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Interactive General-Purpose Function Minimization for the Analysis of Neutron Scattering Data

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Abstract

An on-line graphic display facility has been employed mainly for the peak analysis of time-of-flight spectra measured by inelastic scattering of thermal neutrons. But it is useful also for the analysis of spectra measured with triple axis spectrometers and of diffraction patterns. The spectral lines may be fitted by the following analytical shape functions: (i) a Gaussian, (ii) a Lorentzian, or (iii) a convolution of a Lorentzian with a Gaussian, plus a background continuum. Data reduction or correction may be invoked optionally. For more general applications in analysing of numerical data there is also the possibility to define the analytical shape functions by the user. Three different minimization methods are available which may be used alone or in combination. The parameters of the shape functions may be kept fixed or variable during the minimization steps. The width of variation may be restricted. Global correlation coefficients, parameter errors and the χ^2 are displayed to inform the user about the quality of the fit. A detailed description of the program operations is given. The programs are written in FORTRAN IV and use an IBM/2250-1 graphic display unit.

Programme interactif pour l'analyse des spectres de neutrons diffusés inélastiquement utilisant la méthode des moindres carrés

Résumé

Nous avons introduit des méthodes graphiques interactives pour déterminer les paramètres des spectres de temps de vol de neutrons diffusés inélastiquement. D'autre part on peut utiliser ce programme pour évaluer des spectres mesurés avec un spectromètre à trois axes ou de diffraction. Les lignes spectrales peuvent être adaptées aux fonctions analytiques suivantes: (i) la fonction de Gauss, (ii) la fonction de Lorentz, et (iii) une convolution de l'une avec l'autre. Différentes corrections des données sont possibles. Pour une application plus générale dans l'analyse de données numériques la fonction analytique peut être définie par l'utilisateur lui-même. On peut se servir de trois méthodes mathématiques que l'on peut appliquer indépendamment ou en combinaisons. Les paramètres de fonction peuvent être fixés ou laissés variables, au choix de l'opérateur. D'autre part l'opérateur peut limiter le changement des paramètres en introduisant des restrictions. Des coefficients de la corrélation globale, les erreurs des paramètres et le χ^2 sont représentés sur l'écran pour informer l'opérateur de la qualité du fit. Nous présentons une description détaillée du dialogue entre l'ordinateur et l'utilisateur. Les programmes sont programmés en FORTRAN IV et utilisent une IBM/2250-1.

Interaktives graphisches Minimalisierungsprogramm
zur Analyse von Neutronenstreuungsspektren

Kurzfassung

Es wird die Anwendung eines Computer-Display Systems zur Peak-Analyse von TOF-Spektren aus Experimenten mit thermischen Neutronen beschrieben. Auswertungen von Messungen an Drei-Achsen-Spektrometern oder Diffraktionsspektrometern sind ebenfalls möglich. Zur Beschreibung der experimentellen Daten stehen die folgenden Funktionen zur Verfügung: (i) Gaussfunktion, (ii) Lorentzfunktion, und (iii) Faltung einer Lorentzfunktion mit einer Gaussfunktion. Als Untergrundfunktion kann eine konstante oder lineare Funktion ausgewählt werden. In Hinblick auf eine allgemeinere Anwendung besteht die Möglichkeit, eine Analyse von anderen numerischen Daten durch Umdefinition der Fit-Funktion durchzuführen. Drei verschiedene Minimierungstechniken stehen zur Verfügung und können einzeln oder in Kombination miteinander aufgerufen werden. Die Funktionsparameter können wahlweise fest, variabel oder limitiert sein. Die globalen Korrelationskoeffizienten, die Parameterfehler und das χ^2 werden zur Beurteilung der Güte des Fits auf dem Bildschirm ausgegeben. Der Dialog zwischen dem Benutzer und dem Rechner wird ausführlich dargestellt. Die Programme sind in FORTRAN IV programmiert und benutzen die graphische Bildschirmeinheit IBM/2250-1.

CONTENTS

Abstract, Résumé, Kurzfassung

1. Introduction	1
2. Minimization Routines	3
3. Mathematical Models	4
3.1 Resolution Function	4
3.2 Analysis of Lorentzians	5
3.3 Analysis of Lorentzians viewed through Gaussians	5
3.3.1 Evaluation of the Voigt Integral	5
3.3.2 Calculation of the Complex Error Function	7
3.4 Chi-Square Minimization	8
4. General Description of Program Operation	9
4.1 Data Reduction and Correction of Input Data	9
4.2 Initial Estimate of the Function Parameters	13
4.3 Local and Global Minimum Search	17
4.4 Plot Output	20
5. Description of the Calling Procedure	22
6. Computer Implementations	24
6.1 General Remarks	24
6.2 Description of the User Function	24
6.3 JCL Requirements for the Program Run	26

Acknowledgement

References

Appendix

1. Introduction

An on-line general purpose least square fit program for the analysis of multichannel data has been developed. The program was primarily written for the evaluation of inelastic neutron magnetic scattering data. The usual approach is to fit a given shape function to the experimental data by minimizing the weighted sum of residuals. Different minimization methods are available which will be briefly outlined in section 2/2/.

The current version of the program is restricted to a maximum of 30 function parameters with 15 of them adjustable. However, a redimensioning for larger problems is straightforward. Depending on the behavior of the function or user requirements the parameters may be fixed or may be restored to the variable status between minimization steps by light pen detect. Furthermore, the allowed values of one or more parameters may be limited to a certain range during the fit. Three kinds of analytical shape functions are provided and will be described in more detail in section 3. An additional background continuum may be approximated by a polynomial of up to the 2nd order.

The minimization includes the evaluation of the Voigt integral. To reduce the calculation time this integral has been written in terms of the complex error function/6/. Gautschi has given an algorithm for calculating this function to a high accuracy using the method of continued fractions/7/.

In case of a convolution the program accepts a resolution peak which is sited on the top of one convoluted line as it appears e.g. on the quasi-elastic peak if the scattering process exhibits a pure elastic component.

The light pen is used to correct the input data and to inform the program of some fundamentals, i.e. the region of the input spectrum and the number of peaks involved. After completion of a minimization step the final parameter values and their uncertainties together with the estimated distance to the minimum are displayed. Based on the covariance matrix, if it exists, global correlation coefficients are calculated and also displayed. The problem is to find out the most representative function of the measured data, and to derive desired physical information from the best fitted values of the function parameters.

Compared to the conventional batch processing methods the presentation of the computed results on the screen and the interactive control of the evaluation steps enable the user to arrive at a most acceptable solution by observing the changes in various parameters of the physical system and, therefore, to avoid as much as possible an inadequate analysis of the scattering data.

To process the graphical information, an IBM/2250-1 display unit is used. The programs are written in FORTRAN IV and use the Graphic subroutine Package (GSP) of IBM/11/. More details about the features of the display unit are given in /12/. However, the user should be familiar with the cursor, light pen and keyboard features of the display unit, which allow him to communicate with the program during execution.

However, in order to make the program flexible enough to be easily

applicable to related problems, the calling procedure/1/ may still offer a suitable organizational framework. A description of the calling sequence is given in section 5. In section 6 some remarks are given on the current computer implementation of the interactive graphic computer code.

2. Minimization Routines

Our aim is not to give a detailed discussion of the mathematical problem of minimization. Nevertheless it seems to be useful to briefly characterize the fitting techniques provided. It should be noted before, that all the present methods are taken from MINUIT/2/ with minor modifications with respect to the on-line facility used. For an underlying description or more general consideration the user is referred to Ref./17/ for example. Furthermore, the user should also keep in mind that all calculations are done in simple precision mainly due to the linking of the GSP routines. In consequence, rounding errors or cumulative effects of rounding may be important. However, in our cases of analyzing spectra no influences on the convergence have been observed.

Random Search

The first fitting "technique" is the Monte Carlo search method/2/ which is less popular than the other non-linear minimization routines. However, this method is especially more efficient in parameter spaces of higher dimensionality and gives sufficiently accurate results within reasonable computing times on a high-speed computer/15/. Nevertheless, this procedure should only be used at the beginning of a fit or when no reasonable starting point is known.

Simplex Method

This stepping method is based on that of Nelder and Mead/3/, which is very "safe" and should work as well in non-quadratic as in quadratic regions of the shape of the function. It should be noted, that no derivatives of the function to be studied are required.

Gradient Method

This variable-metric method of the fit uses Fletchers "switching"/4/ variation of the original Davidon-Fletcher-Powell algorithm/5/. The gradient of the function may be supplied analytically. In cases where no derivatives are provided the program estimates the derivatives by finite differences. Whereas the simplex method only gives (good) estimates of the diagonal elements, here a full covariance matrix is produced.

3. Mathematical Models

Though the program is optimized for a specific family of functional forms, it is not specifically designed for a single type of experiment. It should be a general tool for the analysis of spectroscopic data, because the function being analyzed may be in those cases supplied by the user as described below in section 6.2. Several shape functions have so far been proposed for spectrum analysis by computer. However, a large class of problems in many different fields of research is the problem of minimizing the difference between theory and experimental data, wherein theoretical shape functions may be represented by a Gaussian, a Lorentzian, or a convolution of both. Therefore, the aim of this chapter is to give a short description of the mathematical models provided.

3.1 Resolution Function

The resolution function in neutron scattering experiments (inelastic and elastic) is usually approximated by a Gaussian. For processing discrete energy spectra, for example, in γ -ray analysis or nuclear spectroscopy, from semiconductor detector systems, Gaussians are used in the least square fit analysis. It should be mentioned that in the photopeak analysis of semiconductor γ -ray spectra the response function shows significant deviations from a Gaussian shape. First, Routti et al./13/ have proposed to use a Gaussian including high and low energy exponential tails matched on to the Gaussian at some point. Second, for example, Roberts et al./14/ have employed a two-Gaussian (double Gaussian line) approach for the instrumental response function to get a better fit in some cases. Nevertheless, in the present program the resolution function is written as the Gaussian

$$G(x) = A \exp[-(x-c)^2/2\sigma^2]$$

wherein A is the amplitude, c the centroid and σ the standard deviation of the Gaussian. The standard deviation σ is related to the full width at half maximum (fwhm) w by

$$w = 2 \sqrt{(2 \ln 2)} \sigma$$

so the function may be rewritten by

$$G(x) = A \exp[-4 \ln 2 (x-c)^2/w^2]$$

The background continuum is given by the polynomial

$$B(x) = b_0 + b_1(x-c) + b_2(x-c)^2$$

where b_0 represents a constant background under the peak and b_1 is a slope parameter.

The simplest form representing a peak on a background is the given by

$$F(x) = \sum_{i=1}^n G_i(x) + B(x) , \text{ where } n \text{ is the number of peaks.}$$

3.2 Analysis of Lorentzians

The second shape function considered in the least square fit analysis is the Lorentzian. It often arises in nuclear physics and solid state physics that the natural line shape is given by Lorentzians (e.g. phonons, magnons, crytalline field transitions and diffusive modes as observable by neutron scattering experiments). The functional form used here is given by

$$L(x) = A \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (x-c)^2}$$

where the parameters A and c have the same meaning as described above. Γ represents the full width at half maximum.

3.3 Analysis of Lorentzians viewed through Gaussians

3.3.1 Evaluation of the Voigt Integral

In many physical problems the observed spectra may be represented by a convolution of a Lorentzian with a Gaussian as resolution function. The use of such a shape function in the least square analysis is well known in astrophysics and atomic physics. In the simplest case it often arises that a signal of Lorentzian form

$$L(x) = A \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (x-c)^2}$$

is detected through a detector-analyser system whose resolution function may be approximated by the Gaussian

$$G(x) = A' \exp[-x^2/2\sigma^2]$$

The detected signal is then given by the convolution

$$C(x) = \int_{-\infty}^{+\infty} L(x-x') \cdot G(x') dx'$$

Using the relation between σ and the Gaussian fwhm one gets

$$C(x) = A \int_{-\infty}^{+\infty} \exp[-4 \ln 2 \frac{x'^2}{w^2}] \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (x-x'-c)^2} dx'$$

This function $C(x)$ is the so-called Voigt profile/14/ the properties of which have been studied extensively by several authors. It is usually evaluated, in practice, by parameterizations/19/ or by using tabulated forms of the function. Defining a new variable ξ by

$$\xi = \frac{x'}{w} \quad 2\sqrt{\ln 2} \quad d\xi = \frac{2\sqrt{\ln 2}}{w} dx'$$

the function C(x) may be rewritten as

$$C(x) = A' \int_{-\infty}^{+\infty} \exp(-\xi^2) \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + [(x-c) - \theta\xi]^2} d\xi$$

where for ease in notation $\theta = w/2\sqrt{\ln 2}$ and $A' = A \theta$

The integration may be done numerically using Gauss-Hermite quadrature. Then, the following functional form can be used for minimization

$$F(x) = \sum_{i=1}^n C_i(x) + B(x), \text{ where } n \text{ is the number of peaks.}$$

However, the integration must be performed for each point in the fitting interval. In a recent paper Batty et al./6/ have discussed various methods for the direct integration of the Voigt integral which will be briefly reviewed in the following. As mentioned above, the integral may be transformed to a functional form, so that Gauss-Hermite quadrature seems to be a suitable numerical procedure. Depending on the order of the quadrature the integral may exhibit wild oscillations giving an incorrect value. On the other hand, alternative methods as the adaptive Simpson's rule or Romberg's integration method give a reasonable answer, but they are connected with a considerable increase in computing time as mentioned later.

If we substitute in the latter form of the integral the variables

$$a = \frac{\Gamma}{2\theta}, \quad v = \frac{x-c}{\theta}$$

then C(x) reduces to

$$C(x) = A' \int_{-\infty}^{+\infty} \exp(-\xi^2) \frac{a^2}{a^2 + (v-\xi)^2} d\xi$$

This integral is directly related to the complex error function $w(z)/8$, No.7.4.13/ and becomes then after replacing of θ

$$C(x) = A \frac{w}{2\sqrt{\ln 2}} a \pi \operatorname{Re} w(z)$$

where $w(z) = \exp(-z^2) \operatorname{erfc}(-iz)$ and $z = v + ia$

The evaluation of the Voigt integral by using this relation has the advantage, that especially in non-linear least square fitting with gradients, the derivatives of the complex error function are combinations of the same function, so it must not be recalculated several times. The partial derivatives with respect to the variables a and v are

$$\operatorname{Re} \frac{\partial w(z)}{\partial a} = - \frac{2}{\sqrt{\pi}} + 2 v \operatorname{Im} w(z) + 2 a \operatorname{Re} w(z)$$

$$\operatorname{Re} \frac{\partial w(z)}{\partial v} = -2v \operatorname{Re} w(z) + 2a \operatorname{Im} w(z)$$

The partial derivatives to each of the adjustable parameters of the shape function may be then derived by implicit differentiation using the above relations:

$$\frac{\partial C(x)}{\partial A} = \frac{w}{2\sqrt{\ln 2}} a \pi \operatorname{Re} w(z)$$

$$\frac{\partial C(x)}{\partial \Gamma} = \frac{A}{2} \pi \left[\operatorname{Re} w(z) + a \operatorname{Re} \frac{\partial w(z)}{\partial a} \right]$$

$$\frac{\partial C(x)}{\partial c} = -A a \pi \operatorname{Re} \frac{\partial w(z)}{\partial v}$$

We have computed the Voigt integral for a 256 point spectrum. The use of the complex error function has led to a considerably reduced computing time by a factor of about 16 or more with respect to an evaluation using Romberg's method.

3.3.2 Calculation of the Complex Error Function

As mentioned previously Gautschi/7/ has developed a recursive procedure which permits to calculate $w(z)$ for any argument z in the first quadrant of the complex plane. The corresponding procedure written in ALGOL/10/ has been translated into FORTRAN (see App. 1). To continue $w(z)$ in the remaining quadrants the following symmetry relations are included in the algorithm/8, No. 7.1.11,12/

$$\operatorname{erf}(-z) = \operatorname{erf}(z)$$

$$\operatorname{erf}(\bar{z}) = \overline{\operatorname{erf}(z)}$$

$$w(z) = \exp(-z^2) \operatorname{erfc}(-iz) \quad \text{for } Q_1$$

$$w(-\bar{z}) = \overline{w(z)} \quad \text{for } Q_2$$

$$w(-z) = 2 \exp(-z^2) w(z) \quad \text{for } Q_3$$

$$w(\bar{z}) = \overline{w(-z)} \quad \text{for } Q_4$$

A certification of the algorithm has been given by Kölbig/9/ who has also tested the procedure for special complex values of z along the real and imaginary axis, or at (critical) different points within the first quadrant.

Generally, it can be concluded that the computation of $w(z)$ may be performed to a high accuracy, i.e. to ten significant digits at least, or better depending on the values of z in Q_1 .

3.4 Chi-Square Minimization

One of the most common situations in least square fitting is the minimization of the following residuals, between experimental data and predictions of a model with variable parameters:

$$\chi^2 = \sum_{k=1}^m w_k [y_k - F(x_k, u)]^2 = \sum_{k=1}^m f_k^2(u)$$

wherein w_k are the weights directly related to the statistical error of the measured values y_k at the k th channel x_k . The value of the function being studied^k is given by $F(x_k, u)$ ($F(x)$ in our context), depending on the parameter vector

$$u = {}^t(u_1, u_2, \dots, u_p),$$

where p denotes the number of the function parameters. The sum is to be taken over the fitting interval (x_1, x_m) .

With respect to the properties of quadratic forms for understanding gradient methods it is in general not simple to state, whether the second-derivative matrix is positive-definite or not especially in many dimensions. The second-derivative (hessian) matrix G may be expressed in terms of $f_k(u)$ /17/:

$$\nabla_i \nabla_j \chi^2 = \sum_k 2 \nabla_i f_k \nabla_j f_k + \sum_k 2 f_k \nabla_i \nabla_j f_k$$

$$G = \text{Mat}(\nabla_i \nabla_j \chi^2)$$

after introducing the notation $\nabla_i \equiv \partial/\partial u_i$.

The second term is usually assumed to be small compared to the first term. The inverse of G is the covariance matrix V , also often called "error matrix".

To develop a stable method guaranteeing monotonic convergence of V toward the true covariance matrix, many efforts have been done in calculating the second-derivative matrix and to retain its positive definiteness. An important assumption is always the function $f_k(u)$ being usually quite quadratic in the immediate vicinity of the minimum. In non-linear least squares the following linearization may offer an effective approximation in many cases:

$$\nabla_i \nabla_j \chi^2 \cong \sum_k 2 \nabla_i f_k \nabla_j f_k$$

This approximation has the advantage to involve first derivatives only and, moreover, to be "always" positive-definite. The calculation of the χ^2 has been done by the internal procedure FCN for all present shape functions as described above. A listing of this subroutine is given in Appendix 2. From this (see also chapter 6.2), the user can extract the calling sequence and other information needed for submitting his own subroutine, if desired. Because the function value and the derivatives are often recalculated, this program should be optimized as much as possible.

4. General Description of Program Operation

This section describes the use of the interactive graphic computer program IGFIT250. The user is able to direct the mode of operation by a choice of several options. The communication with the computer takes place by means of a light pen, an alphanumeric keyboard and a function keyboard. A survey of the general function keys is given in Table 1. Messages or requests from the program are displayed on the 2250-screen and are given in capital letters in the following.

TABLE 1

Key No.	Function ⁺
1	NO for questions
2	YES for questions or continue processing
28	Equivalent to the END key for keyboard input
30	EXIT or end of program

⁺ Notice that function keys are not always active though their lights are switched on. To use these keys correctly, the user is referred to the description given below.

The program is primarily assigned to analyse neutron time-of-flight (TOF) data. The input spectra may be analysed directly or may be converted to the energy scale before fitting. For general application the x-values must be put in additionally.

4.1 Data Reduction and Correction of Input Data

As already mentioned, the data reduction part is taken from/1/ and is not described in detail here. By inclusion of the graphical representation of the computed results, the experimenter arrives at a most acceptable solution, when he observes the consequences of changes in relevant evaluation steps. Some of them are summarized below.

1. Determination of the range of evaluation in the TOF-spectra.
2. Correction for experimental resolution before fitting.
3. Correction for time-dependent background.
4. Correction for constant background.
5. Correction for detector efficiency.

After initiation of the program (see section 5) the user starts processing by a light pen detect on EVALUATION OF NEUTRON DATA of the SELECT frame. There are two data structures provided for the TOF-data. Therefore, the next frame asks the type of the given input data.

THE DETECTOR SPECTRA ARE GIVEN
SINGLE TOF-SPECTRUM EXISTS

After selection the screen goes blank and the program begins processing. If data of several detectors (DETECTOR SPECTRA) have been saved on a system device, the user is now requested to identify his data set by entering the volume and the fully qualified data set name from the keyboard. Formatting of this input must be a variable record format and must be identical to that of the TIFLIS code/16/. After completing the user must perform the END function with depressing of key 28 or the END key on the keyboard. This action indicates in every input request that the user has finished entering information.

This name is then used to locate the data set and make it available for processing. If the data set is not found on the specified volume, the request is repeated.

On the other hand, if a SINGLE TOF-SPECTRUM EXISTS, the data may be supplied from disk or from cards. For processing more than one spectrum the input card decks may follow each other. In both cases, the session may be canceled using key 30, whereas depressing key 2 continues processing.

Depending on the selected input mode, the data are read in from a system device (disk) or from cards as described below. If the detector spectra are given, the message READ INPUT SPECTRA is displayed on the lower area of the screen while the data are transferred.

If a single TOF-spectrum exists, the user is first requested to define the length of the spectrum by a light pen detect on the appropriate option message in the next frame. If ALL CHANNELS are given, the number of channels must be entered from the alphameric keyboard as indicated by the cursor. A light pen detect on FIXED REGION invokes the requests of the FIRST CHANNEL and LAST CHANNEL. A new scale may be now defined after touching OTHER with the light pen. However, only an equidistant scale is allowed: The user is requested to input the first value and the increment on the scale. Otherwise the x-values must be put in first from the data file.

DESCRIBE TYPE OF X-SCALE
CHANNELS OTHER INPUT X

Then the message READ INPUT TOF-SPECTRUM appears on the screen during input operation. Next, some experimental parameters are expected to be entered from the alphameric keyboard together with additional parameters for the spectrum as specified from external programs generating the TOF-spectrum.

After the input of the TOF-data has been completed, a list of some relevant experimental parameters will be displayed. In the lower area of the screen the cursor indicates that the user is requested to accomplish a title to identify the particular run. The length of this additional information is restricted by an asterisk displayed to avoid an overwriting of the subsequent information in the same line.

The next frame contains a cumulative list of the variable parameters involved in the evaluation of the TOF-data. As explained later, a choice of a symbolic textual element allows the user to change one or more of these parameters. To specify an initial choice of the parameters, the appropriate line will be displayed at the bottom of the screen, requesting the user to enter the data from the keyboard.

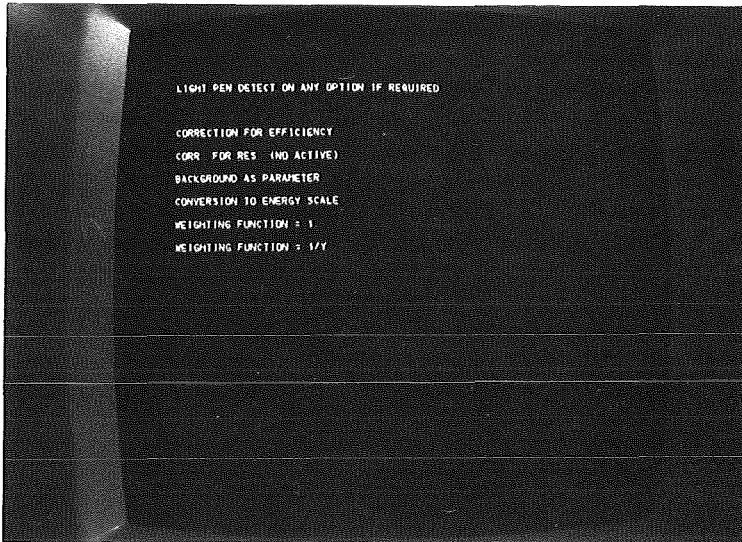


Fig. 1: Program options to be selected

The input values will then be displayed in a column at the right of the actual parameter line. When the list has been completed, depressing key 1 enables the user to change an incorrect value by a light pen detect on the appropriate text as indicated by the heading information message LIGHT PEN DETECT ON THE REQUIRED ELEMENT. Finally, key 2 must be depressed to proceed with the evaluation. Next, the user is requested to select some of the program options with the light pen (Fig.1), if desired. The end of a choice must be signaled by depressing key 2.

The most frequent situation is that no correction for background will be done, because an underlying background must be treated as parameter. Two weighting functions are available.

If the TOF-spectrum exists for all channels, the user can now inspect the whole spectrum on the screen. Scaling of the vertical axis is performed by depressing key 26 or key 27 to expand or contract vertically.

The request SELECT RANGE OF EVALUATION indicates that two points must be touched with the light pen. After selection the channel numbers and the related energy transfers are displayed in the lower area of the screen. Answering RANGE O.K. ? with key 1, a new range can be determined. After depressing key 2 an enlarged display of the selected range of the TOF-spectrum is shown.

Answering DATA CORRECTIONS OR ZOOMING by depressing key 15, a data correction may be included at this point of evaluation.

The next stage of evaluation is the correction for background, time-dependent as well as constant. If no correction whatsoever is desired, processing continues by answering CORRECTION FOR BACKGROUND ?

by depressing of key 1. If the appropriate option BACKGROUND AS PARAMETER has been selected previously, this evaluation step will be skipped automatically.

Otherwise the user is requested to select either of the options given below:

LIGHT PEN DETECT ON THE TYPE OF BACKGROUND
TIME-DEPENDENT CONSTANT

In the case of a time-dependent background, a correction for the constant background is initiated automatically. However, only a short description of this procedure will be given here. Nevertheless, there are few operations which are applicable. The data for the time-dependent background must be supplied from cards or, in principle, can be generated by using the correction option (key 19). The time factor can be entered from the keyboard after depressing key 21. Smoothing by polynomials is included optionally and will be processed after depressing key 20.

In many cases the most important correction to be applied to the data, is the correction for constant background. A constant background can be defined initially by a light pen detect on either of the options listed in the lower area of the screen. However, without answering one of the requests the constant background may be directly determined by touching a representative point in the spectrum with the light pen. Then a line is drawn according to the selection. Depressing key 1 causes the removal of this line, indicating that the selection may be repeated. It is not necessary to do this, because the initial value can be changed by function key attentions as described below. Depressing key 2 causes display of the corrected spectrum on the screen as a first estimation.

At this point, the user has several function key options at his disposal, to adjust the correction for constant background. They are given in Table 2.

TABLE 2

Key No.	Function ⁺
1	Repeat the correction
2	End of correction, continue the evaluation run
7	Smoothing of the spectrum will be initiated
25	Keyboard entry of the reduction factor (default value: 10 %)
26	Decrease constant background
27	Increase constant background

As shown in Table 2 repeated depression of key 26 or key 27 increases or decreases the value of the constant background by 10% and results in the redisplay of the corrected spectrum. Also an information message is issued which contains the current value of the constant background.

However, correction or 'smoothing' of the spectrum may be sometimes desirable. Thus, depressing key 7 invokes a display of two further options. First, by pointing at POINTS, individual channel contents can be replaced by new values after the selection of an appropriate point in response to LIGHT PEN DETECT ON POINT. The new value can be entered by light pen selections on a vertical line. Since the request is repeated automatically, the user must stop this loop by depressing key 1 whenever desired. If, on the other hand, the over-all display should be changed, the selection of SMOOTHING BY LINE ELEMENTS invokes the request of a starting point where smoothing would begin. By indicating the END POINT OF NEW LINE ELEMENT on the vertical line displayed at the identified position, several line elements will be created to represent the new curve. Depressing key 8 allows backward erasion of line elements just generated, element by element. Since usually more than one channel falls into a line element, a linear interpolation is performed. This loop must also be terminated by depressing key 1. In both cases, if no further corrections or graphical smoothing are needed, depressing key 9 results in the termination of this operation.

The end of the data reduction run as described above must be signaled by depressing key 2.

4.2 Initial Estimate of the Function Parameters

In cases where no correction for resolution would be applied to the data, the next main task in program operation is the estimation of the function parameters. A general subroutine suitable for TOF-spectra has been developed for the first determination of starting parameter list by light pen detect on the spectrum or by keyboard entry of the centroids or widths of the spectral lines. First the user must select the type of fit, i.e. one of the four shape functions included in the present program.

SELECT SHAPE FUNCTION

GAUSSIAN CONVOLUTION
LORENTZIAN CONVOLUTION + RESOLUTION PEAK

Depending on the selected option (Fig.1) a redisplay of the spectrum after a conversion to the energy scale will be initiated. At this stage the experimental data are also multiplied by weighting factors normally used for spectra with counting statistics.

SELECT RANGE FOR FIT

Now the user may choose a special range of the spectrum, so that a desired number of peaks may be included in the fitting process. Depressing key 2 accepts the whole spectrum as displayed. Scaling of the spectrum is possible, if desired, by depressing key 20 or key 21.

SELECT PEAK POSITION

The peak position may be determined by light pen detect or by entering the centroid of the peak from the alphanumeric keyboard. The appropriate positions are shown by short vertical bars on the base line. Answering ACCEPTABLE ? by depressing key 2 the user is then requested to

SELECT RANGE FOR FULL WIDTH READ IN FROM KEYBOARD

The next parameter is the fwhm (w or Γ) which may be selected by pointing at two representative points of the spectrum. On the other hand, if no two points may be chosen (in case of overlapping peaks or closely spaced spectral lines), the width may be entered numerically directly from keyboard. After answering ACCEPTABLE the user is now requested to define the status of the peak parameters (Fig.2) by first pointing on the appropriate parameter line and then selecting one of the displayed options. If the user has pointed at LIMITED the values of the parameters may be limited during the fitting process by indicating the LOWER and UPPER bounds given in % of their initial estimates. If all parameters may be left free, key 2 may be depressed. Now the first estimation of the parameters may be completed by taking into account a desired conversion to the energy scale. After answering the next question ARE ALL PEAKS SELECTED ? by depressing key 1 another peak may be selected in the same manner as described above.

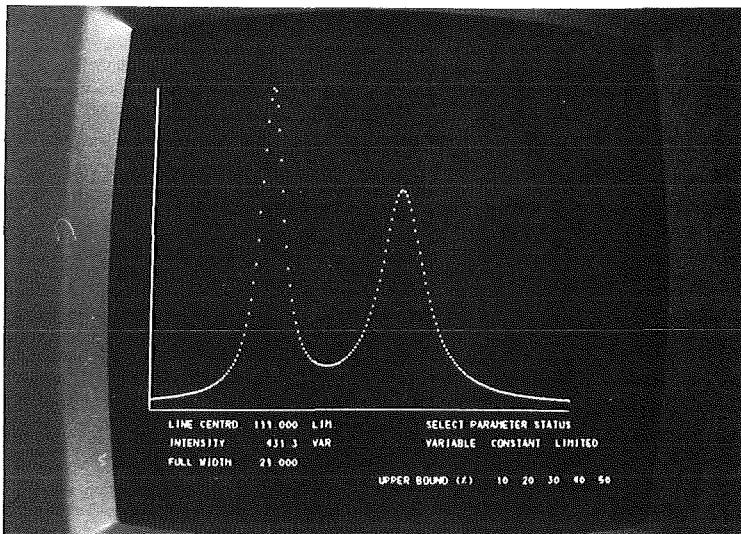


Fig.2: Determination of the parameter status

If no further peak shall be included in the current run, key 2 must be depressed.

The next step is the estimation of the background parameter. First the type of the background must be selected:

LIGHT PEN DETECT OF TYPE OF BACKGROUND
CONSTANT BACKGROUND
LINEAR BACKGROUND

For a linear background two points must be selected by light pen detect. Answering DISPLACEMENT by depressing key 4 the line may be adjusted by shifts in parallel or by 'rotating' using the function keys as given in Table 3.

TABLE 3

Key No.	Function ⁺
4	Correction of the line parameters by moving the line
5	No correction of the displayed line or end of correction
10	Parallel displacement of the line in upward direction
11	Parallel displacement of the line in downward direction
13	Keyboard entry of the shift increment, if desired
14	Increase shift increment by factor 2
15	Decrease shift increment by factor 2
16	Clockwise rotation of the straight line
17	Counter-clockwise rotation of the straight line
19	Keyboard entry of the increment for rotation steps
20	Increase rotation increment
21	Decrease rotation increment

The status of the background parameters is determined in the same way as described above.

For a convolution the fwhm of the Gaussian must now be defined by input or by an estimation using the resolution parameters of the spectrometer.

FIRST ESTIMATION OF THE GAUSSIAN FWHM
FROM RESOLUTION PARAMETERS
READ IN FROM KEYBOARD

If it seems to be useful to determine the fwhm from resolution parameters such as primary energy resolution, flight time uncertainty, and flight path uncertainty, the user must select the appropriate option. In the lower right area of the screen three options are displayed which enable the user to perform another estimation, CONTINUE, or to terminate this calculation, END, if it was successful. Many attempts can be made to arrive at a most acceptable result by changing one or more of the relevant parameters by light pen detects

on the appropriate parameter lines. Then, the cursor appears in the entry area at the right, indicating that a new value can be typed in from the keyboard. The CONTINUE option must be used to signify the completion of a parameter choice for a new estimation. The CANCEL option can be used to finish this calculation. Then, the program returns to read in the Gaussian fwhm.

```
SELECT TYPE OF INPUT OF THE GAUSSIAN FWHM  
WIDTH GIVEN IN MILLI-EV  
WIDTH GIVEN IN X-UNITS(CHANNELS OR OTHER)
```

Depending on the type of x-scale(channels or energy) a conversion of the input value will be done automatically.

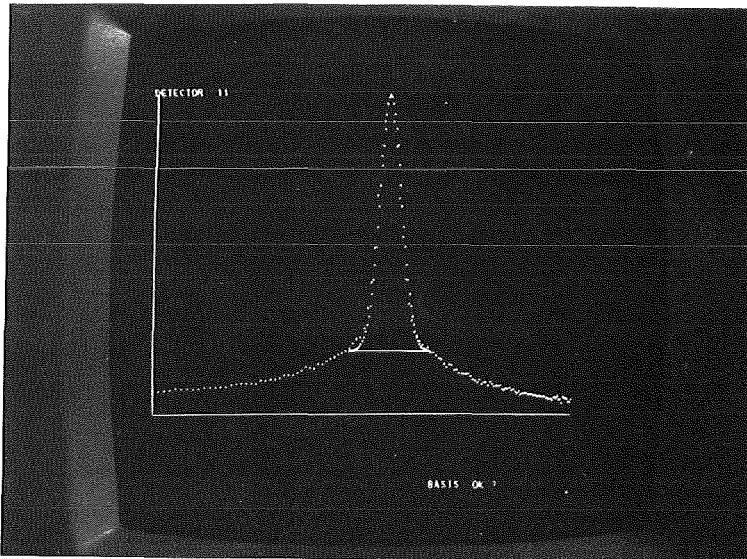


Fig.3: Separation of a resolution peak sited on a TOF-spectrum

If a resolution peak is sited on the top of the spectrum, a separation of this peak will be done approximately. The Gaussian is calculated within a range of 1.5 half widths around the centroid with the half width w as given from experiment. The so-estimated resolution peak will be then displayed for inspection (Fig.3). After answering BASIS OK. ? the user must now

```
SELECT THE HEIGHT OF THE CONVOLUTION PEAK
```

on a vertical line by light pen detect on the representative line segment.

After defining of all involved parameters their values are now stored into the internal parameter list and converted to internal values. Parameters are stored in blocs of three, followed either by the resolution peak height, if any, or either by the one or two parameters describing the background continuum, or both in this order. A quadratic subtraction of the Gaussian line width w from the width of the convoluted signal is used to get a better guess for the starting value/19/. Furthermore, a division of the peak height by w is done to get in this case a value nearer to the optimum. At last, step sizes for parameter variations are calculated from an estimated error of the parameters of 10 %.

4.3 Local and Global Minimum Search

Once the initial values have been calculated, a displayed list informs the user about his selection. At this point, the user is faced with a choice of many options as shown in Fig.4. He may change, for example, the status of one or more parameters between minimization steps, or he may initiate a display of numerical information, or produce a hard copy output of the fitted spectrum. The functions of these options are explained in more detail in Table 4. The selection of one of the fitting options invokes a redisplay of the parameter list and some relevant informations after the particular program has completed. The remaining CPU-time will be displayed. To decide whether the new run has been led to an improved result, depressing key 4 causes the curves as determined with the previous set of parameters to be displayed on the screen.

As already mentioned three different minimization techniques may be used independently of each other in the fitting process. Commonly the SIMPLEX command may be chosen for minimum search. To test, whether convergence is reached or not, a tolerance level EPS on the function value must be put in before. In processing counting spectra it seems to be better to start with a larger tolerance than displayed and to continue with a successively reduced value. The estimated distance to minimum (EDM) will be displayed after each fitting cycle on the screen together with the new parameter set(Fig.4). That is, EDM is twice the expected (vertical) distance to the minimum if the Chi-square function would be quadratic. This important scale-free criterion is given by

$$EDM = \sqrt{(\nabla\chi^2)^T V (\nabla\chi^2)}$$

On the other hand, after selecting MIGRAD the user is requested to enter an additional convergence criterion concerning the stability of the covariance matrix, i.e. a measure for the average fractional change in the diagonal elements of V from one iteration to the next. Both criteria must be satisfied simultaneously or the convergence is attained for EDM less than 10^{-5} EPS. Though MIGRAD often returns without convergence, the fitted curves give reasonable results. However, if convergence is reached, global correlation coefficients will be automatically displayed in an additional column. For the kth parameter we have

$$\rho_k^2 = 1 - [V_{kk}(V^{-1})_{kk}]^{-1}$$

After a SIMPLEX minimization step the HESSE command may be used to estimate the covariance matrix. If successful, global correlation coefficients are also provided in this case. The full covariance matrix is then printed on output device.

Individual correlation coefficients are given by the normalized off-diagonal elements of the covariance matrix as follows

$$\rho_{ij} = V_{ij} / \sqrt{(V_{ii} V_{jj})}$$

The whole fitting process may be recalled after selecting the REPEAT command, whereas the VALUE option serves to reset the parameter values to their initial guess, especially in cases far from minimum (out of radius of convergence). Additional changes may be done. Depressing key 2 must be used to cancel or end this procedure.. Furthermore, if

the user wants to know whether the found minimum is the only one (if more than one are suspected at all), a global minimum search may be started by pointing at IMPROVE. This algorithm is based on that of Goldstein and Price/18/. It is assumed that the function can be represented as Taylor series about the minimum point. Mapping the function using the CONTOUR option may be helpful in those cases (print out only). An appropriate message informs the user whether a truly new minimum has been found or the program has been returned to the original minimum.

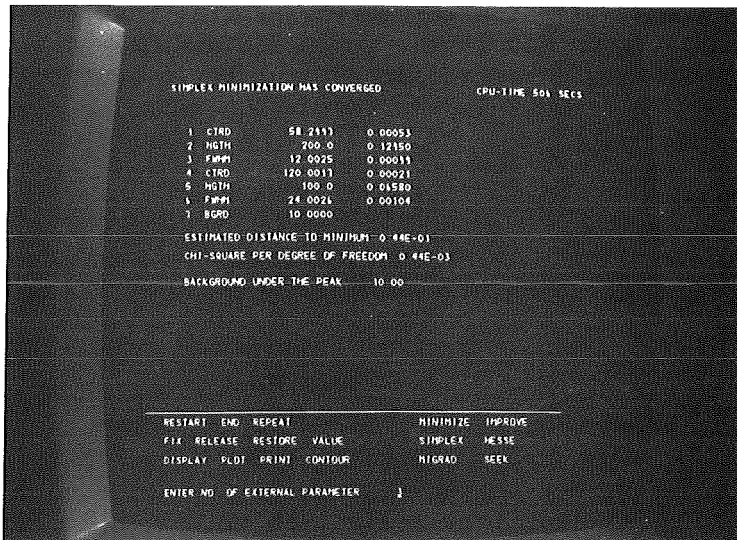


Fig.4: Display of the parameter list after a SIMPLEX call. The FIX option has been selected in order to keep a parameter constant in the next fitting cycle.

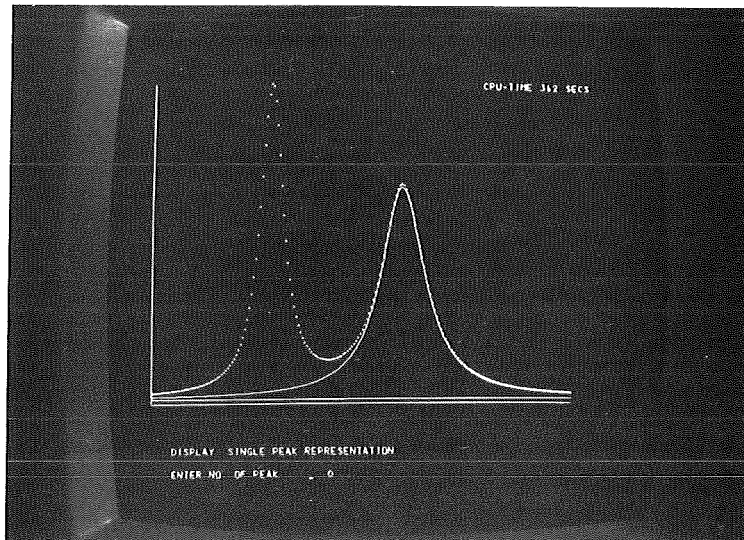


Fig.5: Display of the single peaks from a simulation call. The peak numbers may be input in any order.

TABLE 4

Option	Function
RESTART	At this point the user has the option to return to a read-in of the problem parameters and of the input spectra. RESTART is also useful when a user wants to run a job again that has just been finished, with or without alteration.
CONTOUR	A contour plot will be issued for two variable parameters assuming a minimized FCN, i.e. an existing covariance matrix.
DETECTOR	This option allows the user to evaluate the next detector spectrum, if the data set contains detector spectra as saved by TIFLIS.
END	End of the current run.
VALUE	The parameters are reset to their initial guess and may be altered after a light pen detect on the appropriate parameter line. Key 2 must be used to indicate the end of this correction.
REPEAT	Execute a new parameter selection or change the type of shape function.
DISPLAY	Here, the user has a lot of information at his disposal which may be called in any order by depressing several function keys: Key 16 envelope (minimized function) Key 17 single peak representation Key 18 residuals in units of standard deviation Key 22 normalized Lorentzian (non convoluted) To return to the calling program, the user must depress key 1. If the single peak representation is used, the peaks may be displayed in any order as given by the number of the peak entered from the keyboard. Entering a peak number of -1 results in an erase of all displayed peaks. The end must be signaled by confirming a peak number of 0 (Fig.5).
RELEASE	This option allows the user to release a parameter being fixed previously.
RESTORE	All or only the last parameter may be restored to the variable status.

TABLE 4 (continued)

FIX	This option allows the user to fix a variable parameter.
PLOT	The PLOT option is used to produce a versatile plot output of the fit. A detailed description is given in section 4.4.
PUNCH	This option is used to produce a punching output of some relevant information.
PRINT	The PRINT option produces a print-out of the analyzed spectrum in tables and as a printer plot.
MINIMIZE	This option may be used to start a minimization step calling first SIMPLEX and then MIGRAD.
SIMPLEX	The SIMPLEX program is called.
MIGRAD	The gradient method is used for fitting.
SEEK	A Monte Carlo search has been initiated.
IMPROVE	Test whether another minimum exists or not.
HESSE	Calculates the second derivatives matrix. If this calculation has been finished successfully, the global correlation coefficients are displayed.

4.4 Plot Output

The user may organize his special plot output by two kinds. First, he can use a fixed format output, which contains (i) the input spectrum, (ii) the envelope and (iii) a single peak representation under the envelope. A background plot will be automatically included, if any. Second, the user may include some plot output in a given frame by light pen detects on a displayed plot menu as described below.

After selecting the PLOT option the user is requested to decide what type of plot he wants to perform. Then the user must enter the length of plot axis from the keyboard (in inch). Adjustment of the plot axis may be performed automatically using the SCALE subprogram; an individual annotation of the axis may be achieved in the following way: In the next frame the user is requested to correct XMIN, the first tic mark on the x-axis, and DELTAX given from the x-array according to the chosen length of the plot axis. Now the user can inspect the range of the scale in the upper part of the screen. In the case of agreement the user must touch the END option at the right with the light pen. Otherwise, he may correct the values of the first tic mark and increment by light pen detects on the appropriate text lines and by entering the new values at the cursor's position. Depressing key 2 or

touching CONTINUE invokes a new calculation of the plot scales. Labelling of the x- and y-axis will be done with text strings as input by the user.

Then the preparation of the plot output will be continued automatically, if the fixed output form has been selected previously. On the other hand, a list of different functional forms may be arranged in one plot, so the user may create several plot menus in a simple way by light pen selection. The end of such a selection must be signaled by touching the END OF MENU option (Fig.6) or depressing key 2.

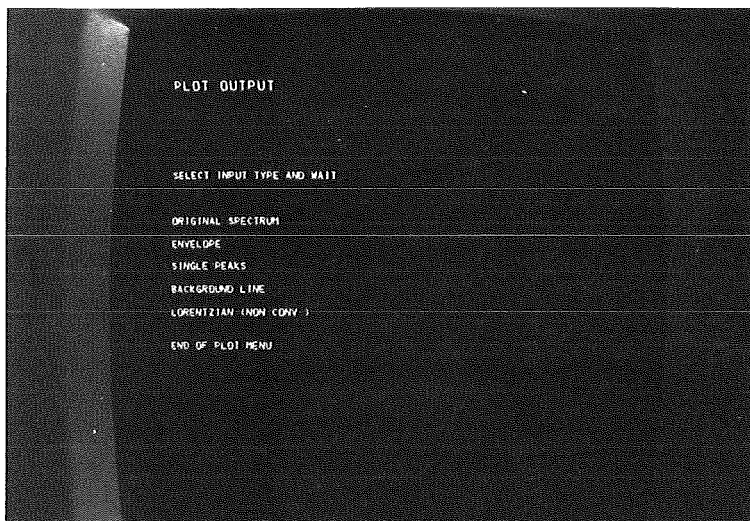


Fig.6: Plot menu selection list

Further arrangements may be processed after answering ANOTHER PLOT MENU ? by depressing key 2. To terminate the plot output at all, FINAL CALL FOR PLOT ? must be answered by depressing key 2 for closing the plot output file. For further PLOT commands key 1 must be depressed.

The program then returns to a redisplay of the actual parameter list and of the program options.

5. Description of the Calling Procedure

With respect to an efficient application of the computer code an interactive graphic main routine has been developed which directs the calling of the evaluation programs. At the beginning of the session an overall title (Fig.7) is displayed on the screen, which must be removed from the screen by depressing key 2 to start processing. First, a SELECT frame appears on the screen and asks the user which one of the programs will be used for processing his data. However, the simulation program serves for testing purposes only.

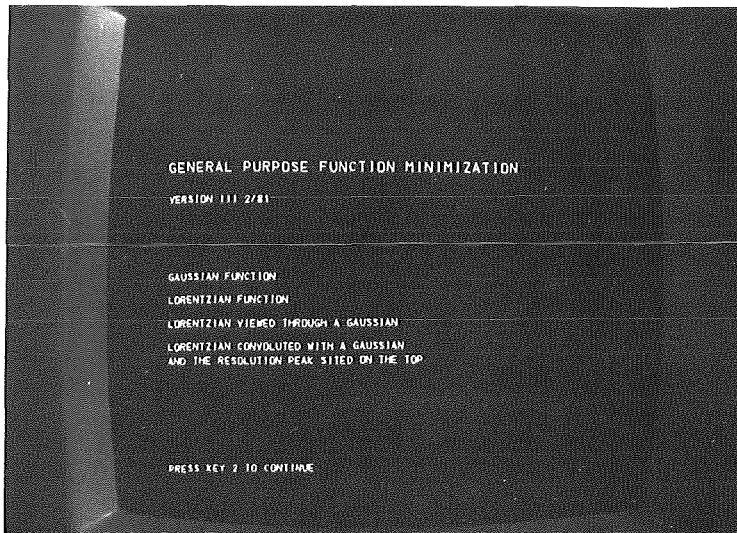


Fig.7: Title after job start

When a program has completed processing as indicated by the user having selected the END option at the end of a particular run, another select frame is displayed together with a history of the current "job" just run as a reminder (Fig.8).

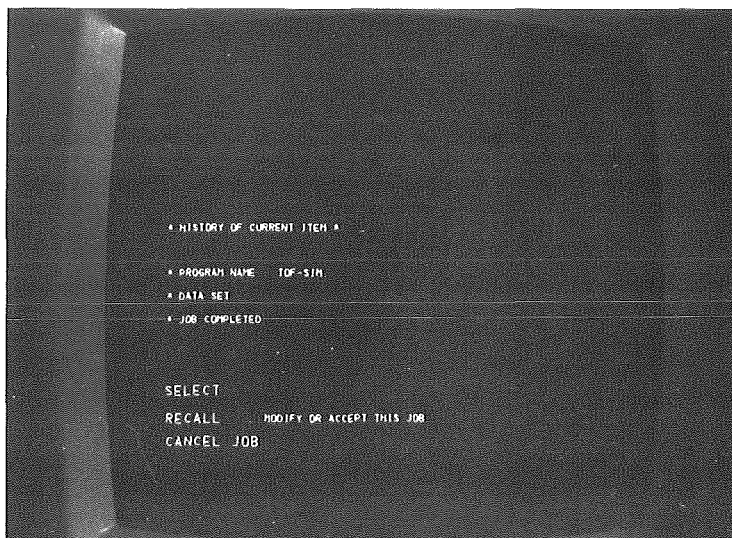


Fig.8: SELECT frame, when a run has completed processing

Since the user has had only one job to process, he selects CANCEL JOB. If he wants to perform further evaluations with or without different data sets, the user must select the RECALL operation from the select frame to continue the session. A recall frame now appears on the screen. After touching the MODIFY option another data set may be selected for processing. If the user has selected the ACCEPT operation, the same job may be called again. At this level, the last operation is equivalent to the RESTART option.

6. Computer Implementations

6.1 General Remarks

The program system is currently implemented on the IBM/370-3033 configuration at the Kernforschungszentrum Karlsruhe(KfK). The programs are written in FORTRAN IV and the IBM GSP package is used for all display management functions. The limit on the array size for formatting the displays is primarily imposed by the display capabilities of the 2250 unit, but also by the wish to minimize the core store requirement. Especially, a substantial fraction of the core requirement is caused by GSP and amounts to about 60K bytes. The size of the complete executable load module is around 300K Bytes. The plot programs are compatible for plotting on XYNETICS, STATOS and VERSATEC plotters.

The CPU time depends upon the number of data points involved in the fit especially in a case of convolution evaluation, because some hundred function calls may be done before reaching the minimum. A solution is obtained in less than 1 minute of elapsed time at the most, and the total session time is typically no more than 30 minutes. Under normal operating conditions in a multiprogramming environment the response time to most actions initiated by the user is of the order of 1 second.

Although large-scale calculations are included, the on-line participation ensures an efficient performance. Due to the implementation of the programs on a high-speed computer the computing time is not too large compared with the normal human conversational time.

6.2 Description of the User Function

The χ^2 function will be calculated in FCN. The parameters of FCN have the following meaning:

NPAR : Number of variable parameters

G : Contains the gradient of the function, if IFLAG=4.

CHISQ : Returns the χ^2 function value as calculated for IMAX points given in the data array E of the labeled common block SQF.

U : External parameter list

IFLAG : Normal entry with IFLAG=1. For IFLAG=4 the derivatives of the function must be supplied.

A listing of the subroutine used here is given in Appendix 2. The user may write his own routine which must then be compiled and linked to separately. However, the structure of FCN is as follows:

```

SUBROUTINE FCN(NPAR,G,CHISQ,U,IFLAG)
COMMON/MUPHV/ HOX,HAX,NPMEXT,NPEAK,DW,IDS1,IDS2,NL,NR,XNEL
COMMON/SQF/   IMAX,Y(512),P(512),NXG,FY,NB,NBG,NF,Q,FC,JST,KFG,
*            E(512),IFALL, X ,DEG,DGG(10),ICHP(10),FFV(5)
DIMENSION U(15),G(15)
C
  GOTO(1,2,3,4), IFLAG
1 CONTINUE
  ...
  calculate the function value (normal entry without gradient)
  ...
  GOTO 5
2 CONTINUE
  ...
  not used
  ...
  GOTO 5
3 CONTINUE
  ...
  not used
  ...
  GOTO 5
4 CONTINUE
  ...
  calculate the function value and the derivatives
  ...
5 CONTINUE
C
  RETURN
  END
```

6.3 JCL Requirements for the Program Run

```
//IAK352GB JOB (0352,143,POA2E),ABEL,CLASS=G,TIME=10
//*MAIN SYSTEM=M3033,LINES=20
//JOB LIB DD UNIT=3350,VOL=SER=GEN002,DISP=SHR,
//          DSN=R216.LINKLIB.GRAPH
// EXEC FGLG,LIB=IAK,PARM.L='LIST,MAP',PLOT=VERSATEC
//L.SYSLIB DD
//          DD
//          DD
//          DD
//          DD
//          DD DSN=SYS2.IMSL.SP,DISP=SHR
//          DD DSN=LOAD.GSP,DISP=SHR
//L.SYSIN DD *
  INCLUDE SYSLIB(IHCGSP03)
  INCLUDE LOAD(IGFIT250)
  INCLUDE LOAD(PRINTP$,ALLOCX,CRDD250,INITDA,TPDSNVOL)
  INCLUDE LOAD(CPUID)
//G.FT10F001 DD UNIT=2250-1
//G.FT20F001 DD DSN=&&TS,SPACE=(2048,(99),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT30F001 DD UNIT=3350,VOL=SER=BAT00F,DISP=SHR
//G.SYSIN DD *

<TOF-spectrum 1 >
<Time-dependent background>
<TOF-spectrum 2 >
<Time-dependent background>
<TOF-spectrum 3 >
...
// EXEC SVPLOT
//
```

Subroutines from LOAD library call

- PRINTP\$ - Printer plot routine
- ALLOCX - Dynamic allocation of data arrays
- CRDD250 - Locates and opens a data set
- INITDA - Defines direct access data sets
- TPDSNVOL - Gets the volume and data set name from the JFCB
- CPUID - Returns the remaining CPU-time/20/ for the job run.

Acknowledgement

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References

- /1/ W.Abel, KfK 2481 (1977)
- /2/ F.James and M.Roos, Comput. Phys. Comm. 10(1975),343
- /3/ J.A.Nelder and R.Mead, Comput. J. 7(1965),308
- /4/ R.Fletcher, Comput. J. 13(1970),317
- /5/ R.Fletcher and M.J.D.Powell, Comput. J. 6(1963),163
- /6/ C.J.Batty,S.D.Hoath and B.L.Roberts, Nucl. Instr. and Meth. 137(1976), 179
- /7/ W.Gautschi, S.I.A.M. J. Numer. Anal., Vol.7, 1(1970), 187
- /8/ W.Gautschi, in Handbook of Mathematical Functions, M.Abramowitz and J.A.Stegun, Eds., NBS Appl. Math. Ser. 55, Washington D.C., 1965, 292
- /9/ K.S.Kölbig, Comm. A.C.M. 15(1972), 465
- /10/ Algorithm 363 Complex Error Function, Comm. A.C.M. 12(1969), 635
- /11/ IBM System /360 OS
Graphic Subroutine Package (GSP)
for FORTRAN IV, COBOL, and PL/I
Form C27-6932-3
- /12/ IBM System /360 Component Description
IBM 2250 Display Unit Model 1
Form A27-2701-2
- /13/ J.Routti and S.Prussia, Nucl. Instr. and Meth., 72(1969), 125
- /14/ B.L.Roberts, R.A.J.Riddle and G.T.A.Squier, Nucl. Instr. and Meth., 130(1975), 595
- /15/ M.Kitamura, Y.Takeda, K.Kawase and K.Sugiyama, Nucl. Instr. and Meth., 136(1976), 363
- /16/ W.Abel, J.B.Suck, KfK 2187(1976)
- /17/ F.James, Function Minimization in Proc. of the 1972 CERN Computing and Data Processing School, CERN 72-21(1972)
- /18/ A.A.Goldstein and J.F.Price, Math. Comp. 25(1971), 569
- /19/ D.A.Wilkinson, Nucl. Instr. and Meth., 95(1971), 259
- /20/ N.Moritz, private communication

Appendix 1

```
      SUBROUTINE WOFZ(X,Y,RE,IM,IQ)
C
C   THIS PROCEDURE EVALUATES THE REAL AND IMAGINARY PART OF THE
C   FUNCTION  $W(Z) = \exp(-Z^2) \operatorname{erfc}(-iZ)$  FOR ARGUMENTS  $Z=X+iY$  IN THE
C   FIRST QUADRANT OF THE COMPLEX PLANE. THE ACCURACY IS 10 DECIMAL
C   PLACES AFTER THE DECIMAL POINT, OR BETTER. FOR THE UNDERLYING
C   ANALYSIS, SEE W. GAUTSCHI, "EFFICIENT COMPUTATION OF THE COMPLEX
C   ERROR FUNCTION", SIAM J. MATH. ANAL., (1969). THE SYMMETRY
C   RELATIONS ARE USED TO CALCULATE THE FUNCTION VALUE IN THE
C   REMAINING QUADRANTS.
C
C   TRANSLATED FROM ALGORITHM 363, COMM. ACM, 12(1969), 635
C   (SINGLE PRECISION VERSION)
C
C   COMPLEX*8 Z,WZ
C   REAL*4 XR,YR,DRE,DIM
C   REAL*4 H,H2,LAMBDA,R1,R2,S,S1,S2,T1,T2,C
C   REAL*4 IM
C   INTEGER CAPN
C   LOGICAL B
C
C   IQ=1
C   IF(X.GE.0..AND.Y.GE.0.) IQ=1
C   IF(X.LT.0..AND.Y.GE.0.) IQ=2
C   IF(X.LT.0..AND.Y.LT.0.) IQ=3
C   IF(X.GE.0..AND.Y.LT.0.) IQ=4
C
C   XR=ABS(X)
C   YR=ABS(Y)
C   Z=CMPLX(XR,YR)
C
C   IF(.NOT.(YR.LT.4.29.AND.XR.LT.5.33)) GOTO 20
C
C   S=(1.-YR/4.29)*SQRT(1.-XR*XR/28.41)
C   H=1.6*S
C   H2=2.*H
C   CAPN=6+23*S
C   LAMBDA=H2**CAPN
C   NU=9+21*S
C   GOTO 30
20 CONTINUE
C   H=0.
C   CAPN=0
C   NU=8
30 CONTINUE
C
C   IN THE FOLLOWING STATEMENT, LAMBDA=0 COVERS THE UNDERFLOW
C   CASE WHEN H>0 IS VERY SMALL.
C
C   B=(H.EQ.0..OR.LAMBDA.EQ.0.)
C   R1=0.
C   R2=0.
C   S1=0.
C   S2=0.
C   NN=NU+1
```

```
DO50 I=1,NN
N=NU-I+1
NP1=N+1
T1=YR+H+NP1*R1
T2=XR-NP1*R2
C=.5/(T1*T1+T2*T2)
R1=C*T1
R2=C*T2
IF(.NOT.(H.GT.0..AND.N.LE.CAPN)) GOTO 70
T1=LAMBDA+S1
S1=R1*T1-R2*S2
S2=R2*T1+R1*S2
LAMBDA=LAMBDA/H2
70 CONTINUE
50 CONTINUE
IF(YR.NE.0.) GOTO 40
DRE=EXP(-XR*XR)
GOTO 45
40 DRE=1.1283792*S1
IF(B) DRE=1.1283792*R1
45 DIM=1.1283792*S2
IF(B) DIM=1.1283792*R2
C
C RETURN REAL AND IMAGINARY PART OF W(Z) IN THE QUADRANT IQ
C
GOTO(1,2,3,4), IQ
C
1 CONTINUE
RE=DRE
IM=DIM
GOTO 5
2 CONTINUE
WZ=CMPLX(DRE,DIM)
WZ=CONJG(WZ)
RE=REAL(WZ)
IM=AIMAG(WZ)
GOTO 5
3 CONTINUE
WZ=CMPLX(DRE,DIM)
WZ=2.*CEXP(-(Z*Z))-WZ
RE=REAL(WZ)
IM=AIMAG(WZ)
GOTO 5
4 CONTINUE
WZ=CMPLX(DRE,DIM)
WZ=2.*CEXP(-(Z*Z))-WZ
WZ=CONJG(WZ)
RE=REAL(WZ)
IM=AIMAG(WZ)
C
5 CONTINUE
C
RETURN
END
```

Appendix 2

```

SUBROUTINE FCN(NPAR,G,QQ,U,IFLAG)
C
C   CALCULATES THE FUNCTION TO BE MINIMIZED, I.E. CHI-SQUARE
C   FUNCTION QQ, AT ALL POINTS X FOR THE ACTUAL PARAMETERS U.
C   FOR IFLAG=4 NO DERIVATIVES G ARE CALCULATED.
C
COMMON/MUPHV/ HOX,HAX,NPMEXT,NPEAK,DW,IDS1,IDS2,NL,NR,XNEL
COMMON /SQF/ IMAX,Y(512),P(512),NXG,FY,NB,NBG,NF,Q,FC,JST,KFG,
*E(512),IFALL, X ,DEG,DGG(10),ICHP(10),FFV(5)
DIMENSION U(15),G(15),F(10),WZR(10),WZI(10)
REAL*4 IM
DATA PI/3.1415927/
C
C   B0   = FIRST PARAMETER FOR BACKGROUND (CONSTANT COEFF.)
C   B1   = SECOND PARAMETER FOR BACKGROUND (SLOPE PARAMETER)
C
C   U(J) = LINE CENTROID
C   U(J+1)= HEIGHT
C   U(J+2)= FULL WIDTH AT HALF MAXIMUM
C
C   IF(KFG-1) 2, 1, 3
C
C
C   GAUSSIAN F(X,U(J),U(J+1),U(J+2))=U(J+1) EXP(-4 LN(2)  $\frac{(X-U(J))^2}{U(J+2)}$ )
C
C
1 CONTINUE
K=3*NPEAK+IFALL+1
B0=U(K)
B1=U(K+1)
QQ=0.
DO100 I=1,IMAX
X=E(I)
FF=0.
FF=FF+B0+B1*(X-E(1))
DO10 M=1,NPEAK
J=3*M-2
DE=X-U(J)
H=DE/U(J+2)
ARG=FC*H*H
IF(ARG.GT.100.) ARG=100.
FG=EXP(-ARG)
F(M)=FG
FF=FF+U(J+1)*FG
10 CONTINUE
Q=Y(I)-FF
QQ=QQ+P(I)*Q*Q
C
C   IF(IFLAG.EQ.4) GOTO 100
C
DO11 J=1,NPAR
11 G(J)=0.
W=P(I)*Q
DO13 M=1,NPEAK

```



```
200 CONTINUE
C
C   RETURN
C
C   CONVOLUTION (LORENTZIAN VIEWED THROUGH A GAUSSIAN)
C   THE INTEGRAL HAS BEEN TRANSFORMED TO THE COMPLEX ERROR FUNCTION.
C   NO NORMALIZATION HAS BEEN DONE.
C
3 CONTINUE
K=3*NPEAK+IFALL+1
L=K-1
B0=U(K)
B1=U(K+1)
C
C   QQ=0.
C   C=SQRT(ALOG(2.))
C   DO300 I=1,IMAX
C   X=E(I)
C   FF=0.
C   FF=FF+B0+B1*(X-E(1))
C   DO25 M=1,NPEAK
C   J=3*M-2
C   DEG=DGG(M)
C   CHANGE OF VARIABLES
C   V=(X-U(J))/DEG * 2.*C
C   A=U(J+2)/DEG * C
C   CALL WOFZ(V,A,RE,IM,IQ)
C   SAVE THE REAL AND IMAGINARY PART
C   WZR(M)=RE
C   WZI(M)=IM
C   V0=0.
C   CALL WOFZ(V0,A,RE0,RIM,IQ)
C   VNORM=PI*RE0
C   FF=FF+U(J+1)* DEG/(2.*C) * A * PI * RE
C   ADD PICK-A-BACK PEAK
C   IF(IFALL.EQ.0) GOTO 25
C   IF(M .NE.NXG) GOTO 25
C   DE=X-U(J)
C   H=DE/DEG
C   ARG=FC*H*H
C   IF(ARG.GT.100.) ARG=100.
C   FG=EXP(-ARG)
C   F(M)=FG
C   FF=FF+U(L)*FG
25 CONTINUE
C   Q=Y(I)-FF
C   QQ=QQ+P(I)*Q*Q
C
C   IF(IFLAG.EQ.4) GOTO 300
C
C   DO30 J=1,NPAR
30 G(J)=0.
C   W=P(I)*Q
C   DO32 M=1,NPEAK
C   J=3*M-2
C   DEG=DGG(M)
C   CHANGE OF VARIABLES
C   V=(X-U(J))/DEG * 2.*C
```

```
A=U(J+2)/DEG * C
C   CALCULATE THE PARTIAL DERIVATIVES OF THE COMPLEX ERROR FUNCTION
    DWZV=2.*V*WZR(M)+2.*A*WZI(M)
    DWZA=-2./SQRT(PI)+2.*V*WZI(M)+2.*A*WZR(M)
C   BUILD DERIVATIVES WITH RESPECT TO THE PARAMETERS
    Q1=-U(J+1)*PI*A*DWZV
    G(J) =Q1 *2.*W + G(J)
    Q1=U(J+1)*DEG/(2.*C)*A*PI*WZR(M)
    G(J+1)=Q1 *2.*W + G(J+1)
    Q1=U(J+1)/2.*PI*(WZR(M)+A*DWZA)
    G(J+2)=Q1 *2.*W + G(J+2)
C   ADD DERIVATIVES OF THE PICK-A-BACK PEAK
    IF(IFALL.EQ.0) GOTO 32
    IF(M .NE.NXG) GOTO 32
    DE=X-U(J)
    FG=F(M)
    G(J) = G(J) + 2.*W*2.*FC*U(L)*DE*FG/(DEG*DEG)
    G(J+1)= G(J+1) + 2.*W*FG
    G(J+2)= G(J+2) + 2.*W*2.*FC*U(L)*DE*DE*FG/(DEG*DEG*DEG)
32 CONTINUE
    IF(B0.EQ.0.) GOTO 301
    G(K)=G(K)+2.*W
301 IF(B1.EQ.0.) GOTO 300
    G(K+1)=G(K+1)+2.*W*(X-E(1))
300 CONTINUE
C
    Q=QQ
C
    RETURN
    END
```