should not occur.

Table 4.3 lists results for the problem [12]

(4.9) $y''(t) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} y(t), \quad y(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad 0 \leq t \leq 100,$

with exact solution $y(t)=(2\cos(t),-\cos(t))^T$. Without preconditioning, the direct three-stage Radau method is unstable for the stepsizes h=1/6 and h=1/15.8, that is at the points z=-69.4 and z=-10 (cf. Table 4.1). These results show that A-stability is retained by preconditioning without reduction of the accuracy. We also applied the indirect version of the three-stage Radau method (which is L-stable and does not need preconditioning). This method is slightly less accurate than its preconditioned, direct counterpart.

Table 4.3. NCD values produced by the three-stage indirect and direct Radau methods for problem (4.9).

Method	ε	σ	h=1/4 z=-156	**h=1/6** **z=-69.4**	h=1/11 z=-20.7	h=1/15.4 z=-10.5	**h=1/15.8** **z=-10**	h=1/16.2 z=-9.5	h=1/20 z=-6.25
Direct three-stage Radau	0		5.2	*	7.4	8.2	*	8.3	8.7
	0.0002	3	5.1	**6.0**	7.4	8.1	**8.2**	8.2	8.7
	0.000015	4	5.2	**6.1**	7.4	8.2	**8.2**	8.3	8.7
Indirect three-stage Radau	-	-	4.6	5.5	6.8	7.6	7.6	7.7	8.1

In addition to the autonomous problem (4.9), we also performed a test with a *nonautonomous* variant of this problem. For that purpose, we added the term $-\gamma\,(y_1-2\cos(t),\ y_2+\cos(t))^T$ to the right-hand side of (4.9). Using the same initial data, this extra term vanishes on the exact solution for all γ. The motivation for this experiment is to get insight into the influence of preconditioning on the accuracy. For a fixed stepsize h=1/10, we applied the unconditionally stable methods of Table 4.3 to this nonautonomous problem. Table 4.4 shows the results for increasing values of γ.

Table 4.4. NCD values obtained by the preconditioned direct Radau method and the indirect Radau method with h=1/10 applied to a nonautonomous variant of problem (4.9).

Method	ε	σ	$\gamma=0$	$\gamma=10$	$\gamma=10^2$	$\gamma=10^3$	$\gamma=10^4$	$\gamma=10^5$	$\gamma=10^6$
Direct three-stage Radau	0.0002	3	7.2	7.5	7.2	3.5	1.5	- 0.6	*
	0.000015	4	7.2	9.2	7.8	3.6	2.0	- 0.4	*
Indirect three-stage Radau	-	-	6.6	7.9	8.0	7.4	6.6	7.9	8.9

Compared with the autonomous case (viz., $\gamma=0$), the preconditioned methods show a similar accuracy for γ-values up to, say, 100, but quickly loose accuracy if γ increases. The reason is, of course, that for such large γ-values the right-hand side is dominated by the nonautonomous term, whereas its influence does not enter into the preconditioning matrix S. The direct method, on the other hand, performs very well, also for large γ-values.

Summarizing, we conclude that the preconditioning technique is a useful tool (i.e., for retaining A-stability without loosing accuracy) for problems where the Jacobian matrix is constant or slowly varying (with respect to the stepsize) and where the nonautonomous (inhomogeneous) term is also of moderate variation.

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A. Appendix

A.1. Derivation of the RKN parameters

The derivation of methods and their stability or periodicity regions becomes increasingly difficult for three-stage and higher-stage methods, and it is not feasible to analyse the stability function of these methods by analytical methods, so that we have to apply numerical techniques. For that purpose, we need a method for explicit evaluation of the stability function for given values of its argument z and given collocation vector **c**. In order to specify such a technique, we derive formulas that express the the RKN parameters explicitly in terms of **c**.

Writing the Lagrange polynomial $L_j(x)$ in the form

$$\text{(A.1a)} \qquad L_j(x) = K_j \sum_{m=0}^{s-1} \gamma_{jm}\, x^m, \quad K_j := \prod_{i=1, i\neq j}^{s} \frac{1}{c_j - c_i},$$

we deduce from the definition of α_j (cf. (3.2)) and β_j (cf. (3.7')) that

$$\text{(A.1b)} \qquad \alpha_j(x) = K_j \sum_{m=0}^{s-1} \frac{\gamma_{jm}}{m+1} x^{m+1}, \qquad \beta_j(x) = K_j \sum_{m=0}^{s-1} \frac{\gamma_{jm}}{(m+1)(m+2)} x^{m+2}.$$

Hence, by defining the s-by-s matrices P, Q and Γ, and the s-dimensional vectors **p** and **q** according to

$$\text{(A.2a)} \qquad \begin{aligned} &\Gamma := (\gamma_{jm}), \quad K = \text{diag}\,(K_j), \quad P = (p_{im}) := \Big(\frac{c_i^{m+1}}{m+1}\Big), \quad Q = (q_{im}) := \Big(\frac{c_i^{m+2}}{(m+1)(m+2)}\Big), \\ &\mathbf{p} := \Big(\frac{1}{m+1}\Big), \quad \mathbf{q} := \Big(\frac{1}{(m+1)(m+2)}\Big), \end{aligned}$$

with j and m+1 running from 1 until s, we may write for the direct collocation method (2.1)

$$\text{(A.2b)} \qquad A = Q(K\Gamma)^T, \quad \mathbf{b} = K\Gamma\mathbf{q}, \quad \mathbf{d} = K\Gamma\mathbf{p},$$

and for the indirect collocation method (3.1)

$$\text{(A.2c)} \qquad \mathring{A} = P(K\Gamma)^T, \quad \mathbf{d} = K\Gamma\mathbf{p}.$$

Since the entries of the matrix $\Gamma=\Gamma_s$ are simple functions of the c_i, (A.2) explicitly expresses the RKN parameters in terms of the collocation vector **c**. For a few values of s, we have listed the matrices Γ:

$$\Gamma_2 := \begin{pmatrix} -c_2 & 1 \\ -c_1 & 1 \end{pmatrix}, \quad \Gamma_3 := \begin{pmatrix} c_2c_3 & -(c_2+c_3) & 1 \\ c_1c_3 & -(c_1+c_3) & 1 \\ c_1c_2 & -(c_2+c_1) & 1 \end{pmatrix}, \quad \Gamma_4 := \begin{pmatrix} -c_2c_3c_4 & c_2c_3+c_2c_4+c_3c_4 & -(c_2+c_3+c_4) & 1 \\ -c_1c_3c_4 & c_1c_3+c_1c_4+c_3c_4 & -(c_1+c_3+c_4) & 1 \\ -c_1c_2c_4 & c_1c_2+c_1c_4+c_2c_4 & -(c_1+c_2+c_4) & 1 \\ -c_1c_2c_3 & c_1c_2+c_1c_3+c_2c_3 & -(c_1+c_2+c_3) & 1 \end{pmatrix}.$$

A.2. Extension of collocation results to higher-order equations

The derivation of collocation methods described in Subsection 3.2.1 can straightforwardly be extended to higher-order equations. The proofs of the superconvergence results such as given in Subsection 3.2.2 can be conveniently based on the following result for interpolatory quadrature formulas (which follows from straightforward Taylor expansions):

Theorem A.2.1. For sufficiently differentiable functions G we have that the s-point quadrature formula

$$\int_{t_n}^{t_{n+1}} G(t)\, dt = \sum_{j=0}^{m-1} \frac{1}{(j+1)!} h^{j+1} G^{(j)}(t_n) + h^{m+1} \mathbf{w}^T G^{(m)}(\mathbf{e}t_n + \mathbf{c}h) + E_s(h)$$

has quadrature error $E_s(h)=O\big(h^{s+i+1}\big)$ if

$$\text{(A.2.1)} \qquad \mathbf{w}^T\mathbf{c}^j = \frac{j!}{(j+m+1)!}, \qquad j = 0, 1, \dots, s+i-m-1. \;\square$$

This theorem can also be used for showing in the proof of Theorem 3.5 that condition (3.4) together with (3.13) implies that $p_1=s+q$ without invoking the lemma of Hairer. This is achieved by observing that the vectors **d** and **b** defined in (3.10) satisfy (A.2.1) for m=i=0 and m=i=1, respectively. Furthermore, it follows from (3.4) that **c** satisfies (A.2.1) also for m=0 and i=q, i.e.,

(A.2.2) $\quad (j+1)\mathbf{d}^T\mathbf{c}^j = 1, \quad j = s, s+1, \dots, s+q-1.$

Now we want to show that **c** satisfies (A.2.1) for m=1 and i=q, i.e.,

(A.2.3) $\quad (j+1)(j+2)\mathbf{b}^T\mathbf{c}^j = 1, \quad j = s, s+1, \dots, s+q-2.$

Since **c** satisfies (3.13), we may write

$$(j+1)(j+2)\mathbf{b}^T\mathbf{c}^j = (j+1)(j+2)\left[\mathbf{d}^T\mathbf{c}^j - (\mathbf{d}.\mathbf{c})^T\mathbf{c}^j\right] = (j+1)(j+2)\left[\mathbf{d}^T\mathbf{c}^j - \mathbf{d}^T\mathbf{c}^{j+1}\right],$$

and using (A.2.2) reveals that (A.2.3) holds, so that $p_1=s+q$.

A.3. Composite methods with nonuniform stepsizes.

The CRKN methods are easily generalized to methods with nonuniform stepsizes. Let us write the RKN method (2.1) in the form

$$w_{n+1} = L(h_n, w_n), \quad w_n := (y_n, y'_n)^T, \quad h_n = t_{n+1} - t_n,$$

where L is a (nonlinear) operator defined by the RKN method. Suppose that we are given ν RKN methods characterzed by operators L_i, then we may define the methods

$$w_{n+i} = L_i(h_{n+i-1}, w_{n+i-1}), \quad n = 0, \nu, 2\nu, \dots, \quad i = 1, \dots, \nu.$$

Let us define

$$h := \frac{h_n + h_{n+1} + \dots + h_{n+\nu-1}}{\nu}, \quad q_i := \frac{h_{n+i-1}}{h}, \quad Q_i := \begin{pmatrix} 1 & 0 \\ 0 & h_{n+i-1} \end{pmatrix},$$

where h denotes the average stepsize of the ν component methods. Applying the CRKN method to the test equation $y''=\lambda y$, we may write

$$w_{n+i} = Q_i^{-1}M_i(q_i^2 z)Q_i w_n, \quad z := \lambda h^2,$$

where the $M_i(z)$ denote the amplification matrices of the individual methods. The stability function of the CRKN method becomes

$$R_C(z) := \rho\Big(\prod_{i=\nu}^{1} Q_i^{-1}M_i(q_i^2 z)Q_i\Big).$$

A.4. A-stable preconditioned methods

It may be recommendable to consider more general preconditioning matrices of the form

(A.4.1) $\quad S = \left[T(h^2 J_n)\right]^{-1}, \quad T(z) := 1 + \varepsilon h^\tau (-z)^\sigma, \quad J_n := \dfrac{\partial f(t_n, y_n)}{\partial y},$

where σ is again a positive integer, and τ and ε are nonnegative parameters. The following theorem can be proved along the same lines as the proof of Theorem 4.2.

Theorem A.4.1. Given an RKN method with step point and stage order p, with stability boundary β_{stab}, and with periodicity boundary β_{per}. The PRKN method generated by (4.6) has step point and stage order p if $\tau+2\sigma\geq p$ (provided that ε, σ and τ do not depend on h), and it is A-stable if

(A.4.2) $\quad \varepsilon h^\tau \geq \dfrac{(\sigma-1)^{\sigma-1}}{(\sigma\beta_{stab})^\sigma}.$

The method is P-stable if in (A.4.2) β_{stab} is replaced by β_{per}, provided that $\beta_{per}\neq 0$. □

The most simple choice is $\tau=0$ leading to the case considered before. However, for $\sigma\geq2$, the stability function $R^*(z)$ converges to 1 as z tends to $-\infty$, so that PRKN methods with $\tau=0$ do not have damping at infinity. It was shown by Hundsdorfer [Numer. Math. 50 (1986), pp.83-95] that generalized RK methods may have a bad convergence behaviour if the stability function approaches 1 too fast as z tends to infinity. This indicates that PRKN methods with $\sigma\geq2$ may be dangerous. In such cases one may choose $\sigma=1$ and $\tau=p-2$, so that $R^*(-\infty)=R(-\varepsilon^{-1}h^{2-p})$, which can be made less than 1 by a judicious choice of ε subject to the condition $\varepsilon^{-1}h^{2-p}<\beta_{stab}$.

A consequence of introducing the preconditioning matrix S, can be seen more clearly by writing out the PRKN method for systems of ODEs. The method then reads

(A.4.3a) $$y_{n+1} = y_n + hy'_n + h^2\sum_{i=1}^{s} b_i\, Sf(t_n + c_ih, Y_i), \quad y'_{n+1} = y'_n + h\sum_{i=1}^{s} d_i\, Sf(t_n + c_ih, Y_i),$$

(A.4.3b) $$Y_i = y_n + c_ihy'_n + h^2\sum_{j=1}^{s} a_{ij}\, Sf(t_n + c_jh, Y_j), \quad i = 1, \dots, s.$$

Defining

(A.4.4) $$X_i := Y_i - y_n - c_ihy'_n,$$

we have to solve the X_i from the system

(A.4.5) $$T(h^2J_n)X_i = h^2 \sum_{j=1}^{s} a_{ij}\, f(t_n + c_jh,\ y_n + c_jhy'_n + X_j), \quad i = 1, \dots, s.$$

From this relation we see that the additional work introduced by the preconditioning matrix is marginal when compared with the amount of work involved in solving this huge nonlinear system.

Finally, after having iterated (A.4.5) until convergence, the new approximations at t_{n+1} are easily found to be

(A.4.6) $$y_{n+1} = y_n + hy'_n + \sum_{i=1}^{s} \beta_i X_i, \quad y'_{n+1} = y'_n + h^{-1}\sum_{i=1}^{s} \delta_i X_i,$$

where (assuming that the matrix A is nonsingular)

(A.4.7) $$(\beta_1,\dots,\beta_s) = (b_1,\dots,b_s)\, A^{-1} \quad \text{and} \quad (\delta_1,\dots,\delta_s) = (d_1,\dots,d_s)\, A^{-1}.$$

In this way the s additional f-evaluations of the stage vectors Y_i (cf. the notation (A.4.3a)) can be avoided.
Notice that the RKN methods with $c_1=0$ possess a singular matrix A. However, changing to the notation (2.7), we have that the resulting A^* matrix is nonsingular and the above technique is straightforwardly extended to this case.

In a forthcoming paper, we shall study the solution of the particular system (A.4.5) by iteration methods that are suitable for use on multi-processor computers, and we anticipate that the preconditioning matrix S will speed up the convergence considerably which compensates the additional effort for computing the matrix $T(h^2J_n)$ and the increased complexity of the system to be solved.

A.5. Butcher arrays for direct collocation methods

3/4	27/32	-9/16
1	4/3	-5/6
	4/3	-5/6
	2	-1

, $p = r = 2$, $k = 2$, $\beta_{stab} = \infty$, $R(\infty) = 1/3$.

1/3	2/27	-1/54
1	1/2	0
	1/2	0
	3/4	1/4

, $p = r = 3$, $k = 2$, $\beta_{stab} \approx 8.61$, $U_1 \approx (-16.73, -8.61)$, $R_{max}(U_1) \approx 1.25$, $R(\infty) = 2$.

-1/5	31/1980	7/275	- 19/900
9/10	2511/17600	4941/4400	- 1377/1600
1	65/396	15/11	- 37/36
	65/396	15/11	- 37/36
	85/396	80/33	- 59/36

, $p = r = 3$, $k = 3$, $\beta_{stab} = \infty$, $R(\infty) \approx 0.67$

0	0	0	0
19/20	22021/96000	2527/1600	- 130321/96000
1	14/57	100/57	- 3/2
	14/57	100/57	- 3/2
	37/114	200/57	- 17/6

, $p = r = 3$, $k = 2$, $\beta_{stab} \approx 11.45$, $U_1 \approx (-12.0, -11.45)$, $R_{max}(U_1) \approx 1.0013$, $R(\infty) \approx 1.32$

$-\frac{1}{4}$	$\frac{1333}{176640}$	$\frac{6673}{262656}$	$-\frac{11575}{158976}$	$\frac{1225}{9728}$	$-\frac{421}{7680}$
0	0	0	0	0	0
$\frac{9}{10}$	$-\frac{29889}{575000}$	$\frac{20763}{76000}$	$\frac{192591}{46000}$	$-\frac{130491}{19000}$	$\frac{286497}{100000}$
$\frac{19}{20}$	$-\frac{8395}{148781}$	$\frac{208819}{710254}$	$\frac{48691}{10472}$	$-\frac{1459523}{192000}$	$\frac{3038709}{959881}$
1	$-\frac{7}{115}$	$\frac{17}{54}$	$\frac{3175}{621}$	$-\frac{25}{3}$	$\frac{52}{15}$
	$-\frac{7}{115}$	$\frac{17}{54}$	$\frac{3175}{621}$	$-\frac{25}{3}$	$\frac{52}{15}$
	$-\frac{4}{45}$	$\frac{427}{1026}$	$\frac{250}{27}$	$-\frac{2500}{171}$	$\frac{181}{30}$

, $p = r = 5$, $k = 4$, $\beta_{stab} = \infty$, $R(\infty) \approx 0.23$.

0	0	0	0	0
$\frac{1}{2}$	$\frac{39}{608}$	$\frac{43}{432}$	$-\frac{100}{513}$	$\frac{5}{32}$
$\frac{19}{20}$	$\frac{14079}{100000}$	$\frac{327349}{875102}$	$-\frac{84113}{216000}$	$\frac{130321}{400000}$
1	$\frac{17}{114}$	$\frac{11}{27}$	$-\frac{200}{513}$	$\frac{1}{3}$
	$\frac{17}{114}$	$\frac{11}{27}$	$-\frac{200}{513}$	$\frac{1}{3}$
	$\frac{1}{6}$	$\frac{2}{3}$	0	$\frac{1}{6}$

, $p = r = 4$, $k = 3$, $\beta_{stab} \approx 9.59$, $U_1 \approx (-9.96, -9.59)$, $R_{max}(U_1) \approx 1.008$, $R(\infty) \approx 1.45$.

0	0	0	0	0
$\frac{9}{10}$	$\frac{63963}{380000}$	$\frac{17037}{2000}$	$-\frac{34992}{2375}$	$\frac{129033}{20000}$
$\frac{19}{20}$	$\frac{194579}{1080000}$	$\frac{29417137}{3145633}$	$-\frac{387353}{24000}$	$\frac{1694173}{240000}$
1	$\frac{197}{1026}$	$\frac{275}{27}$	$-\frac{1000}{57}$	$\frac{23}{3}$
	$\frac{197}{1026}$	$\frac{275}{27}$	$-\frac{1000}{57}$	$\frac{23}{3}$
	$\frac{9}{38}$	$\frac{50}{3}$	$-\frac{1600}{57}$	$\frac{73}{6}$

, $p = r = 4$, $k = 3$, $\beta_{stab} \approx 9.19$, $U \approx (-9.57, -9.19)$, $R_{max}(U) \approx 1.004$, $R(\infty) \approx 0.21$.

$$
\begin{array}{c|cccc}
\frac{1}{10} & \frac{5319}{782000} & -\frac{2189}{665343} & \frac{2195}{283024} & -\frac{1217}{194183} \\
\frac{26}{53} & \frac{15894}{164203} & \frac{11209}{390355} & -\frac{3733}{170869} & \frac{5845}{350736} \\
\frac{19}{20} & \frac{96066}{442813} & \frac{130751}{589037} & \frac{235}{519458} & \frac{4019}{338340} \\
1 & \frac{2425}{10557} & \frac{148877}{604854} & \frac{200}{8279} & 0 \\
\hline
 & \frac{2425}{10557} & \frac{148877}{604854} & \frac{200}{8279} & 0 \\
 & \frac{24250}{95013} & \frac{154483}{319736} & \frac{4000}{8279} & -\frac{323}{1458}
\end{array}
$$

, $p = r = 5,\ k = 4,\ \beta_{stab} \approx 9.77,$

$U_1 \approx (-9.96, -9.77)$, $R_{max}(U_1) \approx 1.007$

$R(\infty) \approx .49$

$$
\begin{array}{c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{4} & \frac{4499}{262656} & \frac{605}{34944} & -\frac{7675}{89856} & \frac{7225}{51072} & -\frac{91}{1536} \\
\frac{9}{10} & \frac{1269}{20000} & \frac{29889}{113750} & \frac{22221}{26000} & -\frac{2187}{1750} & \frac{9477}{20000} \\
\frac{19}{20} & \frac{47913}{722393} & \frac{195916}{686879} & \frac{35596}{34471} & -\frac{505039}{336000} & \frac{182117}{319417} \\
1 & \frac{71}{1026} & \frac{4}{13} & \frac{425}{351} & -\frac{100}{57} & \frac{2}{3} \\
\hline
 & \frac{71}{1026} & \frac{4}{13} & \frac{425}{351} & -\frac{100}{57} & \frac{2}{3} \\
 & \frac{59}{1026} & \frac{368}{819} & \frac{1250}{351} & -\frac{2000}{399} & \frac{35}{18}
\end{array}
$$

, $p = r = 5,\ k = 4,\ \beta_{stab} \approx 9.82,$

$U_1 \approx (-9.90, -9.82)$, $R_{max}(U_1) \approx 1.001$

$R(\infty) \approx .62$