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A program for the numerical solution of large sparse systems of algebraic and implicitly defined stiff differential equations

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A PROGRAM FOR THE NUMERICAL SOLUTION OF LARGE SPARSE SYSTEMS OF ALGEBRAIC AND IMPLICITLY DEFINED STIFF DIFFERENTIAL EQUATIONS

by

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ABSTRACT

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of storage requirements and execution times.

1.0 Introduction

This report documents a program for the solution of algebraic and implicitly defined stiff differential equations. We were particularly interested in solving very large systems of differential equations arising from partial differential equations where the finite element method has been applied in the space variables.

Our original goal was to use a compact storage scheme for the large matrices involved and to use iteration to solve the linear algebraic systems which occur. However, the resulting program is easily adapted to different applications through user modifications accomplished by replacement of one or two relatively simple subroutines. Thus the program is a powerful one which can be used in a variety of applications. Four examples, illustrating different matrix storage techniques and different linear equation solvers are given in the appendix. Other storage schemes and solution methods, e.g. symmetric Jacobian with Cholesky decomposition, are relatively simple to implement.

In Section 2 a brief review of the integration scheme is given. In Section 3 a discussion of differences between this program and the one from which it was adapted is given. Section 4 is devoted to a discussion of information concerning the use of this package.

2.0 Theoretical Background

Consider the system of $N = m + \ell$ differential and algebraic equations in $y_1,\ldots,y_m,v_1,\ldots,v_\ell$,

$$F(y,\dot{y},t) + P(t)\ V = 0\ , \tag{1}$$

with all or some of the initial values $y_1(t_0),\ldots,y_m(t_0),v_1(t_0),\ldots,v_\ell(t_0)$ specified. Enough of the above values must be given in order to determine the remaining values and initial values for any of the derivatives, $\dot{y}_1,\ldots,\dot{y}_m$ which appears in equation (1). In equation (1), $P(t)$ is an $N \times \ell$ matrix, F is a vector with N components, and V is a vector.

The program documented here is a modification of a program due to Brown and Gear [1]. The method of solution is a modification of Gear's method for stiff differential equations [2]. The application to differential algebraic systems was given by Gear [3]. We will briefly describe the method here for completeness, and refer the reader to the references for more details.

Suppose that approximate solution values are known at a number of equally spaced points, $t_{n-1},t_{n-2},\ldots,t_{n-k}$, and are represented by $y^{(n-1)},\ldots,y^{(n-k)}$ respectively. Let $V(t_{n-1})$ be represented by $V^{(n-1)}$. Use of a backward differentiation formula gives

$$h\,\dot{y}^{(n)} = \frac{1}{\beta_0}\left(\alpha_0\, y^{(n)} + \alpha_1\, y^{(n-1)} + \ldots + \alpha_k\, y^{(n-k)}\right),$$

where $h = t_{i+1} - t_i$. The coefficients α_i and β_0 are from Gear [2], p. 217. Substitution of this into (1) gives

$$F\left(y^{(n)}, -\frac{\alpha_0}{\beta_0 h}\, y^{(n)} + \sum_n, t_n\right) + P(t_n)\, V^{(n)} = 0 \qquad (2)$$

as the equation which $y^{(n)}$ and $V^{(n)}$ must satisfy. In equation (2),

$$\sum_n = \frac{1}{\beta_0 h}\left(\alpha_1\, y^{(n-1)} + \ldots + \alpha_k\, y^{(n-k)}\right).$$

In general, equation (2) represents a system of nonlinear equations for $y^{(n)}$ and $V^{(n)}$. The method used for solving this system of algebraic equations is a variant of Newton's method. The initial guess, $y^{(n),0}$, is obtained by polynomial extrapolation using a Hermite polynomial interpolating the known values $\dot{y}^{(n-1)}$, $y^{(n-1)}$, ..., $y^{(n-k)}$. Thus the predicted values has the form

$$(3)\quad y^{(n),0} = h\,\bar{\beta}_1\,\dot{y}^{(n-1)} + \bar{\alpha}_1\,y^{(n-1)} + \ldots + \bar{\alpha}_{n-k}\,y^{(n-k)} .$$

The application of Newton's Method to equation (2) then yields the corrector equation

$$(4)\quad J \cdot \begin{pmatrix} y^{(n),i+1} - y^{(n),i} \\ V^{(n),i+1} - V^{(n),i} \end{pmatrix} = -F\left(y^{(n),i},\ -\frac{\alpha_0}{\beta_0 h}\,y^{(n),i},\ t_n\right) + P(t_n)\,V^{(n),i} ,$$

where J is the Jacobian matrix,

$$(5)\quad J = \begin{pmatrix} \dfrac{\partial F}{\partial y} - \dfrac{\alpha_0}{\beta_0 h}\dfrac{\partial F}{\partial \dot{y}} & \vdots & \\ & & P \\ & & \end{pmatrix} .$$

Gear shows that the initial guess for $V^{(n)}$ is not important, and thus $V^{(n-1)}$ is used. Up to three iterations are performed on the corrector equation. The matrix J is not evaluated at each iteration, nor even at each timestep. J is evaluated whenever (i) the timestep or order is changed, or (ii) the corrector iteration fails to converge in three iterations.

If the corrector iteration fails to converge, the J matrix is evaluated, unless it had already been evaluated at the current time.

If it has been evaluated at the current time, the timestep is reduced by a factor of 4. In either case the step is then retired.

If the corrector iteration converges, the local error is estimated, based on the fact that the local error is approximately proportional to the difference between the predicted and corrected values of $y^{(n)}$. For this purpose a relative error tolerance is used for large solutions and an absolute error tolerance for small solutions. The root-mean-square norm (Euclidean norm divided by the square root of the number of components) is used for the vector with components $e_i/ymax_i$, where e_i is the estimated local error in $y_i^{(n)}$ and $ymax_i = \max_{0 \le k \le n} (|y_i^{(k)}|, 1)$. If the error is larger than that specified by the user, an acceptable timestep is estimated for the current order or order one lower, and the step repeated. Up to three such failures are permitted, after which an attempt is made to start over with a first order method.

When using a method of order q, the program takes at least $q + 1$ steps before changing the timestep. Changes in timestep are preceeded by calculation of the predicted timestep at current order and order one higher and one lower. If the timestep can be increased by more than 10%, the order corresponding to the largest possible timestep is used. If the timestep cannot be increased by at least 10%, the current order and stepsize are retained for at least 10 more steps.

After each step a test is made to determine whether time has advanced to or beyond the input end time. Control is returned to the calling program if it has.

At the initial call, no history of the solution is available, so the program must begin with a first order method, taking two such steps in accordance with the above description. The timestep must be suitably small, again in accordance with the above. At the point the program can begin to increase the order of the method and the timestep. Because the Jacobian matrix must be generated whenever the timestep is changed, it is not efficient to try too large a timestep initially. Because the program rapidly finds the best order and timestep, it is relatively cheap to underestimate the initial timestep compared to the cost of overestimating it.

3.0 Differences compared with DFASUB

The principal differences between the SDESOL/LDASUB package and DFASUB, and the reasons for incorporating them are as follows.

(i) The main goal of this revision was to generate a program which could solve very large sparse systems of differential equations efficiently, both in terms of storage requirements and execution time. We are particularly interested in the solution of ordinary differential equations arising from partial differential equations where the finite element method has been used to discretize the problem in space.

Large sparse problems require at least a different system of storing the Jacobian matrix and possibly the use of iteration to solve for the quasi-Newton iterates in equation (2.4). Two such subroutine packages, to be used with the basic subroutines, have been provided. Another package using standard elimination techniques is also provided and is convenient for smaller systems of equations. Use of any of these

options requires the user to supply a subroutine to evaluate his form of the equations (1), and for efficiency, a subroutine to explicitly evaluate the Jacobian. A subroutine to approximate a full Jacobian through numerical differencing has been provided. With the exception of a minor correction, this is the same as given in [1]. While use of this routine is convenient, it is inefficient and should be avoided for large systems. It is anticipated that the user can provide his own subroutine package, using his own storage scheme for the Jacobian, and with a suitable equation solver for the Newton iterates. There should be no need to disturb the basic package which carries out the time integration.

(ii) For user convenience, without a major rewrite of DFASUB, a driver routine, SDESOL, to be referenced by the user and which then communicates with LDASUB was written. The chief function of SDESOL is to set up a number of references to work storage areas required by LDASUB. In addition, some testing of parameters is accomplished, and a subroutine to calculate initial values of derivatives is called.

(iii) A subroutine to calculate initial values of derivatives, DERVAL, has been provided. The routine provided requires that the first m rows of $\frac{\partial F}{\partial \dot{y}}$ be nonsingular, which does not need to be true in the general case. For this reason, and others discussed in Section 4, the user may need to provide either his own version of DERVAL to evaluate the derivatives initially, or else he may supply initial values and a dummy version of DERVAL.

(iv) Other changes made in generating LDASUB from DFASUB were to simplify the code for the particular type of problem we wish to solve, while

others were to enhance the usability of the code. Some errors were also corrected, notably two errors in coefficients for the fifth and sixth order methods. DFASUB had the capability of computing various elements of the Jacobian at different times if they had different dependencies, with the possibility of inverting that part of the matrix at that time, if it could be done. This could result in increased efficiency in certain problems, at some expense in convenience, but for our purposes it was not considered useful, and was removed. Therefore only one call is made to evaluate the Jacobian. The Jacobian was evaluated at the beginning of each timestep in DFASUB, but this has been eliminated in LDASUB, in accordance with the description in Section 2. A subroutine, S2, was called from DFASUB to evaluate time dependent terms whenever time was changed. This is reasonable, since the function evaluation routine may be called several times at a given value of the independent variable. We have removed this, preferring to test for a new time in the routines where time dependent terms appear, then evaluating and storing them internally to that routine when necessary. This helps make the function evaluation more self contained, as well.

In DFASUB extra parameters in the calling sequence allowed the user to communicate constants to the function evaluation and Jacobian subroutines via DFASUB. We believe this is inefficient and confusing, and removed this capability, preferring to communicate from the main program to these subroutines via Common, or possibly through multiple entry points.

The norm used for error tests in DFASUB is the Euclidean norm. This has the undesirable property that for large systems the allowable

error criterion may be large. We therefore changed to the root-mean-square norm in LDASUB, which is simply the Euclidean norm divided by the square root of the number of components. One other change was made in the error tests. As noted in Section 2, the error vector has components $e_i/ymax_i$, where e_i is the estimated local error in the $i^{\underline{th}}$ variable y_i, and $ymax_i = \max_{0 \le k \le n} (|y_i^{(k)}|, 1)$. In DFASUB the maximum was taken only up to the previous timestep, n-1. This change was incorporated because some of the problems in which we were interested began with many components at zero, but which very rapidly became large, around 10^{12} or more. Without updating the value of $ymax_i$, the size of the timestep was artificially kept extremely small in order to satisfy an unreasonable error tolerance. For this reason, the maximum value of the component was updated before the norm of the relative errors was computed. For problems where values range near to one, the modification will result in no appreciable change in performance.

The printout of counters, timestep, time, and values of the dependent variables was made an option through a parameter in the calling sequence. An additional value printed is the order of the method being used.

DFASUB incorporated the capability of terminating if a certain number of floating point overflows had occurred. This capability was removed from LDASUB.

The final modification to the program was the incorporation of a restart capability without having to begin again with a first order method. This was accomplished by adding two entry points to LDASUB. One, LDASAV, saves values internal to LDASUB, returning them to the main program, where they can be saved for the time at which the calculation

is to be resumed. At that time, another entry point, LDARST, restores those values internal to LDASUB, while other necessary values are restored through the calling sequence.

4.0 Subroutine Descriptions

The description of subroutines is divided into two subsections. The first deals with the basic integration routine and other subroutines which make up the core package, and which should not be modified by the casual user. The second deals with a set of supporting subroutines, at least one of which must be supplied by the user since it defines his system of equations. The others may be usable in the form given in one of the examples, or can be defined by the user to accomplish his desired implementation.

4.1 Basic Subroutine Package

4.1.1 Subroutine SDESOL

This routine is the only one which needs to be referenced by most users. It serves as a driver for the integration routine, LDASUB. SDESOL has a simpler calling sequence than LDASUB and relieves the user of having to set up a number of auxiliary storage arrays. In addition, the routine calls DERVAL to calculate the values of the derivatives on the initial call.

The calling sequence is

```
CALL  SDESOL(Y,YL,T,TEND,NY,NL,M,JSKF,MAXDER,IPRT,H,HMIN,HMAX,RMSEPS,W)
```

where the parameters are defined as follows.

Y - Input and output. An array dimensioned (7,NY). On the initial call this array contains the initial values of the dependent variables y_i, i=1, ..., m in Y(1,i) . During execution of the program the approximate values of $\frac{d^j y_i}{dt^j} \cdot \frac{h^j}{j!}$ is stored in Y(j+1,i) . Here h is the current stepsize. These values must not be changed between returns to the calling program and subsequent entries to SDESOL. It is possible to interpolate for values of the dependent variables at times other than those calculated by using the formula $y_i(t+s) = \sum_{j=0}^{q} Y(j+1,i) \left(\frac{s}{h}\right)^j$, where q is the order formula currently in use, and is obtained as $q = |JSKF/10|$.

YL - input and output. Array of linear variables, v_i, i=1, ..., ℓ . The user supplies initial values for these variables, and during execution it contains current values of the linear variables.

T - input and output. The user supplies the initial time, which is updated to current time during execution.

TEND -input. Time at which the integration is to end. This is the only parameter normally changed by the user between successive entries to SDESOL.

NY - input. The number of differential and nonlinear variables, m .

NL - input. The number of linear variables, ℓ . This may be zero.

M - input. The number of variables to be included in the local error test. The error test will be performed for the variables y_i, i=1, ..., M . The M used is no greater than NY .

JSKF -input and output. An indicator: on input,

JSKF = 0 indicates that this is the initial call to SDESOL. Initial values of the derivatives are calculated and auxiliary storage references are set up. This also indicates to subroutine LDASUB to initialize parameters and begin with a first order integration method.

JSKF > 0 indicates a continuation of a previous call to SDESOL .

JSKF = - 1 indicates a restart call. This is discussed further in Section 4.1.2.

JSKF < - 1 may result from the user neglecting to test for error returns from SDESOL. Because of this possibility, the run is terminated with an appropriate comment when JSKF < - 1 is input.

On output, JSKF normally is a two digit number, $\pm$ qp . q is the order of the formula currently being used for the integration. p is an indicator determining the type of return. JSKF > 0 , p = 1 is the normal return. Note that SDESOL may be re-entered to continue the solution without changing JSKF. JSKF < 0 is an error return, with the value of p indicating the error, as follows.

p = 1 error test failure for H $\geq$ HMIN

p = 3 corrector failed to converge for H > HMIN

p = 4 corrector failed to converge for a first order method

p = 5 error return from subroutine NUITSL

p = 6 error return from subroutine DERVAL

MAXDER-input. Maximum order method which should be used. The highest order possible is six.

IPRT- input. Print control indicator.

≤ 0 , no print from LDASUB

> 0 , at each step, print number of steps, number of Jacobian evaluations, current order being used, stepsize for next step, current time, and current values of the dependent variables.

H - input and output. On initial call it is an estimate of the timestep. During execution it is updated to the current value, and on return contains the stepsize to be tried for the next step. The input value need not be accurate. It is better to underestimate than to overestimate the initial value. The stepsize and order are varied to meet the local error tolerance specified. The user does not normally change the stepsize between entries to SDESOL.

HMIN- input. The minimum stepsize to be allowed.

HMAX- input. The maximum stepsize to be allowed.

RMSEPS-input. The error test constant. The values of the relative local errors must have root-mean-square norm less than RMSEPS.

W - an array of auxiliary storage required by LDASUB. This array must contain a total number of locations equal to the sum of (i) 13*NY + 5*NL for arrays used in LDASUB, (ii) storage for the Jacobian matrix, and (iii) any locations used in processing the Jacobian, e.g., scratch storage used by an equation solver.

4.1.2 Subroutine LDASUB

This subroutine is the basic integration routine and performs the process in essentially the same manner as subroutine DFASUB. A brief description is given in Section 2 and differences between this routine and DFASUB are outlined in Section 3. Parameters in this routine in which the user may be interested are stored in the W array, an argument of subroutine SDESOL.

YMAX - array of maximum magnitudes of the independent variables, y_i, up to the current time (or one, if less than one). This is stored beginning at location 7*NY + NL + 1 of the W array.

ER - This is the array of differences between the predicted and corrected values of the variables, y_i, and is proportional to the estimated error. This array is stored beginning in location 8*NY + NL + 1 of the W array.

This subroutine incorporates a restart capability. In order to restart from a previous point without beginning again with a first order method, it is necessary to have saved a number of variables internal to LDASUB, and then restore them before calling SDESOL again. To save the internal parameters, the user calls subroutine LDASAV(SAV). Here SAV is an array of length 29 in which the values to be saved will be stored. In addition to SAV, the user must also save a number of arrays in the calling sequence of LDASUB, and this is most easily accomplished by saving the W array in the calling sequence for SDESOL. Once these arrays have been saved, along with the other simple parameters in the calling sequence (Y and YL need not be saved), the user is free to

use the package to solve a different problem, or to terminate the computer run, to be restarted later.

At the time the problem is to be restarted, the user calls subroutine LDARST(SAV), where SAV is the array of values obtained previously by calling LDASAV. This restores internal values in LDASUB. The user then calls SDESOL with the same simple parameters and the W array as before, except that JSKF = - 1 and a new end time, TEND, is provided. Restoration of values (including Y and YL) in LDASUB is completed and solution of the problem resumes.

If the user desires to change the error tolerance, number of variables in the error test, or maximum order to be used, the user must make a new initial call to SDESOL, that is, set JSKF = 0 .

4.1.3 Subroutine COPYZ

This subroutine simply transfers the contents of one array into another array.

4.2 Supporting Subroutines

This group of subroutinesmust, at least in part, be supplied by the user. The user must supply at least one subroutine, DIFFUN. For better efficiency, the user should supply a subroutine, JACMAT, to explicitly evaluate the Jacobian, although a version which approximates the Jacobian by numerical differencing is given in the appendix. To take advantage of sparsity or other features of his problem, the user will need to supply the subroutine NUITSL to solve the systems of equations (2.4). For certain problems the user may have to supply

subroutine DERVAL to calculate the initial values of the derivatives. We discuss the requirements of these subroutines in turn.

4.2.1 Subroutine DIFFUN

This subroutine simply evaluates the equations (2.1) at a given time and yalues of y, $\dot{y}$, and V. Other parameters in the function definition must be transmitted from the calling program via COMMON or some other device, determined by the user.

The calling sequence is

CALL DIFFUN (Y, YL, T, HINV, DY), where the parameters are defined as follows.

- Y - input. Same as in SDESOL. This array contains the current values of the variables y_i and their (scaled) derivatives.
- YL - input. Same as in SDESOL. This array contains the current values of the linear variables.
- T - input. Current time.
- HINV - input. $1/h$, where h is the current stepsize.
- DY - output. Array of function values.

4.2.2 Subroutine JACMAT

This subroutine evaluates the Jacobian matrix J, equation (2.5) at the given time and current values of the dependent variables, order, and stepsize. A version of JACMAT which approximates J by numerical differencing is given in the appendix. For maximum efficiency, the user should supply the explicit representation of the Jacobian. Because the Jacobian is used to solve for the quasi-Newton iterates, it is not

necessary for the Jacobian to be exact. Thus the user should consider the possibility of approximations which reduce the total number of computations in this step, with due regard for the fact that a smaller timestep may be required to obtain convergence of the corrector within three iterations.

The calling sequence for this subroutine is
CALL JACMAT (Y, YL, T, HINV, A2, N, NY, EPS, DY, F1, PW), where the parameters are defined as follows.

Y - input. Same as in SDESOL, Y contains the current values of the variables y_i and their (scaled) derivatives.

YL - input. Same as in SDESOL. This array contains the current values of the linear variables.

T - input. Current time.

HINV - input. 1/h , where h is the current stepsize.

A2 - input. The constant α_0/β_0 from LDASUB.

N - input. Total number of variables.

NY - input. Number of differential and nonlinear variables.

EPS - input. Error constant from LDASUB, $\sqrt{M}$ ·RMSEPS.

DY - input. Array of current function values.

F1 - scratch array of N locations available for use by this routine.

PW - output. The Jacobian matrix J , or an approximation, calculated in JACMAT and returned to calling program. This matrix is used in subroutine NUITSL and the storage mode must agree between the two subroutines.

4.2.3 Subroutine NUITSL

This subroutine solves the equations (2.4) for the quasi-Newton iterates. This subroutine will normally be supplied by the user, although versions which solve the system by elimination methods and iterative methods, respectively, are given in the examples in the appendix. This subroutine will often be modified or replaced by the user to take advantage of sparsity or other features of his problem in connection with JACMAT, of course.

The calling sequence for this subroutine is
CALL NUITSL (PW, DY, F1, N, NY. EPS, YMAX, NEWPW, KRET), where the parameters are defined as follows.

PW - input. The Jacobian matrix J computed in JACMAT.

DY - input. Right hand side of the linear system to be solved.

F1 - output. The solution is returned in the array F1 .

N - input. Total number of variables.

NY - input. Number of differential and nonlinear variables.

EPS - input. Error constant from LDASUB, $\sqrt{M}$ · RMSEPS .

YMAX - input. Array of maximum magnitudes of y_i up to the current time (or one if maximum magnitude is less than one).

NEWPW - input. Indicates whether a new J matrix has been computed since the last entry to NUITSL.

= 1, indicates this is a new J matrix. If any preprocessing, such as LU decomposition is to be done, the preprocessing should be done and NEWPW set to zero.

= 0, indicates the J matrix is the same as on the previous entry to NUITSL.

KRET - output. Return indicator.

= 0 , normal return

= 1 , error return, solution of equations not obtained.

Note that the parameters EPS and YMAX are useful if an iterative method is used for solutuon of the equations. Because the solution represents corrections to the predicted value, and corrections to that, the solution is small compared to the dependent variable values. Hence, compared to the YMAX array, the error tolerance can be fairly large. The following convergence criteria have been used, with great success. Let δu_i denote the $i^{\underline{th}}$ component of the difference between successive iterates, with u_i being the $i^{\underline{th}}$ component of the current iterate. Then the iteration is considered to have converged whenever

$$\text{(i)} \qquad \sum_{i=1}^{NY} \left(\frac{\delta u_i}{Ymax_i} \right)^2 < \left(\varepsilon/100 \right)^2 , \text{ or}$$

$$\text{(ii)} \qquad \sum_{i=1}^{NY} \left(\frac{\delta u_i}{\max(|u_i|,\varepsilon)} \right)^2 < \varepsilon^2 .$$

Condition (i) requires convergence to 2 digits more accuracy than the user has asked for in the solution of the system (2.1), relative to YMAX. Condition (ii) requires the same relative accuracy in u_i as is asked for by the user in the solution of the system (2.1), unless the solution is smaller than ε , in which case the change is compared to ε rather than $|u_i|$. This avoids difficulty if u_i is close to zero. The ε above is EPS = $\sqrt{M}$·RMSEPS, where M and RMSEPS are inputs to SDESOL. Two versions of NUITSL incorporating iteration and this convergence test are given in the appendix.

4.2.4 Subroutine DERVAL

This subroutine solves for, or otherwise supplies the initial values of the derivatives, and possibly other variables. In some instances it may need to be supplied by the user. The standard version of DERVAL given in the appendix uses Newton's method to solve the first m (=NY) of the equations (2.1) for $\dot{y}(t_o)$, assuming values for $y(t_o)$ and $V(t_0)$ have been supplied. To accomplish this, the matrix $\frac{\partial F}{\partial \dot{y}}$ is needed, and this is obtained by calling JACMAT with $h = 16^{-20}$, A2 = -1, and N = NY, implying NL = 0 for this call. Special care must be taken if in fact NL is not zero to assure that the matrix is computed and stored properly. The matrix returned is then $16^{20} \frac{\partial F}{\partial \dot{y}}$. A call to DIFFUN yields the function values $F(y(t_0), \dot{y}(t_0), t_0) + PV(t_0)$ where $\dot{y}(t_0)$ is the current iterate. Multiplication of the function values by 16^{20} and a call to NUITSL (again with N = NY) gives the Newton iterate. Of course, the same sort of special care as necessary in JACMAT is necessary in NUITSL.

Obviously the above scheme cannot work if $\frac{\partial F}{\partial \dot{y}}$ is singular, such as it would be if one of the equations is algebraic. In this instance the user must either devise his own version of DERVAL, or supply the values along with a dummy version of DERVAL. In an extreme case the user may simply set initial derivatives to zero. This will provide a poor predicted value on the first step, and will force an artificially small timestep for the first two steps. However, the overall penalty is generally small, as appropriate (corrected) values are computed at the first step, and after two steps the program quickly increases the timestep.

The calling sequence for this subroutine is

CALL DERVAL (Y, YL, T, N, NY, DY, KERET) , where the parameters are defined as follows.

Y - input and output. Same as in SDESOL. On entry Y(1,i) contains the initial values of the variables y_i . On return, the values of the derivatives are stored in Y(2 i) .

YL - input. Same as in SDESOL. This array contains the initial values of the linear variables.

T - input. initial time

N - input. Total number of variables.

NY - input. Number of differential and nonlinear variables.

W - The scratch array from SDESOL, can be used in any way needed by this subroutine.

KERET - output. Return indicater

= 0 normal return

= 1 error return, initial values were not obtained.

5.0 Acknowledgement

The author wishes to express his thanks to Professors David Salinas and Dong Nguyen of the Mechanical Engineering Department at the Naval Postgraduate School. They supplied the initial applications and encouragement for this work. They have continued to support it through valuable discussions with the author throughout the development period.

Appendix 1: Program Listings

The following are listings of the basic subroutine package and supporting subroutines which are of general use. For simple problems the user only needs to supply a calling program and a subroutine, DIFFUN, to evaluate the equations. Use of the NUITSL routine in computer facilities which do not subscribe to the IMSL package will necessitate modifications to replace LUDATF with another LU decomposition routine, and LUELMF with another forward and backward substitution routine.

```
      SUBROUTINE SDESOL (Y,YL,T,TEND,NY,NL,M,JSKF,MAXDER,IPRT,H,HMIN,    SDE   10
     1HMAX,RMSEPS,W)                                                     SDE   20
C                                                                        SDE   30
C     ------------------------------------------------------------------SDE   40
C                                                                        SDE   50
C     SUBROUTINE SDESOL IS A DRIVER ROUTINE FOR SUBROUTINE LDASUB.       SDE   60
C     ITS PURPOSE IS TO SET UP THE NECESSARY REFERENCES TO A LARGE       SDE   70
C     BLOCK OF AUXILLARY STORAGE, AND  OBTAIN INITIAL VALUES OF          SDE   80
C     DERIVATIVES.                                                       SDE   90
C     THE CALLING SEQUENCE FOR SDESOL IS                                 SDE  100
C                                                                        SDE  110
C CALL SDESOL(Y,YL,T,TEND,NY,NL,M,JSKF,MAXDER,IPRT,H,HMIN,HMAX,RMSEPS,W)SDE  120
C                                                                        SDE  130
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                       SDE  140
C                                                                        SDE  150
C        Y        - ARRAY DIMENSIONED (7,NY).  THIS ARRAY CONTAINS THE   SDE  160
C                   DEPENDENT VARIABLES AND THEIR SCALED DERIVATIVES.    SDE  170
C                   Y(J+1,I) CONTAINS THE J-TH DERIVATIVE OF THE I-TH VARSDE  180
C                   IABLE TIMES H**J/J-FACTORIAL, WHERE H IS THE CURRENT SDE  190
C                   STEPSIZE.  ON FIRST ENTRY THE CALLER SUPPLIES THE    SDE  200
C                   INITIAL VALUES OF EACH VARIABLE IN Y(1,I).  ON SUB-  SDE  210
C                   SEQUENT ENTRIES IT IS ASSUMED THE ARRAY HAS NOT      SDE  220
C                   BEEN CHANGED.  TO INTERPOLATE TO NON-MESH POINTS,    SDE  230
C                   THESE VALUES CAN BE USED AS FOLLOWS.  IF H IS THE    SDE  240
C                   CURRENT STEPSIZE AND VALUES AT TIME  T+E  ARE        SDE  250
C                   NEEDED, LET  S = E/H  AND THEN                       SDE  260
C                                                                        SDE  270
C                                                  JS                    SDE  280
C                        I-TH VARIABLE AT  T+E IS  SUM Y(J+1,I)*S**J     SDE  290
C                                                  J=0                   SDE  300
C                                                                        SDE  310
C                   THE VALUE OF JS IS OBTAINED IN THE CALLING PROGRAM   SDE  320
C                   BY  JS = IABS(JSKF/10)                               SDE  330
C        YL       - ARRAY OF NL VARIABLES WHICH APPEAR LINEARLY.         SDE  340
C        T        - CURRENT VALUE OF THE INDEPENDENT VARIABLE (TIME)     SDE  350
C        TEND     - END TIME                                             SDE  360
C        NY       - NUMBER OF DIFFERENTIAL EQUATIONS AND NONLINEAR       SDE  370
C                   VARIABLES.                                           SDE  380
C        NL       - NUMBER OF LINEAR VARIABLES                           SDE  390
C        M        - NUMBER OF VARIABLES INCLUDED IN THE ERROR TEST       SDE  400
C        JSKF     - AN INDICATOR USED BOTH ON INPUT AND OUTPUT           SDE  410
C                   ON INPUT, JSKF = -1 INDICATES A RESTART CALL TO      SDE  420
C                   SDESOL.  JSKF = 0 INDICATES AN INITIAL CALL TO       SDE  430
C                   SDESOL.  JSKF > 0 INDICATES A CONTINUATION OF THE    SDE  440
C                   PREVIOUS CALL TO SDESOL.  JSKF < -1 MAY HAVE RESULTEDSDE  450
C                   FROM THE USER NEGLECTING TO TEST FOR ERROR RETURNS   SDE  460
C                   FROM SDESOL.  BECAUSE OF THIS POSSIBILITY, JSKF < -1 SDE  470
C                   RESULTS IN TERMINATION OF THE RUN WITH THE           SDE  480
C                   APPROPRIATE COMMENT.                                 SDE  490
C                   ON OUTPUT, JSKF CONSISTS OF TWO DIGITS AND SIGN,     SDE  500
C                   + OR - QP.  Q IS THE ORDER OF THE FORMULA CURRENTLY   SDE  510
C                   BEING USED.  P INDICATES THE TYPE OF RETURN, AS      SDE  520
C                   FOLLOWS.                                             SDE  530
C                   JSKF > 0, P = 1 IS THE NORMAL RETURN                 SDE  540
C                   JSKF < 0 IS AN ERROR RETURN, WITH THE FOLLOWING      SDE  550
C                   MEANINGS.                                            SDE  560
C                        P = 1  ERROR TEST FAILURE FOR H > HMIN          SDE  570
C                        P = 3  CORRECTOR FAILED TO CONVERGE FOR H > HMINSDE  580
C                        P = 4  CORRECTOR FAILED TO CONVERGE FOR FIRST   SDE  590
C                               ORDER METHOD                             SDE  600
C                        P = 5  ERROR RETURN FROM SUBROUTINE NUITSL      SDE  610
C                        P = 6  ERROR RETURN FROM SUBROUTINE DERVAL      SDE  620
C        MAXDER   - MAXIMUM ORDER DERIVATIVE THAT SHOULD BE USED IN      SDE  630
C                   METHOD.  IT MUST BE NO GREATER THAN SIX.             SDE  640
C        IPRT     - INTERNAL PRINT CONTROL INDICATOR FOR LDASUB.         SDE  650
C                        IPRT = 0  NO PRINT                              SDE  660
C                        IPRT > 0  PRINT COUNTERS, STEPSIZE, CURRENT TIMESDE  670
C                                  AND VALUES OF DEPENDENT VARIABLES AT  SDE  680
C                                  EACH STEP.                            SDE  690
C        H        - CURRENT STEPSIZE.  AN INITIAL VALUE MUST BE SUPPLIED SDE  700
C                   BUT NEED NOT BE THE ONE WHICH MUST BE USED, SINCE THISDE  710
C                   SUBROUTINE WILL CHOSE A SMALLER ONE IF NECCESSARY TO SDE  720
C                   KEEP THE ERROR PER STEP SMALLER THAN THE SPECIFIED   SDE  730
C                   VALUE.  IT IS BETTER TO UNDERESTIMATE THE INITIAL    SDE  740
C                   STEPSIZE THAN TO OVERESTIMATE IT.  THE STEPSIZE IS   SDE  750
```

```
C                 NORMALLY NOT CHANGED BY THE USER.                                    SDE   760
C         HMIN    - MINIMUM STEPSIZE ALLOWED                                           SDE   770
C         HMAX    - MAXIMUM STEPSIZE ALLOWED                                           SDE   780
C         RMSEPS  - THE ERROR TEST CONSTANT.  THE ROOT-MEAN-SQUARE OF                  SDE   790
C                   THE SINGLE STEP ERROR ESTIMATES, ER(I), DIVIDED BY                 SDE   800
C                   YMAX(I) = (MAXIMUM TO CURRENT TIME OF Y(I) ) MUST BE               SDE   810
C                   LESS THAN EPS.  THE STEPSIZE AND/OR THE ORDER                      SDE   820
C                   ARE VARIED TO ACHIEVE THIS.                                        SDE   830
C         W       - SCRATCH STORAGE ARRAY.  MUST BE AT LEAST 13*NY + 5*NL            SDE   840
C                   LOCATIONS, PLUS THOSE REQUIRED FOR STORAGE OF THE                  SDE   850
C                   MATRIX  PW (SEE DESCRIPTION OF SUBROUTINE JACMAT).                 SDE   860
C                   THE STORAGE OF PW WILL NORMALLY REQUIRE NO MORE THAN               SDE   870
C                   N**2 + 2*N LOCATIONS, AND IF COMPACT STORAGE TECH-                 SDE   880
C                   NIQUES ARE USED, CAN BE MUCH FEWER.                                SDE   890
C                                                                                      SDE   900
C     ------------------------------------------------------------------               SDE   910
      DIMENSION Y(7,1), YL(1), W(1)                                                    SDE   920
      IF (JSKF.GT.0) GO TO 120                                                         SDE   930
      IF (JSKF.LT.-1) GO TO 140                                                        SDE   940
      N = NY+NL                                                                        SDE   950
      IF (JSKF.LT.0) GO TO 110                                                         SDE   960
C                                                                                      SDE   970
C     IF THIS IS THE FIRST ENTRY, OBTAIN VALUES OF THE DERIVATIVES.                    SDE   980
      CALL DERVAL (Y,YL,T,N,NY,W,KRETR)                                                SDE   990
      IF (KRETR.NE.0) GO TO 130                                                        SDE  1000
C                                                                                      SDE  1010
C     NOW SET UP STORAGE BLOCKS IN THE W ARRAY.  THIS NEEDS TO BE DONE                 SDE  1020
C     ONLY INITIALLY AND ON RESTARTS.                                                  SDE  1030
C                                                                                      SDE  1040
C        THE ARRAY   SAVE   STARTS AT LOCATION  1     IN THE W ARRAY                  SDE  1050
C        THE ARRAY   YLSV   STARTS AT LOCATION  NSVL  IN THE W ARRAY                  SDE  1060
C        THE ARRAY   YMAX   STARTS AT LOCATION  NYMAX IN THE W ARRAY                  SDE  1070
C        THE ARRAY   ER     STARTS AT LOCATION  NER   IN THE W ARRAY                  SDE  1080
C        THE ARRAY   ESV    STARTS AT LOCATION  NESV  IN THE W ARRAY                  SDE  1090
C        THE ARRAY   F1     STARTS AT LOCATION  NF1   IN THE W ARRAY                  SDE  1100
C        THE ARRAY   DY     STARTS AT LOCATION  NDY   IN THE W ARRAY                  SDE  1110
C        THE MATRIX  PW     STARTS AT LOCATION  NPW   IN THE W ARRAY                  SDE  1120
C                                                                                      SDE  1130
  110 NSVL = 7*NY+1                                                                    SDE  1140
      NYMAX = NSVL+NL                                                                  SDE  1150
      NER = NYMAX+NY                                                                   SDE  1160
      NESV = NER+NY                                                                    SDE  1170
      NF1 = NESV+NY                                                                    SDE  1180
      NDY = NF1+N                                                                      SDE  1190
      NPW = NDY+N                                                                      SDE  1200
  120 JS = JSKF                                                                        SDE  1210
      CALL LDASUB (Y,YL,T,TEND,N,NY,1,JS,KF,MAXDER,IPRT,H,HMIN,HMAX,                   SDE  1220
     1RMSEPS,W,W(NSVL),W(NYMAX),W(NER),W(NESV),W(NF1),W(NDY),W(NPW))                   SDE  1230
C                                                                                      SDE  1240
C     CODE JSKF ON RETURN FROM LDASUB                                                  SDE  1250
C                                                                                      SDE  1260
      JSKF = ISIGN(JS*10+IABS(KF),KF)                                                  SDE  1270
      RETURN                                                                           SDE  1280
  130 JSKF = -6                                                                        SDE  1290
      RETURN                                                                           SDE  1300
  140 PRINT 1, JSKF                                                                    SDE  1310
      STOP                                                                             SDE  1320
C                                                                                      SDE  1330
C                                                                                      SDE  1340
    1 FORMAT ('0IT IS AN ERROR TO ENTER SDESOL WITH JSKF = ',I10//                     SDE  1350
     1 '    RUN HAS BEEN TERMINATED.')                                                SDE  1360
      END                                                                              SDE  1370


      SUBROUTINE LDASUB (Y,YL,T,TEND,N,NY,M,JSTART,KFLAG,MAXDR,IPRT,H,                 LDA    10
     1HMIN,HMAX,RMSEPS,SAVE,YLSV,YMAX,ER,ESV,F1,DY,PW)                                 LDA    20
C                                                                                      LDA    30
C     SUBROUTINE LDASUB IS A MODIFICATION OF SUBROUTINE DFASUB                         LDA    40
C     WHICH IS DUE TO R. L. BROWN AND C. W. GEAR.  DFASUB IS DOCUMENTED                LDA    50
C     IN THE REPORT                                                                    LDA    60
C        DOCUMENTATION FOR DFASUB--                                                    LDA    70
C        BY R. L. BROWN AND C. W. GEAR                                                 LDA    80
C        REPORT UILCDCS-R-73-575, JULY 1973                                            LDA    90
C        UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN                                    LDA   100
C        URBANA, ILLINOIS  61801                                                       LDA   110
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C     THIS REPORT IS AVAILABLE FROM THE NATIONAL TECHNICAL INFORMATION  LDA  120
C     SERVICE OF THE U. S. DEPARTMENT OF COMMERCE UNDER ACCESSION NUMBERLDA  130
C     COO-1469-225.                                                     LDA  140
C                                                                       LDA  150
C     THE MODIFICATION HERE IS DOCUMENTED IN THE REPORT                 LDA  160
C        A PROGRAM FOR THE NUMERICAL SOLUTION OF LARGE SPARSE SYSTEMS OFLDA  170
C        ALGEBRAIC AND IMPLICITLY DEFINED STIFF DIFFERENTIAL EQUATIONS  LDA  180
C        BY RICHARD FRANKE                                              LDA  190
C        REPORT NPS53FE76051, MAY 1976                                  LDA  200
C        NAVAL POSTGRADUATE SCHOOL                                      LDA  210
C        MONTEREY, CALIFORNIA  93940                                    LDA  220
C                                                                       LDA  230
C     ------------------------------------------------------------------LDA  240
C                                                                       LDA  250
C     THE CALLING SEQUENCE FOR LDASUB IS                                LDA  260
C                                                                       LDA  270
C     CALL LDASUB(Y,YL,T,TEND,W,NY,M,JSTART,KFLAG,MAXOR,IPRT,H,HMIN,    LDA  280
C     HMAX,RMSEPS,SAVE,YLSV,YMAX,ER,ESV,F1,DY,PW)                       LDA  290
C                                                                       LDA  300
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                      LDA  310
C        Y        - ARRAY DIMENSIONED (7,NY).  THIS ARRAY CONTAINS THE  LDA  320
C                   DEPENDENT VARIABLES AND THEIR SCALED DERIVATIVES.   LDA  330
C                   Y(J+1,I) CONTAINS THE J-TH DERIVATIVE OF THE I-TH VARLDA  340
C                   IABLE TIMES H**J/J-FACTORIAL, WHERE H IS THE CURRENT LDA  350
C                   STEPSIZE.  ON FIRST ENTRY THE CALLER SUPPLIES THE   LDA  360
C                   INITIAL VALUES OF EACH VARIABLE IN Y(1,I) AND AN    LDA  370
C                   ESTIMATE OF THE INITIAL VALUES OF THE DERIVATIVES   LDA  380
C                   IN Y(2,I).  ON SUBSEQUENT ENTRIES IT IS ASSUMED THAT LDA  390
C                   THE ARRAY HAS NOT BEEN CHANGED.  TO INTERPOLATE TO  LDA  400
C                   NON-MESH POINTS, THESE VALUES CAN BE USED AS FOLLOWS.LDA  410
C                   IF H IS THE CURRENT STEPSIZE AND VALUES AT TIME T+E  LDA  420
C                   NEEDED, LET S = E/H  AND THEN                       LDA  430
C                                                                       LDA  440
C                                                    NQ                 LDA  450
C                        I-TH VARIABLE AT  T+E IS   SUM Y(J+1,I)*S**J   LDA  460
C                                                   J=0                 LDA  470
C                                                                       LDA  480
C                   THE VALUE OF NQ IS OBTAINED IN THE CALLING PROGRAM  LDA  490
C                   BY  NQ = JSTART.                                    LDA  500
C                                                                       LDA  510
C        YL       - ARRAY OF NL = N - NY VARIABLES WHICH APPEAR LINEARLY.LDA  520
C                   THE USER SUPPLIES INITIAL VALUES FOR THESE VARIABLES.LDA 530
C        T        - CURRENT VALUE OF THE INDEPENDENT VARIABLE (TIME)    LDA  540
C        TEND     - END TIME                                            LDA  550
C        N        - TOTAL NUMBER OF VARIABLES                           LDA  560
C        NY       - NUMBER OF DIFFERENTIAL EQUATIONS AND NONLINEAR      LDA  570
C                   VARIABLES.                                          LDA  580
C        M        - NUMBER OF VARIABLES INCLUDED IN THE ERROR TEST.     LDA  590
C                   THIS NUMBER CAN BE NO GREATER THAN NY.  IF IT IS    LDA  600
C                   GREATER THAN NY, NY VARIABLES ARE USED IN THE ERROR LDA  610
C                   TEST.                                               LDA  620
C        JSTART   - INPUT AND OUTPUT INDICATOR.                         LDA  630
C                   ON INPUT JSTART HAS THE FOLLOWING MEANINGS.         LDA  640
C                        <0  THIS INDICATES A RE-START FROM A PREVIOUS  LDA  650
C                            POINT FOLLOWING TERMINATION OF THE RUN OR  LDA  660
C                            SOLUTION OF ANOTHER PROBLEM DURING THE SAMELDA  670
C                            RUN.  PARAMETERS IN THE CALLING SEQUENCE   LDA  680
C                            MUST HAVE BEEN PRESERVED FROM THE PREVIOUS LDA  690
C                            USE, PARTICULARLY THE ARRAYS               LDA  700
C                                 SAVE, YLSV, ESV, AND PW.              LDA  710
C                            THESE ARRAYS MUST BE SAVED AFTER A CALL    LDA  720
C                            TO SUBROUTINE LDASAV, WHICH ALSO SAVES     LDA  730
C                            NECESSARY PARAMETERS INTERNAL TO LDASUB.   LDA  740
C                        =0  INDICATES AN INITIAL CALL TO LDASUB.  THE  LDA  750
C                            ROUTINE INITIALIZES ITSELF, SCALES THE     LDA  760
C                            DERIVATIVES IN Y(2,I) AND THEN PERFORMS THE LDA 770
C                            INTEGRATION UNTIL T > TEND.                LDA  780
C                        >0  INDICATES THE SOLUTION IS TO BE CONTINUED.  LDA  790
C                            AFTER THE INITIAL ENTRY IT IS NEITHER      LDA  800
C                            DESIRABLE NOR NECESSARY TO RE-ENTER WITH   LDA  810
C                            JSTART = 0, SINCE THIS RE-INITIALIZES      LDA  820
C                            THE CODE, BEGINNING WITH A FIRST ORDER     LDA  830
C                            METHOD AGAIN.                              LDA  840
C                   ON OUTPUT, JSTART IS SET TO THE VALUE OF NQ, THE    LDA  850
C                   ORDER OF THE FORMULA CURRENTLY BEING USED.          LDA  860
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C        KFLAG   - THE COMPLETION CODE INDICATOR, WITH THE FOLLOWING      LDA  970
C                  MEANINGS                                              LDA  980
C                       +1  THE INTEGRATION WAS SUCCESSFUL               LDA  990
C                       -1  ERROR TEST FAILURE FOR H > HMIN              LDA 1000
C                       -3  CORRECTOR FAILED TO CONVERGE FOR H > HMIN    LDA 1010
C                       -4  CORRECTOR FAILED TO CONVERGE FOR FIRST       LDA 1020
C                           ORDER METHOD                                 LDA 1030
C                       -5  ERROR RETURN FROM SUBROUTINE NUITSL          LDA 1040
C        MAXDR   - MAXIMUM ORDER DERIVATIVE THAT SHOULD BE USED IN THE   LDA 1050
C                  METHOD.  IT MUST BE NO GREATER THAN SIX.  IF IT IS    LDA 1060
C                  GREATER THAN SIX, THE MAXIMUM ORDER USED WILL BE SIX. LDA 1070
C        IPRT    - INTERNAL PRINT CONTROL INDICATOR                      LDA 1080
C                       = 0  NO PRINT                                    LDA 1090
C                       > 0  PRINT COUNTERS, STEPSIZE, CURRENT TIME      LDA 1000
C                            AND VALUES OF DEPENDENT VARIABLES AT        LDA 1010
C                            EACH STEP.                                  LDA 1020
C        H       - CURRENT STEPSIZE.  AN INITIAL VALUE MUST BE SUPPLIED  LDA 1030
C                  BUT NEED NOT BE THE ONE WHICH WILL BE USED, SINCE THE LDA 1040
C                  SUBROUTINE WILL CHOOSE A SMALLER ONE IF NECCESSARY TO LDA 1050
C                  KEEP THE ERROR PER STEP SMALLER THAN THE SPECIFIED    LDA 1060
C                  VALUE.  IT IS BETTER TO UNDERESTIMATE THE INITIAL     LDA 1070
C                  STEPSIZE THAN TO OVERESTIMATE IT.  THE STEPSIZE IS    LDA 1080
C                  NORMALLY NOT CHANGED BY THE USER.                     LDA 1090
C        HMIN    - MINIMUM STEPSIZE ALLOWED                              LDA 1100
C        HMAX    - MAXIMUM STEPSIZE ALLOWED                              LDA 1110
C        RMSEPS  - THE ERROR TEST CONSTANT.  THE ROOT-MEAN-SQUARE OF     LDA 1120
C                  THE SINGLE STEP ERROR ESTIMATES, ER(I), DIVIDED BY    LDA 1130
C                  YMAX(I) = (MAXIMUM TO CURRENT TIME OF Y(I)) MUST BE   LDA 1140
C                  LESS THAN RMSEPS.  THE STEPSIZE AND/OR ORDER ARE      LDA 1150
C                  VARIED TO ACHIEVE THIS.                               LDA 1160
C        SAVE    - AN ARRAY OF LENGTH AT LEAST 7*NY                      LDA 1170
C        YLSV    - AN ARRAY OF LENGTH AT LEAST NL                        LDA 1180
C        YMAX    - A VECTOR OF LENGTH NY WHICH CONTAINS THE MAXIMUM      LDA 1190
C                  OF EACH Y SEEN SO FAR.  ON THE FIRST CALL, THESE WILLLDA 1200
C                  BE INITIALIZED AS YMAX(I) = MAX(1,|Y(1,I)|)           LDA 1210
C        ER      - A VECTOR OF LENGTH NY                                 LDA 1220
C        ESV     - A VECTOR OF LENGTH NY                                 LDA 1230
C        F1      - A VECTOR OF LENGTH N = NY + NL                        LDA 1240
C        DY      - A VECTOR OF LENGTH N = NY + NL                        LDA 1250
C        PW      - AN ARRAY IN WHICH THE  J  MATRIX COMPUTED             LDA 1260
C                  IN SUBROUTINE JACMAT WILL BE STORED.  SIZE WHICH      LDA 1270
C                  MUST BE ALLOWED IS DETERMINED BY THE STORAGE TECH-    LDA 1280
C                  NIQUE USED FOR IT, BUT NORMALLY WON'T BE MORE THAN    LDA 1290
C                  N**2 + 2*N LOCATIONS, THE LATTER 2*N BEING REQUIRED   LDA 1300
C                  BY THE LINEAR EQUATION SOLVER.                        LDA 1310
C                                                                        LDA 1320
C     ------------------------------------------------------------------LDA 1330
      DIMENSION Y(7,1), YL(1), SAVE(7,1), YMAX(1), ER(1), YLSV(1), F1(1)LDA 1340
     1, PERT(6,3), COF(21), ESV(1), DY(1), PW(1), SAV(1), A(29)         LDA 1350
      EQUIVALENCE (A(8),BND), (A(9),BR), (A(10),F), (A(11),EDWN),       LDA 1360
     1(A(12),ENQ1), (A(13),ENQ2), (A(14),ENQ3), (A(15),EPS), (A(16),EUP)LDA 1370
     2,(A(17),HNEW), (A(18),PEPSH), (A(19),IDOUB), (A(20),IWEVAL),      LDA 1380
     3(A(21),K), (A(22),LCOPYL), (A(23),LCOPYY), (A(24),MAXDER),        LDA 1390
     4(A(25),M1), (A(26),NL), (A(27),NQ), (A(28),NS), (A(29),NW)        LDA 1400
C                                                                        LDA 1410
C     ------------------------------------------------------------------LDA 1420
C                                                                        LDA 1430
C     THE COEFFICIENTS IN THE PERT ARRAY ARE USED FOR ERROR TESTING AND  LDA 1440
C     CHANGING STEPSIZE AND NEED TO BE ACCURATE TO ONLY A FEW DIGITS.    LDA 1450
C                                                                        LDA 1460
C     ------------------------------------------------------------------LDA 1470
      DATA PERT/4.,9.,16.,25.,36.,49.,9.,16.,25.,36.,49.,64.,1.,1.,.25, LDA 1480
     12.7889E-2,1.7C569E-3,6.83929E-5/                                  LDA 1490
C     ------------------------------------------------------------------LDA 1500
C                                                                        LDA 1510
C     THE ENTRIES IN THE COF ARRAY ARE THE COEFFICIENTS FOR THE STIFFLY  LDA 1520
C     STABLE METHODS USED IN THIS PROGRAM AND ARE TO BE THE MACHINE      LDA 1530
C     PRECISION EQUIVALENTS OF THE FOLLOWING CONSTANTS.                  LDA 1540
C                                                                        LDA 1550
C     -1                                                                 LDA 1560
C     -3/2 , -1/2                                                        LDA 1570
C     -11/6 , -1 , -1/6                                                  LDA 1580
C     -25/12 , -35/24 , -5/12 , -1/24                                    LDA 1590
C     -137/60 , -15/8 , -17/24 , -1/8 , -1/120                           LDA 1600
C     -147/60, -203/90 , -49/48 , -35/144 , -7/240 , -1/720              LDA 1610
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C                                                                       LDA 1620
C     ------------------------------------------------------------------LDA 1630
      DATA COF/-1.,-1.5,-.5,-1.833333,-1.,-.1666667,-2.083333,-1.458333,LDA 1640
     1-.4166667,-.04166667,-2.283333,-1.875,-.7083333,-.125,-.008333333,LDA 1650
     2-2.45,-2.255556,-1.020833,-.2430556,-.02916667,-.001388889/       LDA 1660
      IF (JSTART) 100,110,150                                           LDA 1670
C     ------------------------------------------------------------------LDA 1680
C     IF THIS IS A RESTART ENTRY, RESTORE Y AND YL FROM THE SAVE AND    LDA 1690
C     YLSV ARRAYS, WHERE THEY WERE SAVED BY A PREVIOUS CALL TO LDASAV.  LDA 1700
C     ------------------------------------------------------------------LDA 1710
  100 CALL COPYZ (Y,SAVE,LCOPYY)                                        LDA 1720
      CALL COPYZ (YL,YLSV,LCOPYL)                                       LDA 1730
      GO TO 150                                                         LDA 1740
C     ------------------------------------------------------------------LDA 1750
C     IF THIS IS THE FIRST CALL, INITIALIZE YMAX, SCALE DERIVATIVES, ANDLDA 1760
C     INITIALIZE INDICATORS AND SET ORDER TO ONE.                       LDA 1770
C     FOR DOUBLE PRECISION, SET LCOPYL = 14*NY AND LCOPYL = 2*NL IF     LDA 1780
C     SUBROUTINE COPYZ IS IN SINGLE PRECISION.                          LDA 1790
C     ------------------------------------------------------------------LDA 1800
  110 NL = N-NY                                                         LDA 1810
      LCOPYY = 7*NY                                                     LDA 1820
      LCOPYL = NL                                                       LDA 1830
      M1 = MIN0(M,NY)                                                   LDA 1840
      EPS = SQRT(FLOAT(M1))*RMSEPS                                      LDA 1850
      MAXDER = MIN0(MAXDR,6)                                            LDA 1860
      IF (IPRT.LE.0) GO TO 120                                          LDA 1870
      PRINT 3, N,NL,RMSEPS,TEND,H                                       LDA 1880
      PRINT 4                                                           LDA 1890
  120 NS = 0                                                            LDA 1900
      NW = 0                                                            LDA 1910
C                                                                       LDA 1920
      DO 130 J=1,NY                                                     LDA 1930
      YMAX(J) = AMAX1(1.,ABS(Y(1,J)))                                   LDA 1940
  130 Y(2,J) = Y(2,J)*H                                                 LDA 1950
C                                                                       LDA 1960
      NQ = 1                                                            LDA 1970
      BR = 1.                                                           LDA 1980
      ASSIGN 190 TO IRET                                                LDA 1990
C     ------------------------------------------------------------------LDA 2000
C     SET COEFFICIENTS FOR THE ORDER CURRENTLY BEING USED.              LDA 2010
C     E IS A TEST FOR ERRORS OF THE CURRENT ORDER NQ                    LDA 2020
C     EUP IS TO TEST FOR INCREASING THE ORDER, EDWN FOR DECREASING THE  LDA 2030
C     ORDER.                                                            LDA 2040
C     ------------------------------------------------------------------LDA 2050
  140 K = NQ*(NQ-1)/2                                                   LDA 2060
      CALL COPYZ (A(2),COF(K+1),NQ)                                     LDA 2070
      K = NQ+1                                                          LDA 2080
      IDOUB = NQ                                                        LDA 2090
      ENQ1 = .5/NQ                                                      LDA 2100
      ENQ2 = .5/K                                                       LDA 2110
      ENQ3 = .5/(NQ+2)                                                  LDA 2120
      EPSH = EPS**2                                                     LDA 2130
      E = PERT(NQ,1)*EPSH                                               LDA 2140
      EUP = PERT(NQ,2)*EPSH                                             LDA 2150
      EDWN = PERT(NQ,3)*EPSH                                            LDA 2160
      BND = (EPS*ENQ3)**2                                               LDA 2170
      IWEVAL = 1                                                        LDA 2180
      GO TO IRET, (190,200,490,570)                                     LDA 2190
  150 IF (H.EQ.HNEW) GO TO 190                                          LDA 2200
C     ------------------------------------------------------------------LDA 2210
C     IF CALLER HAS CHANGED H, RESCALE DERIVATIVES TO REFLECT THAT HNEW LDA 2220
C     WAS USED ON THE LAST CALL.                                        LDA 2230
C     ------------------------------------------------------------------LDA 2240
      R = H/HNEW                                                        LDA 2250
      ASSIGN 190 TO IRET                                                LDA 2260
      GO TO 610                                                         LDA 2270
C     ------------------------------------------------------------------LDA 2280
C     SET JSTART TO NQ, THE CURRENT ORDER OF THE METHOD, BEFORE EXIT,   LDA 2290
C     AND SAVE THE CURRENT STEPSIZE IN HNEW.                            LDA 2300
C     ------------------------------------------------------------------LDA 2310
  160 JSTART = NQ                                                       LDA 2320
      HNEW = H                                                          LDA 2330
      RETURN                                                            LDA 2340
  170 NS = NS+1                                                         LDA 2350
      IF (IPRT.LE.0) GO TO 180                                          LDA 2360
```

```
C     ------------------------------------------------------------------LDA 2370
C     PRINT DATA IF DESIRED BY USER                                     LDA 2380
C     ------------------------------------------------------------------LDA 2390
      PRINT 1, NS,NW,NQ,H,T,(Y(1,I),I=1,NY)                             LDA 2400
      IF (NL.GT.0) PRINT 2, (YL(I),I=1,NL)                              LDA 2410
  180 CONTINUE                                                          LDA 2420
      IF (KFLAG.LT.0) GO TO 160                                         LDA 2430
      IF (T.GE.TEND) GO TO 160                                          LDA 2440
C     ------------------------------------------------------------------LDA 2450
C     TAKE ANOTHER STEP IF T < TEND                                     LDA 2460
C     ------------------------------------------------------------------LDA 2470
      JSTART = 1                                                        LDA 2480
C     ------------------------------------------------------------------LDA 2490
C     SAVE DATA FOR TRIAL WITH A SMALLER TIMESTEP IF THIS STEP FAILS    LDA 2500
C     ------------------------------------------------------------------LDA 2510
  190 CALL COPYZ (SAVE,Y,LCOPYY)                                        LDA 2520
      CALL COPYZ (YLSV,YL,LCOPYL)                                       LDA 2530
      RACUM = 1.                                                        LDA 2540
      KFLAG = 1                                                         LDA 2550
      HOLD = H                                                          LDA 2560
      NQOLD = NQ                                                        LDA 2570
      TOLD = T                                                          LDA 2580
  200 T = T+H                                                           LDA 2590
      HINV = 1./H                                                       LDA 2600
C     ------------------------------------------------------------------LDA 2610
C     COMPUTE PREDICTED VALUES BY EFFECTIVELY MULTIPLYING DERIVATIVE    LDA 2620
C     VECTOR BY PASCAL TRIANGLE MATRIX                                  LDA 2630
C     ------------------------------------------------------------------LDA 2640
C                                                                       LDA 2650
      DO 210 J=2,K                                                      LDA 2660
      J3 = K+J-1                                                        LDA 2670
C                                                                       LDA 2680
      DO 210 J1=J,K                                                     LDA 2690
      J2 = J3-J1                                                        LDA 2700
C                                                                       LDA 2710
      DO 210 I=1,NY                                                     LDA 2720
  210 Y(J2,I) = Y(J2,I)+Y(J2+1,I)                                       LDA 2730
C                                                                       LDA 2740
C                                                                       LDA 2750
      DO 220 I=1,NY                                                     LDA 2760
  220 ER(I) = 0.                                                        LDA 2770
C                                                                       LDA 2780
C     ------------------------------------------------------------------LDA 2790
C     DO UP TO THREE CORRECTOR ITERATIONS.  CONVERGENCE IS OBTAINED WHENLDA 2800
C     CHANGES ARE LESS THAN BND WHICH IS DEPENDENT ON THE ERROR TEST    LDA 2810
C     CONSTANT.  THE SUM OF CORRECTIONS IS ACCUMULATED IN ER(I).  IT IS LDA 2820
C     EQUAL TO THE K-TH DERIVATIVE OF Y TIMES H**K/(K-FACTORIAL*A(K)),  LDA 2830
C     AND THUS IS PROPORTIONAL TO THE ACTUAL ERRORS TO THE LOWEST POWER LDA 2840
C     OF H PRESENT, WHICH IS H**K.                                      LDA 2850
C     ------------------------------------------------------------------LDA 2860
C                                                                       LDA 2870
      DO 270 L=1,3                                                      LDA 2880
      CALL DIFFUN (Y,YL,T,HINV,DY)                                      LDA 2890
      IF (IWEVAL.LT.1) GO TO 230                                        LDA 2900
C     ------------------------------------------------------------------LDA 2910
C     IF THERE HAS BEEN A CHANGE OF ORDER OR THERE HAS BEEN TROUBLE     LDA 2920
C     WITH CONVERGENCE, PW IS RE-EVALUATED PRIOR TO STARTING THE        LDA 2930
C     CORRECTOR ITERATION.  IWEVAL IS THEN SET TO -1 AS AN INDICATOR    LDA 2940
C     THAT IT HAS BEEN DONE.  NEWPW IS SET NONZERO TO INDICATE TO       LDA 2950
C     SUBROUTINE NUITSL THAT A NEW PW HAS BEEN PROVIDED.                LDA 2960
C     ------------------------------------------------------------------LDA 2970
      CALL JACMAT (Y,YL,T,HINV,A(2),N,NY,EPS,DY,F1,PW)                  LDA 2980
      KFLAG = 1                                                         LDA 2990
      IWEVAL = -1                                                       LDA 3000
      NW = NW+1                                                         LDA 3010
      NEWPW = 1                                                         LDA 3020
  230 CALL NUITSL (PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRRET)                  LDA 3030
      IF (KRRET.NE.0) GO TO 600                                         LDA 3040
      IF (NL.LE.0) GO TO 250                                            LDA 3050
C                                                                       LDA 3060
      DO 240 I=1,NL                                                     LDA 3070
  240 YL(I) = YL(I)-F1(I+NY)                                            LDA 3080
C                                                                       LDA 3090
  250 CONTINUE                                                          LDA 3100
      DEL = 0.                                                          LDA 3110
```

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C                                                                       LDA 3120
      DO 260 I=1,NY                                                     LDA 3130
      Y(1,I) = Y(1,I)-F1(I)                                             LDA 3140
      Y(2,I) = Y(2,I)+A(2)*F1(I)                                        LDA 3150
      ER(I) = ER(I)+F1(I)                                               LDA 3160
      DEL = DEL+(F1(I)/AMAX1(YMAX(I),ABS(Y(1,I))))**2                   LDA 3170
  260 CONTINUE                                                          LDA 3180
C                                                                       LDA 3190
      IF (L.GE.2) BR = AMAX1(.9*BR,DEL/DEL1)                            LDA 3200
      DEL1 = DEL                                                        LDA 3210
      IF (AMIN1(DEL,BR*DEL*2.).LE.BND) GO TO 330                        LDA 3220
  270 CONTINUE                                                          LDA 3230
C                                                                       LDA 3240
C     ------------------------------------------------------------------LDA 3250
C     THE CORRECTION ITERATION FAILED TO CONVERGE IN 3 TRIES.  VARIOUS  LDA 3260
C     POSSIBILITIES ARE CHECKED FOR.  IF H IS ALREADY HMIN AND PW HAS   LDA 3270
C     ALREADY BEEN RE-EVALUATED, A NO CONVERGENCE EXIT IS TAKEN.        LDA 3280
C     OTHERWISE THE MATRIX PW IS RE-EVALUATED AND/OR (IN THAT ORDER) THELDA 3290
C     STEP IS REDUCED TO TRY AND GET CONVERGENCE.                       LDA 3300
C     ------------------------------------------------------------------LDA 3310
      T = TOLD                                                          LDA 3320
      IF (IWEVAL) 280,300,290                                           LDA 3330
  280 IF (H.LE.HMIN*1.00001) GO TO 310                                  LDA 3340
  290 RACUM = RACUM*.25                                                 LDA 3350
  300 CONTINUE                                                          LDA 3360
      GO TO 560                                                         LDA 3370
  310 KFLAG = -3                                                        LDA 3380
C     ------------------------------------------------------------------LDA 3390
C     RESTORE Y AND YL AFTER CONVERGENCE FAILURE                        LDA 3400
C     ------------------------------------------------------------------LDA 3410
  320 CALL COPYZ (Y,SAVE,LCOPYY)                                        LDA 3420
      CALL COPYZ (YL,YLSV,LCOPYL)                                       LDA 3430
      H = HOLD                                                          LDA 3440
      NQ = NQOLD                                                        LDA 3450
      GO TO 170                                                         LDA 3460
C     ------------------------------------------------------------------LDA 3470
C     THE CORRECTOR CONVERGED, SO NOW THE ERROR TEST IS MADE.           LDA 3480
C     ------------------------------------------------------------------LDA 3490
  330 D = 0.                                                            LDA 3500
C                                                                       LDA 3510
      DO 340 I=1,M1                                                     LDA 3520
      YM = AMAX1(ABS(Y(1,I)),YMAX(I))                                   LDA 3530
  340 D = D+(ER(I)/YM)**2                                               LDA 3540
C                                                                       LDA 3550
      IWEVAL = 0                                                        LDA 3560
      IF (D.GT.E) GO TO 380                                             LDA 3570
C     ------------------------------------------------------------------LDA 3580
C     THE ERROR TEST IS OKAY, SO THE STEP IS ACCEPTED.  IF IDOUB        LDA 3590
C     NOW BECOMES NEGATIVE, A TEST IS MADE TO SEE IF THE STEP SIZE      LDA 3600
C     CAN BE INCREASED AT THIS ORDER OR ONE HIGHER OR ONE LOWER.        LDA 3610
C     THE CHANGE IS MADE ONLY IF THE STEP CAN BE INCREASED BY AT        LDA 3620
C     LEAST 10%.  IDOUB IS SET TO NQ TO PREVENT FURTHER TESTING         LDA 3630
C     FOR A WHILE.  IF NO CHANGE IS MADE, IDOUB IS SET TO 9.            LDA 3640
C     ------------------------------------------------------------------LDA 3650
      IF (K.LT.3) GO TO 360                                             LDA 3660
C                                                                       LDA 3670
      DO 350 J=3,K                                                      LDA 3680
C                                                                       LDA 3690
      DO 350 I=1,NY                                                     LDA 3700
  350 Y(J,I) = Y(J,I)+A(J)*ER(I)                                        LDA 3710
C                                                                       LDA 3720
  360 KFLAG = 1                                                         LDA 3730
      IDOUB = IDOUB-1                                                   LDA 3740
      IF (IDOUB) 410,370,510                                            LDA 3750
  370 CALL COPYZ (ESV,ER,M1)                                            LDA 3760
      GO TO 510                                                         LDA 3770
C     ------------------------------------------------------------------LDA 3780
C     THE ERROR TEST FAILED.  IF JSTART = 0, THE DERIVATIVES IN THE     LDA 3790
C     SAVE ARRAY ARE UPDATED.  TESTS ARE THEN MADE TO FIX THE STEPSIZE  LDA 3800
C     AND PERHAPS REDUCE THE ORDER.  AFTER RESTORING AND SCALING THE    LDA 3810
C     Y VARIABLES, THE STEP IS RETRIED.                                 LDA 3820
C     ------------------------------------------------------------------LDA 3830
  380 IF (JSTART.GT.0) GO TO 400                                        LDA 3840
C                                                                       LDA 3850
      DO 390 I=1,NY                                                     LDA 3860
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  390 SAVE(2,I) = Y(2,I)                                                    LDA 3870
C                                                                           LDA 3880
  400 KFLAG = KFLAG-2                                                       LDA 3890
      IF (H.LE.HMIN) GO TO 550                                              LDA 3900
      T = TOLD                                                              LDA 3910
      IF (KFLAG.LE.-5) GO TO 530                                            LDA 3920
  410 PR2 = (C/E)**ENQ2*1.2                                                 LDA 3930
      L = 0                                                                 LDA 3940
      IF (NQ.LE.1) GO TO 430                                                LDA 3950
      C = 0.                                                                LDA 3960
C                                                                           LDA 3970
      DO 420 J=1,M1                                                         LDA 3980
      YM = AMAX1(ABS(Y(1,J)),YMAX(J))                                       LDA 3990
  420 C = C+(Y(K,J)/YM)**2                                                  LDA 4000
C                                                                           LDA 4010
      PR1 = (C/EDWN)**ENQ1*1.3                                              LDA 4020
      IF (PR1.GE.PR2) GO TO 430                                             LDA 4030
      PR2 = PR1                                                             LDA 4040
      L = -1                                                                LDA 4050
  430 IF (KFLAG.LT.0.OR.NQ.GE.MAXDER) GO TO 450                             LDA 4060
      C = 0                                                                 LDA 4070
C                                                                           LDA 4080
      DO 440 J=1,M1                                                         LDA 4090
      YM = AMAX1(ABS(Y(1,J)),YMAX(J))                                       LDA 4100
  440 C = C+((ER(J)-ESV(J))/YM)**2                                          LDA 4110
C                                                                           LDA 4120
      PR1 = (C/EUP)**ENQ3*1.4                                               LDA 4130
      IF (PR1.GE.PR2) GO TO 450                                             LDA 4140
      PR2 = PR1                                                             LDA 4150
      L = 1                                                                 LDA 4160
  450 R = 1./AMAX1(PR2,1.E-5)                                               LDA 4170
      IF (KFLAG.LT.0.OR.R.GE.1.1) GO TO 460                                 LDA 4180
      IDOUB = 9                                                             LDA 4190
      GO TO 510                                                             LDA 4200
  460 NEWQ = NQ+L                                                           LDA 4210
      K = NEWQ+1                                                            LDA 4220
      IF (NEWQ.LE.NQ) GO TO 480                                             LDA 4230
      R1 = A(NEWQ)/FLOAT(NEWQ)                                              LDA 4240
C                                                                           LDA 4250
      DO 470 J=1,NY                                                         LDA 4260
  470 Y(K,J) = ER(J)*R1                                                     LDA 4270
C                                                                           LDA 4280
  480 CONTINUE                                                              LDA 4290
C     ------------------------------------------------------------------    LDA 4300
C     IF THE STEP WAS OKAY, SCALE THE Y VARIABLES IN ACCORDANCE             LDA 4310
C     WITH THE NEW VALUE OF H.  IF KFLAG < 0, HOWEVER, USE THE              LDA 4320
C     SAVED VALUES (IN SAVE AND YLSV).  IN EITHER CASE, IF THE ORDER        LDA 4330
C     HAS CHANGED IT IS NECESSARY TO FIX CERTAIN PARAMETERS BY CALLING      LDA 4340
C     THE PROGRAM SEGMENT AT STATEMENT NUMBER 140.                          LDA 4350
C     ------------------------------------------------------------------    LDA 4360
      IDOUB = NQ                                                            LDA 4370
      IF (NEWQ.EQ.NQ) GO TO 490                                             LDA 4380
      NQ = NEWQ                                                             LDA 4390
      ASSIGN 490 TO IRET                                                    LDA 4400
      GO TO 140                                                             LDA 4410
  490 IF (KFLAG.GT.0) GO TO 500                                             LDA 4420
      RACUM = RACUM*R                                                       LDA 4430
      GO TO 560                                                             LDA 4440
  500 R = AMAX1(AMIN1(HMAX/H,R),HMIN/H)                                     LDA 4450
      H = H*R                                                               LDA 4460
      IWEVAL = 1                                                            LDA 4470
      ASSIGN 510 TO IRET                                                    LDA 4480
      GO TO 610                                                             LDA 4490
C                                                                           LDA 4500
  510 DO 520 I=1,M1                                                         LDA 4510
  520 YMAX(I) = AMAX1(ABS(Y(1,I)),YMAX(I))                                  LDA 4520
C                                                                           LDA 4530
      GO TO 170                                                             LDA 4540
C     ------------------------------------------------------------------    LDA 4550
C     THE ERROR TEST HAS NOW FAILED THREE TIMES, SO THE DERIVATIVES ARE     LDA 4560
C     IN BAD SHAPE.  RETURN TO FIRST ORDER METHOD AND TRY AGAIN.  OF        LDA 4570
C     COURSE, IF NQ = 1 ALREADY, THEN THERE IS NO HOPE AND WE EXIT WITH     LDA 4580
C     KFLAG = -4.                                                           LDA 4590
C     ------------------------------------------------------------------    LDA 4600
  530 IF (NQ.EQ.1) GO TO 540                                                LDA 4610
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      NC = 1                                                            LDA 4620
      ICOUB = 1                                                         LDA 4630
      ASSIGN 570 TO IRET                                                LDA 4640
      GO TO 140                                                         LDA 4650
  540 NOLD = 1                                                          LDA 4660
      KFLAG = -4                                                        LDA 4670
      GO TO 220                                                         LDA 4680
  550 KFLAG = -1                                                        LDA 4690
      GO TO 170                                                         LDA 4700
C     ------------------------------------------------------------------LDA 4710
C     THIS SECTION RESTORES THE SAVED VALUES OF Y AND YL, SCALING THE   LDA 4720
C     Y DERIVATIVES AS NECESSARY, AND THEN RETURNS TO THE PREDICTOR LOOPLDA 4730
C     ------------------------------------------------------------------LDA 4740
  560 H = HOLD*RACUM                                                    LDA 4750
      H = AMAX1(HMIN,AMIN1(H,HMAX))                                     LDA 4760
  570 RACUM = H/HOLD                                                    LDA 4770
      R1 = 1.                                                           LDA 4780
C                                                                       LDA 4790
      DO 580 J=2,K                                                      LDA 4800
      R1 = R1*RACUM                                                     LDA 4810
C                                                                       LDA 4820
      DO 580 I=1,NY                                                     LDA 4830
  580 Y(J,I) = SAVE(J,I)*R1                                             LDA 4840
C                                                                       LDA 4850
C                                                                       LDA 4860
      DO 590 I=1,NY                                                     LDA 4870
  590 Y(1,I) = SAVE(1,I)                                                LDA 4880
C                                                                       LDA 4890
      CALL COPYZ (YL,YLSV,LCOPYL)                                       LDA 4900
      IWEVAL = 1                                                        LDA 4910
      GO TO 200                                                         LDA 4920
  600 KFLAG = -5                                                        LDA 4930
      GO TO 160                                                         LDA 4940
C     ------------------------------------------------------------------LDA 4950
C     THIS SECTION SCALES THE Y DERIVATIVES BY R**J                     LDA 4960
C     ------------------------------------------------------------------LDA 4970
  610 R1 = 1.                                                           LDA 4980
C                                                                       LDA 4990
      DO 620 J=2,K                                                      LDA 5000
      R1 = R1*R                                                         LDA 5010
C                                                                       LDA 5020
      DO 620 I=1,NY                                                     LDA 5030
  620 Y(J,I) = Y(J,I)*R1                                                LDA 5040
C                                                                       LDA 5050
      GO TO IRET, (190,510)                                             LDA 5060
C     ------------------------------------------------------------------LDA 5070
C     THIS SECTION ALLOWS FOR RESTARTS AFTER SOLVING ANOTHER PROBLEM, ORLDA 5080
C     HAVING TERMINATED THE CURRENT COMPUTER RUN.  SUBROUTINE LDASAV    LDA 5090
C     SAVES THE NECESSARY VALUES WHICH ARE INTERNAL TO LDASUB.  FOR     LDA 5100
C     DOUBLE PRECISION, WITH COPYZ IN SINGLE PRECISION, THE NUMBER OF   LDA 5110
C     LOCATIONS TO BE SAVED AND RESTORED, LCOPYS AND LCOPYR. MUST BE    LDA 5120
C     SET TO 58.                                                        LDA 5130
C     IT IS ASSUMED THAT IN ADDITION TO THE VARIABLES IN THE ARRAY A    LDA 5140
C     SAVED BY CALLING LDASAV, THE USER ALSO SAVES THE ARRAYS SAVE,     LDA 5150
C     YLSV, YMAX, ESV, AND PW.                                          LDA 5160
C                                                                       LDA 5170
C     TO RESTART THE USER FIRST CALLS LDARST TO RESTORE THE VALUES SAVEDLDA 5180
C     BY LDASAV, THEN RE-ENTERS LDASUB WITH JSTART < 0, AND WITH THE    LDA 5190
C     OTHER PARAMETERS THE SAME AS RETURNED FROM THE LAST ENTRY TO      LDA 5200
C     LDASUB, PARTICULARLY THOSE ARRAYS MENTIONED ABOVE.                LDA 5210
C     ------------------------------------------------------------------LDA 5220
      ENTRY LDASAV(SAV)                                                 LDA 5230
      LCOPYS = 29                                                       LDA 5240
      CALL COPYZ (SAV,A,LCOPYS)                                         LDA 5250
      CALL COPYZ (SAVE,Y,LCOPYY)                                        LDA 5260
      CALL COPYZ (YLSV,YL,LCOPYL)                                       LDA 5270
      RETURN                                                            LDA 5280
C                                                                       LDA 5290
      ENTRY LDARST(SAV)                                                 LDA 5300
      LCOPYR = 29                                                       LDA 5310
      CALL COPYZ (A,SAV,LCOPYR)                                         LDA 5320
      RETURN                                                            LDA 5330
C                                                                       LDA 5340
C     ------------------------------------------------------------------LDA 5350
C                                                                       LDA 5360
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C                                                                               LDA 5370
    1 FORMAT (2I5,I2,1P2E10.2,7E14.6/(32X,7E14.6))                              LDA 5380
    2 FORMAT (32X,1P7E14.6)                                                     LDA 5390
    3 FORMAT ('1  N =',I3,'    NL =',I3,'    RMSEPS =',1PE9.2,'    TEND ='  LDA 5400
     1   ,E9.2,'    H =',E9.2//)                                              LDA 5410
    4 FORMAT ('    NS    NW Q     H',8X,'T    ',8X,'Y(1,*) AND YL(*)'//)     LDA 5420
      END                                                                       LDA 5430

      SUBROUTINE COPYZ(S,Y,L)                                                   COP   10
      DIMENSION S(1),Y(1)                                                       COP   20
C     ----------------------------------------------------------------------    COP   30
C                                                                               COP   40
C     THIS SUBROUTINE COPIES THE ARRAY Y, OF LENGTH L, INTO THE ARRAY S         COP   50
C                                                                               COP   60
C     ----------------------------------------------------------------------    COP   70
      IF(L.LE.0)RETURN                                                          COP   80
      DO 100 J=1,L                                                              COP   90
  100 S(J) = Y(J)                                                               COP  100
      RETURN                                                                    COP  110
      END                                                                       COP  120

      SUBROUTINE DERVAL (Y,YL,T,N,NY,W,KERET)                                   DER   10
C                                                                               DER   20
C     THIS SUBROUTINE CALCULATES THE INTIAL VALUES OF THE DERIVATIVES           DER   30
C     IN THE GENERAL CASE.  IT IS WRITTEN SO THAT IT SHOULD WORK IF THE         DER   40
C     FIRST NY EQUATIONS ALL INVOLVE DERIVATIVES.  IT ATTEMPTS TO SOLVE         DER   50
C     THE FIRST NY EQUATIONS USING NEWTON'S METHOD, BUT SINCE IT TRIES          DER   60
C     TO EVALUATE DF/DY' BY CALLING JACMAT IN SUCH A WAY AS TO MAKE THE         DER   70
C     DF/DY TERM INSIGNIFICANT, IT IS POSSIBLE THAT IT MAY FAIL FOR THAT        DER   80
C     REASON.  IT MAY FAIL FOR OTHER REASONS, AS WELL.  IF IT DOES FAIL         DER   90
C     THE USER CAN SUPPLY HIS OWN VERSION OF DERVAL, OR MODIFY THIS             DER  100
C     ROUTINE IN SUITABLE FASHION.  THIS ROUTINE ASSUMES THAT VALUES OF         DER  110
C     THE LINEAR VARIABLES HAVE BEEN SUPPLIED PREVIOUSLY.  IF THOSE             DER  120
C     MUST BE SOLVED FOR SIMULTANEOUSLY WITH THE DERIVATIVES, THE USER          DER  130
C     MUST SUPPLY HIS OWN VERSION OF DERVAL.                                    DER  140
C                                                                               DER  150
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS                               DER  160
C                                                                               DER  170
C     CALL DERVAL(Y,YL,T,N,NY,W,KERET)                                          DER  180
C                                                                               DER  190
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS                               DER  200
C                                                                               DER  210
C        Y        - SAME AS IN LDASUB AND SDESOL.  Y(1,I) CONTAINS THE         DER  220
C                   INITIAL VALUES OF THE DEPENDENT VARIABLES.  THE           DER  230
C                   VALUES OF THE DERIVATIVES ARE RETURNED IN Y(2,I).         DER  240
C        YL       - SAME AS IN LDASUB AND SDESOL.  THE INITIAL VALUES OF      DER  250
C                   THE LINEAR VARIABLES MUST BE SUPPLIED TO THIS VERSION     DER  260
C        T        - INITIAL TIME                                              DER  270
C        N        - SAME AS IN LDASUB, TOTAL NUMBER OF VARIABLES              DER  280
C        NY       - SAME AS IN LDASUB, NUMBER OF DIFFERENTIAL EQUATIONS       DER  290
C                   AND NONLINEAR VARIABLES                                   DER  300
C        W        - SCRATCH ARRAY W FROM THE CALLING SEQUENCE OF SDESOL.      DER  310
C                   THIS CAN BE USED AS NEEDED IN THIS SUBROUTINE.            DER  320
C        KERET    - RETURN INDCATOR                                           DER  330
C                        =0  NORMAL RETURN                                    DER  340
C                        =1  ERROR RETURN                                     DER  350
C                                                                               DER  360
C     ----------------------------------------------------------------------    DER  370
      DIMENSION Y(7,1), YL(1), W(1)                                             DER  380
C                                                                               DER  390
      DO 100 I=1,NY                                                             DER  400
      W(2*N+I) = AMAX1(ABS(Y(1,I)),1.)                                          DER  410
  100 Y(3,I) = 0.                                                               DER  420
C                                                                               DER  430
      HINV = 10.**20                                                            DER  440
      KERET = 0                                                                 DER  450
      EPS2 = NY/1.E8                                                            DER  460
      EPS = SQRT(EPS2)                                                          DER  470
C                                                                               DER  480
      DO 140 IT=1,10                                                            DER  490
C                                                                               DER  500
      DO 110 I=1,NY                                                             DER  510
  110 Y(2,I) = Y(3,I)/HINV                                                      DER  520
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C                                                                       DER   530
      CALL DIFFUN (Y,YL,T,HINV,W)                                       DER   540
      CALL JACMAT (Y,YL,T,HINV,-1.,NY,NY,EPS,W,W(N+1),W(3*N+1))         DER   550
      NEWPW = 1                                                         DER   560
C                                                                       DER   570
      DO 120 I=1,NY                                                     DER   580
  120 W(I) = W(I)*HINV                                                  DER   590
C                                                                       DER   600
      CALL NUITSL (W(3*N+1),W,W(N+1),NY,NY,EPS,W(2*N+1),NEWPW,KRET)     DER   610
      IF (KRET.NE.0) GO TO 170                                          DER   620
      ER = 0.                                                           DER   630
C                                                                       DER   640
      DO 130 I=1,NY                                                     DER   650
      Y(3,I) = Y(3,I)-W(N+I)                                            DER   660
  130 ER = ER+(W(N+I)/AMAX1(ABS(Y(3,I)),1.))**2                         DER   670
C                                                                       DER   680
      IF (ER.LT.EPS2) GO TO 150                                         DER   690
  140 CONTINUE                                                          DER   700
C                                                                       DER   710
      GO TO 170                                                         DER   720
C                                                                       DER   730
  150 DO 160 I=1,NY                                                     DER   740
  160 Y(2,I) = Y(3,I)                                                   DER   750
C                                                                       DER   760
      RETURN                                                            DER   770
  170 KRET = 1                                                          DER   780
      RETURN                                                            DER   790
      END                                                               DER   800

      SUBROUTINE JACMAT (Y,YL,T,HINV,A2,N,NY,EPS,DY,F1,PW)              JAC    10
C     ----------------------------------------------------------------JAC    20
C                                                                       JAC    30
C     SUBROUTINE JACMAT IS (USUALLY) SUPPLIED BY THE USER.  ITS PURPOSE JAC    40
C     IS TO EVALUATE THE  J  MATRIX NEEDED WHEN THE CORRECTOR EQUATION  JAC    50
C     IS SOLVED BY NEWTON'S METHOD.  THIS VERSION APPROXIMATES          JAC    60
C     J  BY NUMERICAL DIFFERENCING AND USES FULL STORAGE MODE           JAC    70
C     IN AN NXN MATRIX.                                                 JAC    80
C                                                                       JAC    90
C                                                                       JAC   100
C     JACMAT CALCULATES THE MATRIX                                      JAC   110
C                                                                       JAC   120
C                DF      A2 DF                                          JAC   130
C        J  =    --  -   -- --                                         JAC   140
C                DY      H  DY'                                         JAC   150
C                                                                       JAC   160
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS                       JAC   170
C                                                                       JAC   180
C     CALL JACMAT(Y,YL,T,HINV,A2,EPS,N,NY,DY,F1,PW)                     JAC   190
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                      JAC   200
C                                                                       JAC   210
C        Y        - SAME AS IN LDASUB AND IN SDESOL.  ON INPUT TO THIS  JAC   220
C                   SUBROUTINE THE ARRAY CONTAINS CURRENT VALUES OF THE JAC   230
C                   DEPENDENT VARIABLES AND THEIR (SCALED) DERIVATIVES. JAC   240
C        YL       - SAME AS IN LDASUB AND IN SDESOL.  ON INPUT TO THIS  JAC   250
C                   SUBROUTINE THE ARRAY CONTAINS CURRENT VALUES OF THE JAC   260
C                   LINEAR VARIABLES.                                   JAC   270
C        T        - CURRENT TIME                                        JAC   280
C        HINV     - 1/H , WHERE H IS THE CURRENT STEPSIZE               JAC   290
C        A2       - A(2) FROM LDASUB.                                   JAC   300
C        N        - SAME AS IN LDASUB, TOTAL NUMBER OF VARIABLES        JAC   310
C        NY       - SAME AS IN LDASUB, NUMBER OF DIFFERENTIAL EQUATIONS JAC   320
C                   AND NONLINEAR VARIABLES                             JAC   330
C        EPS      - L2 ERROR CONSTANT USED IN LDASUB.                   JAC   340
C        DY       - ARRAY OF FUNCTION VALUES AT CURRENT VALUES OF THE   JAC   350
C                   VARIABLES, INPUT TO JACMAT.                         JAC   360
C        F1       - SCRATCH ARRAY OF N LOCATIONS WHICH CAN BE USED BY   JAC   370
C                   THIS SUBROUTINE IN ANY WAY NEEDED.                  JAC   380
C        PW       - J  MATRIX, OR APPROXIMATION, CALCULATED IN JACMAT ANDJAC   390
C                   RETURNED TO CALLING PROGRAM.  THIS MATRIX IS USED IN JAC   400
C                   SUBROUTINE NUITSL AND STORAGE MODE MUST AGREE BETWEENJAC   410
C                   THE TWO SUBROUTINES.                                JAC   420
C                                                                       JAC   430
C     ----------------------------------------------------------------JAC   440
      DIMENSION DY(1), Y(7,1), YL(1), F1(1), PW(1)                      JAC   450
```

```
      NL = N-NY                                                          JAC  460
      NN = N*N                                                           JAC  470
C                                                                        JAC  480
      DO 100 I=1,NN                                                      JAC  490
  100 PW(I) = 0.                                                         JAC  500
C                                                                        JAC  510
C                                                                        JAC  520
      DO 120 J=1,NY                                                      JAC  530
      F = Y(1,J)                                                         JAC  540
      E = Y(2,J)                                                         JAC  550
      R = EPS*AMAX1(EPS,ABS(F),ABS(E))                                   JAC  560
      Y(1,J) = Y(1,J)+R                                                  JAC  570
      Y(2,J) = Y(2,J)-A2*R                                               JAC  580
      CALL DIFFUN (Y,YL,T,HINV,F1)                                       JAC  590
C                                                                        JAC  600
      DO 110 I=1,N                                                       JAC  610
  110 PW(I+(J-1)*N) = (F1(I)-DY(I))/R                                    JAC  620
C                                                                        JAC  630
      Y(2,J) = E                                                         JAC  640
  120 Y(1,J) = F                                                         JAC  650
C                                                                        JAC  660
      IF (NL.EQ.0) GO TO 150                                             JAC  670
C                                                                        JAC  680
      DO 140 J=1,NL                                                      JAC  690
      F = YL(J)                                                          JAC  700
      R = EPS*AMAX1(EPS,ABS(F))                                          JAC  710
      YL(J) = YL(J)+R                                                    JAC  720
      CALL DIFFUN (Y,YL,T,HINV,F1)                                       JAC  730
C                                                                        JAC  740
      DO 130 I=1,N                                                       JAC  750
  130 PW(I+(J+NY-1)*N) = (F1(I)-DY(I))/R                                 JAC  760
C                                                                        JAC  770
  140 YL(J) = F                                                          JAC  780
C                                                                        JAC  790
  150 CONTINUE                                                           JAC  800
      RETURN                                                             JAC  810
      END                                                                JAC  820


      SUBROUTINE NUITSL (PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)              NUI   10
C     ------------------------------------------------------------------NUI   20
C     THE PURPOSE OF THIS SUBROUTINE IS TO SOLVE A                       NUI   30
C     LINEAR SYSTEM OF EQUATIONS FOR THE NEWTON ITERATES WHEN THE        NUI   40
C     CORRECTOR EQUATION IS BEING SOLVED.  UPON ENTRY TO THIS SUBROUTINENUI   50
C     THE SYSTEM OF EQUATIONS TO BE SOLVED IS    J W = -F   , WHERE      NUI   60
C        J  IS STORED IN PW UPON ENTRY                                   NUI   70
C        W  IS RETURNED IN F1                                            NUI   80
C        -F IS STORED IN DY UPON ENTRY                                   NUI   90
C                                                                        NUI  100
C     THIS SUBROUTINE IS GENERALLY SUPPLIED BY THE USER, ALTHOUGH THERE  NUI  110
C     ARE SOME STANDARD FORMS AVAILABLE.  FOR EXAMPLE, THIS VERSION      NUI  120
C     ASSUMES THAT PW IS STORED IN FULL STORAGE MODE IN AN NXN MATRIX.   NUI  130
C     IF NEWPW = 1, AN LU DECOMPOSITION IS DONE, NEWPW IS SET TO ZERO    NUI  140
C     AND FORWARD AND BACKWARD SUBSTITUTION FOR THE SOLUTION IS DONE.    NUI  150
C     IF NEWPW = 0, ONLY FORWARD AND BACKWARD SUBSTITUTION FOR THE       NUI  160
C     SOLUTION IS NECESSARY.                                             NUI  170
C                                                                        NUI  180
C     NOTE THAT THIS VERSION OF NUITSL REQUIRES THAT PW HAVE N**2 + 2*N  NUI  190
C     LOCATIONS SINCE 2*N LOCATIONS ARE USED BY THE IMSL LINEAR EQUATIONNUI  200
C     SOLVER.                                                            NUI  210
C                                                                        NUI  220
C     NOTE THAT THE PARAMETERS EPS AND YMAX ARE USEFUL IF AN ITERATIVE   NUI  230
C     METHOD IS USED TO SOLVE THE SYSTEM OF EQUATIONS.                   NUI  240
C                                                                        NUI  250
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS                        NUI  260
C                                                                        NUI  270
C     CALL NUITSL(PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)                     NUI  280
C                                                                        NUI  290
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                       NUI  300
C                                                                        NUI  310
C        PW       - THE J MATRIX CALCULATED IN SUBROUTINE JACMAT         NUI  320
C        DY       - THE RIGHT HAND SIDE OF THE LINEAR SYSTEM TO BE SOLVEDNUI  330
C        F1       - THE SOLUTION IS RETURNED IN THE ARRAY F1            NUI  340
C        N        - SAME AS IN LDASUB, TOTAL NUMBER OF VARIABLES        NUI  350
C        NY       - SAME AS IN LDASUB, NUMBER OF DIFFERENTIAL EQUATIONS NUI  360
```

```
C                AND NONLINEAR VARIABLES                                    NUI  370
C        EPS     - L2 ERROR CONSTANT USED IN LDASUB                         NUI  380
C        YMAX    - MAXIMUM VALUES OF Y(1,I) SEEN UP TO THE CURRENT TIME     NUI  390
C        NEWPW   - INDICATES WHETHER A NEW J MATRIX HAS BEEN COMPUTED       NUI  400
C                  =1  INDICATES A NEW J MATRIX HAS BEEN COMPUTED           NUI  410
C                      SINCE THE LAST ENTRY TO NUITSL.  NEWPW               NUI  420
C                      SHOULD BE SET TO ZERO IF SOME PREPROCESSING          NUI  430
C                      SUCH AS LU DECOMPOSITION MUST BE DONE ON A           NUI  440
C                      NEW  J  MATRIX.                                      NUI  450
C                  =0  INDICATES THE J MATRIX IS THE SAME AS WHEN           NUI  460
C                      NUITSL WAS LAST ENTERED                              NUI  470
C        KRET    - RETURN INDICATOR                                         NUI  480
C                  =0  NORMAL RETURN                                        NUI  490
C                  =1  ERROR RETURN.  SOLUTION OF EQUATIONS COULD           NUI  500
C                      NOT BE OBTAINED.                                     NUI  510
C                                                                           NUI  520
C     ------------------------------------------------------------------    NUI  530
      DIMENSION PW(1), DY(1), F1(1), YMAX(1)                                NUI  540
      NL = N-NY                                                             NUI  550
      IF (NEWPW.EQ.0) GO TO 100                                             NUI  560
      NEWPW = 0                                                             NUI  570
      NN = N**2+1                                                           NUI  580
      NNN = NN+N                                                            NUI  590
      CALL LUCATF (PW,PW,N,N,0,D1,D2,PW(NN),PW(NNN),F1,IER)                 NUI  600
      IF (IER.EQ.0) GO TO 100                                               NUI  610
      KRET = 1                                                              NUI  620
      RETURN                                                                NUI  630
  100 CALL LUELMF (PW,DY,PW(NN),N,N,F1)                                     NUI  640
      KRET = 0                                                              NUI  650
      RETURN                                                                NUI  660
      END                                                                   NUI  670

      SUBROUTINE DIFFUN(Y,YL,T,HINV,DY)
C     ------------------------------------------------------------------
C     SUBROUTINE DIFFUN IS SUPPLIED BY THE USER.  ITS PURPOSE IS TO
C     EVALUATE THE FUNCTIONS AT CURRENT VALUES OF THE VARIABLES.
C
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS
C
C     CALL DIFFUN(Y,YL,T,HINV,DY)
C
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.
C
C        Y       - SAME AS IN LDASUB AND SDESOL.  ON INPUT TO THIS
C                  SUBROUTINE THE ARRAY CONTAINS CURRENT VALUES OF THE
C                  DEPENDENT VARIABLES AND THEIR (SCALED) DERIVATIVES.
C        YL      - SAME AS IN LDASUB AND SDESOL.  ON INPUT TO THIS
C                  SUBROUTINE THE ARRAY CONTAINS CURRENT VALUES OF THE
C                  LINEAR VARIABLES.
C        T       - CURRENT TIME
C        HINV    - 1/H , WHERE H IS THE CURRENT STEPSIZE
C        DY      - RETURNED ARRAY OF FUNCTION VALUES.
C
C     ------------------------------------------------------------------
      DIMENSION Y(7,1),YL(1),DY(1)
C
C     DEFINE YOUR FUNCTION HERE

      RETURN
      END
```

Appendix 2: Examples

Example 1: This example is the problem proposed by Gear [3]. The system of equations is

$$\dot{y}_i - S + (R-y_i)^2 + \sum_{j=1}^{4} b_{ij}\, y_j = 0 \ , \ i = 1, 2, 3, 4$$

where $R = \frac{1}{2} \sum_{i=1}^{4} y_i$ and

$$S = \frac{1}{2} \sum_{i=1}^{4} (R-y_i)^2 \ , \ \text{and}$$

$$\dot{y}_5 + y_1 \dot{y}_6 + \dot{y}_1 y_6 = 0$$

$$2y_6 + y_6^3 - y_1 + V_1 - 1 - e^{-t} = 0$$

$$V_1 - V_2 + y_1 y_6 = 0$$

$$V_1 + V_2 + 5y_1 y_2 = 0 \ .$$

In the above $b_{11} = b_{22} = b_{33} = b_{44} = 447.501$

$$b_{12} = -b_{34} = b_{21} = -b_{43} = -\ 452.499$$

$$b_{13} = -b_{24} = b_{31} = -b_{42} = -\ 47.499$$

$$b_{14} = -b_{23} = b_{41} = -b_{32} = -\ 52.501 \ .$$

The initial conditions are

$$y_i = 1 \ , \ i=1, 2, 3, 4 \ .$$

$$y_5 = y_0 = 1$$

$$V_1 = -\ 2 \ , \ V_2 = -\ 3 \ .$$

Note that a different version of DERVAL is necessary since $\frac{\partial F}{\partial \dot{y}}$ is singular.

```
      DIMENSION Y(7,6),YL(2),W(150),GI(16)
      COMMON /DAT/G(16)
      DATA GI/447.501,-452.499,-47.499,-52.501,-452.499,447.501,52.501,
     1 47.499,-47.499,52.501,447.501,452.499,-52.501,47.499,452.499,
     2 447.501/
      DATA N,NY,NL,M,REPS,HMAX,HMIN,H,T,TEND/8,6,2,6,1.E-3,5.E2,1.E-10,
     1 1.E-4,0.,1.E3/
      CALL ERRSET(207,256,-1,1)
      CALL ERRSET(208,256,-1,1)
      DO 8 I=1,16
    8 G(I) = GI(I)
      DO 10 I=1,4
   10 Y(1,I) = -1.
      Y(1,5) = 1.
      Y(1,6) = 1.
      YL(1) = -2.
      YL(2) = -3.
      JSKF = 0
      CALL SDESOL(Y,YL,T,TEND,NY,NL,M,JSKF,6,1,H,HMIN,HMAX,REPS,W)
      PRINT 6,JSKF
    6 FORMAT('0   JSKF =',I4)
      STOP
      END

      SUBROUTINE DIFFUN (Y,YL,T,HINV,DY)
      COMMON /DAT/G(4,4)
      DATA TOLD/-13.459/
      DIMENSION Y(7,1),YL(1),DY(1)
      IF(T.EQ.TOLD)GO TO 10
      TMTERM = EXP(-T)
      TOLD = T
   10 CONTINUE
      R = (Y(1,1) + Y(1,2) + Y(1,3) + Y(1,4))/2.
      S = 0.
      DO 20 I=1,4
   20 S = S + (R - Y(1,I))**2/2.
      DO 30 I=1,4
      DY(I) = HINV*Y(2,I) - S +(R - Y(1,I))**2
      DO 25 J=1,4
   25 DY(I) = DY(I) + G(I,J)*Y(1,J)
   30 CONTINUE
      DY(5) = HINV*(Y(2,5) + Y(1,1)*Y(2,6) + Y(2,1)*Y(1,6))
      DY(6) = 2.*Y(1,6) + Y(1,6)**3 - Y(1,1) + YL(1) - 1.-TMTERM
      DY(7) = YL(1) - YL(2) + Y(1,1)*Y(1,6)
      DY(8) = YL(1) + YL(2) + 5.*Y(1,1) * Y(1,2)
      RETURN
      END

      SUBROUTINE CERVAL(Y,YL,T,N,NY,W,KERET)
      DIMENSION Y(7,1),YL(1),W(1)
      KERET = 0
      DO 50 I=1,NY
   50 Y(2,I) = 0.
      HINV = 1.
      CALL DIFFUN(Y,YL,T,HINV,W)
      DO 100 I=1,NY
  100 Y(2,I) = -W(I)
      RETURN
      END
```

Example 2: This example is a small one, contrived to illustrate the possibility of derivatives entering in a nonlinear fashion. The equations are

$$\dot{y}_1 - 98y_1 + 98y_2 = 0$$

$$(\dot{y}_1)^2 + \dot{y}_2 - 198y_1 + e^{-t}\, y_1 + 199y_2 = 0$$

$$V_1 - y_1 - y_2 = 0$$

The initial conditions are

$$y_1 = y_2 = 1 \ , \ V_1 = 2 \ .$$

Note that we have supplied the explicit expression for the Jacobian. Either JACMAT or a modified version of DERVAL must be supplied as the numerical difference approximation to the Jacobian causes DERVAL to fail.

```
      DIMENSION Y(7,2),YL(1),W(50)
      DATA N,NY,NL,M,REPS,HMAX,HMIN,H,T,TEND/3,2,1,2,1.E-5,25.,1.E-10,
     1 1.E-4,0.,50./
      Y(1,1) = 1.
      Y(1,2) = 1.
      YL(1) = 2.
      JSKF = 0
      CALL SDESCL(Y,YL,T,TEND,NY,NL,M,JSKF,6,1,H,HMIN,HMAX,REPS,W)
      PRINT 6,JSKF
    6 FORMAT('0 JSKF =',I4)
      STOP
      END

      SUBROUTINE DIFFUN (Y,YL,T,HINV,DY)
      DIMENSION Y(7,1),YL(1),DY(1)
      DATA TOLD/-79.03/
      IF(T.EQ.TOLD)GO TO 10
      TMTERM = EXP(-T)
      TOLD = T
   10 CONTINUE
      DY(1) = Y(2,1)*HINV - 98.*Y(1,1) + 99.*Y(1,2)
      DY(2) = (Y(2,1)*HINV)**2 + Y(2,2)*HINV - (198. - TMTERM)*Y(1,1) +
     1 199.*Y(1,2)
      DY(3) = YL(1) - Y(1,1) - Y(1,2)
      RETURN
      END

      SUBROUTINE JACMAT(Y,YL,T,HINV,A2,N,NY,EPS,DY,F1,PW)
      DIMENSION Y(7,1),YL(1),F1(1 ),DY(1),PW(N,1)
      AH = A2*HINV
      DO 100 I=1,N
      DO 100 J=1,N
  100 PW(I,J) = 0.
      PW(1,1) = -AH - 98.
      PW(1,2) = 99.
      PW(2,1) = -2.*AH*Y(2,1)*HINV - 198. + EXP(-T)
      PW(2,2) = -AH + 199.
      IF(NL.LE.0)RETURN
      PW(3,1) = -1.
      PW(3,2) = -1.
      PW(3,3) = 1.
      RETURN
      END
```

Example 3: This is another contrived example, this one to illustrate the use of one type of sparse matrix storage, along with the use of iteration to solve the equations (2.4). The system of equations is

$$\overline{A}\,\dot{y} + \overline{B}\,y = 0 \ ,$$

where

$$\overline{A} = \begin{pmatrix} 7 & 0 & 0 & -3 & 0 & -1 \\ 2 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -3 & 0 & 0 & 5 & 0 & 0 \\ 0 & -1 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & -2 & 0 & 6 \end{pmatrix}$$

$$\overline{B} = \begin{pmatrix} .3 & 0 & 0 & .1 & 0 & -.2 \\ 1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 10 & 0 & 0 & 20 & 0 & 0 \\ 0 & 5 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 57 & 0 & 100 \end{pmatrix}$$

The initial conditions are

$$y_1 = 1000$$

$$y_2 = 0$$

$$y_3 = -25$$

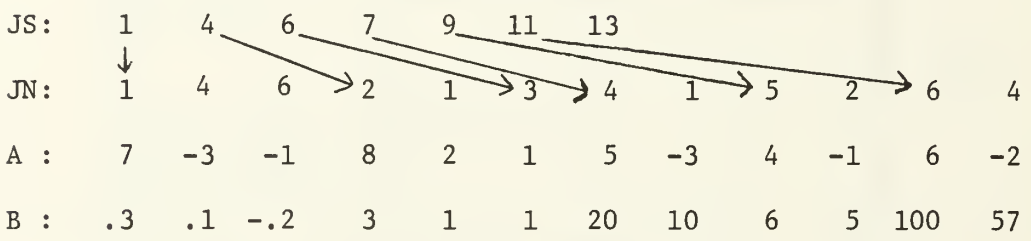
$$y_4 = 10$$

$$y_5 = 0$$

$$y_6 = -1000$$

The matrix storage scheme used for A, B, and the Jacobian, since it has nonzero elements in the same positions as A and B, is that outlined by Gustavson [4]. Briefly, one stores a pointer array (here called JS) which indicates the initial position of new elements in two other arrays, one of which (here called JN) gives the column number of the element stored in the corresponding position of the coefficient arrays (here called A and B).

Thus, for the above problem the arrays stored are



The elements of the $i^{\underline{th}}$ row are stored beginning at location JS(i) of the array A, and in particular A(JS(i) + k) is the element in the $i^{\underline{th}}$ row and JN(JS(i) + k) $^{\underline{th}}$ column of $\overline{A}$, for k = 0, 1, ..., JS(i+1) - JS(i) - 1. For our purposes it is necessary to access the diagonal element easily, so we have required that the diagonal element be the first element stored for a given row. This means that JN(JS(i)) = i, i=1, ..., n. Note that JS(i) is the number of nonzero elements in rows 1 through i - 1, and that JS(n+1) must be defined as the total number of nonzero elements.

Problems similar to the above arise when the finite element method is used to discretize the space domain for time dependent partial differential equations. Simple modifications to the subroutines given below should permit solution of large problems arising in that fashion. We

note, however, that it is not convenient to store synmetric matrices in this form unless all nonzero elements are stored. Storage of only the elements of the lower triangular matrix requires one to reference columns of the matrix, which are not readily accessible. Even if the entire matrix is stored, total storage requirements for matrices arising in finite element applications is still considerably less with this scheme than that required by symmetric band storage mode [5].

```
      DIMENSION Y(7,6),W(126),YI(6),AD(12),BD(12),JSD(7),JND(12)
      COMMON /DATA/A(12),B(12),N,JS(7),JN(12)
      INTEGER*2 JS,JN
      DATA T,TEND,H,JSKP / 0.,250.,1.E-5,0 /
      DATA JSD/1,4,6,7,9,11,13/
      DATA JND/1,3,5,2,1,3,4,1,5,2,6,4/
      DATA AD/7.,-3.,-1.,8.,2.,1.,5.,-3.,4.,-1.,6.,-2./
      DATA BD/.3,.1,-.2,3.,1.,1.,20.,10.,3.,5.,100.,57./
      DATA YI/1000.,0.,-25.,10.,3.,-1000./
      N = 6
      NP1 = N + 1
      JE = JSD(NP1) - 1
      DO 100 I=1,N
100   Y(1,I) = YI(I)
      DO 110 I=1,JE
      A(I) = AD(I)
      B(I) = BD(I)
110   JN(I) = JND(I)
      DO 120 I=1,NP1
120   JS(I) = JSD(I)
      PRINT 4,N,(JS(I),I=1,NP1)
      PRINT 5,(JN(I),I=1,JE)
      PRINT 7,(A(I),I=1,JE)
      PRINT 6,(B(I),I=1,JE)
      CALL SDESOL(Y,YL,T,TEND,N,0,N,JSKP,6,1,H,1.E-6,1.E5,1.E-4,W)
      PRINT 3,JSKP
      STOP
  3   FORMAT('0RETURN FROM SDESOL WITH JSKP =',I4)
  4   FORMAT(' FOR THIS CASE N=',I3//' THE JS ARRAY'//(12I10))
  5   FORMAT(/'0THE JN ARRAY'//(12I10))
  6   FORMAT(/'0THE B ARRAY'//(12F10.2))
  7   FORMAT(/'0THE A ARRAY'//(12F10.2))
      END


      SUBROUTINE DIFFUN (Y,YL,T,HINV,DY)
      COMMON /DATA/A(12),B(12),N,JS(7),JN(12)
      INTEGER*2 JS,JN
      DIMENSION Y(7,1),YL(1),DY(1)
      DO 400 I=1,N
      DY(I) = 0.
      JB = JS(I)
      JE = JS(I+1) - 1
      DO 300 J=JB,JE
      DY(I) = DY(I) + Y(2,JN(J))*A(J)*HINV + B(J)*Y(1,JN(J))
300   CONTINUE
400   CONTINUE
      RETURN
      END


      SUBROUTINE NUITSL (PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)
      COMMON /DATA/A(12),B(12),ND,JS(7),JN(12)
      INTEGER*2 JS,JN
      DIMENSION PW(1),DY(1),F1(1),YMAX(1)
      DATA OMEG,OMEGM1 /1.05,.05/
      KRET = 0
      EPSS = EPS**2
      EPSA2 = EPSS*.0001
      NCIT = N
      DO 100 I=1,NY
100   F1(I) = DY(I)/PW(JS(I))
      DO 300 IT=1,NCIT
      RCH = 0.
      CH = 0.
      DO 200 I=1,NY
      JB = JS(I) + 1
      JE = JS(I+1) - 1
      FN = DY(I)
      IF(JB.GT.JE)GO TO 180
      DO 150 J=JB,JE
150   FN = FN - PW(J)*F1(JN(J))
180   FN = FN/PW(JB-1)
      FN = FN*OMEG - F1(I)*OMEGM1
      ACH = F1(I) - FN
```

```
      CH = CH + (ACH/YMAX(I))**2
      RCH = RCH + (ACH/AMAX1(ABS(FN),EPS))**2
  200 F1(I) = FN
      IF(RCH.LT.EPSS) RETURN
      IF(CH.LT.EPSA2) RETURN
  300 CONTINUE
      KRET = 1
      RETURN
      END

      SUBROUTINE JACMAT(Y,YL,T,HINV,A2,N,NY,EPS,DY,F1,PW)
      COMMON /DATA/A(12),B(12),NDUM,JS(7),JN(12)
      INTEGER*2 JS,JN
      DIMENSION Y(7,1),YL(1),F1(1),DY(1),PW(1)
      AH = -A2*HINV
      JE = JS(N+1) - 1
      DO 100 J=1,JE
  100 PW(J) = AH*A(J) + B(J)
      RETURN
      END
```

Example 4: This example arises from a nonlinear reactor dynamics problem where the finite element method is used to discretize the space domain. The resulting system of equations has the form

$$\bar{A}\,\dot{y} - \bar{B}\,y + w(\bar{C}\,y)\,y = 0 \ ,$$

where $\bar{C}$ is a matrix with three subscripts. The $i^{\underline{th}}$ equation can be expressed as

$$\sum_{j=1}^{N} (\bar{a}_{ij}\,\dot{y}_j - \bar{b}_{ij}\,y_j) + w \sum_{j=1}^{N} \sum_{k=1}^{N} \bar{c}_{ijk}\,y_j\,y_k = 0 \ .$$

In this example $N = 28$, and there are at most seven nonzero elements per row in $\bar{A}$ and $\bar{B}$. The nonlinear term $y_j\,y_k$ appears only if both $\bar{a}_{ij}$ and $\bar{a}_{ik}$ are nonzero. Therefore a different type of sparse matrix storage is used for this problem.

An array, K, dimensioned (28, 7) is used to store (for each row), the columns subscripts for the nonzero elements. For convenience in accessing the diagonal element, we require that $K(i,1) = i$. We can note this matrix is simply the connectivity matrix for the finite element grid. Then the nonzero elements of $\bar{A}$ and $\bar{B}$, are stored in the corresponding portions of the arrays A and B respectively. If there are in fact less than seven nonzero coefficients in a row, the remaining $K(i,j)$ are set to zero.

The storage for $\bar{C}$ is somewhat more complicated. $\bar{C}$ is symmetric (invariant under any permutation of subscripts). The nonlinear term of the $i^{\underline{th}}$ equation was rewritten as

$$w \sum_{j=1}^{N} \sum_{k=1}^{N} \bar{c}_{ijk}\, y_j\, y_k = w \sum_{j=1}^{N} \sum_{k=j}^{N} \bar{d}_{ijk}\, y_j\, y_k \ ,$$

where

$$\bar{d}_{ijk} = \begin{cases} 0 & k < j \\ \bar{c}_{ijk} & k = j \\ \bar{c}_{ijk} + C_{ikj} & k > j \ . \end{cases}$$

The coefficients $\bar{d}_{ijk}$ are then stored in a (28,28) array C in the order the second and third subscripts are given here.
(K(i,1), K(i,1)), ..., (K(i,1), K(i,7)), (K(i,2), K(i,2)), ..., (K(i,2), K(i,7)), ..., (K(i,7), K(i,7)) .

The equations can then be written in the form

$$\sum_{j=1}^{7} [A_{ij}\, \dot{y}_{K(i,j)} - B_{ij}\, y_{K(i,j)}] + \sum_{j=i}^{7} \sum_{k=j}^{7} C_{im_{jk}}\, y_{K(i,j)}\, y_{K(i,k)} = 0$$

where

$$m_{jk} = k + \frac{(j-1)(14-j)}{2} \ .$$

Because of the large amount of data for this problem the input arrays K, A, B, and C are simply listed along with the programs for this example.

```
      DIMENSION Y(7,28),WS(560)
      COMMON /DATA/A(28,7),B(28,7),C(28,28),N,NNZ,K(28,7)
      INTEGER*2 K
      DATA TEND,HMIN,HMAX,EPS,ZOMEGA/.1,1.E-12,.1,.01,650.903E-14/
      DATA NN,NY,NL/28,28,0/
      NNZ = 7
      CALL ERRSET(207,256,-1,1)
      CALL ERRSET(208,256,-1,1)
      N = NN
      M = N
      NEND = NNZ*(NNZ + 1)/2
      PRINT 10
      DO 110 I=1,NN
      READ 1,(K(I,J) ,J=1,NNZ)
  110 PRINT 11,(K(I,J),J=1,NNZ)
      PRINT 12
      DO 120 I=1,NN
      READ 2,(A(I,J),J=1,NNZ)
      Y(1,I) = 0.
  120 PRINT 15,(A(I,J),J=1,NNZ)
      Y(1,1) = 1.E16
      PRINT 13
      DO 130 I=1,NN
      READ 2,(B(I,J),J=1,NNZ)
  130 PRINT 15,(B(I,J),J=1,NNZ)
      PRINT 14
      DO 140 I=1,NN
      READ 2,(C(I,J),J=1,NEND)
      DO 135 J=1,NEND
  135 C(I,J) =  C(I,J) *ZOMEGA
  140 PRINT 15,(C(I,J),J=1,NEND)
      JSKF = 0
      T = 0.
      H = HMIN*1000.
      CALL SDESOL(Y,YL,T,TEND,NY,NL,M,JSKF,6,1,F,HMIN,HMAX,  EPS,WS)
      PRINT 3,JSKF
      STOP
    1 FORMAT(16I5)
    2 FORMAT(7E11.4)
    3 FORMAT('0 JSKF = ',I3)
   10 FORMAT('1K ARRAY'/)
   11 FORMAT(8X,14I8)
   12 FORMAT(///'0A(I,J)'/)
   13 FORMAT(///'0B(I,J)'/)
   14 FORMAT(///'0C(I,J)'/)
   15 FORMAT(8X,1P7E16.6)
      END

      SUBROUTINE DIFFUN(Y,YL,T,HINV,DY)
      COMMON /DATA/A(28,7),B(28,7),C(28,28),N,NNZ,K(28,7)
      INTEGER*2 K
      DIMENSION Y(7,1),YL(1),DY(1)
      DO 400 I=1,N
      DY(I) = 0.
      DO 300 J=1,NNZ
      IF(K(I,J).LE.0)GO TO 310
      DY(I) = DY(I) + Y(2,K(I,J))*A(I,J)*HINV - B(I,J)*Y(1,K(I,J)) +
     1 C(I,J)*Y(1,K(I,J))*Y(1,K(I,1))
  300 CONTINUE
  310 L = NNZ
      DO 360 J1=2,NNZ
      IF(K(I,J1).LE.0)GO TO 400
      DO 350 J2=J1,NNZ
      L = L + 1
      IF(K(I,J2).LE.0)GO TO 350
      DY(I) = DY(I) + C(I,L)*Y(1,K(I,J1))*Y(1,K(I,J2))
  350 CONTINUE
  360 CONTINUE
  400 CONTINUE
      RETURN
      END

      SUBROUTINE JACMAT(Y,YL,T,HINV,A2,N,NY,EPS,DY,F1,PW)
```

```
      COMMON /DATA/A(28,7),B(28,7),C(28,28),ND,NNZ,K(28,7)
      INTEGER*2 K,P
      DIMENSION Y(7,1),YL(1),F1(1 ),DY(1),PW(NY,1)
      DIMENSION P(7,7)
      DATA P/49*0/,INITP/0/
      IF(INITP.EQ.NNZ)GO TO 99
      INITP = NNZ
      DO 98 L=1,NNZ
      DO 98 M = L,NNZ
   98 P(L,M) = M + (L - 1)*(2*NNZ - L)/2
   99 CONTINUE
      AH =-A2*HINV
      DO 300 I=1,NY
      DO 300 J=1,NNZ
      PW(I,J) = AH*A(I,J) - B(I,J)
       DO 100 L=1,J
      IF(K(I,L).LE.0)GO TO 295
  100 PW(I,J) = PW(I,J) + C(I,P(L,J))*Y(1,K(I,L))
      DO 200 M=J,NNZ
      IF(K(I,M).LE.0)GO TO 295
  200 PW(I,J) = PW(I,J) + C(I,P(J,M))*Y(1,K(I,M))
  295 CONTINUE
  300 CONTINUE
      RETURN
      END


      SUBROUTINE NUITSL(PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)
      DIMENSION PW(NY,1),DY(1),F1(1),YMAX(1)
      COMMON /DATA/A(28,7),B(28,7),C(28,28),ND,NNZ,K(28,7)
      DATA  SPC,SPCM1/1.05,.05/
      INTEGER*2 K
      KRET = 0
      EPSS = EPS**2
      EPSA2 = EPSS*.0001
      NOIT = N
  280 DO 281 I=1,NY
  281 F1(I) = DY(I)/PW(I,1)
      DO 287 IT=1,NOIT
      RCH = 0.
      CH = 0.
      DO 285 I=1,NY
      FN = DY(I)
      DO 284 J=2,NNZ
      IF(K(I,J).LE.0.OR.K(I,J).GT.NY)GO TO 284
      FN = FN - PW(I,J)*F1(K(I,J))
  284 CONTINUE
      FN = FN/PW(I,1)
      FN = FN*SPC - SPCM1*F1(I)
      ACH = F1(I) - FN
      CH = CH + (ACH/YMAX(I))**2
      RCH = RCH + (ACH/AMAX1(ABS(FN),EPS))**2
  285 F1(I) = FN
      IF(RCH.LT.EPSS)GO TO 288
      IF(CH.LE.EPSA2)GO TO 288
  287 CONTINUE
      KRET = 3
  288 CONTINUE
      RETURN
      END
```

INPUT DATA FOR EXAMPLE 4

```
    1     6     2
    2     1     6     7     8     3
    3     2     8     4
    4     3     8     9    10     5
    5     4    10    21
    6    11     7     2     1
    7     2     6    11    12    13     8
    8     3     2     7    13     9     4
    9     4     8    13    14    15    10
   10     5     4     9    15    22    21
   11     6    16    12     7
   12     7    11    16    17    18    13
   13     8     7    12    18    14     9
   14     9    13    18    19    20    15
   15    10     9    14    20    23    22
   16    11    28    17    12
   17    12    16    28    27    18
   18    13    12    17    27    26    19    14
   19    14    18    26    25    20
   20    15    14    19    25    24    23
   21     5    10    22
   22    21    10    15    23
   23    22    15    20    24
   24    23    20    25
   25    20    19    26    24
   26    19    18    27
   27    18    17    28    26
   28    16    27    17
 8.3776E 02 8.3776E 02 4.1888E 02 0.0          0.0          0.0          0.0
 5.0265E 03 4.1888E 02 2.0944E 03 2.5133E 03 2.0944E 03 4.1888E 02 0.0
 1.6755E 03 4.1888E 02 1.6755E 03 4.1888E 02 0.0          0.0          0.0
 5.0265E 03 4.1888E 02 2.0944E 03 2.5133E 03 2.0944E 03 4.1888E 02 0.0
 1.4661E 03 4.1888E 02 1.4661E 03 3.1416E 02 0.0          0.0          0.0
 1.0891E 04 2.9322E 03 4.1888E 03 2.0944E 03 8.3776E 02 0.0          0.0
 2.8484E 04 2.5133E 03 4.1888E 03 6.2832E 03 6.7021E 03 6.2832E 03 4.1888E 03
 2.1782E 04 1.6755E 03 2.0944E 03 4.1888E 03 5.8643E 03 4.1888E 03 2.0944E 03
 2.8484E 04 2.5133E 03 4.1888E 03 6.2832E 03 6.7021E 03 6.2832E 03 4.1888E 03
 1.9059E 04 1.4661E 03 2.0944E 03 4.1888E 03 5.1313E 03 3.1416E 03 1.5708E 03
 2.3457E 04 2.9322E 03 5.0265E 03 8.3776E 03 6.2832E 03 0.0          0.0
 5.3616E 04 6.7021E 03 8.3776E 03 1.0472E 04 1.0891E 04 1.0472E 04 8.3776E 03
 4.6914E 04 5.8643E 03 6.2832E 03 8.3776E 03 1.0053E 04 8.3776E 03 6.2832E 03
 5.3616E 04 6.7021E 03 8.3776E 03 1.0472E 04 1.0891E 04 1.0472E 04 8.3776E 03
 4.4663E 04 5.1313E 03 6.2832E 03 8.3776E 03 8.9535E 03 8.4823E 03 6.2046E 03
 3.2515E 04 5.0265E 03 5.1836E 03 1.0812E 04 1.0472E 04 0.0          0.0
 5.6208E 04 1.0891E 04 1.0812E 04 1.1958E 04 1.1958E 04 1.0812E 04 0.0
 8.0582E 04 1.0053E 04 1.0472E 04 1.0812E 04 1.3312E 04 1.3312E 04 2.1284E 04
 5.6208E 04 1.0891E 04 1.0812E 04 1.1958E 04 1.1958E 04 1.0812E 04 0.0
 6.0750E 04 8.9535E 03 1.0472E 04 1.0812E 04 9.2481E 03 1.0348E 04 9.8764E 03
 3.7699E 03 3.1416E 02 1.5708E 03 1.8850E 03
 2.9531E 04 1.8850E 03 3.1416E 03 6.2046E 03 8.7179E 03
 6.1889E 04 8.7179E 03 8.4823E 03 9.8764E 03 1.2468E 04
 6.3303E 04 1.2468E 04 1.0348E 04 8.8357E 03
 5.7962E 04 9.2481E 03 1.1958E 04 1.4726E 04 8986575 03
 3.4719E 04 1.1958E 04 1.3312E 04 1.7671E 04
 9.4719E 04 1.3312E 04 1.1958E 04 1.4726E 04 1.7671E 04
 5.3014E 04 5.1836E 03 1.4726E 04 1.1958E 04
-1.5816E 09 1.1720E 09 1.0449E 09 0.0          0.0          0.0          0.0
-3.9622E 09 1.0449E 09 6.3535E 08 4.4338E 09 6.3535E 08 1.0449E 09 0.0
-3.1631E 09 1.0449E 09 2.3440E 09 1.0449E 09 0.0          0.0          0.0
-3.9622E 09 1.0449E 09 6.3535E 08 4.4338E 09 6.3535E 08 1.0449E 09 0.0
-4.3361E 09 1.0449E 09 1.8355E 09 1.4879E 09 0.0          0.0          0.0
-6.7925E 09 4.5609E 09 6.7778E 09 6.3535E 08 1.1720E 09 0.0          0.0
-1.5223E 10 4.4338E 09 6.7778E 09 1.9061E 09 1.1212E 10 1.9061E 09 6.7778E 09
-1.3585E 10 2.3440E 09 6.3535E 08 6.7778E 09 9.1218E 09 6.7778E 09 6.3535E 08
-1.5223E 10 4.4338E 09 6.7778E 09 1.9061E 09 1.1212E 10 1.9061E 09 6.7778E 09
-2.4104E 10 1.8355E 09 6.3535E 08 6.7778E 09 7.3355E 09 8.4446E 09-6.0318E 08
-1.3995E 10 4.5609E 09 7.9498E 09 1.3556E 10 1.9041E 09 0.0          0.0
-2.9627E 10 1.1212E 10 1.3556E 10 3.1768E 09 1.7989E 10 3.1768E 09 1.3556E 10
-2.7989E 10 9.1218E 09 1.9061E 09 1.3556E 10 1.5900E 10 1.3556E 10 1.9061E 09
-2.9627E 10 1.1212E 10 1.3556E 10 3.1768E 09 1.7989E 10 3.1768E 09 1.3556E 10
-4.8828E 10 7.3355E 09 1.9061E 09 1.3556E 10 1.0212E 10 1.1621E 10 2.0408E 09
-3.5210E 10 7.9498E 09 1.3692E 10 1.6043E 10 3.1768E 09 0.0          0.0
-8.2408E 10 1.7989E 10 1.6043E 10-3.6945E 08 2.4060E 10 1.3103E 10 0.0
```

```
-7.2321E 10  1.5900E 10  3.1768E 09  1.3103E 10 1.1476E 10  1.1476E 10  1.6280E 10
-8.2408E 10  1.7989E 10  1.3103E 10  2.4060E 10-3.6945E 08  1.6043E 10  0.0
-8.7119E 10  1.0212E 10  3.1768E 09  1.6043E 10  2.4798E 10  3.4658E 09  1.3398E 10
-8.2837E 09  1.4879E 09-6.0318E 08  2.8953E 09
-4.7095E 10  2.8953E 09  8.4446E 09  2.0408E 09  6.4005E 08
-1.0136E 11  6.4005E 08  1.1621E 10  1.3398E 10  4.6822E 09
-1.3280E 11  4.6822E 09  3.4658E 09  2.3750E 10
-1.3548E 11  2.4798E 10-3.6945E 08  7.2533E 09  2.3750E 10
-1.5263E 11  2.4060E 10  1.1476E 10-3.5688E 09
-1.4877E 11  1.1476E 10  2.4060E 10  3.3929E 09-3.5688E 09
-7.4644E 10  1.3692E 10  3.3929E 09-3.6945E 08
 4.1888E 02  5.5850E 02  2.7925E 02  0.0          0.0          0.0          0.0
 4.1888E 02  2.7925E 02  0.0          0.0          0.0          0.0          1.3963E 02
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
 2.5133E 03  0.0          8.3776E 02  0.0          0.0          5.5850E 02  0.0          0.0
 1.3963E 02  2.7925E 02  0.0          0.0          0.0          2.7925E 02  9.7738E 02
 0.0          0.0          0.0          5.5850E 02  1.1170E 03  5.5850E 02  0.0
 2.2340E 03  9.7738E 02  0.0          8.3776E 02  1.3963E 02  5.5850E 02  0.0
 8.3776E 02  2.7925E 02  1.1170E 03  2.7925E 02  0.0          0.0          0.0
 1.3963E 02  2.7925E 02  0.0          0.0          0.0          0.0          8.3776E 02
 2.7925E 02  0.0          0.0          0.0          1.3963E 02  0.0          0.0
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
 2.5133E 03  0.0          8.3776E 02  0.0          5.5850E 02  0.0          0.0
 1.3963E 02  2.7925E 02  0.0          0.0          0.0          2.7925E 02  9.7738E 02
 0.0          0.0          0.0          5.5850E 02  1.1170E 03  5.5850E 02  0.0
 2.2340E 03  9.7738E 02  0.0          8.3776E 02  1.3963E 02  5.5850E 02  0.0
 4.1888E 02  2.7925E 02  5.5850E 02  0.0          0.0          0.0          0.0
 1.3963E 02  2.7925E 02  0.0          0.0          0.0          0.0          4.1888E 02
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
 6.7021E 03  2.2340E 03  1.9548E 03  8.3776E 02  0.0          0.0          0.0
 1.2566E 03  1.1170E 03  0.0          0.0          0.0          0.0          1.6755E 03
 5.5850E 02  0.0          0.0          1.3963E 03  6.9813E 02  0.0          0.0
 1.1170E 03  2.7925E 02  0.0          1.1170E 03  0.0          0.0          0.0
 1.6755E 04  2.2340E 03  1.3963E 03  2.5133E 03  0.0          0.0          2.2340E 03  1.3963E 03
 8.3776E 02  5.5850E 02  0.0          0.0          0.0          0.0          1.6755E 03
 1.1170E 03  0.0          0.0          1.9548E 03  2.6529E 03  0.0          0.0
 2.2340E 03  2.7925E 03  1.3963E 03  6.4228E 03  2.6529E 03  2.5133E 03  5.3058E 03
 6.7021E 03  0.0          1.1170E 03  1.9548E 03  2.2340E 03  0.0          0.0
 2.7925E 02  2.7925E 02  0.0          0.0          0.0          8.3776E 02  6.9813E 02
 0.0          0.0          0.0          8.3776E 02  1.6755E 03  1.1170E 03  0.0
 1.9548E 03  1.2566E 03  0.0          0.0          0.0          0.0          0.0
 1.4242E 04  0.0          3.9095E 03  3.6303E 03  2.5133E 03  0.0          0.0
 1.1170E 03  0.0          0.0          1.1170E 03  0.0          2.5133E 03  2.0944E 03
 1.9548E 03  0.0          0.0          0.0          3.3510E 03  1.3963E 03  0.0
 3.0718E 03  2.3736E 03  0.0          2.7925E 03  0.0          0.0          0.0
 3.1835E 04  5.5850E 03  3.0718E 03  4.1888E 03  0.0          3.9095E 03  3.0718E 03
 2.5133E 03  1.3963E 03  0.0          0.0          0.0          0.0          3.3510E 03
 1.9548E 03  0.0          0.0          3.6303E 03  4.3284E 03  0.0          0.0
 3.9095E 03  4.4680E 03  2.2340E 03  1.0612E 04  4.3284E 03  4.1888E 03  1.0332E 04
 2.8484E 04  0.0          2.7925E 03  3.6303E 03  7.8191E 03  3.6303E 03  2.5133E 03
 2.2340E 03  1.1170E 03  0.0          0.0          0.0          6.1436E 03  2.3736E 03
 0.0          0.0          0.0          2.5133E 03  3.3510E 03  1.9548E 03  0.0
 4.4680E 03  4.1888E 03  1.9548E 03  0.0          3.3510E 03  4.4680E 03  5.1662E 03
 3.1835E 04  5.5850E 03  3.0718E 03  4.1888E 03  0.0          3.9095E 03  3.0718E 03
 2.5133E 03  1.3963E 03  0.0          0.0          0.0          0.0          3.3510E 03
 1.9548E 03  0.0          0.0          3.6303E 03  4.3284E 03  0.0          0.0
 3.9095E 03  4.4680E 03  2.2340E 03  1.0612E 04  4.3284E 03  4.1888E 03  1.0332E 04
 1.4242E 04  0.0          2.7925E 03  3.6303E 03  3.9095E 03  0.0          0.0
 1.1170E 03  1.1170E 03  0.0          0.0          0.0          2.5133E 03  2.3736E 03
 0.0          0.0          0.0          2.5133E 03  3.3510E 03  1.9548E 03  0.0
 4.4680E 03  2.0944E 03  0.0          0.0          0.0          0.0          0.0
 1.3823E 04  0.0          0.0          0.0          4.1888E 03  0.0          0.0
 1.9548E 03  0.0          0.0          1.9548E 03  0.0          4.1888E 03  0.0
 0.0          0.0          0.0          0.0          2.3736E 03  2.2340E 03  0.0
 4.7473E 03  4.0492E 03  0.0          4.4680E 03  0.0          0.0          0.0
```

1.4242E 04	8.9361E 03	4.7473E 03	0.0	0.0	4.7473E 03	0.0
4.1888E 03	2.2340E 03	0.0	0.0	0.0	0.0	2.3736E 03
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	2.3736E 03	2.2340E 03	0.0
2.7646E 04	0.0	4.4680E 03	0.0	0.0	0.0	4.1888E 03
3.9095E 03	1.9548E 03	0.0	0.0	0.0	1.0332E 04	4.0492E 03
0.0	0.0	0.0	4.1888E 03	2.3736E 03	0.0	0.0
6.9813E 03	0.0	0.0	0.0	0.0	0.0	1.7872E 04
1.4242E 04	8.9361E 03	4.7473E 03	0.0	0.0	4.7473E 03	0.0
4.1888E 03	2.2340E 03	0.0	0.0	0.0	0.0	2.3736E 03
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	2.3736E 03	2.2340E 03	0.0
1.3823E 04	0.0	4.4680E 03	0.0	0.0	0.0	0.0
1.9548E 03	1.9548E 03	0.0	0.0	0.0	4.1888E 03	4.0492E 03
0.0	0.0	0.0	4.1888E 03	2.3736E 03	0.0	0.0
6.9813E 03	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
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0.0	0.0	0.0	0.0	0.0	0.0	0.0
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0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0

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