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A NONLINEAR LEAST-SQUARE PROGRAM FOR THE
DETERMINATION OF PARAMETERS OF PHOTOPEAKS
BY THE USE OF A MODIFIED-GAUSSIAN FUNCTION

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**PHILLIPS
PETROLEUM
COMPANY**

ATOMIC ENERGY DIVISION

**NATIONAL REACTOR TESTING STATION
US ATOMIC ENERGY COMMISSION**

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ABSTRACT

A computer program has been written to perform a nonlinear, least-squares fit to a set of data points with one or more Gaussian, or "modified-Gaussian", functions. This program was designed for the analysis of gamma-ray spectra obtained with NaI(Tl) scintillation detectors and lithium-drifted germanium detectors. It is used to determine the photopeak positions (gamma-ray energies) and areas for peaks which contain one or more unresolved photopeaks. The functional form used is

$$y(x) = \sum_{j=1}^J y_{oj} e^{-\left(\frac{x - x_{oj}}{w_{oj}/2\sqrt{\ln 2}}\right)^2} \left[1 + \alpha_{1j} (x - x_{oj})^{m_1} + \alpha_{2j} (x - x_{oj})^{m_2} \right] + a x + b$$

where the fit determines the parameters a , b , y_{oj} , x_{oj} , w_{oj} , and α_{ij} . Here m_1 and m_2 are given, even integers. The coefficients a and b describe a straight-line component which may be utilized to represent Compton distributions or background which may underlie the photopeak of interest. Several options are included in the program to facilitate its application to different problems. For example, some of the parameters may be fixed at their initial values and any of the w_{oj} , α_{1j} , or α_{2j} may be given as functions of x_{oj} . The input subroutine has been arranged so that a minimal amount of input information is needed when a series of similar fits are to be carried out in succession. Complete listings of the FORTRAN IV program are included along with samples of input to the program and complete instructions for preparing input.

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I. INTRODUCTION

This computer program has been written to aid in analysis of gamma-ray spectra measured on NaI(Tl) scintillation spectrometers and lithium-ion-drifted germanium detectors. The program is used to determine the parameters of a Gaussian, or a "modified Gaussian", which best fits the data points of a photopeak, or full-energy peak, associated with a single gamma ray as well as to decompose complex peaks into individual photopeaks. Estimates are calculated for the standard deviations associated with the computed parameters. These results are used to obtain the following information:

Peak position for the calculation of the

- (a) energy of gamma ray, or
- (b) relative pulse heights for determination of pulse height versus energy relationship.

Peak area from which can be determined the

- (a) gamma-ray intensity, or
- (b) peak-to-total ratio (area of photopeak ÷ area of spectrum) for single gamma rays.

Peak shape:

A study of photopeak shapes was carried out so that the best determination of the position and area could be made. This information makes the analysis of complex peaks more valid.

Analysis of complex peaks to determine

- (a) energies of gamma rays whose photopeaks make up the peak, or
- (b) intensities of these gamma rays.

It has been found that the photopeaks measured with one particular spectrometer deviate noticeably from a Gaussian function. Therefore, a "modified-Gaussian" function of the form

$$\bar{y}(x) = y_0 e^{-\left(\frac{x - x_0}{w_0/2 \sqrt{\ln 2}}\right)^2} \left[1 + \alpha_1 (x - x_0)^4 + \alpha_2 (x - x_0)^{12} \right]$$

is used to represent the photopeaks. The reasons for the use of this function are discussed in Reference 1. The parameters x_0 (center of photopeak in channels), y_0 (count at peak or x_0), w_0 (full width of photopeak at $y_0/2$, in channels), and α_1 and α_2 can be calculated in the fit. The terms containing α_1 and α_2 represent the deviation from a Gaussian function.

A conventional nonlinear least-squares procedure^[2] can be used in the calculation, or a modified method can be employed. In either case, the parameters are determined by minimizing the function

$$R^2 = \sum_i w_i (y_i - \bar{y}_i)^2$$

where w_i is a set of weights, y_i is the experimental count in the channel i , and $\bar{y}_i$ is the calculated count.

In order to provide a versatile program that can handle many experimental problems, a large number of options have been incorporated. A few of these are as follows:

- (1) Choice of various weighting functions w_i .
- (2) Choice of allowing any parameter to be calculated in the fit, to be fixed at a specified value, or in the case of w_0 , α_1 , and α_2 , to be given by a function of x_0 .
- (3) Choice of standard or modified nonlinear fitting procedure.
- (4) Channels to be used in fit.
- (5) Number of Gaussians to be fitted to the counts in one set of channels.
- (6) Use of line, $ax + b$, to represent the spectral distribution underlying the photopeaks.

Item (2) is performed by providing a set of three polynomial functions which relate w_0 , α_1 , and α_2 to x_0 . Since a given set of polynomials is valid for only one experimental situation [one NaI(Tl) crystal and one gain], several such sets can be stored in the program.

Although this program was written for analysis of gamma-ray spectra, it could be used for any Gaussian, or nearly Gaussian, fitting problem.

The basic mathematics of the nonlinear least-squares method and the specialization to this problem are discussed in the next section. In Section III the input formats and options are described. Examples of the results are given in Section IV. In Section V the modified fitting procedure is discussed, and the descriptions of the operation of the subroutines are presented in Section VI. The FORTRAN listings are given in the Appendix.

The program is written in FORTRAN IV and has been compiled for use on an IBM 7040 computer. Typical running times are 10 to 90 seconds per fit for one or two Gaussians. The program is dimensioned to handle 10 Gaussians and a line, or up to 52 variable parameters. About 13,000 memory locations are required for the program.

II. MATHEMATICS

1. THE THEORY OF LEAST SQUARES

The purpose of a least-squares fit is to find the values of the variable parameters, p_j , which minimize the sum of the squares of the deviations of the data from their estimate; that is,

$$R^2 = \sum_i w_i [N_i - \bar{N}_i(p_j)]^2 \text{ is minimized.} \quad (1)$$

The N_i are the experimental data points, the w_i are the weights associated with the N_i , and the $\bar{N}_i(p_j)$ are the values calculated from a theoretical expression. (The summation is over all the points used in the fit.)

A necessary and sufficient condition for R^2 to be a minimum, as a function of p_j , is that the set of equations

$$\frac{\partial R^2}{\partial p_j} = 0 \quad (2)$$

hold simultaneously for all values of j .

If $\bar{N}$ is a linear function of the parameters p_j , expressions can be derived for the "best" value for each of the parameters. However, if the function is not linear in the parameters, no explicit solution of Equation (2) exists. However, in this case a method of "linearization" can be used.

Such a method is that of Gauss[2]. This method consists of linearizing the function with respect to each of the parameters by use of a truncated Taylor's series. Initial estimates, p_j^0 , of the parameters must be available in order to evaluate the derivatives in the expansion. That is, if $p_j = p_j^0 + \delta p_j$,

$$\begin{aligned} \bar{N}_i(p_j) = \bar{N}(p_j^0) + \sum_j \left(\frac{\partial \bar{N}_i}{\partial p_j} \right)_0 \delta p_j \\ + \frac{1}{2} \sum_k \sum_\ell \left(\frac{\partial^2 \bar{N}_i}{\partial p_k \partial p_\ell} \right)_0 \delta p_k \delta p_\ell + \dots \end{aligned} \quad (3)$$

where the derivatives are evaluated at the initial values of the parameters.

The function $\bar{N}(p_j)$ is a linear function of the δp_j if all derivatives beyond the first are neglected. This gives

$$R'^2 = \sum_i w_i \left[N_i - \bar{N}(p_j^0) - \sum_j \left(\frac{d\bar{N}_i}{dp_j} \right)_0 \delta p_j \right]^2 \quad (4)$$

In this expression the δp_j are the parameters to be computed. The conditions which now determine the minimum are

$$\frac{dR'^2}{d(\delta p_j)} = 0 \quad . \quad (5)$$

The solution of this set of linear equations gives the values δp_j . Since the higher order derivatives have been neglected in Equation (4), this process does not yield the solution of Equation (2). Therefore, Equation (5) is solved again with the p_j^0 replaced by $(p_j^0 + \delta p_j)$. This process is continued until all the δp_j approach zero (or some predetermined convergence criterion).

For a more complete and rigorous discussion of this method, the reader is referred to a report by Moore and Zeigler[2] and the references therein.

2. NONLINEAR LEAST-SQUARES FIT TO A MODIFIED-GAUSSIAN FUNCTION

In the program under discussion it is desirable to compare a set of experimental data, y_i , with the function

$$\bar{y}_i = \sum_{j=1}^J y_{ij} + y_{li}$$

where

$$\bar{y}_{ij} = y_{oj} e^{-\left(\frac{x_i - x_{oj}}{w_{oj}/2 \sqrt{\ln 2}}\right)^2} \left[1 + \alpha_{1j} (x_i - x_{oj})^{m_1} + \alpha_{2j} (x_i - x_{oj})^{m_2} \right] \quad (6)$$

and

$$y_{li} = a + bx_i \quad .$$

The powers m_1 and m_2 are predetermined, even, positive integers. The parameters y_o , x_o , w_o , α_1 , and α_2 can be determined in the fit. The line parameters b (line slope) and a (line intercept) can also be determined in the fit. The subscript j identifies the Gaussian ($j \leq 10$).

In this case for one Gaussian, Equation (4) becomes explicitly

$$R'^2 = \sum_i w_i \left[y_i - \bar{y}_i(p_j^0) - \frac{\partial \bar{y}_i}{\partial y_o} \delta y_o - \frac{\partial \bar{y}_i}{\partial x_o} \delta x_o - \frac{\partial \bar{y}_i}{\partial w_o} \delta w_o - \frac{\partial \bar{y}_i}{\partial \alpha_1} \delta \alpha_1 - \frac{\partial \bar{y}_i}{\partial \alpha_2} \delta \alpha_2 \right]^2 \quad (4a)$$

where w_i is the weighting factor associated with y_i and it is assumed that $\underline{a}$ and $\underline{b}$ are not variables.

For one Gaussian, Equation (5) becomes explicitly (with summation index i and the bar over y_i dropped)

$$\delta y_o \sum w \left(\frac{\partial y}{\partial y_o} \right)^2 + \delta x_o \sum w \frac{\partial y}{\partial y_o} \frac{\partial y}{\partial x_o} + \delta w_o \sum w \frac{\partial y}{\partial y_o} \frac{\partial y}{\partial w_o} + \delta \alpha_1 \sum w \frac{\partial y}{\partial y_o} \frac{\partial y}{\partial \alpha_1} + \delta \alpha_2 \sum w \frac{\partial y}{\partial y_o} \frac{\partial y}{\partial \alpha_2} = \sum w(y - y_o) \frac{\partial y}{\partial y_o} , \quad (5a)$$

$$\delta y_o \sum w \frac{\partial y}{\partial x_o} \frac{\partial y}{\partial y_o} + \delta x_o \sum w \left(\frac{\partial y}{\partial x_o} \right)^2 + \delta w_o \sum w \frac{\partial y}{\partial x_o} \frac{\partial y}{\partial w_o} + \delta \alpha_1 \sum w \frac{\partial y}{\partial x_o} \frac{\partial y}{\partial \alpha_1} + \delta \alpha_2 \sum w \frac{\partial y}{\partial x_o} \frac{\partial y}{\partial \alpha_2} = \sum w(y - y_o) \frac{\partial y}{\partial x_o} , \quad (5b)$$

$$\delta y_o \sum w \frac{\partial y}{\partial w_o} \frac{\partial y}{\partial y_o} + \delta x_o \sum w \frac{\partial y}{\partial w_o} \frac{\partial y}{\partial x_o} + \delta w_o \sum w \left(\frac{\partial y}{\partial w_o} \right)^2 + \delta \alpha_1 \sum w \frac{\partial y}{\partial w_o} \frac{\partial y}{\partial \alpha_1} + \delta \alpha_2 \sum w \frac{\partial y}{\partial w_o} \frac{\partial y}{\partial \alpha_2} = \sum w(y - y_o) \frac{\partial y}{\partial w_o} , \quad (5c)$$

$$\delta y_o \sum w \frac{\partial y}{\partial \alpha_1} \frac{\partial y}{\partial y_o} + \delta x_o \sum w \frac{\partial y}{\partial \alpha_1} \frac{\partial y}{\partial x_o} + \delta w_o \sum w \frac{\partial y}{\partial \alpha_1} \frac{\partial y}{\partial w_o} + \delta \alpha_1 \sum w \left(\frac{\partial y}{\partial \alpha_1} \right)^2 + \delta \alpha_2 \sum w \frac{\partial y}{\partial \alpha_1} \frac{\partial y}{\partial \alpha_2} = \sum w(y - y_o) \frac{\partial y}{\partial \alpha_1} , \quad (5d)$$

$$\delta y_o \sum w \frac{\partial y}{\partial \alpha_2} \frac{\partial y}{\partial y_o} + \delta x_o \sum w \frac{\partial y}{\partial \alpha_2} \frac{\partial y}{\partial x_o} + \delta w_o \sum w \frac{\partial y}{\partial \alpha_2} \frac{\partial y}{\partial w_o} + \delta \alpha_1 \sum w \frac{\partial y}{\partial \alpha_2} \frac{\partial y}{\partial \alpha_1} + \delta \alpha_2 \sum w \left(\frac{\partial y}{\partial \alpha_2} \right)^2 = \sum w(y - y_o) \frac{\partial y}{\partial \alpha_2} . \quad (5e)$$

This is, in general, a system of k simultaneous linear equations in k unknowns (in this case, k is 5). In matrix notation, the terms on the right side of the set are represented by a vector with five components, for one Gaussian,

$$\vec{B} = (B_1, B_2, B_3, B_4, B_5) = \left[\sum_i w_i (y_i - \bar{y}_i^o) \frac{\partial \bar{y}_i}{\partial y_o} , \dots , \sum_i w_i (y_i - \bar{y}_i^o) \frac{\partial \bar{y}_i}{\partial \alpha_2} \right] . \quad (7a)$$

Similarly, the changes in the parameters are given by the vector

$$\vec{\Delta p} = (\delta p_1, \delta p_2, \delta p_3, \delta p_4, \delta p_5) = (\delta y_o, \delta x_o, \delta w_o, \delta \alpha_1, \delta \alpha_2) \quad (7b)$$

The coefficients of the δp_j are represented by, for one Gaussian, a 5 x 5 symmetric matrix with the elements

$$A1_{j,k} = \sum_i w_i \frac{\partial y_i}{\partial p_j} \frac{\partial y_i}{\partial p_k} \quad (7c)$$

Equation (5) can now be written

$$A1 \cdot \vec{\Delta p} = \vec{B} \quad (8a)$$

where $\vec{\Delta p}$ and B are column vectors. The solution is

$$\vec{\Delta p} = A \cdot \vec{B} \quad (8b)$$

where the matrix $A = A1^{-1}$. ($A1$ is assumed nonsingular.) The generalization of these equations for several Gaussians is straight forward.

Basically, the process of solving for $\delta y_o, \dots, \delta \alpha_2$ is to form the matrix $A1$, invert it, and multiply by the vector B . The process is repeated until each δp_j is smaller than a number (convergence criterion) which is part of the input. At this point, the fitting process is concluded and a number of quantities (see II-4) are calculated.

3. MODIFICATIONS OF BASIC METHOD

3.1 Fixed Parameters

Any of the parameters involved in a fit may be fixed at their original input value. This is accomplished by setting $\delta p_j = 0$ in Equation (5).

3.2 Parameters as Functions of x_o

For a given scintillation spectrometer and a given gain scale, the photopeak width w_o and α , and α_2 are unique functions of x_o . Once these functional relationships are known they can be used to reduce the number of variables in a fit. This is especially important if an observed peak is made up of several Gaussians. Therefore, the program provides the option of calculating w_o , α_1 , and α_2 as functions of x_o . That is, as x_o varies, new values of these parameters are calculated.

The functional forms are

$$w_o = \sum_{k=0}^6 a_k x_o^{k/2} \quad , \quad (9)$$

$$\log \alpha_1 = \sum_{k=0}^6 b_k (\log x_o)^k, \text{ and} \quad (10)$$

$$\log \alpha_2 = \sum_{k=0}^6 c_k (\log x_o)^k. \quad (11)$$

The constants a_k , b_k , and c_k are stored in the program (in subroutines ALPHA1, ALPHA2, and OMEGA). Up to 10 such sets of coefficients of each type can be kept in the program so that data can be stored for different gains and different detectors.

The use of these relationships necessitates a modification of the equations used for the partial derivatives in Equation (4). For a single Gaussian with $\alpha_1 = \alpha_2 = 0$, one has

$$\bar{y}(x) = y_o e^{-\left(\frac{x - x_o}{w_o/2 \sqrt{\ln 2}}\right)^2} = y_o e^{-\left(\frac{4 \ln 2}{w_o^2} (x - x_o)^2\right)}.$$

If w_o varies independently

$$\frac{d\bar{y}}{dx_o} = 2 \cdot \frac{4 \ln 2}{w_o} (x - x_o) y_o e^{-\left(\frac{x - x_o}{w_o/2 \sqrt{\ln 2}}\right)^2} \quad (12a)$$

and

$$\frac{d\bar{y}}{dw_o} = 2 \cdot \frac{4 \ln 2}{w_o^3} (x - x_o)^2 y_o e^{-\left(\frac{x - x_o}{w_o/2 \sqrt{\ln 2}}\right)^2}. \quad (12b)$$

If w_o is a function of x_o , then

$$\frac{d\bar{y}}{dx_o} = \frac{\partial \bar{y}}{\partial x_o} + \frac{\partial \bar{y}}{\partial w_o} \frac{dw_o}{dx_o}.$$

Or,

$$\frac{d\bar{y}}{dx_o} = \frac{8 \ln 2}{w_o^2} (x - x_o) y_o e^{-\left(\frac{x - x_o}{w_o/2 \sqrt{\ln 2}}\right)^2}$$

$$+ \frac{8 \ln 2}{w_o^3} (x - x_o) y_o e^{-\left(\frac{x - x_o}{w_o/2 \sqrt{\ln 2}}\right)^2} \left[\sum_{k=1}^5 \frac{k}{2} a_k x_o \left(\frac{k}{2} - 1\right) \right], \quad (12c)$$

and

$$\frac{d\bar{y}}{dw_o} = 0. \quad (12d)$$

Similar modifications are made if $\alpha_1(x_o)$ and $\alpha_2(x_o)$ are used.

3.3 Limits of Variation of Parameters

As part of the input, upper and lower limits, p_j^u , and p_j^l , are supplied. The parameter p_j is then restricted to the range $p_j^l \leq p_j \leq p_j^u$. If, in the course of the fit, a δp_j is such that $p_j + \delta p_j$ is outside of this range, this value is rejected and the corresponding limiting value is used.

This feature is used to restrict parameters to ranges of validity. Also, it is used to prevent the positions of two Gaussians from interchanging positions and thereby preventing convergence.

3.4 Parabolic Fitting Method

In the above procedure, a set of values, δp_j , are obtained and $p_j' = p_j + \delta p_j$. Instead, it is possible to set

$$p_j' = p_j + \lambda \delta p_j \quad \text{for all } j \quad (13)$$

where λ is a constant. The program allows two methods for determining λ . First, it can be given as part of the input in which case it remains the same throughout the fit. In this case a value at, or near, 1 is usually used. Other values can be used to prevent oscillations in reruns of particular problems.

The other option is to allow the program to choose the "best" value of λ . Although $\lambda = 1$ provides the minimum of R'^2 , Equation (5), it does not necessarily provide the minimum of R^2 , Equation (2). Therefore, the usual nonlinear least-squares method is supplemented by a routine which searches for the minimum of R^2 as a function of λ . The method is to calculate the δp_j which minimize R'^2 . Then $R^2(p_j + \lambda \delta p_j)$ is calculated for $\lambda = 1, \lambda = 1/2, \dots$. The particular values of λ used depend on the relative values of $R^2(\lambda = 1)$ and $R^2(\lambda = 1/2)$. This technique is used to find the value of λ which gives a minimum of R^2 . This procedure is described in detail in Chapter V.

4. QUANTITIES CALCULATED AFTER COMPLETION OF FIT

4.1 Errors in the Parameters

After the final values of the parameters have been determined, the estimated uncertainties σ_j in these parameters are evaluated. From statistical arguments it can be shown[2] that

$$\sigma_j = \sqrt{\frac{R_{\min}^2}{n-m} A_{jj}} \quad (14)$$

where A_{jj} is the diagonal element of the inverse matrix $A = A_1^{-1}$, $R_{\min}^2$ is the value for R^2 for the final parameters, n is the number of data points, m is the number of independently variable parameters, and $(n-m)$ is the number of degrees of freedom.

4.2 Quality of Fit

The quality of the fit can be evaluated quantitatively by means of the quantity $\chi^2 = R_{\min}^2$. It can be shown by statistical arguments that if (a) $\bar{N}(p_j)$ is a linear function of the parameters p_j , (b) the experimental points are actually represented by a function of the form $\bar{N}_i(p_j)$, and (c) $\frac{1}{\sqrt{w_i}}$ is a good estimate of the standard deviation of N_i , the values of $R_{\min}^2$ for a large number of identical measurements should have a chi-square distribution with $(n-m)$ degrees of freedom. That is, $R_{\min}^2 / (n-m)$ should be about 1. In the case of nonlinear functions it is common to assume that the values of $R_{\min}^2$ will have a chi-square distribution, although this is not exactly true. Since conditions (b) and (c) are also not strictly valid, $R_{\min}^2$ will only be approximately chi-square distributed in any case [3].

4.3 Photopeak Areas

The area of each photopeak is determined. The modified Gaussian is represented by

$$y(x) = y_0 e^{-\left[\frac{(x_i - x_{oj})}{w_0/2 \sqrt{\ln 2}}\right]^2} \left[1 + \alpha_1 (x - x_0)^{m_1} + \alpha_2 (x - x_0)^{m_2}\right].$$

The area then is

$$A = \int_{-\infty}^{\infty} y(x) dx = A_0 + A_1 + A_2 \quad (15a)$$

where

$$A_0 = \int_{-\infty}^{\infty} y_0 e^{-\left[\frac{(x_i - x_{oj})}{w_0/2 \sqrt{\ln 2}}\right]^2} dx = \sqrt{\frac{\pi}{\ln 2}} \frac{w_0}{2} y_0, \quad (15b)$$

$$\begin{aligned} A_1 &= \int_{-\infty}^{\infty} y_0 \alpha_1 e^{-\left[\frac{(x_i - x_{oj})}{w_0/2 \sqrt{\ln 2}}\right]^2} (x_i - x_{oj})^{m_1} dx \\ &= \frac{(m_1 - 1)!!}{2^{m_1/2}} \left(\frac{w_0}{2 \sqrt{\ln 2}}\right)^{m_1} \alpha_1 A_0, \end{aligned} \quad (15c)$$

$$\begin{aligned}
A_2 &= \int_{-\infty}^{\infty} y_o \alpha_2 e^{-\left[\frac{(x_i - x_{oj})}{w_o/2 \sqrt{\ln 2}}\right]^2} (x_i - x_{oj})^{m_2} dx \\
&= \frac{(m_2 - 1)!!}{2^{m_2/2}} \left(\frac{w_o}{2 \sqrt{\ln 2}}\right)^{m_2} \alpha_2 A_o
\end{aligned} \tag{15d}$$

where $K!! = 1 \cdot 3 \cdot 5 \cdot 7 \cdot \dots \cdot K$, and K is odd.

4.4 Estimated Uncertainty in Area

The errors in the photopeak areas are evaluated by summing the products of the pertinent partial derivatives and variances or covariances. The variances and covariances are determined from the inverse matrix A from the iteration on which the fit converged.

For any one Gaussian, it is possible to get

$$\begin{aligned}
\text{var } A_o &= \left(\frac{\partial A_o}{\partial w_o}\right)^2 \text{var } w_o + 2 \left(\frac{\partial A_o}{\partial y_o}\right) \left(\frac{\partial A_o}{\partial w_o}\right) \text{covar}(w_o, y_o) \\
&\quad + \left(\frac{\partial A_o}{\partial y_o}\right)^2 \text{var } y_o \\
&= \epsilon^2 \left[\frac{1}{2} \sqrt{\frac{\pi}{\ln 2}} \right] \left[y_o^2 A_{33} + w_o^2 A_{11} + 2y_o w_o A_{13} \right]
\end{aligned}$$

where $\epsilon^2 = \frac{R^2_{\min}}{n-m}$, and (16a)

$$\begin{aligned}
\text{var } A_1 &= \left(\frac{\partial A_1}{\partial y_o}\right)^2 \text{var } y_o + \left(\frac{\partial A_1}{\partial w_o}\right)^2 \text{var } w_o + \left(\frac{\partial A_1}{\partial \alpha_1}\right)^2 \text{var } \alpha_1 \\
&\quad + 2 \left(\frac{\partial A_1}{\partial y_o}\right) \left(\frac{\partial A_1}{\partial w_o}\right) \text{covar}(y_o, w_o) + 2 \left(\frac{\partial A_1}{\partial y_o}\right) \left(\frac{\partial A_1}{\partial \alpha_1}\right) \text{covar}(y_o, \alpha_1) \\
&\quad + 2 \left(\frac{\partial A_1}{\partial w_o}\right) \left(\frac{\partial A_1}{\partial \alpha_1}\right) \text{covar}(w_o, \alpha_1)
\end{aligned}$$

$$\begin{aligned}
&= \epsilon^2 C_1^2 w_o^{2m_1} \left[\alpha_1^2 w_o^2 A_{11} + (m_1+1)^2 y_o^2 \alpha_1^2 A_{33} + y_o^2 w_o^2 A_{44} \right. \\
&\quad \left. + 2(m_1+1) y_o w_o \alpha_1^2 A_{13} + 2 y_o w_o^2 \alpha_1 A_{14} + 2(m_1+1) y_o^2 w_o \alpha_1 A_{34} \right] \quad (16b)
\end{aligned}$$

where $C_1^2 = \frac{\pi(m_1+1)!! (m_1-1)!!}{(\ell n 2)^{\frac{m_1+1}{2}} 2^{\frac{3m_1+2}{2}}}$, and

$$\begin{aligned}
\text{var } A_2 &= \left(\frac{\partial A_2}{\partial y_o} \right)^2 \text{var } y_o + \left(\frac{\partial A_2}{\partial w_o} \right)^2 \text{var } w_o + \left(\frac{\partial A_2}{\partial \alpha_2} \right)^2 \text{var } \alpha_2 \\
&\quad + 2 \left(\frac{\partial A_2}{\partial y_o} \right) \left(\frac{\partial A_2}{\partial w_o} \right) \text{covar } (y_o, w_o) + 2 \left(\frac{\partial A_2}{\partial y_o} \right) \left(\frac{\partial A_2}{\partial \alpha_2} \right) \text{covar } (y_o, \alpha_2) \\
&\quad + 2 \left(\frac{\partial A_2}{\partial w_o} \right) \left(\frac{\partial A_2}{\partial \alpha_2} \right) \text{covar } (w_o, \alpha_2) \\
&= \epsilon^2 C_2^2 w_o^{2m_2} \left[\alpha_2^2 w_o^2 A_{11} + (m_2+1)^2 y_o^2 A_{33} + y_o^2 w_o^2 A_{55} \right. \\
&\quad \left. + 2(m_2+1) y_o w_o \alpha_2^2 A_{13} + 2 y_o w_o^2 \alpha_2 A_{15} + 2(m_2+1) y_o^2 w_o \alpha_2 A_{35} \right] \quad (16c)
\end{aligned}$$

where $C_2^2 = \frac{\pi(m_2+1)!! (m_2-1)!!}{(\ell n 2)^{\frac{m_2+1}{2}} 2^{\frac{3m_2+2}{2}}}$,

and finally

$$\begin{aligned}
\text{var } A &= \left(\frac{\partial A}{\partial y_o} \right)^2 \text{var } y_o + \left(\frac{\partial A}{\partial w_o} \right)^2 \text{var } w_o + \left(\frac{\partial A}{\partial \alpha_1} \right)^2 \text{var } \alpha_1 \\
&\quad + \left(\frac{\partial A}{\partial \alpha_2} \right)^2 \text{var } \alpha_2 \quad (16d) \\
&\quad + 2 \left(\frac{\partial A}{\partial y_o} \right) \left(\frac{\partial A}{\partial w_o} \right) \text{covar } (y_o, w_o) + 2 \left(\frac{\partial A}{\partial y_o} \right) \left(\frac{\partial A}{\partial \alpha_1} \right) \text{covar } (y_o, \alpha_1)
\end{aligned}$$

$$\begin{aligned}
& + 2 \left(\frac{\partial A}{\partial y_o} \right) \left(\frac{\partial A}{\partial \alpha_2} \right) \text{covar} (y_o, \alpha_2) + 2 \left(\frac{\partial A}{\partial w_o} \right) \left(\frac{\partial A}{\partial \alpha_1} \right) \text{covar} (w_o, \alpha_1) \\
& + 2 \left(\frac{\partial A}{\partial w_o} \right) \left(\frac{\partial A}{\partial \alpha_2} \right) \text{covar} (w_o, \alpha_2) + 2 \left(\frac{\partial A}{\partial \alpha_1} \right) \left(\frac{\partial A}{\partial \alpha_2} \right) \text{covar} (\alpha_1, \alpha_2) .
\end{aligned}$$

It should be noted that $\text{var } A \neq \sum_{i=0}^2 \text{var } A_i$ due to the presence of additional covariance terms. If a parameter p_k is fixed, then $\text{var } p_k = 0$ and $\text{covar} (p_k, p_j) = 0$ for all j . The variance and covariance terms are given by

$$\text{var } y_o = \epsilon^2 A_{11} , \quad (17a)$$

$$\text{covar} (y_o, x_o) = \epsilon^2 A_{12} , \text{ etc.} \quad (17b)$$

III. INPUT FORMAT AND OPTIONS

1. GENERAL

This program is coded in FORTRAN IV for use on an IBM 7040 computer. The input data are initially punched into cards and then transferred to magnetic tape for input to the computer. The code is a collection of subroutines, since this form allows for ease in making program changes. The function of each subroutine is discussed in Section VI-1. GAUSS can handle a maximum of ten Gaussians in one fit, any number of successive fits to one spectrum, and fits to any number of different spectra.

Any of the five parameters associated with each modified-Gaussian function can be held constant or varied, and the values of α_1 , α_2 , and w_0 can be computed as functions of x_0 . A line can be used to represent the spectral distribution underlying a photopeak. The slope and intercept of the line can vary or remain constant throughout the iteration process. An initial estimate, upper limit, lower limit, and convergence criterion must be supplied for each parameter (see Section III-4.1). The initial estimate is used to start the iteration process. The limits are used to restrict the parameters to regions of validity or reasonableness. Convergence is tested by means of the convergence criterion.

The input is written so as to permit maximum flexibility in running a series of similar problems. Each fixed- and floating-point control word is assigned a unique address which serves to identify the word to the program. After the first fit, only those control words which differ from the preceding case need be entered.

2. GENERAL FORMATS FOR INPUT INFORMATION

Basically, there are four sections of input for each problem,

- (1) Alphanumeric title card
- (2) Fixed-point card(s) -- with control information
- (3) Floating-point card(s) -- with control information
- (4) Spectral data cards.

The cards must always be entered in the program in the above order. (See Figure 1.) In this section a description of the general form of each type of input is given. The meaning of the specific input addresses is discussed in the following section (III-3).

2.1 Alphanumeric Title Card

This card may contain any desired alphanumeric information in columns 6 - 78. This card must be the first card in every fit. The information is printed on the output listing.

Fig. 1 Arrangement of input cards for GAUSS.

2.2 Fixed-Point Control Information

The format of each card is as follows: (All words must be right-adjusted.)

<u>CARD</u> <u>COLUMN</u>	<u>MNEMONIC</u> <u>NAME</u>	<u>FORMAT</u>	<u>ITEM</u>
1-2	NPD	I2	Number of items of control information on this card. (i. e., the number of NF items), $1 \leq \text{NPD} \leq 23$.
3	NOL	I1	0 (or blank), this is not the last fixed-point information card. 1, this is the last fixed-point information card.
4-6	NAD	I3	Address of first item on the card. (These addresses are explained in the next section).)
7	----	--	Blank

<u>CARD COLUMN</u>	<u>MNEMONIC NAME</u>	<u>FORMAT</u>	<u>ITEM</u>
8-10	NF	I3	The control information with addresses NAD to NAD + NPD-1. (The card can contain a maximum of 23 pieces of integer information.)
11-13			
.			
.			
.			
74-76			

2.3 Floating-Point Control Information

The format of each card is as follows: (All words must be right-adjusted.)

<u>CARD COLUMN</u>	<u>MNEMONIC NAME</u>	<u>FORMAT</u>	<u>ITEM</u>
1-2	NPD	I2	Number of items of control information (i.e., the number of FF items) on this card, $1 \leq \text{NPD} \leq 7$.
3	NOC	I1	0 (or blank), this is not the last floating-point information card. 1, this is the last floating-point information card.
4-6	NAD	I3	Address of first item on the card. (These addresses are explained in the next section.)
7	- - -	--	Blank
8-17	FF	E10.5	The control information with addresses NAD to NAD + NPD-1. (The card can contain a maximum of 7 pieces of information.)
18-27			
.			
.			
.			
68-77			

2.4 Spectral Data Cards

The spectrum to which the fit is to be made is entered in the following card format:

<u>CARD COLUMN</u>	<u>MNEMONIC NAME</u>	<u>FORMAT</u>	<u>ITEM</u>
1-2	NOCARD	I2	Card number with zero for the number of the first card. All cards must be numbered in sequence.
3-12	YDATA	F7.0	Input data y_i in counts per channel. The first channel is called channel zero and is not used or kept. The following channels are labelled 1, 2, 3, . . . The last data card must have a card number of 51 or less.
13-22			
.			
.			
63-72			

The last card in each data deck must have "60" in columns 1 and 2.

3. EXPLANATION OF INPUT

An explicit enumeration of the fixed-point and floating-point control information and associated addresses follows. An example of the input, showing the cards for three fits to a peak with two Gaussians, is given in Figure 2. A sample input is also listed in the Appendix.

3.1 Fixed-Point Control Information

<u>FIXED-POINT ADDRESS</u>	<u>MNEMONIC NAME</u>	<u>MEANING</u>
1	IGAUSS	Number of Gaussians to be fitted, $1 \leq \text{IGAUSS} \leq 10$.
2	ISTART	First channel in fit, $1 \leq \text{ISTART} \leq \text{IEND}$.
3	IEND	Last channel in fit, $\text{IEND} \leq 511$.
4	ICON1	This variable determines the iteration process used. 0 - Lambda computed in program (see Chapter V). 1 - Lambda supplied as input (see Section II-3.4).
5	IWEIT	This determines the weight to be used (see Section III-4.32). 1 - $w_i = 1.0$ 2 - $w_i = 1/y_i$ 3 - $w_i =$ input list with $1/w_i$ supplied as input 4 - $w_i = 1/y_i$ if $y_{\min} \leq y_i \leq y_{\max}$ $w_i = 1/y_{\min}$ if $y_i < y_{\min}$ $w_i = y_i^2/y_{\max}$ if $y_{\max} < y_i$ 5 - input list with w_i supplied as input.

Title Card																																																																																																													
6.5, DAY										ZIRCONIUM, 9.5										SAMPLE OF										COMPLETE INPUT										12-8										-6.4																																																											
NPD NOL NAD 1GAUSS										ISTART IEND ICON1										IWEIT NOIT ITEST										IOUTPT M1ALF M2ALF KONST										ILINE ILINE IPARIN (1,1)										IPARIN (1,2) IPARIN (1,3) IPARIN (1,4)										IPARIN (1,5) IPARIN (2,1) IPARIN (2,2) IPARIN (2,3)										IPARIN (2,4) IPARIN (2,5)																																							
2,3,1 1 1 2										7,0 8,2 1										2 1,0 1										1 4 1,2 2										2										2 3 3										3 2 2 3										3 3 3																																							
λ Value										E+0,0																																																																																																			
1 3 1 0										E+0,0																																																																																																			
Initial Values										Upper Limits										Lower Limits										Convergence Criteria																																																																															
4 1,2 4,0										E+0,4,6,0										E+0,4,2,0										E+0,4,1,0										E+0,0										First Gaussian										- Y ₀																																																	
4 1,6 7,2										4 E+0,1,7,4										E+0,1,7,0										E+0,1,1,0										E-0,3																				- X ₀																																																	
1 2,0 6,0										E+0,0										Note: Since W ₀ (X ₀), α ₁ (X ₀), and α ₂ (X ₀)																														- W ₀																																																											
1 2,4 2,0										E-0,4										Are Used, The Quantities In This																														- α ₁																																																											
1 2,8 1,0										E-1,1										Region Are Not Needed.																														- α ₂																																																											
4 3,2 5,0										E+0,4,7,0										E+0,4,2,0										E+0,4,1,0										E+0,0										Second Gaussian										- Y ₀																																																	
4 3,6 7,5										7 E+0,4,7,8										E+0,1,7,4										E+0,1,1,0										E-0,3																				- X ₀																																																	
1 4,0 6,0										E+0,2																																								- W ₀																																																											
1 4,4 2,0										E-0,4																																								- α ₁																																																											
1 4,8 1,0										E-1,1																																								- α ₂																																																											
0,0, C,5,2,0,0,0										0,0,1,0,5,2, 0,0,0										9,8,7, 0,0,0,8,5,2										0,0,0,8,0,0, 0,0										1,0,7,5, 0,0,1,4,5										2, 0,0,2,5,9,7, 0										0,2,2,4,3, 0,0,1,4										9,8																																							
0,1, C,0,0,8,7,3																																																																																																													
3,7, C,0,0,7,5,2										0,0,0,5,1,0, 0,0,0										2,1,1, 0,0,0,0,9,2										0,0,0,0,3,7, 0,0										0,0,1,0																																																																					
6,0																																																																																																													
6.5, DAY										ZIRCONIUM, 9.5										FIT WITH W ₀										FREE TO VARY FOR FIRST GAUSSIAN																																																																															
NPD NOL NAD IPARIN (1,3)																																																																																																													
1 1 1,6 2																																																																																																													
4,1 2,0 6,0										Initial Value 0,0,0,E+0,0,1, 0										Upper Limit 0,0,0,E+0,1,3, 0										Lower Limit 0,0,0,E+0,0,1, 0										Convergence Criteria 0,0,0,E-0,3, 1										First Gaussian-W ₀																																																											
6.5, DAY										ZIRCONIUM, 9.5										SAME AS FIRST SAMPLE										WITH SHORT INPUT																																																																															
2,3,1 1 1 2										7,0 8,2 1										2 1,0 1										1 4 1,2 1,2										2										2 3 3										3 2 2 3										3 3 3																																							
1 3 1,0										E+C,0																																																																																																			
1 1,6 7,2										4 E+0,1										Initial Value of X ₀ - First Gaussian																																																																																									
1 1 3,6 7,5										7 E+C,1										Initial Value of X ₀ - Second Gaussian																																																																																									
1 2 3 4 5 6 7 8 9 10										11 12 13 14 15 16 17 18 19 20										21 22 23 24 25 26 27 28 29 30										31 32 33 34 35 36 37 38 39 40										41 42 43 44 45 46 47 48 49 50										51 52 53 54 55 56 57 58 59 60										61 62 63 64 65 66 67 68 69 70										71 72 73 74 75 76 77 78 79 80																																							
PPC-0-D-668R																																																																																																													

PPC-0-6688

Fig. 2 Three sample input decks for GAUSS showing the card formats. The first case illustrates the complete input for a fit to two Gaussians. The second fit is to the same data, but with a w_0 varying. The third case is the same as the first one except the short input form is used.

<u>FIXED-POINT ADDRESS</u>	<u>MNEMONIC NAME</u>	<u>MEANING</u>
6	NOIT	Maximum number of iterations. This is used to prevent excessive use of computer time for non-convergent fits.
7	ITEST	Number of after convergence iterations, usually set equal to 1. This is used to check for possible anomalous convergences.
8	IOUTPT	Output options (see Section III-5). 1 - Short form 2 - Regular form 3 - Diagnostic form
9	M1ALF	Power of alpha 1 term, i.e., m_1 in Equation (6). It must be an even, positive integer.
10	M2ALF	Power of alpha 2 term, i.e., m_2 in Equation (6). It must be an even, positive integer.
11	KONST	Determines which set of coefficients is to be used to compute the functional forms of α_1 , α_2 , and/or w_0 . These relationships are expressed as polynomial equations. The coefficients are stored as functions of the KONST variable. There are two sets of coefficients at present: 5 keV and 10 keV which have been assigned the values of 1 and 2, respectively. 1 - 10 - Compute functional forms (see Section II-3.2). 11 - 20 - compute functional forms and use short input form (see Section III-4.1).
12	ILINE (1)	Line slope control option. 0 - No line slope to be used 1 - Line slope constant 2 - Line slope allowed to vary in fit
13	ILINE (2)	Line intercept control option. 0 - No line intercept to be used 1 - Line intercept constant 2 - Line intercept allowed to vary in fit

The following fixed-point control information all refers to the method in which the Gaussian parameters are to be treated. They can have the values

- 1 - hold parameters constant
- 2 - vary independently
- 3 - use functional form -- this does not apply to y_0 or x_0 (see Section II-3.2).

<u>FIXED-POINT ADDRESS</u>	<u>MNEMONIC NAME</u>	<u>MEANING</u>
14	IPARIN (1,1)	y_0 of first Gaussian
15	IPARIN (1,2)	x_0 of first Gaussian
16	IPARIN (1,3)	w_0 of first Gaussian
17	IPARIN (1,4)	α_1 of first Gaussian
18	IPARIN (1,5)	α_2 of first Gaussian
19-23		Same as above for second Gaussian
24-63		Control constants for Gaussians 3-10.

3.2 Floating-Point Control Information

<u>FLOATING-POINT ADDRESS</u>	<u>MNEMONIC NAME</u>	<u>MEANING</u>
1	YMAX	Maximum y_i value. Required for weighting option 4. (See Section 4.32)
2	YMIN	Minimum y_i value. Required for weighting option 4. (See Section 4.32)
3	HCONT	Value of lambda, present when ICON1 = 1. (See Chapter V and Section II-3.4)
4	XLINE(1,1)	Line slope -- initial value upper limit lower limit convergence criterion
5	XLINE(1,2)	
6	XLINE(1,3)	
7	XLINE(1,4)	
8	XLINE(2,1)	Line intercept -- initial value upper limit lower limit convergence criterion
9	XLINE(2,2)	
10	XLINE(2,3)	
11	XLINE(2,4)	
12	PARIN(1,1,1)	First Gaussian -- initial estimate of y_0 upper limit of y_0 lower limit of y_0 convergence criterion of y_0
13	PARIN(1,1,2)	
14	PARIN(1,1,3)	
15	PARIN(1,1,4)	
16	PARIN(1,2,1)	First Gaussian -- initial estimate of x_0 value upper limit of x_0 lower limit of x_0 convergence criterion of x_0
17	PARIN(1,2,2)	
18	PARIN(1,2,3)	
19	PARIN(1,2,4)	

<u>FLOATING-POINT ADDRESS</u>	<u>MNEMONIC NAME</u>	<u>MEANING</u>
20	PARIN(1,3,1)	First Gaussian -- initial estimate of w_0
21	PARIN(1,3,2)	upper limit of w_0
22	PARIN(1,3,3)	lower limit of w_0
23	PARIN(1,3,4)	convergence criterion of w_0
24	PARIN(1,4,1)	First Gaussian -- initial estimate of α_1
25	PARIN(1,4,2)	upper limit of α_1
26	PARIN(1,4,3)	lower limit of α_1
27	PARIN(1,4,4)	convergence criterion of α_1
28	PARIN(1,5,1)	First Gaussian -- initial estimate of α_2
29	PARIN(1,5,2)	upper limit of α_2
30	PARIN(1,5,3)	lower limit of α_2
31	PARIN(1,5,4)	convergence criterion of α_2
32-51		Same information for second Gaussian
52-211		Gaussian parameter information for Gaussians 3 - 10.

4. VARIATIONS OF THE STANDARD INPUT FORM

To reiterate, a standard input deck consists of four types of cards which must be in the following order:

- (1) Alphanumeric title card
- (2) Fixed-point control information card(s)
- (3) Floating-point control information card(s)
- (4) Spectral data card(s)

However, in many cases the complete input described above is not necessary.

4.1 Short Input Option

An input option has been incorporated whereby the initial estimate of x_0 can be supplied rather than all of the Gaussian parameter information (floating-point addresses 12-31). The program then determines the initial estimates of the remaining four parameters, as well as the upper and lower limits and convergence criteria of all of the parameters. An example of this input form is given in the third part of Figure 2. This option can be exercised by allowing the value of the fixed-point variable KONST (address 11) to be a number greater than 10.

The necessary quantities are taken to be:

4.11 Initial Values (prime indicates initial estimate)

$$x_0' = \text{input value}$$

$$y_0' = y_i - (a x_i + b) \text{ where } y_i \text{ is experimental count in channel nearest to } x_0'.$$

$$w_o' = w_o(x_o') \text{ from Equation (9)}$$

$$\alpha_1' = \alpha_1(x_o') \text{ from Equation (10)}$$

$$\alpha_2' = \alpha_2(x_o') \text{ from Equation (11)}$$

4.12 Upper Limits

$$y_o^u = 2.0 \cdot y_o'$$

$$x_o^u = 2.0 + x_o'$$

$$w_o^u = 2.0 \cdot w_o'$$

$$\alpha_1^u = 1.0 \times 10^2 \cdot \alpha_1'$$

$$\alpha_2^u = 1.0 \times 10^2 \cdot \alpha_2'$$

4.13 Lower Limits

$$y_o^l = 0.3 \cdot y_o'$$

$$x_o^l = x_o' - 2.0$$

$$w_o^l = 0.5 \cdot w_o'$$

$$\alpha_1^l = 1 \times 10^{-3} \cdot \alpha_1'$$

$$\alpha_2^l = 1 \times 10^{-3} \cdot \alpha_2'$$

4.14 Convergence Criteria

$$y_o^c = 1.0$$

$$x_o^c = 1 \times 10^{-3}$$

$$w_o^c = 1 \times 10^{-3}$$

$$\alpha_1^c = 1 \times 10^{-4} \cdot \alpha_1'$$

$$\alpha_2^c = 1 \times 10^{-4} \cdot \alpha_2'$$

4.2 Subsequent Fits

Another input option is the "change case" option. A "change case" is one which is the same, except for minor changes, as the one preceding it in a set of problems run serially on the computer. In order to run change cases, only those control words which are different from the preceding case need be entered.

However, when running change cases caution should be exercised because unwanted data from preceding cases may be carried over. Since FORTRAN considers blanks to be zeros, care must be taken so that the number of words specified in columns 1 and 2 actually appear on the card, or zeros may be stored in locations where they are not wanted.

If more than one control word is entered on a card, the words succeeding the first are stored in consecutive addresses. Therefore, if the values to be changed do not have consecutive addresses they should be entered on separate cards.

4.21 Fixed- and Floating-Point Control Information. If more than one fixed- or floating-point card is to be read, the associated cards may be in any order. The only requirement is that the last card of each type have a "1" punch in column 3. However, the fixed-point information cards must appear before the floating-point cards in the deck.

4.22 Spectral Data. Data cards must be entered in consecutive order with the first card numbered "00" in columns 1-2. The last card must be a "60" card ("60" in columns 1-2). However, when running change cases for fits to the same data, only a "60" card is needed in place of the entire data deck. (See Figure 2.)

4.3 Weighting

Normally, the program determines the weighting factors from the data. However, there are two options for which the information necessary to determine the weight factors are read in on cards. These are the weighting options 3 or 5 (IWEIT = 3 or 5).

4.31 Reading Weights. For these two options the weights are on cards in the following format.

<u>CARD COLUMN</u>	<u>MNEMONIC NAME</u>	<u>FORMAT</u>	<u>ITEM</u>
1-2	I1	I2	Card number, must be 1 on first card
3-10	--	--	Blank
11-20	WDATA	E10.5	Weighting data Values of weights w_i or $1/w_i$ depending on option chosen
21-30			
.			
.			
.			
71-80	WDATA		

The last card of each weight deck must have "80" in columns 1-2. When running change cases utilizing the same weight deck, an "80" card may be substituted for the entire deck.

4.32 Weighting. The weighting vector w_i in Equation (1) should be chosen such that $\sqrt{1/w_i}$ is a good estimate of the standard deviation associated with the experimental count y_i . If this condition is satisfied and the y_i do, in fact, represent a Gaussian function, an estimate of the standard deviations associated with the calculated parameters (y_0 , x_0 , w_0 , α_1 , and α_2) can be made. Although there is always some doubt about the validity of these estimates, the use of other weights makes the error estimates more questionable. Therefore, the user should exercise some caution in the selection of the weights to be used.

If the y_i are counts for fixed time of random events they are expected to have a Poisson probability distribution. In this case the standard deviation associated with the y_i is approximately $\sigma_i = \sqrt{y_i}$. Then the best weight would be $1/\sigma_i^2 = 1/y_i$. (This assumes y_i is a good estimate of the mean for a large number of similar counts.) Therefore, the option $IWEIT = 2$ is usually used.

The options $IWEIT = 3$ and $IWEIT = 5$ allow the user to supply weights if the internal formulas are not satisfactory. This may be the case if a large background has been subtracted from the original data, or other manipulations of the original data have been made.

The $IWEIT = 0$ option for which all weights are the same is only used for exploring the effect on the results of variations in the weights.

The option $IWEIT = 4$ is an intermediate case between options $IWEIT = 2$ and $IWEIT = 3$ or 5. This allows the user to use the $1/y_i$ option except for very small and/or very large counts. For large counts, the statistical uncertainty may become smaller than the systematic errors of the counting system. In this case it is possible to set a minimum fractional error. For example, if $y_{max} = 10^4$, then the percentage error is $\sigma_i/y_i = (y_i/\sqrt{y_{max}})(1/y_i) = 10^{-2}$ or 1 percent for all $y_i \geq 10^4$. For small values of y_i , two effects may be present. As pointed out by Ferguson^[4], the $\sqrt{y_i}$ does not represent a good estimate of σ_i since y_i is not a good estimate of the mean value of the pertinent Poisson distribution. Ferguson^[4] has solved this problem by setting σ_i equal to the square root of the calculated count $\bar{y}_i$. This method requires an iteration procedure in which the weights vary as the Gaussian parameters vary. The option available herein can be used to achieve approximately the same effect for any particular fit. Secondly, spectra are often fitted after the subtraction of backgrounds or other components. In this case, σ_i is much larger than $\sqrt{y_i}$, but it may be possible to satisfactorily approximate it by the use of this option.

4.4 Summary

Table I contains a summary of the information required to run the GAUSS program using either the standard input or the change case option.

TABLE I

SUMMARY OF INPUT DECK FORMS

Type Case	Type Cards						
	[1] Title Card	[2] Fixed-Point Information	[3] Floating- Point Information	[4] Spectra		[5] Weighting	
				Data	"60"	Data	"80"
Standard	X	X	X	X	X	X*	X*
Change fixed-point only	X	X	B	--	X	--	X*
Change floating-point only	X	B	X	--	X	--	X*
Change fixed and floating	X	X	X	--	X	--	X*
Change data only	X	B	B	X	X	--	X*

Table Note: 1. X = input required

B = blank card only

-- = no input required

X* = required only when IWEIT = 3 or 5

2. The bracketed numbers [n] indicate the required order of the various types of data. The last card of the fixed-point data and the last card of the floating-point data must have a "1" in column 3. The data cards and the weighting data cards must be in consecutive order.

5. OUTPUT DESCRIPTION

5.1 Output Edit

IOUTPT governs the output as follows:

Value of
IOUTPT

0

Short form:

1. Output of all of the input data.
2. Weighting factors for channels fitted.
3. Parameter values for the iteration at which convergence took place, χ^2 , and $\chi^2/(n-m)$.
4. Estimated errors in the final parameters.
5. Areas and estimated errors in the areas of the photopeaks.
6. A channel listing of x_i , y_i , $\bar{y}_i$, $\bar{y}_i - y_i$, $\sigma_i = 1/\sqrt{w_i}$, $\frac{y_i - \bar{y}_i}{\sigma_i}$, and $\left(\frac{y_i - \bar{y}_i}{\sigma_i}\right)^2$.

Value of
IOUTPT

- 1 Regular form:
1. All items of the short form.
 2. Parameter values, χ^2 , and $\chi^2/(n-m)$ at the end of each iteration.
- 2 Diagnostic form:
- In addition to the regular form, the normalized normal equation matrix, the inverse matrix, and the product of these matrices are listed for each iteration.

An example of the regular output form is shown in the Appendix.

5.2 Error Indicators

The following error messages are printed as a result of input errors or singular matrices. When such an error is detected the comment is written on the output tape and the problem and all succeeding cases are skipped, except in the case of a singular matrix. In this case the program skips to the next case.

5.21 Error Comments Pertinent to Fixed-Point Input.

Comment - INPUT ERROR -- NUMBER OFFIXED-POINTVALUES
 TOO LARGE, NUMBER = XXX.

Meaning - The number of fixed-point control words on one card
 is greater than 23. NUMBER identifies the erroneous
 value.

Comment - INPUT ERROR -- XXX IS NOT A FIXED-POINT
 ADDRESS.

Meaning - A fixed-point address larger than 63 (NAD) is indicated.
 The numeric field identifies the input value of the
 address.

5.22 Error Comments Pertinent to Floating-Point Input

Comment - INPUT ERROR -- NUMBER OF FLOATING-POINT
 VALUES TOO LARGE, NUMBER = XXX.

Meaning - If NPF is greater than 7, an error exit occurs.
 The item NUMBER identifies erroneous value.

Comment - INPUT ERROR -- XXX IS NOT A FLOATING-POINT
 ADDRESS.

Meaning - A floating-point address (columns 4-6) which is zero,
 negative, or greater than 211, occurs. The numeric
 field indicates the value of the address.

5.23 Error Comments Pertinent to Data Input

Comment - INPUT ERROR -- FIRST YDATA CARD IS MISSING
 (CARD NUMBER 00).

Meaning - The first card must be "00" (columns 1-2). If this error occurs and it has been ascertained that the "00" card is present, it is advisable to check the fixed- and/or floating-point cards. Check to make certain that the last floating-point card contains a "1" in column 3.

Comment - INPUT ERROR -- YDATA CARDS ARE NOT IN PROPER SEQUENCE. THE CARD NUMBER SHOULD BE XXX.

Meaning - The analyzer data cards must be in ascending order (beginning with 00) with respect to card number. The numeric field identifies the true card number.

5.24 Error Comment Pertinent to Weighting Data Input

Comment - INPUT ERROR -- WDATA CARDS ARE NOT IN PROPER SEQUENCE. THE CARD NUMBER SHOULD BE XXX.

Meaning - The weighting data cards must be in ascending order with respect to card number (columns 1-2). The numeric field identifies the true card number.

5.25 Error Comment Pertinent to Computation

Comment - ERROR - PARTIAL DERIVATIVE MATRIX SINGULAR. CONTINUATION NOT POSSIBLE.

Meaning - A singular matrix is one that has no inverse. When the program encounters a singular matrix, the program prints out the comment and skips to the next problem.

IV. EXAMPLES OF PROBLEMS

1. USES

This program has been used for several different nuclear physics problems. Although the mathematical aspects of these examples are similar, they are described to demonstrate the usefulness of the program and its options.

There are three main types of problems for which the program has been used. These are the determination (a) of photopeak positions, and thereby gamma-ray energies, (b) of the shapes of photopeaks, and (c) of the areas and positions of the components of photopeaks containing more than one gamma ray. All three of these uses have been applied to gamma-ray spectra from both NaI(Tl) scintillation spectrometers and lithium-drifted germanium detectors. Samples of each of these problems are given in the next three sections.

2. PHOTOPEAK POSITIONS AND GAMMA-RAY ENERGIES

The two spectra shown in Figure 3 were used for the determination of the energy of the 269-keV gamma ray from the decay of Pt^{197} . The positions of the four photopeaks above 200 keV were determined. The positions from one spectrum were then multiplied by a constant so that the two Cs^{137} photopeaks were at the same channel. The energy of the gamma-ray from Pt^{197} was then determined from that of the gamma-ray of Hg^{203} and the difference in their positions. The results of two such comparisons are given in Table II. The uncertainties given are the estimated standard deviations obtained from the fit and do not contain any estimate of the systematic errors involved. These data would indicate that it is possible, under ideal conditions, to determine gamma-ray energies to an accuracy of about 0.1 percent.

A gamma-ray spectrum from a Ca^{47} sample is shown in Figure 4. A series of such spectra were taken over a period of four weeks or seven half-lives. For each spectrum the four photopeaks were fitted to determine their positions and areas. The Compton distribution under the lower energy gamma rays were approximated by straight lines of zero slope. The results for the positions are given in Table III. The ratios of the photopeak positions are given to indicate their consistency. It is of interest to note that these ratios vary by about the same amount as their estimated uncertainties. The last entry in the table is from a spectrum which included Cs^{137} . The position of its photopeak can be used to establish the pulse-height scale. If the energy pulse-height relationship were known with sufficient accuracy, these results would again be consistent with the determination of gamma-ray energies with an accuracy of about 0.1 percent.

The ratios of the Ca^{47} photopeak areas are shown in Table IV. Here the variation from the mean is a few percent and is somewhat larger than the estimated uncertainties. The intensity of the 0.16-MeV peak is not included because it is associated with the daughter, Sc^{47} , activity and, therefore, changes relative intensity.

Fig. 3 Spectra used to determine the energy of the 269-keV gamma ray from the decay of Pt-197.

TABLE II

COMPARISON OF ENERGIES OF Hg-203 AND Pt-197 GAMMA RAYS

Experimental Data	Run No. 1		Run No. 2	
	Hg-203 + Cs-137	Pt-197 + Cs-137	Hg-203 + Cs-137	Pt-197 + Cs-137
Cs-137 peak (channels)	131.16 $\pm$ 0.04	131.11 $\pm$ 0.05	131.60 $\pm$ 0.03	131.42 $\pm$ 0.06
Hg-203 peak (channels)	57.17 $\pm$ 0.01		57.43 $\pm$ 0.01	
Pt-197 peak (channels)		55.14 $\pm$ 0.03		55.30 $\pm$ 0.07
<u>Comparison of 269- and (279.12 $\pm$ 0.05)-keV Transitions</u>				
keV/channel at 279 and 269 keV		4.88 $\pm$ 0.01		4.86 $\pm$ 0.01
Difference Hg-203 - Pt-197				
(channels)		2.02 $\pm$ 0.04		2.08 $\pm$ 0.08
(keV)		9.86 $\pm$ 0.20		10.11 $\pm$ 0.40
Average energy of Pt-197 transition			269.17 $\pm$ 0.2	

3. PHOTOPEAK SHAPES

In connection with a general interest in the analysis of gamma-ray spectra, a study has been made of the shapes of photopeaks from a particular NaI scintillation spectrometer. From the results of the first part of this study it was decided to use the powers $m_1 = 4$ and $m_2 = 12$ in Equation (6). Then the variation in α_1 , α_2 , and w_0 as a function of x_0 was determined. The results are shown in Figures 5 and 6. The associated curves represent the functions given by Equations (9), (10), and (11). These are the relationships which are built into the program. (See Section II-3.2.)

In Table V a comparison is given between the quality of the fit number $\chi^2/(n-m)$ for fits to several photopeaks with a Gaussian and with two modified-Gaussian expressions. The added terms are seen to improve the fits significantly. For one peak the three corresponding fits are shown in Figure 7.

4. DECOMPOSITION OF COMPLEX PEAKS

In Figure 8 is shown a spectrum of Sc^{48} . The three gamma rays at 0.99, 1.04, and 1.31 MeV are known to represent gamma-ray transitions of equal intensity. The relative gamma-ray intensities computed from fits to the peaks of this spectrum are shown in column 4 of Table VI. The accuracy of the results is affected adversely by the Compton edge of the 1.31-MeV gamma ray which lies under the 1.0-MeV peak and by the presence of some Sc^{46} contaminant. However, the calculated intensities are within five percent of being equal which is considered satisfactory in the analysis of a complex photopeak.

In the analysis of the 1.0-MeV peak, the values of α_1 , α_2 , and w_0 were determined from the relationships in Equations (9), (10), and (11). For a complex

Fig. 4 One of a series of Ca^{47} spectra used to determine gamma-ray energies and relative intensities.

TABLE III

RESULTS OF FITS TO Cs-47 SPECTRA-PHOTOPEAK POSITIONS

Spectrum	Peak Areas (In units of 10^4 counts)			Relative Peak Areas (1300-keV peak taken as 1.00)	
	1300 keV	800 keV	500 keV	800 keV	500 keV
1	52.58 ± 0.08	7.40 ± 0.03	11.61 ± 0.01	0.141 ± 0.001	0.221 ± 0.001
2	45.13 ± 0.07	6.17 ± 0.03	9.39 ± 0.03	0.137 ± 0.001	0.208 ± 0.001
3	28.49 ± 0.05	4.07 ± 0.03	6.06 ± 0.03	0.143 ± 0.002	0.213 ± 0.001
4	12.39 ± 0.07	1.61 ± 0.02	2.73 ± 0.04	0.130 ± 0.002	0.220 ± 0.004
5	0.80 ± 0.01	---	---	---	---

TABLE IV

RESULTS OF FITS TO Cs-47 SPECTRA-PHOTOPEAK AREAS

Spectrum	Peak Positions				Relative Peak Positions (1300 position taken as 1.00)		
	1300 keV	800 keV	500 keV	160 keV (From Sc-47)	800 keV	500 keV	160 keV
1	126.96 ± 0.01	80.33 ± 0.02	49.31 ± 0.01	16.60 ± 0.02	0.6327 ± 0.0002	0.3884 ± 0.0001	0.1307 ± 0.0002
2	126.02 ± 0.01	79.66 ± 0.02	48.93 ± 0.01	16.48 ± 0.01	0.6321 ± 0.0002	0.3883 ± 0.0001	0.1308 ± 0.0001
3	126.40 ± 0.01	79.88 ± 0.04	49.08 ± 0.02	16.54 ± 0.01	0.6320 ± 0.0004	0.3883 ± 0.0002	0.1309 ± 0.0001
4	126.82 ± 0.02	80.11 ± 0.06	49.21 ± 0.04	16.57 ± 0.01	0.6317 ± 0.0007	0.3880 ± 0.0004	0.1307 ± 0.0001
5	125.62 ± 0.07	Very Weak	Very Weak	16.48 ± 0.01	---	---	0.1312 ± 0.0002
6	127.16 ± 0.01	80.36 ± 0.05	49.23 ± 0.05	16.73 ± 0.01	0.6320 ± 0.0005	0.3871 ± 0.0005	0.1316 ± 0.0001

peak this is generally necessary since the data do not uniquely determine these quantities. Thus, if they are allowed to vary independently, the resulting values will often not be physically reasonable.

Three other spectra for which fits to photopeaks with two Gaussians were carried out are shown in Figure 9. The results for the relative gamma-ray intensities are given in Table VII along with the values previously reported. Only in the case of Sb^{125} has a good determination been made previously. For all three cases, and especially Mo^{99} , the values computed here are probably as accurate as any previous values.

Fig. 5 Variation of α_1 and α_2 with photopeak positions for a scintillation spectrometer on the 5- and 10-keV per channel gain scales.

Fig. 6 Variation of w_0 with photopeak position on 5- and 10-keV gain scales.

TABLE V

COMPARISON OF THE QUALITY OF FITS FOR A GAUSSIAN
AND MODIFIED GAUSSIANS WITH ONE OR TWO α TERMS

Isotope	Number of Data Points Used	Gaussian	$\frac{R^2_{\min}}{n - m}$	
			One α Term $m_1 = 8$ $\alpha_2 = 0$	Two α Terms $m_1 = 4$ $m_2 = 12$
In-115m	10	2.1	1.2	0.9
In-113m	10	8.4	1.3	1.2
Be-7	12	14	1.4	1.5
Sr-85	12	19	2.3	1.7
Y-91m	13	5.9	0.4	0.4
Cs-137	15	25	2.7	1.7
Nb-95	17	35	2.4	1.1
Mn-54	17	61	3.6	2.3
Nb-92	19	40	2.4	1.6
Zn-65	18	47	5.2	1.2
A-41	20	136	7.5	2.0
V-52	22	70	5.7	1.6
K-42	22	45	5.2	1.1
Al-28	25	36	4.9	1.0
Y-88	24	---	---	2.3
Na-24	30	43	6.4	1.5

Fig. 7 Comparison of fits with zero, one, and two α -terms to photopeak of Cs-137 spectrum.

Fig. 8 Spectrum from Sc-48 sample. Peaks are labeled in MeV and the pulse height (ordinate) is in units such that channel 20 is called 200.

TABLE VI
RESULTS FOR Sc-48 SPECTRUM

Energy (MeV)	Photopeak Area	Photopeak Efficiency Correction	Relative Gamma-Ray Intensity	$\chi^2/(n-m)$
0.99	$(154.7 \pm 2.7) \times 10^3$	1.408	$0.954 \pm 0.025[a]$	2.9
1.04	$(155.2 \pm 2.7) \times 10^3$	1.471	1.000	
1.31	$(127.2 \pm 0.5) \times 10^3$	1.852	1.032 ± 0.015	1.2

[a] These uncertainties are computed from the errors in the areas only. That is, for this purpose the photopeak efficiency correction is assumed to be exact.

Fig. 9 Other spectra in which a peak was fitted with two Gaussians. Results are in Table VII.

TABLE VII
ANALYSIS OF COMPLEX PEAKS

Spectrum	Positions	Peak Areas	Photopeak Efficiency Correction	Relative Gamma-Ray Intensity		$\chi^2/(n-m)$
				These Data[a]	Previous Report	
Mo-99	74.93 ± 0.06	$(11.16 \pm 0.21) \times 10^3$	110.5	3.09 ± 0.24	[b]	0.4
	79.00 ± 0.14	$(3.45 \pm 0.22) \times 10^3$	115.6	1.0		
Zr-95	72.53 ± 0.03	$(23.73 \pm 0.38) \times 10^4$	106.4	1.0	[c]	0.9
	75.71 ± 0.02	$(30.53 \pm 0.41) \times 10^4$	110.5	1.34 ± 0.04		
Sb-125	42.88 ± 0.04	$(96.7 \pm 1.4) \times 10^3$	65.4	2.76 ± 0.14	3.1[d]	5.5
	46.42 ± 0.08	$(37.7 \pm 1.5) \times 10^3$	70.4	1.0		

[a] These uncertainties included only the errors in the areas. That is, for this purpose the correction for photopeak efficiency is assumed to be exact.

[b] Values in Reference 5 range from 2.0 to 9.1.

[c] Beta-ray branching data in Reference 5 yields 1.0, 1.25, 1.56, and 0.78 for this ratio.

[d] See Reference 5.

V. PARABOLIC-FITTING MODIFICATION OF LEAST-SQUARES METHOD

1. GENERAL PROCEDURE

The factor λ in Equation (13) may be used in an attempt to speed up the process of finding the best values of the parameters. Normally, it is entered as input and has a value ≈ 1.0 . However, it is possible to have the program determine the value of λ . In this case, at each iteration an optimum value is calculated.

Assume that the program is at the n th iteration and the values Δp_j , ($j = 1, 2, \dots$), have been computed. The old parameter estimates are $p_{j,n-1}$ and the new ones are

$$p_{j,n}(\lambda) = p_{j,n-1} + \lambda \Delta p_j.$$

Then for a prescribed set of values of λ , the function

$$Q(\lambda) = \sum_i w_i (y_i - \bar{y}_i)^2$$

where $\bar{y}_i = \bar{y}_i(p_{j,n}(\lambda))$ is calculated. The value of λ is then taken as that at which $Q(\lambda)$ is a minimum.

2. APPROXIMATION OF THE MINIMUM

The procedure for approximating the minimum is as follows. Initially the function $Q(\lambda)$ is calculated with $\lambda = 1.0$ and $\lambda = 0.5$. Then, if $Q(0.5) \leq Q(1.0)$, the λ value is halved again and the new function, $Q(0.25)$, is compared with $Q(0.5)$. If $Q(0.25) > Q(0.5) \leq Q(1.0)$, these three Q values are fitted with a second degree polynomial $Q(\lambda) = a_0 + a_1\lambda + a_2\lambda^2$. The value of λ at the minimum of this parabola, $\bar{\lambda} = -a_1/2a_2$, is used to calculate the initial parameters for the next iteration. If $Q(0.25) < Q(0.5)$, the process of halving λ is repeated until Q increases or $\lambda = 1/64$. In either case, the last three values are fitted with a second degree polynomial, and the value of λ at the minimum is used.

However, if $Q(0.5) > Q(1.0)$, the function $Q(2.0)$ is compared with $Q(1.0)$. In an analogous manner λ is doubled until the last $Q(\lambda)$ is greater than the previous one or until $\lambda = 2^5$. As in the previous case, the last three values of $Q(\lambda)$ are used to determine a second degree polynomial whose minimum provides the value of $\bar{\lambda}$.

3. TESTS FOR VALIDITY OF CALCULATED λ

The value of $Q(\bar{\lambda})$ computed above should be smaller than any $Q(\lambda)$ computed in the process of reaching the minimum. A comparison is made and if this is not true the value of λ which did, in fact, yield the smallest Q is used.

If, for any λ , $a_{p_j, n}$ is outside its allowed range, it is set at the corresponding limit. $Q(\lambda)$ is calculated with this limiting parameter value.

If the doubling process ($\lambda > 1$) is used, a check is made to determine if all the parameters, $p_{j, k}$, exceed their limits. When this condition occurs, the value of λ is set equal to one.

VI. SUBROUTINES AND FLOW CHARTS

1. SUBROUTINE

The GAUSS program is written as a package of subroutines. The purpose of each subroutine is summarized below. Pertinent data are transferred from one subroutine to another by means of "COMMON" storage.

It is not necessary to have the subroutine decks in any special order. However, it is advisable to have the "INPUT subroutine" as the first deck unless the \$ENTRY control card specifies "INPUT" as being the entry point for the program (INPUT starting in column 16).

<u>Subroutine</u>	<u>Description</u>
-------------------	--------------------

INPUT	This subroutine is the entry point for the GAUSS program. It reads the input information from the tape, stores it in work areas, checks it, and starts the execution of the fit.
-------	--

GAUSS	The purpose of this subroutine is to perform the iterations and test for convergence. The calculation of the partial derivatives and formation of the partial derivative matrix is accomplished here. The parabolic process of determining $\bar{\lambda}$ is incorporated in this subroutine.
-------	--

ERREA	Computes the area of the photopeak and the estimated error in the area.
-------	---

PARMTR	Calculates the necessary Gaussian parameter information as a function of channel, x_0 , if the variable KONST is ≥ 11 .
--------	--

PART1 } PART2 } PART3 }	Evaluates $\partial \alpha_1 / \partial x_0$, $\partial \alpha_2 / \partial x_0$, and $\partial w_0 / \partial x_0$, respectively.
-------------------------------	---

COEFF	Storage area for coefficients of the functional forms $\alpha_1(x_0)$, $\alpha_2(x_0)$, and $w_0(x_0)$.
-------	--

MATMPY	Matrix multiplication subroutine.
--------	-----------------------------------

MAINS } DPSUB }	Double precision matrix inversion subroutine package.
--------------------	---

BOUND	Tests parameters to determine if they are within the prescribed upper and lower limits.
-------	---

XOVARI	A composite subroutine which evaluates the functional forms of $\alpha_1(x_0)$, $\alpha_2(x_0)$, and $w_0(x_0)$ by calling the following subroutines:
--------	---

ALPHA1	Evaluates $\alpha_1(x_0)$
ALPHA2	Evaluates $\alpha_2(x_0)$
OMEGA	Evaluates $w_0(x_0)$

<u>Subroutine</u>	<u>Description</u>
-------------------	--------------------

FCN	Evaluates the modified-Gaussian function to determine y values; that is, it evaluates Equation (6).
-----	---

OUTPUT	Output routine which prints out input data and iteration data, computes and prints estimated errors in fitted parameters, computes and prints $\bar{y}$, $(y-\bar{y})$, $\sigma_i = 1/\sqrt{w_i}$, $(y_i-\bar{y}_i)/\sigma_i$, and $\left(\frac{y_i-\bar{y}_i}{\sigma_i}\right)^2$ for each data point in the fit.
--------	--

2. FLOW CHARTS

PPCo.-C-6825

PPCo.-C-6827

PPCo.-C-6828

PPCo.-8-6829

PPCo -C-6830

PPCo-C-6831

PPCo.-C-6832

PPCo.-C-6833*

PPCo. - C-6834

VII. REFERENCES

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APPENDIX

SAMPLE INPUT, OUTPUT, AND FORTRAN LISTINGS

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1. SAMPLE INPUT -- SHORT FORM

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65 DAY ZIRCONIUM 95
231 1 2 70 82 1 2 10 1 1 4 12 12 2 2 3 3 3 2 2 3 3 3
1 3 1.0 E+00
1 16 7.24E+01
11 36 7.57E+01
0 000000 012500 011833 010478 010102 009645 009353 009252 009453 009438
1 009188 009201 009144 009329 009385 009612 009715 010013 010767 011641
2 011852 011438 010627 010196 010203 010393 010346 010522 010580 010291
3 010215 010348 010076 010131 010173 010013 010005 009975 010045 010004
4 010090 010169 010036 010141 010168 010443 010485 010575 010706 010832
5 011039 010933 010504 009893 008661 007584 006150 004955 004117 003346
6 002756 002402 002268 002233 002282 002556 003441 005395 009441 016705
7 026936 039891 053267 062623 068258 067456 060212 048693 035246 022388
8 012793 006598 003000 001337 000648 000322 000181 000100 000092 000052
9 000047 000063 000051 000050 000049 000040 000049 000020 000039 000043
10 000035 000033 000027 000045 000037 000030 000040 000015 000021 000036
60

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2. SAMPLE OUTPUT

7040 NON-LINEAR MULTIPLE-MODIFIED GAUSSIAN-FITTING PROGRAM

65 DAY ZIRCONIUM 95

PROGRAM CONTROL DATA
NUMBER OF GAUSSIANS***** 2
FIRST CHANNEL IN FIT 70
LAST CHANNEL IN FIT***** 82
MAXIMUM NUMBER OF ITERATIONS 10
NUMBER OF ITERATIONS AFTER CONVERGENCE* 1
WEIGHTING***** 1/Y
ITERATION PROCESS LAMBDA =1.000
OUTPUT***** REGULAR

POWERS OF THE ALPHA TERMS***** 4 AND 12

GAUSSIAN PARAMETER INFORMATION

COEFFICIENTS FOR COMPUTING THE FUNCTIONAL FORMS OF THE PHOTOPEAK PARAMETERS

	HALF-WIDTH	-1.4816000E 00	1.0785000E 00	-2.7944000E-02	1.2692000E-03	0.	0.
ALPHA1	-1.1535900E 01	1.1495400E 01	-5.1163000E 00	6.4880000E-01	0.	0.	0.
ALPHA2	1.4652300E 01	-3.1613800E 01	1.4415000E 01	-2.6263000E 00	0.	0.	0.

GAUSSIAN PARAMETER VALUES

GAUSSIAN	PARAMETER	OPTION	INITIAL VALUE	UPPER LIMIT	LOWER LIMIT	CONVERGENCE CRITERION
1	HEIGHT	VARIED	5.32670E 04	1.06534E 05	1.59801E 04	1.00000E 00
1	CHANNEL	VARIED	7.24000E 01	7.44000E 01	7.04000E 01	1.00000E-03
1	HALF-WIDTH	CALCULATED	5.85827E 00	1.17165E 01	2.92914E 00	1.00000E-03
1	ALPHA1	CALCULATED	2.09092E-04	2.09092E-02	2.09092E-07	2.09092E-08
1	ALPHA2	CALCULATED	6.64164E-12	6.64164E-10	6.64164E-15	6.64164E-16
2	HEIGHT	VARIED	6.02120E 04	1.20424E 05	1.80636E 04	1.00000E 00
2	CHANNEL	VARIED	7.57000E 01	7.77000E 01	7.37000E 01	1.00000E-03
2	HALF-WIDTH	CALCULATED	6.01351E 00	1.20270E 01	3.00675E 00	1.00000E-03
2	ALPHA1	CALCULATED	2.01485E-04	2.01485E-02	2.01485E-07	2.01485E-08
2	ALPHA2	CALCULATED	5.25515E-12	5.25515E-10	5.25515E-15	5.25515E-16

DATA

	0	1	2	3	4	5	6	7	8	9
0	0.	12500.	11833.	10478.	10102.	9645.	9353.	9252.	9453.	9438.
10	9188.	9201.	9144.	9329.	9385.	9612.	9715.	10013.	10767.	11641.
20	11852.	11438.	10677.	10196.	10203.	10383.	10346.	10522.	10580.	10291.
30	10215.	10348.	10076.	10131.	10173.	10013.	10005.	9975.	10045.	10004.
40	10090.	10169.	10076.	10141.	10168.	10443.	10485.	10575.	10706.	10832.
50	11039.	10933.	10574.	9893.	8661.	7584.	6150.	4955.	4117.	3346.
60	2756.	2402.	2268.	2233.	2282.	2556.	3441.	5395.	9441.	16705.
70	26936.	39891.	53267.	62623.	68258.	67456.	60212.	48693.	35246.	22388.
80	12793.	6598.	3070.	1337.	648.	322.	181.	100.	92.	52.
90	47.	63.	27.	50.	49.	40.	49.	20.	39.	43.
100	35.	33.	27.	45.	37.	30.	40.	15.	21.	36.

WEIGHTING VALUES FORMAT = CHANNEL,WEIGHT

70	3.71250E-05	71	2.50683E-05	72	1.87733E-05	73	1.59686E-05	74	1.46503E-05
75	1.48245E-05	76	1.66080E-05	77	2.05368E-05	78	2.83720E-05	79	4.46688E-05
80	7.81677E-05	81	1.51561E-04	82	3.33333E-04				

ITERATION CALCULATIONS (** INDICATES FITTED LAMBDA VALUE)

ITERATION	LAMBDA	CHI**2	CHI**2/NDF	GAUSSIAN***	HEIGHT	CHANNEL	HALF-WIDTH	ALPHA1	ALPHA2
0.		6.406660E 04	7.118511E 03						
				1	5.326700E 04	7.240000E 01	5.858274E 00	2.0909E-04	6.6416E-12
				2	6.021200E 04	7.570000E 01	6.013506E 00	2.0149E-04	5.2552E-12

ITERATION	LAMBDA	CHI**2	CHI**2/NDF				
1	1.000E 00	1.922120E 01	2.135689E 00				
	GAUSSIAN*** PARAMETERS*	GAUSSIAN 1 2	HEIGHT 3.643471E 04 4.684018E 04	CHANNEL 7.246742E 01 7.568902E 01	HALF-WIDTH 5.861477E 00 6.012995E 00	ALPHA1 2.0894E-04 2.0151E-04	ALPHA2 6.6093E-12 5.2592E-12

* ITERATION 1 COMPLETED *

ITERATION	LAMBDA	CHI**2	CHI**2/NDF				
2	1.000E 00	1.199782E 01	1.333092E 00				
	GAUSSIAN*** PARAMETERS*	GAUSSIAN 1 2	HEIGHT 3.649092E 04 4.678840E 04	CHANNEL 7.250122E 01 7.568693E 01	HALF-WIDTH 5.863082E 00 6.012848E 00	ALPHA1 2.0886E-04 2.0152E-04	ALPHA2 6.5931E-12 5.2599E-12

* ITERATION 2 COMPLETED *

ITERATION	LAMBDA	CHI**2	CHI**2/NDF				
3	1.000E 00	1.199729E 01	1.333032E 00				
	GAUSSIAN*** PARAMETERS*	GAUSSIAN 1 2	HEIGHT 3.649474E 04 4.678545E 04	CHANNEL 7.250128E 01 7.568695E 01	HALF-WIDTH 5.863085E 00 6.012898E 00	ALPHA1 2.0886E-04 2.0152E-04	ALPHA2 6.5931E-12 5.2599E-12

* ITERATION 3 COMPLETED *

ITERATION	LAMBDA	CHI**2	CHI**2/NDF				
4	1.000E 00	1.199730E 01	1.333034E 00				
	GAUSSIAN*** PARAMETERS*	GAUSSIAN 1 2	HEIGHT 3.649473E 04 4.678546E 04	CHANNEL 7.250128E 01 7.568695E 01	HALF-WIDTH 5.863085E 00 6.012898E 00	ALPHA1 2.0886E-04 2.0152E-04	ALPHA2 6.5931E-12 5.2599E-12

* CONVERGENCE CRITERION HAS BEEN MET. 1 ITERATIONS WILL BE RUN WITH LAMBDA=1.0 *

ITERATION	LAMBDA	CHI**2	CHI**2/NDF				
4	1.000E 00	1.199729E 01	1.333033E 00				
	GAUSSIAN*** PARAMETERS*	GAUSSIAN 1 2	HEIGHT 3.649473E 04 4.678546E 04	CHANNEL 7.250128E 01 7.568695E 01	HALF-WIDTH 5.863085E 00 6.012898E 00	ALPHA1 2.0886E-04 2.0152E-04	ALPHA2 6.5931E-12 5.2599E-12

* ITERATION CALCULATIONS COMPLETED *

ESTIMATED ERROR IN FITTED PARAMETERS

GAUSSIAN*** PARAMETERS*	GAUSSIAN	HEIGHT	CHANNEL	HALF-WIDTH	ALPHA1	ALPHA2
	1	6.939361E 02	4.194010E-02	0.	0.	0.
	2	7.368736E 02	2.501591E-02	0.	0.	0.

AREA OF MODIFIED-GAUSSIAN PHOTOPEAKS

GAUSSIAN	AREA(0)	AREA(1)	AREA(2)	AREA
1	2.277657E 05	5.484434E 03	8.859742E 02	2.341361E 05
2	2.994517E 05	7.695895E 03	1.257888E 03	3.084055E 05

ERROR IN THE PHOTOPEAK AREAS

GAUSSIAN	VARA(0)	VARA(1)	VARA(2)	VARA
1	4.330097E 03	1.042851E 02	1.684663E 01	4.452029E 03
2	4.716383E 03	1.212111E 02	1.981193E 01	4.857406E 03

YDATA AND YBAR CALCULATIONS

CHANNEL	YDATA	YBAR	DELTA	1/SIG(Y1)	DELTA/SIG	(DELTA/SIG)2
70	2.693600E 04	2.698020E 04	-4.419800E 01	6.093032E-03	-0.269	0.073
71	3.989100E 04	3.998965E 04	-9.864941E 01	5.006826E-03	-0.494	0.244
72	5.326700E 04	5.287405E 04	3.929468E 02	4.332822E-03	1.703	2.899
73	6.262300E 04	6.294737E 04	-3.243696E 02	3.996070E-03	-1.296	1.680
74	6.825800E 04	6.815351E 04	1.044893E 02	3.827571E-03	0.400	0.160
75	6.745600E 04	6.736030E 04	9.570215E 01	3.850257E-03	0.368	0.136
76	6.021200E 04	6.045823E 04	-2.462339E 02	4.075290E-03	-1.003	1.007
77	4.869300E 04	4.876288E 04	-6.988135E 01	4.531758E-03	-0.317	0.100
78	3.524600E 04	3.502857E 04	2.174336E 02	5.326539E-03	1.158	1.341
79	2.238800E 04	2.235887E 04	2.913110E 01	6.683321E-03	0.195	0.038
80	1.279300E 04	1.275212E 04	4.087976E 01	8.841253E-03	0.361	0.131
81	6.598000E 03	6.572472E 03	2.552832E 01	1.231101E-02	0.314	0.099
82	3.000000E 03	3.110774E 03	-1.107740E 02	1.825742E-02	-2.022	4.090

NORMAL RETURN--PROBLEM COMPLETED

END-OF-DATA ENCOUNTERED ON SYSTEM INPUT FILE.

3. LISTING OF FORTRAN PROGRAM DECK

<pre> C C *GAUSS* A NON-LINEAR MULTIPLE MODIFIED GAUSSIAN FITTING SUBROUTINE C M.H.PUTNAM PHILLIPS PETROLEUM CO. SEPTEMBER, 1963 C COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),ALCOE(6),A2COE(6),YDATA(1511),WDATA(511),TPAR(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION 2(3,2),LINALB(2),GASPAR(5,2),XL(INE(2,4),IGAUSS,ISTART,IEND,ICCN1, 3IWEIT,NCIT,ITEST,IOUTPT,MIALF,M2ALF,KGNST,TLINE(2),YMAX,YMIN,HCCNT COMMON TPARE(10,5),ALINE(2),A(100,50),B(50),VECT(50),A1(50,50), 1B1(3),C(50,50),S(3),XL(3),CONI(10),LL,JP,A2(3,3),MATIND(10,5) COMMON TITLE(13),IKONST COMMON EE(211) DIMENSION LF(68),NF(23),FF(7),LFDUM(13) DIMENSION TEMP(9) EQUIVALENCE (LFDUM(1),IGAUSS) C C IFLA = 0 C C***** C READ IN PROBLEM IDENTIFICATION CARD C***** C***** C 1 READ(5,300)(TITLE(I),I=1,13) C***** C ZER0 OUT THE LF AND EE VECTOR AREAS C***** C IF(IFLA.EQ.0)GO TO 2 C GO TO 6 C C 2 DO 3 I = 1,68 C 3 LF(I)=0 C C DO 4 K = 1,211 C 4 EE(K)=0.0 C***** C ZER0 OUT THE WDATA AREA AT THE BEGINNING OF EACH JOB C***** C DO 5 I = 1,START,IEND C 5 WDATA(I) = 0.0 C C IFLA = 1 C C***** C READ IN AND CHECK THE FIXED POINT CONTROL INFORMATION C***** C 6 REAC(5,305)NPD,NOL,NAD,(NF(I),I=1,23) C IF(NPD.EQ.0)GO TO 15 C IF(NPD.GT.23)GO TO 200 C IF(NAD.GT.63)GO TO 202 C DO 7 I = 1,NPD C 7 I=NAD-1 C 7 LF(J)=NF(I) C IF(NOL.EQ.0)GO TO 6 C C STORE FIRST THIRTEEN WORDS IN DUMMY ARRAY L=DUM C C DO 8 I=1,13 </pre>	<pre> INPUT001 INPUT002 INPUT003 INPUT004 INPUT005 INPUT006 INPUT007 INPUT008 INPUT009 INPUT010 INPUT011 INPUT012 INPUT013 INPUT014 INPUT015 INPUT016 INPUT017 INPUT018 INPUT019 INPUT020 INPUT021 INPUT022 INPUT023 INPUT024 INPUT025 INPUT026 INPUT027 INPUT028 INPUT029 INPUT030 INPUT031 INPUT032 INPUT033 INPUT034 INPUT035 INPUT036 INPUT037 INPUT038 INPUT039 INPUT040 INPUT041 INPUT042 INPUT043 INPUT044 INPUT045 INPUT046 INPUT047 INPUT048 INPUT049 INPUT050 INPUT051 INPUT052 INPUT053 INPUT054 INPUT055 INPUT056 INPUT057 </pre>	<pre> 8 LFDUM(I)=LF(I) C***** C STORE FIXED POINT CONTROL INFORMATION IN IPARIN ARRAY C***** C IF(IGAUSS.EQ.0)GO TO 15 C DO 10 I = 1,IGAUSS C DO 10 J = 1,5 C N=5*(I-1)+(J+13) C 10 IPARIN(I,J) = LF(N) C***** C REAC IN AND CHECK THE FLOATING POINT CONTROL INFORMATION C***** C 15 REAC(5,310)NPF,NOC,NAF,(FF(I),I=1,7) C IF(NPF.EQ.0)GO TO 92 C IF(NPF.GT.7)GO TO 204 C IF(NAF.GT.21)GO TO 206 C DO 20 I = 1,NPF C 20 J=1+NAF-1 C 20 EE(J)=FF(I) C IF(NOC.EQ.0)GO TO 15 C YMAX=EE(1) C YMIN=EE(2) C HCONT=EE(3) C IF(ILINE(1).EQ.0.AND.ILINE(2).EQ.0)GO TO 23 C C STORE LINE PARAMETERS IN *XLIN* ARRAY C C DO 22 I = 1,2 C DO 22 J = 1,4 C K=4*(I-1)+(J+3) C 22 XLINE(I,J)=EE(K) C C STORE GAUSSIAN PARAMETERS IN *PARIN* ARRAY C C 23 IF(IGAUSS.EQ.0)GO TO 92 C DO 25 I = 1,IGAUSS C DO 25 J = 1,5 C DO 25 K = 1,4 C M=20*(I-1)+4*(J-1)+(K+11) C 25 PARIN(I,J,K)=EE(M) C***** C READ IN THE ANALYZER DATA C***** C TEMPORARILY STORED THE FIRST DATA UNTIL THE CARD NUMBER HAS C BEEN CHECKED, IF IT IS *60* TRANSFER. C C 92 REAC(5,311)NOCARD,(TEMP(J),J=1,9) C IF(NOCARD.EQ.60)GO TO 101 C IF(NOCARD.NE.0)GO TO 250 C DO 93 J = 1,9 C 93 YDATA(J) = TEMP(J) C J=10 C 94 DO 98 I = 2,53 C L=J+9 C IF(J.EQ.510)L=511 C 96 REAC(5,312)NOCARD,(YDATA(K),K=J,L) </pre>	<pre> INPUT058 INPUT059 INPUT060 INPUT061 INPUT062 INPUT063 INPUT064 INPUT065 INPUT066 INPUT067 INPUT068 INPUT069 INPUT070 INPUT071 INPUT072 INPUT073 INPUT074 INPUT075 INPUT076 INPUT077 INPUT078 INPUT079 INPUT080 INPUT081 INPUT082 INPUT083 INPUT084 INPUT085 INPUT086 INPUT087 INPUT088 INPUT089 INPUT090 INPUT091 INPUT092 INPUT093 INPUT094 INPUT095 INPUT096 INPUT097 INPUT098 INPUT099 INPUT100 INPUT101 INPUT102 INPUT103 INPUT104 INPUT105 INPUT106 INPUT107 INPUT108 INPUT109 INPUT110 INPUT111 INPUT112 INPUT113 INPUT114 </pre>
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      IF(NOCARD.EQ.60)GO TO 100
      IF(I-1.NE.NOCARD)GO TO 255
98  J=J+10
      LL=L
      GO TO 101
100  LL=L-10
C*****
C      REAC IN WEIGHTING DATA IF IWEIT = 3 OR 5
C*****
101  GO TO(120,120,102,120,102),IWEIT
102  J=1
      CO IC6 I = 1, 74
      L=J+6
      IF(L.EQ.510)L=511
104  READ(5,314)I1,(WDATA(K),K=J,L)
      IF(I1.EQ.80)GO TO 107
      IF(I1.NE.I1)GO TO 265
106  J=J+7
107  IF(IWEIT.EQ.5)GO TO 120
108  DO 109 I=ISTART,IEND
109  WDATA(I)=1.0/WDATA(I1)
C*****
C      ALL DATA HAS BEEN READ, BEGIN COMPUTATIONS
C*****
120  CALL GAUSS(IFLAG)
C
110  IF(IFLAG-1)112,114,116
112  WRITE(6,343)
      GO TO 1
114  WRITE(6,344)
      GO TO 1
116  WRITE(6,345)
      GO TO 1
C*****
C      COMMENTS CONCERNING PROBLEM TERMINATION
C*****
200  WRITE(6,316)INPD
      GO TO 295
202  WRITE(6,318)NAD
      GO TO 295
204  WRITE(6,320)NPF
      GO TO 295
206  WRITE(6,322)NAF
      GO TO 295
250  WRITE(6,336)
      GO TO 295
255  WRITE(6,338)NOCARD
      GO TO 295
265  WRITE(6,342)I
295  CALL EXIT
C
C      FORMAT STATEMENTS
C
300  FORMAT(13A6)
305  FORMAT(12,I1,I3,1X,23I3)
310  FORMAT(12,I1,I3,1X,7E10.5)
311  FORMAT(12,7X,9F7.0)

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INPUT115
INPUT116
INPUT117
INPUT118
INPUT119
INPUT120
INPUT121
INPUT122
INPUT123
INPUT124
INPUT125
INPUT126
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INPUT156
INPUT157
INPUT158
INPUT159
INPUT160
INPUT161
INPUT162
INPUT163
INPUT164
INPUT165
INPUT166
INPUT167
INPUT168
INPUT169
INPUT170
INPUT171
312  FORMAT(12,10F7.0)
314  FORMAT(12,8X,7E10.5)
316  FORMAT(67H0 INPUT ERROR--NUMBER OF FIXED POINT VALUES TOO LARGEINPUT172
      1, NUMBER = I3) INPUT173
318  FORMAT(18H0 INPUT ERROR--I3,29H IS NOT A FIXED POINT ADDRESS) INPUT174
320  FORMAT(70H0 INPUT ERROR--NUMBER OF FLOATING POINT VALUES TOO LAINPUT175
      1RGE, NUMBER = I3) INPUT176
322  FORMAT(18H0 INPUT ERROR--I3,32H IS NOT A FLOATING POINT ADDRESSINPUT177
      1) INPUT178
336  FORMAT(60H0 INPUT ERROR--FIRST YDATA CARD IS MISSING(CARD NUMBEINPUT179
      1R OC) INPUT180
338  FORMAT(77H0 INPUT ERROR--YDATA CARDS ARE NOT IN PROPER SEQUENCEINPUT181
      1, THE CARD NUMBER IS I3,1H.) INPUT182
342  FORMAT(84H INPUT ERROR--WDATA CARDS ARE NOT IN PROPER SEQUENCEINPUT183
      1, THE CARD NUMBER SHOULD BE I3) INPUT184
343  FORMAT(3740 NORMAL RETURN--PROBLEM COMPLETED) INPUT185
344  FORMAT(7440 ERROR--PARTIAL DERIVATIVE MATRIX SINGULAR. CCNTINUINPUT186
      1ATICN NOT POSSIBLE) INPUT187
345  FORMAT(7140 PROBLEM DISCONTINUED--MAXIMUM NUMBER OF ITERATIONS INPUT188
      1HAVE BEEN TAKEN) INPUT189
      END INPUT190
      INPUT191
      INPUT192

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C
C
C      SUBROUTINE GAUSS(IFLAG)
C
COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),ALCOE(6),A2COE(6),YDATA(GAUSS006
1511),WDATA(511),TPARI(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION(GAUSS007
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, GAUSS008
3IWEIT,NOIT,ITEST,IOUTPT,MIALF,M2ALF,KONST,ILINE(2),YMAX,YMIN,HCONTGAUSS009
COMMON TPARI(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), GAUSS010
1B1(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,AZ(3,3),MATIND(10,5) GAUSS011
COMMON TITLE(13),IKONST GAUSS012
DIMENSION SRDIA(50) GAUSS013
C***** GAUSS014
C      GENERATE PARAMETER DATA AS FUNCTION OF *XD* OR USE INPUT VALUES GAUSS015
C***** GAUSS016
C      IF(KONST.GT.10)CALL PARMTR GAUSS017
C
C      DETERMINE WEIGHTING FUNCTIONS - WDATA GAUSS018
C
C      GO TO (15,5,15,10,15),IWEIT GAUSS019
C      DO 8 I=ISTART,IEND GAUSS020
C      IF(YDATA(I).LT.1.0)GO TO 7 GAUSS021
C      WDATA(I)=1.0/YDATA(I) GAUSS022
C      GO TO 8 GAUSS023
C      WDATA(I)=1.0 GAUSS024
C      8 CONTINUE GAUSS025
C
C      GO TO 15 GAUSS026
C      DO 14 I=ISTART,IEND GAUSS027
C      IF(YDATA(I).LE.YMAX)GO TO 12 GAUSS028
C      WDATA(I)=YMAX/(YDATA(I)+YDATA(I)) GAUSS029
C      GO TO 14 GAUSS030
C      12 IF(YMIN.LE.YDATA(I))GO TO 13 GAUSS031
C      WDATA(I)=1.0/YMIN GAUSS032
C      GO TO 14 GAUSS033
C      13 WDATA(I)=1.0/YDATA(I) GAUSS034
C      14 CONTINUE GAUSS035
C
C      STORE LINE FIT PARAMETERS IN TLINE GAUSS036
C
C      15 TLINE(1)=XLINE(1,1) GAUSS037
C      TLINE(2)=XLINE(2,1) GAUSS038
C***** GAUSS039
C      DETERMINE AND STORE GAUSSIAN PARAMETERS(OMEGA, ALPHA1, ALPHA2) GAUSS040
C      COMPUTE PARAMETERS USING FUNCTIONAL FORMS WHEN XD VARIES GAUSS041
C***** GAUSS042
C      20 IF(IGAUSS.EQ.0)GO TO 70 GAUSS043
C      DO 65 K1=1,IGAUSS GAUSS044
C      TPARI(K1,1)=PARIN(K1,1,1) GAUSS045
C      TPARI(K1,2)=PARIN(K1,2,1) GAUSS046
C
C      25 IF(IPARIN(K1,3).EQ.3)GO TO 35 GAUSS047
C      TPARI(K1,3)=PARIN(K1,3,1) GAUSS048
C      30 GO TO 40 GAUSS049
C      35 CALL OMEGA(TPARI(K1,2),TPARI(K1,3),K1) GAUSS050
C
C      40 IF(IPARIN(K1,4).EQ.3)GO TO 45 GAUSS051
C      TPARI(K1,4)=PARIN(K1,4,1) GAUSS052
C      GO TO 50 GAUSS053
C      45 CALL ALPHA1(TPARI(K1,2),TPARI(K1,4),*1) GAUSS054
C
C      50 IF(IPARIN(K1,5).EQ.3)GO TO 60 GAUSS055
C      TPARI(K1,5)=PARIN(K1,5,1) GAUSS056
C      GO TO 65 GAUSS057
C      60 CALL ALPHA2(TPARI(K1,2),TPARI(K1,5),*1) GAUSS058
C      65 CONTINUE GAUSS059
C
C      70 ITERAT=1 GAUSS060
C      INIT=0 GAUSS061
C      V=2.77258872 GAUSS062
C      IFLAG=0 GAUSS063
C***** GAUSS064
C      DETERMINE NUMBER OF PARAMETERS BEING VARIED (JP) GAUSS065
C***** GAUSS066
C      80 IF(ILINE(1).EQ.2)GO TO 85 GAUSS067
C      JP=0 GAUSS068
C      GO TO 87 GAUSS069
C      85 JP=1 GAUSS070
C      87 IF (ILINE(2).EQ.2)JP=JP+1 GAUSS071
C      90 IF (IGAUSS.EQ.0)GO TO 100 GAUSS072
C      DO 95 K1=1,IGAUSS GAUSS073
C      DO 95 K2=1,5 GAUSS074
C      IF(IPARIN(K1,K2).NE.2)GO TO 92 GAUSS075
C      JP=JP+1 GAUSS076
C
C      SET UP *MATIND* ARRAY TO INDICATE WHICH MATRIX ELEMENTS ARE ZERO GAUSS077
C
C      MATIND(K1,K2)=JP GAUSS078
C      GO TO 95 GAUSS079
C      92 MATIND(K1,K2)=0 GAUSS080
C      95 CONTINUE GAUSS081
C
C      CALCULATE NUMBER OF DEGREES OF FREEDOM GAUSS082
C
C      NDF=IEND-ISTART+1-JP GAUSS083
C
C      INITIALIZE ITERATION CONTROLS GAUSS084
C
C      100 ISWTC=0 GAUSS085
C      110 SSY=0.0 GAUSS086
C      ISET=0 GAUSS087
C
C      ZERO OUT MATRIX AREA GAUSS088
C
C      120 DO 130 M = 1,JP GAUSS089
C      B(M)=0.0 GAUSS090
C      DO 130 N = 1,JP GAUSS091
C      A(M,N)=0.0 GAUSS092
C      130 CONTINUE GAUSS093
C
C      BEGIN ITERATION CALCULATIONS GAUSS094
C
C      135 DO 470 I = ISTART,IEND GAUSS095

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      XI=I
137 IF(ILINE(1)-2) 14C,150,140
140 J=0
      GO TO 160
150 VECT1(I)=XI
      J=1
160 IF(ILINE(2)-2) 180,170,180
170 J=J+1
      VECT1(J)=1.0
C
180 IF(IGAUSS.EQ.0)GO TO 400
190 DO 390 K1 = 1,IGAUSS
195 IF(IJ.GE.JP)GO TO 400
C*****
C      COMPUTE COMMON VALUES USED IN CALCULATING PARTIAL DERIVATIVES
C*****
200 XIR=XI-TPARI(K1,2)
      XIRS=XIR*XIR
      OMEGA2=TPARI(K1,3)*TPARI(K1,3)
      OMEGA3=TPARI(K1,3)*OMEGA2
      OMEGA4=TPARI(K1,3)*OMEGA3
      Z=(V+XIRS)/OMEGA2
      IF(XIR.NE.0.0)GO TO 202
      XIRM1 = 0.0
      XIRM2 = 0.0
      GO TO 206
202 XIRM1 = XIR**MIALF
      XIRM2=XIR**M2ALF
206 FK1 = 1.0 + TPARI(K1,4)*XIRM1 + TPARI(K1,5)*XIRM2
      EK1=EXP(-Z)
C
C      COMPUTE PARTIAL DERIVATIVES
C
210 IF(IPARIN(K1,1).EQ.1)GO TO 220
      J=J+1
      VECT1(J)=EK1*FK1
220 IF(IPARIN(K1,2).EQ.1)GO TO 330
225 IF(IPARIN(K1,3).EQ.3)GO TO 240
230 POMEGA=0.0
      GO TO 250
240 CALL PART1(TPARI(K1,2),POMEGA,K1)
C
250 IF(IPARIN(K1,4).EQ.3)GO TO 270
260 PAL1=0.0
      GO TO 280
270 CALL PART2(TPARI(K1,2),PAL1,K1)
C
280 IF(IPARIN(K1,5).EQ.3)GO TO 300
290 PAL2=0.0
      GO TO 310
300 CALL PART3(TPARI(K1,2),PAL2,K1)
C
C      SETTING UP TERMS OF THE PARTIAL EQUATION-PARTIAL WITH RESPECT TO
C      1XO(K1)
C
310 J=J+1
      XMIALF=MIALF

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      XM2ALF=M2ALF
      PZ=(-2.0*V*(TPARI(K1,3)*XIR+XIRS*POMEGA))/OMEGA3
      PEK1=-EK1*PZ
315 PFK1=(-XMIALF*TPARI(K1,4)/XIR+PAL1)*XIRM1+(-XM2ALF*TPARI(K1,5)/
      1XIR+PAL2)*XIRM2
320 VECT1(I)= TPARI(K1,1)*(EK1*PFK1 + FK1*PEK1)
C
330 IF(IPARIN(K1,3)-2) 350,340,350
340 J=J+1
      PZ=-2.0*V*XIRS/OMEGA3
      PEK1=-EK1*PZ
      VECT1(J)= TPARI(K1,1)*FK1*PEK1
C
350 IF(IPARIN(K1,4)-2) 370,360,370
360 J=J+1
      VECT1(J)= TPARI(K1,1)*EK1*XIRM1
C
370 IF(IPARIN(K1,5)-2) 390,380,390
380 J=J+1
      VECT1(J)= TPARI(K1,1)*EK1*XIRM2
390 CONTINUE
C*****
C      FORM THE PARTIAL DERIVATIVE MATRIX
C*****
400 CALL FCN1SET,XI,YBAR,TPARI,TLINE)
405 DELTY=YDATA(I)-YBAR
C
C      FORM UPPER TRIANGULAR MATRIX
C
410 DO 450 M=1,JP
415 IF(IWEIT.EQ.1) GO TO 420
417 B(M)=B(M)+WDATA(I)*DELTY*VECT1(M)
      GO TO 430
420 B(M)=B(M)+DELTY*VECT1(M)
430 DO 450 N=M,JP
435 IF(IWEIT.EQ.1) GO TO 440
437 A(M,N)=A(M,N)+WDATA(I)*VECT1(M)*VECT1(N)
      GO TO 450
440 A(M,N)=A(M,N)+VECT1(M)*VECT1(N)
450 CONTINUE
C
455 IF(IWEIT.EQ.1) GO TO 460
457 SSY=SSY+WDATA(I)*DELTY*DELTY
      GO TO 470
460 SSY=SSY+DELTY*DELTY
470 CONTINUE
C
C      FORM COMPLETE MATRIX
C
475 L=JP-1
480 DO 490 N=1,L
      J=N+1
485 DO 490 M = J,JP
490 A(M,N)=A(M,M)
C
C*****

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C      IF INIT = 0, PRINT INPUT, INITIAL ESTIMATES, CHI**2 AND CHI**2/NDFGAUSS229
C***** GAUSS230
540 IF(INIT.NE.0)GO TO 561 GAUSS231
C      GAUSS232
550 ISTEP=0 GAUSS233
555 XNDF=NDF GAUSS234
      XLAMB=0 GAUSS235
      SIG=SSY/XNDF GAUSS236
      INIT=1 GAUSS237
560 CALL OUTPUT(ITERAT,ISTP,TPARI,SSY,SIG,XLAMB,TLINE) GAUSS238
C***** GAUSS239
C      SCALING THE NORMAL EQUATION MATRIX BEFORE INVERSION GAUSS240
C***** GAUSS241
561 DO 562 I =1,JP GAUSS242
562 SRDIA(I)=SQRT(A(I,I)) GAUSS243
      DO 566 J = 1,JP GAUSS244
564 B(I)=B(I)/SRDIA(I) GAUSS245
      DO 566 J = 1,JP GAUSS246
566 A(I,J)=A(I,J)/(SRDIA(I)*SRDIA(J)) GAUSS247
C      GAUSS248
      STORE NORMALIZED NORMAL EQUATION MATRIX IN A1 AREA GAUSS249
C      GAUSS250
      DO 567 M = 1,JP GAUSS251
      DO 567 N = 1,JP GAUSS252
567 A1(M,N)=A(M,N) GAUSS253
C      GAUSS254
      INVERT MATRIX GAUSS255
C      GAUSS256
570 CALL MAINS(A,JP,B,1,DET,IFS) GAUSS257
C      GAUSS258
      IS MATRIX SINGULAR GAUSS259
C      GAUSS260
580 IF(IFS.EQ.0)GO TO 660 GAUSS261
C      GAUSS262
      MATRIX MULTIPLICATION (C=A*A1) GAUSS263
C      GAUSS264
      IF(IOUTPT.EQ.2)CALL MATMPY(A,JP,JP,A1,JP,C) GAUSS265
C      GAUSS266
      DETERMINE THE ORIGINAL MATRIX AFTER INVERTING THE SCALED MATRIX GAUSS267
C      GAUSS268
581 DO 583 I=1,JP GAUSS269
      B(I)=B(I)/SRDIA(I) GAUSS270
      DO 583 J=1,JP GAUSS271
583 A(I,J)=A(I,J)/(SRDIA(I)*SRDIA(J)) GAUSS272
C      GAUSS273
      TEST TO SEE IF CONVERGENCE CRITERION HAS BEEN MET GAUSS274
C      GAUSS275
590 IF(ILINE(1).LE.1)GO TO 610 GAUSS276
      M=1 GAUSS277
500 IF(ABS(B(M)).LE.XLINE(1,4))GO TO 620 GAUSS278
      GO TO 820 GAUSS279
510 M=0 GAUSS280
520 IF(ILINE(2).LE.1)GO TO 630 GAUSS281
525 M=M+1 GAUSS282
527 IF(ABS(B(M)).GT.XLINE(2,4))GO TO 820 GAUSS283
C      GAUSS284
530 IF(IGAUSS.EQ.0)GO TO 670 GAUSS285

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632 DO 650 K1=1,IGAUSS GAUSS286
634 DO 650 K2=1,5 GAUSS287
636 IF(M.EQ.JP)GO TO 670 GAUSS288
638 IF(IPARIN(K1,K2).NE.2)GO TO 650 GAUSS289
640 M=M+1 GAUSS290
      IF(ABS(B(M)).GT.PARIN(K1,K2,4))GO TO 820 GAUSS291
650 CONTINUE GAUSS292
      GO TO 670 GAUSS293
C      GAUSS294
C      IF MATRIX IS SINGULAR, SET IFLAG = 1 AND RETURN GAUSS295
C      GAUSS296
660 IFLAG=1 GAUSS297
      RETURN GAUSS298
C***** GAUSS299
C      CONVERGENCE CRITERION HAS BEEN MET,MORE ITERATIONS WILL BE RUN GAUSS300
C      WITH LAMBDA=1.0 GAUSS301
C      GAUSS302
C      IF ISWTCH = 0 COMPUTE CHI**2 AND CHI**2/NDF FOR PARAMETER VALUES GAUSS303
C      ON WHICH THE CONVERGENCE CRITERION HAS BEEN MET. GAUSS304
C      IF ISWTCH = 1 REPEAT ITERATION PROCESS UNTIL REQUIRED NUMBER OF GAUSS305
C      AFTER CONVERGENCE ITERATIONS HAS BEEN SATISFIED. GAUSS306
C***** GAUSS307
670 IF(ISWTCH.EQ.0)GO TO 690 GAUSS308
675 ISTEP=7 GAUSS309
680 GO TO 700 GAUSS310
690 ISWTCH=1 GAUSS311
      NOT=ISTEP+1 GAUSS312
      ISTEP=6 GAUSS313
700 XLAMB=1.0 GAUSS314
702 CALL BOUND(TLINE,TLINE,TPARI,TPARI,XLAMB,NLIM) GAUSS315
704 IF(IOUTPT.NE.0)GO TO 720 GAUSS316
710 IF((NOT-1).NE.0)GO TO 770 GAUSS317
720 X1=1START GAUSS318
      ISET=0 GAUSS319
722 CALL FCN(ISET,X1,YBAR,TPARI,TLINE) GAUSS320
724 DFF=YDATA(1START)-YBAR GAUSS321
726 IF(IWEIT.EQ.1)GO TO 730 GAUSS322
728 SUM=YDATA(1START)*DFF*DFF GAUSS323
      GO TO 740 GAUSS324
730 SUM=DFF*DFF GAUSS325
740 I1=1START+1 GAUSS326
742 DO 760 I=I1,IEND GAUSS327
      X1=1 GAUSS328
744 CALL FCN(ISET,X1,YBAR,TPARI,TLINE) GAUSS329
      DFF=YDATA(I1)-YBAR GAUSS330
745 IF(IWEIT.EQ.1)GO TO 750 GAUSS331
747 SUM=SUM+YDATA(I1)*DFF*DFF GAUSS332
      GO TO 760 GAUSS333
750 SUM=SUM+DFF*DFF GAUSS334
760 CONTINUE GAUSS335
763 SIG=SUM/XNDF GAUSS336
766 CALL OUTPUT(ITERAT,ISTP,TPARI,SUM,SIG,XLAMB,TLINE) GAUSS337
770 NOT=NOT-1 GAUSS338
775 IF(NOT.NE.0)GO TO 110 GAUSS339
C***** GAUSS340
C      CALCULATION OF ESTIMATED ERROR IN ALL PARAMETERS FITTED GAUSS341
C***** GAUSS342

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780 SIGMA=SQRT(SIG)
M=0
782 DO 790 L=1,2
784 IF(ILINE(L).NE.2)GO TO 787
P=M+1
786 ERESTL(L)= SIGMA*SQRT(A(M,M))
GO TO 790
787 ERESTL(L)=0.0
790 CONTINUE
C
792 IF(IGAUSS.EQ.0)GO TO 810
M=0
794 DO 800 K1=1,IGAUSS
796 DO 800 K2=1,5
798 IF(IPARIN(K1,K2).NE.2)GO TO 799
M=M+1
ERESTG(K1,K2)= SIGMA * SQRT(A(M,M))
GO TO 800
799 ERESTG(K1,K2)= 0.0
800 CONTINUE
C
C CONVERGENCE CRITERIA HAS BEEN, PROBLEM COMPLETED. NORMAL RETURN
C
810 ISTOP=8
CALL OUTPUT(ITERAT,ISTP,TPAR1,SUM,SIG,XLAMB,TLINE)
IFLAG=0
RETURN
C.....
C CONVERGENCE CRITERION HAS NOT BEEN MET, COMPUTE LAMBDA VALUES
C COMPUTE NEW PARAMETER ESTIMATES WITH LAMBDA = 1.0
C.....
820 IF(ICON1.EQ.0)GO TO 830
825 XLAMB=HCONT
GO TO 2810
C
C PARABOLIC FITTING PROCESS WILL BE USED TO DETERMINE LAMBDA
C CHECK TO SEE IF PARAMETERS ARE WITHIN LIMITS, IF NOT, SET TO LIMITS
C
830 M=0
832 DO 880 L=1,2
834 IF(ILINE(L).EQ.2)GO TO 840
836 ALINE(L)=TLINE(L)
GO TO 880
840 M=M+1
844 ALINE(L)=TLINE(L)+B(M)
848 IF(ALINE(L)-XLINE(L,2)) 860,880,850
850 ALINE(L)=XLINE(L,2)
855 B(M)=XLINE(L,2)-TLINE(L)
GO TO 880
860 IF(ALINE(L)-XLINE(L,3)) 870,880,880
870 ALINE(L)=XLINE(L,3)
875 B(M)=XLINE(L,3)-TLINE(L)
880 CONTINUE
C
882 IF(IGAUSS.EQ.0)GO TO 950
884 DO 930 K1=1,IGAUSS
GAUSS343
GAUSS344
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GAUSS398
GAUSS399
885 DO 930 K2=1,5
886 IF(IPARIN(K1,K2).EQ.2)GO TO 890
888 TPARE(K1,K2)=TPAR1(K1,K2)
GO TO 930
890 M=M+1
892 TPARE(K1,K2)=TPAR1(K1,K2)+B(M)
895 IF(TPARE(K1,K2)-PARIN(K1,K2,2))910,930,900
900 TPARE(K1,K2)=PARIN(K1,K2,2)
B(M)=TPARE(K1,K2)-TPAR1(K1,K2)
GO TO 930
910 IF(TPARE(K1,K2)-PARIN(K1,K2,3))920,930,930
920 TPARE(K1,K2)=PARIN(K1,K2,3)
B(M)=TPARE(K1,K2)-TPAR1(K1,K2)
930 CONTINUE
C
940 CALL KOVAR1(TPARE)
950 XI=ISTART
ISET=0
955 CALL FCN(ISET,XI,YBAR,TPARE,ALINE)
OFF=YDATA(ISTART)-YBAR
960 IF(INEIT.EQ.1)GO TO 970
965 S(1)=WDATA(ISTART)*OFF*OFF
GO TO 980
970 S(1)=OFF*OFF
C
980 I1=ISTART+1
981 DO1000 I=I1,IEND
XI=I
982 CALL FCN(ISET,XI,YBAR,TPARE,ALINE)
984 OFF=YDATA(I)-YBAR
986 IF(INEIT.EQ.1)GO TO 990
988 S(1)=S(1)+WDATA(I)*OFF*OFF
GO TO 1000
990 S(1)=S(1)+OFF*OFF
1000 CONTINUE
SUM=S(1)
1010 IF(OUTPUT-1) 1030,1030,1020
C
1020 ISTOP=1
1022 SIG=S(1)/XNDF
XL(1)=1.0
1025 CALL OUTPUT(ITERAT,ISTP,TPARE,S(1),SIG,XL(1),ALINE)
C
C COMPUTE NEW PARAMETER ESTIMATES WITH LAMBDA = 0.5
C
1030 M=0
1035 DO 1050 L=1,2
1037 IF(ILINE(L).NE.2)GO TO 1050
1040 M=M+1
ALINE(L)=TLINE(L)+0.5*B(M)
1050 CONTINUE
C
1055 IF(IGAUSS.EQ.0)GO TO 1084
1060 DO 1080 K1=1,IGAUSS
1062 DO 1080 K2=1,5
1064 IF(M.EQ.J)GO TO 1084
1065 IF(IPARIN(K1,K2).NE.2)GO TO 1080
GAUSS400
GAUSS401
GAUSS402
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GAUSS407
GAUSS408
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GAUSS456

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1070 M=M+1
      TPAR2(K1,K2)=TPAR1(K1,K2)+0.5*B(M)
1080 CONTINUE
C
1082 CALL XOVARI(TPAR2)
1084 XI=ISTART
      ISET=0
1086 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
1087 DFF=YDATA(IISTART)-YBAR
1090 IF(IWEIT.EQ.1)GO TO 2030
1095 S(2)=WDATA(IISTART)*DFF*DFF
      GO TO 2010
2000 S(2)=DFF*DFF
C
2010 I1=ISTART+1
2012 DO 2040 I=I1,IEND
      XI=I
2014 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2016 DFF=YDATA(I)-YBAR
2020 IF(IWEIT.EQ.1)GO TO 2030
2025 S(2)=S(2)+WDATA(I)*DFF*DFF
      GO TO 2040
2030 S(2)=S(2)+DFF*DFF
2040 CONTINUE
2045 IF(OUTPUT-1)2070,2070,2050
C
2050 ISTEP=2
2055 SIG=S(2)/XNDF
      XL(2)=0.5
2060 CALL OUTPUT(ITERAT,ISTEP,TPAR2,S(2),SIG,XL(2),ALINE)
C*****
C      COMPARE SUM OF SQUARES. IF THAT FOR LAMBDA=C.5 IS GREATER THAN
C      THAT FOR LAMBDA=1.0 TRANSFER TO DOUBLING PROCESS OTHERWISE
C      CONTINUE WITH HALVING PROCESS
C*****
2070 J=2
2080 IF(S(2).GT.S(1))GO TO 2510
2090 DO 2500 L=1,5
2092 SS=S(J)
      TEMP=0.5*XL(J)
      J=J+1
2095 IF(J.GT.3)J=1
2097 XL(J)=TEMP
      M=0
2100 DO 2300 I=1,2
2150 IF(ILINE(I).NE.2)GO TO 2300
2200 M=M+1
      ALINE(I)=TLINE(I)+XL(J)*B(M)
2300 CONTINUE
C
2350 IF(IGAUSS.EQ.0)GO TO 2424
2400 DO 2410 K1=1,IGAUSS
2402 DO 2410 K2=1,5
2404 IF(M.EQ.JP)GO TO 2420
2406 IF(IPARIN(K1,K2).NE.2)GO TO 2410
2408 M=M+1
      TPAR2(K1,K2)=TPAR1(K1,K2)+XL(J)*B(M)
      GAUSS457
      GAUSS458
      GAUSS459
      GAUSS460
      GAUSS461
      GAUSS462
      GAUSS463
      GAUSS464
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      GAUSS471
      GAUSS472
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      GAUSS510
      GAUSS511
      GAUSS512
      GAUSS513
2410 CONTINUE
2420 CALL XOVARI(TPAR2)
C
2424 XI=ISTART
      ISET=0
2428 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2430 DFF=YDATA(IISTART)-YBAR
2434 IF(IWEIT.EQ.1)GO TO 2450
2436 S(J)=WDATA(IISTART)*DFF*DFF
2440 GO TO 2460
2450 S(J)=DFF*DFF
C
2460 I1=ISTART+1
2464 DO 2490 I=I1,IEND
      XI=I
2466 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2467 DFF=YDATA(I)-YBAR
2470 IF(IWEIT.EQ.1)GO TO 2480
2472 S(J)=S(J)+WDATA(I)*DFF*DFF
      GO TO 2490
2480 S(J)=DFF*DFF+S(J)
2490 CONTINUE
2492 IF(OUTPUT.NE.2)GO TO 2498
2494 SIG=S(J)/XNDF
2496 CALL OUTPUT(ITERAT,ISTEP,TPAR2,S(J),SIG,XL(J),ALINE)
2498 IF(S(J).GT.SS)GO TO 2620
2500 CONTINUE
      GO TO 2620
C
C      COMPUTE NEW ESTIMATES USING LAMBDA DOUBLING PROCEDURE
C
2510 TEMP=S(1)
      S(1)=S(2)
      S(2)=TEMP
      XL(1)=0.5
      XL(2)=1.0
2520 DO 2610 L=1,5
2522 SS=S(J)
      TEMP=2.0*XL(J)
      J=J+1
2524 IF(J.GT.3)J=1
2526 XL(J)=TEMP
2528 CALL BOUNDITLINE,ALINE,TPAR1,TPAR2,XL(J),NLIM)
2530 IF(NLIM.EQ.0)GO TO 2540
C
C      IF ONE OR MORE PARAMETERS EXCEED LIMITS(NLIM=1)*SET LAMBDA = 1.0
C
2535 XLAMB=1.0
      GO TO 2810
2540 XI=ISTART
      ISET=0
2550 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2554 DFF=YDATA(IISTART)-YBAR
2556 IF(IWEIT.EQ.1)GO TO 2570
2558 S(J)=WDATA(IISTART)*DFF*DFF
2560 GO TO 2580
2570 S(J)=DFF*DFF
      GAUSS514
      GAUSS515
      GAUSS516
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C
2580 I1=ISTART+1
2582 DO 2600 I=I1,IEND
      XI=I
2584 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
      DFF=YDATA(I)-YBAR
2586 IF(IWEIT.EQ.1)GO TO 2590
2587 S(I)=S(I)+WDATA(I)*DFF*DFF
      GO TO 2600
2590 S(I)=S(I)+DFF*DFF
2600 CONTINUE
C
2602 IF(IOUTPT.NE.2)GO TO 2603
2604 SIG=S(I)/XNDF
2606 CALL OUTPUT(ITERAT,ISTP,TPAR2,S(I),SIG,XL(J),ALINE)
2608 IF(S(I).GT.SS)GO TO 2620
2610 CONTINUE
C
      COMPUTE INTERPOLATED POINT LAMBDA-MINIMUM
C
2620 DO 2622 I= 1,3
      A2(I,1)=1.0
      A2(I,2)=XL(I)
      A2(I,3)=XL(I)*XL(I)
2622 B1(I)=S(I)
C
      SOLUTION OF THE THREE SIMULTANEOUS EQUATIONS
C
      DO 2625 I= 1,3
      A2(I,1)=1.0/A2(I,1)
      B1(I)=B1(I)*A2(I,1)
      IF(I.GE.3)GO TO 2628
      L=I+1
      DO 2623 J= L,3
      A2(I,J)=A2(I,J)*A2(I,1)
2623 DO 2625 K= L,3
      B1(K)=B1(K)-A2(K,I)*B1(I)
      DO 2625 J= L,3
2625 A2(K,J)=A2(K,J)-A2(K,I)*A2(I,J)
2628 I=I-1
      DO 2630 K= 1,1
2630 B1(K)=B1(K)-A2(K,I+1)*B1(I+1)
      IF(I.GT.1)GO TO 2628
C*****
C
      COMPUTE LAMBDA, TEST TO SEE IF PARAMETERS ARE WITHIN LIMITS,IF NOT
C
      SET TO LIMITS, COMPUTE SUM OF SQUARES,CHI**2,CHI**2/NDF
C*****
2636 XLAMB=-B1(2)/(2.0*B1(3))
2640 CALL BOUND(TLINE,ALINE,TPAR1,TPAR2,XLAMB,NLIM)
2642 XI=ISTART
      ISET=0
2644 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2646 DFF=YDATA(ISTART)-YBAR
2648 IF(IWEIT.EQ.1)GO TO 2660
2650 SUML=WDATA(ISTART)*DFF*DFF
      GO TO 2664
2660 SUML=DFF*DFF

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2664 I1=ISTART+1
      DO 2690 I=I1,IEND
      XI=I
2666 CALL FCN(ISET,XI,YBAR,TPAR2,ALINE)
2668 DFF=YDATA(I)-YBAR
2670 IF(IWEIT.EQ.1)GO TO 2680
2675 SUML=SUML+WDATA(I)*DFF*DFF
      GO TO 2690
2680 SUML=SUML+DFF*DFF
2690 CONTINUE
C
      COMPARE SUM OF SQUARES USED IN PARABOLIC FIT WITH THAT COMPUTED
      USING MINIMUM LAMBDA
C
2692 SUM=SUML
      J1=0
2694 DO 2710 J=1,3
2700 IF(SUM.LE.S(J))GO TO 2710
2705 SUM=S(J)
      J1=J
2710 CONTINUE
C
2712 IF(J1.EQ.3)GO TO 2730
2714 IF(IOUTPT.NE.2)GO TO 2720
C
      ONE OF THE S(I) IS LESS THAN SUM, PRINT PARAMETERS VALUES USING
      FITTED LAMBDA VALUE, THEN COMPUTE VALUES BASED ON LAMBDA(J1)
C
2716 ISTP=3
2717 SIG=SUML/XNDF
2718 CALL OUTPUT(ITERAT,ISTP,TPAR2,SUML,SIG,XLAMB,ALINE)
2720 XLAMB=XL(J1)
      SUM=S(J1)
      GO TO 2810
C
      SUM IS LESS THAN ANY S(I), PRINT PARAMETER VALUES USING FITTED
      LAMBDA VALUE
C
2730 IF(IOUTPT.EQ.0)GO TO 2740
2732 ISTP=4
2733 SIG=SUML/XNDF
C
2734 CALL OUTPUT(ITERAT,ISTP,TPAR2,SUML,SIG,XLAMB,ALINE)
C
      TRANSFER PARAMETER VALUES TO STORAGE ARRAY FOR FIT PARAMETERS
C
2740 M=0
2742 DO 2750 L=1,2
2744 IF(TLINE(L).NE.2)GO TO 2750
2746 M=M+1
      TLINE(L)=ALINE(L)
2750 CONTINUE
2752 IF(IGAUSS.EQ.0)GO TO 2930
2753 DO 2770 K1=1,1GAUSS
      DO 2770 K2=1,5
2756 IF(M.EQ.JP)GO TO 2930
2760 IF(IPARIN(K1,K2).NE.2)GO TO 2770

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2764 M=M+1
      TPAR1(K1,K2)=TPAR2(K1,K2)
2770 CONTINUE
      GO TO 2930
C
2810 CALL BOUND(TLINE,TLINE,TPAR1,TPAR1,XLAMB,NLIM)
2820 IF(IOUTP1.EQ.0)GO TO 2930
2830 IF(ICON1.EQ.0)GO TO 2925
2834 X1=ISTART
      ISET=0
2840 CALL FCN(ISET,X1,YBAR,TPAR1,TLINE)
2844 OFF=YDATA(ISTART)-YBAR
2850 IF(IWEIT.EQ.1)GO TO 2860
      SUM=WDATA(ISTART)*OFF*OFF
      GO TO 2870
2860 SUM=OFF*OFF
C
2870 I1=ISTART+1
2875 DO 2920 I=I1,IEND
      XI=I
2880 CALL FCN(ISET,XI,YBAR,TPAR1,TLINE)
      OFF=YDATA(I)-YBAR
2890 IF(IWEIT.EQ.1)GO TO 2910
2900 SUM=SUM+WDATA(I)*OFF*OFF
      GO TO 2920
2910 SUM=SUM+OFF*OFF
2920 CONTINUE
C
2925 ISTEP=5
2927 SIG=SUM/XNOF
2928 CALL OUTPUT(ITERAT,ISTP,TPAR1,SUM,SIG,XLAMB,TLINE)
C
2930 IF(ITERAT.EQ.NOIT)GO TO 2935
C
      CONTINUE ITERATION PROCESS
C
      ITERAT=ITERAT+1
      GO TO 100
C*****
C  MAXIMUM NUMBER OF ITERATIONS TAKEN, PRINT EST. ERRORS, AREAS AND
C  ERRORS IN AREAS, SET FLAG AND RETURN
C*****
2935 ISTEP=9
C
      CALCULATION OF ESTIMATED ERROR IN ALL PARAMETERS FITTED
C
2950 SIGMA=SQRT(SIG)
      M=0
      DO 2955 L = 1,2
        IF(ILINE(L).NE.2)GO TO 2952
        M=M+1
        ERESTL(L) = SIGMA*SQRT(A(M,M))
        GO TO 2955
2952 ERESTL(L)=0.0
2955 CONTINUE
C

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      IF(IGAUSS.EQ.0)GO TO 2940
      M=0
      DO 2960 K1 = 1,IGAUSS
        DO 2960 K2 = 1,5
          IF(IPARIN(K1,K2).NE.2)GO TO 2957
          M=M+1
          ERESTG(K1,K2)=SIGMA*SQRT(A(M,M))
          GO TO 2960
2957 ERESTG(K1,K2)=0.0
2960 CONTINUE
C
      CALL OUTPUT(ITERAT,ISTP,TPAR1,SUM,SIG,XLAMB,TLINE)
2940 IFLAG=2
      RETURN
      END

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C      SUBROUTINE WHICH STORES THE COEFFICIENTS REQUIRED TO COMPUTE
C      THE FUNCTIONAL FORMS OF OMEGA, ALPHA1 AND ALPHA2
C
C      SUBROUTINE COEFF(XWCOE,XA1COE,XA2COE)
C
C      COMMON PARIN(10,5,4),IPARIN(10,5),XWCOE(6),XA1COE(6),XA2COE(6),YDATA(COEFF007
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION(COEFF008
213,2),LINALB(2),GASPAR(5,2),XLINE(2,4),EGAUSS,ISTART,IEND,ICON1, COEFF009
31WEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,KONST,TLINE(2),YMAZ,YMIN,HCCNT(COEFF010
COMMON TPAR2(10,5),ALINE(2),A(100,50),R(50),VECT(1,50),A(150,50), COEFF011
1B1(3),C(50,50),S(3),XL(3),CDN1(10),LI,JP,A2(3,3),PATIND(10,5) COEFF012
COMMON TITLE(13),IKONST
DIMENSION XWCOE(6),XA1COE(6),XA2COE(4)
C
C      IF(KONST.GT.10)GO TO 2
C      IKONST = KONST
C      GO TO 5
C      2 IKONST = KONST - 10
C      5 GO TO (10,20,30,40,50,60,70,80,90,100),IKONST
C
C      STORAGE AREA FOR THE 5-KEV SCALE PHOTOPEAK PARAMETERS
C
C      OMEGA COEFFICIENTS
C
10 XWCOE(1)= 5.282
XWCOE(2)=-2.3721
XWCOE(3)= 0.59365
XWCOE(4)=-0.042602
XWCOE(5)= 0.0010922
XWCOE(6)= 0.0
C
C      ALPHA1 COEFFICIENTS
C
XA1COE(1)=-11.4868
XA1COE(2)= 7.6339
XA1COE(3)= 2.5126
XA1COE(4)= .1864
XA1COE(5)= 0.0
XA1COE(6)= 0.0
C
C      ALPHA2 COEFFICIENTS
C
XA2COE(1)=- 740.8588
XA2COE(2)= 2079.0172
XA2COE(3)=-2293.7513
XA2COE(4)= 1235.7398
XA2COE(5)=- 327.1203
XA2COE(6)= 34.12756
RETURN
C
C      STORAGE AREA FOR THE 10-KEV SCALE PHOTOPEAK PARAMETERS
C      OMEGA COEFFICIENTS
C
20 XWCOE(1)=-1.4816
XWCOE(2)= 1.00850
XWCOE(3)=-0.027944
C
C      COEFF001
C      COEFF002
C      COEFF003
C      COEFF004
C      COEFF005
C      COEFF006
C      COEFF007
C      COEFF008
C      COEFF009
C      COEFF010
C      COEFF011
C      COEFF012
C      COEFF013
C      COEFF014
C      COEFF015
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C      COEFF048
C      COEFF049
C      COEFF050
C      COEFF051
C      COEFF052
C      COEFF053
C      COEFF054
C      COEFF055
C      COEFF056
C      XWCOE(4)= 0.0012692
C      XWCOE(5)= 0.0
C      XWCOE(6)= 0.0
C
C      ALPHA1 COEFFICIENTS
C
XA1COE(1)=-11.5359
XA1COE(2)= 11.4554
XA1COE(3)=- 5.1163
XA1COE(4)= 0.6488
XA1COE(5)= 0.0
XA1COE(6)= 0.0
C
C      ALPHA2 COEFFICIENTS
C
XA2COE(1)= 14.6523
XA2COE(2)=-31.6138
XA2COE(3)= 14.4150
XA2COE(4)=- 2.6263
XA2COE(5)= 0.0
XA2COE(6)= 0.0
RETURN
C
C
30 WRITE(6,200)KONST
GO TO 400
40 WRITE(6,200)KONST
GO TO 400
50 WRITE(6,200) KONST
GO TO 400
60 WRITE(6,200)KONST
GO TO 400
70 WRITE(6,200)KONST
GO TO 400
80 WRITE(6,200)KONST
GO TO 400
90 WRITE(6,200)KONST
GO TO 400
100 WRITE(6,200)KONST
GO TO 400
200 FORMAT(54H- NO CONSTANTS ARE PRESENTLY AVAILABLE FOR KONST =
113)
400 CALL EXIT
RETURN
END
C
C      COEFF057
C      COEFF058
C      COEFF059
C      COEFF060
C      COEFF061
C      COEFF062
C      COEFF063
C      COEFF064
C      COEFF065
C      COEFF066
C      COEFF067
C      COEFF068
C      COEFF069
C      COEFF070
C      COEFF071
C      COEFF072
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C      COEFF100
C      COEFF101

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C          SUBROUTINE TO COMPUTE THE FUNCTIONAL FORM OF ALPHA2          ALPH2001
C          SUBROUTINE ALPHA2(XD,ALPH2,K1)                                ALPH2002
C                                                                           ALPH2003
C          SUBROUTINE ALPHA2(XD,ALPH2,K1)                                ALPH2004
C                                                                           ALPH2005
C          COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),A1COE(6),A2COE(6),YDATA(10,5,4),
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONALPH2006
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, ALPH2008
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,VONST,ILINE(2),YMAX,YMIN,HCCNTALPH2009
COMMON TPARG(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), ALPH2010
181(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5) ALPH2011
COMMON TITLE(13),IKONST ALPH2012
C          XOLOG=ALOG10(XD) ALPH2013
CALL COEFF(WCOE,A1COE,A2COE) ALPH2014
2 A2LOG=A2COE(1)+XOLOG*(A2COE(2)+XOLOG*(A2COE(3)+XOLOG*(A2COE(4)+ ALPH2015
1XOLOG*(A2COE(5)+XOLOG*(A2COE(6)))))) ALPH2016
4 ALPH2=EXP(2.30258509*A2LOG) ALPH2017
RETURN ALPH2018
END ALPH2019
ALPH2020

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C          SUBROUTINE TO COMPUTE THE FUNCTIONAL FORM OF HALF-WIDTH          OMEGA001
C          SUBROUTINE OMEGA(XD,OMEGA,K1)                                OMEGA002
C                                                                           OMEGA003
C          SUBROUTINE OMEGA(XD,OMEGA,K1)                                OMEGA004
C                                                                           OMEGA005
C          COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),A1COE(6),A2COE(6),YDATA(10,5,4),
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONALPH2006
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, OMEGA008
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,VONST,ILINE(2),YMAX,YMIN,HCCNTOMEGA009
COMMON TPARG(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), OMEGA010
181(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5) OMEGA011
COMMON TITLE(13),IKONST OMEGA012
C          XOH=SQRT(XD) OMEGA013
CALL COEFF(WCOE,A1COE,A2COE) OMEGA014
2 OMEGA=WCOE(1)+XOH*(WCOE(2)+XOH*(WCOE(3)+XOH*(WCOE(4)+XOH*(WCOE(5) OMEGA015
1+XOH*(WCOE(6)))))) OMEGA016
RETURN OMEGA017
END OMEGA018
OMEGA019

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C          SUBROUTINE TO COMPUTE THE FUNCTIONAL FORM OF ALPHA1          ALPH1001
C          SUBROUTINE ALPHA1(XD,ALPH1,K1)                                ALPH1002
C                                                                           ALPH1003
C          SUBROUTINE ALPHA1(XD,ALPH1,K1)                                ALPH1004
C                                                                           ALPH1005
C          COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),A1COE(6),A2COE(6),YDATA(10,5,4),
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONALPH1006
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, ALPH1008
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,VONST,ILINE(2),YMAX,YMIN,HCCNTALPH1009
COMMON TPARG(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), ALPH1010
181(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5) ALPH1011
COMMON TITLE(13),IKONST ALPH1012
C          XOLOG=ALOG10(XD) ALPH1013
CALL COEFF(WCOE,A1COE,A2COE) ALPH1014
2 A1LOG=A1COE(1)+XOLOG*(A1COE(2)+XOLOG*(A1COE(3)+XOLOG*(A1COE(4)+ ALPH1015
1XOLOG*(A1COE(5)+XOLOG*(A1COE(6)))))) ALPH1016
4 ALPH1=EXP(2.30258509*A1LOG) ALPH1017
RETURN ALPH1018
END ALPH1019
ALPH1020

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C          SUBROUTINE TO COMPUTE THE PARTIAL DERIVATIVE--DALPHA1/DXD          PART1001
C          SUBROUTINE PART1(XD,POMEGA,K1)                                PART1002
C                                                                           PART1003
C          SUBROUTINE PART1(XD,POMEGA,K1)                                PART1004
C                                                                           PART1005
C          COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),A1COE(6),A2COE(6),YDATA(10,5,4),
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONPART1006
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, PART1008
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,VONST,ILINE(2),YMAX,YMIN,HCCNTPART1009
COMMON TPARG(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), PART1010
181(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5) PART1011
COMMON TITLE(13),IKONST PART1012
C          XOH=SQRT(XD) PART1013
CALL COEFF(WCOE,A1COE,A2COE) PART1014
2 POMEGA=0.5*WCOE(2)/XOH+WCOE(3)+1.5*WCOE(4)+XOH+2.0*WCOE(5)+XOH+ PART1015
12.5*WCOE(6)+XOH*XC PART1016
RETURN PART1017
END PART1018
PART1019

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C
C SUBROUTINE TO COMPUTE THE PARTIAL DERIVATIVE.--DALPHA2/DX0
C
C SUBROUTINE PART2(X0,PALPH1,K1)
C
COMMON PARIN(10,5,4),IPARIN(10,5),WC0E(6),A1C0E(6),A2C0E(6),YDATA(
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1,
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,KONST,ILINE(2),YMAX,YMIN,HCCNT
COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50),
1B1(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5)
COMMON TITLE(13),IKONST
C
XLOG=ALOG10(X0)
CALL COEFF(WC0E,A1C0E,A2C0E)
2 PALPH1=TPAR1(K1,4)*(A1C0E(2)+XLOG*(2.0*A1C0E(3)+XLOG*(3.0*A1C0E
1(4)+XLOG*(4.0*A1C0E(5)+XLOG*(5.0*A1C0E(6)))))/X0
RETURN
END

```

```

PART2001
PART2002
PART2003
PART2004
PART2005
PART2006
PART2007
PART2008
PART2009
PART2010
PART2011
PART2012
PART2013
PART2014
PART2015
PART2016
PART2017
PART2018
PART2019

```

```

C
C SUBROUTINE TO COMPUTE OMEGA,ALPHA1 AND ALPHA2 WHEN X0 IS VARYING
C
C SUBROUTINE XQVAR1 (TPAR)
C
COMMON PARIN(10,5,4),IPARIN(10,5),WC0E(6),A1C0E(6),A2C0E(6),YDATA(XQVAR007
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONXQVAR008
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, XQVAR009
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,KONST,ILINE(2),YMAX,YMIN,HCCNTXQVAR010
COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), XQVAR011
1B1(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5) XQVAR012
COMMON TITLE(13),IKONST XQVAR013
DIMENSION TPAR(10,5) XQVAR014
C
DO 50 K1= 1,IGAUSS XQVAR015
10 IF(IPARIN(K1,2).NE.2)GO TO 50 XQVAR016
20 IF(IPARIN(K1,3).EC.3)CALL OMEGA(TPAR(K1,2),TPAR(K1,3),K1) XQVAR017
30 IF(IPARIN(K1,4).EC.3)CALL ALPHA1(TPAR(K1,2),TPAR(K1,4),K1) XQVAR018
40 IF(IPARIN(K1,5).EC.3)CALL ALPHA2(TPAR(K1,2),TPAR(K1,5),K1) XQVAR019
50 CONTINUE XQVAR020
RETURN XQVAR021
END XQVAR022
XQVAR023

```

```

C
C SUBROUTINE TO COMPUTE THE PARTIAL DERIVATIVE.--DOMEGA/DX0
C
C SUBROUTINE PART3(X0,PALPH2,K1)
C
COMMON PARIN(10,5,4),IPARIN(10,5),WC0E(6),A1C0E(6),A2C0E(6),YDATA(
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1,
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,KONST,ILINE(2),YMAX,YMIN,HCCNT
COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50),
1B1(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3),MATIND(10,5)
COMMON TITLE(13),IKONST
C
XLOG=ALOG10(X0)
CALL COEFF(WC0E,A1C0E,A2C0E)
2 PALPH2=TPAR1(K1,5)*(A2C0E(2)+XLOG*(2.0*A2C0E(3)+XLOG*(3.0*A2C0E
1(4)+XLOG*(4.0*A2C0E(5)+XLOG*(5.0*A2C0E(6)))))/X0
RETURN
END

```

```

PART3001
PART3002
PART3003
PART3004
PART3005
PART3006
PART3007
PART3008
PART3009
PART3010
PART3011
PART3012
PART3013
PART3014
PART3015
PART3016
PART3017
PART3018
PART3019

```

```

C
C
C SUBROUTINE FOR DETERMINING IF PARAMETERS ARE BETWEEN LIMITS
C
C SUBROUTINE BOUND(TLIN,ALIN,TPA1,TPA2,EXLAM,NLIM)
C
  DIMENSION TLIN(2),ALIN(2),TPA1(10,5),TPA2(10,5)
  COMMON PARIN(10,5,4),IPARIN(10,5),WCQE(6),ALCOE(6),A2COE(6),YDATA(800008
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTION8CUND009
2(3,2),LINALB(2),GASPAR(5,2),XLIN(2,4),IGAUSS,ISTART,IEND,ICON1, ACUND010
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,MONST,ILINE(2),YMAX,YMIN,HCCNT8CUND011
  COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), BUND012
181(3),C(50,50),S(3),XL(3),CON1(10),L1,JP,A2(3,3),MATIND(10,5)
  COMMON TITLE(13),IKONST
C
  NLIM=1
C
  M=0
  1 DO 40 I= 1,2
  2 IF(ILINE(I).NE.2)GO TO 40
  3 M=M+1
  4 ALIN(I)=TLIN(I)+EXLAM*B(M)
  5 IF(ALIN(I)-XLIN(I,2))15,40,10
  10 ALIN(I)=XLIN(I,2)
  GO TO 40
  15 IF(ALIN(I)-XLIN(I,3))20,40,25
  20 ALIN(I)=XLIN(I,3)
  GO TO 40
C
  ONE OF THE LIMITS HAS BEEN EXCEEDED
C
  25 NLIM=0
  40 CONTINUE
C
  41 IF(IGAUSS.EQ.0)GO TO 90
  45 DO 80 K1=1,IGAUSS
  DO 80 K2=1,5
  50 IF(IPARIN(K1,K2).NE.2)GO TO 80
  55 M=M+1
  56 TPA2(K1,K2)=TPA1(K1,K2)+EXLAM*B(M)
  58 IF(TPA2(K1,K2)-PARIN(K1,K2,2))65,80,60
  60 TPA2(K1,K2)=PARIN(K1,K2,2)
  GO TO 80
  65 IF(TPA2(K1,K2)-PARIN(K1,K2,3))70,80,75
  70 TPA2(K1,K2)=PARIN(K1,K2,3)
  GO TO 80
  75 NLIM=0
  80 CONTINUE
  85 CALL XOVARI(TPA2)
  90 RETURN
  END

```

```

BCUND001
BCUND002
BCUND003
BCUND004
BCUND005
BCUND006
BCUND007
BCUND008
BCUND009
ACUND010
BCUND011
BCUND012
BCUND013
BCUND014
BCUND015
BCUND016
BCUND017
BCUND018
BCUND019
BCUND020
BCUND021
BCUND022
BCUND023
BCUND024
BCUND025
BCUND026
BCUND027
BCUND028
BCUND029
BCUND030
BCUND031
BCUND032
BCUND033
BCUND034
BCUND035
BCUND036
BCUND037
BCUND038
BCUND039
BCUND040
BCUND041
BCUND042
BCUND043
BCUND044
BCUND045
BCUND046
BCUND047
BCUND048
BCUND049
BCUND050
BCUND051

```

```

C
C MATRIX MULTIPLICATION SUBROUTINE
C
C SUBROUTINE MATMPY(A,M,N,B,L,C)
C
  DIMENSION A(100,50),B(50,50),C(50,50)
C
  DO 1 I=1,M
  DO 1 J=1,L
  C(I,J)=0.0
  DO 1 K=1,N
  1 C(I,J)=C(I,J)+A(I,K)*B(K,J)
  RETURN
  END

```

```

C
C SUBROUTINE FOR COMPUTING YBAR(I,J)-MODIFIED GAUSSIAN
C
C SUBROUTINE FCN (ISET,XI,YBAR,TPAR,TLIN)
C
  COMMON PARIN(10,5,4),IPARIN(10,5),WCQE(6),ALCOE(6),A2COE(6),YDATA(FCN66007
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONFCN66008
2(3,2),LINALB(2),GASPAR(5,2),XLIN(2,4),IGAUSS,ISTART,IEND,ICON1, FCN66009
3IWEIT,NOIT,ITEST,IOUTPT,M1ALF,M2ALF,MONST,ILINE(2),YMAX,YMIN,HCCNTFCN66010
  COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), FCN66011
181(3),C(50,50),S(3),XL(3),CON1(10),L1,JP,A2(3,3),MATIND(10,5)
  COMMON TITLE(13),IKONST
  DIMENSION TPAR(10,5),TLIN(2)
C
  IF(ILINE(1).NE.0.AND.ILINE(2).NE.0)GO TO 3
  YBAR = 0.0
  GO TO 5
  3 YBAR= TLIN(1)*XI+TLIN(2)
  5 IF(IGAUSS.EQ.0)GO TO 50
C
  IF(ISET) 30,10,30
  10 DO 20 I = 1,IGAUSS
  20 CON1(I)=2.77258872/(TPAR(I,3)*TPAR(I,3))
  ISET=1
  30 DO 40 I = 1,IGAUSS
  40 YBAR=YBAR+TPAR(I,1)*EXP(-CON1(I)*(XI-TPAR(I,2))**2*(1.0+TPAR(I,4)
1*(XI-TPAR(I,2))*M1ALF+TPAR(I,5)*(XI-TPAR(I,2))*M2ALF)
  50 RETURN
  END

```

```

MATMP001
MATMP002
MATMP003
MATMP004
MATMP005
MATMP006
MATMP007
MATMP008
MATMP009
MATMP010
MATMP011
MATMP012
MATMP013
MATMP014
MATMP015

```

```

FCN66001
FCN66002
FCN66003
FCN66004
FCN66005
FCN66006
FCN66007
FCN66008
FCN66009
FCN66010
FCN66011
FCN66012
FCN66013
FCN66014
FCN66015
FCN66016
FCN66017
FCN66018
FCN66019
FCN66020
FCN66021
FCN66022
FCN66023
FCN66024
FCN66025
FCN66026
FCN66027
FCN66028
FCN66029
FCN66030

```

C		PARMT001			
C	SUBROUTINE TO GENERATE INPUT PARAMETER DATA	PARMT002	DO 30 K = 1,4		PARMT058
C		PARMT003	M = 20*(I-1) + 4*(J-1) + (K+11)		PARMT059
	SUBROUTINE PARMT	PARMT004	30 EE(M) = PARIN(I,J,K)		PARMT060
C		PARMT005	RETURN		PARMT061
	COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(16),A1COE(4),A2COE(6),YDATA(PARMT006		END		PARMT062
	1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),EREI:TL(2),OPTION(PARMT007				
	2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,IS'ART,LEND,ICCN1, PARMT008				
	3IWEIT,NCIT,ITEST,IOUTPT,M1ALF,M2ALF,KONST,ILINE(2),YMAX,YMIN,HCCNT(PARMT009				
	COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT.(50),A1(50,50), PARMT010				
	1E1(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,A2(3,3) MAT1.D(10,5) PARMT011				
	COMMON TITLE(13),IKONST PARMT012				
	COMMON EE(211) PARMT013				
C	IF(ILINE(1).NE.0.AND.ILINE(2).NE.0)GO TO 5 PARMT014				
	XLINE(1,1) = 0.0 PARMT015				
	XLINE(2,1) = 0.0 PARMT016				
C	5 DO 20 K1 = 1,IGAUSS PARMT017				
	JJ = PARIN(K1,2,1) + 0.5 PARMT018				
C	DETERMINE INITIAL HEIGHT VALUE PARMT019				
C	PARIN(K1,1,1) = YDATA(JJ)-(XLINE(1,1)*PARIN(K1,2,1)*XLINE(2,1)) PARMT020				
C	DETERMINE INITIAL VALUES OF HALF-WIDTH, ALPHA1, AND ALPHA2 PARMT021				
C	CALL OMEGA(PARIN(K1,2,1),PARIN(K1,3,1),K1) PARMT022				
C	CALL ALPHA1(PARIN(K1,2,1),PARIN(K1,4,1),K1) PARMT023				
C	CALL ALPHA2(PARIN(K1,2,1),PARIN(K1,5,1),K1) PARMT024				
C	DETERMINE UPPER LIMITS FOR ALL PARAMETERS PARMT025				
	PARIN(K1,1,2) = 2.0 * PARIN(K1,1,1) PARMT026				
	PARIN(K1,2,2) = 2.0 * PARIN(K1,2,1) PARMT027				
	PARIN(K1,3,2) = 2.0 * PARIN(K1,3,1) PARMT028				
	PARIN(K1,4,2) = 1.E+02 * PARIN(K1,4,1) PARMT029				
	PARIN(K1,5,2) = 1.E+02 * PARIN(K1,5,1) PARMT030				
C	DETERMINE LOWER LIMITS FOR ALL PARAMETERS PARMT031				
	PARIN(K1,1,3) = 0.3 * PARIN(K1,1,1) PARMT032				
	PARIN(K1,2,3) = PARIN(K1,2,1) - 2.0 PARMT033				
	PARIN(K1,3,3) = 0.5 * PARIN(K1,3,1) PARMT034				
	PARIN(K1,4,3) = 1.E-03 * PARIN(K1,4,1) PARMT035				
	PARIN(K1,5,3) = 1.E-03 * PARIN(K1,5,1) PARMT036				
C	DETERMINE CONVERGENCE CRITERION PARMT037				
	PARIN(K1,1,4) = 1.E+00 PARMT038				
	PARIN(K1,2,4) = 1.E-03 PARMT039				
	PARIN(K1,3,4) = 1.E-03 PARMT040				
	PARIN(K1,4,4) = 1.E-04 * PARIN(K1,4,1) PARMT041				
	PARIN(K1,5,4) = 1.E-04 * PARIN(K1,5,1) PARMT042				
20	CONTINUE PARMT043				
	DO 30 I = 1,IGAUSS PARMT044				
	DO 30 J = 1,5 PARMT045				
		PARMT046			
		PARMT047			
		PARMT048			
		PARMT049			
		PARMT050			
		PARMT051			
		PARMT052			
		PARMT053			
		PARMT054			
		PARMT055			
		PARMT056			
		PARMT057			

```

C          SUBROUTINE TO COMPUTE THE AREA OF THE MODIFIED GAUSSIAN PHOTOPEAKS
C          AND ERRORS IN THE AREAS
C          SUBROUTINE ERREA(TPAM,SIG)
C
COMMON PARIN(10,5,4),IPARIN(10,5),WCNE(6),ALCOE(6),AZCOE(6),YDATA(EREA007
1511),WDATA(511),TPAR1(10,5),TLINE(2),ERESTG(10,5),ERESTL(2),OPTIONEREA008
2(3,2),LINALB(2),GASPAR(5,2),XLINE(2,4),IGAUSS,ISTART,IEND,ICON1, EREA009
3WEIT,NOIT,ITEST,IOUPT,IALF,M2ALF,WONST,I LINE(2),YMAX,YMIN,HCCNTEREA010
COMMON TPAR2(10,5),ALINE(2),A(100,50),B(50),VECT1(50),A1(50,50), EREA011
1B1(3),C(50,50),S(3),XL(3),CON1(10),L1,JP,A2(3,3),MATIND(10,5) EREA012
COMMON TITLE(13),ICONST EREA013
DIMENSION M(2),MH(2),XMFAC(2),XMHFAC(2),FACCON(2),TPAM(10,5) EREA014
C*****
C      DETERMINE CONSTANTS ERROR IN AREA CALCULATIONS
C*****
CONS1 = 1.06446655 EREA015
CONS2 = 1.13309005 EREA016
CONS3 = SIG*CONS2 EREA017
Y=1.665110 EREA018
XLN2 = 0.6931471806 EREA019
PI = 3.1415927 EREA020
C
C      DETERMINE FACTORIAL VALUES
C
M(1)=M1ALF EREA021
M(2)=M2ALF EREA022
DO 20 K = 1,2 EREA023
XMFAC(K)=M(K) EREA024
N=M(K)-1 EREA025
DO 20 I = 1,N EREA026
XM=M(K)-I EREA027
20 XMFAC(K) = XMFAC(K)*XM EREA028
C
C      M/2 FACTORIAL
C
DO 40 K = 1,2 EREA029
IF(M(K).EQ.2)GO TO 39 EREA030
MH(K)= M(K)/2 EREA031
NN=MH(K)-1 EREA032
XMHFAC(K)=MH(K) EREA033
DO 38 I = 1,NN EREA034
XMH=MH(K)-I EREA035
XMHFAC(K)=XMHFAC(K)*XMH EREA036
38 CONTINUE EREA037
GO TO 40 EREA038
39 XMHFAC(K)=1.0 EREA039
40 CONTINUE EREA040
DO 45 J = 1,2 EREA041
45 FACCON(J) = XMFAC(J)/XMHFAC(J) EREA042
C
C      XM1ALF=M1ALF EREA043
C      XM2ALF=M2ALF EREA044
C
55 CONE = PI*XMFAC(1)*XMFAC(1)/(2.0**(4*M1ALF+2)*(XLN2**(M1ALF+1)) + EREA045
1(XMHFAC(1)*XMHFAC(1))) EREA046
C
C      CTWO = PI*XMFAC(2)*XMFAC(2)/(2.0**(4*M2ALF+2)*(XLN2**(M2ALF+1)) + EREA058
1(XMHFAC(2)*XMHFAC(2))) EREA059
C
DO = 0.5*SQRT(PI/XLN2) EREA060
D1 = XMFAC(1)/(2.0**(2*M1ALF) * XMHFAC(1) * XLN2 ** (M1ALF/2)) EREA061
D2 = XMFAC(2)/(2.0**(2*M2ALF) * XMHFAC(2) * XLN2 ** (M2ALF/2)) EREA062
C
C      COMPUTE PHOTOPEAK AREAS
C
WRITE(6,500) EREA063
WRITE(6,502) EREA064
DO 65 K1 = 1,IGAUSS EREA065
WCON = TPAM(K1,3)/Y EREA066
C
AREA0 = CONS1*TPAM(K1,3)*TPAM(K1,1) EREA067
AREA1 = AREA0 * TPAM(K1,4) * WCON ** M1ALF * (FACCON(1)/2.0 ** M1ERRFA073
1ALF) EREA068
AREA2 = AREA0 * TPAM(K1,5) * WCON ** M2ALF * (FACCON(2)/2.0 ** M2ERRFA075
1ALF) EREA069
C
TAREA = AREA0 + AREA1 + AREA2 EREA070
65 WRITE(6,504)K1,AREA0,AREA1,AREA2,TAREA EREA071
C
C      DETERMINATION OF ERRORS IN THE PHOTOPEAK AREA
C
WRITE(6,506) EREA072
WRITE(6,508) EREA073
DO 400 K1 = 1,IGAUSS EREA074
YOSQ = TPAM(K1,1)*TPAM(K1,1) EREA075
WOSQ = TPAM(K1,3)*TPAM(K1,3) EREA076
AL1SQ= TPAM(K1,4)*TPAM(K1,4) EREA077
AL2SQ= TPAM(K1,5)*TPAM(K1,5) EREA078
C
C      DETERMINE ERROR IN AREA0
C
70 TERM1=0.0 EREA079
TERM2=0.0 EREA080
TERM3=0.0 EREA081
C
I3=0 EREA082
I1=0 EREA083
75 IF(MATIND(K1,3).EQ.0)GO TO 80 EREA084
I3 = MATIND(K1,3) EREA085
TERM1 = YOSQ * A(I3,I3) EREA086
80 IF(MATIND(K1,1).EQ.0)GO TO 90 EREA087
I1 = MATIND(K1,1) EREA088
TERM2 = WOSQ * A(I1,I1) EREA089
85 IF(I3.EQ.0)GO TO 90 EREA090
TERM3 = TPAM(K1,1)*TPAM(K1,3)*A(I1,I3) EREA091
C
90 ERRAO = CONS3 *(TERM1 + TERM2 + 2.0*TERM3) EREA092
C
C      DETERMINE ERROR IN AREA1
C
TERM4=0.0 EREA093
TERM5=0.0 EREA094
TERM6=0.0 EREA095

```

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C

C

2

* 7040 DOUBLE PRECISION DOUBLE PIVOTAL GAUSS-JORDAN MATRIX
 * INVERSION AND SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS
 * MAP SUBROUTINE
 * D.H. GIPSON PHILLIPS PETROLEUM CO. NOV. 1963

PMC ON
 EXTERN DFADS
 EXTERN DFMP
 EXTERN DFDP
 NOCRS

* DCLA MACRO X,T
 CLA X,T
 LDQ X+1,T
 ENDM DCLA

* DSTO MACRO X,T
 STO X,T
 STO X+1,T
 ENDM DSTO

* DFAD MACRO X,T
 TSL DFADS
 PZE X,T
 ENDM DFAD

* DFMP MACRO X,T
 TSL DFMP
 PZE X,T
 ENDM DFMP

* DFOP MACRO X,T
 TSL DFDP
 PZE X,T
 ENDM DFOP

* DCLS MACRO X,T
 CLS X,T
 LDQ X+1,T
 LRS 0
 ENDM DCLS

* MAINS ENTRY MAINS
 ENTRY MAIND
 TRA **
 CLA =0
 STO CHK
 SXA IND1,1
 SXA IND2,2
 SXA IND4,4
 LAC MAINS,1
 CLA 2,4
 STO A
 CLA* 3,4
 STO M
 CLA 4,4
 STO B

ADDRESS OF A

VALUE OF M

ADDRESS OF B

002MAINS CLA* 5,4
 003MAINS STO N
 004MAINS CLA 6,4
 005MAINS STO DET
 006MAINS CLA 7,4
 007MAINS STO IFS
 008MAINS
 009MAINS
 010MAINS
 011MAINS
 012MAINS
 013MAINS
 014MAINS
 015MAINS
 016MAINS
 017MAINS
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 049MAINS
 050MAINS
 051MAINS
 052MAINS
 053MAINS
 054MAINS
 055MAINS
 056MAINS
 057MAINS
 058MAINS

* UNPACK THE MATRIX
 CLA M
 STO J
 CLA A
 ADD M
 STA INS1
 ADD M
 STA INS2
 STA INS3
 BL1 AXT 0,1
 AXT 0,2
 LXA M,4
 BL2 TXI **1,2,1
 INS2 STZ **2
 TXI **1,1,1
 TXI **1,2,1
 INS1 CLA **1
 INS3 STO **2
 TXI BL2,4,1
 CLA J
 SUB =1
 TZE BL3
 STO J
 CLA INS1
 ADD CCN1
 STO INS1
 CLA INS2
 ADD CCN1
 STO INS2
 STA INS3
 TRA BL1
 CLA N
 TZE BL6
 STO J
 CLA B
 ADD M
 STA INS4
 ADD M
 STA INS5
 STA INS6
 BL4 AXT 0,1
 AXT 0,2
 LXA M,4
 BL5 TXI **1,2,1
 INS5 STZ **2
 TXI **1,1,1
 TXI **1,2,1
 INS4 CLA **1
 INS6 STO **2

VALUE OF N

ADDRESS OF DET

ADDRESS OF IFS

***A+2*M

***A+M

***A+2*M

***B+2*M

***B+M

***B+2*M

059MAINS
 060MAINS
 061MAINS
 062MAINS
 063MAINS
 064MAINS
 065MAINS
 066MAINS
 067MAINS
 068MAINS
 069MAINS
 070MAINS
 071MAINS
 072MAINS
 073MAINS
 074MAINS
 075MAINS
 076MAINS
 077MAINS
 078MAINS
 079MAINS
 080MAINS
 081MAINS
 082MAINS
 083MAINS
 084MAINS
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 086MAINS
 087MAINS
 088MAINS
 089MAINS
 090MAINS
 091MAINS
 092MAINS
 093MAINS
 094MAINS
 095MAINS
 096MAINS
 097MAINS
 098MAINS
 099MAINS
 100MAINS
 101MAINS
 102MAINS
 103MAINS
 104MAINS
 105MAINS
 106MAINS
 107MAINS
 108MAINS
 109MAINS
 110MAINS
 111MAINS
 112MAINS
 113MAINS
 114MAINS
 115MAINS


```

MAIND   TRA      00
        CLA      =1
        STO      CHK
        SXA      IND1,1
        SXA      IND2,2
        SXA      IND4,4
        LAC      MAIND,4
        CLA      2,4
        STO      A
        CLA*     3,4
        STO      M
        CLA      4,4
        STO      B
        CLA*     5,4
        STO      N
        CLA      6,4
        STO      DET
        CLA      7,4
        STO      IFS

```

ADDRESS OF A
VALUE OF M
ADDRESS OF B
VALUE OF N
ADDRESS OF DET
ADDRESS OF IFS

```

•
•
•
BL6      LXA      M,4
          AXI      0,1
LOOP      TXI      =+1,1,-1
          STZ      IRON-1,1
          STZ      JCOL-1,1
          TIX      LOOP,4,1
          LAC      CCN1,2
          SXO      INS7,2
          SXO      INS8,2
          SXO      INS9,2
          SXO      INS10,2
          SXO      INS11,2
          SXO      INS12,2
          CLA      A
          STA      INA1
          STA      INA2
          SUB      =1
          STA      INA3
          SUB      =1
          STA      INA4
          STA      INA5

```

116MAINS
117MAINS
118MAINS
119MAINS
120MAINS
121MAINS
122MAINS
123MAINS
124MAINS
125MAINS
126MAINS
127MAINS
128MAINS
129MAINS
130MAINS
131MAINS
132MAINS
133MAINS
134MAINS
135MAINS
136MAINS
137MAINS
138MAINS
139MAINS
140MAINS
141MAINS
142MAINS
143MAINS
144MAINS
145MAINS
146MAINS
147MAINS
148MAINS
149MAINS
150MAINS
151MAINS
152MAINS
153MAINS
154MAINS
155MAINS
156MAINS
157MAINS
158MAINS
159MAINS
160MAINS
161MAINS
162MAINS
163MAINS
164MAINS
165MAINS
166MAINS
167MAINS
168MAINS
169MAINS
170MAINS
171MAINS
172MAINS

STA	INA6
STA	INA7
STA	INA8
STA	INA9
STA	INA10
STA	INA11+1
STA	INA12+1
STA	INA13
STA	INA14+1
STA	BL27
STA	INA15
STA	INA16
STA	INA17
STA	INA18
STA	INA19
STA	INA20
STA	INA21
ADD	=1
STA	INA5+1
STA	INA6+1
STA	INA7+1
STA	INA8+1
STA	INA10+1
STA	INA13+1
STA	BL27+1
STA	INA15+1
STA	INA16+1
STA	INA17+1
STA	INA18+1
STA	INA19+1
STA	INA20+1
STA	INA21+1
CLA	8
STA	INB1
STA	INB2
SUB	=1
STA	INB3
SUB	=1
STA	BL20
STA	INB4
STA	INB5+1
STA	INB6
STA	BL28
STA	INB7
STA	INB8
STA	INB9
ADD	=1
STA	INB4+1
STA	INB6+1
STA	BL28+1
STA	INB7+1
STA	INB8+1
STA	INB9+1

FIND THE PIVOT ELEMENT
CLA = 1.0

173MAINS
174MAINS
175MAINS
176MAINS
177MAINS
178MAINS
179MAINS
180MAINS
181MAINS
182MAINS
183MAINS
184MAINS
185MAINS
186MAINS
187MAINS
188MAINS
189MAINS
190MAINS
191MAINS
192MAINS
193MAINS
194MAINS
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208MAINS
209MAINS
210MAINS
211MAINS
212MAINS
213MAINS
214MAINS
215MAINS
216MAINS
217MAINS
218MAINS
219MAINS
220MAINS
221MAINS
222MAINS
223MAINS
224MAINS
225MAINS
226MAINS
227MAINS
228MAINS
229MAINS

INA10	DSTO	00,1	000A-2	344MAINS	CLA	=1	401MAINS
	LAC	TEMP,2		345MAINS	STO	I	402MAINS
	CLA	J		346MAINS	BL21	TXI 001,2,-2	403MAINS
	SUB	=1		347MAINS	TXI	001,4,-2	404MAINS
	LRS	35		348MAINS	CLA	I	405MAINS
	MPY	CON1		349MAINS	SUB	IP	406MAINS
	LLS	35		350MAINS	TZE	BL22	407MAINS
	PAC	,4		351MAINS	DCLA	ALPHA	408MAINS
	CLA	=1		352MAINS	INA14	DFMP 00,2	000A-2
	STO	I		353MAINS	INB5	DFAD 00,4	000B-2
BL16	TXI	001,2,-2		354MAINS	INB6	DSTO 00,4	000B-2
	TXI	001,4,-2		355MAINS	BL22	CLA I	412MAINS
	CLA	I		356MAINS	CAS	M	413MAINS
	SUB	IP		357MAINS	TRA	BL23	414MAINS
	TZE	BL17		358MAINS	TRA	BL23	415MAINS
	DCLA	ALPHA		359MAINS	ADD	=1	416MAINS
INA11	DFMP	00,2	000A-2	360MAINS	STO	I	417MAINS
INA12	DFAD	00,4	000A-2	361MAINS	TRA	BL21	418MAINS
INA13	DSTO	00,4	000A-2	362MAINS	BL23	CLA J	419MAINS
BL17	CLA	I		363MAINS	CAS	N	420MAINS
	CAS	M		364MAINS	TRA	BL24	421MAINS
	TRA	BL18		365MAINS	TRA	BL24	422MAINS
	TRA	BL18		366MAINS	ADD	=1	423MAINS
	ADD	=1		367MAINS	STO	J	424MAINS
	STO	I		368MAINS	INS8	TXI BL20,1,00	000 -MMAX
	TRA	BL16		369MAINS	BL24	CLA K	426MAINS
BL18	CLA	J		370MAINS	CAS	M	427MAINS
	CAS	M		371MAINS	TRA	BL25	428MAINS
	TRA	BL19		372MAINS	TRA	BL25	429MAINS
	TRA	BL19		373MAINS	ADD	=1	430MAINS
	ADD	=1		374MAINS	STO	K	431MAINS
	STO	J		375MAINS	TRA	BL7	432MAINS
INS7	TXI	BL15,1,00	000 -MMAX	376MAINS	.		433MAINS
.				377MAINS	.	ROW PERMUTATIONS	434MAINS
.				378MAINS	.		435MAINS
.				379MAINS	BL25	CLA =1	436MAINS
BL19	CLA	N		380MAINS	STO	K	437MAINS
	TZE	BL24		381MAINS	BL26	LAC K,1	438MAINS
	CLA	IP		382MAINS	CLA	IROW-1.1	439MAINS
	ADD	IP		383MAINS	STO	I	440MAINS
	PAC	,1		384MAINS	CAS	K	441MAINS
	CLA	=1		385MAINS	TRA	002	442MAINS
	STO	J		386MAINS	TRA	BL30	443MAINS
BL20	CLA	00,1	000B-2	387MAINS	CLS	DET	444MAINS
	TZE	BL23		388MAINS	STO	DET	445MAINS
	STO	ALPHA		389MAINS	LXA	M,4	446MAINS
INB3	LDQ	00,1	000B-1	390MAINS	CLA	K	447MAINS
	STQ	ALPHA+1		391MAINS	ADD	K	448MAINS
	DFDP	PIVOT		392MAINS	PAC	,1	449MAINS
INB4	DSTO	00,1	000B-2	393MAINS	CLA	I	450MAINS
	LAC	TEMP,2		394MAINS	ADD	I	451MAINS
	CLA	J		395MAINS	PAC	,2	452MAINS
	SUB	=1		396MAINS	BL27	DCLA 00,2	000A-2
	LRS	35		397MAINS	DSTO	TEMP1	453MAINS
	MPY	CON1		398MAINS	INA15	DCLA 00,1	000A-2
	LLS	35		399MAINS	INA16	DSTO 00,2	000A-2
	PAC	,4		400MAINS	DCLA	TEMP1	457MAINS

ARITHMETIC OPERATIONS ON THE COLUMNS OF (B)

```

INA17 DSTO 00,1      ***A-2
INS9 TXI 001,1,00    *** -MMAX
INS10 TXI 001,2,00    *** -MMAX
      TIX BL27,4,1
      CLA N
      TZE BL29
      PAX ,4
      CLA K
      ADD K
      PAC ,1
      CLA I
      ADD I
      PAC ,2
BL28 DCLA 00,2      ***B-2
      DSTO TEMP1
IN87 DCLA 00,1      ***B-2
IN88 DSTO 00,2      ***B-2
      DCLA TEMP1
IN89 DSTO 00,1      ***B-2
INS11 TXI 001,1,00    *** -MMAX
INS12 TXI 001,2,00    *** -MMAX
      TIX BL28,4,1
BL29 LAC K,1
      LAC I,2
      CLA IROW-1,2
      STO IROW-1,1
      CLA I
      STO IROW-1,2
      TRA BL26
BL30 CLA K
      CAS M
      TRA BL31
      TRA BL31
      ADD =1
      STO K
      TRA BL26
*
*
*
BL31 CLA =1
      STO K
BL32 LAC K,1
      CLA JCOL-1,1
      STO J
      CAS K
      TRA 002
      TRA BL34
      SUB =1
      LRS 35
      MPY CON1
      LLS 35
      PAC ,1
      CLA K
      SUB =1
      LRS 35
      MPY CON1
      LLS 35

```

```

458MAINS PAC ,2
459MAINS LXA M,4
460MAINS BL33 TXI 001,1,-2
461MAINS TXI 001,2,-2
      INA13 DCLA 00,1      ***A-2
      DSTO TEMP1
      INA19 DCLA 00,2      ***A-2
      INA20 DSTO 00,1      ***A-2
      DCLA TEMP1
      INA21 DSTO 00,2      ***A-2
      TIX BL33,4,1
      LAC J,1
      LAC K,2
      CLA JCOL-1,1
      STO JCOL-1,2
      CLA J
      STO JCOL-1,1
      TRA BL32
BL34 CLA K
      CAS M
      TRA BL35
      TRA BL35
      ADD =1
      STO K
      TRA BL32
BL35 CLA CHK
      TNZ BL41
*
*
*
      PACK THE MATRICES
      CLA =1
      STO J
BL36 CLA M
      SUB =1
      PAX ,4
      CLA J
      SUB =1
      LRS 35
      MPY CON1
      LLS 35
      PAC ,1
      PAC ,2
BL37 TXI 001,1,-2
      TXI 001,2,-1
      INA1 CLA 00,1      ***A
      INA2 STO 00,2      ***A
      TIX BL37,4,1
      CLA J
      CAS M
      TRA BL38
      TRA BL38
      ADD =1
      STO J
      TRA BL36
BL38 CLA N
      TZE BL41
      CLA =1

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515MAINS
516MAINS
517MAINS
518MAINS
519MAINS
520MAINS
521MAINS
522MAINS
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524MAINS
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526MAINS
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531MAINS
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566MAINS
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568MAINS
569MAINS
570MAINS
571MAINS

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BL39	STO	J		572MAINS	CON1	PZE	MMA	629MAINS
	CLA	M		573MAINS	MMA	EQU	100	
	SUB	=1		574MAINS		END		631MAINS
	PAX	,4		575MAINS				
	CLA	J		576MAINS				
	SUB	=1		577MAINS				
	LRS	35		578MAINS				
	MPY	CON1		579MAINS				
	LLS	35		580MAINS				
	PAC	,1		581MAINS				
	PAC	,2		582MAINS				
BL40	TXI	++1,1,-2		583MAINS				
	TXI	++1,2,-1		584MAINS				
INB1	CLA	++,1	==B	585MAINS				
INB2	STO	++,2	==B	586MAINS				
	TIX	BL40,4,1		587MAINS				
	CLA	J		588MAINS				
	CAS	N		589MAINS				
	TRA	BL41		590MAINS				
	TRA	BL41		591MAINS				
	ADC	=1		592MAINS				
	STO	J		593MAINS				
	TRA	BL39		594MAINS				
.				595MAINS				
.	RESET	INDEX REGISTERS AND RETURN		596MAINS				
.				597MAINS				
BL41	LXA	IND1,1		598MAINS				
	LXA	IND2,2		599MAINS				
	LXA	IND4,4		600MAINS				
	CLA	CHK		601MAINS				
	TZE	MAINS		602MAINS				
	TRA	MAIND		603MAINS				
.				604MAINS				
.	RESERVED AREAS			605MAINS				
.				606MAINS				
A	BSS	1		607MAINS				
ALPHA	BSS	2		608MAINS				
B	BSS	1		609MAINS				
CHK	BSS	1		610MAINS				
DET	BSS	1		611MAINS				
I	BSS	1		612MAINS				
IFS	BSS	1		613MAINS				
IND1	BSS	1		614MAINS				
IND2	BSS	1		615MAINS				
IND4	BSS	1		616MAINS				
IP	BSS	1		617MAINS				
IR0W	BSS	MMA/2		618MAINS				
J	BSS	1		619MAINS				
JCOL	BSS	MMA/2		620MAINS				
JP	BSS	1		621MAINS				
K	BSS	1		622MAINS				
M	BSS	1		623MAINS				
N	BSS	1		624MAINS				
ONE	DEC	1.0,		625MAINS				
PIVOT	BSS	2		626MAINS				
TEMP	BSS	1		627MAINS				
TEMP1	BSS	2		628MAINS				

• DOUBLE PRECISION SUBROUTINES FOR THE 7040 D SPEAS, L GANNON 9-63 0010PSUB
 • MODIFICATION OF THE 7090 FORTRAN II SUBROUTINES FOR USE WITH 7040 MAP0020PSUB
 •
 • MS MOST SIGNIFICANT 0030PSUB
 • LS LEAST SIGNIFICANT 0040PSUB
 • ACH PSEUDO ACCUMULATOR MS 41 FORTRAN II 0050PSUB
 • ACL PSEUDO ACCUMULATOR LS 41-1 0060PSUB
 • ACH MQ MS 41-2 0070PSUB
 • ACL MQ LS 41-3 0080PSUB
 • Z= Y OP X YMS AND YLS MUST BE IN THE AC AND MQ, X IS 0090PSUB
 • SPECIFIED BY THE OP CODE, ZMS AND ZLS WILL BE 0100PSUB
 • IN THE AC AND MQ 0110PSUB
 •
 • ENTRY DFA0S 0120PSUB
 • ENTRY DFS0S 0130PSUB
 • ENTRY DFMS 0140PSUB
 • ENTRY DFDP 0150PSUB
 •
 • DFAD ROUTINE 0160PSUB
 • DFA0S PZE ** 0170PSUB
 • TSL SETADD 0180PSUB
 • CLA ACH MOST SIG. AC 0190PSUB
 • FAD* XMS MOST SIG. VARIABLE 0200PSUB
 • STQ ACH SAVE MOST SIG. SUM 0210PSUB
 • STQ ERASE3 LEAST SIG. PART OF SUM TO AC 0220PSUB
 • CLA ERASE3 0230PSUB
 • UFA ACL 0240PSUB
 • UFA* XLS ADD LEAST SIG. PART OF VARIABLE 0250PSUB
 • FAD ACH ADD MOST SIG. SUM 0260PSUB
 • TRA* DFA0S RETURN TO CALLING PROGRAM 0270PSUB
 •
 • DFSB ROUTINE 0280PSUB
 • DFSB PZE ** 0290PSUB
 • TSL SETADD 0300PSUB
 • CLA ACH MOST SIG. AC 0310PSUB
 • FSB* XMS MOST SIG. PART OF VARIABLE 0320PSUB
 • STQ ACH SAVE MOST SIG. DIFFERENCE 0330PSUB
 • STQ ERASE3 LEAST SIG. DIFFERENCE TO AC 0340PSUB
 • CLA ERASE3 0350PSUB
 • UFA ACL PLUS LEAST SIG. AC 0360PSUB
 • UFA* XLS LESS LEAST SIG. PART OF VARIABLE 0370PSUB
 • FAD ACH PLUS DIFFERENCE OF MOST SIG. PARTS 0380PSUB
 • TRA* DFSB RETURN TO CALLING PROGRAM 0390PSUB
 •
 • DFMP ROUTINE 0400PSUB
 • DFMP PZE ** 0410PSUB
 • TSL SETADD 0420PSUB
 • LDQ ACH MOST SIG. AC 0430PSUB
 • FMP* XMS MOST SIG. PART OF VARIABLE 0440PSUB
 • STQ ERASE1 MOST SIG. PART OF PRODUCT 0450PSUB
 • STQ ERASE2 LEAST SIG. PART OF PRODUCT 0460PSUB
 • LDQ ACH MOST SIG. AC 0470PSUB
 • FMP* XLS LEAST SIG. PART OF VARIABLE 0480PSUB
 • UFA ERASE2 PLUS LEAST SIG. PART OF FIRST PRODUCT 0490PSUB
 • STQ ERASE2 SAVE 0500PSUB
 • LDQ* XMS MOST SIG. PART OF VARIABLE 0510PSUB
 • FMP ACL LEAST SIG. AC 0520PSUB
 • 0530PSUB
 • 0540PSUB
 • 0550PSUB
 • 0560PSUB
 • 0570PSUB

UFA ERASE2 PLUS PREVIOUS PRODUCT OF LEAST PARTS 0580PSUB
 FAD ERASE1 PLUS PRODUCT OF MOST PARTS 0590PSUB
 TRA* DFMS RETURN TO CALLING PROGRAM 0600PSUB
 • 0610PSUB
 • DFDP ROUTINE 0620PSUB
 • PZE ** 0630PSUB
 • TSL SETADD 0640PSUB
 • CLA ACH MOST SIG. AC 0650PSUB
 • FDP* XMS / MOST SIG. PART OF VARIABLE 0660PSUB
 • STQ ERASE1 SAVE MOST SIG. QUOTIENT 0670PSUB
 • UFA ACL REMAINDER PLUS LEAST SIG. PART OF VARIABLE 0680PSUB
 • FDP* XMS / MOST SIG. PART OF VARIABLE 0690PSUB
 • STQ ERASE2 SAVE MOST SIG. PART 0700PSUB
 • CLS* XLS 0710PSUB
 • FDP* XMS $(A+B)/(C+D) = ((A+B)/C) \cdot (1-C/C)$ 0720PSUB
 • FMP ERASE1 0730PSUB
 • UFA ERASE2 0740PSUB
 • FAD ERASE1 0750PSUB
 • TRA* DFDP RETURN TO CALLING PROGRAM 0760PSUB
 • 0770PSUB
 • SUBROUTINE TO SET THE RETURN ADDRESS AND THE ADDRESSES OF XMS AND 0780PSUB
 • XLS WHICH ARE USED INDIRECTLY IN THE ARITHMETIC SUBROUTINES 0790PSUB
 • AND STORE THE AC AND MQ IN ACH AND ACL. 0800PSUB
 • 0810PSUB
 • XMS ADDRESS OF ADDRESS OF MOST SIGNIFICANT PART OF VARIABLE 0820PSUB
 • XLS ADDRESS OF ADDRESS OF LEAST SIGNIFICANT PART OF VARIABLE 0830PSUB
 • SETADD PZE ** 0840PSUB
 • SXA XA,4 0850PSUB
 • STQ ACH 0860PSUB
 • STQ ACL 0870PSUB
 • LAC SETADD,4 0880PSUB
 • CLA* -2,4 0890PSUB
 • STQ XMS 0900PSUB
 • ADD =1 0910PSUB
 • STQ XLS 0920PSUB
 • CLA -2,4 0930PSUB
 • ADD =1 0940PSUB
 • STQ -2,4 0950PSUB
 • XA AXT **4 0960PSUB
 • TRA* SETADD 0970PSUB
 • 0980PSUB
 • 0990PSUB
 • XMS PZE ADDRESS OF MS 1000PSUB
 • XLS PZE ADDRESS OF LS 1010PSUB
 • ACH BSS 1 1020PSUB
 • ACL BSS 1 1030PSUB
 • ERASE1 PZE 1040PSUB
 • ERASE2 PZE 1050PSUB
 • ERASE3 PZE 1060PSUB
 • END 1070PSUB

```

C      SUBROUTINE WHICH PRINTS OUTPUT AS A FUNCTION OF *IOUTPT* AND      OUTPT001
C      *ISTP*                                                             OUTPT002
C      OUTPT003
C      SUBROUTINE OUTPUT(ITERAT,ISTP,TPAR,SUM,SIG,XLAMB,TLIN)           OUTPT004
C                                                                           OUTPT005
C                                                                           OUTPT006
C      COMMON PARIN(10,5,4),IPARIN(10,5),WCOE(6),AICOE(6),A2COE(6),YDATA(OUTPT007
1511),WDATA(511),TPAR(10,5),TLIN(2),EREST(10,5),ERESTL(2),OPTION(OUTPT008
2(3,2),LINALB(2),GASPAR(5,2),XLIN(2,4),IGAUSS,ISTART,IEND,ICON1, OUTPT009
3IWEIT,NOIT,ITEST,IOUTPT,MIALF,M2ALF,YMST,ILINE(2),YMAX,YMIN,HCCNT(OUTPT010
COMMON TPAR(10,5),ALINE(2),A(100,50),B(50),VECT(1,50),A1(50,50), OUTPT011
181(3),C(50,50),S(3),XL(3),CON1(10),LL,JP,AZ(3,3),MATING(10,5)
COMMON TITLE(13),IKONST
C
C      DIMENSION TPAR(10,5),TLIN(2)
C
C      5 INTEGER OPTION,GASPAR
10 IF(ISTP.NE.0)GO TO 160
  ASSIGN 160 TO YMAT
C
C      DECIMAL REPRESENTATION OF *VARIED*,*CALCULATED*,AND *CONSTANT*
C      OPTIONS
C
C      15 OPTION(1,1)=-17508752563
  OPTION(1,2)= 18887933952
  OPTION(2,1)=-17599141465
  OPTION(2,2)= 22896902144
  OPTION(3,1)= 20695563555
  OPTION(3,2)= 19114835968
C
C      DECIMAL REPRESENTATION OF *LINE(1)* AND *LINE(2)*
C
C      LINALB(1)=18253611008
  LINALB(2)=19327352832
C
C      DECIMAL REPRESENTATION OF *HEIGHT*, *CHANNEL*, *HALF-WIDTH*.
C      *ALPHA1* AND *ALPHA2*.
C
C      GASPAR(1,1)=-17991554647
  GASPAR(1,2)= 26638224432
  GASPAR(2,1)=-17504999781
  GASPAR(2,2)= 23148563504
  GASPAR(3,1)= 26064283702
  GASPAR(3,2)= 27192560688
  GASPAR(4,1)=-1798977788C
  GASPAR(4,2)= 18283170864
  GASPAR(5,1)=-17989777880
  GASPAR(5,2)= 18299948080
C.....
C      PRINT THE INPUT DATA
C.....
C      20 WRITE(6,1000)
  WRITE(6,1001)(TITLE(I),I=1,13)
  WRITE(6,1002)
  WRITE(6,1003)IGAUSS
  WRITE(6,1004)ISTART
  WRITE(6,1005)IEND
  WRITE(6,1006)NOIT
  WRITE(6,1007)ITEST
  GO TO (21,22,23,24,25),IWEIT
21 WRITE(6,1008)
  GO TO 26
22 WRITE(6,1009)
  GO TO 26
23 WRITE(6,1010)
  GO TO 26
24 WRITE(6,1011)
  GO TO 26
25 WRITE(6,1012)
26 IF(ICON1.EQ.0)GO TO 27
  WRITE(6,1013)HCONT
  GO TO 28
27 WRITE(6,1014)
28 KOUTPT=IOUTPT+1
  GO TO (29,30,31),KOUTPT
29 WRITE(6,1015)
  GO TO 32
30 WRITE(6,1016)
  GO TO 32
31 WRITE(6,1017)
32 WRITE(6,1018)MIALF,M2ALF
  IF(IWEIT.NE.4)GO TO 35
  WRITE(6,1019)YMAX
  WRITE(6,1020)YMIN
35 IF(ILINE(1).EQ.0.AND.(ILINE(2).EQ.0)GO TO 42
  WRITE(6,1021)
  WRITE(6,1022)
  DO 40 I = 1,2
    J=ILINE(I)
40 WRITE(6,1023)LINALB(I',OPTION(J,1),OPTION(J,2),(XLIN(I,K),K=1,4)
42 WRITE(6,1024)
  IF(IGAUSS.EQ.0)GO TO 120
  IF(IPARIN(1,3).LE.2.AND.IPARIN(1,4).LE.2.AND.IPARIN(1,5).LE.2)GO
  1 TO 80
  WRITE(6,1025)
50 IF(IPARIN(1,3).NE.3)GO TO 60
  WRITE(6,1026)(WCOE(I),I=1,6)
60 IF(IPARIN(1,4).NE.3)GO TO 70
  WRITE(6,1027)(AICOE(I),I=1,6)
70 IF(IPARIN(1,5).NE.3)GO TO 80
  WRITE(6,1028)(A2COE(I),I=1,6)
C
C      WRITE GAUSSIAN PARAMETER OPTIONS
C
C      80 WRITE(6,1029)
85 WRITE(6,1030)
  DO 90 K1 = 1,IGAUSS
    DO 90 K2 = 1,5
      K=IPARIN(K1,K2)
90 WRITE(6,1031)K1,GASPAR(K2,1),GASPAR(K2,2),OPTION(K,1),OPTION(K,2),
  1(PARIN(K1,K2,K3),K3=1,4)
C
C      WRITE OUT YDATA
C
  WRITE(6,1006)NOIT
  WRITE(6,1007)ITEST
  GO TO (21,22,23,24,25),IWEIT
  WRITE(6,1008)
  GO TO 26
  WRITE(6,1009)
  GO TO 26
  WRITE(6,1010)
  GO TO 26
  WRITE(6,1011)
  GO TO 26
  WRITE(6,1012)
  IF(ICON1.EQ.0)GO TO 27
  WRITE(6,1013)HCONT
  GO TO 28
  WRITE(6,1014)
  KOUTPT=IOUTPT+1
  GO TO (29,30,31),KOUTPT
  WRITE(6,1015)
  GO TO 32
  WRITE(6,1016)
  GO TO 32
  WRITE(6,1017)
  WRITE(6,1018)MIALF,M2ALF
  IF(IWEIT.NE.4)GO TO 35
  WRITE(6,1019)YMAX
  WRITE(6,1020)YMIN
  IF(ILINE(1).EQ.0.AND.(ILINE(2).EQ.0)GO TO 42
  WRITE(6,1021)
  WRITE(6,1022)
  DO 40 I = 1,2
    J=ILINE(I)
  WRITE(6,1023)LINALB(I',OPTION(J,1),OPTION(J,2),(XLIN(I,K),K=1,4)
  WRITE(6,1024)
  IF(IGAUSS.EQ.0)GO TO 120
  IF(IPARIN(1,3).LE.2.AND.IPARIN(1,4).LE.2.AND.IPARIN(1,5).LE.2)GO
  1 TO 80
  WRITE(6,1025)
  IF(IPARIN(1,3).NE.3)GO TO 60
  WRITE(6,1026)(WCOE(I),I=1,6)
  IF(IPARIN(1,4).NE.3)GO TO 70
  WRITE(6,1027)(AICOE(I),I=1,6)
  IF(IPARIN(1,5).NE.3)GO TO 80
  WRITE(6,1028)(A2COE(I),I=1,6)
  WRITE GAUSSIAN PARAMETER OPTIONS
  WRITE(6,1029)
  WRITE(6,1030)
  DO 90 K1 = 1,IGAUSS
    DO 90 K2 = 1,5
      K=IPARIN(K1,K2)
  WRITE(6,1031)K1,GASPAR(K2,1),GASPAR(K2,2),OPTION(K,1),OPTION(K,2),
  1(PARIN(K1,K2,K3),K3=1,4)
  WRITE OUT YDATA

```

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120 WRITE(6,1032)
WRITE(6,1087)
JJ=0
WRITE(6,1036)JJ,(YDATA(I),I=1,9)
JJ=10
NLL=LL-9
DO 125 K=10,LL,10
KK = K+9
IF(KK.EQ.NLL)GO TO 125
WRITE(6,1033)JJ,(YDATA(I),I=K,KK)
JJ = JJ+10
125 CONTINUE
E
WRITE OUT WDATA VALUES
E
130 WRITE(6,1034)
IF(IWEIT.NE.1)GO TO 137
DO 135 K = ISTART,IEND
135 WDATA(K) = 0.0
137 WRITE(6,1035)(K,WDATA(K),K=ISTART,IEND)
IF(ISTP.EQ.0.AND.IOUTPT.EQ.0)RETURN
C
START THE OUTPUT OF THE ITERATION CALCULATIONS
C
WRITE(6,1053)
C
140 GO TO NSTAT,(160,245)
160 ISTP=ISTP+1
173 GO TO(180,213,180,185,185,177,175,174,250,178),ISTP1
175 IF(ISTP.EQ.6.AND.IOUTPT.EQ.2)GO TO 213
176 IF(ISTP.EQ.6.OR.ISTP.EQ.7).AND.(IOUTPT.EQ.0)GO TO 245
177 IF(ISTP.EQ.5.AND.(COM1.NE.0.AND.IOUTPT.EQ.2)GO TO 213
178 IF(ISTP.EQ.9.AND.IOUTPT.NE.0)GO TO 250
C
180 WRITE(6,1054)
IF(ISTP.NE.0)GO TO 132
WRITE(6,1056)XLAMB,SUM,SIG
GO TO 190
182 WRITE(6,1055)ITERAT,(LAMB,SUM,SIG
GO TO 190
185 WRITE(6,1057)
WRITE(6,1055)ITERAT,(LAMB,SUM,SIG
C
190 IF(ILINE(1).EQ.0.AND.ILINE(2).EQ.0) GO TO 195
WRITE(6,1060)
WRITE(6,1061)(TLIN(L),L=1,2)
C
195 IF(IGAUSS.EQ.C)GO TO 205
WRITE(6,1062)
DO 200 K1=1,IGAUSS
IF(K1.GT.1)GO TO 197
WRITE(6,1063)M1,(TPAR(K1,K2),K2=1,5)
GO TO 200
197 WRITE(6,1064)M1,(TPAR(K1,K2),K2=1,5)
200 CONTINUE
C
IF(NOIT.EQ.0)GO TO 295

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OUTPT112
OUTPT113
OUTPT114
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OUTPT166
OUTPT167
OUTPT168

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C
205 GO TO(207,206,206,206,210,212,240,206,250,280),ISTP1
207 WRITE(6,1091)
206 RETURN
210 IF(ISTP.EQ.4.AND.IOUTPT.NE.0)GO TO 235
211 GO TO 206
212 IF(ISTP.EQ.5.AND.IOUTPT.EQ.0)RETURN
GO TO 235
C
OUTPUT THE NORMALIZED NORMAL EQUATION MATRIX
C
213 WRITE(6,1050)
WRITE(6,1051)
DO 215 I= 1,JP
J=1
214 L=J+4
IF(JP.LT.L)L=JP
WRITE(6,1052)I,(A1(I,K),K=J,L)
IF(L.EQ.JP)GO TO 215
J=J+5
GO TO 214
215 CONTINUE
C
OUTPUT THE INVERSE MATRIX
C
216 WRITE(6,1065)
WRITE(6,1051)
DO 220 I=1,JP
J=1
217 L=J+4
IF(JP.LT.L)L=JP
WRITE(6,1052)I,(A1(I,K),K=J,L)
IF(L.EQ.JP)GO TO 220
J=J+5
GO TO 217
220 CONTINUE
C
OUTPUT THE IDENTITY MATRIX
C
WRITE(6,1066)
WRITE(6,1051)
DO 230 I=1,JP
J=1
225 L=J+4
IF(JP.LT.L)L=JP
WRITE(6,1052)I,(C1(I,K),K=J,L)
IF(L.EQ.JP)GO TO 230
J=J+5
GO TO 225
230 CONTINUE
C
IF(ISTP.EQ.1.AND.IOUTPT.EQ.2)GO TO 190
IF(ISTP.EQ.6.AND.IOUTPT.EQ.2)GO TO 190
232 IF(ISTP.EQ.5.AND.(COM1.NE.0.AND.IOUTPT.EQ.2)GO TO 180
C
235 WRITE(6,1067)
WRITE(6,1068)ITERAT

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OUTPT169
OUTPT170
OUTPT171
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OUTPT221
OUTPT222
OUTPT223
OUTPT224
OUTPT225

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      WRITE(6,1069)
      RETURN
240  WRITE(6,1070)
C
      WRITE(6,1071)ITEST
      WRITE(6,1072)
      RETURN
C
245  ASSIGN 250 TO MSTAT
      WRITE(6,1073)
      GO TO 180
250  WRITE(6,1074)
260  WRITE(6,1075)
270  WRITE(6,1076)
C
C   PRINT OUT ESTIMATED ERRORS IN FITTED PARAMETERS
C
280  WRITE(6,1077)
      IF(ILINE(1).EQ.0.AND.ILINE(2).EQ.0)GO TO 285
      WRITE(6,1060)
      WRITE(6,1061)(ERESTL(L),L=1,2)
285  WRITE(6,1062)
      DO 290 K1 = 1,IGAUSS
      IF(K1.GT.1)GO TO 287
      WRITE(6,1063)K1,(ERESTG(K1,K2),K2=1,5)
      GO TO 290
287  WRITE(6,1064)K1,(ERESTG(K1,K2),K2=1,5)
290  CONTINUE
C
C   COMPUTE AND OUTPUT THE PHOTOPEAK AREAS AND ERRORS IN THE AREAS
C
      CALL ERREA(TPAR1,SIG)
C
C   PRINT OUT YBAR AND YDATA CALCULATIONS
C
295  WRITE(6,1084)
      WRITE(6,1085)
296  XI=ISTART
      ISET=0
      CALL FCN(ISET,XI,YBAR,TPAR1,ILINE)
      DELTY=YDATA(ISTART)-YBAR
      SIGM = SQRT(WDATA(ISTART))
      DYSIG = DELTY * SIGM
      DYSIG2 = (DYSIG*DYSIG)
      WRITE(6,1086)ISTART,YDATA(ISTART),YBAR,DELTY,SIGM,DYSIG,DYSIG2
C
      I1=ISTART+1
300  DO 320 I = I1,IEND
      XI=I
      CALL FCN(ISET,XI,YBAR,TPAR1,ILINE)
      DELTY=YDATA(I)-YBAR
      SIGM = SQRT(WDATA(I))
      DYSIG = DELTY * SIGM
      DYSIG2 = (DYSIG*DYSIG)
320  WRITE(6,1086)I,YDATA(I),YBAR,DELTY,SIGM,DYSIG,DYSIG2
      RETURN

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      OUTPUT226
      OUTPUT227
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      OUTPUT281
      OUTPUT282

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C
C   FORMAT STATEMENTS.
C
1000 FORMAT(63H1 7040 NON-LINEAR MULTIPLE-MODIFIED GAUSSIAN-FITTING
      1PROGRAM/)
1001 FORMAT(13A6)
1002 FORMAT(25H0
      PROGRAM CONTROL DATA)
1003 FORMAT(45H
      NUMBER OF GAUSSIANS***** 13)
1004 FORMAT(45H
      FIRST CHANNEL IN FIT ***** 13)
1005 FORMAT(45H
      LAST CHANNEL IN FIT***** 13)
1006 FORMAT(45H
      MAXIMUM NUMBER OF ITERATIONS ***** 13)
1007 FORMAT(45H
      NUMBER OF ITERATIONS AFTER CONVERGENCE* 13)
1008 FORMAT(57H
      WEIGHTING***** NOT WEIGHTED)
1009 FORMAT(48H
      WEIGHTING***** 1/Y)
1010 FORMAT(52H
      WEIGHTING***** 1/WDATA)
1011 FORMAT(57H
      WEIGHTING***** F(YMAX/YMIN)
      1)
1012 FORMAT(55H
      WEIGHTING***** INPUT LIST)
1013 FORMAT(53H
      ITERATION PROCESS
      13)
1014 FORMAT(60H
      ITERATION PROCESS
      LUTED)
1015 FORMAT(50H
      OUTPUT***** SHORT)
1016 FORMAT(52H
      OUTPUT***** REGULAR)
1017 FORMAT(55H
      OUTPUT***** DIAGNOSTIC)
1018 FORMAT(45H0
      POWERS OF THE ALPHA TERMS***** 12,5H AND
      12)
1019 FORMAT(45H
      VALUE OF YMAX ***** 1PE13.6)
1020 FORMAT(45H
      VALUE OF YMIN***** 1PE13.6)
1021 FORMAT(48H0
      STRAIGHT LINE PARAMETER INFORMATION Y=AX+B)
1022 FORMAT(11H 5X,9HPARAMETER,7X,6HOPTION,7X,13HINITIAL VALUE,5X,11HUPPER
      1ER LIMIT,5X,11HLOWER LIMIT,5X,21HCONVERGENCE CRITERION)
1023 FORMAT(10X,A1,5X,A6,A4,1PE17.5,1PE17.5,1PE16.5,1PE21.5)
1024 FORMAT(35H0
      GAUSSIAN PARAMETER INFORMATION)
1025 FORMAT(80H
      COEFFICIENTS FOR COMPUTING THE FUNCTIONAL FORMS OF
      THE PHOTOPEAK PARAMETERS)
1026 FORMAT(18H
      HALF-WIDTH1PE17.7)
1027 FORMAT(14H
      ALPH14X1PE17.7)
1028 FORMAT(14H
      ALPH24X1PE17.7)
1029 FORMAT(30H0
      GAUSSIAN PARAMETER VALUES)
1030 FORMAT(11H 5X,8HGAUSSIAN,7X,9HPARAMETER,8X,6HOPTION,7X,13HINITIAL
      VALUE,5X,11HUPPER LIMIT,6X,11HLOWER LIMIT,4X,21HCONVERGENCE CRITERIUM)
1031 FORMAT( 9X,I2, 9X,A6,A4,6X,A6,A4,1PE17.5,1PE17.5,1PE20.5)
1032 FORMAT(10H0
      DATA )
1033 FORMAT(110,2X,10F11.0)
1034 FORMAT(49H0
      WEIGHTING VALUES
      1)
1035 FORMAT(517X,I3,3X,1PE2.5)
1036 FORMAT(7X,I3,11X,2H0.-9F11.0)
1050 FORMAT(38H0
      NORMAL ZED NORMAL EQUATION MATRIX)
1051 FORMAT(15X,3HROW,47X,3HMATRIX VALUE)
1052 FORMAT(117,1PE18.7)
1053 FORMAT(62H1
      ITERATION CALCULATIONS (** INDICATES FITTED LAMBDA
      1VALUE)
1054 FORMAT(14H0
      ITERATION,32,6HLAMBDA,9X,6HCHI**2, 9X,10HCHI**2/NDOF)

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      OUTPUT283
      OUTPUT284
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105E FORMAT(8X,12,5X,1PE9.3,1P2E17.6)          OUTPUT340
105E FORMAT(15X,1PE9.3,1P2E17.6)                OUTPUT341
105I FORMAT(14HO      ITERATION,3X,3HLAMBDAA*,7X,6HCHI**2, 9X,10HCHI**2/NO)OUTPUT342
106I)                                           OUTPUT343
106C FORMAT(/14X,11HLINE*****8X,1H4,16V,1H6)   OUTPUT344
106I FORMAT(14X,11HPARAMETERS*,1PE15.6,1P17.6)   OUTPUT345
106Z FORMAT(/14X,11HGAUSSIAN***5X,8HGAUSSIAN,10X,6HHEIGHT,10X,7HCHANNEL)OUTPUT346
11,9X,10HHALF-WIDTH,8X,6HALPHA1,9X,6HALPHA2)      OUTPUT347
106S FORMAT(14X,11HPARAMETERS*,8X,12,5X,1P3E17.6,1P2E15.4) OUTPUT348
1064 FORMAT(33X,12,5X,1P3E17.6,1P2E15.4)         OUTPUT349
106S FORMAT(19HO      INVERSE MATRIX)            OUTPUT350
1066 FORMAT(20HO      IDENTITY MATRIX)            OUTPUT351
1067 FORMAT(///52X,29H*****))                   OUTPUT352
1068 FORMAT(52X,13H*  ITERATION13,13H COMPLETED *) OUTPUT353
1069 FORMAT(52X,29H*****))                       OUTPUT354
1070 FORMAT(///22X,82H*****))                   OUTPUT355
1*****))                                         OUTPUT356
107I FORMAT(22X,38H*  CONVERGENCE CRITERION HAS BEEN MET.13,41H ITERATION)OUTPUT357
IONS WILL BE RUN WITH LAMBDA=1.0 *)              OUTPUT358
107Z FORMAT(22X,82H*****))                   OUTPUT359
1*****))                                         OUTPUT360
107J FORMAT(27HO      FINAL PARAMETER VALUE*)    OUTPUT361
1074 FORMAT(///49X,34H*****))                   OUTPUT362
107S FORMAT(49X,34H*ITERATION CALCULATIONS COMPLETED*) OUTPUT363
1076 FORMAT(49X,34H*****))                   OUTPUT364
107* FORMAT(41HO      ESTIMATED ERROR IN FITTED PARAMETERS) OUTPUT365
107# FORMAT(20HO      LINE PARAMETERS)            OUTPUT366
1079 FORMAT(30HO      A                          B) OUTPUT367
1080 FORMAT(3X,1P2E17.6)                          OUTPUT368
108: FORMAT(24HO      GAUSSIAN PARAMETERS)         OUTPUT369
108Z FORMAT(99H      GAUSSIAN          Y0          X0          OUTPUT370
1      OMEGA          ALPHA1          ALPHA2)      OUTPUT371
108J FORMAT(11X,12,6X,1P5E17.6)                  OUTPUT372
108+ FORMAT(32H-      YDATA AND YBAR CALCULATIONS) OUTPUT373
108% FORMAT(15X,7HCHANNEL,9X,5HYDATA,12X,4HYBAR,12X,5HDELTA,10X, 9H1/SI)OUTPUT374
1G(Y1),8X,9HDELTA/SIG,2X,12HIDELTA/SIG)2)        OUTPUT375
108= FORMAT(17X,13,2X,1P4E17.6,0P2F13.3)         OUTPUT376
108T FORMAT(20X,1H0,10X,1H1,10X,1H2,10X,1H3,10X,1H4,10X,1H5,10X,1H6,10X)OUTPUT377
1,1H7,10X,1H8,10X,1H9)                          OUTPUT378
1G90 FORMAT(13A6)                                  OUTPUT379
1C9I FORMAT(///52X,28H*****))                   OUTPUT380
END                                                  OUTPUT381

```

**PHILLIPS
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ATOMIC ENERGY DIVISION