

THE MOST STORAGE ECONOMICAL RUNGE-KUTTA METHODS FOR THE SOLUTION OF LARGE SYSTEMS OF COUPLED FIRST-ORDER DIFFERENTIAL EQUATIONS (1)

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ABSTRACT

It is shown how the attainable minimum for the memory requirements of Runge-Kutta methods can be realised for methods of the third order. These economisable third order methods belong to a one parameter sub-family from which two particular members with low error bound are selected.

1. INTRODUCTION

The disposal of an economical computational technique for the solution of systems of differential equations is indispensable either when the systems are very large as in the case of discretised integro-differential equations, semi-discretised partial differential equations and in some physical problems as the calculation of structure images in electron microscopy [1], or when the computer storage capabilities are limited (e.g. desk or hand calculators). For this purpose, Runge-Kutta (RK) methods are preferred, which have the advantage of being self starting and less memory consuming at the expense of stability and calculation time.

When in the course of a fourth order RK calculation, the intermediate computed vectors are linearly dependent, it can be shown that the memory requirements can be reduced to $3N + P$, N being the number of equations and P the storage required by the program. Substitution of this condition into the 4th order RK equation generates a one parameter family [e.g. 2] of fourth order RK methods, from which the methods of Gill [3] and Blume [4] are special members. However, the memory requirements cannot be further reduced as long as the computation of the derivative $Y' = f(x, Y)$ (with Y a column vector) requires two column vectors ($2N$) of storage registers. In this work it is suggested that if the elements $Y'(i)$ of the vector Y' can be computed individually, the storage can be

reduced to the minimum $2N + P$ for RK methods up to the third order. Extension to higher order methods however is proved to be impossible.

2. GENERAL EXPRESSIONS

The basis of all RK methods for the solution of a system of N differential equations in vector form :

$$Y' = f(x, Y) \quad (2.1)$$

with given boundary condition :

$$Y(0) = Y_0$$

is to express the difference between values of the function Y at x_{n+1} and x_n as a linear combination of intermediate computed vectors K_i [e.g. 2, 3].

$$Y_{n+1} - Y_n = \sum_{i=1}^m \omega_i K_i \quad (2.2)$$

with

$$K_i = hf(x_n + a_i h, Y_n + \sum_{j=1}^{i-1} \beta_{ij} K_j) \quad (2.3)$$

and where

$$h = x_{n+1} - x_n \text{ and } a_1 = 0$$

Y and K are column vectors of dimension N .

A Runge-Kutta method of the k th order can be constructed by identification of (2.2) and (2.3) with the

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corresponding Taylor series, expanded to the same order, yielding a number of equations from which the coefficients a_i , β_{ij} and ω_i can be determined. The minimal number of elements in (2.2) is given by $m=k$ for $k \leq 4$ and $m > k$ for $k > 4$. The $(k+1)$ th order term can be used for a rough estimation of the truncation error bound. In the explicit case of third order RK methods, the Runge-Kutta equations can be reduced to a two parameter family of the form [3] :

$$\begin{aligned} \omega_1 &= 1 + \frac{2-3(a_2+a_3)}{6a_2a_3}, & \omega_2 &= \frac{3a_3-2}{6a_2(a_3-a_2)}, \\ \omega_3 &= \frac{2-3a_2}{6a_3(a_3-a_2)}, \\ \beta_{21} &= a_2, & \beta_{31} &= \frac{3a_2a_3(1-a_2)-a_3^2}{a_2(2-3a_2)}, \\ \beta_{32} &= \frac{a_3(a_3-a_2)}{a_2(2-3a_2)} \end{aligned} \quad (2.4)$$

with $a_2 \neq a_3$; $a_2, a_3 \neq 0$; $a_2 \neq 2/3$.

The truncation error $|\gamma|h^3$ can be bounded by using $|\gamma| < \Delta ML^3$

with

$$\begin{aligned} \Delta &= \left\{ 8 \left| \frac{1}{24} - \frac{1}{6}(a_2^3\omega_2 + a_3^3\omega_3) \right| + 4 \left| \frac{1}{24} - \frac{1}{2}a_2^2\beta_{32}\omega_3 \right| \right. \\ &\quad \left. + 4 \left| \frac{1}{8} - a_2a_3\beta_{32}\omega_3 \right| + \frac{1}{12} \right\} \end{aligned} \quad (2.5)$$

where M and L are defined by the assumptions :

$$|f(x, y)| < M, \quad \left| \frac{\partial^{i+j} f}{\partial x^i \partial y^j} \right| < \frac{L^{i+j}}{M^{j-1}} \quad (2.6)$$

for $i + j \leq 3$.

3. REDUCTION OF THE STORAGE REQUIREMENTS

In a general third order RK method, the column vectors to be computed and stored successively are :

$$\begin{aligned} A &: Y_n \\ B &: Y_n + \beta_{21}K_1 \\ C &: Y_n + \beta_{31}K_1 + \beta_{32}K_2 \\ D &: Y_n + \omega_1K_1 + \omega_2K_2 + \omega_3K_3 \end{aligned} \quad (3.1)$$

where A is needed for the computation of K_1 , B for K_2 and C for K_3 using (2.3). When a derivative K vector is computed in its entirety, it cannot be stored without destroying the content of the storage vector. Obviously, this content cannot be used to carry intermediate results, making it impossible to reduce the storage to $2N + P$.

This reduction can be achieved when the elements of a derivative vector are computed individually and combined properly with the content of the storage vector, provided that the vectors : $Y_n + \beta_{21}K_1$, $Y_n + \beta_{31}K_1 + \beta_{32}K_2$, $Y_n + \omega_1K_1 + \omega_2K_2$ are linearly dependent irrespective of the values of Y_n, K_1 and K_2 .

A necessary and sufficient condition is that :

$$\begin{vmatrix} 1 & \beta_{21} & 0 \\ 1 & \beta_{31} & \beta_{32} \\ 1 & \omega_1 & \omega_2 \end{vmatrix} = 0 \quad (3.2)$$

Substitution of (2.4) into (3.2) yields :

$$6a_2^2a_3 - 6a_2a_3^2 + 3a_2a_3 - 3a_2 + 6a_3^2 - 6a_3 + 2 = 0 \quad (3.3)$$

which restricts the number of economisable RK methods to a one-parameter family. This extra parameter can then be used for the minimization of the error-bound coefficient (2.5). Extension of this technique to fourth order RK methods leads to three equations of the type (3.2). Unfortunately, substitution of these equations into the two parameter family of all possible 4th order RK methods leads to inconsistencies.

4. CONSTRUCTION OF TWO PARTICULAR ECONOMICAL RUNGE-KUTTA METHODS WITH MINIMAL ERROR BOUND

In figure 1 the contours of the error bound coefficients Δ of all the 3th order RK methods are plotted in the (a_2, a_3) plane. It can be seen that the method with minimal Δ value corresponds to $a_2 = 1/2$, $a_3 = 3/4$.

The one-parameter family of memory-economical 3th order methods corresponding to equation (3.3) is also indicated as a dashed curve. It is clear that among these, the methods with a minimal Δ value are situated somewhere around $a_2 = 1/2$.

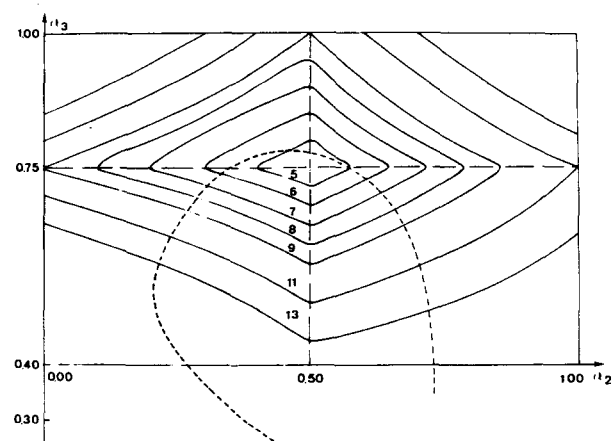


Fig. 1.

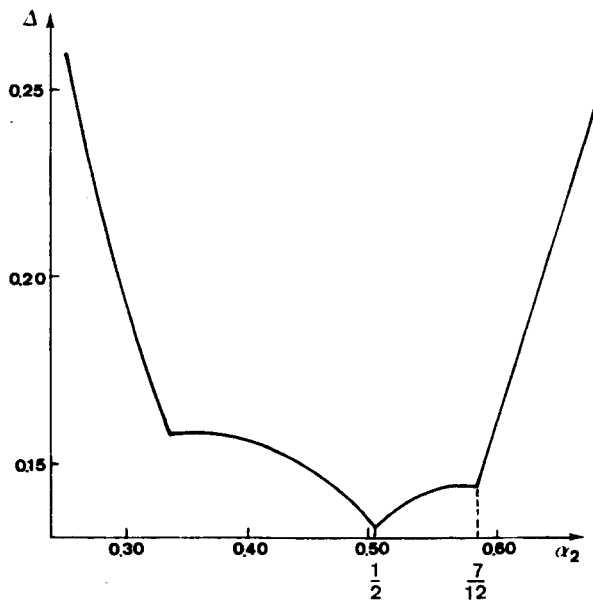


Fig. 2.

In figure 2 the error bound coefficient Δ of the one parameter family of economical 3th order RK methods is plotted in more detail as a function of the independent parameter a_2 . As expected from figure 1 the error bound is minimal in the neighbourhood of $a_2 = \frac{1}{2}$ with two pronounced minima at $a_2 = \frac{1}{2}$ and $a_2 = \frac{7}{12}$ respectively corresponding to $\frac{1}{24} - \frac{1}{2} a_2^2 \beta_{32} \omega_3 = 0$ and $\frac{1}{8} - a_2 a_3 \beta_{32} \omega_3 = 0$ in expression (2.5).

The RK coefficients can be calculated by substitution of $a_2 = 1/2$ resp. $7/12$ into (3.3) and (2.4).

Hence the first RK method ($a_2 = \frac{1}{2}$) takes the explicit form

$$\begin{aligned} K_1 &= hf(x_n, Y_n) \\ K_2 &= hf(x_n + \frac{1}{2}h, Y_n + \frac{1}{2}K_1) \\ K_3 &= hf(x_n + \frac{3+\sqrt{3}}{6}h, Y_n + \frac{(1-\sqrt{3})}{6}K_1 + \frac{\sqrt{3}+1}{3}K_2) \\ Y_{n+1} &= Y_n + (\frac{3-\sqrt{3}}{6})K_1 + (\frac{3-\sqrt{3}}{3})K_2 + (\frac{\sqrt{3}-1}{2})K_3 \end{aligned} \quad (4.1)$$

$$\text{with the error bound from (2.5)} \quad \Delta = \left[\frac{10\sqrt{3}-3}{108} \right] = 0.1326 \quad (4.2)$$

For the second RK method ($a_2 = 7/12$) we obtain :

$$\begin{aligned} K_1 &= hf(x_n, Y_n) \\ K_2 &= hf(x_n + \frac{7}{12}h, Y_n + \frac{7}{12}K_1) \\ K_3 &= hf(x_n + \frac{3}{4}h, Y_n - \frac{3}{28}K_1 + \frac{6}{7}K_2) \\ Y_{n+1} &= Y_n + \frac{5}{21}K_1 + \frac{3}{7}K_2 + \frac{1}{3}K_3 \end{aligned} \quad (4.3)$$

$$\text{with an error coefficient } \Delta = \frac{31}{216} = 0.1435. \quad (4.4)$$

The Δ values of both economised methods are not much larger than the theoretical minimum $\Delta = 0.111$ corresponding with the well known $a_2 = \frac{1}{2}$, $a_3 = \frac{3}{4}$ RK method, which however cannot be economised. Also when applied to concrete problems, the same degree of accuracy was obtained. An extra computational advantage arises from the fact that the coefficients are non-transcendental real numbers.

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