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AN ORDER SIX RUNGE-KUTTA PROCESS WITH EXTENDED REGION OF STABILITY*

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1. Introduction. In this paper we consider the numerical solution of the initial value problem for a system of ordinary differential equations:

$$\frac{dy}{dx} = f(x, y), \qquad y(x_0) = y_0 . \tag{1.1}$$

We consider the family of order six Runge-Kutta increment functions. Such a function requires at least seven derivative evaluations [2] as follows:

$$g_1 = f(x, y), \tag{1.2}$$

$$g_i = f(x + c_i h, \quad y + h \sum_{j=1}^{i-1} a_{ij} g_j), \qquad i = 2, 3, \cdots, 7, \tag{1.3}$$

$$y_{n+1} = y_n + h \sum_{i=1}^{7} b_i g_i, \quad x_{n+1} = x_n + h, \qquad n = 0, 1, \cdots . \tag{1.4}$$

Butcher [1] presents the system of 37 algebraic equations which constrain the selection of the 28 parameters $\{a_{ij}\}, \{b_i\}$. The c_i satisfy

$$c_i = \sum_{j=1}^{i-1} a_{ij} , \qquad i = 2, 3, \cdots, 7. \tag{1.5}$$

He deduces the existence of a four-parameter family of solutions to these equations and exhibits a two-parameter family explicitly, along with several other particular solutions.

2. Optimization. We consider the problem $y' = Ay$, $y(0) = y_0$, where A is a real square matrix. The exact solution at $h, 2h, \cdots$ is given by $y_{n+1} = \exp(hA)y_n$. An order six Runge-Kutta process using seven substitutions gives the approximate solution $y_{n+1} = E(k; hA)y_n$, where

$$E(k; hA) = \sum_{i=0}^{6} \frac{(hA)^i}{i!} + \frac{k}{7!}(hA)^7, \tag{2.1}$$

$$k = 7!b_7 \sum_{i=2}^{7} a_{i,i-1} . \tag{2.2}$$

We define, as in [3], the region of stability of such a Runge-Kutta process

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to be the connected set S of complex z with the properties $0 \in S$, $\mathrm{Re}\,(z) \leqq 0$ and $|E(k;z)| \leqq 1$. If the eigenvalues of hA are contained in the region of stability, then the matrices $E(k; hA)$ and $\exp(hA)$ share the property that all eigenvalues lie within or on the unit circle. We attempt to find a value of k which makes this region as large as possible. We then attempt to find solutions of the 37 Runge-Kutta equations for $\{a_{ij}\}$, $\{b_i\}$, subject to this additional constraint.

To gain some idea of the behavior of $E(k; z)$, its graph is given in Fig. 1 for negative real z and several values of k. If we restrict our consideration to the real axis, $k \approx .544$ is optimal, and the interval $[-6.6, 0]$ (approximately) of the negative real axis is included in the region of stability. This value of k, however, should be slightly increased to avoid excessive narrowing of the region of stability in the complex plane near the value of z for which $E(k; z)$ has a local maximum on the negative real axis. For $k = .55$, the boundary of the corresponding region of stability is plotted in Fig. 2 and labeled RK6ES. The boundaries of the regions of stability of the order five process of [3] and of the classical order four process, as given in [4], are also plotted and are labeled RK5ES and RK4, respectively. The boundaries are symmetric with respect to the real axis, and so the region $\mathrm{Im}\,(z) < 0$ is omitted from Fig. 2.

In the absence of a criterion for a truly optimal region of stability, we shall now attempt to find a Runge-Kutta process with $k = 0.55$.

Inspection of the two-parameter family of processes given explicitly by

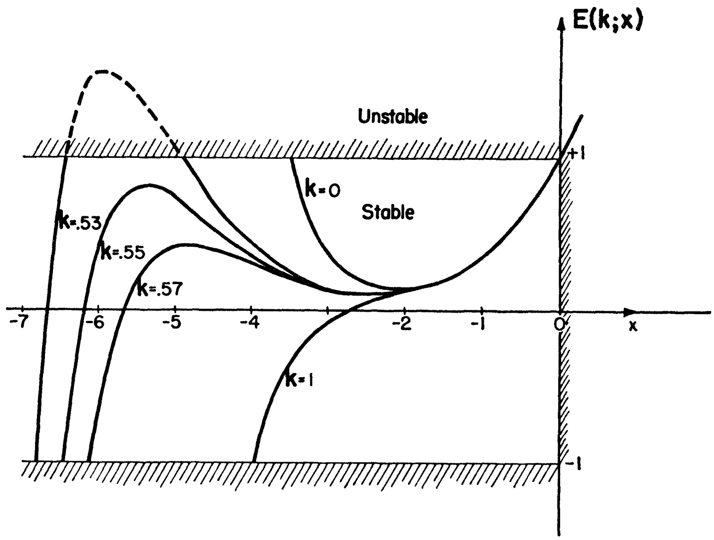

FIG. 1. $E(k; x)$ *for* x *real*

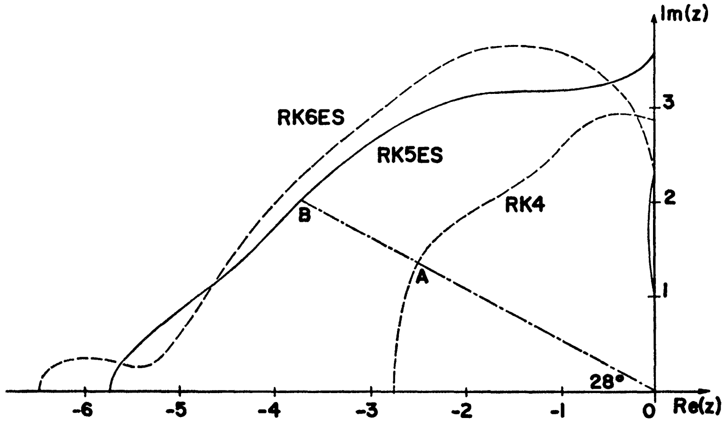

FIG. 2. *Stability regions for Runge-Kutta processes of orders* 4, 5 *and* 6

Butcher in [1] shows that all members have $k = -\frac{7}{3}$. There is thus no optimal member of the two-parameter family, and we therefore examine his four-parameter family in which c_2, c_4, c_5 and c_6 are arbitrary, apart from certain degenerate combinations. Some restrictions inherent in this family are: $b_2 = 0$, $c_7 = 1$ and $2c_4 - (1 + 10c_4)c_3 + 15c_4c_3^2 = 0$. We arbitrarily impose the additional restrictions: $c_2 = \frac{2}{3}c_3$, $c_5 = \frac{1}{2}$, and $c_6 = 1 - c_4$. A consequence of these restrictions is $b_3 = 0$.

Thus, c_1, c_4, c_5, c_6 and c_7 may be considered to be the abscissas and b_1, b_4, b_5, b_6 and b_7 the weights of a member of the one-parameter (c_4) family of closed, symmetric, five-point quadrature formulas. The family of Runge-Kutta processes within which we perform the optimization then reduces to this family of quadrature formulas if $f(x, y)$ in (1.1) is independent of y. Numercial investigation of the solutions to the 37 equations of [1] as a function of c_4 shows that $c_4 = \frac{7}{8}$ gives a process with $k = 0.5497$. Numerical values of $\{c_i\}$, $\{b_i\}$, $\{a_{ij}\}$ for $c_4 = \frac{7}{8}$ are recorded in Table 1. Calculations were performed in FORTRAN II on an IBM 1710 computer using 28S arithmetic. Entries in Table 1 are rounded to 24D.

3. Test problems. In this section we consider the numerical solution of three test problems, by the process developed in §2, which we call RK6ES, by the order five process of [3] called RK5ES, and by the classical order four formula, called RK4.

Problem 1.

$$\begin{aligned} y_1' &= -y_1 + 23y_2, \qquad & y_1(0) &= 1, \\ y_2' &= -y_1 - 25y_2, \qquad & y_2(0) &= 1. \end{aligned} \tag{3.1}$$

Problem 2.

TABLE 1

i	c_i	b_i
1	0.0000000000000000000000	.014285714285714285714286
2	.202276644898140634933337	0.0000000000000000000000
3	.303414967347210952400006	0.0000000000000000000000
4	.8750000000000000000000	.270899470899470899470899
5	.5000000000000000000000	.429629629629629629629630
6	.1250000000000000000000	.270899470899470899470899
7	1.0000000000000000000000	.014285714285714285714286

i	j	a_{ij}
2	1	.202276644898140634933337
3	1	.075853741836802738100001
3	2	.227561225510408214300004
4	1	1.359282217283300317252891
4	2	−5.237885702628806615657060
4	3	4.753603485345506298404170
5	1	−.321092002258021684715280
5	2	1.651353127922382381290896
5	3	−.905286676763720493279991
5	4	.075025551099359796704375
6	1	.292321839349363565719798
6	2	−.748269386089829516522437
6	3	.592470844966485039986419
6	4	−.039554538849143620302490
6	5	.028031240623124531118711
7	1	−20.662761894904085188637368
7	2	63.852320946332118743247958
7	3	−74.151750947688834248615863
7	4	.864117644373384395219349
7	5	14.505481659294823706193336
7	6	16.592592592592592592592588

$$
\begin{aligned}
y_1' &= (-1 - y_2^2)y_1 + 20y_2\,, & y_1(0) &= 0,\\
y_2' &= -20y_1 + (-1 - y_1^2)y_2\,, & y_2(0) &= 1.
\end{aligned}
\tag{3.2}
$$

Problem 3.

$$
\begin{aligned}
y_1' &= (-1 + y_2^2)y_1 + y_2(1 + y_2), & y_1(0) &= -1,\\
y_2' &= -y_1 + (-19 + y_1^2 + 2y_1)y_2\,, & y_2(0) &= 1.
\end{aligned}
\tag{3.3}
$$

Double precision FORTRAN IV programs were written for these problems and were executed on an IBM 7040 computer. In Fig. 3, the error at $t = 1$ is plotted for step-sizes $h = 2^{-m}$, $m = 8, 7, \cdots, 2$. Values of h for which the solutions were unstable are of course, omitted. The error was com-

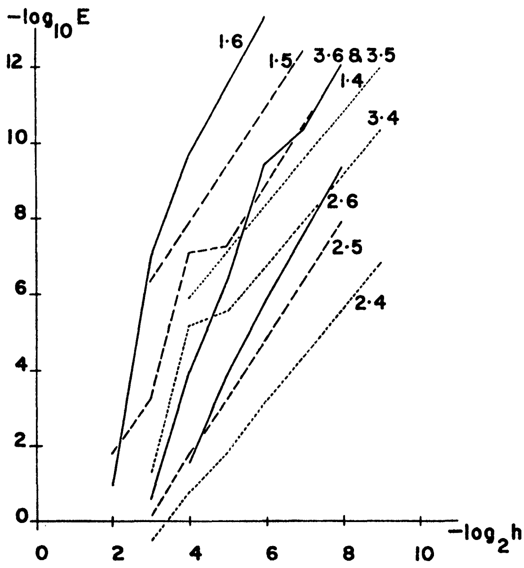

FIG. 3. *Error as a function of step-size. The first digit specifies the problem and the second digit the order of the Runge-Kutta process used.*

puted as the sum of the absolute values of the errors in y_1 and y_2. The numerical solutions produced by RK6ES for $h = 2^{-9}$ were used as approximations to the exact solutions in these comparisons.

Problem 1 is a simple constant coefficient linear system of the form $y' = Ay$, in which matrix A has eigenvalues -2 and -24. By examining the regions of stability for the three Runge-Kutta processes, as given in Fig. 2, we expect to observe instability in RK4 at $h = \frac{1}{8}$, in RK5ES at $h = \frac{1}{4}$, and in RK6ES at $h = \frac{1}{2}$. The numerical experiments confirm this. For this problem, RK6ES is the most efficient, if solutions of relatively high accuracy (say 9S) are desired. Compared to RK4, RK5ES permits a fourfold step-size increase, and RK6ES an eightfold increase. Since the amount of computation per step for the three methods is in the ratio 5:14:24 for trivial derivative evaluations requiring no arithmetic, and approaches the ratio 4:6:7 as the derivative evaluations become arduous, the higher efficiency of RK6ES is apparent.

These observations also hold for Problem 2, namely, RK6ES is most efficient. However, this problem has a lightly damped, highly oscillatory solution for which $y_1(t)$ and $y_2(t)$ have asymptotic values of zero for large t. The corresponding linearized problem, in which the terms y_1^2 and y_2^2 are neglected, may be represented as $y' = Ay$, with A having eigenvalues $-1 \pm 20i$. We see from Fig. 2 that, for problems of this type, the maximum stable step-sizes should be comparable for all three methods. In fact, RK6ES was unstable at $h = \frac{1}{8}$, although RK4 and RK5ES were both stable. This was attributed to the nonlinearity of (3.2), since the point $-0.125 \pm 2.5i$ lies within the region of stability of each of the three formulas, but is very close to the boundary of the region of stability of RK6ES.

For Problem 3, we observe that RK5ES is more efficient than either RK4 or RK6ES. Further, RK5ES is stable at $h = \frac{1}{4}$, but RK6ES is unexpectedly not, presumably because of the nonlinearity of (3.3). The irregular shape of the error graph in this case is perhaps worthy of note. This shows clearly the hazards of the assumption that $E = Ch^K$ for a method of order K, merely because a solution with halved step-size is in agreement to several decimals with a trial solution. We note, however, the validity of the assumption *for h sufficiently small.*

4. Conclusions. If the step-size is constrained solely by stability considerations, the author draws the following conclusions:

(a) For trivial derivative evaluations, RK4 is superior to the new formulas.

(b) For arduous derivative evaluations, RK5ES is more efficient than RK4 if the dominant eigenvalue of the Jacobian matrix has argument in the range $180° \pm 28°$ (approximately), since $OA = (2/3)OB$ in Fig. 2 and RK4 requires two thirds of the number of substitutions per step as RK5ES.

(c) RK5ES is usually more efficient than RK6ES.

If accuracy is the sole arbiter of step-size, then RK6ES and RK5ES seem to be much more efficient than RK4, regardless of derivative complexity or of required accuracy. RK6ES is most efficient for small enough step-sizes, but, as in Problem 3, may be less efficient for step-sizes of practical interest.

In the author's opinion, RK5ES is much superior to RK4 for general use. Any advantages of RK6ES over RK5ES are marginal.

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