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# Automated Heuristic Stability Analysis for Nonlinear Equations 

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# AUTOMATED HEURISTIC STABILITY ANALYSTS FOR NONLINEAR EQUATIONS 

by<br>L. D. Cloutman and L. W. Fullerton




#### Abstract

The modified equation method of heuristic stability analysis has proved to be a useful tool for the prediction of instabilities of nonlinear finite difference equations that are - used in numerical fluid dynamics. The need to calculate and manipulate multi-dimensional Taylor series expansions is a serious disadvantage of this technique, and for many problems of interest, it is difficult to obtain a reliable result by hand. We have, therefore, written general purpose programs to do the algebra by computer, for both the series expansions and elimination of time derivatives from the truncation error terms of the modified equation. We discuss some important features of the procedure and present examples of how the results may be used to design and improve difference methods.


I. INTRODUCTION

Heuristic stability analysis (e.g., Hirt ${ }^{1}$ ) consists of examining the lowest order truncation errors of a finite difference equation (FDE). These errors are obtained from Taylor series expansions, sometimes multi-dimensional, of the solution of the FDE about a suitably chosen point. Often simple examination of the expansion can reveal undesirable properties of the FDE , such as zeroth or negative order errors and diffusional instabilities. In principle, these expansions can also be used to help design difference methods by eliminating inaccurate or unstable forms before performing a series of numerical tests. Heuristic analysis also has been useful in predicting some of the stability requirements of nonlinear finite difference methods used for numerical fluid dynamics calculations. In particular, Rivard et al. ${ }^{2}$ have recently used such truncation error expansions (TEE's) as the basis of a technique to stabilize and improve the accuracy of the ICE algorithm orginally described by Harlow and Amsden. ${ }^{3}$ Warming and Hyett ${ }^{4}$ discuss a procedure for analyzing linear problems using a program written in

FORMAC, but they did not treat nonlinear equations.
The massive amount of algebra involved in carrying out the expansions and time derivatives eliminations for many problems of interest is a hindrance to applying the heuristic technique. Indeed, even relatively simple FDE's may be impractical to analyze by hand, because one cannot be sure there are no blunders in the derived result. We have, therefore, implemented the heuristic technique in an algebraic computer language, and this implementation is discussed in the next section. In Sec. III, we give several examples which illustrate how the results of our program may be used.

## II. METHODOLOGY

In order to illustrate the heuristic technique, we first carry out an analysis of a typical FDE from the field of numerical fiuid dynamics. The onedimensional continuity equation in Cartesian coordinates is

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}+\frac{\partial p u}{\partial x}=\frac{\partial}{\partial x}\left(\xi \frac{\partial \rho}{\partial x}\right) \tag{1}
\end{equation*}
$$

where $\rho$ is the fluid density, $u$ is the velocity, and $\xi$ is an artificial mass diffusion coefficfent that may be needed for stability. For the ICE method, we approximate Eq. (1) by

$$
\begin{align*}
\frac{\rho_{i}^{n+1}-\rho_{i}^{n}}{\delta t} & +\frac{\theta}{2 \delta x}\left[\left(\rho_{i+1}^{n+1}+\rho_{i}^{n+1}\right) u_{i+\frac{1}{2}}^{n+1}-\left(\rho_{i}^{n+1}\right.\right. \\
& \left.\left.+\rho_{i-1}^{n+1}\right) u_{i-\frac{1}{2}}^{n+1}\right]+\frac{(1-\theta)}{2}\left[\left(\rho_{i+1}^{n}\right.\right. \\
& \left.\left.+\rho_{i}^{n}\right) u_{i+\frac{3}{2}}^{n}-\left(\rho_{i}^{n}+\rho_{i-1}^{n}\right) u_{i-\frac{1}{2}}^{n}\right] \\
& =\frac{1}{\delta x^{2}}\left[\xi_{i+\frac{1}{2}}\left(\rho_{i+1}^{n}-\rho_{i}^{n}\right)-\xi_{i-\frac{1}{2}}\left(\rho_{i}^{n}\right.\right. \\
& \left.\left.-\rho_{i-1}^{n}\right)\right], \tag{2}
\end{align*}
$$

where a superscript denotes the time level and a subscript denotes the mesh cell number. Figure 1 shows the kind of staggered grid used by ICE, The time centering parameter $\theta$ assumes values between zero and unity. We now choose a point, say time level $n$ and cell center $i$, about which to expand the dependent variables. Next we calculate the truncated Taylor series expansion

$$
\begin{equation*}
y_{i+k}^{n+h}=\sum_{m=0}^{M} \frac{1}{m!}\left(h \delta t \frac{\partial}{\partial t}+k \delta x \frac{\partial}{\partial x}\right)^{m} y \tag{3}
\end{equation*}
$$

where $y$ is either $\rho$ or $u$ in our example. Because we want truncation errors through $O(\delta t)$ and $O\left(\delta x^{2}\right)$ in the final result, we must, in this case, keep terms in Eq. (3) through $O\left(\delta t^{2}\right)$ and $O\left(\delta x^{4}\right)$. When


Fig. 1 Fragment of the computing mesh for the thermal diffusion example, Eq. (15). The $T_{i}$ are defined on the cell centers $r_{i}$, and the $r_{i-\frac{1}{2}}$ are the cell edges. The same subscripting notation is used in the ICE difference equations, where $\rho$ is defined at $x_{i}=r_{i}$ and $u$ is defined on the cell edges.
we substitute Eq. (3) for each of the variables in Eq- (2) and drop high-order terms, we obtain the original differential equation plus extra terms that we call truncation errors:

$$
\begin{align*}
\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x} & =\frac{\partial}{\partial x}\left(\xi \frac{\partial \rho}{\partial x}\right)-\frac{\delta t}{2}\left[\frac{\partial^{2} \rho}{\partial t^{2}}+2 \theta \cdot\left(u \frac{\partial^{2} \rho}{\partial t \partial x}\right.\right. \\
& \left.\left.+\frac{\partial u}{\partial t} \frac{\partial \rho}{\partial x}+\frac{\partial u}{\partial x} \frac{\partial \rho}{\partial t}+\rho \frac{\partial^{2} u}{\partial t \partial x}\right)\right] \\
& -\frac{\delta x^{2}}{24}\left[4 u \frac{\partial^{3} \rho}{\partial x^{3}}+6 \frac{\partial u}{\partial x} \frac{\partial^{2} \rho}{\partial x^{2}}+3 \frac{\partial^{2} u}{\partial x^{2}} \frac{\partial \rho}{\partial x}\right. \\
& +\rho \frac{\partial^{3} u}{\partial x^{3}}-2 \xi \frac{\partial^{4} \rho}{\partial x^{4}}-4 \frac{\partial \xi}{\partial x} \frac{\partial^{3} \rho}{\partial x^{3}} \\
& \left.-3 \frac{\partial^{2} \xi}{\partial x^{2}} \frac{\partial^{2} \rho}{\partial x^{2}}-\frac{\partial^{3} \xi}{\partial x^{3}} \frac{\partial \rho}{\partial x}\right] \tag{4}
\end{align*}
$$

This result is called the modified equation. This expansion procedure, we see, is simple, well defined and very tedious. It is, therefore, ideally suited for implementation in an algebraic language. We chose to code the heuristic algorithm in ALTRAN, ${ }^{5,6}$ because ALTRAN is designed for massive algebraic operations on rational polynomial expressions. Moreover, it contains a number of routines which manipulate truncated power series efficiently. The list of the expansion code is given in Appendix A. The algorithm could be implemented in a number of other algebraic languages including MACSYMA, REDUCE, and FORMAC, provided they are available on a sufficiently large computer.

The most important consideration in designing this code was to minimize the work space (i.e., core) needed. Even though we use the LCM version of ALTRAN, which has 131000 words of workspace, the explosive growth of intermediate terms can cause memory overflow even for fairly simple difference equations unless care is taken to make the most efficient use of the memory. Running time is usually no problem on the CDC 7600 although the efficient use of memory also tends to reduce run times.

The program uses indeterminant arrays to represent dependent variables and their partial deriv-
atives. For example, $\partial^{(i+j)} u / \partial x^{1} \partial t^{j}$ is represented by the array element $U(I, J)$. The code is set up to handle four such variables; $P, T, R H O$, and $U$. More variables can be added to the layout if needed, although they would increase memory requirements. The maximum order of the expansions is set by the integer variable $O R D$, currently set to a value of six. The maximum value of $I$ or $J$ is set by the integer variable $N$, also currently set equal to six. If higher order derivatives or expansions are needed at any point in the calculation, $N$ and/or ORD must be increased, with a corresponding increase in memory requirements and running time. In practice, however, even large, high-order problems are practical on the LASL 7600's.

The Taylor series expansions are done by the LONG ALGEBRAIC ALTRAN PROCEDURE TE, which is invoked as a function. Suppose we choose (i $\delta r, n \delta t$ ) as the point about which we want to perform the expansions. A single call to TE can expand a product of up to four variables. The calling sequence $\operatorname{TE}\left(f_{1}, a_{1}, b_{1}, f_{2}, a_{2}, b_{2}, f_{3}, a_{3}, b_{3}, f_{4}, a_{4}, b_{4}\right)$ expands
 both $\delta r$ and $\delta t$. For example, $u_{i-1 / 2}^{n+1}$ is represented by TE( $\mathrm{U},-1 / 2,1$ ). It is more efficient to compute products with a single call than to make separate calls and multiply the results. That is, use TE(RHO, $0,1, U, 1 / 2,0)$ for $\rho_{i}^{n+1} u_{i+\frac{1}{2}}^{n}$, not $\operatorname{TE}(\mathrm{RHO}, 0,1) * \operatorname{TE}(\mathrm{U}, 1 / 2,0)$. The first method computes only terms of order ORD. The latter method expands each variable to order ORD, and the multiplication generates many terms through order $2 * O R D$ that are eventually discarded.

Since there is no simple way to specify the difference equation on data cards, all input data is specified in executable ALTRAN statements in a special section of the program. RORD and TORD are the maximum orders of $\delta r$ and $\delta t$, respectively, to be retained in the final result. DERMOD is the lefthand side of the modified equation, and it will be explained in more detail in the example. DE is the differential equation, and $F D E$ is the finite difference equation expressed in terms of TE . The listing of the code in Appendix A contains Eq. (2) as an example. Note that DE and FDE are always written in the form such that they are equal to zero.

We want the truncation errors to $O(\delta t)$ and $O\left(\delta r^{2}\right)$, so $\operatorname{RORD}=2$ and $T O R D=1$. Since the expansions are divided by $\delta t$ and $\delta r^{2}$, they must be carried out to at least order 2 and 4 in $\delta t$ and $\delta r$ respectively. Therefore, ORD must be at least 4.

This example is a trivial problem -- only 14
seconds of central processor time and 37000 words of workspace were required on a CDC 7600. Although 131000 words of workspace are available in our version of ALTRAN, memory space, not running time, still limits the size of the largest problem that can be run. Very large problems often can be run piecemeal, however.

Appendix A consists of a complete listing of the expansion code, plus a sample problem. Appendix B contains a detailed flow chart of the ALTRAN coding, definition of all variables, and a description of the purpose and operation of every procedure.

For some purpose it is necessary to eliminate all time derivatives from the modified equation. In our example, we need $\partial \rho / \partial t$ and $\partial u / \partial t$ and their derivatives with respect to both $r$ and $t$. Therefore, the modified equation is punched out in the form

$$
\begin{align*}
\operatorname{DERMOD}=\operatorname{RHO}(0,1) & =\frac{\partial \rho}{\partial t}=-\frac{\partial u}{\partial x}-\rho \frac{\partial u}{\partial x}+\xi \frac{\partial^{2} \rho}{\partial x^{2}} \\
& +\frac{\partial \xi}{\partial r} \frac{\partial \rho}{\partial r}-\text { TER. } \tag{5}
\end{align*}
$$

The time derivative elimination code then differentiates the right-hand side and eliminates the time derivative from the truncation error terms TER. It is necessary to use the modified equation for the momentum equation to eliminate the time derivatives of $u$. We will return this example in the next section.

A simpler example will suffice to illustrate the complexities of automating the general procedure for eliminating time derivatives. The modified equation for the difference approximation,

$$
\begin{equation*}
\frac{T_{i}^{n+1}-T_{i}^{n}}{\delta t}=\frac{K}{\delta x^{2}}\left(T_{i+1}^{n}-2 T_{i}^{n}+T_{i-1}^{n}\right) \tag{6}
\end{equation*}
$$

to

$$
\begin{equation*}
\frac{\partial T}{\partial t}=K \frac{\partial^{2} T}{\partial x^{2}} \tag{7}
\end{equation*}
$$

expanded about time $n$ and space point $i$ is

$$
\begin{equation*}
\frac{\partial T}{\partial t}=K \frac{\partial^{2} T}{\partial x^{2}}-\frac{\delta t}{2} \frac{\partial^{2} T}{\partial t^{2}}+\frac{\delta x^{2} K}{6} \frac{\partial^{4} T}{\partial x^{4}}+O\left(\delta t^{2}, \delta x^{4}\right) \tag{8}
\end{equation*}
$$

We will keep error terms of order $\delta t$ and $\delta x^{2}$. Begin the elimination of $\partial^{2} T / \partial t^{2}$ by differentiating Eq. (8) with respect to $t$,

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial t^{2}}=K \frac{\partial^{3} T}{\partial x^{2} \partial t}-\frac{\delta t}{2} \frac{\partial^{3} T}{\partial t^{3}}+\frac{\delta x^{2} K}{6} \frac{\partial^{5} T}{\partial x^{4} \partial t} . \tag{9}
\end{equation*}
$$

Substitute Eq. (9) into Eq. (8) and discard high-order terms:

$$
\begin{equation*}
\frac{\partial T}{\partial t}=K \frac{\partial^{2} T}{\partial x^{2}}-\frac{\delta t K}{2} \frac{\partial^{3} T}{\partial x^{2} \partial t}+\frac{\delta x^{2} K}{6} \frac{\partial^{4} T}{\partial x^{4}} \tag{10}
\end{equation*}
$$

Note that we have lowered the order of time derivative in the error terms by one. Now we can differenlate Eq. (8) with respect to x to obtain

$$
\begin{equation*}
\frac{\partial^{3} T}{\partial x^{2} \partial t}=K \frac{\partial^{4} T}{\partial x^{4}}-\frac{\delta t}{2}-\frac{\partial^{4} T}{\partial x^{2} \partial t^{2}}+\frac{\delta x^{2} K}{6} \frac{\partial^{6} T}{\partial x^{6}} \tag{11}
\end{equation*}
$$

which we substitute into Eq. (10):

$$
\begin{equation*}
\frac{\partial T}{\partial t}=K \frac{\partial^{2} T}{\partial x^{2}}+\frac{K \delta x^{2}}{2}\left(\frac{1}{3}-\frac{K \delta t}{\delta x^{2}}\right) \frac{\partial^{4} T}{\partial x^{4}} \tag{12}
\end{equation*}
$$

It is obvious from this trivial example that the elimination of time derivatives from the truncation error terms of the modifed equation is, in general, a very messy algebraic problem for the general case of coupled nonlinear partial differential equations. The code and flow charts listed in Appendixes $C$ and D describe a first attempt to solve this problem. Although this program is capable of handling very large problems in a reasonable amount of central processor time, a clever programmer should be able to improve its efficiency. For this and other reasons to be discussed later, this code should be considered a useable but unpolished tool. The elimination code reads its input from cards punched either by itself or the expansion code. The elimination code only makes a single pass at elim-
inating the time derivatives, lowering the order of the time derivatives by at most one per run. Thus, our simple example would require two runs. The first run would read cards punched by the expansion code, and the next run (and all subsequent runs if necessary) would read the cards punched by the expansion code on the previous run. This multiple run procedure is inefficient in terms of the human intervention and turn around time involved, and we intend to eventually combine the expansion and elimination codes into a single completely automated code.

The elimination code can also handle simple systems of equations. It can read a second modified equation and substitute derivatives of the first, or primary, modified equation into the second, or secondary, modified equation. Our limited experience with systems of modified equations suggests that improving the efficiency of workspace utilization should receive high priority in the list of improvements to this code. The memory problem is not serious with the LCM version of ALTRAN available on the CROS operating system, where 131000 decimal words of workspace are available, but it is likely to be quite limiting at installations with smaller workspaces. Some steps for reducing memory requirements and the number of runs are described in Appendix C.

## III. APPLICATIONS

Truncation error expansions may be employed in three ways. First, they indicate the order and accuracy of FDE's, and so they may be used to help choose the best form for a particular problem. Second, they may be used to find stability conditions for some problems. And finally, they may be employed as the basis of a new method for stabilizing some finite difference algorithms. In this section we discuss examples of each of these applications. We emphasize that although most of our examples are relatively simple and could be done by hand, the ALTRAN programs are powerful tools that can do and have done expansions much too large and complicated to do reliably by hand in a reasonable amount of time.
a. Comparison of Errors of Difference Equations

The TEE's easily indicate some undesirable properties of FDE's, such as zeroth-or negative-
order errors. Such information is quite useful, for it may rule out use of a particular FDE before it is coded and subjected to numerical tests. But beyond such simple observations, FDE's are not easily compared. The next example illustrates the type of analysis frequently necessary to determine which one of several FDE's is more accurate. Consider the onedimensional diffusion problem in spherical coordinates

$$
\frac{\partial T}{\partial t}=\phi \frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial T}{\partial r}\right) \text { for } 0 \leqslant t \leqslant \infty, 0 \leqslant r \leqslant \pi
$$

$$
\begin{equation*}
T(r, 0)=\frac{\sin r}{r}, \tag{13}
\end{equation*}
$$

$$
T(\pi, t)=0,
$$

and

$$
\frac{\partial T}{\partial t}(0, t)=0
$$

where $\phi$ is a constant. The analytic solution is

$$
\begin{equation*}
T(r, t)=\exp (-\phi t) \sin (r) / r \tag{14}
\end{equation*}
$$

Now consider the explicit FDE

$$
\begin{align*}
\frac{T_{1}^{n+1}-T_{i}^{n}}{\delta t} & =\frac{\phi}{V_{i}}\left[\frac{r_{i+\frac{1}{2}}^{2}\left(T_{i+1}^{n}-T_{i}^{n}\right)}{r_{i+1}-r_{1}}\right. \\
& \left.-\frac{r_{i-\frac{3}{2}}^{2}\left(T_{i}^{n}-T_{i-1}^{n}\right)}{r_{i}-r_{i-1}}\right] \tag{15}
\end{align*}
$$

The computing mesh is illustrated in Fig. 1. We compare the accuracy of two different definitions of $V_{i}$ in Eq. (15):

$$
\begin{equation*}
v_{i}=\left(r_{i+\frac{1}{2}}^{3}-r_{i-\frac{1}{2}}^{3}\right) / 3 \tag{16a}
\end{equation*}
$$

and

$$
\begin{equation*}
v_{i}=r_{i}^{2}\left(r_{i+\frac{1}{2}}-r_{i-\frac{1}{2}}\right) \tag{16b}
\end{equation*}
$$

Note that the cells are spherical shells, and $V_{i}$ is the volume of one steradian of the ith cell.

Heuristically we expect Eq. (16a) to be more
accurate than Eq. (16b) near the origin, because the former volume elements exactly fill space. The latter volume elements are all smaller than the former for the same set of mesh points, and the effect is most pronounced at small $r$. Both volume elements give conservative $F D E^{\prime} s$, but they conserve different amounts of the conserved quantity. For constant $T$, volume elements in Eq. (16a) lead to conservation of the correct amount of the conserved quantity
$4 \pi \int_{0}^{\pi / 2} \mathrm{Tr}^{2} \mathrm{dr}$, but Eq. (16b) conserves the wrong amount.

We can use the expansions to determine which volume element is more accurate. The TEE's for Eq. (15) with Eqs. (16a) and (16b), respectively, are equivalent to

$$
\begin{align*}
\frac{\partial T}{\partial t} & =\phi \frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial T}{\partial r}\right) \\
& -\left[\frac{\phi^{2} \delta t}{2}-\frac{\phi \delta r^{2}}{12}\right]\left[\frac{\partial^{4} T}{\partial r^{4}}+\frac{4}{r} \frac{\partial^{3} T}{\partial r^{3}}\right]  \tag{17a}\\
& +\frac{\phi \delta r^{2}}{6 r^{2}}\left[\frac{\partial^{2} T}{\partial r^{2}}-\frac{1}{r} \frac{\partial T}{\partial r}\right]+O\left(\delta t^{2}, \delta r^{4}\right)
\end{align*}
$$

and

$$
\begin{align*}
\frac{\partial T}{\partial t} & =\phi \frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial T}{\partial r}\right)-\left[\frac{\phi^{2} \delta t}{2}-\frac{\phi \delta r^{2}}{12}\right]\left[\frac{\partial^{4} T}{\partial r^{4}}\right. \\
& \left.+\frac{4}{r} \frac{\partial^{3} T}{\partial r^{3}}\right]+\frac{\phi \delta r^{2}}{4 r^{2}} \frac{\partial^{2} T}{\partial r^{2}}+O\left(\delta t^{2}, \delta r^{4}\right) \tag{17b}
\end{align*}
$$

for a uniform mesh.
At first glance, Eq. (17b) appears better than Eq. (17a) because the coefficient of $\frac{\partial T}{\partial r}$ in Eq. (17a) is proportional to $1 / r^{3}$. Furthermore, unlike Eq. (16a), Eq. (16b) leads to a difference scheme which is exact for a solution $T$, linear in $r$. Thus, our earlier arguments about volume elements in Eq. (16a) being better appear to be wrong. However, as we shall show, our superficial examination of Eqs. (17a) and (17b) is at fault.

Currently, there is no general procedure for
choosing the more accurate of several FDE's, based on Taylor series expansions. But we now present a procedure which works many problems, and we hope it will provide a basis for an even more general procedure. The cursory examination above is misleading, because $\frac{\partial T}{\partial r}=0$ at the origin and because some error terms partially cancel each other. We expand $T$ in Taylor series about $r=0$ for some $\eta, 0<\eta<r_{5 / 2}$, and a time $\tau, t_{n}<\tau<t_{n+1}$ :

$$
\begin{equation*}
T(\eta, \tau)=\sum_{i=0}^{\infty} \frac{\partial^{(i)} T(0, \tau)}{\partial r^{(i)}} \frac{n^{i}}{i!} . \tag{18}
\end{equation*}
$$

After differentiating Eq. (18) and substituting into the space errors of Eqs. (17a) and (17b), we find

$$
\begin{align*}
\frac{\phi \delta r^{2}}{12}\left[\frac{\partial^{4} T}{\partial r^{4}}\right. & \left.+\frac{4}{r} \frac{\partial^{3} T}{\partial r^{3}}+\frac{2}{r^{2}} \frac{\partial^{2} T}{\partial r^{2}}-\frac{2}{r^{3}} \frac{\partial T}{\partial r}\right]_{r=\eta, t=\tau} \\
& =\frac{\phi \delta r^{2}}{12}\left[-\frac{2}{n^{3}} \frac{\partial T(0, \tau)}{\partial r}+\frac{5}{\eta} \frac{\partial^{3} T(0, \tau)}{\partial r^{3}}\right. \\
& \left.+0\left(n^{0}\right)\right] \tag{19a}
\end{align*}
$$

and

$$
\begin{align*}
\frac{\phi \delta r^{2}}{12}\left[\frac{\partial^{4} T}{\partial r^{4}}\right. & \left.+\frac{4}{r} \frac{\partial^{3} T}{\partial r^{3}}+\frac{3}{r^{2}} \frac{\partial^{2} T}{\partial r^{2}}\right]_{r=\eta} \\
& =\frac{\phi \delta r^{2}}{12}\left[\frac{3}{2 n^{2}} \frac{\partial^{2} r(0, \tau)}{\partial r^{2}}+\frac{7}{\eta} \frac{\partial^{3} T(0, \tau)}{\partial r^{3}}\right. \\
& \left.+0\left(n^{0}\right)\right] \tag{19b}
\end{align*}
$$

Because $\frac{\partial T(0, \tau)}{\partial r}=0$ for most physical problems, the $1 / \eta^{2}$ error in Eq. (19b) dominates all others in Eqs. (19), and so Eq. (16a) actually leads to errors smaller than Eq. (16b) near the origin.

The boundary conditions are imposed by

$$
\begin{equation*}
\mathrm{r}_{1}^{\mathrm{n}+1}=\mathrm{T}_{2}^{\mathrm{n}+1} \tag{20}
\end{equation*}
$$

and either

$$
\begin{equation*}
T_{N+1}=-T_{N}+2 T_{b} \tag{21a}
\end{equation*}
$$

or

$$
\begin{equation*}
T_{N+1}=-2 T_{N}+\frac{1}{3} T_{N-1}+\frac{8}{3} T_{b}, \tag{21b}
\end{equation*}
$$

where $T_{b}=0$ is the boundary value. For boundary conditions in Eqs. (21a) and (21b), respectively, th right side of Eq. (15) is equivalent to

$$
\begin{equation*}
\phi\left\{\frac{3}{4} \frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial T}{\partial r}\right)-\frac{\delta r}{8}\left[\frac{\partial^{3} T}{\partial r^{3}}+\frac{2}{r} \frac{\partial^{2} T}{\partial r^{2}}\right]+O\left(\delta r^{2}\right)\right\} \tag{22a}
\end{equation*}
$$

and

$$
\begin{equation*}
\phi\left\{\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial T}{\partial r}\right)-\frac{\delta r}{6} \frac{\partial^{3} T}{\partial r^{3}}+O\left(\delta r^{2}\right)\right\} \tag{22b}
\end{equation*}
$$

Each equation is valid for both volume elements in (16a) and (16b). Note that the simpler Eq. (21a) ha a large zeroth-order in the diffusion term. Theref we expect the first-order boundary conditions in Eq (21b) to be more accurate in the outer part of the mesh where the boundary treatment dominates the accuracy of the solution.

In order to substantiate our deductions based on TEE's, we numerically solved Eq. (15) using several combinations of Eqs. (16) and (21). Figure 2 shows the relative errors as a function of $r$ at tim $t=0.23687$ for several of these calculations. We see that the best accuracy obtains from volume element in Eq. (1 $\dot{6} a$ ) and boundary condition in Eq. (2 as predicted.

## b. Truncation Error Cancellation Algorithms

The second application of TEE's is important 1 the field of numerical fluid dynamics. A number of instabilities that arise in such calculations are due to diffusional truncation errors with negative diffusion coefficients. An obvious application of TEE's is to find stability conditions for numerical algorithms that are subject to diffusion instabilities. On a higher level, these expansions can be used as the basis of new method for stabilizing the FDE's as reported by Rivard et $a l^{2}$. Both of these uses are illustrated with a one-dimensional


Fig. 2. Relative truncation errors vs. radius at a fixed time for five solutions to Eq. (15). Curves 1,3 and 5 use volume elements (16a), and curves 2 and 4 use volume elements (16b). Curve 1 used boundary condition (21a). All others use boundary condition (21b). Curves 1,2 , and 3 were computed using 10 cells, and curves 4 and 5 were computed with 20 cells.
version of the ICE method ${ }^{3}$ that requires much less artificial diffusion to obtain stability than many other methods. Again, we emphasize that our simple example is chosen for clarity of presentation, and the programs are useful for much more complicated FDE's.

We describe the truncation error cancellation (TEC) technique in detail only for the continuity equation (1), but the same procedure is applied to the momentum and energy equations, as well. It is possible, however, to improve the algorithm by applying the procedure only to one or two of the equations. We use the FDE given by Eq. (2). The truncation error expansion is given in Eq. (4), but the time derivatives must be converted to space derivatives by using the continuity and momentum modified equations. We obtain for the diffusional errors

$$
\begin{equation*}
\zeta \frac{\partial^{2} \rho}{\partial x^{2}}=\left[(2 \theta-1) \frac{\delta t}{2}\left(u^{2}+c^{2}\right)-\frac{\delta x^{2}}{4} \frac{\partial u}{\partial x}\right] \frac{\partial^{2} \rho}{\partial x^{2}} \tag{23}
\end{equation*}
$$

where $\zeta$ is the diffusion coefficient of the truncation errors and $c$ is the local sound speed. We have neglected the $\partial^{2} \xi / \partial x^{2}$ term in Eq. (4); as we shall see, it is a higher order term in the TEC algorithm. If $\xi=0$ in Eq. (1), the FDE is unstable whenever $\zeta<0$. In the original version of ICE, a constant global artificial mass diffusion coefficient $\xi \geqslant 0$ is used to stabilize the algorithm. It is necessary to choose $\xi$ large enough that $\xi+\zeta \geqslant 0$ for all cells at every time step, and so a large amount of global diffusion is needed to stabilize many problems. Because the diffusion term is explicit, a necessary condition for stability is

$$
\begin{equation*}
\xi \delta t<\frac{1}{2} \delta x^{2} \tag{24}
\end{equation*}
$$

Artificial viscosity plays a similar role in the momentum equation and imposes a separate requirement analogous to Eq. (24). Although these artificial diffusion parameters stabilize the algorithm, they decrease the accuracy of the solution and introduce time step limits that can be so small as to preclude the solution of some problems.

The basic idea of the TEC algorithm is to replace the artificial diffusion parameter with a variable $\xi(x, t)$ which is chosen so that it locally cancels the destabilizing effects of diffusion truncation errors. Consequently, much less diffusion is needed for stability (often several orders of magnitude less in parts of the mesh), and so accuracy is improved and diffusional time step limits are relaxed.

The first step in deriving a TEC scheme is to evaluate algebraically the diffusion coefficient $\zeta$. Expansion yields a result of the form

$$
\begin{align*}
\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x} & =\frac{\partial}{\partial x}\left(\xi \frac{\partial \rho}{\partial x}\right)+\zeta \frac{\partial^{2} \rho}{\partial x^{2}}=\frac{\partial \rho}{\partial x}\left(\xi \frac{\partial \rho}{\partial x}\right) \\
& +\frac{\partial}{\partial x}\left(\zeta \frac{\partial \rho}{\partial x}\right)-\frac{\partial \zeta}{\partial x} \frac{\partial \rho}{\partial x} \tag{25}
\end{align*}
$$

The algorithm for carrying out the expansion gives the nonconservative form $\zeta \frac{\partial^{2} \rho}{\partial x^{2}}$, but we convert it to the conservation form in $\mathrm{x}^{2}$ the right-hand side of Eq. (25). In some cases, usually in the momemtum equation, $\frac{\partial \zeta}{\partial x}$ will contribute additional diffusional
errors that should be included in TEC as discussed by Rivard et al. In our continuity equation, however, $\frac{\partial \zeta}{\partial x}$ does not produce additional diffusional errors, and the $\frac{\partial \zeta}{\partial x} \frac{\partial \rho}{\partial x}$ truncation error is neglected. In order to obtain an improved $F D E$, Eq. (23) is differenced to yield

$$
\begin{align*}
& \zeta_{i-\frac{k_{2}}{}}=(2 \theta-1) \frac{\delta t}{2}\left[\left(u_{i-\frac{3}{2}}^{n}\right)^{2}+\frac{1}{2}\left(c^{2}+c_{i-1}^{2}\right)\right] \\
& -\frac{\delta x}{8}\left(u_{i+\frac{1}{2}}^{n}-u_{i-3 / 2}^{n}\right) . \tag{26}
\end{align*}
$$

Next we choose

$$
\xi_{i-\frac{1}{2}}^{n}=\left\{\begin{array}{l}
-(1+\beta) \zeta_{i-\frac{3}{2}} \text { if } \zeta_{i-\frac{3}{2}}<0 \\
-(1-\beta) \zeta_{i-\frac{1}{2}} \text { if } \zeta_{i-\frac{1}{2}} \geqslant 0
\end{array}\right.
$$

which is then incorporated in the finite difference form of Eq. (1). The constant $\beta, 0 \leqslant \beta \leqslant 1$, is a free parameter that determines the degree to which the diffusional truncation errors are cancelled. If $\beta$ is too small, the FDE's will have so little diffusion that dispersively generated ripples destroy accuracy. If, on the other hand, $\beta$ is too large, unnecessary artifical diffusion reduces the accuracy of the solution. The optimum value of $\beta$ is problem dependent and must be found by trial and error. In practice, $\beta=1$ is frequentiy an adequate value.

Although the derivation of the diffusion errors for the TEC scheme requires extra work, the modified FDE's yield substantially better solutions. TEC has been installed in several programs, and the scheme works well except in problems with very strong shocks where higher order errors are significant. We now briefly compare several TEC and non-TEC solutions in order to show the advantage that may be expected from using TEC.

Consider Fig. 3, which shows the run of density for three one-dimensional shock tube calculations, as well as the analytic solution. The initial condition is a $5: 1$ pressure and density jump at cell 90. All solutions coincide at the left and right bound-
aries; the solutions have been displaced vertically for clarity. The bottom curve is the analytic solution. The top solution is an artificial viscosity solution with nearly the minimum diffusion needed for stability. The right density jump is a shock wave, and the left discontinuity is a contact surface. Both discontinuities move to the right. The shock is smooth, but the contact surface has dispersively driven ripples behind it. TEC. with the same viscosity $\mu$ as the conventional method, was used in the second solution from the top. The shock is unchanged, but the ripples behind the contact surface are stronly damped. The third numerical solution is also TEC run, but the viscosity is reduced by a factor of ten. The shock is significant sharper, but it shows a little overshoot. The first peak behind the contact surface is as high as in the artificial viscosity run, but the damping behind the contact is much stronger. The artificial viscosity scheme is unstable with this little viscosity.

The TEC algorithm readily generalizes to multidimensional flows. As an example, consider a Mach 0.1 wind blowing over a pair of walls as shown in Fig. 4. Shown there are the velocity vectors and isotherms of a TEC solution obtained from the twodimensional RICE program. ${ }^{7}$ The comparison solution with normal artificial viscosity stabilization was obtained with 100 times as much viscosity, because


Fig. 3. One dimensional shock tube calculations. All four solutions coincide at the left and right ends, but the three numerical solutions have been displaced vertically for clarity.
the conventional method was unstable with less viscosity. The two velocity solutions are similar, although the TEC solution shows more shear in the vortex, and the weak Helmholtz instability in the upper right quadrant is somewhat stronger, an indication that viscous forces are relatively small in this problem. The isotherms, however, are much different. The TEC solution shows steeper gradients across the vortex, because there is less diffusion and less viscous heating in the energy equation.

Experience indicates that TEC is quite general in its range of applicability and that it provides significant improvement in the accuracy of numerical fluid dynamics calculations. The use of ALTRAN to compute the TEE's is proving to be extremely helpful.

## IV. SUMMARY

We have shown that the Taylor series expansions needed for Hirt's heuristic stability analysis can be easily generated by a program written in a comput-

Specific Internal Energy


Artificial Viscosity


Truncation Error Cancellation
Velocity Vectors


Artificial Viscosity


Truncation Error Concellotion

Fig. 4. A two-dimensional flow with and without TEC. The TEC run has $1 \%$ as much viscosity as the artificial viscosity run. A Mach 0.1 wind enters the mesh across the upper half of the left boundary, and it leaves across the upper half of the right boundary.
er algebraic language such as ALTRAN. The truncation error expansions have proved quite useful in choosing optimum finite difference equations, in deriving some necessary conditions for stability, and assisting in the design of truncation error cancellation algorithms. The ability to derive the truncation errors automatically is essential for all but the simplest difference equations. The extension of these codes to include more dimensions is straightforward, and present computers are adequate to handle many problems of interest. We expect the use of such algebraic computations to increase and become a much more important part of numerical analysis as algebraic systems become more common on large computers and as potential users become familiar with the language and come to appreciate the potential of algebraic systems for accurately and quickly solving massive problems.

## REFERENCES

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## APPENDIX A

## THE EXPANSION CODE LISTING

This appendix gives instructions for running the code that computes the Taylor series expansions, a listing of the code, and a sample problem. This particular problem was run on a CDC 7600 under the CROS operating system using the LCM version of ALTRAN.

Lines 19 through 27 provide the input for this run. RORD and TORD are the maximum orders of the expansions in $\delta r$ (denoted by $D R$ ) and $\delta t$ (denoted by DT), respectively. This run expands the difference equation (2) for the differential equation (1) using the subscript notation for derivatives and the expansion PROCEDURE TE described in the text. DERMOD is the time derivative we want to eliminate using the second code, and it is not limited to a first derivative in time. For example, $\operatorname{DERMOD}=\mathrm{RHO}(1,2)$ would be appropriate for $\rho_{x t t}=A \rho+B \rho_{x x}$. DE is the differential equation, where we have represented $\xi$ by $T$ in this run. Note that we have shifted the term on the right-hand side of equation (1) over to the lefthand side so $\mathrm{DE}=0$. This must always be done for both $D E$ and the finite difference equation $F D E$. In FDE we have represented $\theta$ by Gl. Note that we have not followed our own advice in the text concerning the efficient use of TE. This problem is small enough to easily run on the LASL LCM version of ALTRAN, but we would have to be more careful with memory utilization with the SCM version or with larger problems. It may be necessary to break large problems into pieces and run them separately. For example, the diffusion term could be deleted from DE and FDE and then computed by itself on a second run.

Most of the output is intermediate results that are sometimes useful if the run terminates abnormally. The final results are printed after the message "CONSTRUCT THE MODIFIED EQUATIONS." The modified equation is given by DERMOD $=$ NUMER/DENOM, and the output beginning with RORD is punched from logical unit 25 by the computer as input for the time derivative elimination code.

In lines 38 and 39, the code checks for the possible existence of errors of order $\delta_{r}^{-1}$ and/or $\delta t^{-1}$ and prints a warning message if appropriate. Some difference equations, such as equations (15) and (16a), will trigger a fictitious warning. However, the truncated power series package cannot han-
dle an error of negative order, and the code will terminate abnormally after the warning message is printed. One example is the Lax method for the diffusion equation:

$$
\begin{align*}
D E & =\frac{\partial T}{\partial t}-D \frac{\partial^{2} T}{\partial X^{2}} \\
& =T(0,1)-D I F * T(2,0) \tag{Al}
\end{align*}
$$

and

$$
\begin{aligned}
\operatorname{FDE} & =\left[T_{i}^{n+1}-\left(T_{i+1}^{n}+T_{i-1}^{n}\right) / 2\right] / \delta t \\
& -D\left[T_{i+1}^{n}-2 T_{i}^{n}+T_{i-1}^{n}\right] / \delta X^{2} \quad(A 2) \\
& =(T E(T, 0,1)-(T E(T, 1,0)+T E(T,-1,0)) / 2) / D T \\
& -D I F *(T E(T, 1,0)-2 * T(0,0)+T E(T,-1,0)) / D R * * 2
\end{aligned}
$$

Lines 33 and 34 contain a possible trap for the unwary user. The use of relations such as $R P=R+D R / 2$ for equations such as Eq. (16a) can simplify the input phase. The user may find other useful substitutions, and these were left in the code as examples of substitutions that we found useful in our test runs. These statements must be removed or replaced before RM and RP can be used for another purpose. 'A similar situation exists for line 55, where F1 and F2 are used as ratios of widths of adjacent cells for cases where $\delta r$ is not constant. That is, FDE may be a (at most) four-point difference scheme over three cells of widths $\mathrm{DR}, \mathrm{F} 1 * \mathrm{DR}$, and $\mathrm{F} 2 * \mathrm{DR}$, with the order being chosen by the user.

```
    PROCEDURE MAIN * TRUNCATION ERRDRS OF DIFFERENCE ERUATIONS.
    EXTERNAL INTEGER ORD=6
    INTEGFR M=31. N=CRN
    INTEGER RORD, TOFD
```



```
        PHI:IM, THETA:M, RP:M, RM:M, GI:M, GZ:M, DIF:M, LAM:M, FI:M, FZ:M,
        TIM&M, |(Q&N, ब;N):XP(N), RHO(Q&N,N:N):XP(N)) ARRAY DETPS, FDFIPS,
        TFR, CONTPS
EXTFRNAI ALGFBRAIC ONR=OR, OHT=DT, LAMZ=LAM
LONG ALGERRAIC FOF, DE, NFRMOD, NUMFR, OENOM
LONG ALGERRAIC ARRAY MODEQ
ALTRAN INTEGER TOSORD
ALTRAN SHORT INTFGER ARRAY XP
ALTRAN ALTEERAIC TE, TPSEVL
ALTRAN ALGERRAIC ARRAY TPS, TPSMUL, TPSSBS, ARRSRS, TETPS, TPSCHOP
```



```
    RORN = 2 TORD = 1
    OERMDD = RHO(A.1)
```



```
        T(1, 日)*RHD(1,㣙
    FNE = (TE(RHO,Q,1)-RHO(㫙暗) / OT + GI*((TE(RMO,1,1) & TE(RHO,A,1)) *
        TE(U,1/2,1) - TE(RHO,&,1) +TE(RMO,-1,1)) * TF(IJ,*1/?,1)) / (Z*NQ) &
        (I-F,1) ((TF(RHO,1,Q) + RHO(Q,a)) * TE(1,,1/2,Q) - (TE(RHO,-1,0) - 
```




```
    WRITE DERMDD, DE, FDF, "END OHASF ONE"
* - - - - . - - 
    FDE = FDE (RP, RM = R* NR/Z, R-DR/?)
    DF = DE (RP, RM = R+DR/Z, R=DR/2)
    FDF=F\capE (DR, OT = LAM*OR,LAM*DT)
    * CHECK FOR TRIJNCATION ERRDRS OF NEGATIVF OROER
    NUMER = ANUM (FDF, OFNOM)
    IF (DEG(NENOM,LAM).GT.(I) WRITF FIF,"MMAY ABORT DJIE TO NEGATIVE DROER ERROR"
    NUMER = O: DENOM = !
* CONVERT DE ANO FDF TO TRUNCATFD POWER SFRIES
    DETPS = TDS ( DEPDR,DT = DR*LAM,DT*LAM), LAM, ORD)
    FDETPS = TPS (FDE, LAM, DRD)
    FDE = D
    WRITE DETPS, FOETPS
# REGIN REDUCTION OF ERRORS
```



| IMAX/S9IMAX | PROC | INT |  | L | S | $x$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| LAM2 | VAR | ALG |  |  | S | $x$ |
| MAIN | PROC |  |  | L. | 5 | K |
| MODEQ | VAR | ALG | A | L |  |  |
| M | VAR | INT |  |  |  |  |
| NIIMER | VAR | ALG |  | 1 |  |  |
| N | VAR | INT |  |  |  |  |
| ORD | VAR | INT |  |  | S | $x$ |
| RORD | VAR | INT |  |  |  |  |
| TETPS | PROC | ALS, | A | L | S | $x$ |
| TE | PROC | ALG |  | L | S | X |
| TORD | VAR | INT |  |  |  |  |
| TPSCHOP | PRDC. | ALG | A | $L$ | S | $x$ |
| TPSEVL | PROC | ALr, |  | L | S | $x$ |
| TPSMUL | PRDC | ALG | A | $L$ | S | $x$ |
| TPSORD | PROC. | INT |  | $L$ | S | X |
| TPSSRS | PROC | ALG | A | L | S | $x$ |
| TPS | PROC | AIS, | A | L | S | X |
| XP | PROC | INT | A |  | S | $x$ |
| L*の日 1 | LAY |  |  |  |  |  |
| CONSTRUCT THE MODIFI | CDNS | CHAR |  |  | S |  |
| FNO PHASE DNE | CONS | CHAP |  |  | S |  |
| INSORRECT OERMOD | CONS | CHAP |  |  | S |  |
| MAY ARORT DUE TI NFG | CONS | CHAR |  |  | S |  |
| TER WITH ALL TIME DE | CONS | CHAD |  |  | 5 |  |
| 9 | CONS | INT |  |  | S |  |
| 1 | CONS | INT |  |  | S |  |
| 25 | CONS | INT |  |  | S |  |
| 2 | C.ONS | INT |  |  | S |  |
| 31 | CONS | INT |  |  | S |  |
| 6 | CONS | INT |  |  | S |  |

ALTRAN VERSION 1 LEVEL 9

PROCEDURE TE ( $A, A X, A T, B, B X, R T, C, C X, C T, O, D X, D T)$
\# 2=0 TAYLOR SERIES FXPANSION OF THE PRODUCT $A * B * C * D$
VALUE $A, A X, A T, R, R X, R T, C, C X, C T, D, D X, D T$
LONG ALGERRAIC ARRAY A,B,C,D
LONG, ALGEBRAIC AX,AT, BX,RT, CX,CT, DX,DT
ALTRAN ALGEBRAIC ARRAY TETPS
ALTRAN ALGEARAIC. TPSFVL
RETURN ( TPSEVL(TFTPS(A,AX,AT, B,BX,BT, C,CX,CT, D,OX,DT), 1) )
END

| AT | VAR | ALG |  | L |  | $V$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AX | VAR | ALG, |  | $L$ |  | $v$ |
| $\Delta$ | VAR | Al C | A | $L$ |  | $v$ |
| AT | VAR | A G |  | L |  | $v$ |
| HX | VAP | $A L G$ |  | L |  | $v$ |
| H | VAR | $A L G$ | A | 1 |  | $v$ |
| CT | VAR | ALG |  | L |  | $v$ |
| CX | VAR | ALG |  | L |  | $v$ |
| C | VAR | ALG | A | L |  | $v$ |
| OT | VAR | ALG |  | L |  | $V$ |
| $0 \times$ | VAR | ALG |  | 1. |  | $v$ |
| D | VAR | ALG | A | L |  | $v$ |
| TETPS | PRDC | ALG | A | L | S | $x$ |
| TE | PROC |  |  | $L$ | S | $x$ |
| TPSEVL | PROC | ALG |  | L | S | $x$ |
| 1 | CONS | INT |  |  | S |  |

ALTRAN VERSION 1 LEVEL 9

```
    PROGEDURE TETPS (A,A\ddot{X,AT, A,RX,BT, C,CX,CT, O,DX,OT)}
```

* 2-0 TPS TAYLOR SERIES OF THE FRQDIJCT $A * B * C * D$
VALIJE $A, A X, A T, G, B X, R T, C, C X, C T, D, D X, \cap T$
LONG ALGERRAIC ARRAY $A, H, C, D$
LONG ALGFRRRAIC AX,AT, BX,RT, CX,CT, ПX, OT
ALTRAN ALGERRAIC ARRAY TETPS, TAYLDR,TPSMUL
IF (NULL(A)) RETURN (TAYLDR(A,AX,AT))
PETIJRN (TPSMUL(TAYLDR(A,AX,AT), TETPS(R,BX,BT, C,CX,CT, D,DX,DT)) )
END
NAMF/FXTNAME IJSE TYPF STRIIC PRFC CLASS SCOPE OB LAY AONR

| AT | VAR | ALT, |  | $L$ | $V$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\Delta X$ | VAR | ALG |  | $L$ | $V$ |
| $A$ | VAR | ALG | A | L | $V$ |
| ET | VAR | ALS, |  | L | $V$ |
| $\mathrm{HX}^{\text {P }}$ | VAR | ALG |  | L | $V$ |
| R | VAR | ALG | A | L | $V$ |
| CT | VAR | ALG |  | 1 | $V$ |
| CX | VAR | ALS, |  | $L$ | $v$ |
| C | VAR | ALG | A | $L$ | $v$ |
| DT | VAR | ALG |  | $L$ | V |
| $13 x$ | VAR | ALG |  | L. | $V$ |


| VAR | ALG | $A$ | $L$ |  | $V$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| PROC | LOG |  |  | $S$ | $x$ |
| PROC | ALG | $A$ | $L$ | $S$ | $x$ |
| PROC | ALG | $A$ | $L$ | $S$ | $x$ |
| OROC ALG | $A$ | $L$ | $S$ | $X$ |  |

ALTRAN VERSION 1 LEVEL 9

PROCEDURE TAYLIAP（F，$A, B$ ）
＊200 TPS TAYLOR SERTES OF THE VARIARLE F
VALUE F，A，B
EXTERNAL ALGERNATC DDR，DDT
EXTFRNAL INTEGEK NRD
INTEGEQ I．J
LONG ALGERRATC A，H
ONG ALGERRAIC ARRAY
LONO ALFERRAIC ARRAY（の\＆ORD）TAY＝（F（Q，日），ORDS日）


IF（A．EA．A）DO \＃OIFFW．R．T．T
IF（B＇EQ，（a）PETURN（TAY）
DO $I=1$ ，ORO
TAY（I）$=($（ $* \cap \cap T) * * I * F($ Q，I）／FACT（I）
OREND
RETURN（TAY）
DOENO

```
IF (B.EQ.Q) DO DIFFW.R.T.R
    DN I=I,ORN
        TAY(I) = (A*ODF)**I*F(I, A)/FACT(I)
    DNEND
```

    RFTIIRN (TAY)
    OOEND
OD $I=1, O R D$ \# DIFF W.R.T. R AND T
D $J=1,1,=1$ : $\operatorname{COF}(J)=C O F(J)+C O F(. J-1):$ DOEND
$20 \mathrm{~J}=0$ •I
TAY(T) $=\operatorname{TAY}(I)+\operatorname{COF}(J) *(A * D D R) * * J *(B * D D T) * *(I-J) * F(J, I-J)$
DEND
TAY(I) $=$ TAY(I)/FACT(I)
DOEND
RF.TURN (TAY)

```
& NAME/EXTNAME IISE TYPF STRUC PREC CLASS SCOPE DG
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline TAY & VAR & \(A L G\) & A & \(L\) & & & D＊日a， \\
\hline FACT & VAR & INT & A & & & &  \\
\hline C．OF & VAR & INT & A & & & & D＊かの3 \\
\hline A & VAR & ALG & & 1 & & V & \\
\hline A & VAR & ALG & & L & & \(v\) & \\
\hline DOR & VAR & ALF， & & & S & \(x\) & \\
\hline DDT & VAR & ALG & & & 5 & \(x\) & \\
\hline \(F\) & VAR & ALG & A & \(L\) & & \(v\) & \\
\hline I & VAR & INT & & & & & \\
\hline \(J\) & VAR & INT & & & & & \\
\hline ORD & VAR & INT & & & S & \(x\) & \\
\hline TAYLDR & DRDC & & & L & S & \(x\) & \\
\hline D＊ の日 \(11^{\text {a }}\) & 08 & & & & & & \\
\hline D＊の日て & DR & & & & & & \\
\hline D＊の日3 & DR & & & & & & \\
\hline \(\square\) & CONS & INT & & & S & & \\
\hline 10 & CONS & INT & & & 5 & & \\
\hline 129 & CONS & INT & & & S & & \\
\hline 1 & CONS & INT & & & 5 & & \\
\hline 24 & CONS & INT & & & S & & \\
\hline 2 & CONS & INT & & & S & & \\
\hline 36？88बの & CONS & INT & & & 5 & & \\
\hline 362889 & CONS & INT & & & S & & \\
\hline 4の32a & CONS & INT & & & S & & \\
\hline 5の4の & CONS & IHT & & & 5 & & \\
\hline 6 & CONS & INT & & & S & & \\
\hline 729 & CONS & INT & & & S & & \\
\hline
\end{tabular}
ALTRAN VERSION 1 LEVFI \(O\)
QROREDIJRE TPSCHOP（A，RORD，TOPD）
＊CHOP THE POD TPS TO GROFP RORO IN DR AND TO DRTER TOQD IN DT
VALIIF A，ROPD，TORO
FXTFRNAL ALGFFRRAIC DDR，OOT，LAMZ
LONG ALGFRRAIC APRAY A
INTEGER I，RDRN，THRD，ORD＝TOSORN（A）
ALTRAN ALGFRRAJC ARRAY TPS
ALTRAN ALFEFRAIC TPSEVI
ALTRAN SHORT INTFGER TPSNRD
ロク \(T=\) の，กRロ
\(A(I)=T P S E V L(T P S(A(I), \cap D R, R O R D), O D R)\)
\(A(I)=T P S F V L(T P S(A(I), D \cap T, T D R D), D D T)\)
DDEAD
RETIRN（A）
END
```

| A | VAR | ALG | A | L |  | $v$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| DDR | VAK | ALS, |  |  | S | $x$ |
| DOT | VAR | ALG |  |  | 5 | X |
| 1 | VAR | INT |  |  |  |  |
| LAM? | VAR | ALG |  |  | S | x |
| ORD | VAR | INT |  |  |  |  |
| RORO | VAR | INT |  |  |  | V |
| TORD | VAR | INT |  |  |  | $v$ |
| TPSCHOP | PROC |  |  | $L$ | S | $X$ |
| TPSEVL | PRDC | A1.G |  | L | S | $x$ |
| TPSORD | PRDC, | INT |  |  | S | $x$ |
| TPS | PRDC | ALG | A | L | 5 | X |
| $\square$ | CONS | INT |  |  | S |  |

```
ALTRAN VERSION 1 LEVEL O
    PROCEOUPE ARRSRS (A, LHS, RHS)
# SURGTTTUTE THE LIST RHS FOR THE LIST LHS IN THE 100 ARRAY A
    VAl.UE A, LHS, RHS
    LONG AlgERRAIC ARRAY A, LHS, RHS
    INTEGFR ARRAY OR=DRINFO(A)
    INTEGER I
    OO I=OR(1, a),DR(1,1)
    A(I)=A(I)(LHS=RHS)
    DOEND
    RETIJRN (A)
    END
```

NAME/EXTNAMF IJSE TYPF STPUC PREC CLASS SCOPF DB LAY ADOR
ARRSBS
A
DRINFO/S ODBIN
DB
I
LHS
RHS
Q
1

| PROC |  |  | $L$ | $S$ |
| :--- | :--- | :--- | :--- | :--- |
| VAR ALG | A | $L$ |  | X |
| PROC INT | A |  | $S$ | $X$ |
| VAR INT | $A$ |  |  |  |
| VAR INT |  |  |  |  |
| VAR ALG | $A$ | $L$ |  | $V$ |
| VAR ALG | $A$ | $L$ |  | $V$ |
| CONS INT |  |  | $S$ |  |
| CONS INT |  |  | $S$ |  |


| 1 | PROCFDURE XP (N) |  |
| :---: | :---: | :---: |
| 2 | VALIJE N |  |
| 3 | INTFGER I, J, N |  |
| 4 |  |  |
| 5 |  |  |
| 6 | $00 \mathrm{I}=0, \mathrm{~N}$ |  |
| 7 | DO $J=\square, N-1$ |  |
| 8 | $\underset{\text { OOEND }}{\text { EXP }}$ (I,J) $=7$ |  |
| 9 |  |  |
| 10 | DOEND |  |
| 11 |  |  |
| 12 | RETIJRN (EXO) |  |
| 13 |  |  |
| 14 | END |  |


| NAME/EXTNAME | USE | TYPE | STPUC | PREC | CLASS | SCDPF | $D B$ | LAY | ADIR |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EXP | VAR | INT | A |  |  |  | $0 * 091$ |  |  |
| 1 | VAR | TNT |  |  |  |  |  |  |  |
| J | VAR | INT |  |  |  |  |  |  |  |
| $N$ | VAR | INT |  |  |  | $v$ |  |  |  |
| XP | PROC |  |  | L | S | x |  |  |  |
| $0 * A Q 1$ | DA |  |  |  |  |  |  |  |  |
| 0 | CONS | INT |  |  | S |  |  |  |  |
| 1 | CONS | INT |  |  | S |  |  |  |  |
| 7 | CONS | INT |  |  | S |  |  |  |  |

- DERMDD

RhD(0,1)

* DE
- $(T(\theta, \theta) * R H D(2, \theta)+T(1, \theta) * R H D(1, \theta)-U(\theta, \theta) * R K D(1, \theta)-U(1, \theta) * R K D(\theta, \theta)-R K O(\theta, 1))$
( FDE














 576A*DR**







 2160*DR**































































































 $\operatorname{RHD}(0,0)+1658880 日 * R K D(0,1)) / 165888$ 日
* End phase one
* OETPS

0 -
0 -
ค.
O.

0 .

- )
n FOETPS



















 5760.




























* FDETPS
- ( $\mathrm{T}(\theta, \theta) * R H D(2, \theta)+\mathrm{T}(1, \theta) * R H D(1, \theta)-U(\theta, \theta) * R K D(1, \theta)-U(1, \theta) * R H D(\theta, \theta)=R H D(\theta, 1))$.

 $\operatorname{RHD}(2, \theta)=3 * U(2, \theta) * R H O(1, \theta)=U(3, \theta) * R H D(\theta, \theta)) / 24)$
* FDETPS




- CONTPS



RHO (2, 日) - $3 * U(2,0) * R H D(1, \theta)-U(3, \theta) \# R H D(0, \theta)) / 24)$
* ter with all time derivatives
* ter

18. 



RHD $(2,0)=3 * U(2,0)=R H D(1,0)=U(3,0) * R H D(0,0)) / 24)$

* Construct the hodified equation
\# RORD
2
* 10.8

1

* numer


 $2 a * U(\theta, \theta) * R H O(i, \theta)=2 a * U(1, \theta) * R H O(\theta, \theta)$
* DENDM

24
*** NORMAL RETIJRN FROM MATN PPOCEDURE
*** RUN STATISTICS
14. 264 SECONOS ELAPSED
$13197 a$ WORDS IM WORKSPACE
14 OIGITS IN SHORT INTEGERS
28 OIGITS IN LONG INTEGERS

- GARQAGE CDLLECTIONS

94557 WORDS OF WORKSPACE NEVER USED
SES

APPENDIX B
FLOW CHARTS FOR THE TRUNCATION ERROR EXPANSION PROGRAM




## APPENDIX C

## Instructions and listing for tee time derivative blimination program

This appendix describes the current form of the code that eliminates time derivatives from the modified equation. This program is continuing to evolve, and our goal is to eventually combine this code with the expansion code to form a completely automated package that we will describe in a future report. However, this first generation program is useful enough to fustify its inclusion in this report.

Input for this program is punched by either itself or the expansion program. If only one equation is being manipulated, there must be a data card setting SDER to zero. If there is a system of two equations, only the first equation read in (the primary equation) is differentiated. However, both the primary and secondary (the second equation read in) equations have derivatives of DERMOD eliminated. For the secondary equation, SDER. SNUM, and SDEN are the analogs of DERMOD, NUMER, and DENOM for the primary equation. RORD and TORD are the same for both equations

A problem is begun by running the expansion code and using its punched output as input for the elimination code. Each run of the elimination code will reduce the order of time derivatives present by at most one. If a given run does not successfully eliminate all the time derivatives, its punched output is used as input for the next run. The optimum strategy for handling systems of equations has not been worked out.

The listings include the setup statements and results from a sample expansion run, a complete listing and first run of the sample problem, and the results of the second elimination run. The input and results for the expansion run are given below.


```
2A (%)
```



```
\3{
```

- Construct the modified equation
* RDRI

2

* TORO

1

* vumer

- DENDM

12*R**2

The remainder of this appendix is a listing of the time derivative elimination program and the output of the two runs needed to complete this sample problem.

1. SAMPLE PROBLEM FROM THE EXPANSION PROGRAM CODE
```
ALTRAN VFRSION 1 LEVFL 9
```

    PROCEDIIRE MAIN \(\Rightarrow\) PROGRAM TO HEAD MODIFIEO EOHATION AND FLIMINATE T DF.RIVS
    FXTERNAL INTEGER \(N 1=7, N: 2=7\)
    INTFCER M=31. MM \(=7\)
    GONG ALGFRRAIC (DT:M, DR;M, R:M, RP;M, RM;N, GI:M, GZ!M, I.AM;M, FI:M,
    

FXTERNAL LNNG ALTFFRRATC LANELAM, $S=R, ~ T I M=T I$
FXTFRNAL LONG AI.RERRAIC ARFAY RI=RMO, PI=P, $T 1=T, 1 J=1 J$
INTEGER I, I, ROPD, TMPO, IT, IR, ISR, IST, NT
INTEGER ARRAY (G:NZ) ISRM
LONG ALGEGPAIC ARRAY (R;AI, Q\&ND) DERIV
LING ALTGERRAIC ARRAY SIIR
LONG AIGERGAIC ALIRAN TIER, GDER
ALGFRRATC ARFAY ALTRAY TFS
ALGFRRATC ALTRAN TDSEVI
RFAL DFLTA, ETIME

```
#.-.- - - - -
```

    rean porn, totari, Dfrandi, mimpr, lifnom, SOFR
    WRITE "INTTIALTZATION", PORC, TORO, DERMOD, NUMER, OFNOM, SOFK
    SinlM = ø
    SDEN \(=1\)
    TF PSDFR.NE. (A) ON
    RFAD SNIJM, SDEN!
    WRTIE SNIMM, STFN
    NOFNT
    \# SFT IIP THE SIRSTITITTION MATRIX
On $T=$ 日, N1
$I R=I$
กロ $J=0, N 2$
$T T=J$
IF (DȨQMOD,NF,.pHO(I,J)) ro TO A
SIIB $=$ QHO
Gก in 1
A1:CONTINUE

$\sin =$ i
COTO 81
AZ:CONTTMAIF
IF (DFRMOH:NF.F(I,J)) GO ID A3
GUR $=P$
COTOR1
A3:CONTIMUE

$S U R=T$
GO) T $\quad$ B
AL:CONTTANJ
DOE NO
NกE.Nก
WRTTF DFRMOI, "IILFGAL DFRMOO, ARORTING"
C.O TO ST
R1: C.ONTI AIJF
WRTTF TG, TT, SUR
ПП $T=T R, N$
กn J = TT, N己
AERTV(I-IR, J-TT) $=\operatorname{SHR}(I, J)$
DFQTV(T,J) $=a$
$\operatorname{SUR}\left(I-I Q_{0} J=I T\right)=$ SURi(I.J)
SUR(T,J) = a
DOENH
DOENE
$T S R=N 1-T R$
JST $=$ NZ -1
WRITF SUM, nERTV, TSH, IST
OFLTA=TTME(FTINF): WIZITF MFLTA,ETIME
\# - - - - - . - - - -
* calcillatf highest norifr derivatives nefift
IP $=a$
IT $=a$
DO J = $\quad$ O, IST
TSRM(J) =
กП $1=1 S R, a,-1$
NT = IMAX: IMAY, DFG(NUMER, SUB(I, J)) DEG(DENOM, SUA(I,JI)),
IMAX(DEG(SNIJN, S!JR(I•J)) OEG(SNEN: SUB(I•J))),
IF (AT.GT.a) An
TR = T
$I T=J$
TSEM(J) $=1$
GOTO NMO
OTEN
DOENT
NMOICONTINIJF

OEG(SDEN, SUR (n, n)
IF IIR.GT: O, OR. IT.GT.N.OR* NT,GT.OS fO TO QS
WRITE 廿NO TIME DERTVATIVES FOUND THAT CAN HE ELIMINATENゅ
GO TO ST
OS:CONTINIF
ISR $=I^{N}$
IST $=I T$
WRITE MMAXIMJM IFRFR OF NFPTVATJVE TO ff. ROMPUTFR", ISR, TST, ISRM
NELTA=TIME(FTINFI: WRITF. JFLTA,FTIMF.

```
# CRFATF HTGHFR ORDER NERTVATIVFS
    MFRTV(GI,O)=N(INER/ MFNON
    WPTTF DFRIV(O,7)
    * PHIRF TIMF NFRIVATIVE DF GROFR IT
    O\cap IT = x, YST
        TF (TT, T,T,F) On
        NIIMER = AMIJM(OFRTV(A,IT=1), OEHOMM)
        OFRIVPO,TT)= (TOFQ(NHMER)*OFNOM - TOFP(OENON)*N!JMED) / OFNON**P
        WRTTE "PIJPF. TIME GFRIVATIVE", IT, NIIMFF, DENOM, GHRIV(F:,IT)
        DNENA
        MRTTE "SQARF NFRIVATTVFS"
        IF (TSRM(TT).GT,O) DO TR = 1, ISRM(TI)
        HIIMFD= ANIIN(DFRTV(TR-1,IT), NENPM)
```



```
        WFTTF IH, PIIMFR, DFNOM, NERIVEIQ,ITI
        DOENT
    OOENT
    WRITE OFRIV
        DFLTA=TTME(FITNEI: WRTTE OFLTA,FTTNF
    H|MFR=?
    OFNOM=O
    * ELTMTNATF TIME NFDIVATTVES FQOM THF PUTMARY MONIFIED FOIATIDN
    On.t = %, 15T
        n\cap 1 = a, TSPM(I)
            DFRTV(a,a)= DFPTV(a,a) (S|R(T,j)= DERIV(I,j))
            OFPTV(O,V) = TPSFVICTPS(OERTV(G,a) (DO, OT`= LAM*OH, LAM*OT).LAM,
            TMAX(RORO, Tח!RD)). 1)
            OERTV(H,A) = TFSFVL(TPS(DFRIV(G,a) (DR = LAN* DR), LAN, RDRD), 1)
```



```
        ONEND
    OOEND
    N(IMER = ANUM (OFRIV(O,N), OFNOM)
    WRITF RODD, TORD, NEEMON, NUNFR, OFNOM
    WRTTF (>5) RORN, THRIG, DERMOR, NJIMFR, DENOM, SUFR
        DFLTA=TIME(ETIMEI: WPITE DFLTA,FTIMF
    NIIMFRR=C
    CENOM=R
    IF (SNFR.FO.O) GO TO ST
    # - - - - - - ....- - - - 
    * ELIHTNATE TIME OFETVATIVES FROM THF SECONOARY IODIFTFO EMUATION
    WRITF "SECONOARY FRUATTON", SDFAR, SNIIM, SNEN
    SECONO = SNIM/ SIFN
    \capQ J = ब. IST
        OD T = f. ISPM(J)
        SECONR = SFCRIJM (SUR(T,J) = MFRIV(T,J))
```

157
158
159
159
169
161
1 1h2
162
143
143
164
145
156
167
168

| 69 |
| :--- | 179

179
SFCOND = TPSFVL (TES (SFCTJNO (OR, DT = LAM* MR, LAM*DT), LAM,
TMAX (ROLDD, TORT)) 1 )
SECO:J) $=$ TPSFVI (TPS (SFCOND (DR $=1 A M * D F), L A M, ~ R O R D), ~ 1$
SECONO $=$ TDSFVL (TOS (SFCOND (IT $=1 A M * D T), L A M, ~ T I R D), ~$
DOEN
DOEND
SNIJM = ANUM (SECOND, SNFN)
WRTTE SNIIM, SDEA
IWRTTE SNIIM, SNEMI
WDTTF (25) STIIM, SNEN
ST: COVTTNIJF
ПELTA=TYME(FTIME): WRITF OFLTA,FTTME
FHO

| NAME／EXTNAMF | IIS ${ }^{\text {F }}$ | TYFF | stolle | PREC | CIASS | SCAPF | OR | LAY | ADIR |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| TSRM | VAR | INT | A |  |  |  |  |  |  |
| DERIV | VAR | A $1 r_{\text {，}}$ | A | L |  |  | $\begin{aligned} n-196 \\ n \end{aligned}$ |  |  |
| DENOM | $\checkmark$ VAR | A！ $0_{0}$ |  | 1 |  |  |  |  |  |
| SERMOT | VAH | $A L C_{0}$ |  | 1 |  |  |  |  |  |
| DIF | IJ） | ALf， |  |  |  |  |  | L＊＊at |  |
| DP | INO | AI．$\%$ |  |  |  |  |  | L＊くッ1 |  |
| Di | TNO | ALT， |  |  |  |  |  | L＊スa） |  |
| F1 | INO | ALC， |  |  |  |  |  | L＊ロッ！ |  |
| F2 | IND | ALC |  |  |  |  |  | $L$＊）${ }_{\text {a }}$ |  |
| 91 | IND | ALG |  |  |  |  |  | L＊いい） |  |
| G2 | TN： | ALC， |  |  |  |  |  | L＊かの1 |  |
| LAM | TND | $\Delta \mathrm{L}$, |  |  |  |  |  | L＊＊から |  |
| NUMER RM | VAR | $A L G$ |  | L |  |  |  | L＊＊＊I |  |
| RP | TVO | $A L F$ |  |  |  |  |  | L＊吅 |  |
| R | IND | ${ }^{\text {AL }}$－$r_{0}$ |  |  |  |  |  | L＊VめI |  |
| SDFN | VAR | 416 |  |  |  |  |  | 1．Ont |  |
| SOFR | VAR | A1．${ }^{\text {A }}$ ， |  | L |  |  |  | L＊ami |  |
| SECOMA | VAR | $A 10$ |  | L |  |  |  | L＊eか！ |  |
| SNUM | VAR | Al $_{\text {a }} r_{0}$ |  | 1 |  |  |  | L＊くら1 |  |
| TI | T：JT | $A L T$. |  |  |  |  |  | －＊以！ |  |
| 1. | INT | $A L T$, | $\wedge$ |  |  |  |  |  |  |
| P | INT | A） 6 | A |  |  |  |  | $L * P D 1$ |  |
| Q H | TAID | A）G | A |  |  |  |  | Lopl |  |
| T | PNAT | $A!r$ | a |  |  |  |  | $L+\operatorname{Cal}$ |  |
| ANIJM／S9ANIMM | PREC | ${ }^{4} \mathrm{~L}$ f， |  | 1. | S | $x$ |  | －＊＊ |  |
| DEFISODFG， | PROT | TNT |  |  | S | $x$ |  |  |  |
| DE．I．TA | VAR | Pral |  |  |  |  |  |  |  |
| ETTME | VAP | REAI |  |  |  |  |  |  |  |
| IMAX／Salmax | GOOC | 1：19 |  | L | $\leqslant$ | x |  |  |  |
| IR | VAR | INT |  |  |  |  |  |  |  |
| $15 R$ | VAR | INT |  |  |  |  |  |  |  |
| IST | VAR | 「リア |  |  |  |  |  |  |  |
| T | VAR | INT |  |  |  |  |  |  |  |
| I | VAR | TNT |  |  |  |  |  |  |  |


| $\stackrel{\omega}{\sim}$ | J | VAR | TA．T |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | LAN | VAR | ALr， |  | 1. | S | $x$ |  |
|  | MAIN | PRDC |  |  | 1 | S | $x$ |  |
|  | MM | VAR | INT |  |  |  |  |  |
|  | M | VAF | INT |  |  |  |  |  |
|  | NT | VAR | INT |  |  |  |  |  |
|  | N1 | VAR | IdT |  |  | S | $x$ |  |
|  | N2 | VAR |  |  |  | S | $x$ |  |
|  | P1 | VAR | ALT | A | L | S | $x$ |  |
|  | RDER | PRDC | ALG |  | L | 5 | X |  |
|  | RORD | VAD | TNT |  |  |  |  |  |
|  | R1 | $V A R$ | ALS， | A | L | S | X |  |
|  | SJ1R | $V A R$ | ALfo | A | $L$ |  |  |  |
|  | 5 | VAR | ALf， |  | L | 5 | $x$ |  |
|  | TOF．R | PROR． | ALC |  | L | $s$ | X |  |
|  | TIME／S9CLTK | OPDC． | QFAL |  | L | S | $x$ |  |
|  | TIM | VAR | ALf， |  | L | 5 | $x$ |  |
|  | TORD | $V A R$ | IMT |  |  |  |  |  |
|  | TPSEVL | PROC | ALG |  | $L$ | S | $x$ |  |
|  | TPS | DRDC | Al． G ， | A | L | S | $x$ |  |
|  | T1 | VAR | Al $\mathrm{F}^{\text {a }}$ | A | $L$ | S | $x$ |  |
|  | 111 | VAh | ALf， | A | L | S | $x$ |  |
|  | 0＊9の6 | nR |  |  |  |  |  |  |
|  | D＊aの7 | DR |  |  |  |  |  |  |
|  | L＊a＠ | L4Y |  |  |  |  |  |  |
|  | A1 | CONS | LAF |  |  | S |  |  |
|  | $A 2$ | COMS | $L \triangle R$ |  |  | S |  | 352 |
|  | 43 | CONS | LAP |  |  | $\leqslant$ |  | 37 h |
|  | A4 | rinns | LAP |  |  | 5 |  | 460 |
|  | R1 | cons | $1 \triangle R$ |  |  | S |  | 427 727 |
|  | NMT | CONS | LAS |  |  | S |  | 727 |
|  | QS | CONS | $l a t i$ |  |  | 5 |  | 757 |
|  | ST | CONS | LAR |  |  | S |  | 1598 |
|  | ILLEGAL DERMON，AROR | Cons | CHAD |  |  | 5 |  |  |
|  | INTTIALTZATION | COHS | C．HAR |  |  | 5 |  |  |
|  | MAXIMIIN DROER OF NFE | coms | Cham |  |  | 5 |  |  |
|  | NO time nertvatives | CONS | CHAR |  |  | S |  |  |
|  | PURE TTME DERIVATIVF． | Coms | chat |  |  | S |  |  |
|  | SFCONOARY FOIIATTMIJ | CONS | CHAR |  |  | 5 |  |  |
|  | SPACE DERIVATIVFS | CONS | CHAD |  |  | $\leqslant$ |  |  |
|  | $a$ | r．nns | TNT |  |  | 5 |  |  |
|  | 1 | coivs | T！ $1 . T$ |  |  | S |  |  |
|  | 25 | Cons | TNT |  |  | S |  |  |
|  | 2 | cons | TNT |  |  | S |  |  |
|  | 31 | CONS | $\mathrm{INT}_{101}^{10}$ |  |  | S |  |  |
|  | 7 | cons | 1ヵT |  |  | S |  |  |

2. LISTING OF THE ELIMINATION PROGRAM AND FIRST RUN OF THE SAMPLE PROBLEM
```
ALTQAN VFGSTON I LEVE! a
```


FXTFANAI TNTEGEE MI, NT
FXTFRNAI. I ONF; ALIFEREATC LAP', S, TIM
EXTFRNAI. JONG, IIGRRGATC AREAYRI, Pi. TI. WI
VALJE A
LONG AIGERRATC, A, DFR
INTFGEP I, .

* DTFFFRFPMTIATE. NITH RFSPFCT TO TTMF. (TIM)
DEQ $=\operatorname{MTFF}(A, T$ TM)
\# CJAIN RULF FOR GMPLIPTT DIFFFGFNTIATION OF DEPENDFNT VARIABLES
กП $T=N 1, \pi,-1$

Dก $J=N 2-1, ~ H,-1$


DOFNO
DOENH
RETIIRN(DER)
KICKOUT;NRITE MFRFGR TN TMER - N JS TIM SMALL", N, DFR, MI. NP. I, J
ENO
NAMF/EXTNAMF. USE TYPE STRUIC PRFC CLASS SCOPF OA IAY AODR

| VAi | ALG: |  | L |  | $v$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| VAF | A C C |  | L |  |  |
| PROC | Alf |  | L | S | x |
| VAR | TNT |  |  |  |  |
| $V A R$ | JNT |  |  |  |  |
| VAR | \&LT, |  | $\downarrow$ | 5 | $x$ |
| $V A Q$ | THT |  |  | 5 | $x$ |
| VAF | INT |  |  | S | $x$ |
| VAR | ALS | $\wedge$ | L | S | $x$ |
| VAR | ALf | A | $L$ | 5 | $x$ |
| VAR | ALS |  | L | S | $x$ |
| PROTI |  |  | L | 5 | $x$ |
| $\checkmark A D$ | ALS. |  | L | S | $x$ |


| $T 1$ |  | VAR | Alf, | A | L |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 111 |  | VAR | ALS, | 1 | L |
| KICKOIT |  | COMS | LAF |  |  |
| ERQOR IN | TOFR - N | CONS | CHAL |  |  |
| ด |  | CONS | TMT |  |  |
| 1 |  | rons | PHT |  |  |

3. RESULTS OF THE SECOND RUN OF THE ELIMINATION PROGRAM
```
ALTRAN VFRSTAN I LEVFL q
    DGOGFOIIRF ROFP (A) F TTMF NFRTVATIVF OF AN AIGFRRATC WITH NENOMTMATOR = I
    EXTFONAL IMTEGFR NI, M!?
FXTFRNAL LOMIG AIIIFKRATC IAN, S, IIM
EXTERNAI LONG ALGFRHAIC ARGAY RI, pl, T1, W!
VAlJF. A
LONG ALGFARATT A, NFE
INTFGER I, J
# OIFFFRFNTIATE WITH QFSPECT TOR (S)
    DEQ = חTFF (A,S)
# CHATN \ULF. FOR TMDLTCIT OIFFFRFNTIATIOF: OF NE゙OENDENI VARIARLFS,
    nn J = NQ, n, -1
```



```
        \cap\cap I=NI=1, u, -1
        DFP= DES + NIFF(A, RI(T,JJ) * RI(J+I,J) + DTFF(A, PI(I,J))*P1(I+I,J)+
            \iFF (A, UI(T,J)) UM(I+I,J) + NIFF(A, TI(T,J)) Ti(I+I,.j)
        DOFNO
    MOENO
    RETURN(NER)
KTCKOUT:WRTTF "FPROR IF' FIDEF= - N TS TOO SMALL", A, OER,NI, NZ, I,J
    F.NO
```

NAME/EXTNAME LISE TYPF STRUC PREC CLASS SCDPF JE LAY ADIDR

| $A$ | $V A P \quad A L C$ | 1 |  | $V$ |
| :--- | :--- | :--- | :--- | :--- |
| OER | VAR ALG | $L$ |  |  |
| DIFF/AGIIFF | PQOC ALG | 1 | $s$ | $x$ |

```
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline I & & & & & & \\
\hline \(j\) & VAR & IA. \({ }^{\text {P }}\) & & & & \\
\hline LAN & \(V A R\) & TNT & & & & \\
\hline N1 & VAD & \(A \backslash r\), & & 1 & 5 & \\
\hline N \({ }^{\text {a }}\) & VAP & INT & & & 5 & \(x\) \\
\hline N & \(V A R\) & INT & & & S & \(x\) \\
\hline PDER & VAF & ALC. & \(\Delta\) & L & S & \(x\) \\
\hline RDER & OROC. & & & L & 5 & \(x\) \\
\hline R1 & VAP & Alf, & A & L & S & X \\
\hline TIM & \(V A P\) & \(A L S\) & & L & 5 & \(x\) \\
\hline T1 & \(V A R\) & ALG, & & \(L\) & S & \(x\) \\
\hline U1 & \(V \triangle R\) & Al. \(G\) & A & L & . & x \\
\hline KICKOUT & VAR & \(\Delta L G\) & A & L. & S & \(x\) \\
\hline
\end{tabular}
KICKOUT
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| $T(4,3)$ | - | T (3,6) | , |  | T(7,1) | , | T(2.4) |
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| $T(a, 4)$ | , | $T(3,7)$ | , |  | r(7, $)$ | , | r(2,5) |
| $T(0,5)$ | , | $T\left(4, \square^{\prime}\right)$ | , |  | T (7,3) | , | T(2,6) |
| $T(A, 6)$ | , | T(4,1) | , |  | T(7,4) | , | T(P,7) |
| $T(4,7)$ | , | T (4, 2 ) | , |  | T(7,5) | , | $\square$. |
| T (1,a) | - | $T(4,3)$ | , |  | T (7,6) | - | T ( 3,1 ) |
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| $T(1,6)$ | , | T (5,1) | , |  | $T(a, 4)$ | , | T(3,7) |
| $T(1,7)$ | , | T(5,2) | - |  | $T(0,5)$ | , | 9 |
| $T(2, a)$ | , | $T(5,3)$ | - |  | $T(a, b)$ | , | T(4,1) |
| $T(2,1)$ | , | $T(5,4)$ | , |  | $T(9,7)$ | , | T(4, 2 ) |
| $T(2,2)$ | , | $T(5,5)$ | - |  | の, |  | T(4, 3) |
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| T(R,4) | , | $T(5,7)$ | - |  | T(1,2) | , | $T(4,5)$ |
| $T(2,5)$ | , | $T(6,9)$ | - |  | T(1,3) | , | $T(4, h)$ |
| $T(2, h)$ | , | $T(6,1)$ | - |  | $T(1,4)$ | , | T(4,7) |
| $T(?, 7)$ | , | $T(6,2)$ | , |  | $T(1,5)$ | - | a. |
| $T(3, a)$ | - | $T(6,3)$ | - |  | T ( 1,6 ) | , | $T(5,1)$ |
| T(3,1) | , | $T(6,4)$ | - |  | T(1,7) | - | T(5,2) |
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| $T(3,3)$ | , | $T(6, b)$ | - |  | $T(?, 1)$ | , | $T(5,4)$ |
| T(3,4) | , | $T(6,7)$ | , |  | T(2, $)$ | , | $T(5,5)$ |
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M OERIV（ $a, P$ ）

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    T(1.1) ,
    T(1,2),
    T(1,3).
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| \& | r(7.1) . | , | T(2.3) | - |  | T(5.6) | - |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | т(7.2) , | , | T (2,4) | - |  | T (5,7) | , |
|  | r(7.3) , | - | T (2.5) | - |  | ค. |  |
|  | T(7.4) , | - | $T(2, t)$ | - |  | T(6.1) | - |
|  | T(7,5) , | , | T(2,7) | - |  | T (6.2) | - |
|  | r(7,6) . | , | $0 \cdot$ |  |  | T(6,2) | - |
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|  | ( T 0,1$)$ | 1 , | T (3.4) | - |  | T (6,7) | - |
|  | T(0.2) | - | T (3,5) | - |  | n , |  |
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|  | $T(0,4)$ | - | T(3,7) | - |  | T(7,2) | - |
|  | - 0.5 ) | - | $n$ - |  |  | T(7.3) | , |
|  | T(n, 6 ) | - | T(4.1) | - |  | T(7,4) | , |
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|  | $\bigcirc$. |  | $T(5,2)$ |  |  | 1.51039 | 95n4 |
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There are three simple modifications that the user can make to improve efficiency. The first change can be made only if all truncation errors containing time derivative are first or higher orderin 0 t or $\delta r$. In that case, we can safely eliminate the highest order errors from the modified equation before differentiating it. This greatly reduces the amount of algebra by disposing of these terms at an early stage rather than waiting until the late stages of the calculation to discard them. To do this, insert the following three statements after Ine 105:
$\operatorname{SEC}$ ND $=\operatorname{DERTV}(0,0)$
$\operatorname{DERIV}(0,0)=\underset{\operatorname{DT})}{\operatorname{TPSEVL}(\operatorname{TPS}(\operatorname{DERIV}(0,0), \operatorname{DT}, \operatorname{TORD}-1), ~}$
$\operatorname{DERTV}(0,0)=\operatorname{TPSEVL}(\operatorname{TPS}(\operatorname{DERIV}(0,0), \operatorname{DR}, \operatorname{RORD}-1)$, DR)
Insert
$\operatorname{DERIV}(0,0)=\operatorname{SECOND}$
SECOND $=0$
after line 129.
The second modification increase the running time of the code for each run, but reduces the number of runs and therefore the amount of human intervention. This modification is recoumended for users who have no difficulty getting the necessary central processor time for a single run. It consists of looping through the code repeatedly until no more eliminations can be made with the current DERM $\varnothing \mathrm{D}$. After line 10 insert the following:

INTEGER NPASS = 1
After line 30 insert the following:
AG: CONTINUE
After line 141 insert the following:
REWIND (25)
Replace lines 145 through 147 with the following:
IF (SDER.EQ.0) G $\emptyset$ T $\emptyset$ BB
Replace Iine 165 with the following:
BB: CONTINUE
WRITE " END OF PASS', NPASS
IF (NPASS .GT. 10) G $\emptyset \square$ ST
NPASS $=$ NPASS +1 GØ Tø AG
After line 167 insert the following:

WRTTE (25) SNUM, SDEN
The third set of changes should improve the core utilization of the frogram enough to avoid running out of workspace if the problem is only slightly too large, and it will reduce the number of passes through the elimination loop for certain problems. After line 133, insert the following: $\operatorname{IF}(\operatorname{SDER} . \operatorname{EQ} \cdot \mathrm{O}$.AND. $\mathrm{I}+\mathrm{J} . \operatorname{NE} .0) \operatorname{DERIV}(\mathrm{I}, \mathrm{J})=0$ After line 139 insert the following: $\operatorname{DERIV}(0,0)=\operatorname{DERIV}(0,0)(\operatorname{SUB}(0,0)=\operatorname{DERIV}(0,0))$

After line 156 insert the following: $\operatorname{IF}(I+J \cdot N E \cdot 0) \operatorname{DERIV}(I, J)=0$

FLOW CHARTS FGR TFE TINE CERIVATIVE ELIMIMATION PROGRAM



The PROCEDURE RDER uses the same algorithm as TDER to differentiate $A$ with respect to $r$.

