BIT 31 (1991), 469–481.

STABILITY OF COLLOCATION-BASED RUNGE-KUTTA-NYSTRÖM METHODS

P. J. VAN DER HOUWEN[1], B. P. SOMMEIJER[1] and NGUYEN HUU CONG*[2]

[1] *Centre for Mathematics and Computer Science, Box 4079, 1009 AB Amsterdam, The Netherlands*

[2] *Faculty of Mathematics, Mechanics and Informatics University of Hanoi, Thuong dinh, Dong Da, Hanoi, Vietnam*

Abstract.

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 $2s$ for all s. 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.

AMS Subject classification: 65M10, 65M20.

1. Introduction.

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

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

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. 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

*) These investigations were supported by the University of Amsterdam who provided the third author with a research grant for spending a total of two years in Amsterdam.

Received September 1990. Revised February 1991.

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. For all s, these methods can be made A-stable and of order $2s$ (Gauss-type methods) or L-stable and of order $2s - 1$ (Radau IIA type methods) by a suitable choice of the collocation parameters. 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 $s \leq 9$ (Newton-Cotes methods [15]) or strongly A-stable for $s \leq 5$ (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] (see also [1]). The main object of the present 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. If the stage order is decreased to s, then infinite stability boundaries 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 right-hand side in (1.1), that is, stiff components in the right-hand 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 relation for the stage vector. The second stabilizing technique is based on the combination 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 $k \leq 4$.

Summarizing, this paper investigates three families of methods based on direct collocation. Assuming that they all use 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 orders):

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

Family		s	p	r	Stability	With preconditioning	Subsections
A. single:	Gauss	k	$2k$	$k+1$	Conditionally stable	Weakly A-stable	4.2.1, 4.3
	Radau	k	$2k-1$	$k+1$	Conditionally stable	Weakly A-stable	4.2.1, 4.3
	Lobatto	$k+1$	$2k$	$k+2$	Conditionally stable	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:	$k \leq 4$		$k+1$	$k+1$	Strongly A-stable	–	4.2.3

2. RKN methods.

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

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

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, $\boldsymbol{b}, \boldsymbol{c}$ and $\boldsymbol{d}$ are s-dimensional vectors, $\boldsymbol{e}$ is the s-dimensional vector with unit entries, A is an $s \times s$ matrix, and, for any pair of vectors $\boldsymbol{v} = (v_i)$, $\boldsymbol{w} = (w_i)$, $f(\boldsymbol{v}, \boldsymbol{w})$ denotes the vector with entries $f(v_i, w_i)$.

If the last row of A equals the row vector $\boldsymbol{b}^T$, i.e., $\boldsymbol{b}^T = \boldsymbol{e}_s^T A$, then, as in the case of RK methods for first-order IVPs, such methods are said to be *stiffly accurate*. In general, stiffly accurate methods perform better on stiff problems than methods that are not stiffly accurate.

2.1. Order of accuracy.

Let $\boldsymbol{Y}(t_{n+1})$ denote the vector with components $y(t_n + c_i h)$ 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

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

then the (global) order of accuracy p and the (global) stage order r are respectively defined by $p = \min\{p_1, p_2\}$ and $r = \min\{p_1, p_2, p_3\}$. Notice that the *local* stage order equals $p_3 + 1$.

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 with their high stage orders are rather accurate for stiff problems. A similar phenomenon occurs in stiff *second-order* equations (cf. Example 2.1 in [10]).

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 $\partial \boldsymbol{f}/\partial \boldsymbol{y}$. This leads to a recursion of the form

$$\boldsymbol{v}_{n+1} = M(z)\boldsymbol{v}_n, \quad \boldsymbol{v}_n := (y_n, hy'_n)^T, \tag{2.3}$$

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

where $z := \lambda h^2$. 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 $\rho(M(z))$ of $M(z)$.

DEFINITION 2.1. The collection of points on the negative real z-axis is called
(i) the region of *stability* if in this region $R(z) := \rho(M(z)) < 1$,
(ii) the region of *periodicity* if $R(z) = 1$ and [trace $M(z)]^2 - 4 \det M(z) < 0$.

If $(-\beta_{\text{stab}}, 0)$ lies in the stability region, then β_{stab} is called the *stability boundary*, and if $(-\beta_{\text{per}}, 0)$ lies in the periodicity region, then β_{per} is called the *periodicity boundary*. *If* $\beta_{\text{stab}} = \infty$, then the RKN method is called *A-stable* and if $\beta_{\text{per}} = \infty$, then it is called *P*-stable. An *A*-stable RKN method is called *L-stable* if $R(-\infty) = 0$.

3. RKN methods based on collocation.

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

$$(1.1') \qquad \boldsymbol{y}'(t) = \boldsymbol{u}(t), \qquad \boldsymbol{u}'(t) = \boldsymbol{f}(t, \boldsymbol{y}(t)), \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \qquad \boldsymbol{u}(t_0) = \boldsymbol{u}_0,$$

and applying an RK method for first-order equations:

$$y_{n+1} = y_n + h\boldsymbol{d}^T f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}), \qquad \boldsymbol{Y} = \boldsymbol{e}y_n + h\mathring{A} f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}),$$

we obtain an RKN method of the form (2.1) with (cf. [6])

$$(3.1) \qquad \boldsymbol{b} = \mathring{A}^T \boldsymbol{d}, \qquad A = \mathring{A}^2.$$

Notice that when the generating RK method has order p and k implicit stages, then this is true for the RKN method as well. Now, let the generating RK method be a collocation method based on the s distinct collocation points $\{t_{nj} := t_n + c_j h, j = 1, \ldots, s\}$, then (see e.g. [7])

$$(3.2) \qquad \mathring{A} = (\mathring{a}_{ij}) := (\alpha_j(c_i)), \quad \boldsymbol{d} = (d_i) := (\alpha_i(1)), \quad \alpha_j(x) := \int_0^x L_j(\xi)\, d\xi,$$

$$L_j(x) := \prod_{i=1, i \neq j}^{s} \frac{x - c_i}{c_j - c_i},$$

where $i, j = 1, \ldots, s$. The family of indirect collocation methods defined by (3.1) and (3.2) has order $p = r = s$ for all collocation vectors $\boldsymbol{c}$ (see e.g. [4]). The RKN method will be called *symmetric* if the location of the collocation points t_{nj} is symmetric with respect 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). The following theorem holds (see e.g. [7, p. 207]):

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. *We have* $p = s + q$ *if, in addition,*

$$P_j(1) = 0, \qquad P_j(x) := \int_0^x \xi^{j-1} \prod_{i=1}^{s} (\xi - c_i)\, d\xi, \qquad j = 1, 2, \ldots, q. \tag{3.3}$$

3.2. Direct collocation methods.

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 $\leq s + 1$ on each interval $[t_n, t_{n+1}]$, $n = 0, \ldots, N - 1$. For such functions u, the second derivative u'' is a polynomial of degree not exceeding $s - 1$ on each of the intervals $[t_n, t_{n+1}]$. Using the $L_j(x)$ defined in (3.2) we may write

$$\begin{gathered} u''(t_n + xh) = \sum_{j=1}^{s} L_j(x) u''(t_{nj}), \qquad u'(t_n + xh) = u'(t_n) + h \sum_{j=1}^{s} \alpha_j(x) u''(t_{nj}), \\ u(t_n + xh) = u(t_n) + xhu'(t_n) + h^2 \sum_{j=1}^{s} \beta_j(x) u''(t_{nj}), \end{gathered} \tag{3.4}$$

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

$$\begin{aligned} \beta_j(x) &:= \int_0^x \int_0^\eta L_j(\xi)\, d\xi\, d\eta = \int_0^x \int_\xi^x L_j(\xi)\, d\eta\, d\xi = \int_0^x (x - \xi) L_j(\xi)\, d\xi \\ &= x\alpha_j(x) - \int_0^x \xi L_j(\xi)\, d\xi. \end{aligned} \tag{3.5}$$

Next, we require that the function u satisfies the collocation equations $u''(t_{nj}) = f(t_{nj}, u(t_{nj}))$ for $j = 1, \ldots, s$. Then (3.4) leads to:

$$\begin{gathered} u(t_{ni}) = u(t_n) + c_i h u'(t_n) + h^2 \sum_{j=1}^{s} \beta_j(c_i) f(t_{nj}, u(t_{nj})), \\ u'(t_{ni}) = u'(t_n) + h \sum_{j=1}^{s} \alpha_j(c_i) f(t_{nj}, u(t_{nj})), \qquad i = 1, \ldots, s, \\ u(t_{n+1}) = u(t_n) + hu'(t_n) + h^2 \sum_{j=1}^{s} \beta_j(1) f(t_{nj}, u(t_{nj})), \\ u'(t_{n+1}) = u'(t_n) + h \sum_{j=1}^{s} \alpha_j(1) f(t_{nj}, u(t_{nj})). \end{gathered} \tag{3.6}$$

By writing $y_n := u(t_n)$, $y'_n := u'(t_n)$ and $\boldsymbol{Y} := (u(t_{ni}))$ and by introducing the quantities

$$\boldsymbol{b} := (b_i), \quad \boldsymbol{d} := (d_i), \quad A = (a_{ij}), \quad b_i := \beta_i(1), \quad d_i := \alpha_i(1), \quad a_{ij} := \beta_j(c_i), \tag{3.7}$$

the method (3.6) is recognized as the s-stage RKN method (2.1). As in the case of indirect collocation methods, the RKN method defined by (3.7) will be called *symmetric* if the location of the collocation points t_{nj} is symmetric with respect to $t_n + h/2$.

Since in the interval $[t_n, t_{n+1}]$ the function u is a polynomial of degree $\leq s + 1$ satisfying the collocation equations, it follows that $p_1 = s + 1$, $p_2 = s$ and $p_3 = s + 1$. Hence, locally, the order of the y'-component is one lower than the order of the other components. Therefore, we have the global order result $p = r = s$ (see also Subsection 2.1).

THEOREM 3.2. *The direct RKN method defined by* (3.7) *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} by writing the local error of y'_{n+1} in the form

$$(3.8) \qquad \int_{t_n}^{t_{n+1}} f(t, y(t))\, dt = y'(t_{n+1}) - y'_n = h\boldsymbol{d}^T f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}) + O(h^{p_2+1}).$$

It can be shown that $\boldsymbol{d}$ generates a quadrature formula with quadrature error of $O(h^{s+q+1})$ whenever the collocation points satisfy the relations (3.3), i.e., $p_2 = s + q$. Thus, setting $q = 1$, we have:

THEOREM 3.3. *If* (3.3) *is satisfied for* $q = 1$, *then the direct RKN method defined by* (3.7) *has global step point order and global stage order* $p = r = s + 1$. *For all symmetric methods with an odd number of stages, condition* (3.3) *is satisfied for* $q = 1$.

EXAMPLE 3.1. For $s = 2$ and $q = 1$ condition (3.3) 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 $\boldsymbol{c} = (0, 2/3)^T$ has order $p = r = 3$ and requires only one implicit stage. Furthermore, for $\boldsymbol{c} = (1/3, 1)^T$ a stiffly accurate method results with order $p = r = 3$.

THEOREM 3.4. *If condition* (3.3) *is satisfied, then the direct RKN method* (3.7) *has global step point order* $p = s + q$.

PROOF. From (3.3) it follows that $p_2 = s + q$ (cf. (3.8)). Furthermore, the condition $P_1(1) = 0$ implies

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

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

$$\int_0^1 \xi L_j(\xi)\,d\xi - \int_0^1 c_j L_j(\xi)\,d\xi = 0. \tag{3.9}$$

By observing that (cf. (3.7))

$$b_i = \beta_i(1) = \alpha_i(1) - \int_0^1 \xi L_i(\xi)\,d\xi, \qquad d_i = \alpha_i(1) = \int_0^1 L_i(\xi)\,d\xi,$$

we derive from (3.9) that $b_i = d_i - d_i c_i$ for $i = 1, \ldots, s$. This condition 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. The stage order of direct collocation methods is one higher whenever* $P_1(1) = 0$.

For a numerical example illustrating this corollary, we refer to [10].

4. Stability of collocation methods.

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 matrix $M(z)$ defined in (2.3) is given by

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

where $R^*(w)$ denotes the stability function of the generating RK method. Hence, the stability function of the generated RKN method is given by $R(z) := \rho(M(z)) = \operatorname{Max}\{R^*(\pm\sqrt{z})\}$. From this formula, we conclude that if, and only if, (2.1) possesses the stability interval $(-\beta_{\text{stab}}, 0)$, then the generating RK method possesses the imaginary stability boundary $(\beta_{\text{stab}})^{1/2}$. Hence, A-stable RK methods (i.e., $(\beta_{\text{stab}})^{1/2} = \infty$) 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 $R^*(w)R^*(-w) = 1$, that is, the collocation points should be distributed symmetrically with respect to 1/2 (see also [16], where an analytical expression for $R^*(w)$ is derived, merely in terms of the collocation points). 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.

Similar to the analysis performed by Wright [16] in the case of first order ODEs, it is possible to derive closed form expressions for the RKN parameters in terms of the collocation vector $\boldsymbol{c}$ (see the Appendix to [10], where full details can be found). With the help of these expressions, the matrix M and its spectral radius can, at least formally, be expressed in terms of $\boldsymbol{c}$. However, the complexity of these expressions is beyond a manageable level. Therefore, we resorted to numerical search techniques. Especially in the derivation of methods with three or more stages, we think this is the only practical approach. As a result of this numerical search, it turned out that the situation for direct collocation methods is less favourable than for indirect methods; 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 is immediate from a result of Kramarz [12], who proved that two-stage, stiffly accurate methods (i.e., $c_2 = 1$) can only be A-stable if $0.7 \leq c_1 < 1$. This conflicts with the requirement to obtain $p = r = 3$ which needs $c_1 = 1/3$ (see Example 3.1).

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 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 $R_{\max}(U_i)$. 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 4.3, we shall describe a stabilizing technique based on preconditioning matrices that removes stiff components from the right-hand side function and transforms conditionally stable methods into A-stable or P-stable methods. By means of this technique the methods from Table 4.1 can be made A-stable or P-stable.

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	cf. [4]	4	3	$(-12, -9)$	1.23	$(-\infty, -35.9)$	13.9	13.9
	Radau	cf. [4]	3	3	$(-16.73, -8.61)$	1.25	$(-\infty, -108)$	2.0	2.0
	Lobatto	cf. [4]	4	4	$(-12.0, -9.6)$	1.17	$(-\infty, -48)$	7.9	7.9
$k = 3$	Gauss	cf. [4]	6	4	$(-10.01, -9.77)$	1.01	$(-60.1, -34.2)$	2.1	26.0
	Radau	cf. [4]	5	4	$(-10.32, -9.55)$	1.04	$(-103.1, -34.9)$	1.97	3.0
	Lobatto	cf. [4]	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

4.2.2. A-stable RKN methods with $p = r = s$. If we drop the additional order condition (3.3), 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 $k = 4$. These are respectively generated by $c^T = (3/4, 1)$, $c^T = (-1/5, 9/10, 1)$ and $c^T = (-1/4, 0, 9/10, 19/20, 1)$ (for more details we refer to the Appendix to [10]). In the following subsection these methods are compared with methods based on composition of RKN methods.

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 (preferably 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 compact form $w_{n+1} = L(h, w_n)$, $w_n := (y_n, y_n')^T$, where L is a (nonlinear) operator defined by the RKN method. Suppose that we are given v 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 $w_{n+i} = L_i(h, w_{n+i-1})$ for $n = 0, v, 2v, \dots$, and $i = 1, \dots, v$. Evidently, these CRKN methods are again of order p. Applying the CRKN method to the equation $y'' = \lambda y$, we may write $w_{n+i} = M_i(z) w_n$ where as before $z := \lambda h^2$ and where the $M_i(z)$ denote the amplification matrices of the individual methods. The stability function becomes the spectral radius of the product of the matrices $M_i(z)$ with $i = v, v - 1, \dots, 1$. Presenting CRKN methods by the formula $\prod c_i^T$, where the c_i correspond to the individual RKN methods, we found three suitable A-stable CRKN methods with $p = r = k + 1$ (family C of Table 1.1). These are generated by: $(1/3, 1) * (0, 19/20, 1)^2$, (0, 1/2, 19/20, 1)∗(0, 9/10, 19/20, 1)^2 and (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 (3.3) for $q = 1$ (for more details we refer to the Appendix to [10]).

EXAMPLE 4.1. The A-stable methods of the families B and C are applied to the semidiscretization of

$$(4.2)\quad \frac{\partial^2 u}{\partial t^2} = \frac{u^2}{1 + 2x - 2x^2}\frac{\partial^2 u}{\partial x^2} + u(4\cos^2(t) - 1), \quad 0 \le t \le 2\pi, \quad 0 \le x \le 1,$$

with initial and Dirichlet boundary conditions such that the solution is given by $u = (1 + 2x - 2x^2)\cos(t)$. Using 3-point symmetric spatial discretization on grid points $x_j = j/20$, we obtain a set of 19 ODEs.

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

	Method	p	r	$h = \pi/15$	$h = \pi/30$	$h = \pi/60$
$k = 2$	(3/4, 1)	2	2	∗	3.6	4.1
	(1/3, 1)∗(0, 19/20, 1)^2	3	3	3.7	4.6	5.5
$k = 3$	(−1/5, 9/10, 1)	3	3	∗	4.4	5.3
	(0, 1/2, 19/20, 1)∗(0, 9/10, 19/20, 1)^2	4	4	6.3	7.3	8.5
$k = 4$	(−1/4, 0, 9/10, 19/20, 1)	5	5	6.9	8.4	9.9
	(1/10, 26/53, 19/20, 1)∗(0, 1/4, 9/10, 19/20, 1)^2	5	5	7.8	9.2	10.8

Table 4.2 lists the number of correct digits (NCD) obtained at the end of the integration interval, i.e., the value defined by $\mathrm{NCD}(h) := -\log_{10}$ (‖ global error (obtained with stepsize h) at $t = t_{\mathrm{end}}$ $\|_\infty$). An asterisk denotes an unstable behaviour.

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 [14] and the Liniger-Willoughby methods [13]. In this paper, we consider generalized RKN methods obtained by replacing in the RKN method all righthand side evaluations $\boldsymbol{f}$ by $S\boldsymbol{f}$ (see also [11] where related right-hand side smoothings are discussed). The preconditioning matrix S is required to be such that $S\boldsymbol{f}$ converges to $\boldsymbol{f}$ as h tends to 0. Furthermore, to be effective,

S should strongly damp the "high frequency (or, stiff) components" (i.e., eigenvectors of the Jacobian corresponding to eigenvalues of large modulus). On the other hand, to preserve accuracy, S should have a negligible effect on the "low frequency components" (eigenvectors corresponding to eigenvalues of small modulus). This leads us to a preconditioning matrix of the form

$$S = [T(h^2 J_n)]^{-1}, \qquad T(z) := 1 + \varepsilon(-z)^\sigma, \qquad J_n := \frac{\partial f(t_n, y_n)}{\partial y}, \tag{4.3}$$

where ε is a small (nonnegative) number, σ is a positive integer, and the minus sign in front of z is added to make T nonsingular for all negative z. The resulting method will be called a *preconditioned* RKN method (PRKN method). The following theorem presents a condition for A- and P-stability.

THEOREM 4.1. *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* (4.3) *has step point and stage order p if* $2\sigma \geq p$, *and it is A-stable if* ε *is bounded below by* $(\sigma - 1)^{\sigma - 1}(\sigma\beta_{\text{stab}})^{-\sigma}$. *The method is P-stable if in this lower bound* β_{stab} *is replaced by* β_{per}, *provided that* $\beta_{\text{per}} \neq 0$.

PROOF. Evidently, by replacing f by Sf, 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 (2.3) assumes the form

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

The corresponding stability function takes the form $R^*(z) := \rho(M(\zeta(z))) = R(\zeta(z))$, where $R(z)$ denotes the stability function of the original RKN method. The stabilized RKN method is A-stable if $\zeta(z)$ satisfies the inequality $-\beta_{\text{stab}} \leq \zeta(z) \leq 0$, where β_{stab} denotes the stability boundary of the original RKN method. It is easily verified that this leads to the lower bound for ε of the theorem. By replacing β_{stab} 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 $(-\beta_{\text{per}}, 0)$ which equal 1, it is immediate that we have P-stability. ■

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 table of results indicated in bold face) the eigenvalues of $h^2 J_n$ 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]

$$(4.4)\quad y''(t) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} y'(t), \quad y(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad 0 \le t \le 100,$$

with exact solution $y(t) = (2\cos(t), -\cos(t))^T$. Without preconditioning, the direct 3-stage Radau method is unstable for the stepsize $h = 1/6$ 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 3-stage Radau method (which is L-stable and does not need preconditioning). It turned out to perform slightly less accurate than its preconditioned, direct counterpart.

Table 4.3. NCD values produced by the 3-stage (A) and indirect (B) Radau methods for Problem (4.4).

Method	ε	σ	$h^{-1} =$ $-z =$	4 156	**6** **69.4**	11 20.7	15.4 10.5	**15.8** **10**	16.2 9.5	20 6.25
A	0			5.2	*	7.4	8.2	*	8.3	8.7
A	0.0002	3		5.1	**6.0**	7.4	8.1	**8.2**	8.2	8.7
A	0.000015	4		5.2	**6.1**	7.4	8.2	**8.2**	8.3	8.7
B	-	-		4.6	5.5	6.8	7.6	7.6	7.7	8.1

In addition to the autonomous problem (4.4), 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 (4.4). Notice that this does not change the exact solution. For γ-values up to, say, 100, the preconditioned methods show a similar accuracy as for the autonomous problem, 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 indirect method, on the other hand, performs very well, also for large γ-values (full details on this experiment can be found in [10]).

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.

REFERENCES

[1] Boor, C. R. de & Swartz, B. (1973): *Collocation at Gaussian points*, SIAM J. Numer. Anal. 10, 582–606.

[2] Brunner, H & Houwen, P. J. van der (1986): *The Numerical Solution of Volterra Equations*, North-Holland, Amsterdam.

[3] Butcher, J. C. (1987): *The Numerical Analysis of Ordinary Differential Equations, Runge-Kutta and General Linear Methods*, Wiley, New York.

[4] Dekker, K. & Verwer, J. G. (1984): *Stability of Runge-Kutta Methods for Stiff Nonlinear Differential Equations*, North-Holland, Amsterdam.

[5] Hairer, E. (1977): *Méthodes de Nyström pour l'équation différentielle $y'' = f(x, y)$*, Numer. Math. 27, 283–300.

[6] Hairer, E. (1979): *Unconditionally stable methods for second order differential equations*, Numer. Math. 32, 373–379.

[7] Hairer, E., Nørsett, S. P. & Wanner, G. (1987): *Solving Ordinary Differential Equations*, I. *Nonstiff Problems*, Springer-Verlag, Berlin.

[8] Houwen, P. J. van der (1977): *Construction of Integration Formulas for Initial Value Problems*, North-Holland, Amsterdam.

[9] Houwen, P. J. van der & Sommeijer, B. P. (1991): *Iterated Runge-Kutta methods on parallel computers*, to appear in SSISC.

[10] Houwen, P. J. van der, Sommeijer, B. P. & Nguyen huu Cong (1990): *Stability of collocation-based Runge-Kutta-Nyström methods*, Report NM-R9016, Centre for Mathematics and Computer Science, Amsterdam.

[11] Jameson, A. (1983): *The evolution of computational methods in aerodynamics*, J. Appl. Mech. 50, 1052–1076.

[12] Kramarz, L. (1980): *Stability of collocation methods for the numerical solution of $y'' = f(x, y)$*, BIT 20, 215–222.

[13] Liniger, W. & Willoughby, R. A. (1970): *Efficient integration methods for stiff systems of ordinary differential equations*, SIAM J. Numer. Anal. 7, 47–66.

[14] Rosenbrock, H. H. (1963): *Some general implicit processes for the numerical solution of differential equations*, Comput. J. 5, 329–330.

[15] Watts, H. A. & Shampine, L. F. (1972): *A-stable block implicit one-step methods*, BIT 12, 252–266.

[16] Wright, K. (1970): *Some relationships between implicit Runge-Kutta, collocation and Lanczos τ methods, and their stability properties*, BIT 10, 217–227.