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Mono-implicit Runge–Kutta schemes for the parallel solution of initial value ODEs

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Abstract

Among the numerical techniques commonly considered for the efficient solution of stiff initial value ordinary differential equations are the implicit Runge–Kutta (IRK) schemes. The calculation of the stages of the IRK method involves the solution of a nonlinear system of equations usually employing some variant of Newton's method. Since the costs of the linear algebra associated with the implementation of Newton's method generally dominate the overall cost of the computation, many subclasses of IRK schemes, such as diagonally implicit Runge–Kutta schemes, singly implicit Runge–Kutta schemes, and mono-implicit (MIRK) schemes, have been developed to attempt to reduce these costs. In this paper we are concerned with the design of MIRK schemes that are inherently parallel in that smaller systems of equations are apportioned to concurrent processors. This work builds on that of an earlier investigation in which a special subclass of the MIRK formulas were implemented in parallel. While suitable parallelism was achieved, the formulas were limited to some extent because they all had only stage order 1. This is of some concern since in the application of a Runge–Kutta method to a system of stiff ODEs the phenomenon of order reduction can arise; the IRK method can behave as if its order were only its stage order (or its stage order plus one), regardless of its classical order. The formulas derived in the current paper represent an improvement over the previous investigation in that the full class of MIRK formulas is considered and therefore it is possible to derive efficient, parallel formulas of orders 2, 3, and 4, having stage orders 2 or 3.

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1. Introduction

In this paper we will be concerned with the numerical solution of systems of initial value ordinary differential equations, i.e. initial value problems (IVPs), of the form

$$y'(t) = f(y(t)), \quad y(t_0) = y_0, \tag{1}$$

where $y \in \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}^m$. When the IVP is stiff, implicit Runge–Kutta (IRK) schemes (see, for example [6] and references therein) are commonly used to provide a numerical solution. For the nth step, using a stepsize h, an s-stage IRK scheme has the form

$$y_{n+1} = y_n + h \sum_{r=1}^{s} b_r f(Y_r), \tag{2}$$

with

$$Y_r = y_n + h \sum_{j=1}^{s} a_{r,j} f(Y_j), \quad r = 1, \ldots, s. \tag{3}$$

Note that each unknown, Y_r, is defined implicitly in terms of itself and the other unknowns. These schemes are normally given in terms of the compact tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}}, \end{array}$$

where $c = Ae$, $c = (c_1, c_2, \ldots, c_s)^{\mathrm{T}}$, $b = (b_1, b_2, \ldots, b_s)^{\mathrm{T}}$ and A is the s by s matrix whose (i,j)th component is $a_{i,j}$, and e is the vector of 1's of length s.

Newton's method is usually employed to solve the system of $s \times m$ nonlinear equations given in (3) in order to determine the intermediate values, Y_r. This leads to an iteration matrix $(I_{ms} - hA \otimes J)$, where J is an approximation to the Jacobian $\partial f / \partial y$. Since the costs of the linear algebra associated with the solution of these linear systems generally dominate the overall cost of the computation, many subclasses of IRK schemes, such as diagonally implicit (DIRK) schemes [11, 1], singly implicit (SIRK) schemes [3], and mono-implicit (MIRK) schemes [7], have been developed to attempt to reduce these costs, usually by decoupling this large system of $s \times m$ equations into s systems each of dimension m. In this paper we are concerned with the design of IRK schemes that are inherently parallel in that the s systems of equations are apportioned to s concurrent processors. To achieve this brand of parallelism across the method we focus on MIRK schemes which, when applied to (1), have the form (for the nth step)

$$y_{n+1} = y_n + h \sum_{r=1}^{s} b_r f(Y_r), \tag{4}$$

where

$$Y_r = (1 - v_r) y_n + v_r y_{n+1} + h \sum_{j=1}^{r-1} x_{r,j} f(Y_j), \quad r = 1, \ldots, s. \tag{5}$$

Thus the stages of a mono-implicit Runge–Kutta scheme are implicit only in y_{n+1}. MIRK schemes are usually represented by the modified tableau

$$\begin{array}{c|c|c} c & v & X \\ \hline & & b^{\mathrm{T}}, \end{array}$$

where $v=(v_1,v_2,\dots,v_s)^{\mathrm{T}}$, $c=v+Xe$, and X, the s by s matrix whose (i,j)th component is $x_{i,j}$, is strictly lower triangular. The MIRK scheme (4), (5) is equivalent to the IRK scheme (2) with $A=X+vb^{\mathrm{T}}$ (see [9]). The stability function, $R(z)$, of a MIRK satisfies (see [9])

$$R(z)=\frac{P(z,e-v)}{P(z,-v)},$$

where

$$P(z,w)=1+zb^{\mathrm{T}}(I-zX)^{-1}w, \quad w\in\mathbb{R}^s.$$

Desirable stability properties for a MIRK scheme are given in terms of this stability function. A-stability requires $|R(z)|\leqslant 1, \forall z\in\mathbb{C}^-$; L-stability requires A-stability and the requirement that $|R(z)|\to 0$ as $\mathrm{Re}(z)\to-\infty$; see e.g. [6].

Parallel MIRK formulas consisting of s implicit stages and $s-1$ explicit stages were investigated by Voss [14]. While achieving order s utilizing s processors, all formulas considered had stage order one. This can be a difficulty because in the presence of order reduction (see, e.g., [10]), the observed order of accuracy of a Runge–Kutta scheme having stage order q can be reduced to order q or $q+1$, regardless of the classical order of the scheme. The main goal of this paper is to derive new MIRK schemes which have the advantage of higher stage order, while retaining desirable stability properties and the property of allowing an efficient parallel implementation. It is shown in [5] that the maximum stage order of a pth-order MIRK scheme is $\min(p,3)$. In this paper, for $p=2,3,4$, we shall derive MIRK schemes having stage order equal to the maximum or within one of the maximum.

There is a considerable amount of literature on parallel Runge–Kutta methods. Examples of recent work include papers on parallel multiply implicit Runge–Kutta (PMIRK) schemes [12], and singly diagonally implicit Runge–Kutta (SDIRK) schemes [8]. See [4] and references within.

Section 2 provides further background details associated with the parallel implementation of the MIRK schemes and with the design of these schemes. In Sections 3, 4, and 5 we present derivations of a number of MIRK schemes of orders 2, 3, and 4 that are suitable for use in parallel methods for IVPs. Section 6 provides a summary of the schemes derived in previous sections and reviews the application of certain optimization criteria in the specification of selected schemes. In Section 7, we present numerical results, based on some of the schemes derived earlier, which confirm the expected efficiency advantages of the new schemes.

2. Background

Within the next three sections of this paper, we will present derivations of MIRK schemes which we will characterize on the basis of several quantities. The notation MIRK*spq* will be used to indicate a MIRK scheme having s stages, of order p, and having stage order q, A MIRK scheme has order p if it local error is $O(h^{p+1})$; for Runge–Kutta schemes this is imposed by requiring the coefficients of the scheme to satisfy a set of equations called order conditions (see [6]). We shall identify specific order conditions, in their MIRK forms, as required, in later sections of this paper. A MIRK scheme has stage order q if it has coefficients which satisfy the conditions,

$$Xc^{r-1} + \frac{v}{r} = \frac{c^r}{r}, \quad r = 1, \ldots, q \tag{6}$$

(see [5]).

We next briefly review the parallel implementation for MIRK schemes, as described in [14]. Rewriting (4), we define

$$F(y_{n+1}) \equiv y_{n+1} - y_n - h \sum_{r=1}^{s} b_r f(Y_r). \tag{7}$$

Setting $F(y_{n+1}) = 0$ gives a system of m nonlinear equations implicitly defining y_{n+1}. The Newton iteration for the solution of this system is

$$J_F(y_{n+1}^{(l)}) \Delta y_{n+1}^{(l)} = -F(y_{n+1}^{(l)}), \qquad y_{n+1}^{(l+1)} = y_{n+1}^{(l)} + \Delta y_{n+1}^{(l)}, \quad l = 0, 1, \ldots. \tag{8}$$

Although the expression for $J_F(y_{n+1}^{(l)})$ involves the evaluation of $\partial f / \partial y$ at several points the usual modification of Newton's method approximates all these partial derivatives with an evaluation at a single point — we will refer to this evaluation as $J(y_{n+1}^{(l)})$. It is then possible to express $J_F(y_{n+1}^{(l)})$ as a polynomial in $J(y_{n+1}^{(l)})$ whose coefficients depend on the coefficients of the MIRK scheme. It is the goal of our work to design MIRK schemes for which we have

$$J_F(y_{n+1}^{(l)}) = \prod_{i=1}^{s} (I - B_i h J(y_{n+1}^{(l)})), \tag{9}$$

i.e., the polynomial expression for $J_F(y_{n+1}^{(l)})$ is factorable into linear factors. It is then possible, assuming the B_i's are distinct, to write $J_F^{-1}(y_{n+1}^{(l)})$ in a partial fraction expansion form as

$$J_F^{-1}(y_{n+1}^{(l)}) = \sum_{i=1}^{s} C_i (I - B_i h J(y_{n+1}^{(l)}))^{-1}, \tag{10}$$

where

$$C_i = \frac{B_i^{s-1}}{\prod_{j=1, j \neq i}^{s} (B_i - B_j)}. \tag{11}$$

Upon rewriting of (8) and substitution of (10), it can be seen that the task of computing $\Delta y_{n+1}^{(l)}$ can be subdivided into the following s independent tasks which can be computed on s processors,

$$(I - B_i h J(y_{n+1}^{(l)})) \Delta_i y_{n+1}^{(l)} = -F(y_{n+1}^{(l)}), \quad i = 1, \ldots, s, \tag{12}$$

and then

$$\Delta y_{n+1}^{(l)} = \sum_{i=1}^{s} C_i \Delta_i y_{n+1}^{(l)}. \tag{13}$$

Note that if for some i, $B_i = 0$, then the degree of $J_F(y_{n+1}^{(l)})$ is reduced by one and one less processor is needed in the computation associated with (12).

Throughout this paper we will express the stability function, $R(z)$, of a scheme in the form $P(z)/Q(z)$, with the numerator $P(z)$ and denominator $Q(z)$, polynomials in z. As noted in [14], the problem of trying to find MIRK schemes that are suitable for the parallel solution of IVPs as described above can be reduced to finding MIRK schemes for which $Q(z)$ can be factored into linear factors, i.e.,

$$Q(z) = (zB_1 - 1) \cdots (zB_s - 1), \tag{14}$$

where the B_i's are real, distinct, and positive. It can be shown (see [9]), that $Q(z)$ for an s-stage MIRK scheme can be expressed in the form

$$(b^{\mathrm{T}}X^{s-1}v)z^s + \cdots + (b^{\mathrm{T}}Xv)z^2 + (b^{\mathrm{T}}v)z - 1. \tag{15}$$

Expanding (14) gives

$$\begin{aligned}&(B_1 \cdot \ldots \cdot B_s)z^s - \cdots + (-1)^{s-2}(B_1 \cdot B_2 + B_1 \cdot B_3 + \cdots B_{s-1} \cdot B_s)z^2\\ &\quad +(-1)^{s-1}(B_1 + \cdots + B_s)z + (-1)^s,\end{aligned} \tag{16}$$

from which a comparison of coefficients of like powers of z in (15) shows that the requirements for the existence of a scheme with a stability function with a $Q(z)$ factorable as in (14) are

$$\begin{aligned}&B_1 + \cdots + B_s = b^{\mathrm{T}}v,\\ &B_1 \cdot B_2 + B_1 \cdot B_3 + \cdots + B_{s-1} \cdot B_s \cdots = -b^{\mathrm{T}}Xv,\\ &\ldots,\\ &B_1 \cdot \ldots \cdot B_s = (-1)^{s-1}b^{\mathrm{T}}X^{s-1}v.\end{aligned} \tag{17}$$

The derivation process to be employed in the next three sections of this paper will begin by selecting or determining families of MIRK schemes with a given number of stages, a given order, and a given stage order. These families usually have several free parameters. We will then apply the factorization conditions (17), and solve them to obtain expressions for the free parameters of the MIRK scheme in terms of the B_i parameters, if possible. A particular MIRK scheme will be obtained by choosing specific values for the free parameters.

Sections 3, 4, and 5, will consider families of MIRK schemes of orders 2, 3, and 4, and, overall, will present nine specific schemes. Sample numerical results will be presented for a selected subset of these schemes in Section 7; similar results could be obtained for the remaining schemes. For the selected schemes, the free parameters are chosen to yield optimal schemes according to the following criteria. Subject to the restrictions that the B_i's be real, distinct, and positive, we will attempt to, firstly, minimize $\|T_{p+1}\|$, the norm of the vector of weighted unsatisfied order conditions for order $p+1$, associated with the local truncation error coefficient of order $p+1$ of a pth-order MIRK scheme (see [6]), subject to the constraint that the ratio $\|T_{p+2}\|/\|T_{p-1}\|$ is not too large, and, secondly, minimize $\|C\|$, the norm of the vector of C_i coefficients arising in (13). Smaller truncation error coefficients will generally lead to more accurate schemes, while bounding the values for the C_i coefficients will tend to contribute to the avoidance of overflow in (13), and will force the B_i values to be distinct as assumed for (11). The details of the optimization process for these schemes are provided in Section 6.

3. Second-order MIRK schemes

3.1. Overview

The maximum stage order of a second-order scheme is stage order two. It is easily shown that such a MIRK scheme must employ at least two stages. We derive the primary scheme of this section, MIRK222, in the next subsection; it is a two-stage, second-order, stage order two MIRK scheme, which turns out to be necessarily L-stable. In the last subsection, we consider two other second-order MIRK schemes. The first, (MIRK221A), is relevant if L-stability, which implies strong damping at infinity, is considered to be undesirable. (For example, in the boundary value ODE context symmetric, A-stable methods, rather than L-stable methods are needed — see [9].) The resultant scheme then necessarily has only stage order one. The second scheme of the last subsection, (MIRK221L), is an L-stable scheme for which the stage order requirement is relaxed to stage order one. This allows us to consider the possibility of deriving a scheme with a smaller $\|T_{p+1}\|$ value; such a scheme would generally be more accurate than MIRK222, in the absence of order reduction.

3.2. Stage order 2

3.2.1. MIRK222 (L-stable)

The order conditions that the coefficient of a MIRK scheme must satisfy for second-order are

$$b^{\mathrm{T}}e = 1, \quad b^{\mathrm{T}}c = \tfrac{1}{2}, \tag{18}$$

and the stage order two conditions are given by (6) with $q = 2$. Solution of these conditions leads to a family which includes A-stable schemes. This family, with free parameter $c_2 \neq 1$, has the tableau and stability function

$$\begin{array}{c|c|cc} 1 & 1 & 0 & 0 \\ c_2 & c_2(2-c_2) & c_2(c_2-1) & 0 \\ \hline & & \dfrac{(c_2-\frac{1}{2})}{(c_2-1)} & \dfrac{1}{2(1-c_2)} \end{array}, \quad R(z) = \frac{z(1-c_2)+2}{z^2c_2-(1+c_2)z+2}. \tag{19}$$

Solving the factorization conditions (17), for c_2 and B_2 yields

$$c_2 = \frac{B_1(2B_1-1)}{B_1-1}, \quad B_2 = \frac{B_1-\frac{1}{2}}{B_1-1}. \tag{20}$$

In order for B_2 to be positive, we must choose $B_1 \in (0, \frac{1}{2}) \cup (1, \infty)$; B_1 and B_2 will be distinct if $B_1 \neq 1 \pm \sqrt{2}/2$. With B_1 and B_2 positive and real, there are no additional requirements for A-stability.

Choosing $B_1 = \frac{1}{10}$ gives $B_2 = \frac{4}{9}$ and $c_2 = \frac{4}{45}$. The tableau and the stability function become

$$\begin{array}{c|c|cc} 1 & 1 & 0 & 0 \\ \frac{4}{45} & \frac{344}{2025} & -\frac{164}{2025} & 0 \\ \hline & & \frac{37}{82} & \frac{45}{82} \end{array}, \quad R(z) = \frac{\frac{41}{4}z + \frac{45}{2}}{(z-\frac{9}{4})(z-10)}. \tag{21}$$

This scheme is L-stable since it is A-stable ($|Q(\mathrm{i}y)|^2 - |P(\mathrm{i}y)|^2 = 16y^4$) and clearly $|R(z)| \to 0$ as $\mathrm{Re}(z) \to -\infty$. (For $Q(z)$ as in (14), with $B_1, B_2 > 0$, the A-stability requirement reduces to the requirement that $|Q(\mathrm{i}y)|^2 - |P(\mathrm{i}y)|^2 > 0, \forall y \in \mathbb{R}$ with $y \neq 0$. See e.g. [6] for details.) It has $\|T_3\| \approx 0.086$, $\|C\| \approx 1.3$, and $\|T_4\| \approx 0.14$, which gives $\|T_4\|/\|T_3\| \approx 1.6$.

3.3. Stage order 1

3.3.1. MIRK221A (A-stable)

The application of the order conditions for order 2, (18), plus the stage order 1 conditions, (6) with $q=1$, to the general family of two stage MIRK schemes leads to a family with three parameters c_1, c_2, and v_2 with the restriction that $c_1 \neq c_2$. The tableau for this scheme is

$$\begin{array}{c|c|cc} c_1 & c_2 & 0 & 0 \\ c_2 & v_2 & c_2 - v_2 & 0 \\ \hline & & \dfrac{(\frac{1}{2} - c_2)}{c_1 - c_2} & \dfrac{(\frac{1}{2} - c_1)}{c_2 - c_1} \end{array}, \qquad (22)$$

and the stability function has

$$R(z) = \frac{\gamma + 2zc_2 + z^2c_2 - z^2v_2 - 3z^2c_2c_1 + 3z^2v_2c_1 - zc_1}{\gamma - z^2c_2c_1 + z^2v_2c_1 + zc_1}, \qquad (23)$$

where

$$\gamma = -2c_1 - zv_2 - 2zc_2c_1 + 2zv_2c_1 + 2c_2 + 2z^2c_2c_1^2 - 2z^2v_2c_1^2.$$

Solving the factorization equations (17), for c_1 and v_2 in terms of c_2, B_1, and B_2 gives

$$c_1 = \frac{B_1B_2}{B_1 + B_2 - \frac{1}{2}}, \qquad (24)$$

and

$$v_2 = \frac{(B_1^2B_2 + B_1B_2^2 - \frac{1}{2}B_1B_2) - c_2(B_1^2 + B_1B_2 + B_2^2 - \frac{1}{2}(B_1 + B_2))}{(2B_1 - 1)(2B_2 - 1)}.$$

An example of a specific A-stable, scheme from this family is obtained by choosing $B_1 = 1$, $B_2 = 2$, and $c_2 = \frac{1}{5}$, which gives a scheme with tableau and stability function

$$\begin{array}{c|c|cc} \frac{4}{5} & \frac{4}{5} & 0 & 0 \\ \frac{1}{5} & \frac{26}{5} & -5 & 0 \\ \hline & & \frac{1}{2} & \frac{1}{2} \end{array}, \quad R(z) = \frac{\frac{-z^2}{4} - z + \frac{1}{2}}{(z - \frac{1}{2})(z - 1)}. \qquad (25)$$

It is A-stable since $|Q(\mathrm{i}y)| - |P(\mathrm{i}y)|^2 = 15y^4$.

3.3.2. MIRK221L (L-stable)

If we now return to the MIRK family (22) and require the degree of $P(z)$ to be less than the degree of $Q(z)$ by setting the coefficient of the z^2 term in $P(z)$ to be zero, we get the requirement that $B_2 = (B_1 - \frac{1}{2})/(B_1 - 1)$. (This is the same expression for B_2 as obtained in a previous subsection; see (20). The two cases are related; this value for B_2 coupled with the factorization condition (24), on c_1, forces $c_1 = 1$, which is the same value required of c_1 from the application of the stage order two conditions, as in the derivation of the MIRK222 scheme, (21).) The requirement that B_2 be positive implies $B_1 \in (0, \frac{1}{2}) \cup (1, \infty)$. The requirement that B_1 and B_2 be distinct implies $B_1 \neq 1 - \sqrt{2}/2$. Then for c_1 and v_2 we have

$$c_1 = 1 \quad \text{and} \quad v_2 = \frac{(2B_1^2 - 2B_1^2 c_2 - B_1 + 2B_1 c_2 - c_2)}{(B_1 - 1)},$$

with $c_2 \neq 1$ still free. Provided B_1 and B_2 are positive and real, there are no additional restrictions for A-stability.

With $B_1 = \frac{3}{25}$, we get $B_2 = \frac{19}{44}$ and the tableau and stability function are

$$\begin{array}{c|c|cc} 1 & 1 & 0 & 0 \\ \frac{1}{3} & \frac{332}{825} & -\frac{19}{275} & 0 \\ \hline & & \frac{1}{4} & \frac{3}{4} \end{array}, \quad R(z) = \frac{493z + 1100}{(19z - 44)(3z - 25)}. \tag{26}$$

This scheme is L-stable since it is A-stable ($|Q(\mathrm{i}y)|^2 - |P(\mathrm{i}y)|^2 = 3249y^4$) and clearly $|R(z)| \to 0$ as $\mathrm{Re}(z) \to -\infty$. It has $\|T_3\| \approx 0.057$, $\|C\| \approx 1.4$, and $\|T_4\| \approx 0.069$, which gives $\|T_4\|/\|T_3\| \approx 1.2$. Comparing these values with those for MIRK222, as discussed in introductory subsection, we see that the $\|T_3\|$ value is about 25% smaller, the $\|T_4\|$ value is about 50% smaller, and the $\|C\|$ value is about the same.

4. Third-order MIRK schemes

4.1. Overview

The next subsection considers schemes with stage order 3. Since there are only two 2-stage, third-order schemes [2], and neither of them have stage order 3, 3-stage schemes are considered first. It is found that it is possible to obtain an A-stable scheme only if one of the abscissa is allowed to be outside the current step, and that even under this relaxed condition, no L-stable schemes are possible. Schemes having 4-stages are then considered and it is found that it is possible to obtain an A-stable scheme with all abscissa within the current step but still no L-stable schemes are possible. It may be possible to employ 5-stages to obtain an L-stable scheme with all abscissa within the current step; this is left for a future study.

In the last subsection of this section, schemes with stage order 2 are considered. Since neither of the two 2-stage, third order, stage order 2 schemes cited above are suitable, 3-stage schemes are considered. It is found that it is possible to obtain a third order, A-stable scheme, with all abscissa within the current step, as well as a third order, L-stable scheme, with all abscissa within the current step.

4.2. Stage order 3

4.2.1. MIRK333 (A-stable)

In [5] the tableau for a two-parameter family of 3-stage, third-order, stage order 2 MIRK schemes is given. Applying the stage order 3 conditions (6) with $q=3$, to this family leads to a family of schemes with the tableau,

$$\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ c_3 & c_3^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 \\ \hline & & \frac{(3c_3-1)}{6} & \frac{(3c_3-2)}{6(c_3-1)} & \frac{1}{6c_3(1-c_3)} \end{array},$$

and the stability function is

$$R(z)=-\frac{z^2(c_3-1)+z(2c_3-4)-6}{z^2c_3-2z(c_3+1)+6}. \tag{27}$$

In this case, the factorization conditions (17), require us to choose one of B_1, B_2, or B_3 equal to zero (since for the above X matrix, $X^2=0$, the coefficient of z^3 in (15), namely, $b^{\mathrm{T}}X^2v$ is zero, requiring the product, $B_1 \cdot B_2 \cdot B_3$ to be zero as well). We choose $B_1=0$ and then solve for c_3 and B_2 in terms of B_3,

$$c_3=\frac{6B_3(B_3-\frac{1}{3})}{(2B_3-1)}, \quad B_2=\frac{(B_3-\frac{1}{3})}{(2B_3-1)}. \tag{28}$$

(Recall that $B_1=0$ implies that only 2 processors can be used.) We see from the above expression for B_2 that we must have

$$B_3 \in (0,\tfrac{1}{3}) \cup (\tfrac{1}{2},\infty) \text{ so that } B_2>0. \tag{29}$$

Also an inspection of the expression for c_3 shows that we must have

$$B_3 \in (0,\tfrac{1}{3}) \text{ so that } c_3 \in (0,1). \tag{30}$$

Unfortunately, for this case, $|Q(\mathrm{i}y)|^2-|P(\mathrm{i}y)|^2<0 \ \forall B_3 \in (0,\frac{1}{3})$ and this scheme cannot be A-stable. However, choosing $B_3=\frac{3}{4}$, we get $B_2=\frac{5}{6}$ and $c_3=\frac{15}{4}$ (outside the current step), and a scheme with tableau and stability function,

$$\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \frac{15}{4} & -\frac{2025}{32} & \frac{1815}{64} & \frac{2475}{64} & 0 \\ \hline & & \frac{41}{90} & \frac{37}{66} & -\frac{8}{495} \end{array}, \quad R(z)=\frac{-11z^2-14z+24}{15(z-\frac{6}{5})(z-\frac{4}{3})}. \tag{31}$$

For this scheme, $|Q(iy)|^2-|P(iy)|^2=104y^4$ and we get an A-stable method. It is not possible to obtain an L-stable scheme within this family.

Since this family of schemes does not have enough freedom to allow us to derive an L-stable scheme, and an A-stable scheme can be obtained only by choosing c_3 outside [0,1], we will turn to four-stage MIRK schemes in an attempt to derive more satisfactory schemes.

4.2.2. MIRK433 (A-stable)

When the order conditions for third order,

$$b^{\mathrm{T}}e=1,\quad b^{\mathrm{T}}c=\tfrac{1}{2},\quad b^{\mathrm{T}}c^2=\tfrac{1}{3},\quad b^{\mathrm{T}}(Xc+\tfrac{1}{2}v)=\tfrac{1}{6},\tag{32}$$

and the stage order conditions up to order 3, (6) with $q=3$, are applied to the general four-stage MIRK family, the resultant four-parameter family has the tableau

$$\begin{array}{c|c|cccc} 0 & 0 & 0 & 0 & 0 & 0\\ 1 & 1 & 0 & 0 & 0 & 0\\ c_3 & c_3^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 & 0\\ c_4 & v_4 & x_{41} & x_{42} & x_{43} & 0\\ \hline & & b_1 & b_2 & b_3 & b_4 \end{array},\tag{33}$$

where

$$x_{41}=-\frac{-6c_4c_3+3c_3v_4+3c_3c_4^2-v_4-2c_4^3+3c_4^2}{6c_3},$$

$$x_{42}=\frac{-3c_4^2+v_4+2c_4^3}{6c_3(c_3-1)},\quad x_{43}=-\frac{-2v_4+2c_4^3+3v_4c_3-3c_4^2c_3}{6(c_3-1)},$$

$$b_1=-\frac{6b_4c_4^2-6b_4c_4+1}{6c_3(c_3-1)},\quad b_2=\frac{-6c_3b_4c_4+3c_3+6b_4c_4^2-2}{6(c_3-1)}$$

and

$$b_3=-\frac{-6c_3b_4c_4+6b_4c_3-3c_3+6b_4c_4^2-6b_4c_4+1}{6c_3}.$$

The four free parameters are c_3, c_4, v_4, and b_4 with the restrictions that $c_3\neq 0,1$. Also, c_4 must be chosen so that the fourth stage is distinct from the first three.

Application of the factorization conditions (17), leads to the requirement that one of B_1, B_2, B_3, and B_4 must be zero (since for the above X matrix, $X^3=0$, the coefficient of z^4 in (15), namely, $b^{\mathrm{T}}X^3v$, is zero, requiring the product, $B_1\cdot B_2\cdot B_3\cdot B_4$ to be zero as well). We set $B_1=0$ and then obtain c_3, v_4, and b_4 in terms of B_2, B_3, B_4, and c_4. (Recall that $B_1=0$ implies that only 3 processors can be used.) After some analysis, we found that we were able to get an A-stable scheme with $c_3\in(0,1)$ by choosing $B_2=\frac{1}{3}$, $B_3=\frac{1}{2}$, and $B_4=\frac{1}{4}$, giving $c_3=\frac{1}{2}$. The choice of $c_4=\frac{3}{4}$, which completes the definition of the scheme, leads to the tableau and stability function,

$$\begin{array}{c|c|cccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{8} & \frac{-1}{8} & 0 & 0 \\ \frac{3}{4} & \frac{45}{32} & \frac{-3}{64} & \frac{-15}{64} & \frac{-3}{8} & 0 \\ \hline & & \frac{5}{18} & \frac{-1}{6} & 0 & \frac{8}{9} \end{array}, \quad R(z)=\frac{z^3+5z^2+2z-24}{(z-2)(z-3)(z-4)}. \tag{34}$$

Since $|Q(\mathrm{i}y)|^2-|P(\mathrm{i}y)|^2=8y^4$, we have an A-stable method. It is not possible to obtain an L-stable scheme from within this family.

4.3. Stage order 2

4.3.1. MIRK332A (A-stable)

In [5] the tableau and stability function for a three-parameter family of 3-stage, third-order, stage order 2, MIRK schemes are given. For general c_2, $P(z)$ is of degree 2 and $Q(z)$ is of degree 3. We choose $c_2=0$ which causes the degree of $Q(z)$ to become 2 as well. The factorization conditions (17) force one of B_1, B_2, or B_3 to be zero, as in previous sections. We choose $B_1=0$ and solve for B_2 and v_3 in terms of B_3 and c_3:

$$B_2=\frac{3B_3-1}{3(2B_3-1)}, \quad v_3=\frac{c_3(12(c_3-1)B_3^2-(6c_3-4)B_3+c_3)}{1-2B_3}.$$

After some analysis, we found that choosing $B_3=\frac{5}{6}$ and $c_3=\frac{5}{6}$ gives a suitable scheme. The tableau and stability function are

$$\begin{array}{c|c|ccc} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{5}{6} & \frac{125}{72} & \frac{-25}{48} & \frac{-55}{144} & 0 \\ \hline & & -\frac{1}{2} & \frac{3}{10} & \frac{6}{5} \end{array}, \quad R(z)=-\frac{11z^2+14z-24}{(5z-6)(3z-4)}. \tag{35}$$

Since $|Q(\mathrm{i}y)|^2-|P(\mathrm{i}y)|^2=104y^4$ it is an A-stable method.

4.3.2. MIRK332L (L-stable)

We begin with the 3-stage, third-order, stage order 2, MIRK family given in [5]. Applying the factorization conditions (17) and solving for v_3, c_2 and B_3 gives

$$B_3=-\frac{B_1+B_2-2B_1B_2-\frac{1}{3}}{2B_1B_2-2B_1-2B_2+1}, \tag{36}$$

and expressions for c_2 and v_3 are too complicated to be given here. The parameter, c_3, is left free, with the requirement that it be distinct from 1 and c_2. Recall also that we must ensure that $c_2\neq 0$ so that the degree of $Q(z)$ is greater than the degree of $P(z)$, since we are looking for an L-stable scheme. We also have B_1 and B_2 free. For this family of MIRK schemes, the fact that B_1, B_2, and B_3 are real and positive is not sufficient to ensure A-stability; in addition we must have $(3c_2-1)\beta/\alpha<\frac{1}{2}$, where $\alpha=(c_3-1)(c_3-c_2)$ and $\beta=\frac{1}{2}(v_3+c_3(c_3-2))(3c_2-1)$ [5].

Choosing $B_1=1$, $B_2=\frac{1}{4}$, and $c_3=\frac{7}{9}$ gives $B_3=\frac{5}{12}$ and the corresponding tableau and stability function are

$$\begin{array}{c|c|ccc} 1 & 1 & 0 & 0 & 0 \\ \frac{5}{24} & \frac{215}{576} & -\frac{95}{576} & 0 & 0 \\ \frac{7}{9} & \frac{241}{81} & -\frac{1414}{1539} & -\frac{656}{513} & 0 \\ \hline & & \frac{1}{76} & \frac{384}{779} & \frac{81}{164} \end{array}, \quad R(z)=\frac{1}{5}\frac{19z^2+32z-48}{(z-1)(z-4)(z-\frac{12}{5})}. \tag{37}$$

This method is L-stable since it is A-stable ($|Q(\mathrm{i}y)|^2-|P(\mathrm{i}y)|^2=208y^4+25y^6$) and clearly $|R(z)|\to 0$ as $\mathrm{Re}(z)\to-\infty$. It has $\|T_4\|\approx 0.064$, $\|C\|\approx 2.9$, and $\|T_5\|\approx 0.16$, which gives $\|T_5\|/\|T_4\|\approx 2.5$.

5. Fourth-order MIRK schemes

5.1. Overview

The next subsection considers stage order 3 schemes. Since the only 3-stage, fourth-order, stage order 3, MIRK scheme [2], does not have a stability function with a factorable denominator, we consider MIRK schemes having 4-stages, and derive a family of suitable fourth-order, stage order 3, MIRK schemes. A specific A-stable scheme from this family is presented; however it is found that one of the abscissa must be outside the current step. It is also found that there are no L-stable schemes in this family. It may be possible to obtain L-stable, fourth-order, stage order 3 schemes with all abscissa within the current step by using 5 stages; this is left for a future study.

The last subsection considers stage order 2 schemes and begins by examining the 3-stage family from [5]. However, it is shown that there are no suitable schemes within this family and the investigation thus turns to 4-stage schemes. The subsection concludes with the derivation of a family of such schemes and a specific A-stable scheme is exhibited. This family does not contain any L-stable schemes.

5.2. Stage order 3

5.2.1. MIRK443 (A-stable)

The family is considered in [5]; it has free parameters c_3, c_4, and v_4. Application of the factorization conditions (17) forces us to choose one of B_1, B_2, B_3, or B_4 equal to zero; we choose $B_1=0$ and solve for v_4, c_3, and B_4, (leaving c_4 free). We get

$$B_4=\frac{12B_2B_3-4B_2-4B_3+1}{4(6B_2B_3-3B_2-3B_3+1)}, \tag{38}$$

$$c_3=\frac{6B_2B_3(12B_2B_3-4B_2-4B_3+1)}{6(B_2+B_3)(4B_2B_3-2B_2-2B_3+1)-24B_2B_3-1}, \tag{39}$$

and a more complicated expression for v_4. After some analysis it was found that it was not possible to obtain an A-stable scheme with $B_4 > 0$ and c_3 within the current step. An example of an A-stable scheme from this family is obtained by choosing $B_2 = 2$ and $B_3 = \frac{3}{2}$. Then $c_3 = \frac{414}{125}$ (outside the current step) and $B_4 = \frac{23}{34}$. The stability function for this scheme is

$$R(z) = \frac{-\frac{289}{414}z^3 - \frac{5}{6}z^2 + \frac{36}{23}z - \frac{34}{69}}{(z - \frac{34}{23})(z - \frac{1}{2})(z - \frac{2}{3})}, \tag{40}$$

for all values of c_4. Since $|Q(iy)|^2 - |P(iy)|^2 = 87875y^6$, this scheme is A-stable. For the choice of $c_4 = \frac{3}{4}$, the tableau is

$$\begin{array}{c|c|ccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ \frac{414}{125} & -\frac{77642388}{1953125} & \frac{34577694}{1953125} & \frac{49533444}{1953125} & 0 & 0 \\ \frac{3}{4} & \frac{881901}{191216} & -\frac{57970637}{35183744} & -\frac{5076616551}{221045696} & \frac{833984375}{10168102016} & 0 \\ \hline & & \frac{1945}{7452} & -\frac{69}{289} & \frac{1953125}{919599156} & \frac{11248}{11529} \end{array}. \tag{41}$$

It is not possible to derive an L-stable scheme within this class of methods.

5.3. Stage order 2

5.3.1. MIRK342

In [5] a family of schemes of this type are presented; it has free parameters c_2 and c_3. Beginning with this family and applying the factorization requirements (17) allows us to solve for c_2, B_2 and B_3 and we get

$$c_2 = \frac{B_1(12B_1^2 - 6B_1 + 1)}{36B_1^3 - 24B_1^2 + 7B_1 - 1}, \tag{42}$$

$$B_2 = -\frac{72B_1^3 - 57B_1^2 + 21B_1 + 3B_1\sqrt{D} - 3 - 2\sqrt{D}}{3(-72B_1^3 + 72B_1^2 - 29B_1 + 5 + \sqrt{D})}, \tag{43}$$

$$B_3 = -\frac{-24B_1^2 + 15B_1 - 3 + \sqrt{D}}{12(6B_1^2 - 4B_1 + 1)}, \tag{44}$$

where

$$D = -288B_1^4 + 288B_1^3 - 135B_1^2 + 30B_1 - 3. \tag{45}$$

Unfortunately, for all positive B_1, D is negative, and thus B_2 and B_3 are complex. Hence, no suitable factorizations are possible for this family. We will thus consider schemes with one extra stage.

5.3.2. MIRK442 (A-stable)

The coefficients of this family are required to satisfy the eight-order conditions,

$$b^{\mathrm{T}}e=1,\quad b^{\mathrm{T}}c=\tfrac{1}{2},\quad b^{\mathrm{T}}c^2=\tfrac{1}{3},\quad b^{\mathrm{T}}(Xc+\tfrac{1}{2}v)=\tfrac{1}{6},\quad b^{\mathrm{T}}c^3=\tfrac{1}{4},$$
$$b^{\mathrm{T}}c(Xc+\tfrac{1}{2}v)=\tfrac{1}{8},\quad b^{\mathrm{T}}(X(Xc+\tfrac{1}{2}v)+\tfrac{1}{6}v)=\tfrac{1}{24},\quad b^{\mathrm{T}}(Xc^2+\tfrac{1}{3}v)=\tfrac{1}{12}, \tag{46}$$

plus the stage order conditions (6) with $q=2$. Solution of these conditions leads to a family of schemes which includes some A-stable schemes. It has $c_1=1$ and free parameters c_2, c_3, c_4, v_3, and v_4. The tableau of this family is somewhat complicated and is not included here. In order to simplify subsequent calculations we choose $c_2=0$. The application of the factorization conditions (17) forces us to choose one of B_1, B_2, B_3, or B_4 equal to zero; we choose $B_4=0$ and then solve us for v_3, v_4 and B_3; we get

$$B_3=\frac{12B_1B_2-4B_1-4B_2+1}{4(6B_1B_2-3B_1-3B_2+1)}, \tag{47}$$

and expressions for the v_3 and v_4 that are too complicated to present here. If we choose $B_1=\frac{3}{4}$ and $B_2=1$, then $B_3=3$ with c_3, c_4 as free parameters; we get the stability function,

$$R(z)=\frac{-\frac{37}{54}z^3-\frac{7}{9}z^2+\frac{5}{3}z-\frac{4}{9}}{(z-1)(z-\frac{1}{3})(z-\frac{4}{3})}, \tag{48}$$

for which $|Q(\mathrm{i}y)|^2-|P(\mathrm{i}y)|^2=1547y^6$, so this scheme is A-stable. Its tableau, for the choices $c_3=\frac{1}{3}$ and $c_4=\frac{2}{3}$, is

$$\begin{array}{c|c|cccc} 1 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ \frac{1}{3} & \frac{233}{153} & -\frac{12}{17} & -\frac{74}{153} & 0 & 0\\ \frac{2}{3} & \frac{1654}{153} & -\frac{719}{306} & \frac{12}{17} & -\frac{17}{2} & 0\\ \hline & & \frac{1}{8} & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} \end{array}. \tag{49}$$

It is not possible to derive an L-stable method within this family.

6. Summary of derived schemes

In this section we summarize the schemes derived in this paper. In Table 1, the number of stages is s, the order is p, the stage order is q, the stability is A, for A-stability, or L, for L-stability, and for convenient reference, the equation number for the tableau of the scheme is given in the final column.

All derived schemes are either A-stable or L-stable and all but two, MIRK333 and MIRK443, have all abscissa within the current step. Recalling that the maximum stage order of a pth-order MIRK scheme is $\min(p,3)$, we observe that all the derived schemes have stage order equal to the maximum or within one of the maximum.

Table 1
Summary of derived schemes

Method	s	p	q	stability	Equation
MIRK222	2	2	2	L	(21)
MIRK221A	2	2	1	A	(25)
MIRK221L	2	2	1	L	(26)
MIRK333	3	3	3	A	(31)
MIRK433	4	3	3	A	(34)
MIRK332A	3	3	2	A	(35)
MIRK332L	3	3	2	L	(37)
MIRK443	4	4	3	A	(41)
MIRK442	4	4	2	A	(49)

In the next section, we provide the results of some numerical testing based on a selected subset of the above schemes. Similar numerical testing could be done for other schemes. We select three L-stable schemes for testing, MIRK222, MIRK221L, and MIRK332L. For each of these schemes, the following subsection provides the details of the optimization process used in the selection of free parameters. Similar optimization analyses could be applied to any of the schemes.

6.1. Optimization of selected schemes

All analyses are performed subject to the constraint that the B_i values be distinct and positive.

6.1.1. Optimization of MIRK222

From the factorization conditions, we have $B_2 > 0 \Rightarrow B_1 \in (0, \frac{1}{2}) \cup (1, \infty)$. If $B_1 = B_2 = 1 - \sqrt{2}/2$ then $\|T_3\|$ reaches the minimum value of approximately 0.057; however this violates the requirement that $B_1 \neq B_2$. If we choose $B_1 = 0$ or $B_1 = \frac{1}{2} \Rightarrow B_2 = 0$ (or $B_1 = 1 \Rightarrow B_2 \to \infty$) then $\|C\|$ reaches the minimum value of 1.0, but there is no opportunity for parallelism. Since minimization according to either of these criteria leads to values for B_1 and B_2 that are problematic, we will choose B_1 so that $\|T_3\|$ and $\|C\|$ are simultaneously close to their respective minimum values. We found that we were able to choose B_1 so that the resultant values were within a ratio of 1.5 of their respective minimums. This optimal value for B_1 is near $\frac{1}{10}$.

6.1.2. Optimization of MIRK221L

Again, $B_2 > 0 \Rightarrow B_1 \in (0, \frac{1}{2}) \cup (1, \infty)$. Optimization with respect to $\|T_3\|$ gives the minimum value of 0.040 but requires $B_1 = B_2 = 1 - \sqrt{2}/2$. Optimization with respect to $\|C\|$ gives the minimum value of 1.0 but requires $B_1 = 0$ or $B_1 = \frac{1}{2} \Rightarrow B_2 = 0$ (or $B_1 = 1 \Rightarrow B_2 \to \infty$) and there is no opportunity for parallelism. Since either minimum taken independently leads to difficulty, we will attempt to simultaneously optimize $\|T_3\|$ and $\|C\|$ with respect to their minimum values. Since only $\|T_3\|$ depends on c_2, we first optimize $\|T_3\|$ with respect to c_2 which gives $c_2 = \frac{1}{3}$. We then simultaneously optimize $\|T_3\|$ and $\|C\|$ with respect to B_1 and find that if we choose B_1 near $\frac{3}{25}$ we get values for $\|T_3\|$ and $\|C\|$ within a ratio of 1.4 of their respective minimums.

6.1.3. Optimization of MIRK332L

We begin the optimization process for this family by observing that of the quantities we are interested in optimizing only $\|T_4\|$ is a function of c_3. We thus first minimize $\|T_4\|$ with respect to c_3, which gives c_3 in terms of B_1 and B_2. Since the expression for c_3 is somewhat complicated we do not include it here. As mentioned previously, A-stability here requires $(3c_2-1)\beta/\alpha<\frac{1}{2}$, where $\alpha=(c_3-1)(c_3-c_2)$ and $\beta=\frac{1}{2}(v_3+c_3(c_3-2))(3c_2-1)$ [5]. An examination of this condition shows that both B_1 and B_2 cannot both be less than approximately 0.4. A subsequent examination of $\|C\|$ then shows that the minimum is obtained only if one of B_1 or B_2 is approximately equal to 1.0. We choose $B_1=1$ and proceed to attempt to simultaneously minimize $\|C\|$ and $\|T_4\|$ with respect to B_2. We note that, in order for B_3 to be positive, we must choose $B_2\in(0,\frac{2}{3})$. We find that $\|C\|$ is then minimized with respect to B_2 when $B_2\approx 0.198$ or $B_2\approx 0.469$, in which case we have $\|C\|\approx 2.81$. $\|T_4\|$ is minimized when $B_2=\frac{1}{3}$; for its minimum value we have $\|T_4\|\approx 0.0589$. However, this choice for B_2 gives B_3 also equal to $\frac{1}{3}$. Thus, we will determine the value to be used for B_2 by requiring both $\|C\|$ and $\|T_4\|$ to be simultaneously minimized with respect to their respective minimums. This calculation leads to the choices $B_2\approx 0.25717$ or $B_2\approx 0.40949$ (either choice leads to the same MIRK scheme), which give $\|T_4\|$ and $\|C\|$ values within 10% of their respective minimums. We conclude by choosing $B_2=\frac{1}{4}$ (close to the first of these two values). This gives $c_3=\frac{7}{9}$.

7. Numerical results

In this section we will report the numerical results obtained by three L-stable MIRK schemes, namely, MIRK222, MIRK221L, and MIRK332L, given, respectively, in tableaus (21), (26), and (37), when implemented on the linear ODE system of Prothero–Robinson-type equations [13] and the nonlinear ODE system arising from a semidiscretized nonlinear convection–diffusion problem discussed by Cong [8]. Cong developed a second order, L-stable, parallel singly diagonally implicit Runge–Kutta (PDIRK_2) method, having stage order 2 and showed its efficient behavior when compared to several higher order sequential DIRK methods, when applied to these two problems. As in [8], all computations were performed using fifteen digit (double precision) arithmetic and the accuracy is given by the number of correct digits, NCD, obtained by writing the maximum norm of the error at the end of the interval of integration in the form $E=10^{-\text{NCD}}$. The sequential computational effort is measured by the number of sequential stages, i.e., the number of stages that cannot be computed in parallel, per unit interval and the stepsize h is chosen such that the number of sequential stages per unit interval equals a prescribed number M. Thus a method that uses fewer sequential stages per step can employ more steps, i.e., smaller steps, per unit subinterval, leading to more accuracy. Using adjacent entries in the tables, we estimate the order as $p=\log(E_1/E_2)/\log(h_1/h_2)$, where the error E_i, defined above, arises using stepsize h_i

PDIRK_2 is a six-stage SDIRK method which, when implemented on a two-processor computer, effectively requires only two implicit stages per step. Similarly, a MIRK*spq* implemented on a s-processor computer effectively requires only one implicit stage per step, i.e., all stages can be computed independently, in parallel. In Tables 2 and 3, s^* denotes the effective number of implicit stages per step required by the various methods. For completeness, the tables also include the results by PDIRK_2 in [8] as well as the four DIRK methods considered in [8]:

- Nørsett_3, Nørsett_4: third and fourth-order A-stable methods of Nørsett,

Table 2
Values of NCD and p for problem (50)

			M							
			120		240		480		960	
Method	Order	s^*	NCD	p	NCD	p	NCD	p	NCD	p
Nørsett_3	3	2	3.3	—	3.9	2.0	4.5	2.0	5.1	2.0
Nørsett_4	4	3	3.1	—	3.7	2.0	4.3	2.0	4.9	2.0
HW_4	4	5	4.5	—	5.5	3.3	6.0	1.7	6.3	1.0
CS_5	5	5	2.2	—	2.6	1.3	2.9	1.0	3.3	1.3
$PDIRK_2$	2	2	5.1	—	5.7	2.0	6.3	2.0	6.9	2.0
MIRK221L	2	1	4.9	—	5.5	2.0	6.1	2.0	6.7	2.0
MIRK222	2	1	5.6	—	6.2	2.0	6.8	2.0	7.4	2.0
MIRK332L	3	1	7.1	—	7.9	2.7	8.7	2.7	9.6	3.0

- HW_4: fourth-order L-stable method of Hairer and Wanner,
- CS_5: fifth-order A-stable method of Cooper and Sayfy.

7.1. Prothero–Robinson-type problem

$$\frac{dy(t)}{dt} = J[y(t) - g(t)] + g'(t), \quad y(0) = g(0), \tag{50}$$
$$J = \text{diag}(-10^{2(j-1)}),$$
$$g(t) = (1 + \sin(jt)), \quad j = 1, \ldots, 6, \quad 0 \leqslant t \leqslant 20.$$

Prothero and Robinson [13] used a problem of this type to show the order reduction phenomenon of Runge–Kutta methods. The exact solution of (50) is $y(t) = g(t)$ which has both slowly and rapidly varying components. For this problem, all methods for which results are presented in Table 2 exhibit at most second-order behavior, except MIRK332L which shows third-order. As noted by Cong [8], order reduction really does occur for the DIRK methods on this problem. However, order reduction did not occur for the parallel MIRK schemes due to their higher stage order and, in particular, MIRK222 gives a superior performance among the second-order schemes.

7.2. Nonlinear partial differential equation

We next consider the convection–diffusion problem [8]

$$\frac{\partial u(t,x)}{\partial t} = u(t,x)\frac{\partial^2 u(t,x)}{\partial x^2} - x\cos(t)\frac{\partial u(t,x)}{\partial x} - x^2\sin(t), \tag{51}$$

with $0 \leqslant x \leqslant 1$, $0 \leqslant t \leqslant 1$, in order to show the performance of the L-stable MIRK methods on problems to be solved with low accuracy demand. The initial and Dirichlet boundary conditions are such that the exact solution is given by $u(t,x) = x^2\cos(t)$. Central finite-difference discretization of the spatial derivatives on a uniform grid with mesh size $\frac{1}{40}$ yields a system of 39 ODEs with exact

Table 3
Values of NCD and p for problem (51)

			M							
			30		60		120		240	
Method	Order	s^*	NCD	p	NCD	p	NCD	p	NCD	p
$Nørsett_3$	3	2	3.8	—	4.4	2.0	5.1	2.0	5.7	2.0
$Nørsett_4$	4	3	3.5	—	4.1	2.0	4.8	2.0	5.4	2.0
HW_4	4	5	3.8	—	4.5	2.0	5.1	2.0	5.8	2.3
CS_5	5	5	2.6	—	3.2	2.0	4.0	2.7	5.0	3.3
$PDIRK_2$	2	2	4.7	—	5.3	2.0	5.9	2.0	6.6	2.3
MIRK221L	2	1	4.4	—	5.0	2.0	5.6	2.0	6.2	2.0
MIRK222	2	1	5.2	—	5.8	2.0	6.4	2.0	7.0	2.0
MIRK332L	3	1	6.3	—	7.1	2.7	7.9	2.7	8.7	2.7

solution $(\frac{1}{40}j)^2\cos(t)$, $j=1,\ldots,39$. An examination of Table 3 again reveals order reduction for the DIRK methods with the parallel methods performing similar to that for (50).

References

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

[2] W.M.G. van Bokhoven, Implicit end-point quadrature formulae, BIT 3 (1980) 87–89.

[3] K. Burrage, A special family of Runge–Kutta methods for solving stiff differential equations, BIT 18 (1978) 22–41.

[4] K. Burrage, Parallel and Sequential Methods for Ordinary Differential Equations, Oxford University Press, New York, 1995.

[5] K. Burrage, F.H. Chipman, P.H. Muir, Order results for mono-implicit Runge–Kutta methods, SIAM J. Numer. Anal. 31 (1994) 876–891.

[6] J.C. Butcher, The Numerical Analysis of Ordinary Differential Equations, Wiley, Chichester, 1987.

[7] J.R. Cash, A. Singhal, Mono-implicit Runge–Kutta formulae for the numerical integration of stiff differential systems, IMA J. Numer. Anal. 2 (1982) 211–217.

[8] N. Cong, A parallel DIRK method for stiff initial-value problems, J. Comp. Appl. Math. 54 (1994) 121–127.

[9] W.H. Enright, P.H. Muir, Efficient classes of Runge–Kutta methods for two-point boundary value problems, Computing 37 (1986) 315–334.

[10] R. Frank, J. Schneid, C.W. Ueberhuber, Order results for implicit Runge–Kutta methods applied to stiff systems, SIAM J. Numer. Anal. 23 (1985) 515–534.

[11] S.P. Nørsett, Semi-explicit Runge–Kutta methods, Report Math. Comput. No. 6/74, Dept. Math. Univ. of Trondheim, 1974.

[12] B. Orel, Parallel Runge–Kutta methods with real eigenvalues, Appl. Numer. Math. 11 (1990) 241–250.

[13] A. Prothero, A. Robinson, On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations, Math. Comp. 28 (1974) 145–162.

[14] D.A. Voss, Parallel mono-implicit Runge–Kutta methods for stiff ODEs, Report, Dept. of Math. Western Illinois University, 1995.