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Floating Point Cowell (Second-Sum), Runge-Kutta Integration of Second-Order Ordinary Differential Equations (Subroutine ASC DEQ4)

Prepared by JAMES F. HOLT
Electronics Division

May 1968

El Segundo Technical Operations
AEROSPACE CORPORATION

Prepared for SPACE AND MISSILE SYSTEMS ORGANIZATION
AIR FORCE SYSTEMS COMMAND
LOS ANGELES AIR FORCE STATION
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47

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FLOATING POINT COWELL (SECOND-SUM), RUNGE-KUTTA INTEGRATION OF SECOND-ORDER ORDINARY DIFFERENTIAL EQUATIONS (SUBROUTINE ASC DEQ4)

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FOREWORD

This report is published by the Aerospace Corporation, El Segundo, California, under Air Force Contract No. F04695-67-C-0158.

This report, which documents research carried out from 1 January 1967 to 1 April 1967, was submitted on 22 July 1968 to Lieutenant Kenneth E. Nelson, SAMSO(SMTTA), for review and approval.

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Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

Kenneth E. Nelson

Kenneth E. Nelson, 2nd Lt, USAF
Project Officer

ABSTRACT

ASC DEQ4 is a floating point subroutine, written in FORTRAN IV source language, which integrates numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i.e., $y_i'' = f(t, y_i, y_i')$ of $y_i'' = f(t, y_i)$, $i = 1, 2, \ldots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations (e. g. , variational equations) then DEQ4 has the capability of integrating the final N-IB equations at a larger step size than the first IB equations, thus saving 2(R-1)(N-IB) derivatives per integration step. This subroutine obsoletes subroutine DEQ2 with the following improvements: better accuracy controls, new starting procedure, improved halving and doubling procedure, reduction in computing time, and reduction in core storage requirements (10N less).

The subroutine is restricted in that it contains 20 digit octal constants (real constants) for the CDC 6000 series machines.

CONTENTS

ABSTRACT iii

I. INTRODUCTION 1

A. Purpose 1

B. Restrictions 1

C. Method 2

II. PROGRAM USAGE 3

A. Calling Sequence 3

B. Multiple Entries 7

C. Two-Group Multi-Step Mode 9

D. Coding Information 10

E. Space Required 11

APPENDIXES

A. MATHEMATICAL METHOD A-1

B. FORTRAN IV SOURCE LANGUAGE FOR DEQ4 (CDC 6400-6600) B-1

TABLES

A-1. Difference Table A-7

A-2. Coefficients for W_i for Eq. (A-5) A-12

A-3. Coefficients for V_i for Eq. (A-6) A-12

A-4. Coefficients for N_i, $\dot{N}_i$, B_i, $\dot{B}_i$, D_i, and C_i A-13

SECTION I

INTRODUCTION

A. PURPOSE

The purpose of ASC DEQ4 is to integrate numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i. e., $y_i'' = f(t, y_i, y_i')$ or $y_i'' = f(t, y_i)$ $i = 1, 2, \ldots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations, then DEQ4 has the capability of integrating the final N-IB equations at a larger step size (ratio = $R = 2^K$, $K \geq 1$) than the first IB equations. This will save $2(R-1)(N-IB)$ derivatives per integration step when operating in the Cowell mode.

B. RESTRICTIONS

The restrictions associated with the use of ASC DEQ4 are as follows:

1. No internal checks are made for overflow or underflow.
2. The user must provide an auxiliary subroutine (DAUX) which evaluates the second-order derivatives and the name of the auxiliary subroutine must be defined as an argument in the calling sequence and also through the use of the EXTERNAL statement in the main program (i. e., EXTERNAL DAUX).
3. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N-IB derivatives when TEST is negative. (See IB, TEST, and VMIN in Section II-A for restrictions on the use of the two-group, multi-step mode.
4. Initial conditions must be stored prior to entering the program.
5. ASC DEQ4 is a single precision subroutine written in Fortran IV Source Language.
6. The subroutine contains 20 digit octal constants (real constants) for the CDC 6000 series machines.

C. METHOD

A fourth-order Runge-Kutta method[1] is used to start the integration and to halve the step size during integration. A Cowell "second-sum" method based on eighth differences is used to continue the integration. Doubling is accomplished in the Cowell mode through the accumulation of alternate steps. Truncation error can be controlled by choosing an appropriate step size, and by using the variable step size mode of operation. DEQ4 has an automatic restart procedure which works as follows:

> After eight Runge-Kutta steps (h = H/IR), an attempt is made to integrate in the Cowell mode (h = H/IR). If the error criterion (see ER in Section II-A) cannot be satisfied for the first IB equations, the initial conditions (i. e., t_0, y'_{i0}, and y''_{i0}) are restored, the step size is reduced to h = h/2*IR), and the integration is restarted. This procedure continues until the error criterion is satisfied, or until h < HMIN. For the latter, the subroutine sets TEST = 13 and exits to the user.
>
> Note: Either I2 < 0, or HMIN = HMAX nullifies the restart procedure as well as the halving procedure.

[1] J. B. Scarborough, Numerical Mathematical Analysis, Third Edition, John Hopkins Press, Baltimore (1955) pp. 301-302.

SECTION II

PROGRAM USAGE

A. CALLING SEQUENCE[1]

CALL DEQ4(N, I1, I2, IA, IB, IR, ER, HMIN, HMAX, YMIN,
DAUX, TEST, IDH, NTRY, JHH, JHD, VMIN, VMAX, T,
H, Y, YP, Y2P, T1, T2, T3, T4, T5, T6, T7, F2P, F1P,
DLT1, DLT2, DLT3, DLT4, DLT5, DLT6, DLT7, DLT8)

The nomenclature is as follows:

N — the number of equations.

I1 — an option, so that if

- $I1 \geq 0$, 1st derivatives are present in the evaluation of the second derivatives, $[y_i'' = f(t, y_i, y_i')]$.
- $I1 < 0$, 1st derivatives are missing in the evaluation of the second derivatives, $[y_i'' = f(t, y_i)]$.

I2 — an option, so that if

- $I2 \geq 0$, variable step size mode of operation is used.
- $I2 < 0$, fixed step size mode of operation is used.
- (Note: For $I2 < 0$, $h = H/IR$ for all steps.)

IA — an indicator switch to the user during exit to DAUX.

- IA = -1 for first (1, 2, 3 if Runge-Kutta) pass through DAUX.
- IA = +1 for final (4th if Runge-Kutta) pass through DAUX.

This applies for each integration step. In the Cowell mode, IA = -1 when the derivatives of the predictor are being asked for, and IA = +1 when the derivatives of the corrector are being asked for.

IB — Only the first IB ($\leq$ N) equations are tested to determine whether it is necessary to halve or possible to double the step size or to proceed with a Cowell integration step. (See Section I-A and Section II-C for an additional use of IB.)

---
[1] See NTRY and Section II-B

IR For a given step-size H, the initial step size for both Runge-Kutta and Cowell will be $h = H/IR$. If halving is required, the current step-size h is reduced to $h = h/(2*IR)$ for all N equations, and the integration procedure returns to the Runge-Kutta mode. (Usually IR = 8 or 16; if IR = 0, DEQ4 sets IR = 16.)

ER The user should set ER = 1E - S (i. e., 10^{-S}), where S is the approximate number of significant figures desired. If ER = 0, DEQ4 sets ER = 1E - 11. (User should test for best ER.) In general, ER ≤ 1E - 11 is recommended.

HMIN the minimum absolute value of the step size allowed when halving is required. During the starting procedure (see Section I-C), if halving is required and $h/(2*IR) < HMIN$, the integration is terminated with TEST = 13.; otherwise, the integration is continued in the Cowell mode with the current step-size h (i. e., halving is not permitted). If HMIN = HMAX, all halving is suppressed during the entire integration procedure. If HMIN = 0, DEQ4 sets HMIN = 1E - 5. Only the first IB equations are tested for halving.

HMAX the maximum absolute value of the step size allowed for the first IB equations. The final N-IB equations may be integrated at a larger step size when operating in the two-group, multi-step integration mode (see Section I-A). If HMAX = 0, DEQ4 sets HMAX = 1. A value of HMAX ≤ 16. is recommended for most problems.

YMIN the minimum absolute value allowed for y_i for the relative error test during the halving and doubling procedure. YMIN prevents unnecessary halving for $y_i \approx 0$. If YMIN = 0, DEQ4 sets YMIN = 1. (User should supply YMIN).

> Note: For the more difficult problems, it may be necessary for the user to modify the subroutine and make YMIN a vector of dimension IB -- thus allowing a different YMIN for the first IB equations.

DAUX the location of the entry point of an external subroutine (supplied by the user) which evaluates and stores (see Y2P) the second-order derivatives y_i''. DAUX must be defined by the user through the use of the EXTERNAL statement in the main program, and COMMON must be used as a means of data linkage. CALL DAUX is used by DEQ4 to enter DAUX. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N-IB derivatives when TEST is negative.

TEST has the following multiple uses:

Initially (i. e., prior to NTRY = 1), the user must set:

TEST = +1., to integrate the N equations at the same step size.

TEST ≥ +2., to use the two-group, multi-step mode. The maximum ratio of the step sizes for the two groups will be R_{MAX} = 2**(TEST -1). Recommend TEST ≤ 5.

After each integration step (NTRY = 2) DEQ4 will set:

TEST = +1., if the integration was a Runge-Kutta step (i. e., during starting procedure, or halving procedure if JHH = 1).

TEST = +2., if the integration has been restarted during the initial starting procedure. Indicates h = h/(2*IR) and Runge-Kutta step.

TEST = +3., if the step size has been reduced [h = h/(2*IR)] and the integration has been returned to a previous step during the halving procedure (possible only if JHH = 3).

TEST = -1., if the integration was a Cowell step.

During the starting procedure (see Section I-C):

TEST = +13., if the integration has been terminated during the restarting procedure. Indicates programming error, or ER, H, or HMIN too restrictive.

During transfers to DAUX (also, see IA and DAUX):

TEST = -1., when the first IB equations are being integrated (at a smaller step-size) in the multi-step Cowell mode.

TEST = +1., when the N equations are being integrated in the Runge-Kutta or Cowell mode.

IDH an indicator switch to the user after each integration step.

IDH = 1, if the step size has not changed

IDH = 2, if the step size of all N equations has been reduced to h = h/(2*IR) where h is the current step size of the first IB equations.

IDH = 3, if the step size of all N equations has been doubled.

IDH = 4, if the step size of the final N-IB equations has been doubled (possible only in multi-step mode).

NTRY a special option to simulate multiple entries. The user must set NTRY prior to using the calling sequence.

NTRY = 1 Setup entry (store all initial conditions first).

NTRY = 2 Normal Runge-Kutta/Cowell integration.

NTRY = 3 Integrate in Runge-Kutta mode exclusively.

(Note: NTRY = 1 must be used prior to the other two values. See Section II-B for further details.)

JHH an option to control the halving procedure.

JHH = 1 Reduce step size and return to Runge-Kutta mode.

JHH = 3 Return to previous step, restore all conditions (i. e., t, $y_i^{\prime}$, and $y_i^{\prime\prime}$) at that step, reduce step size and return to Runge-Kutta mode.

(Note: See Section II-C for exception to JHH = 3 option.)

JHD (No longer used in DEQ4)

All doubling is performed in the Cowell mode through the accumulation of alternate steps.

VMIN the location of one cell used by DEQ4 for the halving and doubling tests.

$VMIN = 10^{-1}\ ER/H^2$ (computed internally, varies with H)

Initially (prior to NTRY = 1) the user must set VMIN ≥ 1. if TEST ≥ 2. (i. e., multi-step mode). This initial value allows the user to control the doubling procedure for the final N-IB equations if the multi-step mode is used. A larger value of VMIN (initially) will reduce the accuracy requirements for the final N-IB equations and thus allow them to be integrated at a larger step-size. A value of $10. \leq VMIN \leq 10.^5$ is recommended.

VMAX the location of one cell used by DEQ4 for the halving and doubling tests. $VMAX = 10.^3\ ER/H^2$ (computed internally, varies with H).

T the location of the independent variable t_n -- stored initially by the user and incremented automatically by the subroutine during the integration procedure. T may be reset to a previous step by the subroutine during the starting procedure or, during the halving procedure when JHH = 3.

H the location of step-size h -- stored initially by the user and modified automatically by the subroutine during the integration procedure. Initially, DEQ4 sets H = H/IR as the initial step-size for both Runge-Kutta and Cowell. If H = 0, DEQ4 sets H = 0.01 (H can be positive or negative). In the multi-step mode, H will contain the current step size of the first IB equations.

Y the location of N dependent variables y_i -- stored initially by the user and modified automatically by the subroutine during the integration procedure.

YP the location of N first derivatives y_i' -- stored initially by the user and modified automatically by the subroutine during the integration procedure.

Y2P the location of N second derivatives y_i'' -- computed and stored by the DAUX subroutine supplied by the user. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N-IB second derivatives when TEST is negative.

T1 through T7, F2P, F1P, and DLT1 through DLT8 are temporary storages used by the subroutine. Each of these temporary storages must have a dimension of N and must be preserved throughout the integration procedure.

B. MULTIPLE ENTRIES

For purposes of compatibility between machines and different versions of Fortran IV, the parameter NTRY is used to simulate multiple entires. This requires the user to change the value of NTRY prior to using the calling sequence. This is done as follows:

NTRY = 1, Setup Entry

The user must set NTRY = 1 and store all initial conditions and options prior to using the calling sequence. This includes N, I1, I2, IB, IR, ER, HMIN, HMAX, YMIN, TEST, NTRY, JHH, VMIN, T, H, Y, and YP.

After setting NTRY = 1, the user must CALL DEQ4(N, I1, . . . , DLT8) for the setup entry. The subroutine performs various tests on parameters (e. g., sets H = 0.01, if H = 0), sets initial switches and options for the integration procedure, calls DAUX to form y_i'' at t_0, and then returns to the user. No integration is performed during the setup entry. The above entry must be performed prior to any other entry (one time only).

NTRY = 2, Integration Entry - Runge-Kutta/Cowell Mode

This is the normal integration entry and should be programmed within a DO loop (to control situations such as maximum steps in case of an error). After setting NTRY = 2, the user must CALL DEQ4(N, I1, . . . , DLT8) to integrate one step in the Runge-Kutta/Cowell mode. The subroutine integrates one step (H/IR initially) and returns to the user. The first eight steps will be in the Runge-Kutta mode; thereafter the subroutine will integrate in the Cowell mode (h = H/IR), doubling approximately every 16 steps until $h \rightarrow H$. If the two-group, multi-step mode is used (TEST ≥ 2. initially) then the step size of the final N-IB equations may continue to double, subject to the restrictions of the initial values of TEST and VMIN. In this case, during each entry to DEQ4, the first IB equations will be integrated R steps (h = H) while the final N-IB equations will be integrated one step (h = R*H). All of this is automatic, and the user need only loop through the calling sequence to integrate from t_0 to t_{END}. The user should test T after each integration step to determine the proper exit procedure, using NTRY = 3 to integrate to a specific time point t_{END}. If output is desired at a particular time point t_i ($t_i \neq t_n$), an interpolation subroutine such as RW NTRP is recommended.

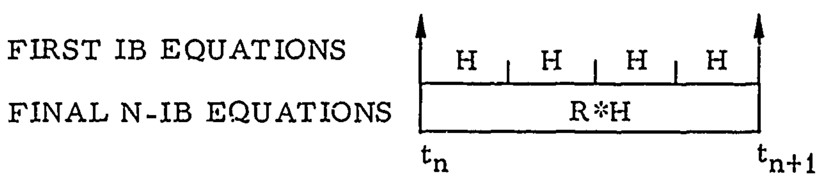
NTRY = 3, Integrate in the Runge-Kutta Mode

After any integration step, or after setup entry, the user can integrate one or more steps in the Runge-Kutta mode. After setting NTRY = 3 (and changing the step-size H if necessary), the user must CALL DEQ4(N, I1, . . . , DLT8) to integrate one step in the Runge-Kutta mode. The step size can be changed after each Runge-Kutta integration step, and negative H is permissible. NTRY = 3 should be used primarily to end the integration at a specific value t_{END}. It can also be used to integrate to a specific output time t_{OUTPUT} (t_n - H < t_{OUTPUT} < t_n + H), where t_n is the current value of the independent variable and H is the current step size, if the regions TEST, T, H, Y, YP, Y2P, and T1 through T4 are saved and restored before continuing the normal integration (i. e., NTRY = 2). Note that the step size for the Runge-Kutta integration should be ≤ H/IR if the same accuracy is desired, where H is the current step size of the Cowell mode. If the two-group multi-step mode is used, then several Runge-Kutta steps may be required to integrate from t_n to t_{OUTPUT} (i. e., t_n - R*H < t_{OUTPUT} < t_n + R*H). (See Section II-C for further details.)

C. TWO-GROUP MULTI-STEP MODE

The subroutine assumes that the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations. This would be the case, for example, for a system of nonlinear differential equations which are integrated simultaneously with the variational equations (i. e., Newton-Raphson Method). Since the variational equations are always linear and also require less accuracy, they can be integrated at a larger step size than the first IB nonlinear differential equations. This is accomplished in DEQ4 through the use of the initial values of TEST and VMIN. TEST controls the maximum ratio of the two step sizes and VMIN controls the accuracy of the final N-IB equations. For example, if TEST = 3. and VMIN = 1000. initially, then the maximum possible ratio of the two groups will be $R_{MAX} = 2^2$ = 2**(TEST -1.) and the accuracy requirements for the final N-IB equations will be ER*1000, where ER determines the accuracy of the first IB equations.

The doubling procedure works as follows: Initially, all N equations are integrated in the Runge-Kutta mode at a step-size H = H_0/IR. After eight Runge-Kutta steps all N equations are integrated in the Cowell mode at a step-size h = H_0/IR. Thereafter (assuming halving is not required), the step size for all N equations will double every 16 steps (in the Cowell mode) until the step size for the first IB equations can no longer be doubled. From that point the step size of the final N-IB equations will continue to double under the restrictions of TEST and VMIN described above. For example, during an entry to DEQ4 (NTRY = 2) if R = 4 the following integration will be performed in the Cowell mode:



Note that during one entry into DEQ4, the first IB equations are integrated R steps with a step size of H while the final N-IB equations are integrated one step with a step size of R*H. Upon the next entry, if halving is required for the first IB equations, then H is reduced to H = H/(2*IR) for all N equations and the above procedure is repeated. If JHH = 1 the integration will continue from T = t_{n+1}. If JHH = 3 the integration will normally continue from T = t_n with all conditions restored at that point. However, if the final N-IB equations were being saved for doubling at T = t_n (i. e., R_{MAX} had not been reached), then the integration will be continued from T = t_{n+1} (same as JHH = 1). Thus, the doubling of the final N-IB equations is given precedent over the halving procedure in regards to the JHH = 3 option. For this reason TEST ≤ 5.is recommended, since the doubling procedure for the final N-IB equations is discontinued when R_{MAX} has been reached.

Since 2(R-1)(N-IB) derivatives are no longer computed during each Cowell step, the use of the two-group multi-step mode will result in a considerable saving of computing time where applicable.

D. CODING INFORMATION

The calling sequence can be simplified to

CALL DEQ4

by placing all parameters of the calling sequence in (labeled or blank) COMMON and using the name DAUX (identical with the name used internally by DEQ4) for the auxiliary subroutine. In additon, all parameters (i.e., Y, YP, Y2P, etc.) must be dimensioned within subroutine DEQ4[1], and the SUBROUTINE statement in DEQ4 must be changed to

SUBROUTINE DEQ4

E. SPACE REQUIRED

In addition to the parameters in the calling sequence, approximately 3571_8 cells are required.

Note: The coefficients required for the Cowell integration mode are stored in DEQ4 as 20 digital octal constants through the use of the DATA declaration. These coefficients were formed in double precision on the CDC 6600 and are the octal equivalent of the 60-bit real floating point constants of the CDC 6000 series machines. See Appendix A for a complete description of the mathematical method.

[1] The Fortran IV Source Language for DEQ4 is provided in Appendix B.

APPENDIX A

MATHEMATICAL METHOD

The ASC DEQ4 subroutine [Floating Point Cowell (Second-Sum) Runge-Kutta Integration of Second-Order Ordinary Differential Equations] is prepared to solve the system of equations defined as

$$\begin{aligned} y_i'' &= f_i(t,\ y_i, \ldots, y_N, y_i', \ldots, y_N') \quad (i = 1, 2, \ldots, N) \\ y_i(t_0) &= y_{i0},\ y_i'(t_0) = y_{i0}' \quad (i = 1, 2, \ldots, N) \end{aligned} \tag{A-1}$$

In case none of the f_i involve the first derivatives y_i', time is saved by indicating this in the set-up (i.e., set I1 = -1). DEQ4 includes a fourth order Runge-Kutta subroutine that is used for the starting procedure and for the halving procedure. The Runge-Kutta subroutine can also be used independently of the main subroutine through the use of NTRY = 3. For the sake of completeness the Runge-Kutta equations are given in the following paragraphs.

A. 1. RUNGE-KUTTA EQUATIONS

Let y_{in} and y_{in}' be the values of y_i and y_i' at $t = t_n$; f_{in} be the second derivative of y_i at $t = t_n$; and h be the increment (step size) of the independent variable t. The Runge-Kutta formulas[1] used in this subroutine are as follows:

[1] J. B. Scarborough, Numerical Mathematical Analysis, Third Edition, John Hopkins Press, Baltimore, Maryland (1955) pp. 300-301.

$$k_{i1} = hf_i(t_n, y_{in}, y'_{in})$$

$$k_{i2} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}, y'_{in} + \frac{k_{i1}}{2}\right)$$

$$k_{i3} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}, y'_{in} + \frac{k_{i2}}{2}\right)$$

$$k_{i4} = hf_i(t_n + h, y_{in} + hy'_{in} + \frac{h}{2}k_{i3}, y'_{in} + k_{i3}) \qquad \text{(A-2)}$$

$$\Delta y_{in} = h\left[y'_{in} + \frac{1}{6}(k_{i1} + k_{i2} + k_{i3})\right]$$

$$\Delta y'_{in} = \frac{1}{6}[k_{i1} + 2k_{i2} + 2k_{i3} + k_{i4}]$$

$$y_{i,n+1} = y_{in} + \Delta y_{in}$$

$$y'_{i,n+1} = y'_{in} + \Delta y'_{in}$$

For the special second-order equation, you have

$$y''_i = f_i(t, y_1, \ldots, y_n) \quad \text{(1st derivatives missing)} \qquad \text{(A-3)}$$

It should be noted that $k_{i2} = k_{i3}$, so that above formulas reduce to the following Runge-Kutta formulas:

$$k_{i1} = hf_i(t_n, y_{in})$$

$$k_{i2} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}\right)$$

$$k_{i3} = hf_i\left(t_n + h, y_{in} + hy'_{in} + \frac{h}{2}k_{i2}\right)$$

$$\Delta y_{in} = h\left[y'_{in} + \frac{1}{6}(k_{i1} + 2k_{i2})\right]$$

(cont.)

$$\Delta y'_{in} = \frac{1}{6}\left[k_{i1} + 4k_{i2} + k_{i3}\right]$$

$$y_{i,n+1} = y_{in} + \Delta y_{in}$$

$$y'_{i,n+1} = y'_{in} + \Delta y'_{in} \qquad \text{(A-4)}$$

where k_{i4} of Eq. (A-2) is now k_{i3} of Eq. (A-4).

The subroutine can be made to take advantage of this fact by a simple change in the calling sequence (i. e., set I1 = -1) and thus save one derivative per integration step in the Runge-Kutta mode.

A. 2 COWELL STARTING PROCEDURE

A Cowell (Second-Sum) method based on eight differences is used to continue the integration after the first eight Runge-Kutta steps. The user must ask for each integration step and the subroutine will follow this sequence:

a. Perform eight Runge-Kutta steps of size $h = H_{start}/IR$ (one Runge-Kutta step for each entry to DEQ4) to obtain y_{i1}, y'_{i1}, y''_{i1} through y_{i8}, y'_{i8}, y''_{i8}.

b. For each of the N equations, that part of the difference table above the diagonal line is constructed in an accumulative manner during the eight Runge-Kutta steps (DEQ4 returns to the user after each Runge-Kutta step).

To start the Cowell integration we need $''F_{i10}$, $'F_{i9}$, y_{i8}, y'_{i8}, y''_{i8}, Δ^{I}_{i7}, Δ^{II}_{i6}, Δ^{III}_{i5}, Δ^{IV}_{i4}, Δ^{V}_{i3}, Δ^{VI}_{i2}, Δ^{VII}_{i1}, and Δ^{VIII}_{i0}. The values y_{i8}, y'_{i8}, and y''_{i8} are available after the eight Runge-Kutta integration step. The other values are computed as follows:

$$\begin{aligned} 'F_{i9} = y'_{i4}/H &+ W_0 y''_{i0} + W_1 y''_{i1} + W_2 y''_{i2} + W_3 y''_{i3} \\ &+ W_4 y''_{i4} + W_5 y''_{i5} + W_6 y''_{i6} + W_7 y''_{i7} + W_8 y''_{i8} \end{aligned} \qquad \text{(A-5)}$$

$$''F_{i10} = y_{i4}/H^2 + 5y'_{i4}/H + V_0 y''_{i0} + V_1 y''_{i1} + V_2 y''_{i2}$$
$$+ V_3 y''_{i3} + V_4 y''_{i4} + V_5 y''_{i5} + V_6 y''_{i6} + V_7 y''_{i7} + V_8 y''_{i8} \qquad \text{(A-6)}$$

$$\Delta^{I}_{i7} = y''_{i8} - y''_{i7} \qquad \text{(A-7)}$$

$$\Delta^{II}_{i6} = y''_{i8} - 2\,y''_{i7} + y''_{i6} \qquad \text{(A-8)}$$

$$\Delta^{III}_{i5} = y''_{i8} - 3\,y''_{i7} + 3\,y''_{i6} - y''_{i5} \qquad \text{(A-9)}$$

$$\Delta^{IV}_{i4} = y''_{i8} - 4\,y''_{i7} + 6\,y''_{i6} - 4\,y''_{i5} + y''_{i4} \qquad \text{(A-10)}$$

$$\Delta^{V}_{i3} = y''_{i8} - 5\,y''_{i7} + 10\,y''_{i6} - 10\,y''_{i5} + 5\,y''_{i4} - y''_{i3} \qquad \text{(A-11)}$$

$$\Delta^{VI}_{i2} = y''_{i8} - 6\,y''_{i7} + 15\,y''_{i6} - 20\,y''_{i5} + 15\,y''_{i4} - 6\,y''_{i3} + y''_{i2} \qquad \text{(A-12)}$$

$$\Delta^{VII}_{i1} = y''_{i8} - 7\,y''_{i7} + 21\,y''_{i6} - 35\,y''_{i5} + 35\,y''_{i4} - 21\,y''_{i3} + 7\,y''_{i2} - y''_{i1} \qquad \text{(A-13)}$$

$$\Delta^{VIII}_{i0} = y''_{i8} - 8\,y''_{i7} + 28\,y''_{i6} - 56\,y''_{i5}$$
$$+ 70\,y''_{i4} - 56\,y''_{i3} + 28\,y''_{i2} - 8\,y''_{i1} + y''_{i0} \qquad \text{(A-14)}$$

Before going to a Cowell step, the step-size $h = H_{start}/IR$ is tested. Only the first IB equations are used to test, where $1 \leq IB \leq N$. For the first

IB equations we determine

$$V = \max_{1 \le i \le IB} \left[\frac{|\Delta_{i1}^{VII}|}{\max(|y_{i8}|,\ \mathrm{YMIN})} \right] \tag{A-15}$$

If $V \ge 10^3 * ER/h^2$, then the ratio of the seventh difference to function is too large. Therefore, h is reduced to $h = h/(2*IR)$, the initial conditions (i.e., t_0, y_{i0}, y'_{i0}, and y''_{i0}) are restored, and the integration procedure is restarted. This procedure is repeated until: (a) $V < 10^3 * ER/h^2$ or (b) h < HMIN. For (a) the routine proceeds to a Cowell integration step with the current value of h. For (b) the routine sets TEST = 13. and returns to the user -- indicating a programming error or that ER, H_{start}, or HMIN are too restrictive. The constant YMIN (equals 1. if unspecified) prevents division by y near a zero; for example, in the sine calculation YMIN = 0.01 avoids difficulty near 180 deg. The value ER (equals 1E - 11 if unspecified) allows a larger h if chosen larger, say ER = 1E - 8.

A.3 COWELL INTEGRATION

If $V < 10^3 * ER/h^2$ after the eighth Runge-Kutta step, we begin the Cowell integration with predictions of

$$\begin{aligned} y_{i9} = h^2\Big(& {''F}_{i10} + N_0 y''_{i8} + N_1\Delta_{i7}^{I} + N_2\Delta_{i6}^{II} + N_3\Delta_{i5}^{III} \\ & + N_4\Delta_{i4}^{IV} + N_5\Delta_{i3}^{V} + N_6\Delta_{i2}^{VI} + N_7\Delta_{i1}^{VII} + N_8\Delta_{i0}^{VIII}\Big) \end{aligned} \tag{A-16}$$

$$\begin{aligned} y'_{i9} = h\Big(& {'F}_{i9} + \dot{N}_0 y''_{i8} + \dot{N}_1\Delta_{i7}^{I} + \dot{N}_2\Delta_{i6}^{II} + \dot{N}_3\Delta_{i5}^{III} \\ & + \dot{N}_4\Delta_{i4}^{IV} + \dot{N}_5\Delta_{i3}^{V} + \dot{N}_6\Delta_{i2}^{VI} + \dot{N}_7\Delta_{i1}^{VII} + \dot{N}_8\Delta_{i0}^{VIII}\Big) \end{aligned} \tag{A-17}$$

These equations use the row of the difference table above the diagonal line; only this row is needed for a Cowell step and is kept up to date as the integration proceeds. The prediction for y'_{i9} is omitted if the option I1 = -1 is used. Now from y_{i9} and y'_{i9}, we obtain y''_{i9} (from DAUX) and then complete the row of differences out to Δ_{i1}^{VIII} under the diagonal line in Table A-1. For example: $\Delta_{i8}^{I} = y''_{i9} - y''_{i8}$; $\Delta_{i7}^{II} = \Delta_{i8}^{I} - \Delta_{i7}^{I}$; and so on.

With this row, we calculate the corrected values:

$$y_{i9} = h^2\Big({''F}_{i10} + B_0 y''_{i9} + B_1\Delta_{i8}^{I} + B_2\Delta_{i7}^{II} + B_3\Delta_{i6}^{III} + B_4\Delta_{i5}^{IV} + B_5\Delta_{i4}^{V} + B_6\Delta_{i3}^{VI} + B_7\Delta_{i2}^{VII} + B_8\Delta_{i1}^{VIII}\Big) \tag{A-18}$$

$$y'_{i9} = h\Big({'F}_{i9} + \dot{B}_0 y''_{i9} + \dot{B}_1\Delta_{i8}^{I} + \dot{B}_2\Delta_{i7}^{II} + \dot{B}_3\Delta_{i6}^{III} + \dot{B}_4\Delta_{i5}^{IV} + \dot{B}_5\Delta_{i4}^{V} + \dot{B}_6\Delta_{i3}^{VI} + \dot{B}_7\Delta_{i2}^{VII} + \dot{B}_8\Delta_{i1}^{VIII}\Big) \tag{A-19}$$

From these we get corrected values for y''_{i9} (from DAUX) and recalculate the entire row under the diagonal line. Using these new values we calculate new values for y_{i9} and y'_{i9} using Eqs. (A-18) and (A-19). Thus, y_{i9} and y'_{i9} are corrected twice; however, new values for y''_{i9} are not computed for these new values. Next we compute ${'F}_{i10} = {'F}_{i9} + y''_{i9}$ and ${''F}_{i11} = {''F}_{i10} + {'F}_{i10}$. This completes the integration step and DEQ4 exits to the user.

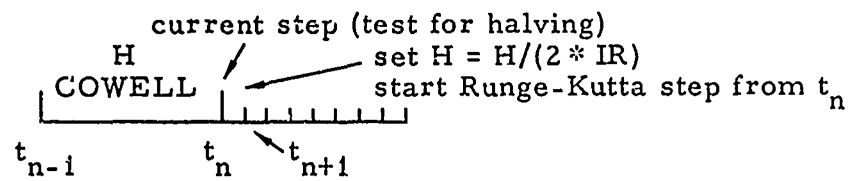
On the next entry we repeat the test for halving [i. e., at Eq. (A-15)]. If halving is not required, we continue the Cowell integration using Eqs. (A-16) through (A-19) as before. If halving is required after at least one Cowell integration step has been completed, we set H = H/(2*IR) and start a new sequence of eight Runge-Kutta steps. If JHH = 1, we do not retrace ground; however, if JHH = 3 (and the final N-IB equations are not being saved for doubling in the two-group multi-step mode) then we return to the previous step, restore the conditions at that point and then start a new sequence of

		y''_{i0}								
			Δ^{I}_{i0}							
		y''_{i1}		Δ^{II}_{i0}						
			Δ^{I}_{i1}		Δ^{III}_{i0}					
		y''_{i2}		Δ^{II}_{i1}		Δ^{IV}_{i0}				
			Δ^{I}_{i2}		Δ^{III}_{i1}		Δ^{V}_{i0}			
		y''_{i3}		Δ^{II}_{i2}		Δ^{IV}_{i1}		Δ^{VI}_{i0}		
			Δ^{I}_{i3}		Δ^{III}_{i2}		Δ^{V}_{i1}		Δ^{VII}_{i0}	
$''F_{i5}$		y''_{i4}		Δ^{II}_{i3}		Δ^{IV}_{i2}		Δ^{VI}_{i1}		Δ^{VIII}_{i0}
	$'F_{i5}$		Δ^{I}_{i4}		Δ^{III}_{i3}		Δ^{V}_{i2}		Δ^{VII}_{i1}	
$''F_{i6}$		y''_{i5}		Δ^{II}_{i4}		Δ^{IV}_{i3}		Δ^{VI}_{i2}		Δ^{VIII}_{i1}
	$'F_{i6}$		Δ^{I}_{i5}		Δ^{III}_{i4}		Δ^{V}_{i3}		Δ^{VII}_{i2}	
$''F_{i7}$		y''_{i6}		Δ^{II}_{i5}		Δ^{IV}_{i4}		Δ^{VI}_{i3}		
	$'F_{i7}$		Δ^{I}_{i6}		Δ^{III}_{i5}		Δ^{V}_{i4}			
$''F_{i8}$		y''_{i7}		Δ^{II}_{i6}		Δ^{IV}_{i5}				
	$'F_{i8}$		Δ^{I}_{i7}		Δ^{III}_{i6}					
$''F_{i9}$		y''_{i8}		Δ^{II}_{i7}						
	$'F_{i9}$		Δ^{I}_{i8}							
$''F_{i10}$		y''_{i9}								
	$'F_{i10}$									
$''F_{i11}$										

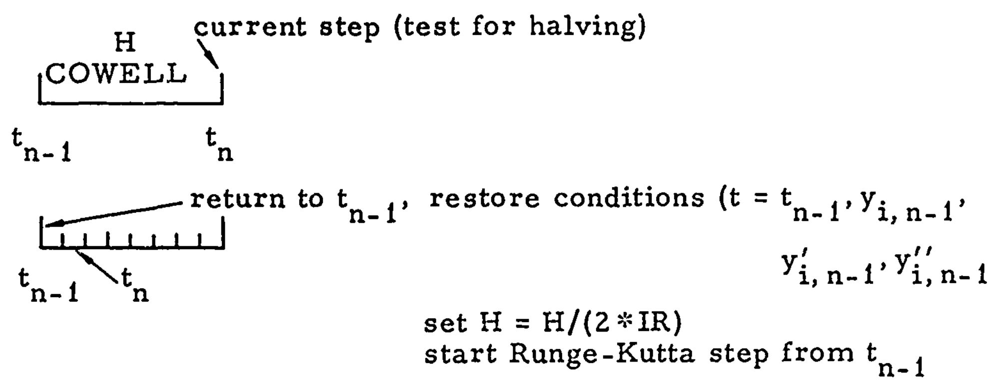
Table A-1. Difference Table

eight Runge-Kutta steps with H = H/(2*IR). This can be shown graphically as

JHH = 1



JHH = 3



During the halving procedure all N equations return to Runge-Kutta with the same step size (i. e., the two-group multi-step mode is temporarily suspended).

If halving is not required, we proceed with a Cowell step, making the following test every other step to determine whether we may be able to double h. If

$$V \le \frac{(10^{-2}) * ER}{h^2} \tag{A-20}$$

we may be able to double h.

We test further to see that

$$W = \max_{1 \le i \le IB} \left[\frac{|\Delta_{i0}^{VIII}|}{\max(|y_{i8}|,\ YMIN)} \right] \le \frac{10^{-2} * ER}{h^2} \tag{A-21}$$

If the conditions of Eqs. (A-20) and (A-21) are satisfied for 16 steps (testing every other step) then the step-size h is doubled for all N equations in the Cowell mode. In addition, all of the data above the diagonal line is doubled in the Cowell mode using Eq. (A-23). We then proceed to a Cowell step using Eqs. (A-16) through (A-19) with step-size 2H. On the next entry, the halving and doubling tests are continued as before.

The doubling procedure requires a counting device and it works as follows. Initially, we set K = 1 at the beginning of the first Cowell step. The counter is advanced every other step if Eqs. (A-20) and A-21) are satisfied for the first IB equations. We accumulate the data required for doubling at alternate steps. If the tests fail at any point (assuming halving is not required) the counter is restarted if all N equations are being integrated at the same step size (i. e., TEST = VMIN = 1. initially). However, if the two-group mode is being used, then the doubling tests for the first IB equations are temporarily suspended (i. e., the step size for the first IB equations remains constant unless halving is later required). Thereafter, the doubling for the final N-IB equations is continued using the following test, that is, if

$$\mathrm{VAR} = \max_{\mathrm{IB} < i \leq N} \left[\frac{|\Delta_{i1}^{\mathrm{VII}}|}{\max\left(|y_{i8}|,\ \mathrm{YMIN}\right)} \right] < \frac{10^{-2} * \mathrm{ER} * \mathrm{VMIN}}{h^2} \qquad \text{(A-22)}$$

for the remaining steps [K = 1(1)9], then the step size for the final N-IB equations is doubled. Also, for the final N-IB equations all of the data above the diagonal line is doubled in the Cowell mode. Note that VMIN of Eq. (A-22) is the initial value of VMIN for NTRY = 1. The counter K will be set to one for the next entry, and the doubling procedure will be restarted for the final N-IB equations.

The equations used for doubling in the Cowell mode are as follows. Let Δ represent a difference (i.e., $\Delta^{I} = \Delta^{I}_{17}$, $\Delta^{II} = \Delta^{II}_{16}$) at step-size h, and $\blacktriangle$ represent a difference at step-size 2b. Then we compute

$$\blacktriangle^{I} = 2\Delta^{I} - \Delta^{II}$$

$$\blacktriangle^{II} = 4\Delta^{II} - (4\Delta^{III} - \Delta^{IV})$$

$$\blacktriangle^{III} = 8\Delta^{III} - (12\Delta^{IV} - 6\Delta^{V} + \Delta^{VI})$$

$$\blacktriangle^{IV} = 16\Delta^{IV} - (32\Delta^{V} - 24\Delta^{VI} + 8\Delta^{VII} - \Delta^{III})$$

$$\blacktriangle^{V} = 5\blacktriangle^{IV} - (10\blacktriangle^{III} - 10\blacktriangle^{II} + 5\blacktriangle^{I}) + (y''_{16} - y''_{6})$$

$$\blacktriangle^{VI} = 6\blacktriangle^{V} - (15\blacktriangle^{IV} - 20\blacktriangle^{III} + 15\blacktriangle^{II} - 6\blacktriangle^{I}) - (y''_{16} - y''_{4})$$

$$\blacktriangle^{VII} = 7\blacktriangle^{VI} - (21\blacktriangle^{V} - 35\blacktriangle^{IV} + 35\blacktriangle^{III} - 21\blacktriangle^{II} + 7\blacktriangle^{I}) + (y''_{16} - y''_{2})$$

$$\blacktriangle^{VIII} = 8\blacktriangle^{VII} - (28\blacktriangle^{VI} - 56\blacktriangle^{V} + 70\blacktriangle^{IV} - 56\blacktriangle^{III} + 28\blacktriangle^{II} - 8\blacktriangle^{I}) - (y''_{16} - y''_{0})$$

$$'F(\blacktriangle) = y'_8/2h + W_0 y''_0 + W_1 y''_2 + W_2 y''_4 + W_3 y''_6 + W_4 y''_8 + W_5 y''_{10} + W_6 y''_{12} + W_7 y''_{14} + W_8 y''_{16}$$

$$''F(\blacktriangle) = y_8/(2h)^2 + 5\, y'_8/2h + V_0 y''_0 + V_1 y''_2 + V_2 y''_4 + V_3 y''_6 + V_4 y''_8 + V_5 y''_{10} + V_6 y''_{12} + V_7 y''_{14} + V_8 y''_{16} \qquad \text{(A-23)}$$

where the values y_8, y'_8, and y''_0, y''_2, ..., y''_{16} are the integrated values saved at alternate steps of the Cowell integration procedure. For the two-group mode h will be the value in cell H when the step size for all N equations is being doubled and R * H when the step size for the final N-IB equations is being dcubled.

A. 4 CALCULATION OF COEFFICIENTS

In a previous version of the subroutine (ASC DEQ2) $''F_{i10}$ and $'F_{i9}$ of Table A-1 were calculated by first forming $''F_{i5}$ and $'F_{i5}$ as follows:

$$'F_{i5} = y'_{i4}/H - D_0 y''_{i4} - D_1\Delta^{I}_{i4} - D_2\Delta^{II}_{i3} - D_3\Delta^{III}_{i3}$$

$$- D_4\Delta^{IV}_{i2} - D_5\Delta^{V}_{i2} - D_6\Delta^{VI}_{i1} - D_7\Delta^{VII}_{i1} - D_8\Delta^{VIII}_{i0} \qquad \text{(A-24)}$$

$$''F_{i5} = y_{i4}/H^2 - C_0 y''_{i4} - C_2\Delta^{II}_{i3} - C_4\Delta^{IV}_{i2} - C_6\Delta^{VI}_{i1} - C_8\Delta^{VIII}_{i0} \qquad \text{(A-25)}$$

Then $''F_{i10}$ and $'F_{i9}$ were calculated through the sequence as

$$'F_{i\,K+1} = 'F_{iK} + y''_{iK} \qquad (K = 5,\ 6, \ldots,\ 8) \qquad \text{(A-26)}$$

$$''F_{i\,K+1} = ''F_{iK} + 'F_{iK} \qquad (K = 5,\ 6, \ldots,\ 9) \qquad \text{(A-27)}$$

However, by substituting ordinates (y''_{iK}) for differences (Δ_{iK}) (e.g., $\Delta^{I}_{i4} = y''_{i5} - y''_{i4}$; $\Delta^{II}_{i3} = y''_{i5} - 2y''_{i4} + y''_{i3}$) in Eqs. (A-24) and (A-25) and through the use of Eqs. (A-26) and (A-27) $'F_{i9}$ and $''F_{i10}$ can be defined by Eqs. (A-5) and (A-6). Tables A-2 and A-3 give the value of V_i and W_i. Table A-4 gives the values of the other coefficients.

The coefficients for V_i and W_i were formed in double precision on the CDC 6600 and are included in subroutine DEQ4 as 20 digit octal constants. For example, using Table A-3

$$V_7 = (2 - 5D5 - 5D6 + 35D7 + 40D8 - C6 + 8C8) \qquad \text{(A-28)}$$

Table A-2. Coefficients for W_i for Eq. (A-5)

	1	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
W_0										-1
W_1								-1	1	8
W_2						-1	1	6	-7	-28
W_3				-1	1	4	-5	-15	21	56
W_4		-1	1	2	-3	-6	10	20	-35	-70
W_5	1		-1	-1	3	4	-10	-15	35	56
W_6	1				-1	-1	5	6	-21	-28
W_7	1						-1	-1	7	8
W_8	1								-1	-1

Table A-3. Coefficients for V_i for Eq. (A-6)

	1	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	C_0	C_2	C_4	C_6	C_8
V_0										-5					-1
V_1								-5	5	40				-1	8
V_2						-5	5	30	-35	-140			-1	6	-28
V_3				-5	5	20	-25	-75	105	280		-1	4	-15	56
V_4		-5	5	10	-15	-30	50	100	-175	-350	-1	2	-6	20	-70
V_5	4		-5	-5	15	20	-50	-75	175	280		-1	4	-15	56
V_6	3				-5	-5	25	30	-105	-140			-1	6	-28
V_7	2						-5	-5	35	40				-1	8
V_8	1								-5	-5					-1

Table A-4. Coefficients for N_i, $\dot{N}_i$, B_i, $\dot{B}_i$, D_i, and C_i

i =	0	1	2	3	4	5	6	7	8
N_i	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{19}{240}$	$\frac{3}{40}$	$\frac{863}{12096}$	$\frac{275}{4032}$	$\frac{33953}{518400}$	$\frac{8183}{129600}$	$\frac{3250433}{53222400}$
$\dot{N}_i$	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\frac{19087}{60480}$	$\frac{5257}{17280}$	$\frac{1070017}{3628800}$	$\frac{25713}{89600}$
B_i	$\frac{1}{12}$	0	$\frac{-1}{240}$	$\frac{-1}{240}$	$\frac{-221}{60480}$	$\frac{-19}{6048}$	$\frac{-9829}{3628800}$	$\frac{-407}{172800}$	$\frac{-330157}{159667200}$
$\dot{B}_i$	$\frac{1}{2}$	$\frac{-1}{12}$	$\frac{-1}{24}$	$\frac{-19}{720}$	$\frac{-3}{160}$	$\frac{-863}{60480}$	$\frac{-275}{24192}$	$\frac{-33953}{3628800}$	$\frac{-8183}{1036800}$
D_i	$-\frac{1}{2}$	$\frac{-1}{12}$	$\frac{1}{24}$	$\frac{11}{720}$	$\frac{-11}{1440}$	$\frac{-191}{60480}$	$\frac{191}{120960}$	$\frac{2497}{3628800}$	$\frac{-2497}{7257600}$
C_i	$\frac{1}{12}$	0	$\frac{-1}{240}$	0	$\frac{31}{60480}$	0	$\frac{-289}{3628800}$	0	$\frac{317}{22809600}$

APPENDIX B

FORTRAN IV SOURCE LANGUAGE FOR DEQ4
(CDC 6400-6600)

```
C     ASC DEQ4  (8TH ORDER) R.K./GAUSS JACKSON (4-18-67) J.F. HOLT       DEQ40001
      SUBROUTINE DEQ4(N,I1,I2,IA,IB,IR,ER,HMIN,HMAX,YMIN,DAUX,TEST,IDH, DEQ40002
     1 NTRY,JHH,JHD,VMIN,VMAX,                                          DEQ40003
     2 T,H,Y,YP,Y2P,T1,T2,T3,T4,                                        DEQ40004
     3T5,T6,T7,                                                         DEQ40005
     4 F2P,F1P,DLT1,DLT2,DLT3,DLT4,DLT5,DLT6,DLT7,DLT8)                 DEQ40006
      DATA A0,A1,A2,A3,A4,A5,A6,A7,A8/01714525252525252525252,01714525252DEQ40007
     *252525252,01714504210421042104210042,0171446314631463146314631,01714444167DEQ40008
     *441671441,0171442727272727272727272,0171441421243454500046,01714402477DEQ40009
     *525655446,01713764235204726027O/                                  DEQ40010
      DATA AP0,AP1,AP2,AP3,AP4,AP5,AP6,AP7,AP8/0171740000000000000000,017DEQ40011
     *1665252525252525,0171660000000000000,0171654476447644764447,017DEQ40012
     *1652161616161616,01716503125037756523l,0171646741521424667 74,017DEQ40013
     *16455743602120766l,0171644567162064523 30/                        DEQ40014
      DATA B0,B1,B2,B3,B4,B5,B6,B7,B8/01714525252525252525252,000000000000DEQ40015
     *000000000,0606735673567356735 67,0606735673567356735 67,0607004103l3DEQ40016
     *556630410,06070144167144167144l,060702347642525026560,0607031322 07DEQ40017
     *010257763,060703607613672523307/                                  DEQ40018
      DATA BP0,BP1,BP2,BP3,BP4,BP5,BP6,BP7,BP8/0171740000000000000000,060DEQ40019
     *6325252525252525,0606425252525252525 25,060651175117511751175,060DEQ40020
     *6531463146314631 46,06066054332706016 0543,06066213406613406613 4,060DEQ40021
     *6631531727250332 57,060663753007252122331/                        DEQ40022
      DATA W0,W1,W2,W3,W4,W5,W6,W7,W8/01704550610074310761 2,0607004235 25DEQ40023
     *521066740,01712463435013346321 3,06063342540014555533 1,01717400000 0DEQ40024
     *000000000,0172042165177715111 22,01717766307057510631 3,017204007354DEQ40025
     *252256711,01717777645635760715 6/                                 DEQ40026
      DATA V0,V1,V2,V3,V4,V5,V6,V7,V8/0170667724065360754 67,0606533052 33DEQ40027
     *301450700,0171457262712357060 17,0606124357566316157 70,0172146342 66DEQ40028
     *567637354,0172242664067115576 15,0172156363635156161 35,0172140226 62DEQ40029
     *701160620,0171777707131442462 12/                                 DEQ40030
C     THE CALLING SEQUENCE CAN BE SIMPLIFIED BY PUTTING ALL PARAMETERS  DEQ40031
C     EXCEPT NTRY AND DAUX IN LABELED COMMON.  (SEE EXAMPLE BELOW)      DEQ40032
C     HOWEVER, THE DIMENSION STATEMENTS MUST BE CHANGED, OR INCLUDED    DEQ40033
C     IN THE LABELLED COMMON STATEMENT.   THE NEW CALLING SEQ. BECOMES  DEQ40034
C     CALL DEQ4 (NTRY,DAUX)                                             DEQ40035
C     ALSO, THE SUBROUTINE STATEMENT (SEE ABOVE) MUST BE CHANGED TO     DEQ40036
C     SUBROUTINE DEQ4(NTRY,DAUX)                                        DEQ40037
C     EXAMPLE FOLLOWING SHOWS LABELED COMMON FOR SIMPLIFIED CALLING SEQ.DEQ40038
C     COMMON/CDEQ/N,I1,I2,IA,IB,IR,ER,HMIN,HMAX,YMIN,TEST,IDH,IRK,JHH,  DEQ40039
C    1              JHD,VMIN,VMAX,T,H,Y,YP,Y2P,T1,T2,T3,T4,T5,T6,T7,    DEQ40040
C    2              F2P,F1P,DLT1,DLT2,DLT3,                             DEQ40041
C    3              DLT4,DLT5,DLT6,DLT7,DLT8                            DEQ40042
```

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C     DIMENSION Y( 63),YP( 63),Y2P( 63),T1( 63),T2( 63),T3( 63),          DEQ40043
C    1          T4( 63),T5( 63),T6( 63),T7( 63),                          DEQ40044
C    2         F2P( 63),F1P( 63),DLT1( 63),DLT2( 63),                     DEQ40045
C    3          DLT3( 63),DLT4( 63),DLT5( 63),DLT6( 63),DLT7( 63),        DEQ40046
C    4          DLT8( 63)                                                 DEQ40047
      DIMENSION Y(2),YP(2),Y2P(2),T1(2),T2(2),T3(2),T4(2)                 DEQ40048
      DIMENSION T5(2),T6(2),T7(2)                                         DEQ40049
      DIMENSION F2P(2),F1P(2)                                             DEQ40050
      DIMENSION DLT1(2),DLT2(2),DLT3(2),DLT4(2),DLT5(2),DLT6(2)           DEQ40051
      DIMENSION DLT7(2),DLT8(2)                                           DEQ40052
C*****NOTE ALL OPTIONS AND INITIAL CONDITIONS (T,H,Y,YP) MUST BE STORED DEQ40053
C*****      PRIOR TO THE SETUP ENTRY TO DEQ4. (DEQ4 ENTRY CALLS DAUX)    DEQ40054
C**** SPECIAL NOTE ********************************* SPECIAL NOTE ****CDEQ40055
C           WITH THE DATA ALLOCATION SCHEME OF DEQ4, IT IS POSSIBLE FOR  DEQ40056
C     THE USER TO INTEGRATE THE FIRST  P EQUATIONS SIMPLY BY CHANGING N.DEQ40057
C     OF COURSE, THIS ASSUMES THAT THE FIRST P EQUATIONS DO NOT DEPEND  DEQ40058
C     ON THE FINAL N-P EQUATIONS.  (SEE WRITE-UP FOR FURTHER DETAILS.)  DEQ40059
C     N     IS THE NUMBER OF EQUATIONS.                                 DEQ40060
C     I1    IS AN OPTION, SUCH THAT IF                                  DEQ40061
C           I1 IS G.E. +0, Y2P = F(X,Y,YP)  (I.E., FUNCTION OF 1ST DERIV.)DEQ40062
C           I1 IS L.T.  0, Y2P = F(X,Y)                                 DEQ40063
C     I2    IS AN OPTION, SUCH THAT IF                                  DEQ40064
C           I2 IS G.E. +0, VARIABLE STEP-SIZE MODE IS USED.             DEQ40065
C           I2 IS L.T.  0, FIXED STEP-SIZE MODE IS USED.                DEQ40066
C     IA    IS AN INDICATOR SWITCH TO THE USER DURING EXIT TO DAUX SUB. DEQ40067
C           IA=-1 FOR 1ST (1,2,3 IF R.K.) PASS THRU DAUX.               DEQ40068
C           IA=+1 FOR FINAL PASS THRU DAUX. (APPLIES FOR EACH STEP.)    DEQ40069
C           NOTE  IN THE COWELL MODE, IA=-1 WHEN THE DERIVATIVES OF THE DEQ40070
C                 PREDICTOR ARE BEING ASKED FOR, AND IA=+1 WHEN THE     DEQ40071
C                 DERIVATIVES OF THE CORRECTOR ARE BEING ASKED FOR.     DEQ40072
C     IB    ONLY THE 1ST IB (L.E. N) EQNS. ARE TESTED DURING ERROR TESTS.DEQ40073
C           FOR THE TWO GROUP MODE, THE FIRST IB EQNS ARE INTEGRATED AT DEQ40074
C           STEP-SIZE H, AND THE FINAL N-IB EQNS ARE INTEGRATED AT STEP- DEQ40075
C           SIZE R*H (R= 1., 2., 4., 8., ETC. DEPENDING ON THE INITIAL  DEQ40076
C           VALUES OF TEST AND VMIN).  (SEE TEST AND VMIN)              DEQ40077
C     IR    FOR A GIVEN STEP-SIZE H, COWELL STEP = H, R.K. STEP = H/IR. DEQ40078
C     ER    RELATIVE ERROR CRITERIA.(SET ER=1.E-9 OR LESS)              DEQ40079
C     HMIN IS THE MINIMUM STEP-SIZE ALLOWED. (ABSOLUTE VALUE)           DEQ40080
C     HMAX IS THE MAXIMUM STEP-SIZE ALLOWED. (ABSOLUTE VALUE)           DEQ40081
C     YMIN IS THE MIN. ABS. VALUE OF Y(I) ALLOWED FOR THE ERROR TEST.   DEQ40082
C     DAUX IS AN EXTERNAL SUB. SUPPLIED BY USER TO EVAL. THE 2ND DERIV. DEQ40083
C     TEST AFTER EACH INTEGRATION STEP,                                 DEQ40084
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C          TEST WILL BE +1. IF THE INTEGRATION WAS A RUNGE-KUTTA STEP.  DEQ40085
C          TEST WILL BE -1. IF THE INTEGRATION WAS A COWELL STEP,       DEQ40086
C          NOTE  INITIALLY SET TEST=1, FOR NORMAL INTEGRATION.  FOR TWO-DEQ40087
C                GROUP MODE SET TEST G.E. 2. (MAX R = 2.**(TEST-1.)     DEQ40088
C     IDH  AFTER EACH INTEGRATION STEP,                                 DEQ40089
C          IDH WILL BE +1 IF THE STEP-SIZE HAS NOT CHANGED.             DEQ40090
C          IDH WILL BE +2 IF THE STEP-SIZE HAS BEEN HALVED.             DEQ40091
C          IDH WILL BE +3 IF THE STEP-SIZE HAS BEEN DOUBLED             DEQ40092
C          IDH WILL BE +4 IF H FOR FINAL N-IB EQNS. DOUBLED.            DEQ40093
C     NTRY IS A SPECIAL OPTION TO ALLOW MULTIPLE ENTRIES.               DEQ40094
C          NTRY=1. SETUP ENTRY.  (STORE INITIAL COND. PRIOR TO ENTRY.)  DEQ40095
C          NTRY=2, NORMAL R.K./GAUSS-JACKSON INTEGRATION.               DEQ40096
C          NTRY=3, INTEGRATE IN R.K. MODE EXCLUSIVELY.                  DEQ40097
C     JHH  IS AN OPTION TO CONTROL THE HALVING PROCEDURE.  IF,          DEQ40098
C          JHH=1, 8*IR R.K. STEPS ARE USED DURING THE HALVING PROCEDURE.DEQ40099
C          JHH=3, RETURN TO T(I) AFTER COWELL ATTEMPT TO T(I+1), 8*IR RKDEQ40100
C          SEE WRITE-UP FOR FURTHER DETAILS CONCERNING HALVING PROCEDUREDEQ40101
C     JHD  IS AN OPTION TO CONTROL THE DOUBLING PROCEDURE.              DEQ40102
C          NOTE  JHD IS NO LONGER USED IN DEQ4.  ALL DOUBLING IS DONE   DEQ40103
C                IN THE COWELL MODE BY THE ACCUM. OF ALTERNATE DATA.    DEQ40104
C     VMIN IS THE LOC OF  1 CELL USED  BY DDEQ FOR HALVING/DOUBLING TESTDEQ40105
C          NOTE  INITIALLY SET VMIN=1.EP (P=2,3,...,5) FOR TWO-GROUP MODEDEQ40106
C     VMAX IS THE LOC OF  1 CELL USED  BY DDEQ FOR HALVING/DOUBLING TESTDEQ40107
C     T    IS THE LOCATION OF THE INDEPENDENT VARIABLE T(I).            DEQ40108
C     H    IS THE LOCATION OF THE INITIAL AND CURRENT STEP-SIZE.        DEQ40109
C     Y    IS THE LOCATION OF N DEPENDENT VARIABLES.                    DEQ40110
C     YP   IS THE LOCATION OF N 1ST DERIVATIVES.                        DEQ40111
C     Y2P  IS THE LOCATION OF N 2ND DERIVATIVES,(COMPUTED BY DAUX)      DEQ40112
C     T1 THRU T7 ARE VECTORS OF DIMENSION N USED BY THE SUBROUTINE.     DEQ40113
C     F2P, F1P, AND DLT1 THRU DLT8 ARE VECTORS OF DIMENSION N.          DEQ40114
C       SETUP FOR DEQ4 SUBROUTINE. CALL DEQ4(N,I1,I2,...,DLT7,DLT8)     DEQ40115
      GO TO (1,2,3),NTRY                                                DEQ40116
 1    IDH=1                                                             DEQ40117
      RXH=TEST                                                          DEQ40118
      IF(RXH-1.)380,381,381                                             DEQ40119
380   RXH=1.                                                            DEQ40120
381   IKR=1                                                             DEQ40121
      IF(VMIN-1.)382,383,383                                            DEQ40122
382   VMIN=1000.                                                        DEQ40123
383   VARX=VMIN                                                         DEQ40124
      RXA=RXH                                                           DEQ40125
      TEST=+1.                                                          DEQ40126
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      TST=+1.                                                   DEQ40127
      NSTRT=-1                                                  DEQ40128
      IF(N)391,390,392                                          DEQ40129
  390 N=1                                                       DEQ40130
  391 N=IABS(N)                                                 DEQ40131
  392 IF(N-IB)393,394,394                                       DEQ40132
  393 IB=N                                                      DEQ40133
  394 IF (IB)400,400,410                                        DEQ40134
  400 IB=N                                                      DEQ40135
  410 IF (IR)420,420,430                                        DEQ40136
  420 IR=16                                                     DEQ40137
  430 IF(H)432,431,432                                          DEQ40138
  431 H=.01                                                     DEQ40139
 C431 H=.01D0                                                   DEQ40140
  432 R=IR                                                      DEQ40141
      H=H/R                                                     DEQ40142
      HA=H                                                      DEQ40143
      IF(ER)433,433,434                                         DEQ40144
  433 ER=1.E-11                                                 DEQ40145
 C433 ER=1.D-11                                                 DEQ40146
  434 HH=H*H                                                    DEQ40147
      N1=N                                                      DEQ40148
      IF (YMIN)439,440,450                                      DEQ40149
  440 YMIN=1.                                                   DEQ40150
 C440 YMIN=1.D0                                                 DEQ40151
  439 YMIN= ABS(YMIN)                                           DEQ40152
 C439 YMIN=DABS(YMIN)                                           DEQ40153
  450 IF (HMAX)460,460,470                                      DEQ40154
  460 HMAX=1.                                                   DEQ40155
 C460 HMAX=1.D0                                                 DEQ40156
  470 IF(HMIN)471,471,472                                       DEQ40157
  471 HMIN=1.E-5                                                DEQ40158
 C471 HMIN=1.D-5                                                DEQ40159
  472 VMIN=ER/(HH*100.)                                         DEQ40160
      VMAX=VMIN*100000.                                         DEQ40161
      IA=-1                                                     DEQ40162
C       IA=-1 FOR 1ST (1,2,3 IF R.K.)PASS THRU DAUX             DEQ40163
      NHH=+1                                                    DEQ40164
      CALL DAUX                                                 DEQ40165
C     SAVE INITIAL CONDITIONS FOR RESTART                       DEQ40166
      TZ=T                                                      DEQ40167
      DO 473 I=1,N1                                             DEQ40168
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      T5(I)=Y(I)
      T6(I)=YP(I)
 473  T7(I)=Y2P(I)
      IF(HMAX-HMIN)261,474,261
 474  NHH=-1
C       EXIT FROM DEQ2 SETUP
      GO TO 261
C       NORMAL INTEGRATION ENTRY.  CALL RKCW
C     ENTRY RKCW
C     INTEGRATE 1 STEP (H OR H/IR) IN THE COWELL/R.K. MODE
 2    N1=N
      IF(TEST)900,500,500
C       R.K. STEP (OR R.K. STEPS)
 500  IDH=1
 501  IF(IKR)505,502,502
C       R.K. STEP (INITIAL STARTING PROCEDURE)
 502  K=1
      TEST=TST
      IKR=-1
 505  GO TO (510,520,530,540,550,560,570,580,590),K
C     K=1
 510  DO 511 I=1,N1
      DLT1(I)=Y2P(I)
      F1P(I)=W0*Y2P(I)
 511  F2P(I)=V0*Y2P(I)
 512  K=K+1
 513  IF(K-10)3,600,3
C       SPECIAL R.K. INTEGRATION ENTRY.   (NTRY=3)
C     ENTRY RK
C       INTEGRATE 1 STEP (H, OR H/IR) IN THE RUNGE-KUTTA MODE.
C       NTRY=3 IS A SPECIAL USAGE. INTEGRATES ONLY IN R.K. MODE
 3    N1=N
      H1=H
      HH=H*H
      H2=H/2.
      H3=HH/2.
      H4=H3/2.
      H5=H4/2.
      H6=H/6.
      DO 100 I=1,N1
      T1(I)=Y(I)
      T2(I)=YP(I)
```

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      T3(I)=Y2P(I)                                                      DEQ40211
  100 T4(I)=Y2P(I)                                                      DEQ40212
  110 T=T+H2                                                            DEQ40213
      IA=-1                                                             DEQ40214
      IF (I1)300,200,200                                                DEQ40215
C       R.K. STEP FOR Y2P=F(X,Y,YP)                                     DEQ40216
  200 DO 210 I=1,N1                                                     DEQ40217
C     Y2P=F(X,Y,YP) IF I1=+                                             DEQ40218
      Y(I)=T1(I)+H2*T2(I)+H5*Y2P(I)                                     DEQ40219
  210 YP(I)=T2(I)+H2*Y2P(I)                                             DEQ40220
      CALL DAUX                                                         DEQ40221
      DO 220 I=1,N1                                                     DEQ40222
      T3(I)=T3(I)+Y2P(I)                                                DEQ40223
      T4(I)=T4(I)+2.*Y2P(I)                                             DEQ40224
  220 YP(I)=T2(I)+H2*Y2P(I)                                             DEQ40225
      CALL DAUX                                                         DEQ40226
      DO 230 I=1,N1                                                     DEQ40227
      T3(I)=T3(I)+Y2P(I)                                                DEQ40228
      T4(I)=T4(I)+2.*Y2P(I)                                             DEQ40229
      Y(I)=T1(I)+H1*T2(I)+H3*Y2P(I)                                     DEQ40230
  230 YP(I)=T2(I)+H1*Y2P(I)                                             DEQ40231
      T=T+H2                                                            DEQ40232
      CALL DAUX                                                         DEQ40233
      DO 240 I=1,N1                                                     DEQ40234
  240 T4(I)=T4(I)+Y2P(I)                                                DEQ40235
  250 DO 260 I=1,N1                                                     DEQ40236
      Y(I) =T1(I)+H1*(T2(I)+H6*T3(I))                                   DEQ40237
  260 YP(I)=T2(I)+H6*(T4(I))                                            DEQ40238
      IA=+1                                                             DEQ40239
C       IA=+1 FOR FINAL PASS THRU DAUX                                  DEQ40240
      CALL DAUX                                                         DEQ40241
  262 TEST=TST                                                          DEQ40242
  261 RETURN                                                            DEQ40243
C       R.K. STEP FOR Y2P=F(X,Y)                                        DEQ40244
  300 DO 310 I=1,N1                                                     DEQ40245
C     Y2P=F(X,Y) IF I1=-                                                DEQ40246
  310 Y(I)=T1(I)+H2*T2(I)+H5*Y2P(I)                                     DEQ40247
      CALL DAUX                                                         DEQ40248
      DO 320 I=1,N1                                                     DEQ40249
      T3(I)=T3(I)+2.*Y2P(I)                                             DEQ40250
  320 T4(I)=T4(I)+4.*Y2P(I)                                             DEQ40251
      T=T+H2                                                            DEQ40252
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```
      DO 330 I=1,N1
  330 Y(I)=T1(I)+H1*T2(I)+H3*Y2P(I)
      CALL DAUX
      DO 340 I=1,N1
  340 T4(I)=T4(I)+Y2P(I)
      GO TO 250
C     K=2
  520 DO 521 I=1,N1
      DLT1(I)=DLT1(I)-8.*Y2P(I)
      DLT2(I)=Y2P(I)
      F1P(I)=F1P(I)+W1*Y2P(I)
  521 F2P(I)=F2P(I)+V1*Y2P(I)
      GO TO 512
C     K=3
  530 DO 531 I=1,N1
      DLT1(I)=DLT1(I)+28.*Y2P(I)
      DLT2(I)=7.*Y2P(I)-DLT2(I)
      DLT3(I)=Y2P(I)
      F1P(I)=F1P(I)+W2*Y2P(I)
  531 F2P(I)=F2P(I)+V2*Y2P(I)
      GO TO 512
C     K=4
  540 DO 541 I=1,N1
      DLT1(I)=DLT1(I)-56.*Y2P(I)
      DLT2(I)=DLT2(I)-21.*Y2P(I)
      DLT3(I)=DLT3(I)-6.*Y2P(I)
      DLT4(I)=Y2P(I)
      F1P(I)=F1P(I)+W3*Y2P(I)
  541 F2P(I)=F2P(I)+V3*Y2P(I)
      GO TO 512
C     K=5
  550 DO 551 I=1,N1
      DLT1(I)=DLT1(I)+70.*Y2P(I)
      DLT2(I)=DLT2(I)+35.*Y2P(I)
      DLT3(I)=DLT3(I)+15.*Y2P(I)
      DLT4(I)=5.*Y2P(I)-DLT4(I)
      DLT5(I)=Y2P(I)
      F1P(I)=F1P(I)+W4*Y2P(I)+YP(I)/HA
  551 F2P(I)=F2P(I)+V4*Y2P(I)+(5.*YP(I)/HA)+(Y(I)/(HA*HA))
      GO TO 512
C     K=6
  560 DO 561 I=1,N1
```

```
      DLT1(I)=DLT1(I)-56.*Y2P(I)
      DLT2(I)=DLT2(I)-35.*Y2P(I)
      DLT3(I)=DLT3(I)-20.*Y2P(I)
      DLT4(I)=DLT4(I)-10.*Y2P(I)
      DLT5(I)=DLT5(I)-4.*Y2P(I)
      DLT6(I)=Y2P(I)
      F1P(I)=F1P(I)+W5*Y2P(I)
  561 F2P(I)=F2P(I)+V5*Y2P(I)
      GO TO 512
C     K=7
  570 DO 571 I=1,N1
      DLT1(I)=DLT1(I)+28.*Y2P(I)
      DLT2(I)=DLT2(I)+21.*Y2P(I)
      DLT3(I)=DLT3(I)+15.*Y2P(I)
      DLT4(I)=DLT4(I)+10.*Y2P(I)
      DLT5(I)=DLT5(I)+6.*Y2P(I)
      DLT6(I)=3.*Y2P(I)-DLT6(I)
      DLT7(I)=Y2P(I)
      F1P(I)=F1P(I)+W6*Y2P(I)
  571 F2P(I)=F2P(I)+V6*Y2P(I)
      GO TO 512
C     K=8
  580 DO 581 I=1,N1
      DLT1(I)=DLT1(I)-8.*Y2P(I)
      DLT2(I)=DLT2(I)-7.*Y2P(I)
      DLT3(I)=DLT3(I)-6.*Y2P(I)
      DLT4(I)=DLT4(I)-5.*Y2P(I)
      DLT5(I)=DLT5(I)-4.*Y2P(I)
      DLT6(I)=DLT6(I)-3.*Y2P(I)
      DLT7(I)=DLT7(I)-2.*Y2P(I)
      DLT8(I)=Y2P(I)
      F1P(I)=F1P(I)+W7*Y2P(I)
  581 F2P(I)=F2P(I)+V7*Y2P(I)
      GO TO 512
C     K=9
  590 DO 591 I=1,N1
      DLT1(I)=DLT1(I)+Y2P(I)
      DLT2(I)=DLT2(I)+Y2P(I)
      DLT3(I)=DLT3(I)+Y2P(I)
      DLT4(I)=DLT4(I)+Y2P(I)
      DLT5(I)=DLT5(I)+Y2P(I)
      DLT6(I)=DLT6(I)+Y2P(I)
```

```
      DLT7(I)=DLT7(I)+Y2P(I)
      DLT8(I)=Y2P(I)-DLT8(I)
      F1P(I)=F1P(I)+W8*Y2P(I)
  591 F2P(I)=F2P(I)+V8*Y2P(I)
      GO TO 512
C     ENTRY CW
  600 K=1
      KC=1
      KS=1
      RAT=1.
      NDUB=+1
      NH2=NHH
      NVR=1
      NJH3=+1
C     TEST FOR HALVING AND DOUBLING
C     IDH=1 IF STEP-SIZE HAS NOT CHANGED.
  900 IDH=1
      IC=IB+1
      IF (I2)1000,901,901
  901 IF(NH2)9011,9010,9010
 9010 DO 902 I=1,IB
      IF( ABS(DLT2(I)/AMAX1( ABS(Y(I)),YMIN)).GE.VMAX) GO TO 1100
C     IF(DABS(DLT2(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMAX) GO TO 1100
  902 CONTINUE
C     IF 2.*H G.T. HMAX, STOP DOUBLING TEST
 9011 IF(NDUB)980,9020,9020
 9020 IF(NVR)980,980,9021
 9021 IF(RAT-1.)9022,9022,980
 9022 IF(KS)954,954,9023
 9023 DO 903 I=1,IB
      IF( ABS(DLT2(I)/AMAX1( ABS(Y(I)),YMIN)).GE.VMIN) GO TO 980
C     IF(DABS(DLT2(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMIN) GO TO 980
  903 CONTINUE
C     TEST FURTHER FOR DOUBLING.
      DO 904 I=1,IB
      IF( ABS(DLT1(I)/AMAX1( ABS(Y(I)),YMIN)).GE.VMIN) GO TO 980
C     IF(DABS(DLT1(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMIN) GO TO 980
  904 CONTINUE
C     IF HERE, CURRENT STEP O.K. FOR DOUBLING.
  950 TMP4=H+H
      IF( ABS(TMP4).GT.HMAX) GO TO 3000
C     IF(DABS(TMP4).GT.HMAX) GO TO 3000
```

```
C     KJ=1 (SAVE ALL EQUATIONS FOR DOUBLING)                            DEQ40379
      KJ=1                                                              DEQ40380
  952 KA=KC                                                             DEQ40381
      KC=KC+1                                                           DEQ40382
      GO TO (2010,2020,2030,2040,2050,2060,2070,2080,2090),KA           DEQ40383
  954 KS=-KS                                                            DEQ40384
      GO TO 1000                                                        DEQ40385
  980 IF(IB-N1)981,3002,981                                             DEQ40386
  981 IF(RXH-1.)3002,3002,990                                           DEQ40387
  990 IF(KS)954,954,992                                                 DEQ40388
  992 KJ=IB+1                                                           DEQ40389
      VAR=VARX*VMIN/RAT                                                 DEQ40390
      DO 991 I=KJ,N1                                                    DEQ40391
      IF( ABS(DLT2(I)/AMAX1( ABS(Y(I)),YMIN)).GE.VAR) GO TO 3002        DEQ40392
  991 CONTINUE                                                          DEQ40393
      NVR=-1                                                            DEQ40394
      GO TO 952                                                         DEQ40395
C     HALVE H, RETURN TO R.K.                                           DEQ40396
 1100 R=IR                                                              DEQ40397
      H=H/(2.*R)                                                        DEQ40398
      IF( ABS(H).LT.HMIN) GO TO 3050                                    DEQ40399
C     IF(DABS(H).LT.HMIN) GO TO 3050                                    DEQ40400
      IDH=2                                                             DEQ40401
      RXH=RXA                                                           DEQ40402
      TST=+1.                                                           DEQ40403
      TEST=3.                                                           DEQ40404
      IF(NJH3)1104,1101,1101                                            DEQ40405
 1101 IF(NSTRT)1102,1106,1106                                           DEQ40406
 1102 TEST=2.                                                           DEQ40407
C     RESTORE INITIAL CONDITIONS AND RESTART.  (TEST=2.)                DEQ40408
 1104 T=TZ                                                              DEQ40409
      TST=TEST                                                          DEQ40410
      DO 1105 I=1,N1                                                    DEQ40411
      Y(I)=T5(I)                                                        DEQ40412
      YP(I)=T6(I)                                                       DEQ40413
 1105 Y2P(I)=T7(I)                                                      DEQ40414
 1106 IKR=+1                                                            DEQ40415
      HA=H                                                              DEQ40416
      VMIN=ER/(H*H*100.)                                                DEQ40417
      VMAX=VMIN*100000.                                                 DEQ40418
      GO TO 502                                                         DEQ40419
C     KA=1  SAVE Y2P(0) IN T2  (ACCUM, F1P(2H), F2P(2H))                DEQ40420
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```
 2010 DO 2011 I=KJ,N1
      T2(I)=Y2P(I)
      T6(I)=W0*Y2P(I)
 2011 T7(I)=V0*Y2P(I)
      GO TO 954
C     K1=2  SAVE Y2P(2) IN T3  (ACCUM. F1P(2H), F2P(2H))
 2020 DO 2021 I=KJ,N1
      T3(I)=Y2P(I)
      T6(I)=T6(I)+W1*Y2P(I)
 2021 T7(I)=T7(I)+V1*Y2P(I)
      GO TO 954
C     K1=3  SAVE Y2P(4) IN T4  (ACCUM. F1P(2H), F2P(2H))
 2030 DO 2031 I=KJ,N1
      T4(I)=Y2P(I)
      T6(I)=T6(I)+W2*Y2P(I)
 2031 T7(I)=T7(I)+V2*Y2P(I)
      GO TO 954
C     K1=4  SAVE Y2P(6) IN T5  (ACCUM. F1P(2H), F2P(2H))
 2040 DO 2041 I=KJ,N1
      T5(I)=Y2P(I)
      T6(I)=T6(I)+W3*Y2P(I)
 2041 T7(I)=T7(I)+V3*Y2P(I)
      GO TO 954
C     K1=5  (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)
 2050 H1=1./(H+H)
      H2=H1*H1
      H3=1./RAT
      H4=H3*H3
      DO 2051 I=KJ,N1
      IF(I-IC)2053,2052,2053
 2052 H1=H1*H3
      H2=H2*H4
 2053 T6(I)=T6(I)+W4*Y2P(I)+YP(I)*H1
 2051 T7(I)=T7(I)+V4*Y2P(I)+5.*YP(I)*H1+Y(I)*H2
      GO TO 954
C     K1=6  (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)
 2060 DO 2061 I=KJ,N1
      T6(I)=T6(I)+W5*Y2P(I)
 2061 T7(I)=T7(I)+V5*Y2P(I)
      GO TO 954
C     K1=7  (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)
 2070 DO 2071 I=KJ,N1
```

```
      T6(I)=T6(I)+W6*Y2P(I)                                              DEQ40463
 2071 T7(I)=T7(I)+V6*Y2P(I)                                              DEQ40464
      GO TO 954                                                          DEQ40465
C     K1=8  (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)                       DEQ40466
 2080 DO 2081 I=KJ,N1                                                    DEQ40467
      T6(I)=T6(I)+W7*Y2P(I)                                              DEQ40468
 2081 T7(I)=T7(I)+V7*Y2P(I)                                              DEQ40469
      GO TO 954                                                          DEQ40470
C     K1=9  (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)                       DEQ40471
 2090 DO 2091 I=KJ,N1                                                    DEQ40472
      F1P(I)=T6(I)+W8*Y2P(I)                                             DEQ40473
      F2P(I)=T7(I)+V8*Y2P(I)                                             DEQ40474
C     DOUBLE H IN COWELL MODE                                            DEQ40475
      DLT8(I)= 2.*DLT8(I)-DLT7(I)                                        DEQ40476
      DLT7(I)= 4.*DLT7(I)-(4.*DLT6(I)-DLT5(I))                           DEQ40477
      DLT6(I)= 8.*DLT6(I)-(12.*DLT5(I)-6.*DLT4(I)+DLT3(I))               DEQ40478
      DLT5(I)=16.*DLT5(I)-(32.*DLT4(I)-24.*DLT3(I)+8.*DLT2(I)-DLT1(I))   DEQ40479
      DLT4(I)= 5.*DLT5(I)-(10.*DLT6(I)-10.*DLT7(I)+5.*DLT8(I))           DEQ40480
     1+(Y2P(I)-T5(I))                                                    DEQ40481
      DLT3(I)= 6.*DLT4(I)-(15.*DLT5(I)-20.*DLT6(I)+15.*DLT7(I)           DEQ40482
     1-6.*DLT8(I))-(Y2P(I)-T4(I))                                        DEQ40483
      DLT2(I)= 7.*DLT3(I)-(21.*DLT4(I)-35.*DLT5(I)+35.*DLT6(I)           DEQ40484
     1-21.*DLT7(I)+7.*DLT8(I))+(Y2P(I)-T3(I))                            DEQ40485
      DLT1(I)= 8.*DLT2(I)-(28.*DLT3(I)-56.*DLT4(I)+70.*DLT5(I)           DEQ40486
     1-56.*DLT6(I)+28.*DLT7(I)-8.*DLT8(I))-(Y2P(I)-T2(I))                DEQ40487
 2091 CONTINUE                                                           DEQ40488
C     END OF DOUBLING                                                    DEQ40489
      IF(NVR)2093,2092,2092                                              DEQ40490
 2092 IDH=3                                                              DEQ40491
      VMIN=VMIN/4.                                                       DEQ40492
      VMAX=VMAX/4.                                                       DEQ40493
      H=H+H                                                              DEQ40494
      HA=H                                                               DEQ40495
      NH2=NHH                                                            DEQ40496
      GO TO 2095                                                         DEQ40497
 3000 NDUB=-1                                                            DEQ40498
 3002 NJH3=+1                                                            DEQ40499
      IF(NH2)2095,3004,3004                                              DEQ40500
 3004 IF(JHH-3)2095,3006,2095                                            DEQ40501
 3006 NJH3=-1                                                            DEQ40502
      TZ=T                                                               DEQ40503
      DO 3010 I=1,N1                                                     DEQ40504
```

```
      T5(I)=Y(I)
      T6(I)=YP(I)
 3010 T7(I)=Y2P(I)
      GO TO 2095
 3050 NH2=-1
      IF(NSTRT)3052,1000,1000
 3052 TEST=13.
      GO TO 261
 2093 RAT=2.*RAT
      K=K+K
      RKH=RKH-1.
      IDH=4
 2095 KC=1
      KS=1
C     STEP-SIZE O.K., PROCEED WITH COWELL STEP.
 1000 TEST=-1.
      H=HA
      NSTRT=+1
      HH=H*H
      NX=IB
C     COMPLETE K STEPS FOR FIRST IB EQNS.
      DO 1022 K1=1,K
      T=T+H
      IF(K-K1)6660,6660,6661
 6660 NX=N1
      TEST=+1.
 6661 DO 1001 I=1,NX
      IF(I-IC)6666,6665,6666
 6665 H=HA*RAT
      HH=H*H
 6666 T1(I)=Y2P(I)
 1001 Y(I) =HH*(F2P(I)+A0*Y2P(I)+A1*DLT8(I)+A2*DLT7(I)+A3*DLT6(I)
     1 +A4*DLT5(I)+A5*DLT4(I)+A6*DLT3(I)+A7*DLT2(I)+A8*DLT1(I))
      H=HA
      IF(I1)1007,1005,1005
 1005 DO 1006 I=1,NX
      IF(I-IC)1006,6667,1006
 6667 H=HA*RAT
 1006 YP(I)=H*(F1P(I)+AP0*Y2P(I)+AP1*DLT8(I)+AP2*DLT7(I)+AP3*DLT6(I)
     1 +AP4*DLT5(I)+AP5*DLT4(I)+AP6*DLT3(I)+AP7*DLT2(I)+AP8*DLT1(I))
 1007 ASSIGN 1015 TO IFLAG
      IA=-1
```

```
1010 CALL DAUX                                                          DEQ40547
     H=HA                                                               DEQ40548
     HH=H*H                                                             DEQ40549
1009 DO 1013 I=1,NX                                                     DEQ40550
     IF(I-IC)6669,6668,6669                                             DEQ40551
6668 H=HA*RAI                                                           DEQ40552
     HH=H*H                                                             DEQ40553
6669 TMP1=Y2P(I)-T1(I)                                                  DEQ40554
     TMP2=TMP1-DLT8(I)                                                  DEQ40555
     TMP3=TMP2-DLT7(I)                                                  DEQ40556
     TMP4=TMP3-DLT6(I)                                                  DEQ40557
     TMP5=TMP4-DLT5(I)                                                  DEQ40558
     TMP6=TMP5-DLT4(I)                                                  DEQ40559
     TMP7=TMP6-DLT3(I)                                                  DEQ40560
     TMP8=TMP7-DLT2(I)                                                  DEQ40561
     Y(I)=HH*(F2P(I)+B0*Y2P(I)+B1*TMP1+B2*TMP2+B3*TMP3+B4*TMP4+B5*TMP5  DEQ40562
    1 +B6*TMP6+B7*TMP7+B8*TMP8)                                         DEQ40563
1011 YP(I)=H*(F1P(I)+BP0*Y2P(I)+BP1*TMP1+BP2*TMP2+BP3*TMP3+BP4*TMP4     DEQ40564
    1 +BP5*TMP5+BP6*TMP6+BP7*TMP7+BP8*TMP8)                             DEQ40565
1013 CONTINUE                                                           DEQ40566
     GO TO IFLAG,(1015,1020)                                            DEQ40567
1015 ASSIGN 1020 TO IFLAG                                               DEQ40568
     IA=+1                                                              DEQ40569
     GO TO 1010                                                         DEQ40570
1020 DO 1021 I=1,NX                                                     DEQ40571
     TMP1=Y2P(I)-T1(I)                                                  DEQ40572
     TMP2=TMP1-DLT8(I)                                                  DEQ40573
     DLT8(I)=TMP1                                                       DEQ40574
     TMP1=TMP2-DLT7(I)                                                  DEQ40575
     DLT7(I)=TMP2                                                       DEQ40576
     TMP2=TMP1-DLT6(I)                                                  DEQ40577
     DLT6(I)=TMP1                                                       DEQ40578
     TMP1=TMP2-DLT5(I)                                                  DEQ40579
     DLT5(I)=TMP2                                                       DEQ40580
     TMP2=TMP1-DLT4(I)                                                  DEQ40581
     DLT4(I)=TMP1                                                       DEQ40582
     TMP1=TMP2-DLT3(I)                                                  DEQ40583
     DLT3(I)=TMP2                                                       DEQ40584
     DLT1(I)=TMP1-DLT2(I)                                               DEQ40585
     DLT2(I)=TMP1                                                       DEQ40586
     F1P(I)=F1P(I)+Y2P(I)                                               DEQ40587
1021 F2P(I)=F2P(I)+F1P(I)                                               DEQ40588
```

```
                                                                    DEQ40589
      TEST=TFST-1.                                                  DEQ40590
      H=HA                                                          DEQ40591
      HH=HA*HA                                                      DEQ40592
 1022 CONTINUE                                                      DEQ40593
      TEST=-1.                                                      DEQ40594
      GO TO 201                                                     DEQ40595
      END
```

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13 ABSTRACT

ASC DEQ4 is a floating point subroutine, written in FORTRAN IV source language, which integrates numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i.e., $y_i'' = f(t, y_i, y_i')$ of $y_i'' = f(t, y_i)$, $i = 1, 2, \ldots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations (e.g., variational equations) then DEQ4 has the capability of integrating the final N-IB equations at a larger step size than the first IB equations, thus saving 2(R-1)(N-IB) derivatives per integration step. This subroutine obsoletes subroutine DEQ2 with the following improvements: better accuracy controls, new starting procedure, improved halving and doubling procedure, reduction in computing time, and reduction in core storage requirements (10N less).

The subroutine is restricted in that it contains 20 digit octal constants (real constants) for the CDC 6000 series machines.

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