Using constrained variables in FITHEO

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Introduction

The standard MINUIT cards allow to define and refine up to 50 (60) parameters:

```
***param-N  *param***  ****value  ****error  ******min  ******max
         1          x      .7000       .010       0.00       1.00
         2         Ao      2.866       .010       2.80       3.50
       ....
```

These parameters are called within FITHEO referring to their number *param-N*. This modification allows to define new variables, functions of the 1...60 MINUIT parameters. These new parameters can be used within FITHEO as the standard MINUIT ones.

Use

The FITHEO **CARD 1** defines the number of XAS files to be analyzed, **NXAS**. If **NXAS**< 0, follow **N_frm** = - **NXAS** cards, each one defining a new "constrained variable" which is a function of the above defined MINUT parameters. The values of each "constrained variable" are defined by a string like:

```
& #1* 1.4142136 + #3 &   ! comment
```

- The function is enclosed between "&", the following is a comment.
- The allowed arithmetic operations are executed in the standard order: `^, * ,/ ,+ ,-`.
- A MINUIT parameter is indicated by "#", the example above means: "the MINUIT parameter **1** multiplied by **1.4142136** is added to the MINUIT parameter **3**". Spaces are ignored (but considered in the total string length, see the limitations section)
- Each "constrained variable" is numbered progressively 61, 62, 63, ... N_frm.
- The new variables are updated at each MINUIT cycle. In this way FITHEO can use either a standard MINUIT parameter (≤ 60) or a new variable ($N > 60$). This can be done either for "structural" cards (R, Debye Waller, Coordination numbers) either for non-structural parameters (E_o, discontinuities, etc...)

Examples:

```
& #1 + 0.5 * #2 +#3^2 &
```

assigns the value: $X(1) + 0.5 * X(2) + X(3) * *2.5$ to the variable ($X(i)$ being MINUIT parameters).

```
& 1.414 &
```

assigns the constant value 1.1414 to the variable.

Limitations:

- $N\_frm \leq 40$.

- Maximum string length = 78 characters.
- No parenthesis are allowed.
- a "constrained variable" cannot refers to one other "constrained variable"

Input file example

Considering a chemically disordered fcc alloy A_xB_{1-x}. The parameter **10** is the lattice parameter. The parameters **11** (x_1) and **12** (x_2) represent the fraction of A atoms in the first and second shell respectively. The parameters GAMMA, Exp. Resolution and S_o^2 are kept fixed.

```
         **EXAFS FITTING PARAMETERS**
         1    Eo       6545.40      0.50    6541.0     6550.
...
        10     A_o       1.980       .00     1.900      2.10
        11     x_1         0.5       .01     0.000     1.000
        12     x_2         0.5       .01     0.000     1.000
...

-9                                  ! 9 c.v. must be defined}
& #10 / 2.0 ^ 0.5 &          I.st shell         parameter 61
& #10 * 1.5 ^ 0.5 &          IInd shell         parameter 62
& #11 * 12        &         N_A   I shell       parameter 63
& 12 - #11 * 12   &         N_B   I shell       parameter 64
& #12 * 6         &         N_A   II shell      parameter 65
& 6 - #12 * 6     &         N_B   II shell      parameter 66
& 0.85            &          So^2               parameter 67
& 0.00            &          gamma              parameter 68
& 0.30            &          exp-res            parameter 69

1        ! number of files (if -1 Energy and Alpha columns can be given)

 LM1_0_2.MU
 pro
 6400.,6500.    !  E MIN E MAX FIT PRE EDGE LINEARE
 6560.,.8      !  E MAX CALCOLO dABS/dE (0->next), TOLLERANZA
 N             !  MESH DK=COST?
 ...
 0             !  MFP:
 68,69         ← ! GAMMA, Exp. Res. fixed values
 ...
```

```
4                    !  Number Coordination numbers
63                  ← C. V. number 63
64                  ← C. V. number 64
65                  ← C. V. number 65
66                  ← C. V. number 66
4                   ! num. g2
'G'
61,15               ← C. V. number 61
1
../der/momg21.der
1,1.                A-A First shell

'G'
61,16               ← C. V. number 61
1
../der/momg22.der
2,1.                A-B First shell

'G'
62,17               ← C. V. number 62
1
../der/momg23.der
3,1.                A-A Second shell

'G'
62,18               ← C. V. number 62
1
../der/momg24.der
4,1.                A-B second shell

...
67                  ←  ! S0**2, constant number 67
...
```