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A STUDY OF SOME NUMERICAL METHODS
FOR THE INTEGRATION OF SYSTEMS OF
FIRST-ORDER ORDINARY DIFFERENTIAL EQUATIONS

by

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ABSTRACT

This study of some numerical methods for the integration of systems of first-order ordinary differential equations describes the extrapolation methods of Bulirsch-Stoer and Neville, presents the results of some tests comparing the extrapolation methods with the Runge-Kutta and Adams-Moulton methods, and shows some of the circumstances under which the extrapolation method may be preferred. Results of double-precision tests of the Bulirsch-Stoer method are presented to show the efficiency of various orders of this method as a function of desired accuracy.

I. INTRODUCTION

The object of this study was to test and compare several methods for integrating systems of coupled first-order ordinary differential equations. The extrapolation methods using the Bulirsch-Stoer extrapolation by rational functions and using Neville's extrapolation by polynomial functions were compared to the widely known Runge-Kutta and Adams-Moulton methods in order to ascertain the merits of the extrapolation methods and to determine the circumstances under which they might be preferable to the more traditional methods.

This work was motivated by the paper¹ presented by Stoer at the IFIP meeting in May 1965 and by a NASA report.² The speed and accuracy of the methods were compared by programming the methods on the same computer and applying each method to the same sets of equations. The number of times the functions to be integrated had to be evaluated to obtain a desired accuracy was used as a computer-independent and program-independent measure of time. The accuracy was compared by using each method to integrate from given initial conditions to some final point at which the relative error was computed.

References for several of the numerical methods used in this report were obtained from Henrici.³

II. COMPUTER CHARACTERISTICS

The computer used was the CDC 3600. Its floating-point operations all round and then normalize the results. The characteristics of the CDC 3600 that greatly affect the time and accuracy of the results are given in the following table:

<u>Characteristic</u>	<u>Single Precision</u>	<u>Double Precision</u>
Word length, bits	48	96
Floating-point fraction length, bits	36	84
Floating-point add time, μsec	4.25	6.38
Floating-point multiply time, μsec	6.4	26.90
Floating-point divide time, μsec	13.0	27.20
Load and Store operations, μsec	1.96	4.75

III. INTEGRATION METHODS USED

The integration methods used are:

- (1) The single-step Runge-Kutta method of order 4.
- (2) The multistep Adams-Moulton method of order 4.
- (3) The single-step method using Bulirsch-Stoer rational-function extrapolation.
- (4) The single-step method using Neville's polynomial extrapolation.

Methods 3 and 4 are of variable order. In the testing of methods 1 and 2, a slightly modified form of the COOP program RKAM,⁴ written at the University of Texas, was used. For methods 3 and 4, the program pair, DIFSUB and DIFSYS,⁵ used was written at Argonne National Laboratory and is based on the algorithm of Bulirsch and Stoer.¹

The following descriptions of the Runge-Kutta and Adams-Moulton methods are adapted from the University of Texas program write-up for RKAM.⁴

IV. RUNGE-KUTTA METHOD

In the Runge-Kutta method, only one initial condition is given for each dependent variable, namely the values at the starting value for the independent variable.

Let the dependent variables be denoted by $y_1, y_2, \dots, y_n$, where n is the order of the system, let x denote the independent variable, and let the differential equations be given by

$$\frac{dy_i}{dx} = F_i(x, y_1, y_2, \dots, y_n),$$

where $i = 1, 2, \dots, n$, for a system of n equations. The formulas are of fourth-order accuracy and have the form

$$y_{i,1} = y_i + \frac{1}{6}(K_{0,i} + 2K_{1,i} + 2K_{2,i} + K_{3,i}),$$

where

$$K_{0,i} = hF_i(x, y_1, y_2, \dots, y_n),$$

$$K_{1,i} = hF_i(x + \frac{1}{2}h, y_1 + \frac{1}{2}K_{0,1}, y_2 + \frac{1}{2}K_{0,2}, \dots, y_n + \frac{1}{2}K_{0,n}),$$

$$K_{2,i} = hF_i(x + \frac{1}{2}h, y_1 + \frac{1}{2}K_{1,1}, y_2 + \frac{1}{2}K_{1,2}, \dots, y_n + \frac{1}{2}K_{1,n}),$$

$$K_{3,i} = hF_i(x + h, y_1 + K_{2,1}, y_2 + K_{2,2}, \dots, y_n + K_{2,n}),$$

$$y_i = y_i(x),$$

and

$$y_{i,1} = y_i(x+h).$$

The above addition is carried out in partial double precision, with y_i in double precision, the increment added in single precision, and $y_{i,1}$, their sum, in double precision.

The new values of the derivatives can now be calculated by

$$F_{i,1} = F_i(x+h, y_{1,1}, y_{2,1}, \dots, y_{n,1}),$$

where $i = 1, 2, \dots, n$.

V. ADAMS-MOULTON METHOD

The method attributed to Adams and Moulton, sometimes known as the modified Adams method, is referred to as one of the closed type of predictor-corrector formulas. When this method is applied to a system of equations, the predicted values are calculated by

$$y_{i,1}^{[p]} = y_i + \frac{h}{24}(55F_i - 59F_{i,-1} + 37F_{i,-2} - 9F_{i,-3}),$$

where

$$y_{i,s} = y_i(x + sh),$$

$$F_{i,s} = F_i(x + sh, y_{1,s}, y_{2,s}, \dots, y_{n,s}),$$

$$y_i = y_i(x),$$

and

$$F_i = F_{i,0},$$

with $i = 1, 2, \dots, n$. The corrected values can now be calculated by

$$y_{i,1}^{[c]} = y_i + \frac{h}{24} (9F_{i,1}^{[p]} + 19F_i - 5F_{i,-1} + F_{i,-2}),$$

where

$$F_{i,1}^{[p]} = F_i(x + h, y_{1,1}^{[p]}, y_{2,1}^{[p]}, \dots, y_{n,1}^{[p]}),$$

with $i = 1, 2, \dots, n$. The corrected values are now accepted as the new values of the dependent variables, with

$$y_{i,1} = y_{i,1}^{[c]}, \quad i = 1, 2, \dots, n.$$

The new values of the derivatives may be found by

$$F_{i,1} = F_i(x + h, y_{1,1}, y_{2,1}, \dots, y_{n,1}),$$

with $i = 1, 2, \dots, n$. Again the addition is performed in partial double-precision arithmetic with y_i in double precision, the increment added in single precision, and $y_{i,1}^{[c]}$ the sum in double precision. The predicted values $y_{i,1}^{[p]}$ are calculated by using floating-point arithmetic.

The three additional starting values needed for this method are supplied by the Runge-Kutta method in Section IV above.

VI. THE EXTRAPOLATION METHODS

The following descriptions of the Stoer and the Neville methods are from the Argonne program write-up of DIFSUB:⁵

Derivation: The system $y' = F(x, y_1), \dots, y_n$ is integrated from x_0 to $x = x_0 + H$ by the modified midpoint rule (see Ref. 1, p. 2) using first a step size h_1 , then a step size h_2 , etc., where

$$h_k = H, \frac{H}{2}, \frac{H}{3}, \frac{H}{4}, \frac{H}{6}, \frac{H}{8}, \frac{H}{12}, \frac{H}{16}, \frac{H}{24}, \frac{H}{32}, \frac{H}{48}, \frac{H}{64} \quad \text{for } k = 1, 2, 3, \dots, 12, \text{ respectively.} \quad (1)$$

The result is a sequence of approximations $T(h_k, x)$ to $y(x)$, such that

$$T(0, x) = \lim_{h_k \rightarrow 0} T(h_k, x) = y(x). \quad (2)$$

A. The Bulirsch-Stoer Method

Interpolation of the first $m + 1$ values $T(h_k, x)$, beginning with $m = 0$, yields a rational function of the form

$$\hat{T}_m(h) = \frac{p_0 + p_1 h^2 + \dots + p_u h^{2u}}{1 + q_1 h^2 + \dots + q_v h^{2v}}, \quad \text{where } u = \left\lfloor \frac{m}{2} \right\rfloor \text{ and } v = m - u, \quad (3)$$

which can be extrapolated to $h = 0$, giving an estimate of $T(0, x)$. Then, for each new approximation $T(h_k, x)$, a new rational function $\hat{T}_m(h)$ is determined and extrapolated to obtain $\hat{T}_m(0)$. Consecutive approximations with $k = m + 1 = 1, 2, 3, \dots$, are obtained until either the desired accuracy is attained, i.e., two consecutive values $\hat{T}_{m-1}(0)$, $\hat{T}_m(0)$ differ by an amount less than the error criterion, or until m has reached a predetermined value M . (Note that M is an input parameter which is allowed to take on the values 4 through 10.) If sufficient accuracy has not yet been attained when m reaches M , then the order of the rational function remains constant at M , and consecutive approximations $\hat{T}_{M,i}(h)$, $i = 1, 2, \dots$, are defined by the requirement $\hat{T}_{M,i}(h_k) = T(h_k, x)$ for $k = i + 1, i + 2, \dots, i + M + 1$. Consecutive approximations $\hat{T}_{M,i}(0)$, $\hat{T}_{M,i-1}(0)$ (where $\hat{T}_{M,0}(0) = \hat{T}_m(0)$) are compared until sufficient accuracy is obtained or until i reaches 3. If sufficient accuracy has not been attained at this point, H is replaced by $H/2$ and the method is repeated for this smaller step. A thorough derivation and justification of the Bulirsch-Stoer method appear in Ref. 1, pp. 2-5.

B. The Neville Method

The interpolation method of Neville,^{6,7} with the same modified midpoint rule for integration, is derived similarly, using instead of Eq. 3 the equation

$$\hat{T}_m(h) = a_0 + a_1 h^2 + \dots + a_m h^{2m}, \quad (4)$$

and substituting the word "polynomial" for the word "rational" in the derivation above. The stability conditions are known, and convergence has been proved for the Neville method.

Although some double-precision arithmetic might have been profitably employed in the Bulirsch-Stoer and Neville methods (as it was in the Runge-Kutta and Adams-Moulton methods), the code used for the single-precision tests of these methods contained no double precision.

Error Analysis

It has been shown (in Ref. 1, p. 8) that if M is the order of the rational extrapolation function, and h_k , $k = 1, 2, \dots$, are the h 's of Eq. 1, then, under certain hypotheses (see Refs. 8-10), the error is of the form

$$\hat{T}_{M,K} - T(0) = (-1)^M h_k^2 \times h_{k+1}^2 \times h_{k+2}^2 \times \dots \times h_{k+M}^2 \left[\tau_{k+1} + o(h_k^2) \right].$$

VII. A COMPARISON OF METHODS IN SINGLE PRECISION

A. On the Negative-exponential Problem

In this first portion of the study of these numerical methods, the comparisons made were based on the performance of the four methods in the solution of several rather arbitrarily chosen problems. The first problem, the negative-exponential equation $y' = -y$, is a traditional test. This problem was chosen as the first test because it is one of the simplest applicable problems, it is naturally a constant-step-size problem, and correct results are easily available for any point.

The initial conditions used were $x = 0$, $y(0) = 1$. Integration steps from the initial conditions out to $x = 20$ ($e^{-20} = 2.06115\ 36224\ 38557\ 828 \times 10^{-9}$) were performed for several step sizes with each method. At $x = 20$, the relative error $[y(20) - e^{-20}] / e^{-20}$ was computed and this error was plotted on a log-log scale versus the number of times the function F was evaluated in reaching $x = 20$ by the particular method. The results of these tests using single-precision arithmetic are shown in Fig. 1. Notice that round-off

Fig. 1. A Comparison of Four Numerical Methods, Using Single Precision to Extrapolate the Negative-exponential Equation

Bulirsch-Stoer method with $M = 6$ were nearly the same. The Adams-Moulton method took about $5/3$ as long as the other three methods per function evaluation.

error effects are appreciable in the results from the Runge-Kutta method when the number of function evaluations is greater than 7000.

Following the example in Ref. 1, the extrapolation methods of Bulirsch-Stoer and Neville were first tested with $M = 6$, that is, with an error of order $H^{14}/(2 \cdot 3 \cdot 4 \cdot 6 \cdot 8 \cdot 12)^2$. This was a rather fortunate choice since 6 proved to be the most efficient choice for M for this problem for the range of relative error from 10^{-10} to 10^{-5} . For relative errors greater than 10^{-5} , greater efficiency can be achieved with a value of M less than 6.

From Fig. 1, we can conclude that the Bulirsch-Stoer method is preferable when we desire relative errors less than 10^{-4} and that the Adams-Moulton method is preferable for larger relative errors. The relative speeds of the four methods will vary for each computer and program. However, with the programs used on the CDC 3600, the speeds (in function evaluations per second) of the Runge-Kutta method, the Neville method with $M = 6$, and the

B. On Euler's Equation of Motion for Rigid Bodies

The second problem chosen was the Euler equation of motion in three-dimensional space for a rigid body without external forces, a system of three coupled first-order differential equations. The equations and initial condition used were as follows:

$$y' = \begin{Bmatrix} y_1' \\ y_2' \\ y_3' \end{Bmatrix} = \begin{Bmatrix} y_2 y_3 \\ -y_1 y_3 \\ -k^2 y_1 y_2 \end{Bmatrix}, \quad x = 0, \quad y(0) = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad k^2 = 0.51, \quad \text{from } x = 0 \text{ to } x = 60.$$

The solution of the Euler equation is a Jacobian elliptic function where $y_1 = \text{sn}(x|k^2)$, $y_2 = \text{cn}(x|k^2)$, and $y_3 = \text{dn}(x|k^2)$. For $k^2 = 0.51$, $x = 60.0$, the values of sn, cn, and dn are $\text{sn} = 0.380572994334$,

cn = 0.92475 0883190, and dn = 0.96235 8425924. A plot of the three components of motion sn, cn, and dn with time is shown in Fig. 2.

Fig. 2

Plot of Components of Motion
(sn, cn, and dn) with Time

The results of tests run, using the same four methods as used for the first problem, are shown in Fig. 3. The error plotted on this graph is the square root of the sum of the squares of the errors in y_1 , y_2 , and y_3 .

For this problem, the results obtained by using the Bulirsch-Stoer method and Neville's method are nearly the same and both are to be preferred over the Runge-Kutta or Adams-Moulton method for relative errors less than 10^{-5} . Round-off error effects can be observed in the results from the Adams-Moulton method for cases with more than 5000 function evaluations, and in the results from the Runge-Kutta method for cases with more than 10,000 function evaluations.

C. On Bessel's Equation

The third problem chosen was the Bessel equation of order 16, with solution J_{16} . This problem was used by Nordsieck to test his method¹¹ and was later used by Gear¹¹ in his test of hybrid methods. The second-order ordinary differential equation

$$y'' + \frac{y'}{x} - \left(\frac{256}{x^2} - 1 \right) y = 0$$

was solved using the pair of first-order equations $y_1' = y_2$ and

$$y_2' = \left(\frac{256}{x^2} - 1 \right) y_1 - \frac{y_2}{x}.$$

Integration proceeded from $x = 6$ to $x = 6138$. The initial conditions used were $y_1(6) = 1.20194993 \times 10^{-6}$, $y_2(6) = 2.98647976 \times 10^{-6}$. J_{16} has its largest magnitude at its first crest at $x \sim 18.1$. The errors given below are

$$y_1' = y_2 y_3, \quad y_2' = -y_1 y_3, \quad y_3' = -0.51 y_2 y_3$$

from $x_0 = 0$, $y(0) = (0, 1, 1)$, to $x = 60$

Fig. 3 Comparison of Four Numerical Methods, Using Single Precision to Extrapolate Euler's Equation

the average of the magnitudes of the errors in y at $x = 6132, 6134, 6136$, and 6138 , relative to the value $y(18.1) \cong 0.2612$. The results at the four values of x are

$$y(6132) = 4.130472 \times 10^{-3},$$

$$y(6134) = 6.749666 \times 10^{-3},$$

$$y(6136) = -9.745831 \times 10^{-3},$$

and

$$y(6138) = 1.362485 \times 10^{-3}$$

Fig. 4. Plot of $J_{16}(x)$ from $x = 0$ to $x = 60$

A plot of $J_{16}(x)$ from $x = 0$ to $x = 60$ is shown in Fig. 4. Notice that at $x = 6$ the solution is still quite small. The test results for the third problem are shown in Fig. 5. This graph indicates that for this problem the Bulirsch-Stoer method with $M = 6$ is again preferable for errors less than 10^{-3} .

VIII. A STUDY OF EXTRAPOLATION METHODS IN DOUBLE PRECISION

A. On the Negative-exponential Problem

In this second portion of this study, comparisons were made within the extrapolation methods, varying the order of the extrapolating function to determine the efficiency of using a particular order method to obtain a particular accuracy. Various orders of the Bulirsch-Stoer and Neville methods, were used to integrate the negative exponential and to integrate the restricted three-body problem. Both the Neville and the Bulirsch-Stoer methods are ideal for this type of study since the order of the extrapolating function is extremely easy to change and can in fact be an input parameter. This type of study would be considerably more difficult for the Adams-Moulton or Runge-Kutta method. All computations in this portion of the study were done in double precision. Relative errors less than 10^{-22} were achieved without appreciable round-off error effects. The negative-exponential problem was integrated from $x = 0$, $y(0) = 1$,

$$y_1' = y_2, \quad y_2' = \left(\frac{256}{x} - 1\right)y_1 - \frac{y_2}{x},$$

from $x_0 = 6$, to $x = 6138$

Fig. 5. A Comparison of Four Numerical Methods, Using Single Precision to Extrapolate Bessel's Equation J_{16}

to $x = 20$ as before. For this part of the study, the step size and the form and order of the extrapolating function were kept constant and the relative error was computed but was not used as a criterion for step-size change or conversion. Several step sizes were used with each value of M from $M = 4$ to $M = 11$ for both the Bulirsch-Stoer rational-function extrapolation and Neville's polynomial extrapolation to produce results shown in Fig. 6. The cases for Neville's method for odd values of M were not computed since there is no reason to suspect an odd/even phenomenon to appear for that method. A minor odd/even phenomenon did appear using the Bulirsch-Stoer method, odd values of M tending to be more efficient for very small relative errors and the even values of M more efficient for relative errors larger than 10^{-16} . On the whole, the Bulirsch-Stoer rational-function method is more efficient than Neville's method. Figure 7 presents cross plots of the same information as was plotted on Fig. 6 with the addition of lines of constant execution time. These figures show, as would be expected, that the order of the optimum method goes up with the number of digits of accuracy needed.

$$\frac{p_0 + p_1 h^2 + p_2 h^4 + \dots + p_u h^{2u}}{q_0 + q_1 h^2 + q_2 h^4 + \dots + q_v h^{2v}}, \quad \frac{p_0 + p_1 h^2 + p_2 h^4 + \dots + p_u h^{2u}}{q_0 + q_1 h^2 + q_2 h^4 + \dots + q_v h^{2v}}, \quad a_0 + a_1 h^2 + a_2 h^4 + \dots + a_M h^{2M}$$

for $u = \frac{M-1}{2}, v = \frac{M+1}{2}$ for $u = v = M/2$

Fig. 6. Number of Function Evaluations vs. Relative Error with Results of Double-precision Tests on the Negative-exponential Problem Using Extrapolating Functions of Varying Order and Form

Fig. 7. Number of Function Evaluations vs. Order of Extrapolating Function with Lines of Constant Relative Error for Rational and Polynomial Extrapolating Functions

B. On the Restricted Three-body Problem

The next problem used to study various orders of the extrapolation methods is described in Ref. 2, p. 5, as follows:

"This problem is known as the restricted three-body problem. Here three masses are assumed to attract each other by an inverse square force but one of the bodies is considered small enough so that its influence on the motion of the other two can be neglected. It is also assumed that the motion takes place in a plane and that the distance between the two massive bodies remains fixed. In the rotating coordinate system in which the two massive bodies appear to be at rest, the equations of motion for the restricted three-body problem are:

$$x'' = x + 2y' - (1 - \mu) \frac{x + \mu}{[(x + \mu)^2 + y^2]^{3/2}} - \mu \frac{x - 1 + \mu}{[(x - 1 + \mu)^2 + y^2]^{3/2}}$$

$$y'' = y - 2x' - (1 - \mu) \frac{y}{[(x + \mu)^2 + y^2]^{3/2}} - \mu \frac{y}{[(x - 1 + \mu)^2 + y^2]^{3/2}}$$

Here the two massive bodies are located on the x axis with the center of mass of the system at the origin, μ is the ratio of the mass of the body located on the positive x axis to the mass of the entire system. The units of distance here are chosen so that the

distance between the two massive bodies is unity, and the unit of time is chosen so that the angular velocity of the rotating reference frame is unity (period 2π)."

The above equations for x'' and y'' , along with the accompanying three sets of initial conditions and parameters, determine the three periodic earth-moon-satellite orbits shown in Fig. 8.

ORBIT 1

$x_0 = 1.2,$
 $y_0 = 0,$
 $\dot{x}_0 = 0,$
 $\dot{y}_0 = -1.04935750983031990726,$
 $\mu = 0.0121285627653123104912068,$
 period = 6.19216933131963970674.

ORBIT 2

$x_0 = 0.994,$
 $y_0 = 0,$
 $\dot{x}_0 = 0,$
 $\dot{y}_0 = -2.0317326295573368357302058,$
 $\mu = 0.012277471,$
 period = 11.124340337266085134999734.

ORBIT 3

$x_0 = 0.994,$
 $y_0 = 0,$
 $\dot{x}_0 = 0,$
 $\dot{y}_0 = -2.1138987966945026682938111,$
 $\mu = 0.012277471,$
 period = 5.4367954392601899689796307.

Fig. 8. Periodic Earth-Moon-Satellite Orbits

The initial conditions for orbit 1 are known to 19 decimal places. The initial conditions for orbits 2 and 3 are believed to be good to 24 significant figures.

The following experiment was performed on the three orbits of the restricted three-body problem to test the interdependency of the single-step errors in the problem. First, a number of orbit calculations were performed using the Bulirsch-Stoer method with a single-step relative error criterion of 10^{-20} using various step sizes and orders of rational extrapolating function so that the errors in the results at the end of one orbit would generally be less than 10^{-18} . Tables I-III in the Appendix, show some of these results. Then an intentional error greater than 10^{-18} was introduced into the initial velocity, $\dot{y}$, and the orbit calculations were redone. For orbit 1, each initial error 10^{-r} ($r = 4, 8, 12$, and 16) in the velocity, $\dot{y}$, resulted in an error of 0.2×10^{-r} in the position, x , and 2.5×10^{-r} in the velocity, $\dot{x}$, at the end of one orbit. These results do not show a serious error-dependency problem for orbit 1. For orbit 2, initial errors in velocity, $\dot{y}$, of 2×10^{-r} ($r = 8, 12$, and 16) resulted in an error of 38.3×10^{-r} in the position, x , an error of 1081×10^{-r} in the x component of the velocity, and an error of 587×10^{-r} in the y component of the velocity at the end of one orbit. For orbit 3, initial errors in velocity, $\dot{y}$, of 2×10^{-r} ($r = 8, 12$, and 16) resulted in an error of 15.0×10^{-r} in the position, x , an error of 705×10^{-r} in the x component of the velocity, and an error of 2215×10^{-r} in the y component of the velocity. These results indicate that for orbits 2 and 3 there is a serious problem of interdependency of single-step errors, and it will therefore be necessary in general to demand that the single-step errors be much smaller than the maximum tolerable error for the orbit. Notice that the errors shown in Tables I-III in the Appendix are less than the errors resulting from these deliberately introduced initial errors, indicating that the errors introduced at each step of the integration are very small.

The restricted three-body, earth-moon-satellite problem formulated as a first-order system was used as a double-precision test of several orders of the Bulirsch-Stoer method. Several cases were also used to test Neville's method of extrapolation using polynomials. In these tests, the Bulirsch-Stoer method generally gave somewhat better results than the Neville method. Therefore the greater part of the double-precision study was performed only with the Bulirsch-Stoer method.

The Bulirsch-Stoer method with rational extrapolating functions of the form

$$\frac{p_0 + p_1 h^2 + \dots + p_u h^{2u}}{q_0 + q_1 h^2 + \dots + q_v h^{2v}},$$

where

$$u = \left\lceil \frac{M}{2} \right\rceil$$

and $v = M - u$, was tested for values of M from 4 through 10 with single-step relative-error criteria ϵ of 10^{-4} , 10^{-8} , 10^{-12} , 10^{-16} , and 10^{-20} . The results of these tests are shown in Tables I-III in the Appendix and in Fig. 9. The order of the method, M , shown is the average order used. In practice, about half the steps taken were of order M , about one-third were of order $M - 1$, about one-sixth were of order $M + 1$, and there were occasionally steps of order $M - 2$ or $M + 2$. The step size of the succeeding step was chosen, dependent upon the order of the rational approximation necessary to satisfy the error criterion, as follows: If the order of the present step was J and the desired order was M , then, if $J > M$, the next step size was computed as $2^{(M-J)/2}$ times the present step size; if $J = M$, the step size remained the same; and if $J < M$, the new step size was computed as $[1 + (M - J)/6]$ times the present step size. This rule for increasing the step size (which is more conservative than the Bulirsch-Stoer rule) was used because the penalty for taking a step that is smaller than optimum is often much less than the penalty for taking a step that is too large. Therefore, it was often necessary to increase the step size in several consecutive steps. Steps that are too small and steps that are too large can cause a time loss due to inefficiency, and both can cause a loss of accuracy; but a small step size causes a loss in accuracy by necessitating more steps and giving more chance for errors to accumulate, while large steps may cause instability or difficulty in convergence due to an accumulation of errors within the step.

Fig. 9. Averages of Results for Tests Made on Earth-Moon-Satellite Orbits 1, 2, and 3 Comparing Various Orders of the Bulirsch-Stoer Method

It is difficult to compare the results of these tests with those done on the same orbits at Georgia Institute of Technology,¹² especially because of the error-dependency problem in orbits 2 and 3. Because the tests were performed on different computers, time cannot be compared. For orbit 1, the number of function evaluations needed to obtain an accuracy of 10^{-12} with the Bulirsch-Stoer method was fewer than the number listed in Table XXII of the Georgia Tech report¹² for the Runge-Kutta-Shanks, Adams-Bashforth-Moulton, Stoermer-Cowell, and Cowell constant, Nth-order-difference methods and was more than for the Runge-Kutta-Fehlberg and Stetter-Gragg-Butcher methods.

According to the results in Table XXIV of Ref. 12, to obtain an accuracy of 10^{-16} on orbit 1, the Bulirsch-Stoer method took fewer function evaluations than the Runge-Kutta-Shanks method and more than the rest of the methods tested. On orbit 2, according to results in Ref. 7, only the Runge-Kutta, Fehlberg method was capable of accuracies of 10^{-16} , while the Bulirsch-Stoer method can attain accuracies greater than 10^{-16} with each of its orders from $M = 6$ through $M = 10$. On orbit 3, the Bulirsch-Stoer method needed fewer function evaluations than the Runge-Kutta-Shanks method, more than the Runge-Kutta-Fehlberg method, and about the same number as the Cowell constant-Nth-order-difference method.

The next experiment compared the accuracy achievable with the Bulirsch-Stoer method using various rules for choosing the step size. By appropriate adjustments of parameters, runs for each of the three orbits were obtained with the variable-step rule previously described, a constant distance step, and a constant time step. Each of these integrations required about 200 steps and used approximately the same number of function evaluations per step.

Figure 10 shows plots of these solutions with scaled velocity vectors emanating from the orbital position at each step. The origin of coordinates is at the center of mass of the earth-moon system, the earth being centered on the negative x-axis near the origin, and the moon on the positive x-axis.

Figure 10 verifies that the choice of either equal time steps or equal distance steps is poor. In each case, the sparseness of steps in the regions of greatest orbital velocity is reflected in the poor overall accuracy of the solution. For constant time steps, the average error for the three orbits was approximately 10^{-6} ; for constant distant steps, it was about 10^{-8} . This should be contrasted with an average error of about 10^{-13} when the routine was allowed to choose its own step size, i.e., to take smaller steps in the regions of greatest change.

Orbit 1, Bulirsch-Stoer Integration Steps,
 $\epsilon = 10^{-14}$, $M = 5$

Orbit 1, with Constant Distance Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 8$

Orbit 1, with Constant Time Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 8$

Orbit 2, Bulirsch-Stoer Integration Steps,
 $\epsilon = 10^{-14}$, $M = 5$

Orbit 2, with Constant Distance Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 9$

Orbit 2, with Constant Time Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 10$

Orbit 3, Bulirsch-Stoer Integration Steps,
 $\epsilon = 10^{-14}$, $M = 5$

Orbit 3, with Constant Distance Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 9$

Orbit 3, with Constant Time Steps,
 $\epsilon = 2.5 \times 10^{-7}$, $M = 9$

Fig. 10. Comparison of Three Algorithms for Choosing Size of Integration Step for Periodic Orbits Shown with Velocity Vectors Emanating from Orbital Position at Each Step

IX. CONCLUSIONS

The results of the cases run on the four methods tested indicate that the efficiency of the solution of systems of differential equations is quite dependent on the proper matching of the order of the method of solution to the desired accuracy. For example, consider the graphs (Figs. 1, 6, and 7) showing the results of tests on the negative-exponential equation. On Fig. 7, to obtain a relative error of 10^{-16} , the Neville method with $M = 4$ takes twice as long as the method with $M = 6$ and about two and one-half times as long as the shortest time, that for $M = 10$. If the lines for the Runge-Kutta fourth-order method and the Adams-Moulton fourth-order method shown on Fig. 1 were extrapolated to the point at which the relative error was 10^{-16} , we could estimate that these fourth-order methods would take about 160 times as long as Neville's method with $M = 10$ or about 250 times as long as the Bulirsch-Stoer method with $M = 10$. Even at relative errors of 10^{-9} , the Adams-Moulton and Runge-Kutta methods take about nine times as long as the Neville and Bulirsch-Stoer methods with $M = 6$. At the other extreme, if a rough estimate is desired and errors up to 10^{-2} could be tolerated, then Neville's method with $M = 10$ would take almost seven times as long as the fourth-order Adams-Moulton method, and the methods of lower order would be preferable.

The double-precision tests of the Bulirsch-Stoer method show it to be quite powerful for high-accuracy work. With the modification described here for a conservative step-increasing rule, and the ease of changing order, this method seemed especially capable of coping with the changing difficulty of solution of the equations presented to it.

APPENDIX

Results of Tests of the Bulirsch-Stoer Method on Periodic OrbitsTABLE I. Results of Tests of the Bulirsch-Stoer
Method on Periodic Orbit 1

Order M	Time, sec	Number of Function Evaluations	Number of Steps	Error at End of One Period, in Units of Allowed Single-step Error		
				For x	For x	For $\dot{y}$
Single-step Relative-error Criterion: 10^{-19}						
6	56.0	19,744	280	0.3	0.3	0.2
7	43.7	15,540	156	0.2	0.9	0.2
8	38.6	15,131	107	0.4	1.4	0.4
9	38.1	15,693	74	0.1	0.7	0.04
10	50.9	21,789	63	0.1	1.2	0.04
Single-step Relative-error Criterion: 10^{-16}						
5	39.9	14,830	310	0.7	4.3	0.8
6	26.9	10,505	153	0.5	2.4	0.5
7	25.5	10,271	103	1.0	0.8	0.8
8	28.2	11,721	75	0.5	0.8	0.6
9	32.3	13,789	59	0.1	0.2	0.06
10	41.0	17,992	48	1.5	1.8	1.3
Single-step Relative-error Criterion: 10^{-12}						
4	22.9	8,387	263	0.2	0.4	0.2
5	15.3	5,788	124	0.9	1.0	0.8
6	14.9	5,803	84	0.5	0.9	0.3
7	17.7	7,153	62	0.8	0.2	0.7
8	20.3	8,442	49	1.8	3.2	2.2
9	23.8	10,139	39	0.1	0.1	0.08
10	24.5	10,785	29	0.2	0.3	0.2
Single-step Relative-error Criterion: 10^{-8}						
4	8.4	3,036	98	4.6	9.6	4.4
5	8.1	3,036	61	3.7	8.9	3.0
6	10.2	4,013	49	4.5	27.7	5.3
7	12.5	5,024	41	0.7	1.5	0.7
8	15.1	6,344	31	5.2	40.2	6.3
9	18.9	8,160	27	0.4	2.4	0.5
10	22.1	9,731	22	1.6	3.8	1.4
Single-step Relative-error Criterion: 10^{-4}						
4	6.1	2,224	64	5.8	47.4	7.1
5	6.7	2,565	42	2.4	6.3	2.2
6	7.0	2,790	30	3.1	4.3	2.7
7	10.4	4,274	27	2.7	15.9	2.8
8	12.0	5,121	21	5.4	34.7	6.2
9	17.3	7,563	21	4.8	8.9	4.3

TABLE II Results of Tests of the Bulirsch-Stoer
Method on Periodic Orbit 2

Order M	Time, sec	Number of Function Evaluations	Number of Steps	Error at End of One Period, in Units of Allowed Single-step Error		
				For x	For x	For y
Single-step Relative-error Criterion 10 ⁻²⁰						
6	74.4	27,626	386	0.5	13.5	74.0
7	51.6	19,210	190	0.4	1.2	7.0
8	43.3	16,934	118	0.9	26.0	143.0
9	44.3	18,170	85	0.4	0.2	1.0
10	49.0	20,894	66	0.3	8.5	46.0
Single-step Relative-error Criterion 10 ⁻¹⁶						
5	42.9	16,319	339	0.1	2.7	14.6
6	30.5	11,915	171	0.2	4.8	26.5
7	25.2	10,158	102	0.2	4.4	23.1
8	27.5	11,376	76	0.2	5.5	30.2
9	30.6	13,033	58	0.2	5.2	28.3
10	33.2	14,467	44	0.04	1.3	6.7
Single-step Relative-error Criterion 10 ⁻¹²						
4	27.4	10,081	313	0.1	2.0	17.0
5	16.8	6,347	135	2.2	61.8	342.0
6	15.0	5,861	85	0.1	2.5	20.0
7	16.0	6,402	62	0.2	4.6	25.0
8	16.7	6,949	45	0.6	16.5	90.0
9	18.9	8,045	37	0.4	12.3	67.0
10	21.7	9,463	31	0.3	8.2	45.0
Single-step Relative-error Criterion 10 ⁻⁸						
4	8.8	3,191	103	0.1	3.7	21.0
5	8.0	2,993	63	0.4	11.6	57.0
6	9.0	3.533	48	1.2	3.5	190.0
7	8.6	3,455	35	1.2	31.1	178.0
8	10.5	4,351	30	0.9	24.5	135.0
9	10.0	4,167	25	0.06	1.7	10.0
10	12.7	5,482	23	0.01	0.0	2.0
Single-step Relative-error Criterion 10 ⁻⁴						
4	5.3	1,923	59	0.5	12.8	80.0
5	4.3	1,573	37	0.08	3.4	13.0
6	3.9	1,460	28	2.7	6.5	509.0
7	6.3	2.527	27	1.0	19.4	164.0
8	7.5	3.110	23	0.7	14.1	120.0
9	8.5	3,605	21	4.1	236.6	479.0

TABLE III Results of Tests of the Bulirsch-Stoer
Method on Periodic Orbit 3

Order M	Time, sec	Number of Function Evaluations	Number of Steps	Error at End of One Period, in Units of Allowed Single-step Error		
				For x	For x	For y
Single-step Relative-error Criterion 10^{-20}						
6	63.6	23,499	331	0.1	3.8	12.0
7	51.2	17,865	177	0.2	8.2	15.0
8	40.6	15,879	111	0.1	2.5	9.0
9	42.7	17,527	81	0.1	6.6	19.0
10	49.2	21,015	63	0.5	28.5	71.0
Single-step Relative-error Criterion 10^{-16}						
5	38.1	14,475	303	0.6	27.3	87.0
6	26.9	10,481	153	0.3	11.8	37.0
7	23.6	9,496	96	0.02	1.1	3.7
8	25.6	10,634	70	0.1	6.6	22.0
9	31.7	13,522	57	0.08	5.9	12.0
10	37.3	16,306	46	0.1	4.8	15.0
Single-step Relative-error Criterion 10^{-12}						
4	22.1	8,119	255	0.08	3.7	11.0
5	15.5	5,854	126	0.01	0.5	1.6
6	14.0	5,477	78	6.1	282.0	894.0
7	16.0	6,435	60	0.01	0.7	2.0
8	18.5	7,688	46	0.02	0.7	2.4
9	19.3	8,301	34	0.09	4.5	13.0
10	22.0	9,649	29	0.02	1.2	3.8
Single-step Relative-error Criterion 10^{-8}						
4	7.9	2,851	93	0.3	10.8	39.0
5	7.9	2,960	61	0.3	13.7	43.0
6	9.6	3,783	47	0.9	46.3	138.0
7	10.2	4,160	35	2.3	107.0	340.0
8	13.6	5,704	31	0.4	19.5	64.0
9	12.6	5,414	24	0.07	3.3	11.0
10	16.3	7,202	22	1.0	47.1	151.0
Single-step Relative-error Criterion 10^{-4}						
4	4.9	1,751	57	1.2	67.0	178.0
5	5.2	1,961	38	0.6	30.5	90.0
6	5.8	2,272	28	0.3	13.0	43.0
7	3.8	1,461	20	0.02	2.0	2.0
8	6.5	2,685	19	1.9	113.0	262.0
9	5.7	2,387	15	2.0	74.4	303.0

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