The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1944-28

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

19 - 30 May 2008

SAMMY Excersises.

MARRONE Stefano

Universita' degli Studi di Bari
Istituto Nazionale di Fisica Nucleare-INFN
Via Orabona, 4
70125 Bari
ITALY

SAMMY EXCERSISES

S. Marrone
Istituto Nazionale Fisica Nucleare &
Dipartimento di Fisica, BARI (ITALY).

OUTLINE

1) SCOPE
2) INSTALLATION and ENVIRONMENT
3) STRUCTURE of the FILES
4) FORMAT of FILES
5) PREREQUISITES
6) EXCERSISES
7) OTHER USEFUL PROGRAMS

SCOPE

- SAMMY code allows the fitting of the reaction data according to the R-Matrix theory.
- The R-Matrix describes the features of the Reaction Cross Section in Resolved Resonance Region.
- SAMMY works both for neutron and for incident charged particles e.g.: (n,α) or (α,n).

PREREQUISTES

- CROSS SECTION calculated according to R-Matrix theory from the resonance parameters (E_r, Γ_n, Γ_γ, Γ_f) in several approximations (Single Level, Multi Level Breit Wigner, Reich-Moore).
- BAYES THEORY to perform the fitting procedure;
- SECONDARY EFFECTS: Flux Normalization, Doppler Effect, Beam Resolution, Self Shielding and Multiple Scattering;
- UNIX/LINUX minimal practice.

INSTALLATION

- 1 tar FILE (sammy-7.0.0.tar) for the installation:
  - `tar -zxf sammy-7.0.0.tar`
  - `cd sammy-7.0.0`
  - `configure`
  - `make`
  - `make install`

  Works Fine on Fedora 6 (or larger) or Scientifix Linux, and gcc version >= 4.0. Available in several UNIX environment. See File INSTALL if you have not the privileges of ADMINISTRATOR.
- Other 2 tar FILES: EXCERSISES (samexm-7.0.0.tar), and TEST CASES (samtry-7.0.0.tar).

ENVIRONMENT

- Add the path of SAMMY executable in your UNIX/LINUX environment to the variable $PATH.
- For BASH-shell in FILE ".bash_profile"
  - `export $PATH:/…/sammy-7.0.0/bin`
- For C-shell in FILE ".cshrc"
  - `set path = ($path /…/sammy-7.0.0/bin)`

STRUCTURE of FILES

- Main INPUT files of 3 types (258): DATA (.dat), PARAMETERS (.par), COMMANDS (.inp).
- .inp 11 Cards (260). Indicate the statements to perform the fit, the spin and channel assignment, miscellaneous;
- .par 16 Cards (329). Provide the Resonance Parameters, Errors, Neutron Beam resolution, Normalization, the Isotopic Composition;
- .dat 2 formats (374). Cross section or Experimental Yield have to be provided;

INPUT CARD FORMAT

Available on Manual Pages 260 – 328

C:L	P,T	Variable name	Meaning (units)	Note
1:1	1-80, A	TITLE		
2:1	1-10, A	ELMNT	Sample element's name	
	11-20, F	AW	Atomic weight (amu)	
	21-30, F	EMIN	Minimum energy for this data set (eV)	These values for E
	31-40, F	EMAX	Maximum energy (eV)	EMAX will be igr are given in the in (see Section VI.E)
	41-45, I	NEPNTS	1. Number of points to be used in generating artificial energy grid (default = 10001) 2. Maximum number of points to be analyzed at one time (default = 500). Use of this option is discouraged.	1. See Section V discussion of t energy grid. 2. NEPNTS is th data points to each region wl DATA INTO specified in card set 3.
	46-50, I	ITMAX	Number of iterations (default = 2)	Use a negative number for values > 9; see Section IV.A.3 for details.
	51-52, I	ICORR	Correlations smaller than this value (divided by 100) are not to be printed. $0 \le ICORR \le 100$ Default = 50	ICORR is ignored unless the phrase "DO NOT PRINT SMALL Correlation coefficients" occurs in card set 3. ICORR relates only to what is printed in SAMMY.LPT, not to what is used in calculations.

```
Example # 004
element         10.000  200.    1200.
use csisrs format for data
do not suppress any intermediate printout
broadening is not wanted
generate odf file automatically

    2.9080
capture
  1       1     0  0.5         1.0    .0
    1     1     0    0         0.5
  2       1     0 -0.5         1.0    .0
    1     1     0    1         0.5
  3       1     0 -1.5         1.0    .0
    1     1     0    1         0.5
```

PAR CARD FORMAT

- Manual Available on pages 329-373;

```
  -1.50000    66.00000      .06000                    0 0 0      1
  18.00000    70.00000    10.00000                    0 0 1      2
  27.00000    80.00000   300.00000                    0 0 1      2
  40.60000    68.00000     2.50000                    0 0 0      2
  46.08000    69.00000   154.00000                    0 0 0      2
  47.80000    78.00000   115.00000                    0 0 0      1
  65.50000   103.00000     2.50000                    0 0 0      2
 101.30000    65.00000   240.00000                    0 0 0      1
 103.80000    66.00000     3.00000                    0 0 0      2
 137.80000    75.00000    10.80000                    0 0 0      1
```

Card set	Alphanumeric header line	No
1		Resonance paramet line; card set ends i
2		Fudge factor for de no header line, no b
3	EXTERnal R-function parameters follow	Only one of card se permitted.
3a	R-EXTernal parameters follow	
4	BROADening parameters may be varied	
5	UNUSEd but correlated variables	Card set is created by SAMAMR run.
6	NORMAlization and background	
7	RADIUs parameters follow (two versions: usual for fewer than 99 channels and spin groups, alternative version for greater than 99 channels or spin groups.	Card set 7a is the preferred method.
7a	RADII are in KEY-WORD format or CHANNel radius parameters follow	

```
RPI RESOLUTION PARAMETERS FOLLOW
burst0        210.000     21.000
TAU  00000      326.      0.025      323.      0.029      240.
TAU
LAMBD000       687.0     -225.0     21.00
LAMBD
A1   00000  -.000990      0.0240  -.000630     3.530  0.001030
A1
EXPON00000      950.    -65.640      0.005   0.39400   0.00080
EXPON
CHANN 0        1.139 16000.000      5.100
CHANN 0       42.064   500.000      0.160
CHANN 0      447.072   125.000      0.040
```

DATA CARD FORMAT

- Manual Available on pages 261-

```
13.500000   .99899149 0.02497479
13.750000   .99892944 0.02497323
14.000000   .99885726 0.02497143
14.250000   .99877232 0.02496931
14.500000   .99867123 0.02496678
14.750000   .99854904 0.02496373
15.000000   .99839842 0.02495996
15.250000   .99820852 0.02495521
15.500000   .99796200 0.02494905
15.750000   .99763000 0.02494075
16.000000   .99716127 0.02492903
16.250000   .99645662 0.02491141
16.500000   .99530137 0.02488253
16.750000   .99315226 0.02482881
17.000000   .98814762 0.02470369
```

Line	Column	Variable	Format	Meaning
1	1-10	VARDAT(1,1)	F10.1	Variance for data point 1
2	1-10	VARDAT(2,1)	F10.1	Covariance between data points 1 and 2
	11-20	VARDAT(2,2)	F10.1	Variance for data point 2
3	1-10	VARDAT(3,1)	F10.1	Covariance between data points 1 and 3
	11-20	VARDAT(3,2)	F10.1	Covariance between data points 2 and 3
	21-30	VARDAT(3,3)	F10.1	Variance for data point 3
4	1-10 ...	VARDAT(4,1) etc.	F10.1	
...				
Last	1-10 ...	VARDAT(Last,1) etc.	F10.1	

EXCERSISE #1

- Look at: …/sammy-7.0.0/samexm/ex001
- Run the simple case;
- Make the plot
- Add a resonance.

EXCERSISE #2

- Look at: …/sammy-7.0.0/samexm/ex002
- RUn the Case
- Run bombs! Why?
- Make the change and run again.

EXCERSISE #4

- Look at: …/sammy-7.0.0/samexm/ex004
- Spin of the Resonance wrong?
- Change the spin of a resonance
- Insert the new sping group

EXCERSISE #5

- Look at: …/sammy-7.0.0/samexm/ex005
- Temperatures wrong?
- Parameter of the resonance wrong?
- How to compare the relative cases?

EXCERSISE #8

- Look at: …/sammy-7.0.0/samexm/ex008
- Introduction to beam resolution
- RPI function
- Another example (ORR function) is provided in Ex. 7.

EXCERSISE #9

- Look at: …/sammy-7.0.0/samexm/ex009
- Normalization
- Background

EXCERSISE #12

- Look at: …/sammy-7.0.0/samexm/ex012
- Isotopic Mass Composition Transmission.

EXCERSISE #13

- Look at: …/sammy-7.0.0/samexm/ex013
- Bayes Method to vary the prior values of the parameters.

EXCERSISE #15

- Look at: …/sammy-7.0.0/samexm/ex015
- Simultaneous Vs Sequential Fit.
- To improve this feature see Exc. 16 & 17.

EXCERSISE #18

- Look at: …/sammy-7.0.0/samexm/ex018
- How to deal with Covariance Matrix.

EXCERSISE #19

- Look at: …/sammy-7.0.0/samexm/ex019
- Self Shielding and Multiple Scattering Correction.

EXCERSISE #20

- Look at: …/sammy-7.0.0/samexm/ex020
- INtegral Quantities
- Unbroadened Cross Section

EXCERSISE #24

- Look at: …/sammy-7.0.0/samexm/ex024
- The LADDER program is used to create a pseudo SAMMY resonance
- parameter file, where the parameters are chosen from a particular
- pdf (probability density function) such as Wigner, Porter-Thomas,
- or Chi-squared distribution.

EXCERSISE #25

- Look at: …/sammy-7.0.0/samexm/ex025
- SAMDIST Program to calculate average quantities of
- D0, G_g, G_N, G_f.

EXCERSISE #27

- Look at: …/sammy-7.0.0/samexm/ex027
- SAMMY can read directly from File 2 of an ENDF file,