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# A-stable Diagonally Implicit Runge-Kutta-Nyström Methods for Parallel Computers

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In this paper, we study diagonally implicit Runge-Kutta-Nyström methods (DIRKN methods) for use on parallel computers. These methods are obtained by diagonally implicit iteration of fully implicit Runge-Kutta-Nyström methods (corrector methods). The number of iterations is chosen such that the method has the same order of accuracy as the corrector, and the iteration parameters serve to make the method at least A-stable. Since a large number of the stages can be computed in parallel, the methods are very efficient on parallel computers. We derive a number of A-stable, strongly A-stable and L-stable DIRKN methods of order p with s*(p) sequential, singly diagonal-implicit stages where s*(p) = [(p+1)/2] or s*(p) = [(p+1)/2]+1, [.] denoting the integer part function.

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## 1. Introduction

Consider the initial-value problem for systems of special second-order, ordinary differential equations (ODEs) of dimension d

$$(1.1) \quad y''(t) = f(y(t)), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \quad y : \mathbb{R} \to \mathbb{R}^d, \quad f : \mathbb{R}^d \to \mathbb{R}^d, \quad t_0 \le t \le t_{end}.$$

One possibility for solving such problems is the use of singly diagonal-implicit Runge-Kutta-Nyström methods (SDIRKN methods). Compared with linear multistep methods (LM methods), SDIRKN methods have the disadvantage of requiring the solution of a sequence of implicit systems of dimension d per step, whereas LM methods require the solution of only one such system per step. On the other hand, a number of SDIRKN methods available in the literature possess excellent stability properties, which are much better than those of the best LM methods. In spite of that, LM methods are still more popular than SDIRKN methods, because of their lower costs on a sequential computer.

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However, on parallel computers, this situation may change. In this paper, we shall construct DIRKN methods tuned to parallel computers, such that each processor has to compute relatively few stages sequentially. We require that on each processor, these stages are *singly diagonal-implicit* , so that effectively the sequential costs of the parallel DIRKN method (PDIRKN method) are equal to those of an SDIRKN method. In fact, these methods are based on a *fixed* number of iterations of k-stage *indirect* RKN methods of Radau IIA and Gauss-Legendre type (methods of *indirect* type are understood to be methods that are derived by applying an RK method for first-order ODEs to the first-order form of (1.1)). Furthermore, the iteration parameters are chosen such that A-stability is obtained as soon as the order of the corrector is reached. The resulting methods require k = [(p+1)/2] processors, where p denotes the order and [·] denotes the integer part function. We present a number of A-stable, strongly A-stable and L-stable PDIRKN methods of order p with s*(p) sequential, singly diagonal-implicit stages, where s*(p) = [(p+1)/2] or s*(p) = [(p+1)/2]+1.

In order to appreciate these methods, we have summarized in Table 1.1 the characteristics of a number of already available SDIRKN-type methods of orders p=3 until p=8. We included DIRKN methods of both *direct* and *indirect* type (for a specification of indirect RKN methods we refer to [10] and to the Appendix of the present paper). Furthermore, we also listed a few indirect parallel DIRKN methods derived from *parallel* DIRK methods. Both the sequential and parallel methods are (effectively) *singly* diagonal-implicit, so that the number of sequential stages s* refer to the number of *singly* diagonal-implicit stages to be computed on each of the k processors.

By means of numerical experiments we will compare the performance of the methods constructed in this paper with that of a number of the methods listed in Table 1.1.

**Table 1.1.** DIRKN methods of order p requiring s* singly diagonal-implicit, sequential stages on k processors.

| Method | p | s* | k | Main properties | Type |
|---|---|---|---|---|---|
| Nørsett [14] | 3 | p-1 | 1 | A-stable | indirect |
| Crouzeix [6] | 3 | p-1 | 1 | Strongly A-stable | indirect |
| Sharp, Fine & Burrage [16] | 3 | p-1 | 1 | A-stable, reduced phaselag | direct |
| Cash [3], Cash & Liem [4] | 3 | p | 1 | S-stable | indirect |
| Burrage [1] | 3 | p+1 | 1 | A-stable, B-convergent | direct |
| Nørsett & Thomsen [15] | 3 | p+1 | 1 | L-stable | indirect |
| Iserles & Nørsett [12] | 4 | p-2 | 2 | L-stable | indirect |
| Nørsett [14] | 4 | p-1 | 1 | A-stable | indirect |
| Sharp, Fine & Burrage [16] | 4 | p-1 | 1 | A-stable, reduced phaselag | direct |
| Cash [3], Cash & Liem [4] | 4 | p+1 | 1 | S-stable | indirect |
| Cooper & Sayfy [5] | 5 | p | 1 | A-stable | indirect |
| v/d Houwen, Sommeijer & Couzy [9] | 5 | p | 3 | L-stable | indirect |
| Cooper & Sayfy [5] | 6 | p-1 | 1 | A-stable | indirect |
| Sommeijer [17] | 6 | p-1 | 3 | A-stable | indirect |
| v/d Houwen, Sommeijer & Couzy [9] | 6 | p | 3 | L-stable | indirect |
| v/d Houwen, Sommeijer & Couzy [9] | 7 | p+1 | 4 | L-stable | indirect |
| | 8 | p | 4 | L-stable | indirect |

## 2. Diagonal-Implicit Iteration

Our starting point is the fully implicit Runge-Kutta-Nyström (RKN) methods of the form

$$y_{n+1} = y_n + hy'_n + h^2\sum_{i=1}^{k} b_i f(Y_i),$$

$$y'_{n+1} = y'_n + h\sum_{i=1}^{k} d_i f(Y_i), \tag{2.1a}$$

$$Y_i = y_n + c_i h y'_n + h^2\sum_{j=1}^{k} a_{ij} f(Y_j), \quad i = 1, \ldots, k,$$

where $\mathbf{b}=(b_i)$, $\mathbf{c}=(c_i)$ and $\mathbf{d}=(d_i)$ are k-dimensional vectors, and $A=(a_{ij})$ is a nonsingular k-by-k matrix. This method will be referred to as the corrector method

We employ a similar iteration technique as applied in [11] which automatically leads to DIRKN methods. However, we now determine the iteration parameters such that the method is A-stable, strongly A-stable or L-stable as soon as the order of the corrector is reached.

Let $Y_i^{(\mu)}$ denote the $\mu$th iterate to $Y_i$, and define the transformed stage vector quantities $X_i$ and $X_i^{(\mu)}$ (cf. [8])

$$X_i := Y_i - x_i, \quad X_i^{(\mu)} := Y_i^{(\mu)} - x_i, \quad x_i := y_n + c_i h y'_n, \quad i = 1, \ldots, k. \tag{2.1b}$$

In terms of $X_i$ and $x_i$, the stage vector equation in (1.2) reads

$$X_i = h^2\sum_{j=1}^{k} a_{ij} f(X_j + x_j), \quad i = 1, \ldots, k.$$

For each of these equations, we define the iteration process

$$X_i^{(\mu)} - \delta_i h^2 f\left(X_i^{(\mu)} + x_i\right) = h^2\Big(\sum_{j=1}^{k} a_{ij} f\left(X_j^{(\mu-1)} + x_j\right) - \delta_i f\left(X_i^{(\mu-1)} + x_i\right)\Big), \tag{2.2a}$$

where $i = 1, \ldots, k$; $\mu = 1, \ldots, m$, and where the $\delta_i$ are positive iteration parameters that will be used to control the stability of the method. In order to start the iteration process, we compute the initial approximations $X_i^{(0)}$ by means of the predictor formula

$$X_i^{(0)} = \theta\delta_i h^2 f(X_i^{(0)}+x_i), \tag{2.2b}$$

where either $\theta = 0$ or $\theta = 1$. These formulas will be referred to as predictor formulas of type I and II, respectively.

In [11] it was shown that the formulas for the step values defined in the corrector (2.1) can be presented in the form

$$y_{n+1} = y_n + hy'_n + \sum_{i=1}^{k} \alpha_i X_i, \qquad y'_{n+1} = y'_n + h^{-1} \sum_{i=1}^{k} \beta_i X_i,$$

where $\alpha_i$ and $\beta_i$ are the components of the vectors $\alpha := \mathbf{b}^T A^{-1}$, $\beta := \mathbf{d}^T A^{-1}$. This suggests defining the step values $y_{n+1}$ and $y'_{n+1}$ corresponding to the iterated method as

$$(2.3) \qquad y_{n+1} = y_n + hy'_n + \sum_{i=1}^{k} \alpha_i X_i^{(m)}, \qquad y'_{n+1} = y'_n + h^{-1} \sum_{i=1}^{k} \beta_i X_i^{(m)}.$$

It is easily seen that for m fixed the method {(2.2),(2.3)} fits into the class of DIRKN methods that can be characterized by the Butcher array

$$(2.4) \qquad \begin{array}{c|cccccc} X^{(0)} & \theta D & & & & & \\ X^{(1)} & A\text{-}D & D & & & & \\ X^{(2)} & O & A\text{-}D & D & & & \\ \vdots & & \ddots & \ddots & \ddots & & \\ X^{(m)} & O & O & O \ \ldots & O & A\text{-}D & D \\ \hline & O & O & O \ \ldots & O & \mathbf{b}^T A^{-1}(A\text{-}D) & \mathbf{b}^T A^{-1} D \\ & O & O & O \ \ldots & O & \mathbf{d}^T A^{-1}(A\text{-}D) & \mathbf{d}^T A^{-1} D \end{array},$$

where D is the diagonal matrix with diagonal entries $\delta_i$.

Since the k systems that are to be solved in each iteration step of (2.2) can be solved *in parallel* and each has a dimension equal to that of the system of ODEs, the iteration process (2.2) is on a k-processor computer of the same computational complexity as an (m+θ)-stage SDIRKN method on a one-processor computer. Thus, the method {(2.2),(2.3)} has only $s^* := m+\theta$ *sequential, singly diagonal-implicit* stages.

**Theorem 2.1.** Let p be the order of the k-stage corrector method (2.1) and let $m := [(p+1)/2]$. Then the method {(2.2),(2.3)} is an s-stage DIRKN method of order p with $s^*$ sequential, singly diagonal-implicit stages, where s and $s^*$ are defined by $s = k[(p+1)/2] + 1 + \theta(k-1)$ and $s^* = [(p+1)/2]+\theta$.

**Proof.** The expressions for s and s* immediately follow from the Butcher array (2.4). The order of the method is obtained by considering the iteration error of the method. Obviously, (2.2b) defines a first-order predictor formula (i.e., $X_i^{(0)} - X_i = O(h^2)$), so that by means of (2.2a)

$$X_i^{(m)} - X_i = O(h^{2+2m}). \tag{2.5}$$

In order to avoid confusion, let us denote the step values associated with the corrector by $u_{n+1}$ and $u'_{n+1}$. Subtracting the corrector step values and the iterated step values shows that

$$u_{n+1} - y_{n+1} = \sum_{i=1}^{k} \alpha_i (X_i - X_i^{(m)}) = O(h^{2+2m}),$$

$$u'_{n+1} - y'_{n+1} = h^{-1} \sum_{i=1}^{k} \beta_i (X_i - X_i^{(m)}) = O(h^{1+2m}).$$

Let y(t) be the local exact solution. Then the local truncation error is given by

$$\begin{aligned} y(t_{n+1}) - y_{n+1} &= y(t_{n+1}) - u_{n+1} + u_{n+1} - y_{n+1} = O(h^{p+1}) + O(h^{2+2m}), \\ y'(t_{n+1}) - y'_{n+1} &= y'(t_{n+1}) - u'_{n+1} + u'_{n+1} - y'_{n+1} = O(h^{p+1}) + O(h^{1+2m}), \end{aligned} \tag{2.6}$$

where p is the order of the corrector. Thus, we need only m = [(p+1)/2] iterations to reach the order of the corrector, so that s* := m+θ = [(p+1)/2]+θ. []

It follows from (2.6) that there three sources of local errors which together constitute the global error, i.e., the truncation error of the corrector (of order p+1) and the iteration errors corresponding to $y_{n+1}$ and $y'_{n+1}$ (of orders 2m+2 and 2m+1). In addition to these orders, the order *constants* also play a role. The magnitude of the order constant associated with the corrector is usually rather small. The order constants of the iteration errors decrease with m and are expected to be rather large for small values of m (see also Table 4.1). As the value of m is relatively small, the iteration errors may easily dominate the global error, so that the order of the corrector is not always shown in actual computation. For example, if the iteration error corresponding to $y_{n+1}$ dominates, then the effective order p* is given by p* = 2m+1 = 2[(p+1)/2] + 1. Likewise, if the iteration error corresponding to $y'_{n+1}$ dominates, then p* = 2m = 2[(p+1)/2].

## 3. Stability

The linear stability of the method {(2.2),(2.3)} is determined by applying it to the scalar test equation $y''=\lambda y$, where $\lambda$ runs through the eigenvalues of $\partial f/\partial y$, which are supposed to be negative. Defining the matrix

$$(3.1)\quad Z(z) := z[I - zD]^{-1}[A - D],\quad P_\theta(z) := z[I - zA]^{-1}[A - \theta D][I - \theta zD]^{-1},\quad z := \lambda h^2,$$

and the vectors

$$(3.2)\quad w_{n+1} := \begin{pmatrix} u_{n+1} \\ hu'_{n+1} \end{pmatrix},\quad v_{n+1} := \begin{pmatrix} y_{n+1} \\ hy'_{n+1} \end{pmatrix},$$

it can be shown (cf. [11]) that the following recursions hold:

$$(3.3)\quad w_{n+1} - v_{n+1} = E_m(z)v_n,\ E_m(z) := \begin{pmatrix} \mathbf{b}^T A^{-1}Z^m(z)P_\theta(z)\mathbf{e} & \mathbf{b}^T A^{-1}Z^m(z)P_\theta(z)\mathbf{c} \\ \mathbf{d}^T A^{-1}Z^m(z)P_\theta(z)\mathbf{e} & \mathbf{d}^T A^{-1}Z^m(z)P_\theta(z)\mathbf{c} \end{pmatrix},$$

$$(3.4)\quad w_{n+1} = M(z)v_n,\quad M(z) := \begin{pmatrix} 1+z\mathbf{b}^T(I-Az)^{-1}\mathbf{e} & 1+z\mathbf{b}^T(I-Az)^{-1}\mathbf{c} \\ z\mathbf{d}^T(I-Az)^{-1}\mathbf{e} & 1+z\mathbf{d}^T(I-Az)^{-1}\mathbf{c} \end{pmatrix}.$$

Hence, by eliminating the corrector values $w_{n+1}$ from (3.3) and (3.4), we find the recursion

$$(3.5)\quad v_{n+1} = [M(z) - E_m(z)]v_n.$$

We shall call the matrix $M(z) - E_m(z)$ the *stability matrix* of the method and its spectral radius the *stability function*, i.e., the function:

$$R_m(z) := \rho([M(z) - E_m(z)]).$$

The method {(2.2),(2.3)} is called A-stable if $R_m(z)$ assumes values in (-1,1) for $z < 0$, strongly A-stable if it is A-stable with $R_m(z)$ is bounded away from 1 outside the neighbourhood of the origin, and L-stable if it is A-stable with $R_m(\infty) = 0$.

Putting $m = [(p+1)/2]$, we obtain pth-order accuracy for any D. We shall exploit the matrix D to obtain pth-order A-stable, strongly A-stable or L-stable methods. However, it turns out that various choices of D generate such highly stable methods. From these methods we selected the methods with smallest truncation error. Recalling that the truncation error of the PDIRKN method will usually be dominated by the iteration error, we are led to consider the iteration error defined by (3.3). Since the nonstiff error components in the iteration error corresponding to small values of $|z|$ are sufficiently damped by the matrix $E_m(z)$ (note that $E_m(z) = O(z^{m+1})$), we shall concentrate on the *stiff* error components. From (3.2), (3.3) and (3.4) it follows that

$$w_{n+1} - v_{n+1} = E_m(z)v_n = E_m(z)[M(z) - E_m(z)]v_{n-1} = E_m(z)[M(z) - E_m(z)]^n v_0.$$

Restricting our considerations to the iteration error associated with $y_{n+1}$, we deduce that $u_{n+1} - y_{n+1}$ can be bounded by

$$(3.6)\qquad \| u_{n+1} - y_{n+1} \| = \| e_1^T E_m(z)[M(z) - E_m(z)]^n v_0 \|$$

$$\leq \| e_1^T E_m(z) \| \, \| [M(z) - E_m(z)]^n \| \, \| v_0 \|$$

$$\approx \text{const. } n^{\nu-1} [R_m(z)]^n \| e_1^T E_m(z) \| \, \| v_0 \| \text{ as } n \to \infty,$$

where $\nu$ denotes the maximum dimension of the Jordan box corresponding to the maximum-modulus-eigenvalues of the matrix $M(z) - E_m(z)$. This estimate shows that the stiff error components can be suppressed if the stability function $R_m(z)$ is small for large $| z |$-values. We remark that a similar estimate can be derived for $u'_{n+1} - y'_{n+1}$. The following theorem may be helpful in selecting methods possessing this property:

**Theorem 3.1.** Let the predictor be given by (2.2b) and let the corrector (2.1) be obtained from a consistent RK method for first-order equations given by the parameter arrays $\{A^*,b^*,c\}$, then the following assertions hold:
**(a)** If $\theta = 0$, then

$$R_m(\infty) = \rho \begin{pmatrix} 1 - (b^*)^T A^* Q_m e & 1 - (b^*)^T A^* Q_m c \\ - (b^*)^T Q_m e & 1 - (b^*)^T Q_m c \end{pmatrix}, \quad Q_m := (A^*)^{-2}[I - [I - D^{-1}(A^*)^2]^m].$$

**(b)** If $\theta = 1$, then $R_m(\infty) = | 1 - (b^*)^T (A^*)^{-1} e |$ for all m and D, and if the RK method $\{A^*,b^*,c\}$ is stiffly accurate, then $R_m(\infty) = 0$ for all m and D.

**Proof.** If the corrector (2.1) is obtained from an RK method for first-order equations $\{A^*,b^*,c\}$, then

$$(3.7)\qquad A = (A^*)^2, \quad b = (A^*)^T b^*, \quad c = A^* e, \quad d = b^*.$$

Furthermore, we have that $Z(\infty) = I - D^{-1}A$ and $P_\theta(\infty) = (\theta - 1)I$, where $\theta$ is either 0 or 1. Hence,

$$(3.8)\qquad M(\infty) - E_m(\infty) = \begin{pmatrix} 1 - b^T Q_{m\theta} e & 1 - b^T Q_{m\theta} c \\ - d^T Q_{m\theta} e & 1 - d^T Q_{m\theta} c \end{pmatrix}, \quad Q_{m\theta} := A^{-1}[I + (\theta - 1)[I - D^{-1}A]^m].$$

**(a)** On substitution of $\theta = 0$ and (3.7) into (3.8), part (a) is immediate.
**(b)** For $\theta = 1$ and using (3.7), we see that (3.8) reduces to

$$(3.8') \quad M(\infty) - E_m(\infty) = \begin{pmatrix} 1 - (b^*)^T(A^*)^{-1}e & 1 - (b^*)^Te \\ -(b^*)^T(A^*)^{-2}e & 1 - (b^*)^T(A^*)^{-1}e \end{pmatrix}.$$

Because of the consistency we have that $(b^*)^Te = 1$, so that the eigenvalues of $M(\infty) - E_m(\infty)$ are given by $1 - (b^*)^T(A^*)^{-1}e$. If the corrector $\{A^*,b^*,c\}$ is stiffly accurate, then

$$(3.9) \qquad e_k^Tc = 1, \ (b^*)^T = e_k^TA^*.$$

so that $R_m(\infty)$ vanishes for all m and D. []

This theorem shows that for *explicit* predictors of type I ($\theta = 0$), the behaviour of the stability function at infinity depends on D, so that we can exploit the matrix D by selecting methods with the smallest value $R_m(\infty)$. It is interesting to note that we obtained strongly A-stable PDIRKN methods although the corrector is only A-stable (e.g., in the case of Gauss-Legendre correctors listed in Table 4.1).

For *implicit* predictors of type II ($\theta = 1$), the behaviour of the stability function at infinity is completely determined by the corrector, so that D cannot be used for selecting small values of $R_m(\infty)$ in the estimate (3.6). However, (3.6) indicates that the iteration error is also influenced by the maginitude of $\| e_1^TE_m(z) \|$. Since $e_1^TE_m(z)$ vanishes at infinity, we selected methods with a small value of $\| e_1^TE_m(z) \|$ in the whole interval $(-\infty,0)$.

## 4. Survey of PDIRKN methods

In Table 4.1, we list the main characteristics of the A-stable, strongly A-stable and L-stable PDIRKN methods we found by means of the approach described in the preceding sections. In this table, $E_{max}$ denotes the maximum value of $\| e_1^TE_m(z) \|_\infty$ in the interval $(-\infty,0)$ and $E_\infty$ denotes the value of $\| e_1^TE_m(\infty) \|_\infty$. The predictors are of the form (2.2b) with $\theta = 0$ (predictor I) and $\theta = 1$ (predictor II), and the correctors used are the indirect collocation-type RKN methods based on the Gauss-Legendre and Radau IIA RK methods for first-order equations. Specification of the parameters of the resulting methods can be found in the Appendix to this paper.

Comparing the main characteristics of the methods listed in Table 4.1 with those listed in Table 1.1, we conclude that the computational costs per step of the lower-order methods (order three or four) are comparable, but the higher-order methods in Table 4.1 are much cheaper. On the other hand, the error constant $E_{max}$ of the iteration error associated with $y_{n+1}$ is relatively large. However, as we have shown in the discussion of Theorem 2.1, the order in h of these iteration errors is also larger, which may compensate the large error constants. Hence, we may hope for improved efficiency for the new PDIRKN methods.

**Table 4.1.** PDIRKN methods of order p requiring s* singly diagonal-implicit, sequential stages on k processors.

| {Predictor - Corrector} | iteration parameters $\delta_i$ | p | s* | k | Stability | $E_{max}$ | $E_\infty$ |
|---|---|---|---|---|---|---|---|
| {I - Radau IIA} | (11/200, 107/225) | 3 | p-1 | 2 | Strongly A-stable | 0.35 | 0.06 |
| {II - Radau IIA} | (1/5, 1/5) | 3 | p | 2 | L-stable | 0.14 | 0.00 |
| {I - Gauss-Legendre} | (1/5, 11/20) | 4 | p-2 | 2 | Strongly A-stable | 1.35 | 1.35 |
| {II - Gauss-Legendre} | (223/10000, 311/1000) | 4 | p-1 | 2 | A-stable | 0.25 | 0.00 |
| {I - Radau IIA} | (1/40, 1/4, 3/5) | 5 | p-2 | 3 | Strongly A-stable | 0.73 | 0.16 |
| {II - Radau IIA} | (639/5000, 17/1250, 409/2500) | 5 | p-1 | 3 | L-stable | 0.51 | 0.00 |
| {I - Gauss-Legendre} | (1/5, 1/2, 3/4) | 6 | p-3 | 3 | Strongly A-stable | 1.44 | 0.51 |
| {II - Gauss-Legendre} | (1/100, 1/5, 9/20) | 6 | p-2 | 3 | A-stable | 1.32 | 0.00 |
| {I - Radau IIA} | (1/5, 4/5, 4/5, 19/20) | 7 | p-3 | 4 | Strongly A-stable | 1.43 | 0.77 |
| {II - Radau IIA} | (9/200, 1/40, 9/40, 91/200) | 7 | p-2 | 4 | L-stable | 1.09 | 0.00 |
| {I - Gauss-Legendre} | (13/20, 13/20, 3/4, 19/20) | 8 | p-4 | 4 | Strongly A-stable | 1.60 | 1.60 |
| {II - Gauss-Legendre} | (1/10, 1/5, 3/10, 2/5) | 8 | p-3 | 4 | A-stable | 1.55 | 0.00 |

## 5. Numerical experiments

We shall numerically investigate the following aspects of the PDIRKN methods: (i) the stability, in particular, the damping of perturbations of the initial conditions, (ii) the effective order, in relation to the order of the generating corrector, (iii) the predictor, mutual comparison of the explicit and implicit prdictor formula, and (iv) the efficiency, in comparison with available sequential SDIRKN methods from the literature.

All problems are taken from the literature and possess exact solutions in closed form. Initial (and boundary) conditions are taken from the exact solution.

### 5.1. Stability test

We first test the stability properties of the various PDIRKN methods by integrating a nonautonomous problem with varying stiffness:

$$y''(t) = \begin{pmatrix} -2\alpha(t)+1 & -\alpha(t)+1 \\ 2(\alpha(t)-1) & \alpha(t)-2 \end{pmatrix} y(t), \quad y(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -1 \\ 2 \end{pmatrix}, \quad 0 \le t \le 4000,$$

(5.1)

$$\alpha(t) = \sqrt{1+t^3} + \frac{1}{\sqrt{1+t^3}}.$$

The Jacobian matrix of the system has the eigenvalues -1 and - $\alpha(t)$, so that the spectral radius, and therefore the stiffness, increases with t. We compared the numerical solution of (5.1) with the numerical solution obtained by perturbing the initial conditions, i. e., instead of the initial conditions y(0) and y'(0) we used the initial conditions y(0) + $\varepsilon e$ and y'(0) + $\varepsilon e$. Denoting the numerical solutions by $y_n$ and $y^*_n$, we may expect from any stable method that $\| y_n - y^*_n \|$ does not increase with n. For various PDIRKN methods, Table 5.1 lists the values $C_n := \| y_n - y^*_n \| / \| y_0 - y^*_0 \| = \| y_n - y^*_n \| / \varepsilon$ for n = 5000. The methods are specified by the generating Predictor-Corrector pair where the predictor is indicated by its type. It turned out that $C_n$ is almost independent of $\varepsilon$ for $\varepsilon \le 1/10$. The results in Table 5.1 demonstrate the strong damping of the initial perturbation by the PDIRKN methods.

**Table 5.1.** Values of the amplification factor $C_n$ for problem (5.1) with n = 5000 for various Predictor-Corrector pairs.

| Type I - Methods | p | s* | k | $C_n$ | Type II - Methods | p | s* | k | $C_n$ |
|---|---|---|---|---|---|---|---|---|---|
| I - Radau IIA | 3 | 2 | 2 | 0.64E-13 | II - Radau IIA | 3 | 3 | 2 | 0.17E-06 |
| I - Gauss-Legendre | 4 | 2 | 2 | 0.27E-05 | II - Gauss-Legendre | 4 | 3 | 2 | 0.11E-01 |
| I - Radau IIA | 5 | 3 | 3 | 0.20E-10 | II - Radau IIA | 5 | 4 | 3 | 0.62E-01 |
| I - Gauss-Legendre | 6 | 3 | 3 | 0.39E-09 | II - Gauss-Legendre | 6 | 4 | 3 | 0.66E-07 |
| I - Radau IIA | 7 | 4 | 4 | 0.43E-07 | II - Radau IIA | 7 | 5 | 4 | 0.41E-02 |
| I - Gauss-Legendre | 8 | 4 | 4 | 0.26E-08 | II - Gauss-Legendre | 8 | 5 | 4 | 0.21E-00 |

## 5.2 Effective order and efficiency of the explicit and implicit predictor

In this section, we show that the effective order of the PDIRKN methods may exceed the order of the corrector. In addition, we compare the efficiency of the explicit and implicit predictor. In all experiments the accuracy is given by means of the number of minimal correct digits (NCD) defined by NCD(h) = -log( || global error at the endpoint of the integration interval $||_\infty$), and the computational effort is measured by the total number of sequential stages per unit interval, that is, by M = Ns*, where N is the number of integration steps per unit interval.

Table 5.2 lists results for the problem (see [13])

$$(5.2)\qquad y''(t) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} y(t),\ 0 \le t \le 100,$$

with exact solution $y(t) = (2\cos(t), -\cos(t))^T$. These results show that for the higher-order methods (i.e., $p \ge 5$), the effective order $p^*$ is usually greater than p (see the discussion of Theorem 2.1). Furthermore, except for the third-order Radau corrector, the superiority of the implicit predictor of type II is clear, inspite of the additional implicit stage. Therefore, in the following, we shall confine our considerations to the type II predictor.

**Table 5.2.** Effective order $p^*$ and values of NCD and M for problem (5.2).

| Predictor - Corrector | p | s* | k | M = 25 | M = 50 | M = 100 | M = 200 | p* |
|---|---|---|---|---|---|---|---|---|
| I - Radau IIA | 3 | 2 | 2 | 2.8 | 3.8 | 4.7 | 5.6 | 3 |
| II- Radau IIA | 3 | 3 | 2 | 2.4 | 3.3 | 4.2 | 5.1 | 3 |
| I - Gauss-Legendre | 4 | 2 | 2 | 3.3 | 4.5 | 5.7 | 6.9 | 4 |
| II - Gauss-Legendre | 4 | 3 | 2 | 4.0 | 5.4 | 6.7 | 8.0 | 4 |
| I - Radau IIA | 5 | 3 | 3 | 4.2 | 6.0 | 7.8 | 9.6 | 6 |
| II - Radau IIA | 5 | 4 | 3 | 5.1 | 6.8 | 8.5 | 10.0 | 5 |
| I - Gauss-Legendre | 6 | 3 | 3 | 3.9 | 5.8 | 7.6 | 9.4 | 6 |
| II - Gauss-Legendre | 6 | 4 | 3 | 4.6 | 6.7 | 8.8 | 11.0 | 7 |
| I - Radau IIA | 7 | 4 | 4 | 4.5 | 6.9 | 9.3 | 12.0 | 8 |
| II - Radau IIA | 7 | 5 | 4 | 5.4 | 8.1 | 10.8 | | 9 |
| I - Gauss-Legendre | 8 | 4 | 4 | 4.4 | 6.8 | 9.2 | 12.8 | 8 |
| II - Gauss-Legendre | 8 | 5 | 4 | 5.2 | 7.7 | 10.1 | | 8 |

## 5.3. Efficiency tests

In this section, we compare the efficiency of the PDIRKN with methods from the literature. We selected the following methods from Table 1.1:

| | |
|---|---|
| Nørsett $_3$ | third-order method of Nørsett |
| Nørsett $_4$ | fourth-order method of Nørsett |
| $SFB_3$ | third-order method of Sharp, Fine & Burrage |
| $SFB_4$ | fourth-order method of Sharp, Fine & Burrage |

| | |
|---|---|
| $B_3$ | third-order method of Burrage |
| $CS_5$ | fifth-order method of Cooper & Sayfy |
| $CS_6$ | sixth-order method of Cooper & Sayfy. |

**5.3.1. Linear Kramarz problem.** Table 5.3 presents results for these sequential methods and for our PDIRKN methods when applied to the Kramarz problem (5.2). In most cases, the PDIRKN methods are by far the most accurate ones. Notice that the $CS_6$ method does not show its order 6 in the high accuracy range. This is caused by an insufficient accuracy of the method parameters

**Table 5.3.** Values of NCD and M for problem (5.2).

| Methods | p | s* | k | M = 25 | M = 50 | M = 100 | M = 200 |
|---|---|---|---|---|---|---|---|
| Nørsett$_3$ | 3 | 2 | 1 | 2.1 | 3.0 | 3.9 | 4.8 |
| SFB$_3$ | 3 | 2 | 1 | 1.8 | 2.7 | 3.6 | 4.5 |
| B$_3$ | 3 | 4 | 1 | 1.2 | 2.1 | 3.0 | 3.9 |
| II- Radau IIA | 3 | 3 | 2 | 2.4 | 3.3 | 4.2 | 5.1 |
| Nørsett$_4$ | 4 | 3 | 1 | 2.8 | 3.8 | 4.9 | 6.1 |
| SFB$_4$ | 4 | 3 | 1 | 3.2 | 4.5 | 5.7 | 6.9 |
| II - Gauss-Legendre | 4 | 3 | 2 | 4.0 | 5.4 | 6.7 | 8.0 |
| $CS_5$ | 5 | 5 | 1 | 4.1 | 5.6 | 7.1 | 8.6 |
| II - Radau IIA | 5 | 4 | 3 | 5.1 | 6.8 | 8.5 | 10.0 |
| $CS_6$ | 6 | 5 | 1 | 5.5 | 7.0 | 8.4 | 9.0 |
| II - Gauss-Legendre | 6 | 4 | 3 | 4.6 | 6.7 | 8.8 | 11.0 |
| II - Radau IIA | 7 | 5 | 4 | 5.4 | 8.1 | 10.8 | |
| II - Gauss-Legendre | 8 | 5 | 4 | 5.2 | 7.7 | 10.1 | |

**5.3.2. Linear Strehmel-Weiner problem.** In [18] we find the following linear, stiff problem:

$$(5.3)\quad y''(t) = \begin{pmatrix} -20.2 & 0 & -9.6 \\ 7989.6 & -10000 & -6004.2 \\ -9.6 & 0 & -5.8 \end{pmatrix} y(t) + \begin{pmatrix} 150\cos(10t) \\ 75\cos(10t) \\ 75\cos(10t) \end{pmatrix}, \quad 0 \le t \le 100$$

with exact solution

$$y(t) = \begin{pmatrix} \cos(t) + 2\cos(5t) - 2\cos(10t) \\ 2\cos(t) + \cos(5t) - \cos(10t) \\ -2\cos(t) + \cos(5t) - \cos(10t) \end{pmatrix}.$$

Unlike the Kramarz problem, this problem has slowly and rapidly oscillating solution components (nonstiff and stiff solution components) which are appearing with comparable weights. This implies a severe test for the PDIRKN methods because of the strong damping, and therefore inaccurate approximation, of the stiff solution components. In spite of that, they are generally superior to the sequential methods.

**Table 5.4.** Values of NCD and M for problem (5.3).

| Methods | p | s* | k | M = 100 | M = 200 | M = 400 | M = 800 |
|---|---|---|---|---|---|---|---|
| $Nørsett_3$ | 3 | 2 | 1 | 1.1 | 2.0 | 2.9 | 3.8 |
| $SFB_3$ | 3 | 2 | 1 | 0.8 | 1.7 | 2.6 | 3.5 |
| $B_3$ | 3 | 4 | 1 | 0.3 | 1.1 | 2.0 | 2.9 |
| II - Radau IIA | 3 | 3 | 2 | 1.4 | 2.3 | 3.2 | 4.1 |
| $Nørsett_4$ | 4 | 3 | 1 | 1.2 | 2.5 | 3.8 | 5.0 |
| $SFB_4$ | 4 | 3 | 1 | 2.3 | 3.4 | 4.7 | 5.9 |
| II - Gauss-Legendre | 4 | 3 | 2 | 3.1 | 4.9 | 6.7 | 7.3 |
| $CS_5$ | 5 | 5 | 1 | 3.0 | 4.5 | 5.9 | 7.4 |
| II - Radau IIA | 5 | 4 | 3 | 4.9 | 6.6 | 7.6 | 9.0 |
| $CS_6$ | 6 | 5 | 1 | 3.6 | 5.5 | 7.5 | 8.2 |
| II - Gauss-Legendre | 6 | 4 | 3 | 3.2 | 5.3 | 7.4 | 9.4 |
| II - Radau IIA | 7 | 5 | 4 | 3.9 | 6.6 | 9.4 | 10.0 |
| II - Gauss-Legendre | 8 | 5 | 4 | 4.4 | 6.5 | 8.8 | 10.0 |

**5.3.3. Nonlinear Strehmel-Weiner problem.** In [18] we also find a nonlinear, stiff problem:

$$\begin{aligned} y''_1(t) &= (y_1(t) - y_2(t))^3 + 6368y_1(t) - 6384y_2(t) + 42\cos(10t), \\ y''_2(t) &= -(y_1(t) - y_2(t))^3 + 12768y_1(t) - 12784y_2(t) + 42\cos(10t), \end{aligned} \qquad 0 \le t \le 10 \tag{5.4}$$

with exact solution $y_1(t) = y_2(t) = \cos(4t) - \cos(10t)/2$. Table 5.5 demonstrates that the PDIRKN methods similarly compare with the sequential methods as for the linear Kramarz and Strehmel-Weiner problems.

**Table 5.5.** Values of NCD and M for problem (5.4).

| Methods | p | s* | k | M = 100 | M = 200 | M = 400 | M = 800 |
|---|---|---|---|---|---|---|---|
| $\text{Nørsett}_3$ | 3 | 2 | 1 | 2.9 | 3.9 | 4.8 | 5.7 |
| $SFB_3$ | 3 | 2 | 1 | 2.7 | 3.6 | 4.5 | 5.4 |
| $B_3$ | 3 | 4 | 1 | 2.3 | 3.6 | 5.2 | 6.2 |
| II - Radau IIA | 3 | 3 | 2 | 3.3 | 4.1 | 5.1 | 6.0 |
| $\text{Nørsett}_4$ | 4 | 3 | 1 | 3.0 | 4.2 | 5.3 | 6.5 |
| $SFB_4$ | 4 | 3 | 1 | 3.7 | 4.9 | 6.1 | 7.3 |
| II - Gauss-Legendre | 4 | 3 | 2 | 4.8 | 6.1 | 7.4 | 8.7 |
| $CS_5$ | 5 | 5 | 1 | 4.9 | 6.4 | 7.9 | 9.4 |
| II - Radau IIA | 5 | 4 | 3 | 5.8 | 7.6 | 9.4 | 11.1 |
| $CS_6$ | 6 | 5 | 1 | 5.9 | 7.6 | 9.2 | 9.9 |
| II - Gauss-Legendre | 6 | 4 | 3 | 5.5 | 7.6 | 9.7 | 11.8 |
| II - Radau IIA | 7 | 5 | 4 | 6.4 | 9.0 | 11.6 | |
| II - Gauss-Legendre | 8 | 5 | 4 | 5.8 | 8.2 | 10.6 | |

**5.3.4. Fehlberg problem.** An often used test problem is the orbit equation (cf. [7])

$$y''_1(t) = -4t^2 y_1(t) - \frac{2y_2(t)}{\sqrt{y_1^2(t) + y_2^2(t)}}$$

$$y''_2(t) = -4t^2 y_2(t) + \frac{2y_1(t)}{\sqrt{y_1^2(t) + y_2^2(t)}} \qquad , \sqrt{\pi/2} \le t \le 3\pi \tag{5.5}$$

with the exact solution $y_1(t) = \cos(t^2)$, $y_2(t) = \sin(t^2)$. In this experiment, the sixth-order method of Cooper & Sayfy can compete with the PDIRKN method of order six.

**Table 5.6.** Values of NCD and M for problem (5.5).

| Methods | p | s* | k | M = 98 | M = 196 | M = 392 | M = 783 |
|---|---|---|---|---|---|---|---|
| $Nørsett_3$ | 3 | 2 | 1 | 0.9 | 1.8 | 2.7 | 3.6 |
| $SFB_3$ | 3 | 2 | 1 | 0.6 | 1.5 | 2.4 | 3.3 |
| $B_3$ | 3 | 4 | 1 | 0.2 | 0.9 | 1.9 | 2.7 |
| II - Radau IIA | 3 | 3 | 2 | 0.9 | 2.0 | 2.9 | 4.0 |
| $Nørsett_4$ | 4 | 3 | 1 | 0.7 | 1.5 | 2.7 | 4.0 |
| $SFB_4$ | 4 | 3 | 1 | 1.2 | 2.4 | 3.6 | 4.8 |
| II - Gauss-Legendre | 4 | 3 | 2 | 1.7 | 3.2 | 4.5 | 5.9 |
| $CS_5$ | 5 | 5 | 1 | 1.7 | 3.1 | 4.7 | 6.2 |
| II - Radau IIA | 5 | 4 | 3 | 2.1 | 3.8 | 5.6 | 7.3 |
| $CS_6$ | 6 | 5 | 1 | 1.9 | 3.5 | 5.3 | 7.1 |
| II - Gauss-Legendre | 6 | 4 | 3 | 1.2 | 3.1 | 5.1 | 7.2 |
| II - Radau IIA | 7 | 5 | 4 | 1.1 | 3.3 | 5.9 | 8.5 |
| II - Gauss-Legendre | 8 | 5 | 4 | 1.1 | 3.2 | 5.6 | 8.0 |

**5.3.5. Semi-discrete partial differential equation.** Consider following initial-boundary-value problem (see [11]):

$$(5.6)\qquad \frac{\partial^2 u}{\partial t^2} = \frac{4\pi^2 u^2}{1 + 2x - 2x^2}\frac{\partial^2 u}{\partial x^2} + 4\pi^2 u[\,4\cos^2(2\pi t) - 1], \quad 0 \le t \le 1, \quad 0 \le x \le 1,$$

with Diriclet boundary conditions and exact solution $u = (1 + 2x - 2x^2)\cos(2\pi t)$. By using second-order symmetric spatial discretization on a uniform grid with mesh $\Delta x = 1/20$ we obtain a set of 19 ODEs. Table 5.7 shows that the PDIRKN methods are at least competitive and often more efficient than the sequential methods of the same order (notice that in Table 5.7 the " * " indicates bad convergence in the Newton iterations ).

**Table 5.7.** Values of NCD and M for problem (5.6)

| Methods | p | s* | k | M = 200 | M = 400 | M = 800 | M = 1600 |
|---|---|---|---|---|---|---|---|
| $Nørsett_3$ | 3 | 2 | 1 | 3.5 | 4.3 | 5.1 | 5.9 |
| $SFB_3$ | 3 | 2 | 1 | 3.6 | 4.5 | 5.4 | 6.3 |
| $B_3$ | 3 | 4 | 1 | * | 4.3 | 5.4 | 6.4 |
| II - Radau IIA | 3 | 3 | 2 | 3.7 | 5.1 | 6.0 | 6.8 |
| $Nørsett_4$ | 4 | 3 | 1 | 3.4 | 4.2 | 5.2 | 5.9 |
| $SFB_4$ | 4 | 3 | 1 | 5.5 | 6.4 | 7.6 | 8.8 |
| II - Gauss-Legendre | 4 | 3 | 2 | 5.0 | 6.3 | 7.8 | 9.2 |
| $CS_5$ | 5 | 5 | 1 | 4.0 | 5.3 | 6.6 | 7.7 |
| II- Radau IIA | 5 | 4 | 3 | 4.2 | 5.2 | 6.3 | 7.7 |
| $CS_6$ | 6 | 5 | 1 | 3.1 | 4.4 | 5.5 | 6.9 |
| II - Gauss-Legendre | 6 | 4 | 3 | 3.8 | 4.7 | 6.2 | 8.1 |
| II - Radau IIA | 7 | 5 | 4 | * | 4.7 | 6.0 | 8.5 |
| II - Gauss-Legendre | 8 | 5 | 4 | 3.6 | 4.4 | 5.5 | 7.0 |

## 6. Concluding remarks

In this paper, we have shown that diagonally implicit iteration of fully implicit, pth-order RKN correctors leads to parallel DIRKN methods of order p with relatively few sequential stages. For Radau IIA and Gauss-Legendre correctors, the iteration parameters are determined in such a way that the methods are A-stable, strongly A-stable or L-stable. Numerical experiments clearly demonstrate the superiority of the parallel methods over the sequential SDIRKN methods available in the literature.

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# A. Appendix

## A.1. Indirect collocation-based Runge-Kutta-Nyström methods

By writing (1.1) in the first-order system of ODEs form and by applying Runge-Kutta methods with Butcher array,

| | |
|---|---|
| c | Å |
| | $d^T$ |

we get indirect Runge-Kutta-Nyström methods with following Butcher array:

| | |
|---|---|
| c | $Å^2$ |
| | $d^T Å$ |
| | $d^T$ |

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

For completeness, we give the Butcher arrays of the indirect RKN methods generated by Radau IIA and Gauss - Legendre RK methods of two, three and four stages together with corresponding vectors $\alpha$ and $\beta$ (see (2.3)), for the stiffly accurate Radau IIA methods $\alpha = e_k^T$.

### A.2.1. The indirect Radau IIA Runge-Kutta-Nyström method with k = 2

| | | |
|---|---|---|
| 0.333333333333 | 0.111111111111 | -0.055555555556 |
| 1.000000000000 | 0.500000000000 | 0.000000000000 |
| | 0.500000000000 | 0.000000000000 |
| | 0.750000000000 | 0.250000000000 |

with $\beta = (-4.500000000000,\ 2.500000000000)^T$

### A.2.2. The indirect Gauss-Legendre Runge-Kutta-Nyström method with k = 2

| | | |
|---|---|---|
| 0.211324865405 | 0.041666666667 | -0.019337567297 |
| 0.788675134595 | 0.269337567297 | 0.041666666667 |
| | 0.394337567297 | 0.105662432703 |
| | 0.500000000000 | 0.500000000000 |

with $\beta = (-16.392304845413,\ 4.392304845413)^T$

$\alpha = (-1.732050807569,\ 1.732050807569)^T$

### A.2.3. The indirect Radau IIA Runge-Kutta-Nyström method with k = 3

| | | | |
|---|---|---|---|
| 0.155051025722 | 0.021835034191 | -0.019857254099 | 0.010042630197 |
| 0.644948974278 | 0.177190587432 | 0.038164965809 | -0.007375963530 |
| 1.000000000000 | 0.318041381744 | 0.181958618256 | 0.000000000000 |
| | 0.318041381744 | 0.181958618256 | 0.000000000000 |
| | 0.376403062700 | 0.512485826188 | 0.111111111111 |

with $\beta$ = (5.531972647422, -7.531972647422, 5.000000000000)$^T$

### A.2.4. The indirect Gauss-Legendre Runge-Kutta-Nyström method with k = 3

| | | | |
|---|---|---|---|
| 0.112701665379 | 0.011111111111 | -0.008288518805 | 0.003528240383 |
| 0.500000000000 | 0.102402546475 | 0.027777777778 | -0.005180324253 |
| 0.887298334621 | 0.218693981839 | 0.163844074360 | 0.011111111111 |
| | 0.246471759617 | 0.222222222222 | 0.031306018161 |
| | 0.277777777778 | 0.444444444444 | 0.277777777778 |

with $\beta$ = ( 1.666666666667, -1.333333333333, 1.666666666667)$^T$

$\alpha$ = (32.909944487358, -16.000000000000, 7.090055512642)$^T$

### A.2.5. The indirect Radau IIA Runge-Kutta-Nyström method with k = 4

| | | | | |
|---|---|---|---|---|
| 0.088587959513 | 0.006728344412 | -0.006260584380 | 0.006465233729 | -0.003009080475 |
| 0.409466864441 | 0.068145660054 | 0.020150312614 | -0.007623261099 | 0.003158844969 |
| 0.787659461761 | 0.155303251991 | 0.142674406078 | 0.013937669505 | -0.001711613723 |
| 1.000000000000 | 0.200931913739 | 0.229241106360 | 0.069826979901 | 0.000000000000 |
| | 0.200931913739 | 0.229241106360 | 0.069826979901 | 0.000000000000 |
| | 0.220462211177 | 0.388193468843 | 0.328844319980 | 0.062500000000 |

with $\beta$ = (-6.923488256444, 6.595237669626, -12.171749413180, 8.499999999998)$^T$

**A.2.6. The indirect Gauss-Legendre Runge-Kutta-Nyström method with k = 4**

| | | | | |
|---|---|---|---|---|
| 0.069431844203 | 0.004038191451 | -0.003295860945 | 0.002644782952 | -0.000976722963 |
| 0.330009478208 | 0.043563580902 | 0.013818951406 | -0.004340134194 | 0.001410729739 |
| 0.669990521792 | 0.105864352634 | 0.106518360965 | 0.013818951406 | -0.001758015359 |
| 0.930568155797 | 0.148798496193 | 0.198470498852 | 0.081671359796 | 0.004038191451 |
| | 0.161851320862 | 0.218465536295 | 0.107607041136 | 0.012076101706 |
| | 0.173927422569 | 0.326072577431 | 0.326072577431 | 0.173927422569 |

with $\beta = ( -1.640705321739,\ 1.214393969799,\ -1.214393969799,\ 1.640705321739)^T$

$\alpha = (-54.681428514064,\ 26.155201475250,\ -22.420557316693\ \ 10.946784355507)^T$