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Embedded Diagonally Implicit Runge-Kutta Algorithms on Parallel Computers

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This paper investigates diagonally implicit Runge-Kutta methods in which the implicit relations can be solved in parallel and are singly diagonally implicit on each processor. The algorithms are based on diagonally implicit iteration of fully implicit Runge-Kutta methods. The iteration scheme is chosen in such a way that the resulting algorithm is A(α)-stable or L(α)-stable with α equal or very close to $\pi/2$. Because of the iterative nature of the methods, embedded formulas of lower orders are automatically available allowing a strategy for step and order variation.

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1. INTRODUCTION

In [8], predictor-corrector (PC) methods for solving the initial-value problem for the system of ordinary differential equations (ODEs)

$$(1.1) \qquad \frac{dy(t)}{dt} = f(y(t)),$$

on parallel computers were developed. These methods are based on functional iteration (or Jacobi iteration) of implicit Runge-Kutta (RK) methods. On sequential computers, implicit RK methods are seldom used as corrector equation, because of the large number of implicit relations to be solved when using these correctors. However, matters are different when parallel computers are used, since functional iteration possesses a high degree of parallelism. These 'parallel, iterated' RK methods (called PIRK methods in [8]) have the attractive feature that embedded formulas of lower orders are automatically available allowing a strategy for step and order variation. On the other hand, due to their explicit character, PIRK methods have rather limited regions of stability and are therefore not suitable for integrating stiff systems. In this paper, we investigate the possibility of constructing highly stable methods by diagonally implicit iteration of fully implicit RK methods. Such methods belong to the class of DIRK methods, but, when run on a parallel computer, they have the same reduced computational complexity as the singly diagonally implicit RK (SDIRK) methods designed for sequential computers. Furthermore, like the PIRK methods, they possess embedded formulas of lower order which make them an ideal starting point for developing variable order/variable step codes. We shall call the 'Parallel, Diagonal-implicitly Iterated' RK methods PDIRK methods.

In the literature various embedded DIRK methods were published for the integration of stiff systems of ODEs on one-processor computers. We mention the L-stable methods of orders 2 and 3 by Nørsett [11], and the strongly S-stable three-stage, third-order and five-stage, fourth-order methods by Cash [3] and by Cash and Liem [4]. In the present paper, the main results are

(i) L-stable, stiffly accurate methods of orders $p \le 8$ and $p=10$ with embedded formulas of orders 1 up to p and requiring p+1 sequential stages
(ii) L-stable, stiffly accurate methods of orders $p \le 6$ and $p=8$ with embedded formulas of orders 1 up to p and requiring p sequential stages (for $p=7$, we found an L(α)-stable method with $\alpha \approx \pi/2$)
(iii) A(α)-stable ($\alpha \approx \pi/2$), stiffly accurate methods of orders $p=5$ and 7 with embedded formulas of orders 2 up to p and requiring p-1 sequential stages.

The number of sequential stages mentioned assumes the availability of [(p+1)/2]-processors, where [x] denotes the integer part of x.

2. PDIRK METHODS

For notational convenience, we shall assume in the following that the equation (1.1) is a scalar equation. However, all considerations below are straightforwardly extended to systems of ODEs, and therefore, also to nonautonomous equations. Our starting point is the s-stage, implicit, one-step RK method

$$(2.1a) \qquad y_{n+1} = y_n + h\mathbf{b}^T\mathbf{r}_{n+1},$$

where $\mathbf{r}_{n+1}$ is implicitly defined by the set of algebraic equations

(2.1b) $\mathbf{r}_{n+1} := f(y_n\mathbf{e} + hA\mathbf{r}_{n+1})$.

Here, h is the integration step, e is a column vector of dimension s with unit entries, **b** is an s-dimensional vector and A is an s-by-s matrix. Furthermore, we use the convention that for any given vector $\mathbf{v}=(v_j)$, $f(\mathbf{v})$ denotes the vector with entries $f(v_j)$.

By iterating, say m times, the equation for $\mathbf{r}_{n+1}$ by diagonally implicit iteration, we obtain the method

(2.2) $\mathbf{r}^{(j)} = f(y_n\mathbf{e} + h[A - D]\,\mathbf{r}^{(j-1)} + hD\mathbf{r}^{(j)}),\quad y^{(j)} = y_n + h\mathbf{b}^T\mathbf{r}^{(j)},\quad j = 1, 2, \ldots, m,$

where D is a diagonal matrix with free diagonal elements and $\mathbf{r}^{(0)}$ denotes an initial approximation to the vector $\mathbf{r}_{n+1}$. Notice that after each iteration the current approximation $y^{(j)}$ to y_{n+1} can be computed. As we shall see in Section 2.1, the order of these approximations increases by 1 in each iteration. Therefore, the mth iterate will be used to continue the integration process and the preceding iterates can be used for error control.

It is sometimes convenient to use an alternative representation of this iteration process. By writing $\mathbf{r}^{(j)}=f(\mathbf{Y}^{(j)})$, (2.2) takes the form

(2.2') $\mathbf{Y}^{(j)} = y_n\mathbf{e} + h[A - D]\,f(\mathbf{Y}^{(j-1)}) + hDf(\mathbf{Y}^{(j)}),\quad y^{(j)} = y_n + h\mathbf{b}^Tf(\mathbf{Y}^{(j)}),\quad j = 1, 2, \ldots, m,$

where now $\mathbf{Y}^{(0)}$ denotes an initial approximation to the solution of $\mathbf{Y} = y_n\mathbf{e} + hAf(\mathbf{Y})$.

Since the matrix D is of diagonal form, the s components of each vector $\mathbf{r}^{(j)}$ can be computed in parallel, provided that s processors are available. Thus, effectively, we obtain a method which requires per integration step the computational time needed for computing one component of the initial approximation $\mathbf{r}^{(0)}$ and the successive solution of m equations. In the following, we always assume that we have s processors at our disposal and we shall speak about computational effort per step when we mean the computational time required per step if s processors are available. We shall call the method providing $\mathbf{r}^{(0)}$ the *predictor method* and (2.1) the *corrector method.*

In this paper, we restrict our considerations to the case where the predictor method is itself an RK-type method. Hence, by performing m iterations with (2.2) and by accepting $y^{(m)}$ as the final approximation to y_{n+1}, we obtain an RK method with a fixed number of stages. Furthermore, we assume that the predictor is explicit or at most diagonally implicit. Then, the resulting parallel RK method belongs to the class of DIRK methods (Diagonally Implicit RK methods), and will be briefly called *PDIRK method.*

2.1. Order of PDIRK Methods

Assuming that the iteration process (2.2) converges as $m\to\infty$, the values $y^{(j)}$ approximate the solution of the corrector method (2.1), i.e., $y^{(\infty)}=y_{n+1}$. The approximation $y^{(j)}$ differs from $y^{(\infty)}$ by the amount

$$y^{(j)} - y^{(\infty)} = y^{(j)} - y_{n+1} = h\mathbf{b}^T[\mathbf{r}^{(j)} - \mathbf{r}_{n+1}].$$

If the right-hand side function is sufficiently smooth, then the iteration error $\mathbf{r}^{(j)} - \mathbf{r}_{n+1}$ satisfies the approximate recursion

$$\mathbf{r}^{(j)} - \mathbf{r}_{n+1} \approx h\,[I - h\frac{\partial f}{\partial y}D]^{-1}\frac{\partial f}{\partial y}[A - D][\mathbf{r}^{(j-1)} - \mathbf{r}_{n+1}] = h^j\left([I - h\frac{\partial f}{\partial y}D]^{-1}\frac{\partial f}{\partial y}[A - D]\right)^j[\mathbf{r}^{(0)} - \mathbf{r}_{n+1}],$$

so that

(2.3) $$y^{(m)} - y_{n+1} = h^{m+1}\mathbf{b}^T\left([I - h\frac{\partial f}{\partial y}D]^{-1}\frac{\partial f}{\partial y}[A - D]\right)^m[\mathbf{r}^{(0)} - \mathbf{r}_{n+1}].$$

Let the predictor be of order q, i.e.,

(2.4) $\mathbf{r}^{(0)} - \mathbf{r}_{n+1} = O(h^q) \;\Rightarrow\; y^{(0)} - y_{n+1} = O(h^{q+1}),$

then

$$y^{(m)} - y_{n+1} = O(h^{q+m+1}),$$

so that $y^{(m)}$ has (global) order q+m.

In this paper, we shall study PDIRK methods with predictors of the form

(2.5) $\mathbf{r}^{(0)} := f(y_n\mathbf{e} + hEf(y_n\mathbf{e}) + hB\mathbf{r}^{(0)})$

or, using the representation (2.2'),

(2.5') $\mathbf{Y}^{(0)} := y_n\mathbf{e} + hEf(y_n\mathbf{e}) + hBf(\mathbf{Y}^{(0)})$.

Because this predictor is *implicit*, we will choose the matrix B of diagonal form in order to exploit parallelism. Since

$$\mathbf{r}^{(0)} - \mathbf{r}_{n+1} = f(y_n\mathbf{e} + hEf(y_n\mathbf{e}) + hBf(y_n\mathbf{e} + hEf(y_n\mathbf{e}) + hBf(y_n\mathbf{e}))) - f(y_n\mathbf{e} + hAf(y_n\mathbf{e} + hAf(y_n\mathbf{e}))) + O(h^3),$$

it is easily verified that the predictor (2.5) is always first-order accurate; it becomes of order two if (E+B-A)e vanishes and of order three if, in addition, $(BA-A^2)\mathbf{e}$, vanishes.

By defining y_{n+1} according to

(2.6) $y_{n+1} := y^{(m)} = y_n + h\mathbf{b}^T\mathbf{r}^{(m)} = y_n + h\mathbf{b}^Tf(\mathbf{Y}^{(m)})$,

the PDIRK method is completely determined. For this method, we summarize the above order considerations in the following theorem:

Theorem 2.1. Let the corrector be of order p*, then the approximation y_{n+1} generated by the PDIRK method {(2.5),(2.2),(2.6)} has order min{p*,m+1} for all matrices B and E, order min{p*,m+2} if (E+B)e=Ae, and order min{p*,m+3} if, in addition, $BA\mathbf{e}=A^2\mathbf{e}$. □

We remark that correctors of any order are explicitly available. Correctors of any even order p* are provided by the p*/2-stage Gauss-Legendre methods and correctors of any odd order p* are provided by the (p*+1)/2-stage Radau methods.

2.2. Stiffly Accurate PDIRK Methods

As was discussed by Alexander [1], when integrating stiff equations it may be advantageous to use RK methods {A,**b**} of which **b** equals the last row of A, i.e., $\mathbf{b}^T=\mathbf{e}_s^TA$, where s is the number of stages of the RK method. Such RK methods were termed *stiffly accurate* in [1]. Therefore, it is of interest to look for PDIRK methods possessing the property of stiff accuracy. Formally, we can associate with any PDIRK method a new PDIRK method possessing the property of stiff accuracy, simply by replacing (2.6) with

(2.7) $y_{n+1} = \mathbf{e}_s^T\mathbf{Y}^{(m)}$.

Of course, this only yields a feasible method if the last component of the vector $\mathbf{Y}^{(m)}$ provides an approximation to y_{n+1}. For example, this is true if the corrector itself is stiffly accurate, i.e., $\mathbf{b}^T=\mathbf{e}_s^TA$. We shall call the two versions corresponding to (2.6) and (2.7) PDIRK methods of Type I and II, and denote them by $PDIRK^I$ and $PDIRK^{II}$, respectively. Thus,

Type I : PDIRK method {(2.5'),(2.2'),(2.6)}
Type II : PDIRK method {(2.5'),(2.2'),(2.7)}.

The following theorem is the analogue of Theorem 2.1:

Theorem 2.2. Let the corrector be stiffly accurate ($\mathbf{b}^T=\mathbf{e}_s^TA$) and be of order p*, then the approximation y_{n+1} generated by the $PDIRK^{II}$ method is also stiffly accurate, and has order min{p*,m} for all matrices B and E, order min{p*,m+1} if (E+B)e=Ae, and order min{p*,m+2} if, in addition, $BA\mathbf{e}=A^2\mathbf{e}$. □

2.3. Various Types of PDIRK Methods and Their Butcher Arrays

Given the generating RK method (corrector) {A,**b**} defined by (2.1), we shall investigate three special families of PDIRK methods, either of Type I or of Type II, which differ from each other by the way in which the predictor is defined, i.e., in choosing the matrices B and E. Let O denote the s-by-s matrix with zero entries, then we distinguish:

Type A : Last-step-value predictor	(E=B=O)	$Y^{(0)} := y_n e$
Type B : Backward Euler predictor	(E=O, B=D)	$Y^{(0)} := y_n e + hDf(Y^{(0)})$
Type C : Theta method predictor	(B=D)	$Y^{(0)} := y_n e + hEf(y_n e) + hDf(Y^{(0)})$.

Notice that the matrix B either vanishes or is chosen equal to D. Although, in general, B and D may be different (diagonal) matrices, the particular choice B=D has advantages with respect to the implementation of the method. Typically for stiff equations, the implicit relations in which the matrix $D=\mathrm{diag}(d_1,d_2,...,d_s)$ is involved, will be solved by some form of Newton iteration, which requires (in the case of systems of ODEs) the LU-decomposition of the matrices $I - d_i\, h\, \partial f/\partial y$. Clearly, if B=D then these decompositions can also be used in solving the predictor (see also the discussion below). In the remainder of this paper, the analysis is performed in terms of a general matrix B and concrete results are only specified for B=O or B=D.

For future reference, we specify the various PDIRK^I families of methods in terms of their Butcher arrays and give the corresponding orders of accuracy p^I:

Type IA

j=0	O
j=1	A-D D
j=2	O A-D D
j=3	O O A-D D
.	. . . .
.	. . . .
.	. . . .
j=m	O . . . O A-D D
	0^T . . . 0^T 0^T b^T

1. $D \neq O$: $p^I = \min\{p^*, m+1\}$

Type IB

j=0	D
j=1	A-D D
j=2	O A-D D
j=3	O O A-D D
.	. . . .
.	. . . .
.	. . . .
j=m	O . . . O A-D D
	0^T . . . 0^T 0^T b^T

1. $D \neq O$: $p^I = \min\{p^*, m+1\}$
2. $D := \mathrm{diag}(Ae)$: $p^I = \min\{p^*, m+2\}$

Type IC

	O
j=0	E D
j=1	O A-D D
j=2	O O A-D D
.	. . . .
.	. . . .
.	. . . .
j=m	O . . . O A-D D
	0^T . . . 0^T 0^T b^T

1. $D \neq O$, $E \neq O$: $p^I = \min\{p^*, m+1\}$
2. $D := \mathrm{diag}(Ae-Ee)$, $E \neq O$: $p^I = \min\{p^*, m+2\}$
3. $D := \mathrm{diag}(Ae-Ee)$, $DAe = A^2e$: $p^I = \min\{p^*, m+3\}$

In these arrays, **0** denotes the s-dimensional nullvector. Type II versions are obtained by defining y_{n+1} by means of (2.7) instead of by (2.6), and, if the weights of the corrector satisfy $\mathbf{b}^T = e_s^T A$, then by virtue of Theorem 2.2, we may replace p^I by p^{II} and m by m-1. Notice that the **b**-vector is not actually needed if the algorithm is based on Type II methods. Furthermore, we remark that methods of Type B.2 are completely determined by the generating corrector, and that those of Type C.3 prescribe the matrix D and the row sums of the matrix E.

As already observed, PDIRK methods all belong to the class of DIRK methods (since the name DIRK is not consistently used in the literature, we remark that we shall call an RK method of DIRK type if the strict upper triangular part of its Butcher tableau vanishes). Moreover, the ith processor (i=1,2,...,s) is faced with solving a sequence

of implicit relations in each of which the decomposition of the matrix $I - d_i h \partial f/\partial y$ is required (in case of systems of ODEs). Since this decomposition can be used in all m iterations in (2.2), we shall say that PDIRK methods are *singly* diagonally implicit RK methods (SDIRK methods). Here we remark that this terminology is often reserved for methods in which *all* stages are implicit with the same diagonal entry in their Butcher array. However, the zero diagonal entries in PDIRK methods of the Types A and C (originating from B=O) do not exclude these methods from the class of SDIRK methods, since these zeros mean that $f(y_n)$ has to be evaluated prior to the iteration process. Because the bulk of the computational effort per step consists in solving the implicit relations, the costs of this explicit stage are relatively negligible.

Therefore, taking parallelism into account, we shall say that PDIRK methods require k *sequential stages* if each processor has to solve k implicit relations per step. Thus, Type A methods require m sequential stages, whereas for Type B and Type C methods this number is given by m+1.

Finally, we observe that if the diagonal matrix D has *equal* diagonal entries, then all processors need the same LU-decomposed matrix in their solution processes. In such cases, this decomposition, as well as the evaluation of the Jacobian matrix $\partial f/\partial y$, may be performed by an additional processor, providing a 'fresh' decomposition for *all* processors as soon as it is available.

3. STABILITY

Applying the PDIRK method to the test equation

$$y'(t) = \lambda y(t), \tag{3.1}$$

yields a relation of the form

$$y_{n+1} = R_m(z) y_n,$$

where $z := \lambda h$ and $R_m(z)$ is a rational function, the so-called *stability function*. The stability functions corresponding to $PDIRK^I$ and $PDIRK^{II}$ methods will be denoted by $R^I_m(z)$ and $R^{II}_m(z)$, respectively. They can be directly derived from the Butcher arrays by using the familiar 'determinant formula' (cf., e.g., [6, p.72]). However, the dimension of these arrays is usually so high that the evaluation of the determinants is rather tedious, even for small values of the number of iterations m. Therefore, we shall derive alternative formulas.

From (2.6) and (2.7) we see that the stability functions are respectively determined by

$$y_{n+1} = y_n + z\mathbf{b}^T\mathbf{Y}^{(m)} = R^I_m(z) y_n \quad \text{and} \quad y_{n+1} = \mathbf{e}_s^T \mathbf{Y}^{(m)} = R^{II}_m(z) y_n. \tag{3.2}$$

In order to derive an expression for $\mathbf{Y}^{(m)}$ we write

$$\mathbf{Y}^{(j)} = [I - zD]^{-1} Q_j y_n \mathbf{e},$$

where the matrix Q_j follows from

$$\mathbf{Y}^{(j)} = [I - zD]^{-1}\left[y_n\mathbf{e} + z(A - D)\mathbf{Y}^{(j-1)}\right] = [I - zD]^{-1}\left[y_n\mathbf{e} + z(A - D)[I - zD]^{-1} Q_{j-1} y_n \mathbf{e}\right].$$

Introducing the matrix function

$$Z = Z(z) := z(A - D)(I - zD)^{-1},$$

we find that Q_j satisfies the recursion

$$Q_0 = [I - zD][I - zB]^{-1}[I + zE], \quad Q_j = I + ZQ_{j-1}.$$

Hence, the stability functions

$$\begin{aligned} &R^I_m(z) = 1 + z\mathbf{b}^T[I - zD]^{-1} Q_m(z)\mathbf{e}, \quad R^{II}_m(z) = \mathbf{e}_s^T[I - zD]^{-1} Q_m(z)\mathbf{e}, \\ &Q_m = Q_m(z) := I + Z + Z^2 + \ldots + Z^{m-1} + Z^m[I - zD][I - zB]^{-1}[I + zE]. \end{aligned} \tag{3.3}$$

We shall separately consider the case where the diagonal matrices B and D have *constant* diagonal elements, and the case where the matrices B and D are *arbitrary* diagonal matrices.

3.1. PDIRK Methods with Constant Diagonal Elements

If B=bI and D=dI, then the matrix $Q_m(z)$ can be written as

$$Q_m(z) = \frac{N_m(z)}{(1 - bz)(1 - dz)^{m-1}},$$

where $N_m(z)$ is a polynomial in z with matrix-valued coefficients. Thus, (3.3) becomes

$$(3.4) \qquad R^{I}_m(z) = 1 + \frac{b^T z N_m(z) e}{(1 - bz)(1 - dz)^m}, \qquad R^{II}_m(z) = \frac{e_s^T N_m(z) e}{(1 - bz)(1 - dz)^m}.$$

This representation shows that both stability functions are of the form

$$(3.5a) \qquad R(z) := (1 - dz)^{-q} P(dz), \qquad P(dz) := \sum_{j=0}^{r} c_j (dz)^j,$$

where the coefficients c_j depend on q and d (recall that either b=0 or b=d). For future reference, it is convenient to specify the values of r and q for the various types of methods. In Table 3.1 these values are listed for general values of d.

Table 3.1. Values of r and q in the stability function (3.5a).

Type	IA	IB	IC	IIA	IIB	IIC
r =	m+1	m+1	m+2	m	m	m+1
q =	m	m+1	m+1	m	m+1	m+1

For an arbitrary given value of d the order of consistency of the stability function (3.5a) cannot exceed r, hence, by choosing m such that the order p of the PDIRK method equals r, we achieve that the number of sequential stages is minimal with respect to the order p.

3.1.1. Derivation of A-acceptable and L-acceptable stability functions. The following theorem defines an explicit representation of the stability function.

Theorem 3.1. Let p be the order of the method and let m be such that r=p, then the coefficients of (3.5a) are given by

$$(3.5b) \qquad c_j = \sum_{i=0}^{j} \binom{q}{j-i} \frac{(-1)^{j-i}}{i! d^i}, \quad j = 0, 1, \ldots, q; \qquad c_j = \sum_{i=0}^{q} \binom{q}{i} \frac{(-1)^i}{(j-i)! d^{j-i}}, \quad j = q+1, q+2, \ldots, p,$$

where 0! := 1.

Proof. Since it is assumed that the method is of order p we necessarily have $R(z)=\exp(z)+O(z^{p+1})$. By expanding the function $(1 - dz)^q \exp(z)$ in a Taylor series at z=0 and by equating corresponding coefficients in this expansion and in the polynomial P(z), defined in (3.5a), we can find the first p+1 coefficients of P. Hence, all coefficients of P are uniquely determined and are given by (3.5b) (see also Nørsett [11] and Butcher [2, p. 246] for expressions in terms of derivatives of Laguerre polynomials). □

Notice that the condition r=p excludes methods of Type C.1, because for Type I and Type II variants the maximal order is m+1 and m, respectively, which is one lower than the corresponding value of r. As a consequence, for methods of Type C with stability functions of the form (3.5) the order should be increased by one, which is obtained by requiring the matrix E to satisfy the condition Ee=Ae-de.

By means of Theorem 3.1 the stability analysis is now rather straightforward. Following Nørsett [12] and Butcher [2], we write $u=y^2$ and define the so-called E-polynomial

$$E(u) := |(1 - iy)^q|^2 [1 - |R(iy/d)|^2] = |(1 - iy)^q|^2 - |P(iy)|^2$$

$$= (1 + u)^q - [c_0 - c_2u + c_4u^2 - \dots]^2 - u[c_1 - c_3u + c_5u^2 - \dots]^2.$$

From the condition $R(z)=\exp(z)+O(z^{p+1})$ it follows that $|R(iy/d)|^2=1+O(y^{p+1})$, so that $E(y^2)=O(y^{p+1})$. Hence, all terms of $E(y^2)$ of degree less than p+1 in y vanish, so that

$$E(u) = \sum_{j=[p/2]+1}^{q} e_j u^j, \quad e_j = e_j(d) := \binom{q}{j} - c_j^2 - 2\sum_{i=1} (-1)^i c_{j-i}c_{j+i}, \quad c_j := 0 \text{ if } j > p \text{ or } j < 0.$$

Because of the maximum principle, we have A-stability if $|R(iy)|$ is bounded by 1 for all real y, so that the method is A-stable if, and only if, E(u) is nonnegative for $u \geq 0$.

Values of d for which R(z) is A-acceptable will be called A-acceptable. Let the range of d-values which are A-acceptable be denoted by I_{pq}, i.e., $I_{pq}:=\{d: E(u)\geq 0 \text{ for all } u\geq 0\}$, then the following survey is easily obtained by using Table 3.1 and the order results obtained for the various types of methods (p* denotes the order of the corrector {A,**b**}):

Table 3.2. Survey of properties of PDIRK methods with constant diagonal elements.

Type	Condition	Order	Sequential stages	A-acceptable d-values
IA.1	$m\leq p^*-1$	m+1	m	$I_{m+1,m}$
IB.1	$m\leq p^*-1$	m+1	m+1	$I_{m+1,m+1}$
IC.2	$m\leq p^*-2$	m+2	m+1	$I_{m+2,m+1}$
IIA.1	$m\leq p^*$	m	m	$I_{m,m}$
IIB.1	$m\leq p^*$	m	m+1	$I_{m,m+1}$
IIC.2	$m\leq p^*-1$	m+1	m+1	$I_{m+1,m+1}$

Notice that R(z) is L-acceptable if R(z) is A-acceptable and if q>p. From Table 3.2 we see that the methods of Type IIB.1 possess L-acceptable stability functions. Since L-stable methods are usually more suitable for integrating stiff equations than A-stable methods, the methods of Type IIB.1 are of interest in spite of the additional sequential stage when compared with the other methods. However, just as in the case of SDIRK methods, it is possible that an A-stable method can be made L-stable if the interval of A-acceptable d-values contains a value for which c_p vanishes. For $q=p\leq 15$, this has been investigated by Wolfbrandt [13] and it was found that such values of d exist for $p\leq 6$ and p=8. This information is summarized in Table 3.3a.

In a similar way, L-acceptable ranges of d-values can be found in the case q=p+1. These ranges turn out to be nonempty for $p\leq 8$ and for p=10, and are given in Table 3.3b. Moreover, we list the values of $d_{p,p+1}$, which are inside these L-acceptable ranges and cause c_p to vanish, resulting in even stronger damping at 'infinity'.

Finally, we considered the case q=p-1, resulting from IA.1 and IC.2 type methods. Since now the degree of the numerator in R(z) is larger than that of the denominator, a necessary condition for this case to yield A-stability, is that c_p vanishes. For p=2,3,...,10 we determined the zeros of $c_p(d)$ and checked the resulting stability function on A-acceptability. Only for p=2 (d=1/2), p=3 ($d=(3+\sqrt{3})/6$) and p=4 (d=1.0685790213) A-stability can be obtained. Hence, in this way we have found A-stable methods of orders p up to 4 requiring p-1 sequential stages. This result is similar to what is possible in the case of RK methods for sequential computers (cf. [1]); however, the present methods contain embedded formulas of lower order.

Table 3.3a. A-acceptable and L-acceptable values of d for p=q.

p = q	Range I_{pp}	d_{pp}
1	[1/2, ∞]	1
2	[1/4, ∞]	$1\pm\sqrt{1/2}$
3	[1/3, 1.068]	0.43586650
4	[0.395, 1.280]	0.5728160625
5	[0.247, 0.361] + [0.421,0.473]	0.2780538410
6	[0.285, 0.54]	0.3341423671
7	empty	
8	[0.218, 0.264]	0.2343731596
9	empty	
10	empty	

Table 3.3b. Ranges of L-acceptable values of d for p=q-1.

p = q -1	Range $I_{p,p+1}$	$d_{p,p+1}$
1	$[1-\sqrt{1/2},\ 1+\sqrt{1/2}]$	0.5
2	[0.181, 2.185]	$0.5\pm\sqrt{1/12}$
3	[0.224, 0.572]	0.3025345782
4	[0.248, 0.676]	0.3888576711
5	[0.184, 0.334]	0.2168805435
6	[0.205, 0.378]	0.2579552416
7	[0.157, 0.2029]+[0.2052, 0.234]	0.1690246379
8	[0.171, 0.259]	0.1929778040
9	empty	
10	[0.147, 0.165]+[0.1938, 0.1961]	0.1541460739

Notice that any s-stage, pth-order corrector (even explicit corrector methods) can be used for generating A-stable methods of Type IB, and any pth-order corrector satisfying the condition $\mathbf{b}^T=\mathbf{e}_s^TA$ for generating the A-stable methods of Type IIA and IIC, or the L-stable methods of Type IIB.

Furthermore, we have seen that the stability can be improved by selecting special d-values. Another possibility, which might be useful in a variable-stepsize implementation, is to exploit the *length* of the A- and L-acceptable ranges: for small changes in the stepsize h, the value of hd could be kept fixed (as long as the corresponding d-value is still in the allowed range, of course), so that a new decomposition of $I - h\,d\,\partial f/\partial y$ can be avoided.

3.1.2. Comparison of diagonally implicit methods. It may be of interest to compare the characteristics of a number of SDIRK methods from the literature with those of the PDIRK methods constructed in this section. In the comparison presented by Table 3.4, DIRKII denote the Type II methods of Iserles and Nørsett [9] which are, like all PDIRK methods of this paper, *effectively* singly diagonally implicit on multi-processor computers. Furthermore, the order range of the embedded methods, if any, is denoted by p_{emb}.

Table 3.4. Comparison of DIRK methods of order p≥3.

Method	Order	Stages	Seq. stages	Processors	Stability	p_{emb}	Reference/Specification
SDIRK	p=3	p-1	p-1	1	A-stable		Nørsett [11]
SDIRK	p=4	p-1	p-1	1	A-stable		Crouzeix [5], Alexander [1]
SDIRK	p=3	p	p	1	S-stable	<p	Cash [3], Cash & Liem [4]
SDIRK	p=4	p+1	p+1	1	S-stable	<p	Cash [3], Cash & Liem [4]
DIRKII	p=4	p	p-2	2	L-stable	p-1	Iserles & Nørsett [9]
PDIRK	p≤4	(p-1)s	p-1	[(p+1)/2]	A-stable	<p	Type IA.1 & IC.2, D=dI
PDIRK	p≤6	ps	p	[(p+1)/2]	L-stable	<p	Type IIA.1, D=dI
PDIRK	p=8	ps	p	[(p+1)/2]	L-stable	<p	Type IIA.1, D=dI
PDIRK	p≤8	(p+1)s	p+1	[(p+1)/2]	L-stable	<p	Type IIB.1, D=dI
PDIRK	p=10	(p+1)s	p+1	[(p+1)/2]	L-stable	<p	Type IIB.1, D=dI

3.1.3. Numerical experiment. It is well known [6] that, when integrating general stiff systems, the actually observed order is usually much lower than the *classical order* p. In fact, the order behaviour is often dictated by the so-called *stage order* r (for a definition of this notion and its consequences the reader is referred to [6]). Since most (P)DIRK methods have stage order r=1, one might question the relevance of PDIRK methods possessing a high classical order. And indeed, for a general stiff problem, this order reduction phenomenon has great impact on the accuracy of this type of methods.

However, in [7], Hairer et al. give a thorough analysis of the behaviour of RK methods when applied to a singular perturbed problem of the form

3.6) $\varepsilon \frac{dy_1}{dt} = f_1(y_1,y_2), \qquad \frac{dy_2}{dt} = f_2(y_1,y_2), \qquad$ with $\varepsilon << 1$,

ınd show that for special RK methods the classical order may still dominate the global error, especially if stiffness ncreases (i.e., if $\varepsilon \to 0$). The motivation to consider this particular problem class is that it has practical significance and ıas been extensively studied in the literature (see the references cited in [7]). An important characteristic of problems of he form (3.6) is that the eigenvalues of the Jacobian matrix can be clustered into two groups, and behave as O(1) and $O(\varepsilon^{-1})$, respectively. Here we summarize the main result of [7] (cf. Theorem 1 on p. 680) concerning the global error:

Let the RK method be A-stable and let $\varepsilon \leq$ Constant·h. Then the global error for the stiff component y_1 behaves as $O(\varepsilon h^r) + O(h^p)$ if $\mathbf{b}^T = \mathbf{e}_s^T A$ and as $O(h^{r+1})$ if $|R(\infty)|<1$. For both cases, the global error for the nonstiff component y_2 behaves as $O(\varepsilon h^{r+1}) + O(h^p)$.

This result indicates that Type II methods are to be preferred if $\varepsilon \to 0$, since then the global error is dominated by the classical order, whereas methods of Type I will behave according to their (low) stage order.

To illustrate these properties, we applied the PDIRK methods listed in Table 3.4 to a problem of the form (3.6), proposed by Kaps [10]:

3.6') $\frac{dy_1}{dt} = -(2 + \varepsilon^{-1})y_1 + \varepsilon^{-1} y_2, \quad \frac{dy_2}{dt} = y_1 - y_2(1 + y_2), \quad y_1(0) = y_2(0) = 1, \ 0 \le t \le 1,$

with the smooth exact solution $y_1 = \exp(-2t)$ and $y_2 = \exp(-t)$ for all values of the parameter ε.
The methods we have used in our tests are based on correctors of different classical order (a specification of these correctors can be found in the Appendix). Moreover, all methods were equipped with the special d_{pp} or $d_{p,p+1}$ values given in the Tables 3.3 and, consequently, are L-stable.

For $\varepsilon = 10^{-8}$ the absolute error for the stiff component y_1 at the end point t=1 is given in Table 3.5; here, the error is written in the form $10^{-\Delta}$ and the values of Δ are listed. Notice that the Type II methods require a stiffly accurate corrector (such as the Radau IIA formulas) and that L-stable, seventh-order PDIRK methods are only possible within the family of Type IIB.1 methods (cf. Tables 3.2 and 3.3b). This table clearly demonstrates the superiority of the stiffly accurate Type II methods over the Type I methods, which show only a second-order behaviour for the global error (recall that r=1 for the Type IB.1 methods). However, the stiffly accurate methods demonstrate the classical order in the error behaviour and thus both results are in perfect agreement with the estimates in the theorem of Hairer et al.

From this experiment we may conclude that it is relevant indeed to have high-order PDIRK methods for integrating stiff systems of the form (3.6), in spite of their low stage order.

Comparing the efficiency of the various parallel methods of Type II, we observe that schemes of Type A and C are equally efficient, since they require the same number of sequential stages (cf. Table 3.2). The Type IIB.2 methods yield slightly more accurate results, but need an additional stage to reach the same order (we remark that the seventh-order method of this type does not show full advantage, since the integration process was impeded by the machine precision which is approximately $7 \cdot 10^{-14}$ on our machine).

Table 3.5. Values of Δ at t=1 for the first component of problem (3.6') with $\varepsilon = 10^{-8}$.

Type	Corrector	Order	h=1/4	h=1/8	h=1/16	h=1/32	h=1/64	Seq. Stages per step	Number of Processors
IB.1	Radau IIA	3	3.7	4.1	4.6	5.2	5.8	3	2
	Gauss-Legendre	4	2.9	3.6	4.2	4.8	5.4	4	2
	Explicit Runge-Kutta	4	3.0	3.7	4.3	4.9	5.5	4	4
	Radau IIA	5	3.6	4.3	4.9	5.5	6.1	5	3
	Gauss-Legendre	6	3.1	3.7	4.4	5.0	5.6	6	3
IIA.1	Radau IIA	3	4.0	4.9	5.8	6.7	7.6	3	2
	Radau IIA	5	6.9	8.4	9.8	10.6	11.0	5	3
IIB.1	Radau IIA	3	4.3	5.2	6.1	7.0	7.9	4	2
	Radau IIA	5	7.2	8.7	10.3	11.8	11.8	6	3
	Radau IIA	7	9.7	10.2	10.6	10.9	11.2	8	4
IIC.2	Radau IIA	3	4.0	4.9	5.8	6.7	7.6	3	2
	Radau IIA	5	6.9	8.4	9.8	10.6	11.0	5	3

3.2. PDIRK Methods with Arbitrary Diagonal Matrices

In the case where B and D are allowed to be arbitrary diagonal matrices, it is convenient to express $Q_m(z)$ in the form

$$Q_m(z) = [I - Z]^{-1}[I - Z^m] + Z^m Q_0 = [I - Z]^{-1}[I - Z^m] + Z^m[I - zD][I - zB]^{-1}[I + zE].$$

Since $[I-zD]^{-1}=[I-zA]^{-1}[I-Z]$, we find

$$Q_m(z) = [I - zD][I - zA]^{-1}\left[I - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right],$$

so that (3.3) yields

$$\begin{aligned} R^I_m(z) &= 1 + z\mathbf{b}^T[I - zA]^{-1}\left[I - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right]\mathbf{e}, \\ R^{II}_m(z) &= \mathbf{e}_s^T[I - zA]^{-1}\left[I - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right]\mathbf{e} \\ &= 1 + \mathbf{e}_s^T[I - zA]^{-1}\left[zA - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right]\mathbf{e}. \end{aligned} \tag{3.3'}$$

In the following two subsections, a representation for the stability functions without inverses of matrices will be given and stability characteristics of PDIRK methods of the Types IB.2, IIB.2 and IIC.3 are presented.

3.2.1. Representation theorems. The following theorem gives a representation of the stability functions in terms of determinants only containing inverses of diagonal matrices:

Theorem 3.2. The stability functions (3.3') can be represented by

$$\begin{aligned} R^I_m(z) &= \frac{\det\left\{I - zA + z\left[I - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right]\mathbf{e}\mathbf{b}^T\right\}}{\det\{I - zA\}}, \\ R^{II}_m(z) &= \frac{\det\{I - zA + \left[zA - Z^m + [I - Z]Z^m[I - zD][I - zB]^{-1}[I + zE]\right]\mathbf{e}\mathbf{e}_s^T\}}{\det\{I - zA\}}. \end{aligned} \tag{3.7}$$

Proof. Applying the identity

$$1 + \mathbf{x}^T N^{-1}\mathbf{y} = \frac{\det\{N + \mathbf{y}\mathbf{x}^T\}}{\det\{N\}},$$

to the stability functions (3.3') straightforwardly leads to the representations (3.7). □

The expressions (3.7) can be simplified for the respective Types A, B and C:

Corollary 3.1. Let the matrix Z be given by $Z = z(A-D)(I-zD)^{-1}$, then the following assertions hold:
(a) The stability function of PDIRK methods of Type A.1 are given by

$$R^I_m(z) = \frac{\det\left\{I - zA + z[I - zZ^m A]\mathbf{e}\mathbf{b}^T\right\}}{\det\{I - zA\}}, \quad R^{II}_m(z) = \frac{\det\left\{I - zA + z[I - Z^m]A\mathbf{e}\mathbf{e}_s^T\right\}}{\det\{I - zA\}}. \tag{3.8a}$$

(b) The stability function of PDIRK methods of Type B are given by

$$R^I_m(z) = \frac{\det\left\{I - zA + z[I - Z^{m+1}]\mathbf{e}\mathbf{b}^T\right\}}{\det\{I - zA\}}, \quad R^{II}_m(z) = \frac{\det\left\{I - zA + [zA - Z^{m+1}]\mathbf{e}\mathbf{e}_s^T\right\}}{\det\{I - zA\}}. \tag{3.8b}$$

(c) The stability function of PDIRK methods of Type C.2 or Type C.3 are given by

$$(3.8c)\qquad R^{I}_{m}(z) = \frac{\det\{I - zA + z[I - zZ^{m+1}A]\mathbf{e}\mathbf{b}^{T}\}}{\det\{I - zA\}}\,,\; R^{II}_{m}(z) = \frac{\det\{I - zA + z[I - Z^{m+1}]A\mathbf{e}\mathbf{e}_{s}^{T}\}}{\det\{I - zA\}}\,. \;\square$$

Notice that these expressions do not explicitly depend on E and B anymore and are completely determined by the corrector and the matrix Z.

3.2.2. Stability characteristics. In this subsection, we consider the stability of PDIRK methods. We shall distinguish between methods based on Radau IIA correctors and on Gauss-Legendre correctors.

The Radau IIA correctors have order p=2s-1, where s is the number of stages, and satisfy the condition $\mathbf{b}^{T}=\mathbf{e}_{s}^{T}A$ (their Butcher arrays for s=1,...,4 are given in the Appendix). Due to this property, PDIRK methods of Type I and Type II are both relevant. We confine our considerations to types which require (with respect to their order) less sequential stages than the corresponding methods indicated in Table 3.2, that is, we consider methods of the Types IB.2, IIB.2 and IIC.3. For these types of methods, the stability functions are completely determined. In Table 3.6, we present a survey of the characteristics of these methods for several orders. Based on the stability functions (3.8), the stability region of the methods was determined numerically. It turned out that some stability functions are only A(α)-acceptable. However, in these cases α is very close to 90° (in the Appendix, a set of stability regions is given, including the regions of the embedded lower order methods).

Furthermore, we considered PDIRK methods based on Gauss-Legendre correctors. Such s-stage correctors have order 2s, but are not stiffly accurate and hence, only Type I methods are relevant. In Table 3.6 we have included the characteristics of fourth- and sixth-order methods of Type IB.2 (the generating correctors can be found in [2, p. 219]).

Table 3.6. Characteristics of PDIRK methods based on arbitrary B and D matrices

Type	Corrector	Order	Seq.Stages	Processors	Stability
IB.2	Radau IIA	3	2	2	Strongly A-stable
	Gauss-Legendre	4	3	2	Strongly A-stable
	Radau IIA	5	4	3	Strongly A-stable
	Gauss-Legendre	6	5	3	Strongly A(α)-stable, α=89.97°
	Radau IIA	7	6	4	Strongly A(α)-stable, α=83.3°
IIB.2	Radau IIA	3	3	2	L(α)-stable, α=89.75°
	Radau IIA	5	5	3	L(α)-stable, α=89.12°
	Radau IIA	7	7	4	L(α)-stable, α=89.02°
IIC.3	Radau IIA	3	2	2	A-stable
	Radau IIA	5	4	3	A(α)-stable, α=89.997°
	Radau IIA	7	6	4	A(α)-stable, α=89.95°

In comparison with the PDIRK methods constructed in Section 3.1, we observe that the above PDIRK methods of Type IB.2 and IIC.3 require one sequential stage less to obtain a given order of accuracy. Moreover, with the exception of the 7th-order method of Type IB.2, these methods possess almost the same good stability properties.

For the methods of Type IIB.2 (for which the order equals the number of sequential stages), only the seventh-order is relevant, since in Section 3.1 it turned out to be impossible to construct an L-stable method of order 7 with 7 sequential stages; the third- and fifth-order methods of Type IIB.2 do not have an advantage over the L-stable methods described in Section 3.1.

3.2.3. Numerical experiment. We conclude this section by applying the methods specified in the above table to the problem (3.6'). Using the same notation as described in Section 3.1.3, the results are given in Table 3.7.

Again, the stiffly accurate Type II methods are much more efficient than the methods of Type I. Moreover, the order behaviour nicely illustrates the results of the theorem of Hairer et al. (cf. Section 3.1.2). Furthermore, within the class of stiffly accurate methods, the C-variant is superior to the B-variant, since it is cheaper and yields, for this example, more accuracy.

Table 3.7. Values of Δ at t=1 for the first component of problem (3.6') with $\varepsilon=10^{-8}$.

Type	Corrector	Order	h=1/4	h=1/8	h=1/16	h=1/32	h=1/64	Seq. Stages per step	Number of Processors
IB.2	Radau IIA	3	2.8	3.8	4.1	4.7	5.3	2	2
	Gauss-Legendre	4	2.7	3.4	4.0	4.6	5.3	3	2
	Radau IIA	5	2.4	2.8	3.4	4.1	4.8	4	3
	Gauss-Legendre	6	3.0	3.5	4.1	4.8	5.4	5	3
	Radau IIA	7	4.2	4.6	5.2	5.8	6.4	6	4
IIB.2	Radau IIA	3	3.4	4.1	4.9	5.8	6.7	3	2
	Radau IIA	5	4.9	6.1	7.5	9.0	10.4	5	3
	Radau IIA	7	6.4	8.2	10.1	11.9	12.5	7	4
IIC.3	Radau IIA	3	4.3	5.2	6.1	7.0	7.9	2	2
	Radau IIA	5	6.6	8.0	9.4	10.8	11.6	4	3
	Radau IIA	7	8.7	10.6	12.0	12.3	12.6	6	4

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REFERENCES

[1] **Alexander, R. (1977)**: Diagonally implicit Runge-Kutta methods for stiff ODEs, SIAM J. Numer. Anal. **14**, 1006-1021.

[2] **Butcher, J.C. (1987)**: The numerical analysis of ordinary differential equations, Runge-Kutta and general linear methods, Wiley, New York.

[3] **Cash, J.R. (1979)**: Diagonally implicit Runge-Kutta formulae with error estimates, J. Inst. Maths. Applics. **24**, 293-301.

[4] **Cash, J.R. & Liem, C.B. (1980)**: On the design of a variable order, variable step diagonally implicit Runge-Kutta algorithm, J. Inst. Maths. Applics. **26**, 87-91.

[5] **Crouzeix, M. (1975)**: Sur l'approximation des équations différentielles opérationnelles lineáires par des méthodes de Runge-Kutta, Ph. D. Thesis, Université de Paris.

[6] **Dekker, K. & Verwer J.G. (1984)**: Stability of Runge-Kutta methods for stiff nonlinear differential equations, CWI Monograph 2, North-Holland, Amsterdam-New York-Oxford.

[7] **Hairer, E., Lubich, Ch. & Roche, M. (1988)**: Error of Runge-Kutta methods for stiff problems studied via differential algebraic equations, BIT **28**, 678-700.

[8] **Houwen, P.J. van der & Sommeijer, B.P. (1988)**: Variable step iteration of high-order Runge-Kutta methods on parallel computers, Report NM-R8817, Centre for Mathematics and Computer Science, Amsterdam (to appear in J. Comp. Appl. Math.).

[9] **Iserles, A. & Nørsett, S.P. (1988)**: On the theory of parallel Runge-Kutta methods, Report DAMTP 1988/NA12, University of Cambridge.

[10] **Kaps, P. (1981)**: Rosenbrock-type methods, in: Numerical methods for stiff initial value problems, G. Dahlquist and R. Jeltsch (eds.), Bericht nr. 9, Inst. für Geometrie und Praktische Mathematik der RWTH Aachen.

[11] **Nørsett, S.P. (1974)**: Semi-explicit Runge-Kutta methods, Report Mathematics and Computation No.6/74, Dept. of Mathematics, University of Trondheim.

[12] **Nørsett, S.P. (1975)**: C-polynomials for rational approximation to the exponential function, Numer. Math. **25**, 39-56.

[13] **Wolfbrandt, A. (1977)**: A study of Rosenbrock processes with respect to order conditions and stiff stability, Ph. D. Thesis, Chalmers University of Technology, Göteborg.

APPENDIX

1. RADAU IIA CORRECTORS

First, we specify the A-matrices of the Radau IIA correctors underlying the Type II methods. For orders p*=3,5,7 and 9, the corresponding matrices are respectively given by

$$\text{(A.1)} \qquad A := \begin{pmatrix} \frac{5}{12} & \frac{-1}{12} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix},$$

$$\text{(A.2)} \qquad A := \begin{pmatrix} \frac{88 - 7\sqrt{6}}{360} & \frac{296 - 169\sqrt{6}}{1800} & \frac{-2 + 3\sqrt{6}}{225} \\ \frac{296 + 169\sqrt{6}}{1800} & \frac{88 + 7\sqrt{6}}{360} & \frac{-2 - 3\sqrt{6}}{225} \\ \frac{16 - \sqrt{6}}{36} & \frac{16 + \sqrt{6}}{36} & \frac{1}{9} \end{pmatrix},$$

$$\text{(A.3)} \qquad A := \begin{pmatrix} .11299947932316 & -.04030922072352 & .02580237742034 & -.0099046765073 \\ .23438399574740 & .20689257393536 & -.04785712804854 & .01604742280652 \\ .21668178462325 & .40612326386737 & .18903651817006 & -.02418210489983 \\ .22046221117677 & .38819346884317 & .32884431998006 & \frac{1}{16} \end{pmatrix},$$

$$\text{(A.4)} \qquad A := \begin{pmatrix} .07299886431790 & -.02673533110795 & .01867692976398 & -.01287910609331 & .00504283923388 \\ .15377523147918 & .14621486784749 & -.03644456890513 & .02123306311930 & -.00793557990273 \\ .14006304568481 & .29896712949128 & .16758507013525 & -.03396910168662 & .01094428874419 \\ .14489430810953 & .27650006876016 & .32579792291042 & .12875675325491 & -.01570891737881 \\ .14371356079123 & .28135601514946 & .31182652297574 & .22310390108357 & \frac{1}{25} \end{pmatrix}.$$

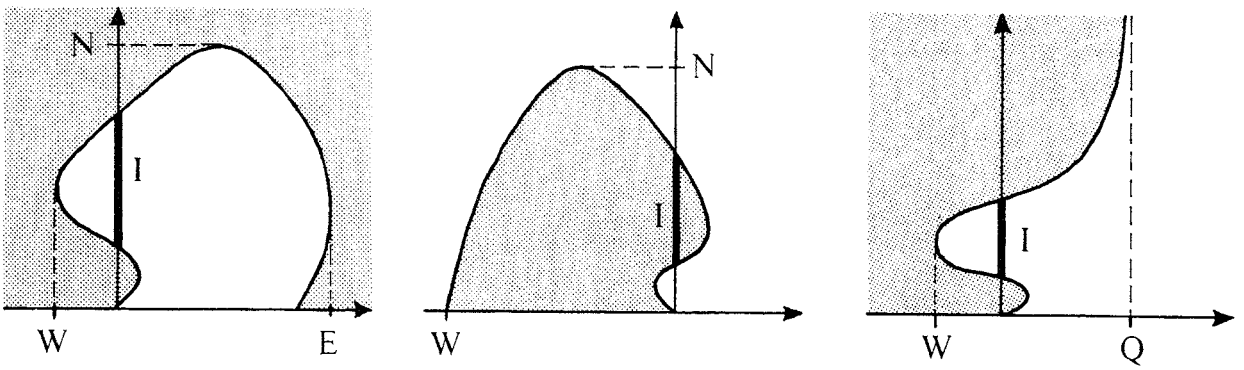
Recall that the weights of these RK methods are given by $\mathbf{b}^T=\mathbf{e}_s^T A$.

2. STABILITY PLOTS OF PDIRK METHODS.

Next, we give plots of the stability region of methods of Type IB.2, IIB.2 and IIC.3 based on Radau IIA correctors up to order seven, and of methods of Type IB.2 based on Gauss-Legendre correctors of order four and six. In these plots, the shaded area indicates the region where the method is stable.

For each method, we first made a plot using a rather coarse scale along the real and imaginary axis. Then, using a much finer scale, a further inspection was made of several parts of the complex plane, with emphasis on the neighbourhood of the origin and on points along the imaginary axis. Following this procedure, several methods were found to be only A(α)- or L(α)-stable, however with α close to 90°. When this situation happened to be the case for a particular method, we also provide a close-up, showing that part of the left half plane where the method is unstable. Moreover, for each method of order≤6, the plot of its stability region is preceded by plots of the stability regions of the embedded formulas. Finally, since the stability regions are symmetric with respect to the real axis, we confine ourselves to the upper halfplane.

It turned out that all stability regions have one of the following three characteristic forms:



Situation 1 Situation 2 Situation 3

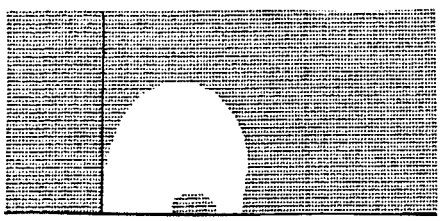
In these pictures some parameters have been introduced in order to adequately describe the size of the stability region:

in case of Situation 1 and 3, N, W and E can respectively be interpreted as the (projections of) the northern, western and eastern point of the region where the method is *unstable*; in the case of Situation 2, N and W have the same interpretation for the *stability* region.
I denotes the interval on the imaginary axis where the method is unstable (Situation 1 and 3) / stable (Situation 2).
Finally, Q is introduced to describe an *asymptotic behaviour* of the stability region (cf. Situation 3).
In the plots, only the relevant parameters will be specified.

2.1. Third-Order Methods Based on the Radau IIA Corrector of Order 3.
For all methods described in this subsection, the corrector is given in (A.1)

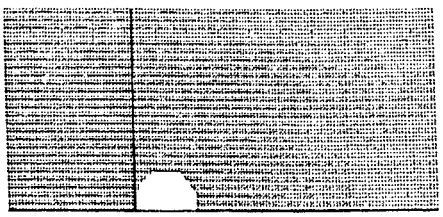
2.1.1. Methods of Type IB.2. For methods of this type the order is given by $p^I = \min\{3,m+2\}$.

m=0, N=5.4, W=-11.0, I=[0,0]

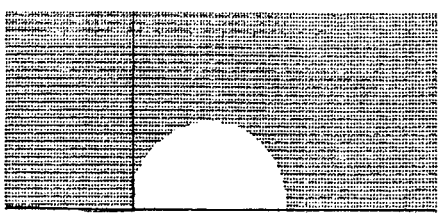


m=1, N=6.6, E=9.2, strongly A-stable

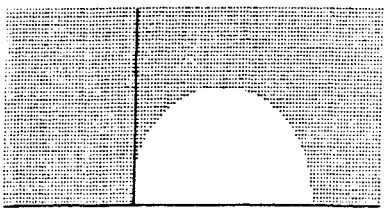
2.1.2. Methods of Type IIB.2. For methods of this type the order is given by $p^{II} = \min\{3,m+1\}$.



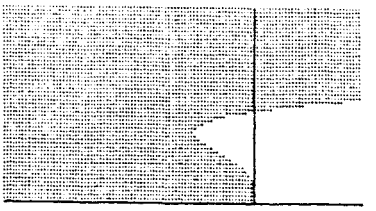
m=0, N=1.0, E=2.0, L-stable



m=1, N=2.3, E=4.6, L-stable

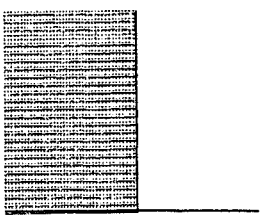


m=2, N=3.0, E=5.6, W=-0.02, I=(0,0.60)
L(α)-stable, α=89.75°

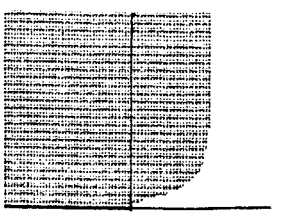


m=2, close-up

2.1.3. Methods of Type IIC.3. For methods of this type the order is given by $p^{II} = \min\{3,m+2\}$.



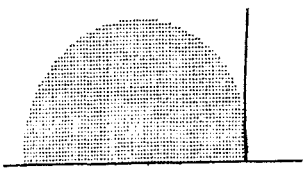
m=0, Q=0.0, A-stable



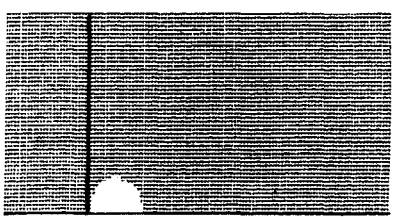
m=1, Q=0.50, A-stable

2.2. Fifth-Order Methods Based on the Radau IIA Corrector of Order 5.
For all methods described in this subsection, the corrector is given in (A.2)

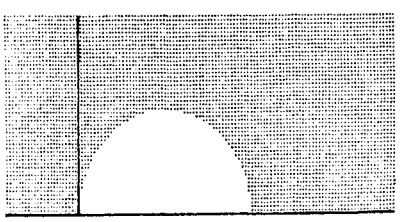
2.2.1. Methods of Type IB.2. For methods of this type the order is given by $p^{I} = \min\{5,m+2\}$.



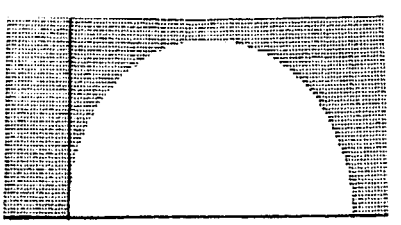
m=0, N=3.6, W=-6.8, I=[0,0]



m=1, N=10, E=17, strongly A-stable

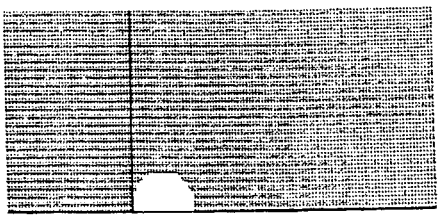


m=2, N=27, E=54, strongly A-stable

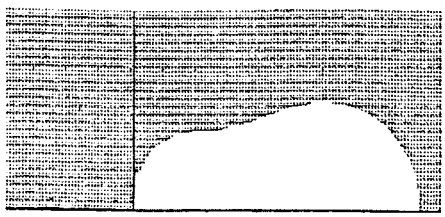


m=3, N=44, E=60, strongly A-stable

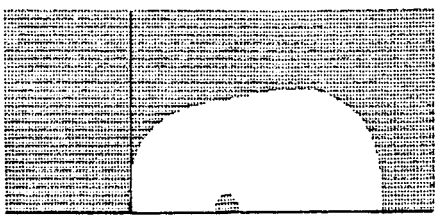
2.2.2. Methods of Type IIB.2. For methods of this type the order is given by $p^{II} = \min\{5,m+1\}$.



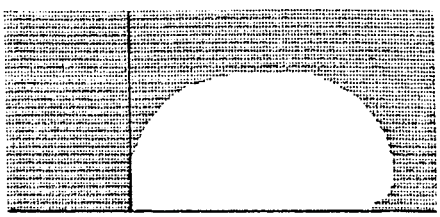
m=0, N=1.0, E=2.0, L-stable



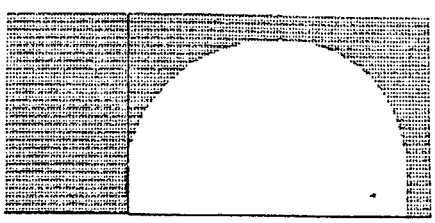
m=1, N=2.8, E=8.9, L-stable



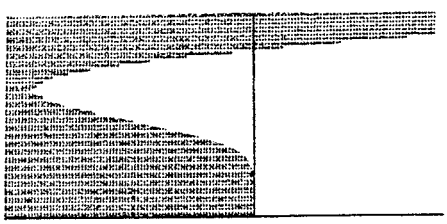
m=2, N=3.1, E=7.9, W=-2.0$_{10}$-4, I=(0,0.58)
L(α)-stable, α=89.98°



m=3, N=3.5, E=8.2, W=-0.008, I=(0,0.94)
L(α)-stable, α=89.31°

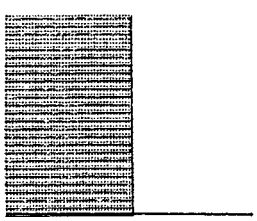


m=4, N=4.5, E=8.8, W=-0.015, I=(0.30,1.26)
L(α)-stable, α=89.12°

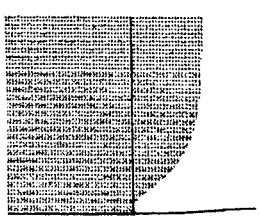


m=4, close-up

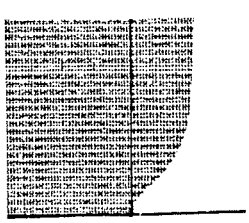
2.2.3. Methods of Type IIC.3. For methods of this type the order is given by $p^{II} = \min\{5,m+2\}$.



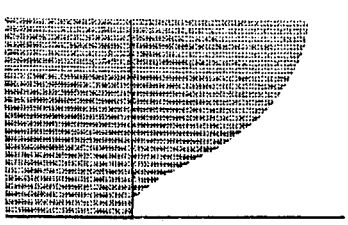
m=0, Q=0.0, A-stable



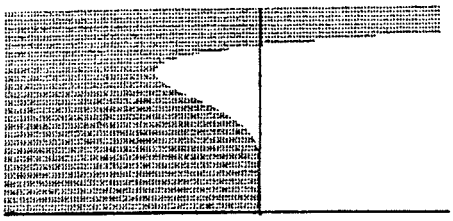
m=1, Q=2.3, A-stable



m=2, Q=2.1, A-stable



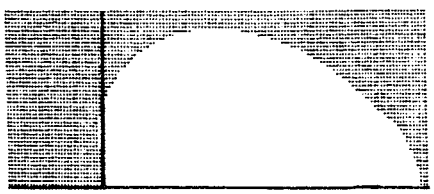
m=3, Q=6.3, W=-3.5$_{10}$-5, I=(0,0.82)
A(α)-stable, α=89.997°



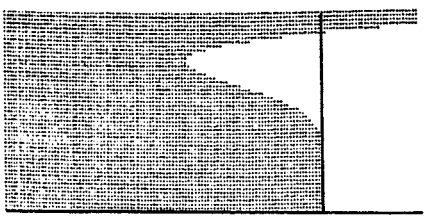
m=3, close-up

2.3. Seventh-Order Methods Based on the Radau IIA Corrector of Order 7.
For all methods described in this subsection, the corrector is given in (A.3)

2.3.1. Methods of Type IB.2. For methods of this type the order is given by $p^{I} = \min\{7,m+2\}$.

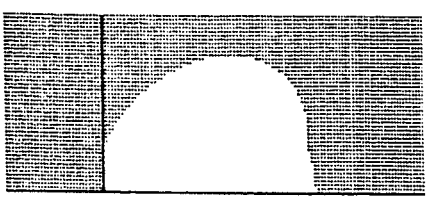


m=5, N=5.4, E=12.6, W=-0.21, I=(1.0,3.0)
strongly A(α)-stable, α=83.3°

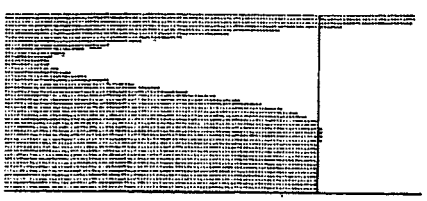


m=5, close-up

2.3.2. Methods of Type IIB.2. For methods of this type the order is given by $p^{II} = \min\{7,m+1\}$.

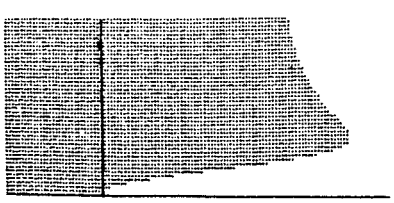


m=6, N=7.0, E=13.4, W=-0.022, I=(0.68,1.68)
L(α)-stable, α=89.02°

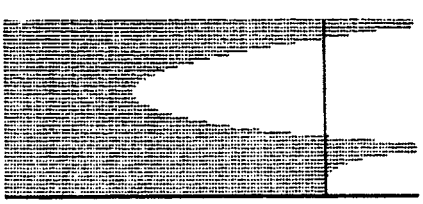


m=6, close-up

2.3.3. Methods of Type IIC.3. For methods of this type the order is given by $p^{II} = \min\{7,m+2\}$.



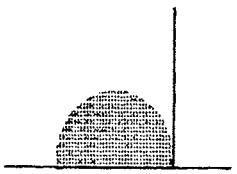
m=5, Q=5.5, W=-0.0011, I=(0.48,1.8)
A(α)-stable, α=89.95°



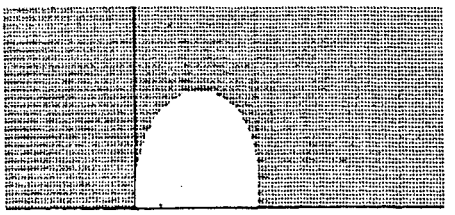
m=5, close-up

2.4. Fourth-Order Methods Based on the Gauss-Legendre Corrector of Order 4.

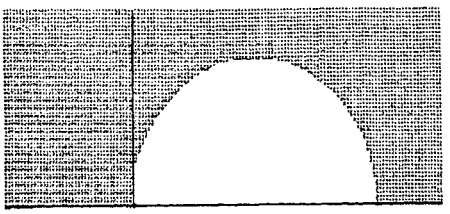
The two-stage, fourth-order corrector can be found in [2, p. 219]. Recall that only methods of Type I are relevant. The order of this type of methods is given by $p^I = \min\{4,m+2\}$.



m=0, N=3.8, W=-7.4, I=[0,0]



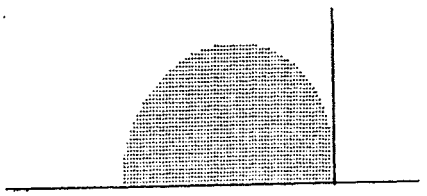
m=1, N=5.8, E=7.8
strongly A-stable



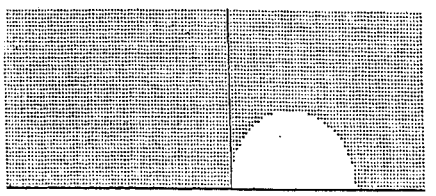
m=2, N=7.6, E=15.0
strongly A-stable

2.5. Sixth-Order Methods Based on the Gauss-Legendre Corrector of Order 6.

The three-stage, sixth-order corrector can be found in [2, p. 220]. Recall that only methods of Type I are relevant. The order of this type of methods is given by $p^I = \min\{6,m+2\}$.



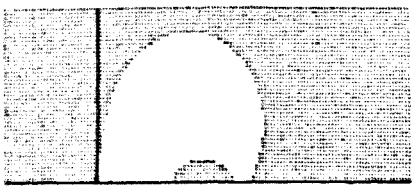
m=0, N=3.2, W=-6.2, I=[0,0]



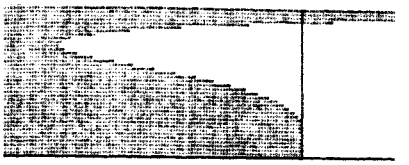
m=1, N=21, E=40
strongly A-stable

m=2, N=55, W=-120, I=[0,8.6]

m=3, N=110, W=-220, I=[0,0]∪[0.49,10.0]



m=4, N=19, E=29, W=-3.3$_{10}$-4, I=(0.16,0.84)
strongly A(α)-stable, α=89.87°



m=4, close-up