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010

TOWARDS EFFICIENT RUNGE-KUTTA METHODS FOR STIFF SYSTEMS*

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Abstract. A special class of implicit Runge-Kutta methods is developed for the numerical solution of stiff initial value problems. These formulae are derived from known singly implicit methods by adding one or more extra diagonally implicit stages. It is hoped that this modification of the original method will lead to an overall gain in efficiency, and an analysis of the advantages of making this enhancement is presented.

Key words. stiff problem, Runge-Kutta method, singly implicit method

AMS(MOS) subject classifications. 65L05, 65L20

1. Introduction. In the search for efficiently implementable Runge-Kutta methods for the initial value problem in stiff ordinary differential equations, it is natural to consider singly implicit methods and, in particular, diagonally implicit methods. Each of these classes has been extensively analysed [1], [3]-[6], [11] and each seems to offer some important advantages over other methods as well as some disadvantages. For diagonally implicit methods, the limitation of the stage-order to 1, and the difficulty of finding high order for the method as a whole, or of constructing realistic local error estimates, makes these methods unlikely candidates for incorporating in highly accurate and efficient software. The limitation of stage-order seems to make the practical effect of whatever higher method-order that can be achieved of dubious value for very stiff problems [9], and this seems to be an insuperable barrier. Allowing the use of general singly implicit methods overcomes these difficulties but introduces other disadvantages. In particular, at least for small problems, the cost of the transformations associated with the singly implicit iterations has a dominant effect on the overall computational costs, even though an asymptotic analysis shows the transformation costs to be of little significance for large problems.

In an attempt to derive high-order highly stable diagonally implicit schemes, the use of block methods has been proposed [7], [8]. These offer an advantage over standard diagonally implicit methods in that they require fewer function evaluations per step to achieve a particular order. The limitation of stage-order to 1 still remains, however.

In the present paper, we consider a combination, in block form, of diagonally implicit with more general singly implicit methods. The first stages are as for a singly implicit method and have an acceptable stage-order. To these are added one or more diagonally implicit stages in such a way that the stage-order is preserved but such that the new method has greater computational efficiency than unmodified singly implicit methods.

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The Runge-Kutta array for the proposed methods thus has the form

$$(1.1)\qquad \begin{array}{c|cccccccc} \bar{c}_1 & \bar{a}_{11} & \bar{a}_{12} & \cdots & \bar{a}_{1p} & 0 & 0 & \cdots & 0 \\ \bar{c}_2 & \bar{a}_{21} & \bar{a}_{22} & \cdots & \bar{a}_{2p} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \bar{c}_p & \bar{a}_{p1} & \bar{a}_{p2} & \cdots & \bar{a}_{pp} & 0 & 0 & \cdots & 0 \\ \bar{c}_{p+1} & \bar{a}_{p+1,1} & \bar{a}_{p+1,2} & \cdots & \bar{a}_{p+1,p} & \lambda & 0 & \cdots & 0 \\ \bar{c}_{p+2} & \bar{a}_{p+2,1} & \bar{a}_{p+2,2} & \cdots & \bar{a}_{p+2,p} & \bar{a}_{p+2,p+1} & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \bar{c}_s & \bar{a}_{s1} & \bar{a}_{s2} & \cdots & \bar{a}_{sp} & \bar{a}_{s,p+1} & \bar{a}_{s,p+2} & \cdots & \lambda \\ \hline & \bar{b}_1 & \bar{b}_2 & \cdots & \bar{b}_p & \bar{b}_{p+1} & \bar{b}_{p+2} & \cdots & \bar{b}_s \end{array},$$

where the submatrix

$$(1.2)\qquad \begin{bmatrix} \bar{a}_{11} & \bar{a}_{12} & \cdots & \bar{a}_{1p} \\ \bar{a}_{21} & \bar{a}_{22} & \cdots & \bar{a}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{a}_{p1} & \bar{a}_{p2} & \cdots & \bar{a}_{pp} \end{bmatrix}$$

has a one-point spectrum $\{\lambda\}$, with λ the same real number that appears on the diagonal of the diagonally implicit block. The intention is that every stage should have order p and that stages $p+1, p+2, \cdots, s$ are added successively to improve the overall performance of the method, above what can be achieved for the p-stage, singly implicit method on which it is built. It is hoped that the method based on (1.1) will integrate further forward than is appropriate for the singly implicit method on its own and the transformation costs will be reduced in comparison with the overall cost of integrating a given distance along a trajectory. Since the stage order will be p for every stage, this will constitute an advantage over diagonally implicit methods.

As a notational convenience, we will write $h\lambda = H$ so that, using H as the unit of distance in the direction of the independent variable, the method takes a form in which the single eigenvalue associated with the method becomes 1, but where we are approximating the solution at a distance of θ units along the trajectory, where $\theta = \lambda^{-1}$. A further effect of this change of scale is that all the elements of the array in (1.1) will be multiplied by λ^{-1}. It thus takes the form

$$(1.3)\qquad \begin{array}{c|cccccccc} c_1 & a_{11} & a_{12} & \cdots & a_{1p} & 0 & 0 & \cdots & 0 \\ c_2 & a_{21} & a_{22} & \cdots & a_{2p} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_p & a_{p1} & a_{p2} & \cdots & a_{pp} & 0 & 0 & \cdots & 0 \\ c_{p+1} & a_{p+1,1} & a_{p+1,2} & \cdots & a_{p+1,p} & 1 & 0 & \cdots & 0 \\ c_{p+2} & a_{p+2,1} & a_{p+2,2} & \cdots & a_{p+2,p} & a_{p+2,p+1} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{sp} & a_{s,p+1} & a_{s,p+2} & \cdots & 1 \\ \hline & b_1 & b_2 & \cdots & b_p & b_{p+1} & b_{p+2} & \cdots & b_s \end{array},$$

with $\{1\}$ the spectrum of the principal $p \times p$ submatrix.

We will be concerned only with methods that are strongly stable at infinity (that is, methods for which A-stability implies L-stability). Hence, we assume that

$$[b_1 \quad b_2 \quad \cdots \quad b_p \quad b_{p+1} \quad b_{p+2} \quad \cdots \quad b_s]$$
$$= [a_{s1} \quad a_{s2} \quad \cdots \quad a_{sp} \quad a_{s,p+1} \quad a_{s,p+2} \quad \cdots \quad 1].$$

Note that this assumption also guarantees that the order of the method is p, the same as the stage order. It is known that for low values of p, the standard p stage singly implicit method can be L-stable. We will investigate to what extent we can add stages at points $\theta_{p+1}, \theta_{p+2}, \cdots, \theta_s$ to maintain L-stability. By adding on these stages, we may be converting existing methods to more complicated methods with more than the minimum number of stages necessary to achieve the required combination of order and L-stability, but it is hoped that there might nevertheless be a gain in the efficacy of the new methods. We will investigate to what extent this hope is realized and attempt to determine the most suitable choice of s for a given value of p.

2. Construction of the formulae with $p=1$. In this and later sections, we will investigate the feasibility of deriving L-stable methods with various orders in the form given by (1.3). In the case of orders less than 7, L-stable singly implicit methods already exist with $s=p$. In the case $p=7$, we will be aiming for something particularly interesting since L-stable methods with $s=7$ do not exist. For the moment, we consider only the case $p=1$.

For the $s=1$ case, the only choice is the backward Euler method given by

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}. \tag{2.1}$$

If we add to this a further stage, we have a method of the form

$$\begin{array}{c|cc} 1 & 1 & 0 \\ \theta & \theta-1 & 1 \\ \hline & \theta-1 & 1 \end{array}. \tag{2.2}$$

The first question we ask about this method is for what set of θ values it is A-stable. We approach this question, and other similar questions in this paper, by making use of the E-polynomial technique [10]. If for a particular Runge-Kutta method, the numerical solution for the scalar test equation $y'=\mu y$ grows by a factor $N(\mu H)/D(\mu H)$ in each integration step, where N and D are polynomials, then A-stability is equivalent to the requirements that D should have no zeros in the left half-plane and that the E-polynomial given by

$$E(y^2)=|D(iy)|^2-|N(iy)|^2$$

should take nonnegative values for all positive real arguments. In the case of the method (2.2), we have $N(z)=1+z(\theta-2)$ and $D(z)=(1-z)^2$. As for all the methods of the form we are considering, there is always a repeated zero of D at 1 and no other zeros. Hence, it will be necessary only to apply the E-polynomial criterion. Writing $t=y^2$, we find

$$E(t)=|(1-iy)^2|^2-|1+iy(\theta-2)|^2=(2-(\theta-2)^2)^2t+t^2.$$

Thus, for A-stability it is necessary and sufficient that the coefficient of t is nonnegative. This means that $2-\sqrt{2} \leqq \theta \leqq 2+\sqrt{2}$. Using the greatest allowed value of θ, we obtain the method

$$\begin{array}{c|cc} 1 & 1 & 0 \\ 2+\sqrt{2} & 1+\sqrt{2} & 1 \\ \hline & 1+\sqrt{2} & 1 \end{array}. \tag{2.3}$$

If we add a third stage and again write θ for the value of this final output point, we have $N(z)=1+(\theta-3)z+\alpha_2 z^2$, $D(z)=(1-z)^3$, where α_2 is an additional constant to be chosen. We will find the greatest θ for which, with a suitable choice of α_2, A-stability is achieved. Writing $\alpha_1=\theta-3$, we have for the E-polynomial

$$E(t)=|(1-iy)^3|^2-|1+iy\alpha_1-\alpha_2 y^2|^2=(3-\alpha_1^2+2\alpha_2)t+(3-\alpha_2^2)t^2+t^3$$

and it can be verified that the optimal choice is given by $\alpha_2=2$, $\alpha_1=(3/2)\sqrt{3}$, leading to $\theta=3+(3/2)\sqrt{3}$. Using the A-stable method with $s=2$ to provide the first and second stages and the value of θ we have just found for the third stage, we arrive at the following combined method:

$$\begin{array}{c|ccc} 1 & 1 & 0 & 0 \\ 2+\sqrt{2} & 1+\sqrt{2} & 1 & 0 \\ 3+\frac{3}{2}\sqrt{3} & a_{31} & a_{32} & 1 \\ \hline & a_{31} & a_{32} & 1 \end{array}, \tag{2.4}$$

where $a_{32}=(3+\frac{3}{2}\sqrt{3})(\sqrt{2}-1)$ and $a_{31}=2+\frac{3}{2}\sqrt{3}-a_{32}$. A further analysis shows that a fourth stage may be added at the point $4+2(2+\sqrt{2})^{1/2}$ and that a fifth stage may be added at a point given approximately by $\theta=9.7652825814$. There is no reason why even further stages should not be added but, for the purpose of illustrating the idea, five stages will suffice.

3. Construction of the formulae with $p=2$. We first consider the question of adding on a single additional stage to the singly implicit method with $p=2$. In the case $p=1$, we saw that L-stability is possible for $\theta\in[2-\sqrt{2}, 2+\sqrt{2}]$. For $p=2$, a similar analysis can be carried out. It is found that

$$N(z)=1+(\theta-3)z+\left(\frac{\theta^2}{2}-3\theta+3\right)z^2, \qquad D(z)=(1-z)^3,$$

so that the E-polynomial is

$$\begin{aligned} E(t) &= (1+t)^3-\left(1-\left(\frac{\theta^2}{2}-3\theta+3\right)t\right)^2-t(\theta-3)^2 \\ &= \left(3-\left(\frac{\theta^2}{2}-3\theta+3\right)^2\right)t^2+t^3, \end{aligned}$$

which is nonnegative for all $t\geqq 0$ if and only if $\theta\in[3-(3+2\sqrt{3})^{1/2}, 3+(3+2\sqrt{3})^{1/2}]$. It is also interesting to consider the possibility of adding on two diagonally implicit stages. We find that

$$N(z)=1+(\theta-4)z+\left(\frac{\theta^2}{2}-4\theta+6\right)z^2+\alpha_3 z^3, \qquad D(z)=(1-z)^4,$$

and that

$$E(t) = (1+t)^4 - \left(1 - \left(\frac{\theta^2}{2} - 4\theta + 6\right)t\right)^2 - t(\theta - 4 - \alpha_3 t)^2$$

$$= \left(6 - \left(\frac{\theta^2}{2} - 4\theta + 6\right)^2 + 2\alpha_3(\theta - 4)\right)t^2 + (4 - \alpha_3^2)t^3 + t^4.$$

It is found that L-stability is possible if and only if $\theta \in [4-(8+4\sqrt{2})^{1/2}, 4+(8+4\sqrt{2})^{1/2}]$.

As for the $p=1$ case, we can also consider the question of adding on a further stage making a total of $s=5$ stages. It is now found that A-stability is possible for $\theta \in [0.2552062669, 9.7447727309]$.

4. *L*-stable methods with $s=p+1$, $s=p+2$, and $s=p+3$. In this section, we summarize in tabular form the choices for θ that are possible for A-stability, and hence L-stability, to be achieved for $s-p \in \{1, 2, 3\}$ and $p = 1, 2, \cdots, 8$. We deal first with the case $s=p+1$. For each value of p, an interval of θ values is tabulated. These are rounded inward so that points in the given intervals guarantee the required stability conditions. Note that with the addition of a single diagonally implicit stage, L-stability is available for all orders up to at least $p=8$, whereas for singly implicit methods with $s=p$, order 7 is not possible. Note also that for $p=7$, $s=8$, there are two disjoint intervals of possible θ values.

We now turn to the case $s=p+2$ with $p = 1, 2, 3, \cdots, 8$ and present Table 4.2 in a form similar to Table 4.1. Note that in the case $p=4$, two nonintersecting intervals are given. As for Table 4.1, the ends of the intervals are rounded inward so that points in the given intervals guarantee the required stability conditions. In addition to the θ

TABLE 4.1
Intervals for L-stability with $s=p+1$.

s	p	θ
2	1	[0.5857864377, 3.4142135623]
3	2	[0.4575402432, 5.5424597568]
4	3	[1.7457611012, 4.4713160416]
5	4	[1.4791971777, 4.0323452767]
6	5	[2.9927363261, 5.4373046411]
7	6	[2.6394633406, 4.8999563246]
8	7	[4.2667001703, 4.8734327612]
		[4.9276895840, 6.3833074203]
9	8	[3.8547453251, 5.8516502767]

TABLE 4.2
Intervals for L-stability for $s=p+2$.

s	p	θ	α_{p+1}
3	1	[0.4019237887, 5.5980762113]	(2.000000, 2.000000)
4	2	[0.3044818700, 7.6955181300]	(−2.613125, 2.613125)
5	3	[1.3947540934, 6.2258427661]	(−1.416535, −2.49275)
6	4	[1.1587465517, 5.6077999145]	(1.60825, 2.09413)
		[6.2252398417, 8.1270286166]	(−4.1399552365, −3.6021217350)
7	5	[2.5494591576, 7.0527426071]	(1.701390, 3.050240)
8	6	[2.2168752644, 6.3842656791]	(−1.759816, −2.68453)
9	7	[3.7667335875, 7.9826328967]	(−2.439684, −3.83114)
10	8	[3.3671496520, 7.2911042513]	(2.361400, 3.47341)

intervals, ordered pairs of α_{p+1} are given. The first member of each pair corresponds to an allowed choice of α_{p+1} for the lower end of the θ interval and the second member to the upper end of the θ interval. The number of digits presented for each α value is determined by the requirement that if the last digit is changed by 1 in either direction, the stability condition is not violated.

Finally, we turn to the case $s=p+3$. For each θ interval it is now necessary to present values of α_{p+2} as well as α_{p+1} and the details are given in Table 4.3. The rounding rules used in the previous tables are also adhered to here.

5. Error constants. In this section we consider the error constants for the results computed at various stages. For a stage value Y, which computes an approximation to $y(x_{n-1}+\theta H)$, write C for the error constant. Thus, assuming sufficient smoothness, and that y_{n-1} exactly equals $y(x_{n-1})$, we see that

$$Y=y(x_{n-1}+\theta H)-CH^{p+1}y^{(p+1)}(x_{n-1})+O(H^{p+2}). \tag{5.1}$$

If the stability function associated with this stage is

$$\frac{N(z)}{D(z)}=\frac{1+\alpha_1 z+\alpha_2 z^2+\cdots+\alpha_{s-1}z^{s-1}}{(1-z)^s}, \tag{5.2}$$

then C can be characterized by

$$\exp(\theta z)-\frac{N(z)}{D(z)}=Cz^{p+1}+O(|z|^{p+2}). \tag{5.3}$$

We will use (5.3) to obtain an expression for C. Multiply both sides by $(1-z)^s$, and we see that C is the coefficient of z^{p+1} in $(1-z)^s\exp(\theta z)-\alpha_{p+1}$. Thus,

$$C=\frac{\theta^{p+1}}{(p+1)!}-\binom{s}{1}\frac{\theta^p}{p!}+\binom{s}{2}\frac{\theta^{p-1}}{(p-1)!}+\cdots+(-1)^{p+1}\binom{s}{p+1}-\alpha_{p+1}. \tag{5.4}$$

For stage numbers $s>p$ this is as convenient a formula for the error constant as we can expect to find. However, for stage number $k\leqq p$, the total number of stages on which this stage depends is $s=p$ and θ is zero number k of the Laguerre polynomial L_p. In this case, $\alpha_{p+1}=0$ and (5.4) reduces to

$$\begin{aligned} C&=(-1)^p\int_0^\theta L_p(x)\,dx=(-1)^p(L_p(\theta)-L_{p+1}(\theta))=(-1)^{p+1}L_{p+1}(\theta)\\ &=(-1)^{p+1}\left(L_p(\theta)+\frac{\theta}{p+1}L'_{p+1}(\theta)\right)=(-1)^{p+1}\frac{\theta}{p+1}L'_{p+1}(\theta)\\ &=(-1)^{p+1}\frac{\theta}{p+1}(L'_p(\theta)-L_p(\theta))=\frac{(-1)^{p+1}}{p+1}\theta L'_p(\theta). \end{aligned} \tag{5.5}$$

TABLE 4.3
Intervals for L-stability for $s=p+3$.

s	p	θ	α_{p+1}	α_{p+2}
4	1	[0.3044818700, 7.6955181300]	(4.8284271247, 4.8284271247)	(−2.61313, 2.61313)
5	2	[0.2552062669, 9.7447727309]	(−7.6787081681, 7.6820157176)	(3.095444431, 3.1118493240)
6	3	[1.1587465519, 8.1380064292]	(0.4145469534, −7.2822985148)	(1.60825, −3.395467336)
7	4	[1.0153730681, 9.9146129154]	(−0.0963690470, −11.0081135283)	(−1.7871334419, −3.5602114153)
8	5	[2.6168752645, 8.8615861154]	(1.0487086198, 10.3920384371)	(−1.759812, 4.335671324)
9	6	[1.9937968171, 8.2595608126]	(0.8240732891, −8.420313758)	(1.856125635, −4.7504819878)
10	7	[3.3671496521, 9.6642701078]	(1.7094396577, −14.4644166239)	(2.36140, −5.0415697842)
11	8	[3.0810618816, 9.0009848319]	(−1.4107171098, 13.128758693)	(−2.371363446, 5.4397003614)

In the steps leading to (5.5) a number of standard results associated with Laguerre polynomials have been used (see, for example, [2]).

In § 6, we will use (5.4) and (5.5) in our discussion of the accuracy of the various methods we have introduced.

6. Selection from alternative methods. For a given order $p \leqq 8$, it is possible to construct methods with various values of s from p upward and still retain L-stability. As we have shown in the last section, there is also a choice as to where the output points are placed. In this section we discuss criteria for choosing amongst this large class of possibilities.

An obvious approach would be to use the magnitude of the error constant for the method as a measure of its inaccuracy. This is not an appropriate choice for a number of reasons. In the first place, the error constant must be normalized to take into account the fact that the stepsize is θH rather than H and therefore a factor $\theta^{-(p+1)}$ must be incorporated into the constant. Also, to adjust for the different costs of different methods with varying values of s, it is necessary to use a further factor s^p.

Even with these normalizations taken into account, we may be faced with the difficulty of dealing with an abnormally low value of the magnitude of the error constant. If the error constant is actually zero, for example, so that the order is really $p+1$, it is not necessarily the case that the method is more accurate than competing methods of order p. It might be possible to carry out a sophisticated analysis of the error in which more than the principal term is taken into account, but conclusions drawn from such an analysis will depend on the problem and the choice of stepsize, and it seems to be very difficult to arrive at any general conclusions.

Among different possible ways out of this dilemma, we will take what seems an easy but reasonable choice. This is to use not simply the error constant associated with the stage from which the output is taken, but rather the greatest in magnitude of the error constants for all the stages. The normalization described above will then be applied to the greatest magnitude amongst the error constants.

While it cannot be claimed that this choice of worst possible error constant amongst all stages takes into account all possible types of complicated interplay between the stages, it does have the advantage of being conservative in expressing the performance of multistage methods.

We look first at the example of first-order methods. With only a single stage the only choice of L-stable method is

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \tag{6.1}$$

and the error constant is $-\frac{1}{2}$. Adding a second stage so as to produce the method

$$\begin{array}{c|cc} 1 & 1 & 0 \\ \theta & \theta-1 & 1 \\ \hline & \theta-1 & 1 \end{array}, \tag{6.2}$$

we find the error constant for the two stages to be, respectively, $-\frac{1}{2}$ and $\frac{1}{2}\theta^2-2\theta+1$. Hence, using the rules that we have described above, we have as a measure of the inaccuracy of the method (6.2),

$$2\max\left(\frac{1}{2}, \left|\frac{\theta^2}{2}-2\theta+1\right|\right)\Big/\theta^2.$$

It is easy to see that within the interval $[2-\sqrt{2}, 2+\sqrt{2}]$, where L-stability is achieved, the optimal result is obtained with $\theta = 2+\sqrt{2}$ giving an adjusted error constant of $3/2-\sqrt{2} \approx 0.0857864376$. Under the assumptions we have been making, this is a considerable improvement over what is obtained using the simple one-stage method (6.1).

We now come to the question of adding a third stage, and we ask whether or not this should be considered an advantage. The method takes the form

$$\begin{array}{c|ccc} 1 & 1 & 0 & 0 \\ 2+\sqrt{2} & 1+\sqrt{2} & 1 & 0 \\ \theta & a_{31} & a_{32} & 1 \\ \hline & a_{31} & a_{32} & 1 \end{array} \tag{6.3}$$

where a_{31} and a_{32} are chosen to satisfy the order and stability requirements as well as the condition that the error constant for the third stage is minimized in absolute value. It is found that the best choice is with the greatest value allowed by Table 4.2 and that an improvement over the two-stage case is then achieved. Similarly, if a fourth stage is to be added, then this should be using the greatest θ allowed by Table 4.3 and the result achieved is even better than for three stages. The results for the various first-order cases are as summarized in Table 6.1.

The phenomenon exhibited here, that additional stages give consistently improved performance, continues at least until $s = 10$, for which the values of θ and the error constant are, respectively, 19.8768834058 and 0.0126553285. Because of the inflexible way in which it is necessary to implement a method with this many stages, it is not recommended that all of them be used. However, something like four or five stages with order 1 seems to be quite reasonable and, under the assumptions inherent in our accuracy comparisons, is certainly an improvement over the single-stage method.

A similar calculation with order 2 does not give the same uniformly improving sequence of normalized error constants when $s \geqq 8$. However, we will present only the results as far as they might seem to be of potential practical interest, that is, for the order 2 cases included within Tables 4.1, 4.2, and 4.3, which takes us as far as $s = 5$ (see Table 6.2).

TABLE 6.1
Error constants with $p = 1$ and $s = 1, 2, 3, 4$.

s	θ	Error constant
1	1.0000000000	0.5000000000
2	3.4142135623	0.0857864376
3	5.5980762113	0.0478645132
4	7.6955181300	0.0337718043

TABLE 6.2
Error constants with $p = 2$ and $s = 2, 3, 4, 5$.

s	θ	Error constant
2	3.4142135624	0.1617604581
3	5.5424597568	0.1096637123
4	7.6955181300	0.1027249960
5	9.7447727309	0.0920589178

Although it is not convenient to reproduce all the results in full detail, it can be reported that for other orders from 3 to 8, the pattern of uniform improvement of normalized error constants persists for very high values of s. For example, in the case $p = 8$, this pattern persists up to at least $s = 17$. For this order the singly implicit method with eight stages has a normalized error constant equal to 587537.0178, whereas for the 17-stage diagonally implicit extension of the method with maximum possible value of θ for L-stability, it is found that $\theta = 21.4915566760$ and the error constant is 117.0374835, an improvement by a factor of more than 5,000. We note that the value of θ quoted here is close to the value of the greatest zero of L_8.

It is the opinion of the authors that the appropriate choice for s corresponding to each order should be at least as great as $s = p + 3$, since this makes it possible to obtain reliable asymptotic error estimates for the method itself and for the method of next highest order. It is also felt that the final output point should be close to, or greater than, the greatest zero of the Laguerre polynomial L_p. This would mean that a characteristic difficulty of singly implicit methods, the amount by which for high-order methods some of the abscissae move further and further out of the integration interval, is avoided. The authors believe that this is a very important property of the block methods proposed in this paper and is likely to give them a considerable advantage over standard singly implicit methods.

Subject to the requirements we have mentioned, and the aim of obtaining a worthwhile reduction in the effective error constant, it seems to be a good design decision to keep the number of stages as low as possible. This and other implementation details are yet to be settled and will hinge on the results of numerical testing presently in progress.

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