

Short User Guide of Generalised Least Squares Code GMAP

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Introduction

GMAP is a generalised least-squares code named after **G**auss, **M**arkov, **A**ikten. It was developed by W. Poenitz and written in Fortran 77 for standard neutron cross section evaluation. GMAP provides non model fit of the experimental data. This short guide covers the basic properties of the GMAP code and gives some examples. It also covers usage of DATP code used for fitting experimental data to energy grid. Few minor modifications of DATP were done during recent evaluation:

- Increased maximum dimension of data set to 600.
- New commenting by using symbol “#” which made the previous commenting obsolete.
- Variable number of priors.

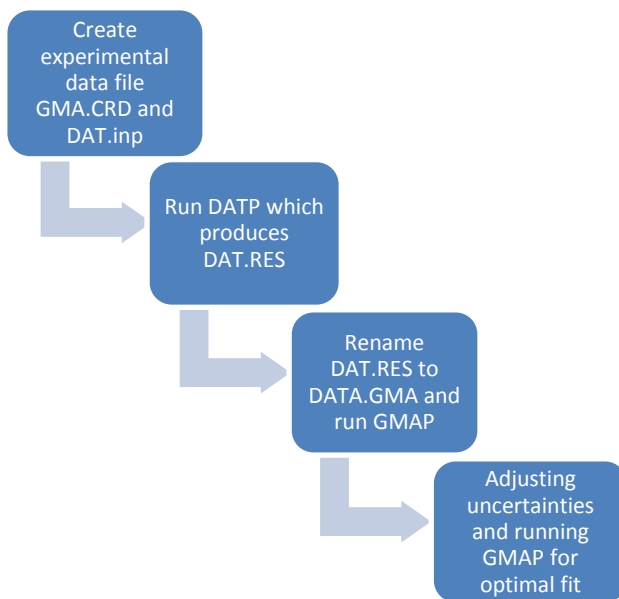


Figure 1. Scheme of GMA code usage

Structure of code and sequence of operations

The procedure of GMA use includes these steps (see in ref. [1])

1. Create two input files:

- DAT.inp - input file of output control parameters, **priors cross sections** for reactions you would like to fit and ²⁵²Cf(s.f.) **standard** prompt fission neutron spectrum if spectrum averaged experimental data will be used in the fit.

- GMDATA.CRD – input file of the reaction experimental data selected for the fit. This file is usually created manually by the evaluator using data from the EXFOR database or primary references and editors allowing to make block operations.

2. Run code DATP to convert all experimental data to the energy grid provided by priors.

3. Rename created file DAT.RES to DATA.GMA.

4. Run the GMAP code, it will produce GMA.RES with all results and plot.dta which contains only the fitted cross section value of every with uncertainties.

Description of DAT.inp

This is the input for the cross section energy grid, *a priori* cross sections and control parameters. DAT.inp begins with control parameters (see Figure 2), californium prompt fission **standard** neutron spectrum (if necessary), followed by the cross sections for evaluated reactions. Line with 0 marks the beginning of the reaction cross section input.

All energies are given in **MeV**, cross sections - in **barn**. The number of *a priori* cross sections should be defined within DAT.inp. Input data have to be provided in fixed format. For more details about the format see DAT.inp file, ref. [1] or Figure 2.

Cross section definition begins with one comment line followed by the energy and cross section values (2E10.4 format) in two columns. The last line of every cross section array should be 0. All the cross sections will be automatically assigned numbers according to the order of appearance in the input file. Reaction which appears first (Pb(n,f) for example) is assigned number one and will be referred as reaction #1 in the GMAP code and GMDATA.CRD file.

```

A2 A2 A1  I5      I5      I5      I5
I/OC  | ..... 1 | ..... 1 | ..... 1 | ..... 0 | ..... 0 ..... 1 ..... 0 ..... 1
MODE  | ..... 3 | ..... 0 | ..... 0 | ..... 6 | ..... 1 ..... 0 ..... 0 ..... 0
..... 0 | ..... 0 | ..... 0 | ..... 0 | ..... 0 ..... 0 ..... 0 ..... 0 ..... 0
Pb (n, f) ← End of control parameters and Cf(s.f.)
3.2000E+01 7.6847E-05 ← comment for reaction nr #1
3.4000E+01 9.5615E-05
3.6000E+01 1.2566E-04 ← Reaction Cross section
3.8000E+01 1.7035E-04
4.0000E+01 2.3284E-04
E10.4      E10.4

```

Figure 2. DAT.inp input format. Information is read in batches A2, A2, A1, 8I5. I/OC is output control, mode controls the correlation matrix construction, etc. Detailed meaning of each parameter and code words are described in [1].

Description of GMDATA.CRD

This fixed format file contains experimental data on various reaction cross sections, see example in Figure 3. “#” - is a comment symbol and everything after it in the line will be treated as a comment. Energies are provided in **MeV**, cross sections in **barn**, uncertainties in %. Data block ends by entry EBEBEB. If data block consists from few correlated datasets, each of them ends with entry ESES. Correlations between datasets are introduced before the ESES entry starting from second dataset. Extensive input definitions are provided in [1], however in this text some of the features will be explained in more detail.

Line 1 contains information about the primary quantity measured in the experiment. It begins with 4 digits unique integer number (arbitrary) as ID for this

Table 1. Type of measurements available in GMAP

Type of measurement (MT)	Measurement type
1	Absolute cross section
2	Cross section shape
3	Absolute cross section ratio
4	Ratio shape
5	Sum of cross sections
6	Spectrum averaged cross section
7	Absolute ratio of cross section vs. sum of cross sections
8	Shape of type 5
9	Shape of type 7

specific data set, followed by 4 digits number

(usually a year of experiment for mnemonic and tracking). After that there is possibility to add relevant labels.

Line 2 provides following information: data set tag for selective purposes (NQ), type of measurement (Table 1.) (MT), source of correlation matrix (NCO), number of preceding data sets for which correlations are given (NCS), number of comment lines (NCCO – **obsolete feature after current update, any integer can be entered**), number of experimental data entries (energy points) (NO), reaction numbers involved in the measurement.

In the provided example (Figure 3) we input the ^{209}Bi (reaction $^{\circ}\#2$) to ^{238}U (reaction $^{\circ}\#5$) fission cross section ratio which is referred in line 2 by the second digit $\#3$ (absolute cross section ratio). The command line 2 also specifies that there are 5 comment lines (obsolete in updated version of DATP) after it and 11 entries of data. Comments follow after this line.

Next command line after the comments specifies 10 uncertainties which are fully correlated in the whole energy range in %. This line should be skipped if the data is shape measurement.

Fully correlated uncertainties are followed by matrix of parameters determining the length of energy correlations for components of uncertainties given in column #11 - #21 below. It is not used for #11 and #12 – incident energy uncertainties, #13 – usually used for presentation of statistical component and #22 where calculated total uncertainty can be given (for information). The first line of the matrix is related to the #11 uncertainty, second - to the #12 and so on (for more details see page 16 of [1]).

```

1 17082004Bi(n,f)/8U(n,f) ..... A.N. Smirnov ..... Phys.Rev. C
2 1 3 0 0 5 11 2 5 0 0 0 0
3 # UNCERTAINTY ..... Ratio of Bi(n,f)/8U(n,f) .....
4 # (ERR-ERG) energy error .....
5 # (ERR-1) total error excluding ERR-2 and ERR-3 .....
6 # (ERR-2) Uncertainty of calculation of relative detection efficiency .....
7 # (ERR-3) Uncertainty of detection efficiency from one sandwich to another in
8 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1 1 1 1 2 2 2 0 0 0
9 .....
10 .....
11 .....
12 .....
13 .....
14 .....
15 .....
16 .....
17 .....
18 .....
19 .....
20 ..... 9 9 1 2 2 2 0 0 1 tags for energy dependat uncertainty components (not used)
21 # As this data set is correlated with preceding data set this numbering will
22 # provide information which columns are correlated
23 # Numbering ..... #11 #12 #13 #14 #15 #16 #17 #18 #19 #20 #21 #22
24 0.3450E+020.1900E-03 4.1 0.0 9.2 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
25 0.4630E+020.1050E-02 2.6 0.0 8.1 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
26 0.6660E+020.5400E-02 1.4 0.0 7.8 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
27 0.7390E+020.8200E-02 1.4 0.0 6.8 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
28 0.8960E+020.1330E-01 0.9 0.0 7.5 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
29 0.9410E+020.1570E-01 1.5 0.0 7.3 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
30 0.1113E+030.2470E-01 1.0 0.0 9.7 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
31 0.1329E+030.3070E-01 1.4 0.0 7.2 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
32 0.1446E+030.3350E-01 1.2 0.0 7.8 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
33 0.1600E+030.4150E-01 1.1 0.0 7.7 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
34 0.1733E+030.4170E-01 1.1 0.0 8.2 5.0 0.6 0.0 0.0 0.0 0.0 0.0 0.0
35 ESESESESES ..... end of data set
36 170920040Pb(n,f)/Bi(n,f) ..... A.N. Smirnov ..... Phys.Rev. C
37 1 3 0 1 6 8 1 2 0 0 0 0

```

Figure 3. Example of GMDATA.CRD input file.

The experimental data is provided in this example in lines from 24 to 34. There are 14 columns in fixed format (2E10.4, 12F5.1). The first column is energy, the second – cross section. The subsequent columns are numbered #11, #12 ... until max #22. Column #11 is the

energy uncertainty in %, #12 – energy resolution in %, #13 – statistical uncertainty of cross section in %, from #14 to - #21 - systemic uncertainties in (medium energy range correlation components) %.

As mentioned before, there is a possibility to add correlation between different datasets (cross-datasets correlations). The example below shows a correlation of the data set 1709 with 1708. A proper command line has to be inserted just after the end of 1709 data entry, but before the data block or data set end:

```
# This instructs code that column #14 in dataset 1708
# correlates with column #14 in dataset 1709 as well as #1:
17081414 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
# this specifies the correlation strength
0.5 0.5 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
EBEBEBEBEB
```

When all uncertainties, energy-energy and cross-datasets correlations are inserted in the input file GMDATA.CRD, DATP should be ran and finally the created DAT.RES file renamed into DATA.GMA.

Description of DATA.GMA

The DATA.GMA is an input file for GMA code (it could be edited to embed additional information).

The beginning of DATA.GMA is the same as provided in DAT.inp except that after the Californium spectrum definition it is specified how many *a priori* cross sections and values are available in the input by line:

```
APRI 529 5
```

In this example there are 5 *a priori* cross sections provided and 529 values of cross section. This command is followed by *a priori* cross section input which is ended by:

```
BLCK 0 0.
```

This is followed by data blocks with experimental data reduced to the energy grid last entry of energy and cross section should be 0.

```

BLCK      0      0
DATA 1720      3      0      2      2      3      0      0
2011      1      0 D.Tarrío                               Phys.Rev. C vol83
  1.2  2.5  3.5  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1  1  1  1  2  2  2  0  0  0
  0.00 0.00 0.00  0
  0.00 0.00 0.00  0
  0.00 0.00 0.00  9
  0.50 0.50 0.50  9
  0.50 0.50 0.50  1
  0.50 0.50 0.50  2
  0.50 0.50 0.50  2
  0.50 0.50 0.50  2
  0.50 0.50 0.50  0
  0.50 0.50 0.50  0
  0.00 0.00 0.00  1
0.4400E+020.9821E-03  0.0  0.0  52.9  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.4800E+020.1177E-02  0.0  0.0  51.7  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.5200E+020.2058E-02  0.0  0.0  36.9  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.5800E+020.3435E-02  0.0  0.0  29.9  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.6400E+020.4614E-02  0.0  0.0  22.7  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.6800E+020.5493E-02  0.0  0.0  16.9  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.7600E+020.8678E-02  0.0  0.0  23.1  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.8400E+020.1082E-01  0.0  0.0  18.9  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.9200E+020.1298E-01  0.0  0.0  15.7  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0

```

Figure 4. DATA.GMA data set input example.

It is important to note that if for a specific energy value of *a priori* there is no experimental value in “DATA.GMA” the code will fail. For this reason the user has to introduce the “dummy” sets into the DATA.GMA which will match energy grid of the *a priori* cross sections. The values of *a priori* cross sections are used for DUMMY sets. They have to be assigned with high uncertainty (e.g., 60%) to make the overall influence on the least squares fit insignificant. The “dummy” values just prevent failure of the code when the energy grid is not optimal for the fit. After producing first fit it can be seen at which energies there are no experimental data as the uncertainty of the fit will be equal to 60%. These energy points can be later removed from *a priori* cross section as insignificant.

When the energy correlation matrix is known it is possible to introduce it into the DATA.GMA file. Example: in the data set 2380 the third number specifies how many lines the correlation matrix has (106 in this example):

```

DATA 2380      1 106      1      5      0      0      0
2001      1      0 STANDARD!!! U8

```

The number of energy correlation matrix elements allowed per line is limited to 10 (format 10F8.5). For more details look into DATA.GMA file datasets 2380, 2350.

References

- [1] W.P.Poenitz, S.E aumeier, “The Simultaneous Evaluation of the Standards and Other Cross Sections of Importance for Technology”, Report ANL/NDM-139 (1997).