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Workshop on

Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

13 March - 14 April 2000

Miramare - Trieste, Italy

Resonance Parameter Analysis with SAMMY

N. M. Larson
Oak Ridge National Laboratory
Oak Ridge, USA

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Dr. Nancy M. Larson
Oak Ridge National Laboratory

Information Please

- To join the SAMMY users' group, visit the web site
  http://www.nea.fr/html/dbdata/sammy.htm
  and fill out the registration form.

- To add you name to the distribution list for ORNL/TM and other reports from the
  Nuclear Data Group (Luiz Leal, Group Leader),
  Radiation Information Analysis Section (Bob Roussin, Section Leader),
  Computational Physics and Engineering Division,
  Oak Ridge National Laboratory
  send e-mail to **nml@ornl.gov** with your return address (include both e-mail and regular mail addresses)

- For those without e-mail, my address is
  Dr. Nancy M. Larson
  Oak Ridge National Laboratory
  Building 6011 MS 6370
  P O Box 2008
  Oak Ridge, TN 37831-6370 USA

- Also please note the Nuclear Data Group web site:
  http//www.cad.ornl.gov/~jzw/NUCDATA/NDgroup.html

  and NML homepage:
  http://www.cad.ornl.gov/~jzw/NUCDATA/STAFF/nml.html

SAMMY WORKSHOP

ICTP March 2000

N. M. Larson

SAMMY References

Users' Manual:

- N. M. Larson, *Updated Users' Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-9179, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (August 1984)
- First revision ORNL/TM-9179/R1 (July 85)
- Second revision ORNL/TM-9179/R2 (June 1989)
- Third revision ORNL/TM-9179/R3 (Sept. 1996)
- Fourth revision ORNL/TM-9179/R4 (Dec. 1998)
- Fifth revision to be published mid-2000

Other documents:

- "Introduction to the Theory and Analysis of Resolved (and Unresolved) Neutron Resonances via SAMMY," N. M. Larson, Proceedings the IAEA Workshop on "Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety" held at the International Centre for Theoretical Physics, Trieste, Italy, 23 February - 27 March 1998, published 1999. Also published as ORNL/M-6576, July, 1998.
- "Covariance Matrices for Use in Criticality Safety Predictability Studies," H. Derrien, N. M. Larson, L. C. Leal, ORNL/TM-13492 (September 1997).
- "Integral Data Analysis for Resonance Parameters Determination," N. M. Larson, L. C. Leal, H. Derrien, ORNL/TM-13495 (September 1997). Also *Nucl. Sci. and Eng.* **131** 254 (February 1999).
- "SAMDIST: A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters", L. C. Leal & N. M. Larson, ORNL/TM-13092 (September 1995).
- "Doppler Broadening Revisited," N. M. Larson, M. C. Moxon, L. C. Leal, H. Derrien, ORNL/TM-13525 (January 1998).
- "Derivation and Implementation of Multiple-Scattering Corrections for Capture and Fission Yields," N. M. Larson, in preparation.
- "Merger of Nuclear Data with Criticality Safety Calculations," N. M. Larson, L. C. Leal, H. Derrien, *Sixth International Conference on Nuclear Criticality Safety*, September 20-24, 1999, Versailles, France.
- "Representation and Processing of Covariance Matrices for Resonance Parameters," N. M. Larson, *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies*, Brookhaven National Laboratory, 22-23 April 1999.

How to obtain the SAMMY code and/or manual

USA Contact

Radiation Safety Information Computational Center
(RSICC)
formerly, Radiation Shielding Information Center (RSIC)
P.O. Box 2008, Oak Ridge, TN 37831-6362 USA

on the web at http://www-rsicc.ornl.gov/rsic.html
telephone at 865-574-6176

Note: "package name" = "SAMMY"
"ID number" = "PSR-158"

European Contact

The OECD Nuclear Energy Agency
Le Seine-St Germain
12, boulevard des Îles
F-92130 Issy-les-Moulineaux, France

Telephone: (33) 1 45 24 10 10
Fax: (33) 1 45 24 11 10
on the web as: http://www.nea.fr/html/dbprog

Biographical Information for Nancy Larson, author of SAMMY code

- PhD, Michigan State University, 1972 (three-body problem)
- Senior Research Staff Member at Oak Ridge National Laboratory (ORNL), 1972-present (part time from 1976 to 1996, currently full time)
- Working on SAMMY since ~1977
- Husband Duane Larson is director or ORELA
- For additional information, visit the web site

IMPORTANT

Nancy has a tendency to speak rapidly; if she should succumb to this habit, please tell her immediately so that she can slow down and you can understand her!

SAMMY Overview

- Is used for analysis of neutron-induced time-of-flight cross-section data in resolved-resonance region, also unresolved-resonance region, integral data
- Uses Bayes' method (generalized least squares) to find parameter values & covariances.
- Uses Reich-Moore approximation to R-matrix theory (default) or multi- or single- level Breit Wigner theory.
- Treats most types of (energy-differential) cross sections.
- Treats (energy- and angle- differential) angular distributions of scattering.
- Treats integral data such as Westcott's g-factor, resonance integral, K1, etc.
- Properly treats samples which contain a mixture of different nuclei (e.g., chemical combinations such as oxides; multiple isotopes; contaminants).
- Includes three options for free-gas model of Doppler broadening, one approximate and two "exact".

- Includes three distinct descriptions of resolution broadening, each of which has several variable parameters.
- Includes self-shielding and multiple-scattering corrections for capture or fission yields.
- Has the ability to reconstruct an energy grid sufficiently dense to properly represent any cross section (but user must exercise caution!).
- Includes an option to generate energy-averaged cross sections and/or Maxwellian (stellar) averages of capture cross sections. Bondarenko narrow-resonance approximation will be available in the next release.
- Has several options for input of experimental data and/or values for resonance parameters.
- Has user-friendly operator commands.
- Contains numerous options for normalization, background corrections, etc.
- Has isolated constant values for physical and mathematical constants in one site within the code to ensure consistency.
- Provides output in ENDF File2 format, with maximum possible number of significant digits.

Example of INPut file

```
Test case number 75 -- mock U235
      u235      235.   2.0     4.
print theoretical values
print varied input parameters
CSISRS
do not suppress any intermediate
values
generate plot file automatically
USE NEW SPIN GROUP FORMAT

   300.0
   9.602
fission
        3.5          0.    0    1
  1       1    2  3.0         1.0  3.5
    1     1    0    0       3.000
    2     0    0    0       3.000
    3     0    0    0       3.000
  2       1    2  4.0         1.0  3.5
    1     1    0    0       4.000
    2     0    0    0       4.000
    3     0    0    0       4.000
```


The PARameter File

1. Values for resonance parameters:
   - resonance energy
   - capture width
   - neutron width
   - other widths: inelastic, fission, ...

2. Values for other parameters:
   - effective temperature
   - resolution parameters
   - normalization & backgrounds
   - nuclear radii
   - nuclide abundances
   - etc.

3. A priori uncertainties on all parameter values

4. Flags to indicate which parameter values are to be varied and which held fixed

Example of PARameter file

Energy in eV	Γ_γ in meV	Γ_n in meV	Γ_α in meV	Γ_p in meV	flags
-2.0383E+03	3.3792E+01	1.9703E+01	-4.6652E+01	-1.0088E+02	0 0 0 0 0 1
-1.8121E+03	3.7445E+01	8.5740E-01	7.3617E+02	-7.4187E+02	0 0 0 0 0 1
-1.5862E+03	3.4439E+01	8.2845E+00	1.5365E+02	-9.9186E+01	0 0 0 0 0 1
-1.3575E+03	3.8506E+01	5.0787E+01	-1.6914E+02	-3.8622E+02	0 0 0 0 0 1
-1.1321E+03	3.9794E+01	1.7144E+03	4.7701E+02	-4.6937E+02	0 0 0 0 0 2
-7.2239E+02	3.6122E+01	2.5036E+03	7.7494E+02	-8.3009E+02	0 0 0 0 0 2
-5.1588E+02	3.8030E+01	2.9884E+03	8.1285E+02	-8.1805E+02	0 0 0 0 0 1
-3.2436E+02	3.8934E+01	1.5196E+02	7.6083E+02	-7.7511E+02	0 0 0 0 0 2
-7.4766E+01	5.2085E+01	3.8375E+02	-8.6440E+02	-7.8652E+02	0 0 0 0 0 1
-3.4098E+00	3.7807E+01	8.5218E-05	-6.8909E+00	1.2977E+01	0 0 0 0 0 1
-2.6993E+00	4.7012E+01	5.6422E+00	2.3596E+02	-1.0107E+02	0 0 0 0 0 2
-1.5027E+00	3.7237E+01	8.7360E-05	-7.2798E+00	1.2287E+01	0 0 0 0 0 1
-9.4548E-01	4.9404E+01	5.7502E-02	1.3397E+03	-2.6963E+00	0 0 0 0 0 1
-1.6052E-01	1.5678E+01	1.1942E-02	1.4586E+01	-8.8782E+00	0 0 0 0 0 2
3.6575[illegible]	4.0000E+01	6.4608E-08	-5.0912E-01	9.3536E-01	0 0 0 0 0 2
.3018[illegible]	4.0705E+01	4.8608E-03	1.2139E+02	1.9661E-01	1 1 1 1 1 1
1.13257[illegible]	3.1770E+01	1.4131E-02	9.8006E-02	1.2898E+02	1 1 1 1 1 2
1.3086[illegible]	4.5120E+01	1.9938E-04	-1.8055E-01	1.8730E+01	1 1 1 1 1 2
2.0[illegible]	3.8027E+01	9.2671E-03	-9.8491E+00	9.3994E-01	1 1 1 1 1 1
2.[illegible]	4.1413E+01	6.6991E-04	1.2854E+02	-1.5081E-01	1 1 1 1 1 2
3.14738[illegible]	4.4826E+01	2.4926E-02	-1.8744E+01	8.7105E+01	1 1 1 1 1 1
3.614400625	3.6904E+01	4.3883E-02	-5.1667E+01	-6.5359E+00	1 1 1 1 1 2
4.850314617	3.7288E+01	5.1995E-02	-1.3173E-01	-4.4703E+00	1 1 1 1 1 2
5.440935612	4.0000E+01	2.4099E-02	-3.0152E+02	-2.0229E+02	1 1 1 1 1 2
6.171471119	4.0000E+01	6.4725E-02	-5.6557E+01	1.5807E+02	1 1 1 1 1 1
6.38[illegible]	3.8969E+01	2.3809E-01	8.4392E-01	1.0962E+01	1 1 1 1 1 2
7.08[illegible]	4.8348E+01	1.1299E-01	3.8625E+00	-3.0033E+01	1 1 1 1 1 2
7.63[illegible]	4.0000E+01	3.0291E-03	5.8333E+01	1.0432E+02	1 1 1 1 1 1
8.76[illegible]	3.3644E+01	9.1148E-01	8.2604E+01	-1.7267E+01	1 1 1 1 1 2
8.87012[illegible]	4.2250E+01	1.5194E-01	-2.3774E+02	9.8369E+01	1 1 1 1 1 1
9.271508217	3.7053E+01	1.1546E-01	3.6473E+01	3.5471E+01	1 1 1 1 1 2
9.705396652	4.0000E+01	3.9228E-02	-3.9107E+00	-2.1639E+02	1 1 1 1 1 1
10.16225243	3.5420E+01	4.6146E-02	4.0219E-04	-5.7414E+01	1 1 1 1 1 2
10.64940071	4.0000E+01	6.4711E-03	-7.0937E+00	-2.7133E+02	1 1 1 1 1 1
11.[illegible]6488934	3.9232E+01	5.0092E-01	1.8671E+00	4.0165E+00	1 1 1 1 1 2
12.38597393	4.0000E+01	1.8982E-01	3.0890E+00	6.9333E+01	1 1 1 1 1 2
12.38910770	4.1078E+01	1.1835E+00	3.1303E+01	-1.5675E+00	1 1 1 1 1 1
12.83880138	3.5900E+01	6.4661E-02	2.4479E+00	1.3452E+02	1 1 1 1 1 2
13.25238991	2.9042E+01	6.3798E-02	-6.6914E+01	1.4372E+02	1 1 1 1 1 2
13.59823513	4.0000E+01	9.1267E-02	-4.3150E+00	-3.5653E+02	1 1 1 1 1 1
13.97505856	4.0000E+01	3.5379E-03	-5.4776E+01	1.0840E+02	1 1 1 1 1 2
13.99681473	2.2570E+01	4.4249E-01	-3.6071E+02	1.4590E+02	1 1 1 1 1 1
14.55182934	4.0794E+01	1.2259E-01	7.4960E+00	1.2983E+01	1 1 1 1 1 1
15.41108990	4.2319E+01	2.0811E-01	-2.5089E+01	2.7595E+01	1 1 1 1 1 2
16.08851242	3.7185E+01	3.2503E-01	7.9401E+00	1.5682E+01	1 1 1 1 1 2

Another Example of PARameter file

```
3.000000000 5.0    E+01 3.0000E-02-4.     E+01 6.5    E+01 1 1 1 1 1 1

0.50
```

And Another

```
-1.0400E+02 1.2000E+02 3.3200E+02                                  0 0 0      1
  1617.0000 8.0000E+01 2.8087E+02                                  1 1 0      1

 0.99
RADIUS PARAMETERS FOLLOW
   5.14000   5.14000 0 0 1 2 3

ISOTOPIC MASSES AND ABUNDANCES FOLLOW
133.904495 0.8420600 0.0000500 0 1 2 3

BROADENING PARAMETERS FOLLOW
  5.140000   300.000  0.001135  0.020000  0.020000  0.000000 0 0-2 0 0 0

ORRESolution function parameters follow
BURST 0          7.000      1.000
WATER 0004       3.614     -0.089      0.037
WATER 0004       0.050      0.002      0.001
LITHI 000        1.000      0.692      1.000
LITHI            0.100      0.000      0.100
CHANN 0          7.482   4096.000      0.100
CHANN 0         14.611   1024.000      0.100
CHANN 0         27.949    512.000      0.100
CHANN 0         58.712    256.000      0.100
CHANN 0        116.675    128.000      0.100
CHANN 0        224.719     64.000      0.100
CHANN 0        415.621     32.000      0.100
CHANN 0       1089.655     16.000      0.100
CHANN 0       3672.072      8.000      0.100
CHANN 0       6540.650      6.000      0.100
CHANN 0      21321.801      4.000      0.100
CHANN 0      59782.000      2.000      0.100

NORMAlization and "constant" background follow
 1.0000000 4.695E-03 0.385      0.000E+00 0.000E+00 0 0 0 0 0 0
```

SAMPLE "LPT" FILE

```
*** M. SAMMY        8- 1-97 ***
Name of user's input file:                                          <<<
   t??sam.inp
Name of user's parameter file:                                      <<<
   t??sam.par
generate plot file a
Name of user's experimental data file is:                           <<<
   t??sam.dat

*********** READY TO RUN SAMOLF *********
                                                    CPU =      .16 sec
### Estimated array size for SAMMY-OLF is      144 ###
                                                    CPU =      .07 sec
*********** READY TO RUN SAMMY VERSION M2 *********

                                                    CPU =      .04 sec
### Estimated array size for SAMMY-INP is      122 ###

*********************************************************************
*****                                                           *****
*****   u235 dummy case                                         *****
*****                                                           *****
*********************************************************************

 Input quantities from card number 2 are:
  sitea1, altomz   ##      u235##       Atomic Weight =   235.0
  energy range =         2.000            4.000
  npoints,itmax,icorr,nxtra,iptdop,iptwid,ixxchn=    0 0  0  0  0  0          0
 adjusted - itmax,icorr,nxtra,iptdop,iptwid     =       2 50  0  4  5


TARGET ELEMENT IS        u235
ATOMIC WEIGHT IS  235.000


*********** Alphanumeric Control Information *********

 ssl??

PRINT THEORETICAL VALUES
PRINT VARIED INPUT PARAMETERS
DO NOT suppress any
use obsolete spin group format
OLF FILE IS WANTED--SAMMY.ODF ,ZERO TH ?
PRINT BAYES CHI SQUARED
SOLVE BAYES EQUATIONS
CHI SQUARED IS WANTED

**** End of Alphanumeric Control Information *********


 EFFECTIVE TEMPERATURE= 300.00000
   FLIGHT PATH=      .00000 METERS +/-      .0000072 METERS
     DELTAE=         .000000    DELTAG=        .00000
     deltt=          .00000     ELOWBR=      .00000000

CHANNEL RADIUS=    9.602
TARGET THICKNESS=     .0000E+00

 Finished

 TARGET SPIN=   3.5
```



```
           # of  # of
group entr  exit  spin*  chan LPENT ISHIFT LSPIN CHSPIN  ENBND     ECHAN
  #   chan  chan abndnc   #
  1    1     2     .438   1     1      0     0     3.0  0.00E+00  0.00E+00
                          2     0      0     0      .0  0.00E+00  0.00E+00
                          3     0      0     0      .0  0.00E+00  0.00E+00
  2    1     2     .562   1     1      0     0     4.0  0.00E+00  0.00E+00
                          2     0      0     0      .0  0.00E+00  0.00E+00
                          3     0      0     0      .0  0.00E+00  0.00E+00


### Array size used for SAMMY-INP is      110 ###
                                                    CPU =      .09 sec
### Estimated array size for SAMMY-PAR is      234 ###

Total  number of resonances is    1
Number of particle channels is    3
Number of varied parameters is    5
Number of spin groups is          2
### Array size used for SAMMY-PAR is      223 ###
                                                    CPU =      .10 sec
### Estimated array size for SAMMY-NEW is      237 ###


*****INITIAL VALUES FOR PARAMETERS

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G=  .4375
                 "true" radius =  9.6020E+00        9.6020E+00        9.6020E+00
             effective radius =  9.6020E+00        9.6020E+00        9.6020E+00

     ENERGY         GAMMA-           GAMMA-            GAMMA-             GAMMA
                    GAMMA          CHANNEL 1         CHANNEL 2          CHANNEL 3
                                 L=0  SPIN= 3.0    L=0  SPIN=  .0     L=0  SPIN=  .0
      (eV)        (MILLI-EV)      (MILLI-EV)        (MILLI-EV)         (MILLI-EV)
 3.00000E+00(  1) 5.0000E+01(  2) 3.0000E-02(  3) -4.0000E+01(  4)  6.5000E+01(  5)


   RADIUS         TEMPERATURE      THICKNESS
 9.6020E+00       3.0000E+02       0.0000E+00

   DELTA-L         DELTA-T-GAUS     DELTA-T-EXP
 0.0000E+00       0.0000E+00       0.0000E+00


***** CORRELATION MATRIX FOR INPUT PARAMETERS


***** STANDARD DEVIATION (SORT OF DIAGONAL OF COV MATRX)
       STD. DEV.              STD. DEV.              STD. DEV.             STD. DEV.
(  1)  8.6638E-02   (  2)   25.00        (  3)  1.5000E-02   (  4)   20.00
(  5)    32.50
### Array size used for SAMMY-NEW is      242 ###
                                                    CPU =      .1. sec

    Emind        Emins        Eminr        Emin
  1.854        2.000        2.000        2.000
    Emax         Emaxr        Emaxs        Emaxd
  4.000        4.000        4.000        4.214

Dopple. Width at Emin =  2.926815E-02 and at Emax =  4.273353E-02
### Estimated array size for SAMMY-DAT is  5833397 ###

Energy range of data is from 2.00000E+00 to 4.00000E+00 eV.
Number of data points is       41

Number of points in auxiliary grid =       46
### Array size used for SAMMY-DAT is  6999973 ###
### Array size used for SAMMY-DAT is      293 ###
                                                    CPU =      .13 sec
 ### Estimated array size for SAMMY-THE is      433 ###
Number of parameters affected by this data set=    5
### Array size used for SAMMY-THE is      433 ###
                                                    CPU =      .09 sec
### Estimated array size for SAMMY-XCT is     1254 ###
### Array size used for SAMMY-XCT is     1192 ###
```

```
                                                    CPU =       .02 sec
### Estimated array size for SAMMY-FGM is      1053 ###
npnts =     46
### Array size used for SAMMY-FGM is      1007 ###
                                                    CPU =       .03 sec

### Estimated array size for SAMMY-INT is       444 ###
 ***** THEORETICAL VALUES (broadnd,normed,...as required)

     ENERGY    THEORY          ENERGY    THEORY          ENERGY    THEORY
( 1)2.000000  .262501    ( 15)2.940000  18.4276    ( 29)3.136610  11.8208
( 2)2.100000  .314482    ( 16)2.960000  22.9661    ( 30)3.154915  9.54598
( 3)2.200000  .386072    ( 17)2.980000  27.5709    ( 31)3.173219  7.79310
( 4)2.300000  .488501    ( 18)3.000000  31.1462    ( 32)3.200000  5.92089
( 5)2.400000  .642406    ( 19)3.015000  32.4276    ( 33)3.250000  3.79555
( 6)2.500000  .889023    ( 20)3.025908  32.3971    ( 34)3.300000  2.60579
( 7)2.600000  1.32021    ( 21)3.030000  32.1712    ( 35)3.400000  1.43058
( 8)2.700000  2.18524    ( 22)3.034092  31.8331    ( 36)3.500000  .891233
( 9)2.800000  4.31323    ( 23)3.040796  31.0522    ( 37)3.600000  .604529
(10)2.843390  6.34194    ( 24)3.047500  30.0202    ( 38)3.700000  .434928
(11)2.865085  7.96804    ( 25)3.065000  26.4668    ( 39)3.800000  .326700
(12)2.886780  9.92321    ( 26)3.092500  22.3460    ( 40)3.900000  .253654
(13)2.900000  11.5228    ( 27)3.100000  18.3549    ( 41)4.000000  .200079
(14)2.920000  14.5637    ( 28)3.118305  14.7390
### Array size used for SAMMY-INT is       356 ###
                                                    CPU =       .10 sec

KNPV,KIPQ,KMPW       563       493       205
                                                    CPU =       .10 sec

USE (I+Q) INVERSION SCHEME
### Estimated array size for SAMMY-IPQ is       554 ###

CUSTOMARY CHI SQUARED =   45514.6
CUSTOMARY CHI SQUARED DIVIDED BY NDAT =    1110.11

BAYESIAN CHI SQUARED =     145.359     -     986224.     -     986078.
BAYESIAN CHI SQUARED DIVIDED BY NDAT =    3.54532
### Array size used for SAMMY-IPQ is       554 ###
                                                    CPU =       .03 sec
### Estimated array size for SAMMY-FIN is       399 ###

*****NEW VALUES FOR RESONANCE PARAMETERS

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G= .4375
                  "true" radius =  9.6020E+00       9.6020E+00       9.6020E+00
                effective radius =  9.6020E+00       9.6020E+00       9.6020E+00

    ENERGY          GAMMA-          GAMMA-          GAMMA-          GAMMA-
                    GAMMA           CHANNEL 1       CHANNEL 2       CHANNEL 3
                                    L=0  SPIN= 3.0  L=0  SPIN=  .0  L=0  SPIN=  .0
      (eV)          (MILLI-EV)      (MILLI-EV)      (MILLI-EV)      (MILLI-EV)
3.03038E+00(  1) 5.1323E+01(  2) 2.1759E-02(  3) -3.6825E+01(  4) 5.6754E+01(  5)
Expected
 Value        +/- 1.9523E+01  +/- 4.3865E-03  +/- 1.7201E+01  +/- 2.1152E+01
EV changed        0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
Parameters   +/- 0.0000E+00  +/- 0.0000E+00  +/- 0.0000E+00  +/- 0.0000E+00

  RADIUS          TEMPERATURE     THICKNESS
9.6020E+00        3.0000E+02      0.0000E+00

  DELTA-L         DELTA-T-GAUS    DELTA-T-EXP
0.0000E+00        0.0000E+00      0.0000E+00

 ***** CORRELATION MATRIX FOR OUTPUT PARAMETERS
  STD.DEV.  (REL.)   CORRELATION*100
                      1   2   3   4   5
1 5.6792E-05 .000 100
2  19.52     .380   0 100
3 4.3865E-03 .202   0 100 100
4  17.20     .467   0 -31 -31 100
5  21.15     .373   0 -66 -66 -51 100
```

```
***** RATIO OF UNCERTAINTIES ON VARIED PARAMETERS
       NEW/OLD              NEW/OLD              NEW/OLD              NEW/OLD
 (  1)   [illegible]E-04   (  2)   .[illegible]   (  3)   .2924    (  4)   .9601
 (  5)    [illegible]

***** RATIO OF UNCERTAINTIES ON VARIED U-PARAMETERS
       NEW/OLD              NEW/OLD              NEW/OLD              NEW/OLD
 (  1)   [illegible]E-04   (  2)   .[illegible]   (  3)   .3425    (  4)   .8964
 (  5)    [illegible]

### Array size used for SAMMY-FIN is       459 ###
                                                   CPU =       .13 sec
*********** READY TO RUN SAMMY VERSION M2 **********
                                                   CPU =       .09 sec
Name of binary parameter covariance file is:
   [illegible].COV                                                    <<<
### Estimated array size for SAMMY-INP is       172 ###

**********************************************************************
*****                                                            *****
*****   u-235 dummy case                                         *****
*****                                                            *****
**********************************************************************


Input quantities from card number 2 are:
  alfnel, alfnm2 - ##        u235##         Atomic Weight =    235.0
  energy range =         2.000             4.000
  ncpnts,itmax,icorr,nxtra,iptdop,iptwid,ixxchn=    0 0  0  0  6  9          0
  (default) - itmax,icorr,nxtra,iptdop,iptwid       =       2 50  0  9  5


TARGET ELEMENT IS          u235
ATOMIC WEIGHT IS   235.000


*********** Alphanumeric Control Information *********

options
PRINT THEORETICAL VALUES
DO NOT PRINT ANY INPUT PARAMETERS
do not suppress any
use obsolete spin group format
ODF FILE IS WANTED--SAMMY.ODF ,FINAL VAL
DO NOT PRINT BAYES CHI SQUARED
DO NOT SOLVE BAYES EQUATIONS
PRINT LS CHI SQUARED

**** end of Alphanumeric Control Information *********

EFFECTIVE TEMPERATURE= 300.00000
   FLIGHT PATH=      .00000 METERS +/-     .00000/2 METERS
     DELTAL=         .00000     DELTAG=        .00000
     deltte=         .00000     ELOWBR=     .00000000

CHANNEL RADIUS=     9.602
TARGET THICKNESS=    .0000E+00

fission

### Array size used for SAMMY-INP is       110 ###
                                                   CPU =       .11 sec
### Estimated array size for SAMMY-PAR is       234 ###

Total  number of resonances is      1
Number of particle channels is      3
Number of flagged parametrs is      5
Number of spin groups is            2
### Array size used for SAMMY-PAR is       223 ###
                                                   CPU =       .12 sec
```



```
### Estimated array size for SAMMY-OLD is       237 ###

Broadening (etc.) parameters actually used for this run
              Radius (CRFN) =     9.60200        9.60200       CYCRFN =  2.1003[illegible]
     Effective Temperature =    300.000        300.000            DO =  1.05338[illegible]
          Sample Thickness =   0.000000E+00   0.000000E+00
FLIGHT PATH LENGTH (DIST) =   0.000000E+00
                    DELTAL =   0.000000E+00   0.000000E+00      BO2 =  0.000000E+00
                    DELTAG =   0.000000E+00   0.000000E+00      AO2 =  0.000000E+00
                    DELTAE =   0.000000E+00   0.000000E+00      CO2 =  0.000000E+00
                                                                DO2 =   .000000E+00
### Array size used for SAMMY-OLD is       263 ###
                                                    CPU =       .05 sec
    Emind        Emins        Eminr        Emin
  1.854        2.000        2.000        2.000
    Emax         Emaxr        Emaxs        Emaxd
  4.000        4.000        4.000        4.214

Doppler Width at Emin =   .926815E-02 and at Emax =  4.273353E-02
### Estimated array size for SAMMY-DAT is  5833397 ###

Energy range of data is from 2.00000E+00 to 4.00000E+00 eV.
Number of data points is      41

Number of points in auxiliary grid =       46
### Array size used for SAMMY-DAT is  6999973 ###
### Array size used for SAMMY-DAT is       293 ###
                                                    CPU =       .07 sec
### Estimated array size for SAMMY-THE is       381 ###
### Array size used for SAMMY-THE is       381 ###
                                                    CPU =       .03 sec
### Estimated array size for SAMMY-XCT is       844 ###
### Array size used for SAMMY-XCT is       782 ###
                                                    CPU =       .07 sec
### Estimated array size for SAMMY-FGM is       622 ###
npnts =     46
### Array size used for SAMMY-FGM is       530 ###
                                                    CPU =       .06 sec
### Estimated array size for SAMMY-INT is       427 ###


***** THEORETICAL VALUES (broadnd,normed,...as required)
      ENERGY       THEORY           ENERGY       THEORY           ENERGY       THEORY
(  1)2.000000    .222991     ( 15)2.940000   15.5858     ( 29)3.136610   12.276
(  2)2.100000    .266693     ( 16)2.960000   20.0715     ( 30)3.154915   9.7254
(  3)2.200000    .326724     ( 17)2.980000   25.1854     ( 31)3.173219   7.8923
(  4)2.300000    .412342     ( 18)3.000000   29.9381     ( 32)3.200000   5.8120
(  5)2.400000    .540472     ( 19)3.015000   32.3733     ( 33)3.250000   3.61538
(  6)2.500000    .744747     ( 20)3.025908   33.1622     ( 34)3.300000   2.43523
(  7)2.600000   1.09956      ( 21)3.030000   33.2130     ( 35)3.400000   1.30785
(  8)2.700000   1.80508      ( 22)3.034092   33.1267     ( 36)3.500000   .804357
(  9)2.800000   3.52445      ( 23)3.040796   32.6945     ( 37)3.600000   .541189
( 10)2.843390   5.16214      ( 24)3.047500   31.9217     ( 38)3.700000   .387191
( 11)2.865085   6.40325      ( 25)3.065000   28.6099     ( 39)3.800000   .289660
( 12)2.886780   8.09625      ( 26)3.082500   24.2292     ( 40)3.900000   .224175
( 13)2.900000   9.43791      ( 27)3.100000   19.7435     ( 41)4.000000   .179191
( 14)2.920000  12.0643       ( 28)3.118305   15.6034
### Array size used for SAMMY-INT is       386 ###
                                                    CPU =       .09 sec

### Estimated array size for SAMMY-NPV is       100 ###

CUSTOMARY CHI SQUARED =    256.132
CUSTOMARY CHI SQUARED DIVIDED BY NDAT =     6.24712
### Array size used for SAMMY-NPV is        98 ###
                                                    CPU =       .05 sec
### Estimated array size for SAMMY-FIN is       342 ###
### Array size used for SAMMY-FIN is       205 ###
                                                    CPU =       .05 sec
                            Total time =      2.98 seconds
```

SAMMY.PAR

- In the same format as the input parameter file
- Contains updated parameter values, plus a message explaining the existence of a covariance file
- May be used as input for another SAMMY run

SAMMY.COV

- Binary file produced by SAMMY, contains
  - Covariance matrix for varied parameters
  - "Exact" values for all parameters
- May be used as input for another SAMMY run

SAMMY.ODF

- In ODF (ORELA Data Format) or "generic" binary (decision to be made by the system manager, depending on the plotting package used at your facility)
- To be used for making plots of data vs theory
- Contains:
  - Energy grid
  - Experimental data
  - Absolute uncertainties for experimental data
  - Initial calculated values for cross section (or whatever the data is)
  - Final calculated values for cross section (ditto)
- May also contain
  - Uncertainties on calculated values
  - Revised energy grid

What to do when SAMMY doesn't work?!

1. Do not panic -- this happens to **everybody**.

2. Is this run *really* the same as the one that worked last week? Think carefully -- *exactly* what did you change?

3. Look at the LPT file **in detail**.
   - Did SAMMY understand all of your instructions? *Maybe you had a typo.*
   - Is SAMMY using the same parameter values that you intended? *Maybe you had a typo. Look for factors-of-ten.*
   - Would additional information help? *Maybe you need to ask SAMMY to print out more initial values, or more intermediate steps.*
   - Did SAMMY give you an error message? *Look at the very end of the file.*

4. Can you simplify and/or isolate the problem?
   - Use a smaller energy range.
   - Vary fewer parameters.
   - Drop normalization & background options.
   - Do no broadening.

   Find the smallest case for which the error occurs, and try to understand what is unique about that case.

5. If the problem persists, ask for help!

Help is available

- Talk to your office-mate. *Maybe you've just been looking at it for too long, and someone else can see immediately what you can no longer see!*

- Talk to the most experienced SAMMY user in the neighborhood. *It does get easier with practice!*

- Talk to me at *nml@ornl.gov*

  - First, send information but not files. Describe the problem in some detail:
    What version of SAMMY are you using?
    What features are in use?
    Did the code bomb or just give wrong answers?
    In which module did the bomb occur?
    Does a minor perturbation of this case work properly?

  - When requested, send very small files from the simplest case which has the problem (as attachments if possible, otherwise as separate e-mail messages): command file, INPut file, PARameter file, and DATa file.

NOTE: If you find and fix a bug in your version of SAMMY, please tell me about it so I can fix it in my version!

ALSO: If you can suggest a more informative error message, I'd be happy to consider using it.

TUTORIAL

Number	Description of feature emphasized in this example
000	use of plotting package RSAP (or FORODF)
001	simple one-resonance non-fissile nucleus, capture experiment
002	fissile nucleus, several resonances, capture experiment
003	different kinds of cross sections
004	$\ell > 0$ (s, p, d waves); $I > 0$
005	Doppler broadening
006	resolution broadening (Gaussian)
007	resolution broadening (ORR)
008	resolution broadening (RPI)
009	normalization
010	backgrounds
011	more than one channel radius
012	multiple nuclides within a single sample
013	uncertainties on parameters
014	angular distributions
015	sequential vs. simultaneous fitting of data
016	sequential fitting of three data sets; parameter covariance matrix as input
017	several data sets; varying data-reduction parameters
018	data covariances (implicit and explicit)
019	self-shielding and multiple-scattering corrections to capture yields
020	integral quantities
021	almost real data: W transmission with many complications
022	almost real data: U235. How to do an evaluation
023	finding input errors
024*	ladder program for generating artificial resonance parameters
025*	samdist program for calculating statistical properties
026*	create ENDF File 2

* Not included with M2 release of SAMMY code

/samexm/README.FIRST

```
##########################################
General instructions:

Begin with example EX000 to learn how to
make plots using the plotting package rsap
(or forodf).

Begin learning to use the SAMMY code by
starting with Example EX001 in
subdirectory ex001, and progressing
through all examples in order from 1 to 23
(or more, if more exist by the time you
are reading this).

In each subdirectory read the README.FIRST
file to obtain instructions re what is to
be done for this example.
##########################################
```

/samexm/ex000/README.FIRST.rsap

NOTE: RSAP is not available at Trieste workshop

```
##############################################################################
Instructions for Example EX000:

This example is a mini-tutorial on how to use the new ORNL plotting
        package "rsap", developed by Royce Sayer.  This program will be
        used throughout this tutorial to produce graphics from SAMMY
        output files.  There may, however, be a need for other plotting
        packages as well; see the other README file for information on
        the older package "forodf".

Please note that rsap is still "under development", so your suggestions
        for improvements would be most appreciated!

To make a simple plot of the file ex000.odf, type the program name
        followed by the input stream as given in file rsap.inp.
Alternatively,
        type "rsap < rsap.inp" .  Either way, an X-terminal window should
        appear on your screen, containing a plot of experimental data with
        uncertainties, plus curves for initial and final cross sections
        (i.e., cross sections generated from original parameter values and
        from final parameter values.)

An explanation of the information in rsap.inp follows:

----

ev  2                          Energies are in eV in the ODF file.
par ex000.par                  The PARameter file is ex000.par.
odf ex000.odf                  The ODF (plot) file is ex000.odf.
tit This is Example 000        This is a title to be placed on the plot.
ops  1 1 0 1 1 1               These are options for plotting:
                                 nxp = number of frames in x-direction.
                                 nyp = number of frames in y-direction.
                                 kstack = number of plots per frame
                                   (default = 1) ["frame" = Energy-grid
                                   (which may have two separate plots)]
                                 kpoints=0 => histogram; =1 => curve.
                                 keres = 1 => show resonance energy on plot.
                                 kgamres = 1 => show resonance width on plot.
x                              The output device is an X-plot on the screen.
1 etb 9.0,11.0,0.,200.         Use the first plot file (but there's only
                                       one in this example);
                                 etb=> put data, errors, initial theory,
                                       and final theory on the plot;
                                 energy limits are 9.0 eV to 11.0 eV;
                                 vertical limits are 0 to 200 barns.
(blank)                        Blank line terminates info about this
                                 plot, and causes the plot to appear.
q                              Quit rsap.
```

Please see the file HELP.RSAP for additional details. Note that typing "h" while in rsap will provide the same information as in that file.

---

1. Try running the program "as is", then make modifications to the energy range or to the y-axis limits.

2. The error bars can be distractive; to get rid of them but keep all other information, change "etb" to "dtb".

3. Add a second frame on the same plot, this one containing the residuals. To do this, change kstack from 0 (=1 by default) to 2 in the "ops" line. Also add a second line of plotter commands, as "1 rb 9.0,11.0,-0.5,0.8"

4. To change from linear to log scale, add a line that says "log 1 0" for the x-axis, "log 0 1" for the y-axis, or "log 1 1" for both.

##

/samexm/ex000/README.FIRST.forodf

```
################################################################################
Instructions for Example EX000:

This example is a mini-tutorial on how to use the ORNL plotting package
        "forodf" to produce simple plots from SAMMY output plot files.
        Only the very basic features are covered here.

The following command stream will permit plotting of file ex000.odf.
        You will type lower-case characters; the code types the upper
        case.  Notes to the right of the page, in square brackets, are
        explanations.  Try the commands as-is first, then vary by changing
        energy-range, setting limits for y-axis, making log-log plots,
        etc...

-----------------
forodf                                                        [run the program]
 FILENAME 1=ex000.odf                                            [name of file]
 RUN 0 7 DATASETS 315 CHANNELS/DATASET MODE 3 (S1=E)
 FILENAME 2=                                                    [no more files]

 *** FORCOM ***   8- 9-95
 TYPE EQUATION                                                    [use S1 for x]
/xsn1
 TYPE EQUATION                                          [print the first channel]
f1s2sc1
 1       .32540001E-01    .80466003E+01
 TYPE EQUATION                                  [print the last channel, # 315]
f1s2sc315
 315     .16050000E-01    .11953890E+02
 TYPE EQUATION                                       [set min x for plot = 8.00]
/xmin 8.00
 TYPE EQUATION                                       [set max x for plot =12.00]
/xmax 12.00
 TYPE EQUATION                                       [plot file 1 section 2 & 4]
dvt f1s2,f1s4                                                    [ends the plot]
carriage return
dvt /sym3 f1s2,/nosy f1s4          [plot file 1 S2 as symbols, S4 as line]
carriage return
dvt /sym3 f1s2,/nosy /dash0.1 f1s4, /nodash f1s5
          [plot file 1 S2 as symbols, S4 as dashed line, S5 as solid line]
carriage return                                                  [end the program]
stop
STOP
-----------------
```

```
Other useful commands:
/reset          [reset all "/" commands]
/ymin 0.01      [sets minimum y-value at 0.01]
/ymax 100.0     [sets maximum y-value]
/noymin         [resets ymin to default: program chooses ymin]
/noymax         [resets ymax]
/ylog           [plot y on log scale]
/noylog         [plot y on linear scale]
/xlog           [plot x on log scale]
/noxlog         [plot x on linear scale]
/ave3           [plots the average of three consecutive points]
stop            [get out of forodf]
------
```

It is possible to use "command files" to store frequently-used commands; the command file is then invoked by typing the "@" sign followed by the file name. For example, all of the initialization commands from the example above might be stored in a file named "x." (the period is necessary), then you can type @x (without the period) to execute, as illustrated below. Similarly, file "y." holds the plot command.

```
-----------------
forodf
 *** FORODF ***   8- 9-1995

 FILENAME 1=ex000.odf
 RUN 0 7 DATASETS 315 CHANNELS/DATASET MODE 3 (S1=E)
 FILENAME 2=

 *** FORCOM ***   8- 9-95
 TYPE EQUATION
@x                                                  [to initialize]
 TYPE EQUATION
@y                                                  [to make plot]

 *** FORPLT ***   8- 9-1995


 *** FORCOM ***   8- 9-95
 TYPE EQUATION
stop
STOP
-----------------
```

You will notice that forodf creates several temporary files in your area. So long as those are not deleted, any switches you may have set (e.g. /xmin8.0) remain active. Also, if you "stop" and then wish to re-enter forodf using the same file, typing "forcom" rather than "forodf" will put you directly into the "TYPE EQUATION" mode.

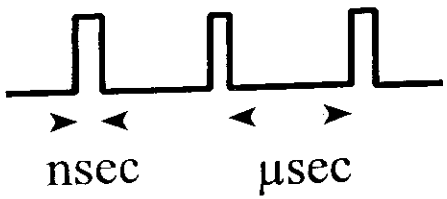
##

WORDS FREQUENTLY USED WITH A SAMMY RUN

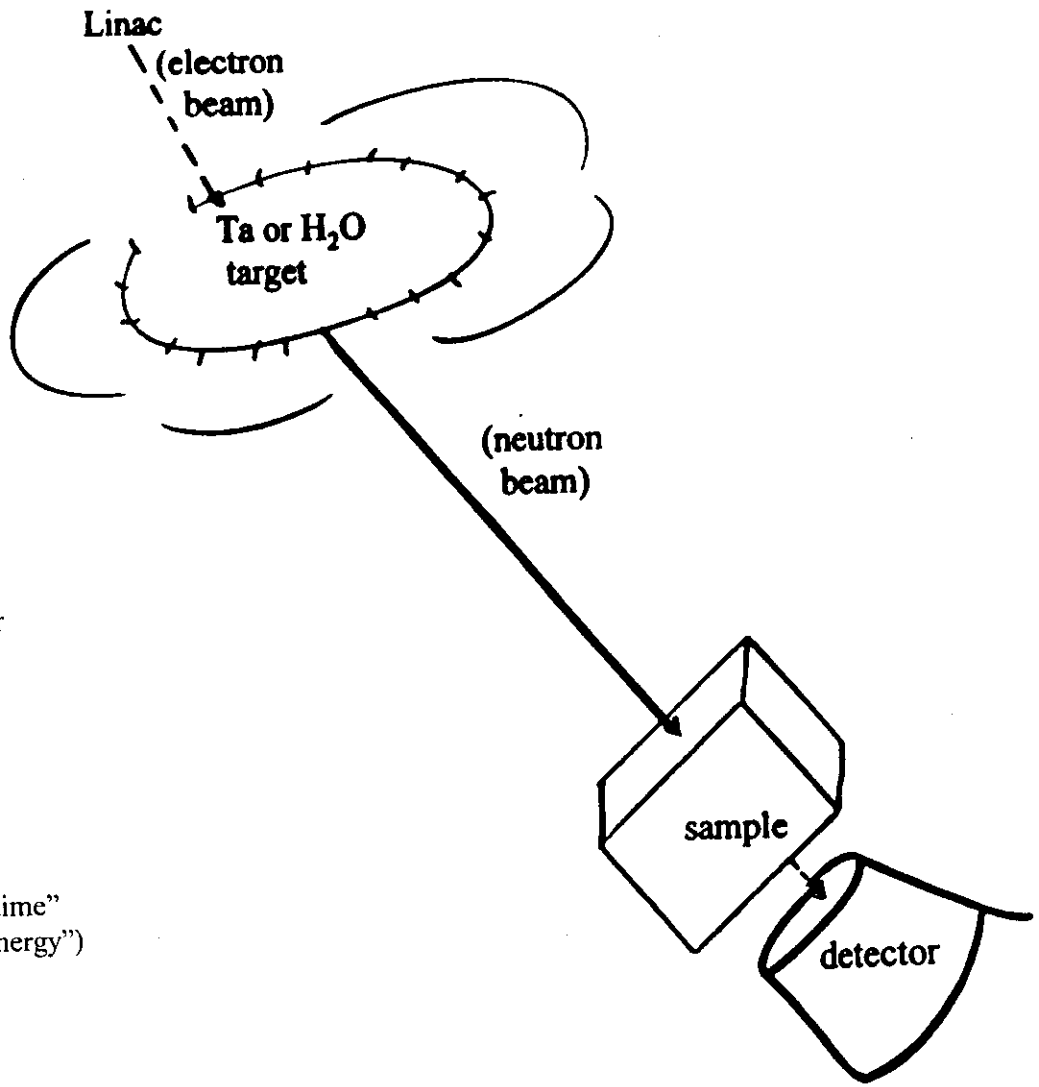
NO BAYES	run SAMMY with no parameter variation (i.e., just calculate the cross section, do not solve Bayes' equations for updated parameter values)
BAYES	run SAMMY and vary some parameters (i.e., solve Bayes' equations)
ODF file	also called "plot file"; binary file generated by SAMMY, from which plots can be made using either FORODF or RSAP
COV file	SAMMY output file which contains (among other things) the calculated parameter covariance matrix
INPut file	SAMMY input file which contains general information such as operator commands, spin and mass for the nuclides in the sample, spin group quantum numbers, etc.
PARameter file	file containing resonance parameters and any other parameters which are to be varied
DATa file	sometimes called "SAM file"; contains experimental data. Several formats are available for this file.
ENDF file	file in the ENDF/B-VI format
FGM	free gas model for Doppler broadening
HEGA	high-energy Gaussian approximation to the free gas model

Time of Flight Experiment

for measuring energy-dependent neutron cross sections



Linac e^- beam



- Measure path length L precisely
- Know time t_0 at which neutron leaves target
- Find time t at which neutron reaches detector
- Therefore know energy E:

$$E = \frac{m}{2}\left(\frac{L}{(t-t_0)}\right)^2$$

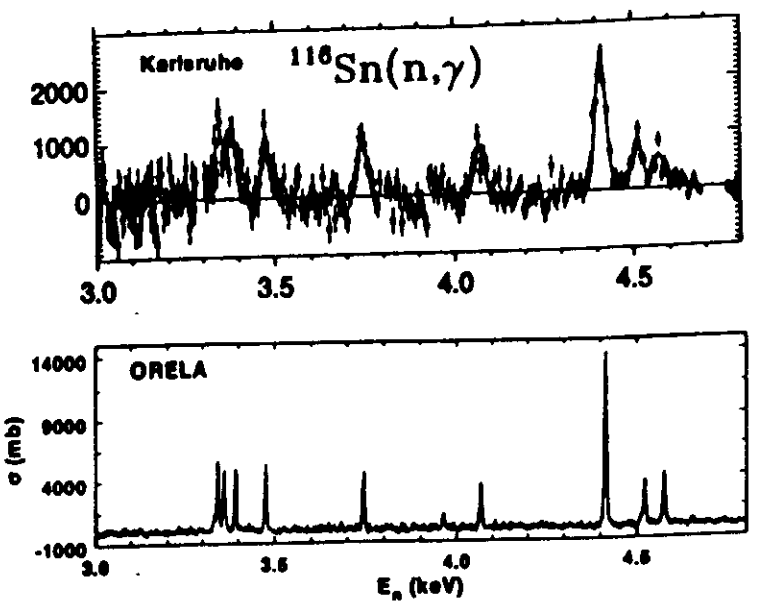
Data are "number of counts reaching detector" vs "time"
(i.e. vs "energy")

Time of Flight Experiments

measure energy-dependent neutron cross sections as follows:

- An accelerator produces a beam of electrons. (Usually this is a linear accelerator such as the Oak Ridge Electron Linear Accelerator (ORELA), the Geel LINAC (GELINA), or the Gaerttner LINAC at Rensselaer Polytechnic Institute.)
- The electrons hit a target (water and/or tantalum at ORELA, Uranium at GELINA).
- This produces neutrons, which fly straight outward in all directions. Shielding is used to collimate the beam.
- The neutrons are used as a probe to study nuclei. Samples of the material to be studied are placed in the beam line where neutrons will interact with nuclei in the sample.
- Detectors literally count the particles that reach them.
- Experimentalists "reduce" the "count" to a quantity which resembles a "cross section." This data-reduction process involves dead-time corrections, background subtraction, normalization, and a host of other operations.
- The next step is to interpret the results in terms of phenomenological scattering theory (R-matrix theory). ***The major emphasis of this class will be on this step.***

Typical ORELA Capture Data at 40 m



The impact of good time-of-flight (TOF) resolution at the example ^{116}Sn

Types of Differential Data

- transmission
- total cross section
- elastic cross section
  (angle-integrated or differential)
- fission
- inelastic
- capture
- absorption
- eta
- self-indication
- combinations of the above

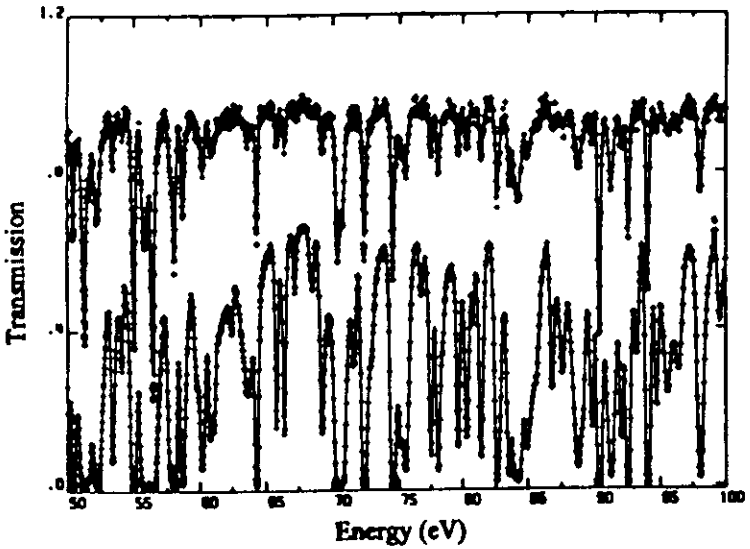
(SAMMY can accommodate all of these.
Other options can be added with relative ease.)

Types of Integral Data

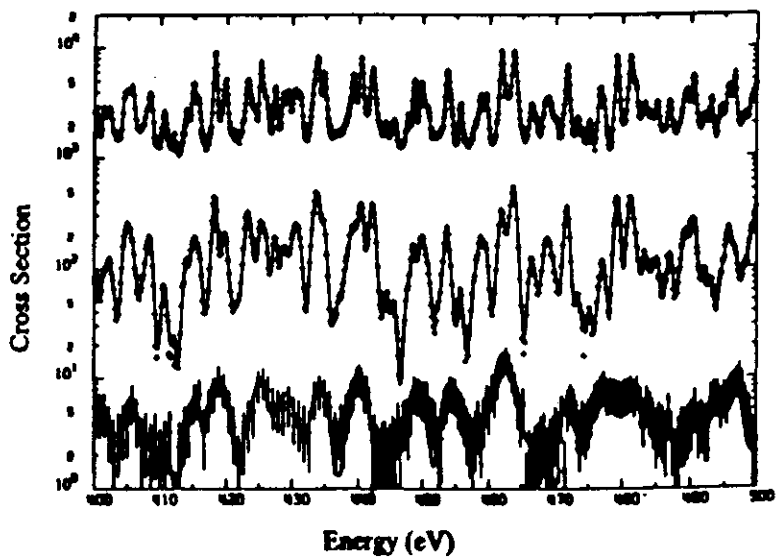
- Thermal cross section
- Average integral
- Maxwellian average
- $K1$, K_{eff}
- Westcott's g-factor
- α
- Resonance integral
- Reaction Rates
- NJOY's α
- NJOY's η

(To be discussed later in detail)

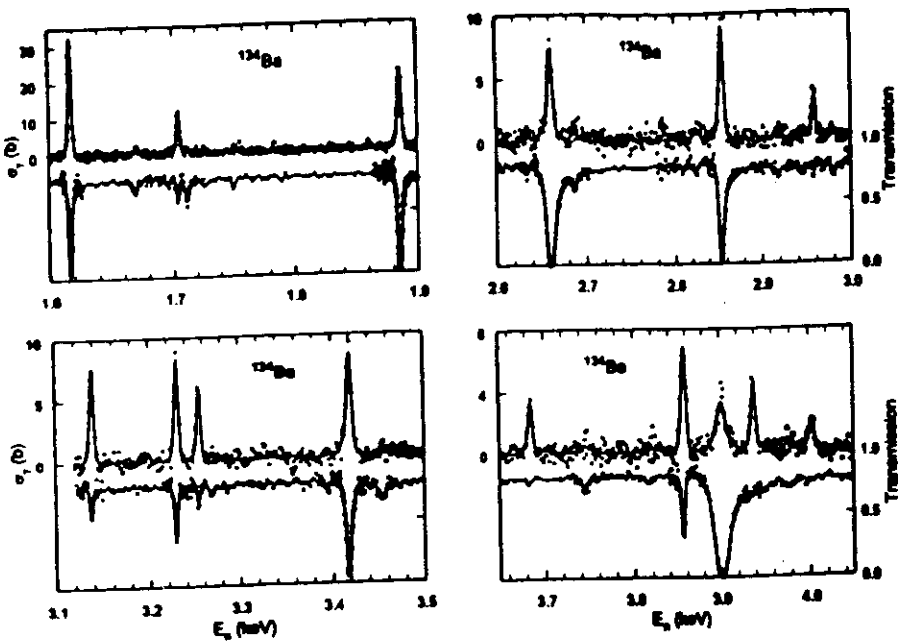
(SAMMY can accommodate all of these.
Other options can be added with relative ease.)



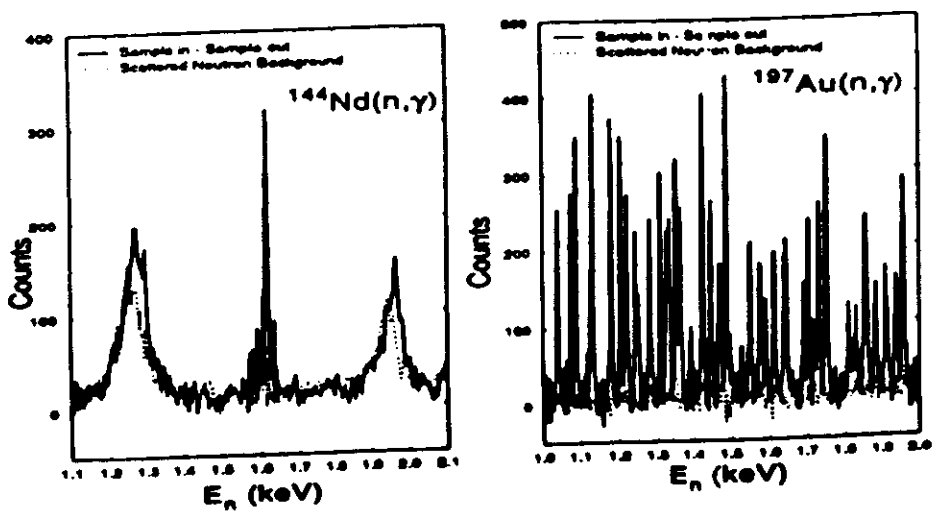
^{235}U experimental and calculated neutron transmission in the energy range from 50 to 100 eV. Results of the two sample thickness transmission experiments of Harvey et al. are displayed.



^{235}U experimental and calculated total cross section, fission cross section, and capture cross section in the energy range from 400 to 500 eV. Harvey et al. total cross section (multiplied by 100), Weston fission (multiplied by 10), and deSaussure capture cross sections are displayed.



Data (points) and SAMMY fits (solid curves) from capture (top) and transmission (bottom) measurements on ^{134}Ba. From "Resonance neutron capture and transmission measurements and the stellar neutron capture cross sections of ^{134}Ba and ^{136}Ba," P. E. Koehler et al., *Phys. Rev. C* 54 (1996), 1463.



Time-of-flight spectrum for ^{144}Nd and ^{197}Au. From "A BaF_2 detector system for (n,γ) cross section measurements at ORELA," K. H. Guber et al, *Nuclear Physics* A621 (1997) 254c.

Analysis of neutron cross-section data in the resolved-resonance region requires:

1. Correct formalism for calculation of cross sections
2. Correct mathematical description of experimental effects
3. Correct fitting procedure, including treatment of covariances

All three are included in SAMMY.

FORMALISM FOR CALCULATION OF CROSS SECTIONS

Scattering Theory:

Also called: Collision Theory or R-Matrix Theory

Definitive Paper: Lane & Thomas, "R-Matrix Theory of Nuclear Reactions", *Reviews of Modern Physics* **30**, 257-353 (1958)

Easier Reading Book: Foderaro, *The Elements of Neutron Interaction Theory*, The MIT Press, Cambridge MA and London, England (1971)

- Is mathematically rigorous (but usually approximated)
- Describes what is actually measured but not what happens inside the nucleus (i.e. the neutron-nucleus interaction is not explicitly included)
- Parameterizes in terms of
  - interaction radii & boundary conditions
  - resonance energies & widths
  - quantum numbers

Other valuable References:

F. H. Fröhner, "Applied Theory of Resolved and Unresolved Resonances," *Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications*, M.K. Mehta and J.J. Schmidt (eds.), World Scientific, Singapore (1989)

- Work was initially presented at ICTP Winter Courses on Nuclear Physics and Reactors, 1978.
- A comprehensive and useful guide to applied neutron resonance theory
- Discusses a variety of topics — preparation of data, the various approximations to R-matrix theory, Doppler broadening, experimental complications, data-fitting procedures, statistical tests

F. H. Fröhner, "Theory of Neutron Resonance Cross Sections for Safety Applications," KFK 5073, Kernforschungszentrum Karlsruhe (1992)

- review paper prepared for the "Workshop on Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety," held at the ICTP, Trieste, Italy, 10 February - 13 March 1992
- updated version of the first paper... covers many of the same topics

Why parameterize the cross sections?

Why not just use the measured data?

1. Too much information, too little understanding
   - cross section vs energy => ~100,000's of numbers
   - angular distributions have even more numbers
   - human minds seldom make sense of this many numbers!

2. Not enough information => extrapolations are needed for practical applications
   - other energies
   - other experimental conditions:
     - temperature (Doppler broadening)
     - geometry (self-shielding calculations, multiple-scattering effects, etc.)
   - other nuclides

(for more details, see Froehner's paper)

Multilevel R-Matrix Theory

- phenomenological
  - describes what is seen (i.e. the measured cross sections)
  - does not describe what is not seen (i.e. the underlying nuclear physics)

- mathematically correct
  - analytic, unitary, rigorous

- based on the following assumptions (re Lane & Thomas):
  - the applicability of nonrelativistic quantum mechanics
  - the absence or unimportance of all processes in which more than two product nuclei are formed
  - the absence or unimportance of all processes of creation or destruction
  - the existence of a finite radial separation beyond which no nuclear interactions occur

DEFINITION OF TERMS

channel = pair of (incoming or outgoing) particles, defined by *mass*, *charge*, and *spin quantum numbers*

mass = atomic mass of the particles

neutron mass = 1.008665 amu

amu = atomic mass unit, from Nuclear Wallet Cards:
= $1.49241909 \times 10^{-3}$ erg
= 9.3149432×10^{8} eV
= $2.25234242 \times 10^{23}$ / sec
= $7.51300563 \times 10^{12}$ /cm
= 1.0809478×10^{13} K
= $1.6605402 \times 10^{-24}$ g

charge = Z for nuclide, 0 for neutron, 1 for proton

spin quantum numbers (Note unprimed → incident, primed → exit):

i = intrinsic spin of incident neutron = ½
I = spin of target nuclide = integer or ½ integer
l = relative orbital angular momentum (s, p, d, f, ...)
(l = 0, 1, 2, 3,...)
s = channel spin; $\vec{s} = \vec{i} + \vec{I}$
J = total spin for channel; $\vec{J} = \vec{s} + \vec{l}$

Required: conservation of spin and parity
(spin of incident channel = $J = J'$ = spin of exit channel)

Elementary angular momentum addition rules:

If vector spin $\vec{a}$ is given by

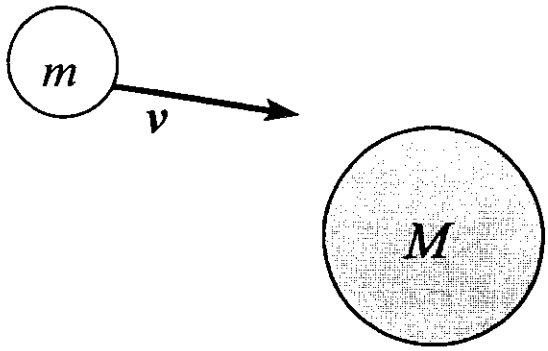
$$\vec{a} = \vec{b} + \vec{c}$$

then the magnitude of $\vec{a}$ is within the limits

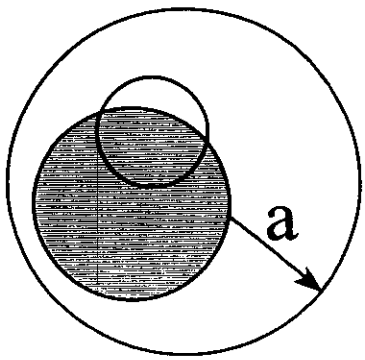
$$|b - c| \le a \le b + c$$

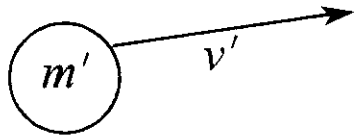
and a is either integer (if b and c are both integer or both half-integer) or half-integer (if one of b and c is integer and the other half-integer).

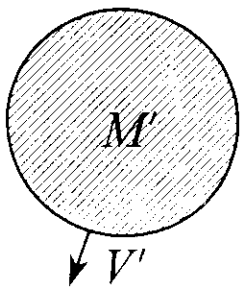
b	c	a
0	0	0
0	1/2	1/2
0	1	1
0	3/2	3/2
0	2	2
1/2	1/2	0, 1
1/2	1	1/2, 3/2
1/2	3/2	1, 2
1/2	2	3/2, 5/2
1	1	0, 1, 2
1	3/2	1/2, 3/2, 5/2
1	2	1, 2, 3
3/2	3/2	0, 1, 2, 3
3/2	2	1/2, 3/2, 5/2, 7/2
2	2	0, 1, 2, 3, 4



Incident Channel







Exit Channel

Multilevel R-Matrix Theory Equations, continued

How to calculate the scattering matrix:

$$U^J_{cc'} = \Omega_l \, W^J_{cc'} \, \Omega_{l'}$$

where l = orbital angular momentum

$$\Omega_l = e^{-i\phi_l}$$

where ϕ = potential phase shift

In matrix notation, with indices suppressed, W is given by

$$W = P^{1/2} (I - RL)^{-1} (I - RL^*) P^{-1/2}$$

$$L = (S - B) + iP$$

with
P = penetrability
S = shift factor
B = arbitrary boundary constant at the channel radius a_c
I = identity matrix
R = R-matrix

Penetrability (penetration factor) P, level shift factor S, and potential scattering phase shift ϕ for orbital angular momentum l, center of mass momentum k, and channel radius a_c, with $\rho = ka_c$.

l	P_l	S_l	ϕ_l
0	ρ	0	ρ
1	$\frac{\rho^3}{(1+\rho^2)}$	$\frac{-1}{(1+\rho^2)}$	$\rho - \tan^{-1}\rho$
2	$\frac{\rho^5}{(9+3\rho^2+\rho^4)}$	$-\frac{(18+3\rho^2)}{(9+3\rho^2+\rho^4)}$	$\rho - \tan^{-1}\left[\frac{3\rho}{(3-\rho^2)}\right]$
3	$\frac{\rho^7}{(225+45\rho^2+6\rho^4+\rho^6)}$	$\frac{-(675+90\rho^2+6\rho^4)}{(225+45\rho^2+6\rho^4+\rho^6)}$	$\rho - \tan^{-1}\left[\frac{\rho(15-\rho^2)}{(15-6\rho^2)}\right]$
4	$\frac{\rho^9}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)}$	$\frac{-(44100+4725\rho^2+270\rho^4+10\rho^6)}{(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)}$	$\rho - \tan^{-1}\left[\frac{\rho(105-10\rho^2)}{(105-45\rho^2+\rho^4)}\right]$
l	$\frac{\rho^2 P_{l-1}}{(l-S_{l-1})^2 + P^2_{l-1}}$	$\frac{\rho^2 (l-S_{l-1})}{(l-S_{l-1})^2 + P^2_{l-1}} - l$	$\phi_{l-1} - \tan^{-1}\left(\frac{P_{l-1}}{l-S_{l-1}}\right)$

Multilevel R-Matrix Theory Equations, continued

W can be modified using

$$L^* = (S - B) - iP = L - 2iP$$

to give

$$W = I + 2iP^{1/2}L^{-1}(L^{-1} - R)^{-1}RP^{1/2}$$
$$= I + 2iX$$

where X is defined by

$$X = P^{1/2}L^{-1}(L^{-1} - R)^{-1}RP^{1/2} \quad .$$

A general description of the matrix R is

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

where c and c' refer to *any* channel (neutron, fission, inelastic, capture [i.e. gamma], etc.)

What is used in SAMMY is the Reich Moore Approximation to Multilevel R-matrix theory, in which we neglect level-level interference for gamma channels:

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\gamma_{\lambda\gamma}^2}$$

where c and c' refer to only *non-capture* channels.
(For algebra, see Section III.A and III.D of SAMMY manual.)

Cross sections in terms of X are then

$$\sigma^{total} = \frac{4\pi}{k^2}\sum_J g_J \sum_{\substack{incident\\channels\ c}} \left(\sin^2(\phi_c) + \cos(2\phi_c)\, Im(X_{cc'}^J) - \sin(2\phi_c)\, Re(X_{cc}^J) \right)$$

$$\sigma^{elastic} = \frac{4\pi}{k^2}\sum_J g_J \sum_{\substack{incident\\channels\ c}} \left(\sin^2(\phi_c)\,(1 - 2\, Im(X_{cc'}^J)) - \sin(2\phi_c)\, Re(X_{cc}^J) \right)$$

$$\sigma^{reaction} = \frac{\pi}{k^2}\sum_J g_J \sum_{\substack{incident\\channels\ c}} \sum_{\substack{exit\\channels\ c'}} |X_{cc'}^J|$$

$$\sigma^{capture} = \frac{\pi}{k^2}\sum_J g_J \sum_{\substack{incident\\channels\ c}} \left(Im(X_{cc}^J) - \sum_{\substack{all\\channels\ c'}} |X_{cc'}^J| \right)$$

SAMMY options

for generation of cross sections:

- Reich-Moore approximation to multilevel multichannel R-matrix

  with contribution from external resonances approximated by

  - "dummy" resonances, or
  - logarithmic R-function

- multilevel Breit Wigner

- single level Breit Wigner

RECOMMENDATION

Use only Reich Moore

(or something better)

- Multilevel Breit Wigner is often wrong. Single-level Breit Wigner is almost always wrong.

- When it's right, MLBW gives identical results to Reich Moore !!

- "Ease of Programming" is no longer a good excuse for using MLBW. Neither is a slow computer.

MATHEMATICAL

DESCRIPTION

OF

EXPERIMENTAL

EFFECTS

MATHEMATICAL DESCRIPTION OF EXPERIMENTAL EFFECTS

1. Calculation of cross sections
2. Mathematical description of experimental effects
3. Fitting procedure

Numbers 1 & 3 are relatively easy.
Number 2 is impossible!

Includes all the complexity from being part of the real world:

- Many neutrons, not just one
- Many nuclei (sample is finite size)
- Many **kinds** of nuclei (isotopes, chemical compounds, impurities)
- Nucleus is moving (finite temperature)
- Time is not exact
- Distance is not exact
- Neutron-producing target is finite size
- Detector is finite size
- etcetera

DOPPLER BROADENING

Doppler broadening is the average over the thermal motion of the particles within the sample.

The nuclei within the sample are not sitting still, but exhibit random thermal motion. In macroscopic terms, the temperature is not absolute zero.

Two options to describe the sample nuclei:

1. Crystal lattice model (the sample is a solid).
2. Free gas model (the sample is a gas).

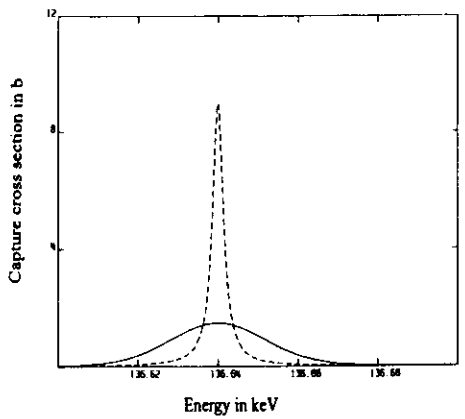
Option 2 works in most physical situations, even for very heavy nuclei (e.g. lead, uranium).

Historically, codes used the *high-energy Gaussian approximation* (HEGA) to the free gas model (FGM) because of its convenient analytical properties:

HEGA + Breit-Wigner => psi,chi functions

Today, one should only use FGM not HEGA.

Re: "Doppler Broadening Revisited," N. M. Larson, M. C. Moxon, L. C. Leal, and H. Derrien, ORNL/TM-13525, Oak Ridge National Laboratory, Oak Ridge, TN (1998)



Capture cross section for ^{58}Ni without Doppler broadening (dashed curve) and with Doppler broadening at 300 L (solid curve)

DERIVATION OF THE FREE GAS MODEL

Definitions:

- a parallel beam of monoenergetic particles with lab velocity $\vec{v}$
- target nuclei whose velocities $\vec{W}$ are distributed in such a way that $p(\vec{W})\, d^3W$ is the fraction with velocities in a small three-dimensional region d^3W around $\vec{W}$
- ρ_1 and ρ_2 are the densities of beam and target particles, respectively
- $\sigma(E)$ is unbroadened cross section
- $\bar{\sigma}(mv^2/2)$ is the effective or Doppler-broadened cross section for incident particles with speed v [laboratory energy $m v^2/2$]

Then:

- the number of reactions occurring per unit time and unit volume is

$$\rho_1 \rho_2 \int d^3W\, p(\vec{W})\, |\vec{v} - \vec{W}|\, \sigma(m|\vec{v} - \vec{W}|^2/2) \equiv \rho_1 \rho_2\, v\, \bar{\sigma}(mv^2/2)$$

Assume:

- target nuclei have same velocity distribution as atoms of ideal [monatomic] gas, i.e. the Maxwell-Boltzmann distribution,

$$p(\vec{W})\, d^3W = \frac{1}{\pi^{3/2}} \exp\left(-\frac{W^2}{u^2}\right) \frac{d^3W}{u^3}$$

with

$$\frac{M}{2} u^2 = kT$$

where M = nuclear mass and k = Boltzmann's constant, T = temperature

Then:

- The Doppler-broadened cross section is given by

$$v\bar{\sigma}(mv^2/2) = \frac{1}{\pi^{3/2}u^3}\int_{\text{all }\vec{W}} d^3W\ \exp\left(-\frac{W^2}{u^2}\right) \times |\vec{v}-\vec{W}|\ \sigma(m|\vec{v}-\vec{W}|^2/2)$$

Simplify:

- change integration variable from $\vec{W}$ to $\vec{w} = \vec{v} - \vec{W}$
- choose spherical coordinates

$$v\bar{\sigma}\left(\frac{mv^2}{2}\right) = \frac{1}{\pi^{3/2}u^3}\int_{\text{all }\vec{w}} d^3w\ \exp\left(-\frac{(v^2-2vw\cos\theta+w^2)}{u^2}\right) w\,\sigma\left(\frac{mw^2}{2}\right)$$

$$= \frac{1}{\pi^{3/2}u^3}\int_0^{\pi} d\phi \int_0^{\infty} w^2\,dw \int_0^{\pi} d(\cos\theta)\ \exp\left(-\frac{(v^2-2vw\cos\theta+w^2)}{u^2}\right) w\,\sigma\left(\frac{mw^2}{2}\right)$$

$$= \frac{1}{\pi^{3/2}u^3}\int_0^{2\pi} d\phi \int_0^{\infty} dw\,w^3\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v^2+w^2)}{u^2}\right)\int_{-1}^{+1} d\mu\ \exp\left(-\frac{2vw\mu}{u^2}\right)$$

$$= \frac{2\pi}{\pi^{3/2}u^3}\int_0^{\infty} dw\,w^3\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v^2+w^2)}{u^2}\right)\left(\frac{-u^2}{2vw}\right)\left[\exp\left(-\frac{2vw}{u^2}\right)-\exp\left(+\frac{2vw}{u^2}\right)\right]$$

$$= \frac{1}{v\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\left[\exp\left(-\frac{(v-w)^2}{u^2}\right)-\exp\left(-\frac{(v+w)^2}{u^2}\right)\right].$$

which may be more familiar as:

$$\bar{\sigma}\left(E=\frac{mv^2}{2}\right) = \frac{1}{v^2\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v-w)^2}{u^2}\right) - \frac{1}{v^2\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v+w)^2}{u^2}\right)$$

Define pseudo cross section s:

$$s(w) = \sigma(m(w)^2/2) \quad \text{for } w>0$$
$$= -\sigma(m(-w)^2/2) \quad \text{for } w<0\ .$$

Simplify:

- Free gas model of Doppler broadening can be written

$$\bar{\sigma}\left(\frac{mv^2}{2}\right) = \frac{1}{v^2\sqrt{\pi}\,u}\int_{-\infty}^{\infty} dw\,w^2\,s(w)\exp\left(-\frac{(v-w)^2}{u^2}\right)$$

DOPPLER BROADENING in SAMMY

(page numbers refer to the SAMMY users' manual)

- via Gaussian (page 61)
  - high energy approximation
  - integrations performed numerically using energy-grid appropriate for resonance structure

- via Leal-Hwang (pages 92a-92c)
  - exact free gas model
  - is solution of partial differential equation having same form as 1-d time-dependent heat equation
  - efficient where cross section is smooth

- via SAMMY's "free gas model" (pages 92q-92r)
  - integrations performed numerically using appropriate velocity-grid
  - relatively accurate and relatively efficient for all energies, even where there is structure

- Crystal-lattice effect
  - may be important for some low-energy cross sections
  - effect in practical applications has yet to be investigated
  - will be added to SAMMY as needed, when time permits

RESOLUTION BROADENING

Resolution broadening is "smearing" due to

- spread in burst width
- finite size of neutron source
- time-of-flight channel width
- finite size of detector
- etc

Mathematically, this smearing can be described by a resolution-broadening function of the form $R(E,E')$,

$$\bar{\sigma}(E) = \int dE'\ R(E,E')\ \sigma(E')$$

where generally $R(E,E')$ depends only on the energy difference $E-E'$.

There is no "standard" resolution broadening function. SAMMY contains three distinct methods and a fourth is contemplated. Values for all parameters can be fitted to data.

Resolution Broadening in SAMMY

(page numbers refer to the SAMMY users' manual)

- via Gaussian and/or exponential (page 63-71)
  - convolution of Gaussian approximation for three components (path length, burst width, channel width)
  - integrations performed numerically using energy-grid appropriate for resonance structure
- via Oak Ridge Resolution Function (pages 92e-92o)
  - analytic convolution (where possible) of four components, with realistic descriptions for all four
- via RPI Resolution Function (pages 92s-92v)
  - ditto, designed for use with data from Linac at Rensselaer Polytechnic Institute
- Numerical description of resolution function
  - will be added to SAMMY as needed, when time permits

Resolution Function # 1

Original Gaussian and/or Exponential

(See pages 63-80 of the SAMMY users' manual)

Gaussian: combination of three components:

- a square function of (flight-path) length
  - input is the full width of a square distribution in length (i.e. $\sqrt{12}$ × standard deviation of a Gaussian)
- burst width, a Gaussian in time
  - input is the full width at half max of Gaussian
- channel width, a square function in time
  - input is full width of square function
  - different values may be specified for different energy ranges

Exponential, or Gaussian plus exponential

- provides asymmetric component to the resolution function

Resolution Function # 2

Oak Ridge Resolution Function

(See pages 92e-92o of the SAMMY users' manual)

A "realistic" resolution function, the convolution of four components:

- electron burst width
- neutron source
- time-of-flight channel width
- detector

Each component is described mathematically as a function of either time t or flight-path-length ℓ, then converted to a function of t using (for fixed E)

$$E = \frac{m}{2}\frac{\ell^2}{t^2}$$

The "complete" resolution function is the convolution of the four individual pieces:

$$r(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3\; I_4(t_3$$

Integrations are analytical where possible (to maximize speed and accuracy), numerical where necessary.

Components of the Oak Ridge Resolution Function

1. electron burst width, a square function in time:

$$I_1(t) = \begin{cases} 1/p & \textit{for } 0 < t < p \\ 0 & \textit{otherwise} \end{cases}$$

where p is the burst width in nanoseconds

2. neutron source, two possibilities:

2a. *ORELA Water Moderator*

χ^2 distribution with $2(m+1)$ degrees of freedom, where $m = 4$ or 5:

$$I'_{2a}(\ell) = \frac{\ell^m}{m!\,\Lambda^{m+1}} \exp\left(-\frac{\ell}{\Lambda}\right)$$

where ℓ = the flight-path-length variable and moderation distance Λ is a mean free path. Value of Λ varies with energy as $\Lambda = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 (\ln(E))^2$.

Note: in the next SAMMY release, any positive integer can be used for m.

2b. tantalum target

$$I'_{2b}(\ell) = \begin{cases} 0 & for \quad \ell < x'_1 \\ u'(\ell) + v'(\ell) & for \; x'_1 < \ell < x'_2 \\ u'(\ell) + w'(\ell) & for \; x'_2 < \ell < x'_3 \\ w'(\ell) & for \; x'_3 < \ell \end{cases}$$

where the functions $u'(\ell)$, $v'(\ell)$, and $w'(\ell)$ are defined as

$$u'(\ell) = N' \exp\{-\epsilon'^2 (\ell - x'_0)^2\} \quad for \; x'_1 < \ell < x'_3$$

$$v'(\ell) = \frac{N'\alpha'\ell}{x'_2} \exp\{-\beta'(\ell - x'_2)\} \quad for \; x'_1 < \ell < x'_2$$

and

$$w'(\ell) = N'\alpha' \exp\{-\beta'(\ell - x'_2)\} \quad for \; x'_2 < \ell$$

3. time-of-flight channel width

$$I_3(t) = \begin{cases} 1/c & for \; 0 < t < c \\ 0 & otherwise \end{cases}$$

where channel width c may be different for different energy-regions.

4. detector

4a. *NE110 Detector*

$$I'_{4a}(\ell) = \begin{cases} \Delta \exp(-\lambda\sigma\ell) & for \; 0 < \ell < \delta \\ 0 & otherwise \end{cases}$$

δ = thickness of the NE110 detector
λ = number of molecules per mm.b of detector (0.0047 for NE110)
$\sigma(E)$ = total cross section of detector material ($CH_{1.104}$ for NE110)
Δ = normalization factor found from $\int I'_{4a} =$ 1:

$$\Delta = \frac{\lambda\sigma}{1 - \exp(-\lambda\sigma\delta)}$$

4b. *Lithium Glass Detector*

$$I_{4b}(t) = \begin{cases} D\,g & for \; 0 < t < d \\ D \exp(-f(t-d)) & for \; d < t \end{cases}$$

g = constant,
D is chosen to give $\int I'_{4b} = 1$:

$$D = \frac{f}{1 + g\,f\,d}$$

Resolution Function # 3

RPI Resolution Function

(See pages 92s-92v of the SAMMY users' manual)

Another "realistic" resolution function, convolution of three components, designed for use with data taken at the Gaerttner LINAC at Rensselaer Polytechnic Institute :

- electron burst width
- neutron source + detector
- time-of-flight channel width

Each component is described mathematically as a function of t.

The "complete" resolution function is the convolution of the three individual pieces:

$$I(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2\; I_3(t_2)$$

Integrations are analytical where possible (to maximize speed and accuracy) and numerical where necessary.

Components of the RPI Resolution Function

1. electron burst width, a Gaussian function in time

$$I_1(t) = \frac{w}{\sqrt{\pi}}\, e^{-w^2 t^2}$$

$2\sqrt{\ln 2}\,/w = p$ is full width at half max of the burst

2. neutron source + detector, chi-squared plus exponentials

$$I_2(t) = A_0 \left\{ \frac{(t+\tau)^2}{2!\,\Lambda^3}\, e^{-(t+\tau)/\Lambda} + A_1 \left[A_2\, e^{-A_3(t+t_0)} + A_4\, e^{-A_5(t+t_0)} \right] \right\}$$

where τ and Λ are functions of energy, A_0 is normalization.

3. time-of-flight channel = square function of time

$$I_3(t) = \begin{cases} 1/c & \text{for } -c/2 < t < c/2 \\ 0 & \text{otherwise} \end{cases}$$

where channel width c may be different for different energy-regions

Resolution Function # 4

Numerical Resolution Function
To be incorporated into SAMMY eventually

Yet another "realistic" resolution function, convolution of several components, designed for use when other forms are not adequate

- electron burst width
- neutron source
- time-of-flight channel width
- detector
- other ?

Each component is described numerically as a function of t.

The "complete" resolution function is the convolution of the individual pieces:

$$I(t) = \int I_1(t - t_1)\,dt_1 \int I_2(t_1 - t_2)\,dt_2 \cdots \int I_{n-1}(t_{n-2} - t_{n-1})\,dt_{n-1}\, I_n(t_{n-1})$$

Integrations are numerical in all cases.

SAMMY's Integration Method for Doppler and Resolution Broadening

see Section IV.B page 73ff SAMMY manual

Wanted: to evaluate integrals of the form

$$\bar{f}(E_i) = \int_{Emin}^{Emax} f(E')\, B(E_i, E')\, dE'$$

where

$\{E_i\}$ is a predetermined set of grid points on which we wish to know the broadened values $\bar{f}(E_i)$

$f(E')$ are the unbroadened theoretical values (for cross section, transmission, etc.)

$B(E_i, E')$ is the Doppler- or resolution-broadening function

$Emin = 0$ and $Emax = \infty$, but in practice smaller range is used

Solution: Choose points $\{E_j'\}$ and associated weights $\{W_j\}$ such that

$$\int_a^b f(E')\, B(E_i, E')\, dE' = \sum_j f(E_j')\, B(E_i, E_j')\, W_j$$

where the approximation is exact if $f(E')\, B(E_i, E')$ is a polynomial of some specified degree

Choice of "auxiliary grid" $\{E_j'\}$ is somewhat arbitrary.

SAMMY's choice (see pages 79-80 in SAMMY users' manual):

- start with experimental grid
- add extra points between each point in grid (optional)
- add points to the extremities (i.e. outside data range) so can broaden the end-points
- add enough points to adequately describe each resonance
- test the resulting grid to be sure spacings do not vary too wildly among neighboring points

Most integrations in SAMMY use four-point progressive interpolation method of Mintz and Jordan [M. D. Mintz and D. P. Jordan, *A 'Progressive' Interpolation Scheme for Hand and Digital Computer Analysis of Tabulated Data*, Lawrence Livermore Laboratory Report UCRL-7681 (1964)]

for which W_j is given by

$$W_j = (E'_{j+1} - E'_{j-1})/3 + (E'_{j+2} - E'_{j-2})/12 + \frac{1}{12}\left[\frac{(E'_j - E'_{j-1})^2 - (E'_{j+2} - E'_{j+1})^2}{(E'_{j+1} - E'_j)} + \frac{(E'_{j+1} - E'_j)^2 - (E'_{j-1} - E'_{j-2})^2}{(E'_j - E'_{j-1})} \right]$$

Explicit Normalization and/or Background Functions

pages 98g, 122c, 122n.1 in R4 of SAMMY Users' Manual

"Corrected" theoretical value T (for cross section, transmission, etc.) is given by

$$T(E) = a\,T_u(E) + b(E)$$

where T_u = uncorrected theoretical value
a = normalization
$b(E)$ = background

In SAMMY, there are three methods of specifying backgrounds:

Method 1. Use any or all of the following (but only one of each):

$$b_1(E) = B_a$$
$$b_2(E) = B_b / \sqrt{E}$$
$$b_3(E) = B_c \times \sqrt{E}$$
$$b_4(E) = B_d \times e^{-B_f/\sqrt{E}}$$

Method 2. Use as many of the following as needed:

$$b_1(E) = A$$
$$b_2(E) = Ae^{-Bt}$$
$$b_3(E) = A\,t^{B}$$
$$b_4(E) = e^{A + Bt + C/\ln(t)}$$

where time t is derived from the energy

$$t = \sqrt{\frac{m L^2}{2E}}$$

where L is the flight-path length.

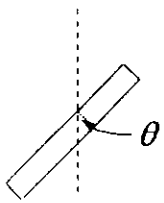
Method 3. The user can provide a point-wise description of the background. Note that this method has been available from the beginning, but has not been used extensively, therefore comes with no guarantees.

Finite Size Corrections for Total Cross Sections

- Measured as transmission through sample of thickness n

$$T = e^{-n\sigma_t}$$

- Sample oriented at angle to beam? Correct by modifying the apparent value of n



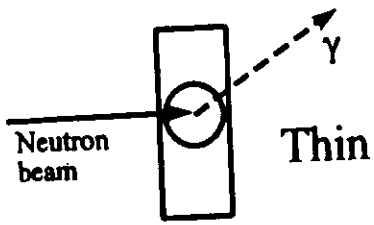
$$n_{apparent} = n / \cos(\theta)$$

- Non-uniform thickness n ? Correct by treating n as variable.
(Pictures are obviously grossly exaggerated!)

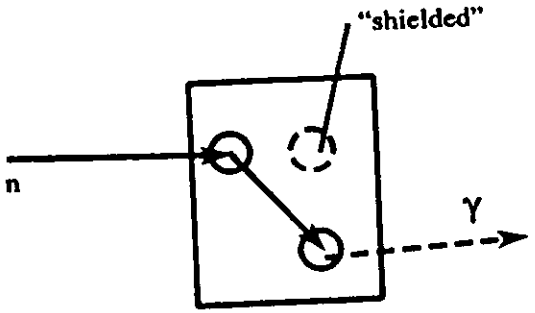
Finite-size Corrections for Capture and Fission Experiments

- self-shielding
  - exact
  - easy
- single-scattering followed by capture
  - exact for simplified geometry
  - complicated mathematics
  - complicated coding
  - simplifies if assume target is infinite slab
- double-scattering followed by capture
  - gross approximation

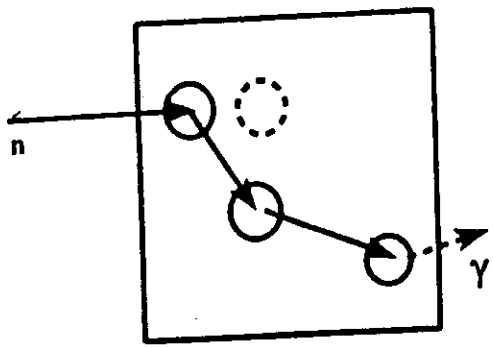
CAPTURE



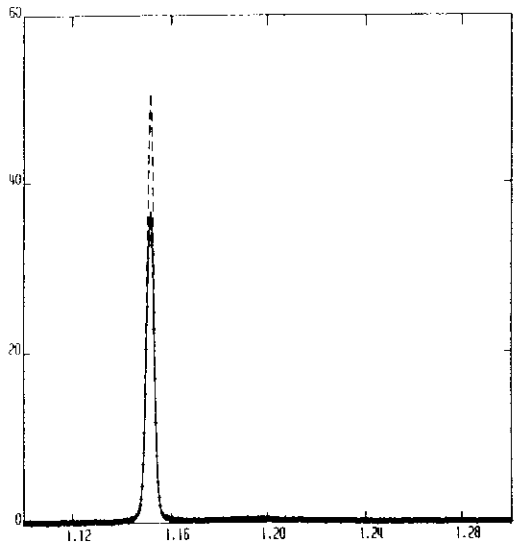
Thin sample



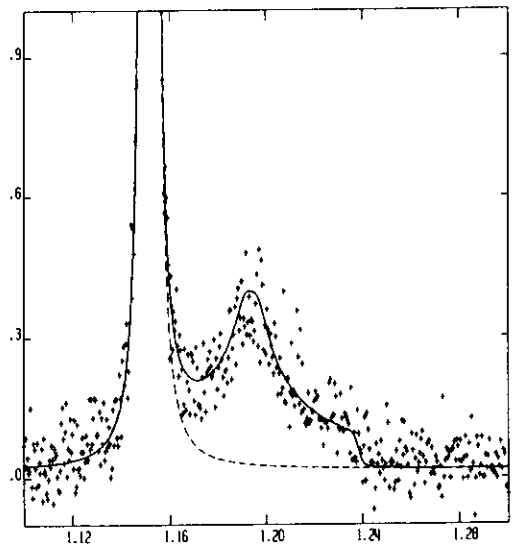
Thicker sample, single scattering



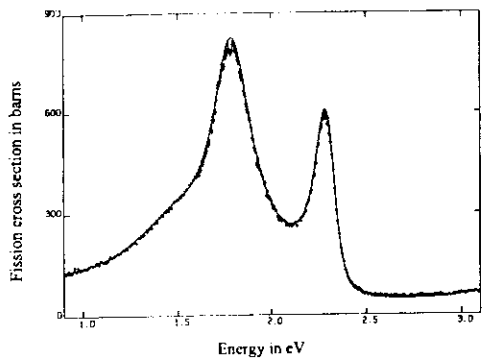
Thicker yet, multiple scattering



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

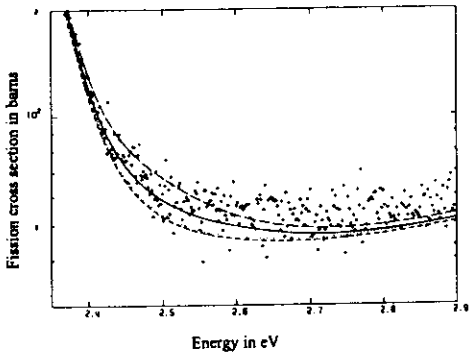


Fission cross section for ^{233}U

++ Measurement of Klaus Guber et al. at ORELA (data averaged by 5)

. Preliminary SAMMY analysis of Herve Derrien

.... Using same resonance parameters without finite-size corrections



Fission cross section for ^{233}U
(including aluminum in the analysis)

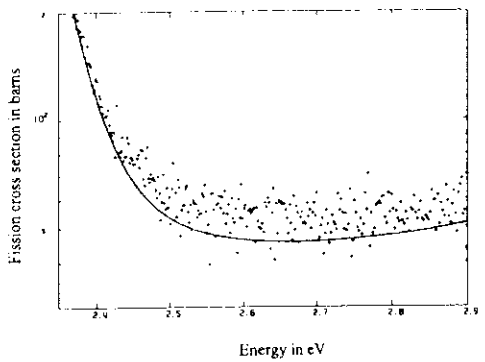
++++++ ORELA measurement

..... No finite-size corrections to calculated cross section

---------- With self-shielding but no multiple scattering

— — — With multiple-scattering corrections but infinite-slab for single-scattering

——— With full multiple-scattering including edge-effects correction



Fission cross section for ^{233}U
(with no aluminum in the analysis)

+ + + + +	ORELA measurement
.....	No finite-size corrections to calculated cross section
----------	With self-shielding but no multiple scattering
	With multiple-scattering corrections but infinite-slab for single-scattering
————	With full multiple-scattering including edge-effects correction

CAUTION

When using more than one nuclide and requiring multiple-scattering corrections, *be sure* to define the isotopes in the PARameter file. It is not sufficient to give abundances only in the INPut file.

The next release of SAMMY is dummy-proofed against this, but the current release will merrily calculate garbage.

Self-Shielding and Multiple-Scattering Corrections

See pages 56o and following in the SAMMY Users' Guide. Complete documentation is in preparation.

Self-shielded capture yield:

$$Y_0 = \left(1 - \exp(-N\sigma_t Z)\right) \frac{\sigma_c}{\sigma_t}$$

N is the density (atoms/volume) of the nuclei in the sample
Z is the thickness of the sample
σ_t is the total cross section
σ_c is the capture cross section

Note that there are other ways to normalize the capture yield; SAMMY has three different options.

Single-scattering correction without edge effects (i.e. infinite-slab approximation):

$$Y_{1\infty} = 2\pi \int_0^1 d\mu \, \frac{\sigma_c'}{\sigma_t'} \, \frac{d\sigma}{d\Omega} \left[\frac{1 - \exp(-N\sigma_t Z)}{\sigma_t} + \frac{\exp(-N\sigma_t Z) - \exp(-N\sigma_t' Z/\mu)}{\sigma_t - \sigma_t'/\mu} \right]$$

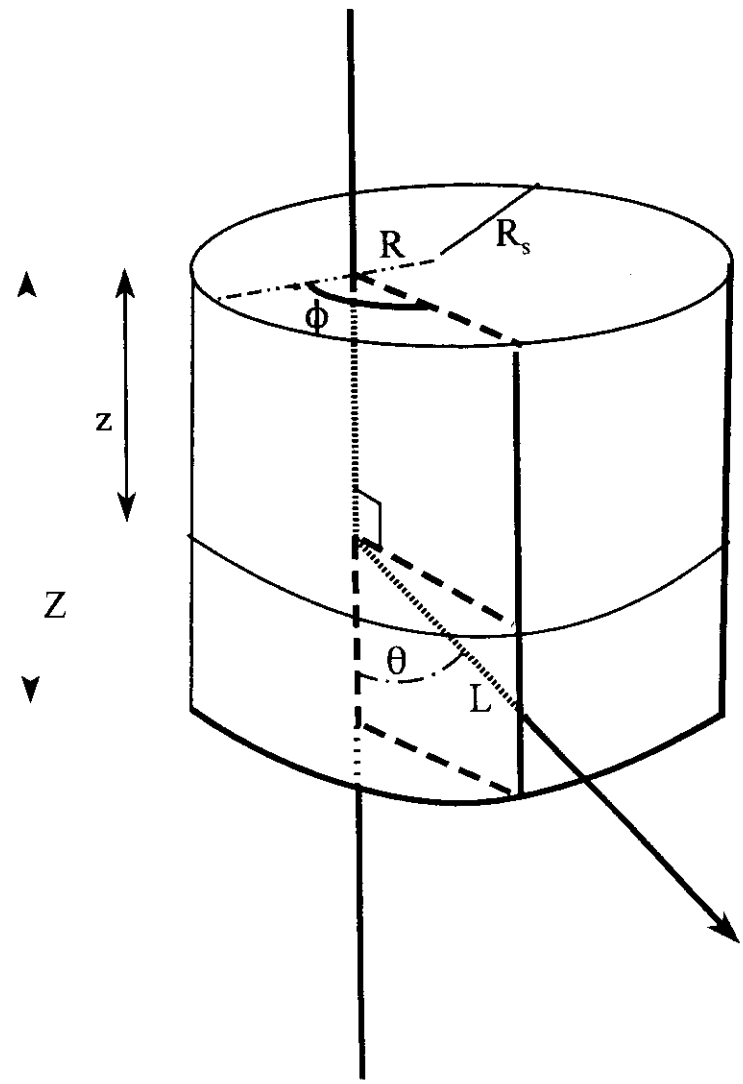
$$+ 2\pi \int_{-1}^{\nu} d\mu \, \frac{\sigma_c'}{\sigma_t'} \, \frac{d\sigma}{d\Omega} \left[\frac{1 - \exp(-N\sigma_t Z)}{\sigma_t} + \frac{\exp\left(-N(\sigma_t - \sigma_t'/\mu)\, Z\right) - 1}{\sigma_t - \sigma_t'/\mu} \right]$$

Primes indicate quantities are to be evaluated at the scattered energy:

$$E' = E \left[\frac{\cos\theta}{(1+r)} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2\theta}{(1+r)^2}} \right]^2$$

where r is the ratio of the mass of the nucleus to the mass of the neutron, and $\cos\theta = \mu$.

Single-scattering correction for a cylindrical sample



Edge-effects correction for Cylinder:

$$Y_{1ec} = \int_0^{\mu_1} d\mu \, \frac{d\sigma}{d\Omega} \, \frac{\sigma_c'}{\sigma_t'} \, Q_f(\mu,\sigma_t,\sigma_t') + \int_{-\mu_1}^{0} d\mu \, \frac{d\sigma}{d\Omega} \, \frac{\sigma_c'}{\sigma_t'} \, Q_b(-\mu,\sigma_t,\sigma_t')$$

where Q_f and Q_b are defined as

$$Q_f(\mu,\sigma_t,\sigma_t') = \int_0^{z_1} dz \, \exp(-N\sigma_t z) \, U(\mu,z,\sigma_t')$$

$$Q_b(\mu,\sigma_t,\sigma_t') = \int_0^{z_1} dz \, \exp\left(-N\sigma_t(Z-z)\right) U(-\mu,z,\sigma_t')$$

with U given by

$$U(\nu,w,s) = -\frac{4N}{R_0^2} \int_{R_1}^{R_0} R\,dR \int_0^{\phi_1} d\phi \left(\exp\left(-\frac{Ns(Z-w)}{\nu} \right) - \exp\left(-\frac{Ns\left(-R\cos\phi + \sqrt{R_s^2 - R^2\sin^2\phi} \right)}{\sqrt{1-\nu^2}} \right) \right)$$

The limits in these expressions are given by

$$\mu_1 = \cos\theta_1 \qquad \tan\theta_1 = (R_s - R_0)/Z$$

$$z_1 = Z - (R_s - R_0)/\tan\theta$$

$$R_1 = R_s - (Z-z)\tan\theta$$

$$\cos\phi_1 = \frac{R_s^2 - R^2 - (Z-z)\tan^2\theta}{2(Z-z)R\tan\theta}$$

Multiple* Scattering Correction for Capture and Fission Yield

* "Multiple" => Double, Triple, etc.

Treatment borrowed from M. Moxon, REFIT

- Assumption: after a few scatterings, neutrons are distributed uniformly throughout the sample, and directions of motion are also distributed uniformly
- Probability of escape for a neutron after k scatters is $e^{-N\sigma^{k}L}$ where L is the distance left to travel
- Average escape probability is therefore

$$p_e(E^{(k)}) = \frac{1}{ZN\sigma^{(k)}}\left[\frac{1}{2} - \int_1^\infty u^{-3}\,du\; e^{-N\sigma^{(k)}Zu}\right]$$

- Correction for capture preceded by 2, 3, 4, ... scatterings is given by

$$\bar{Y}_2(E) = N\int dz\; e^{-N\sigma_t z}\; 2\pi N\int d\mu_1\;\frac{d\sigma}{d\Omega_1}\;y_1\;\int dq_1\; e^{-N\sigma_t' q_1}$$

where y_i are found iteratively from

$$y_{j+1} = 2\pi\int d\mu_j\;\frac{d\sigma^{(j-1)}}{d\Omega_j}\left(\sigma_c^{(j)} + y_j\right)\left(1 - p_e(E^{(j)})\right)$$

(Superscript j on cross sections indicates that the cross section is to be evaluated at the energy after j scatters.)

More than One Type of Nuclide in Sample

- Multiple isotopes
- Chemical compounds (e.g. oxides)
- Contaminants

What do YOU do about these?

- specify each nuclide independently
  - spin and parity (in INPut file)
  - mass and abundance (in PARameter file)

What does SAMMY do about these?

- includes appropriate angular momentum algebra for each nuclide
- includes proper kinematics for each nuclide

Details are given in the computer exercises
(see Exercise ex012)

FITTING

PROCEDURE

(Bayes' Method)

SAMMY's fitting procedure uses Bayes' Equations rather than least squares.

See page 3 *ff* in R3 or R4 of SAMMY Users' Manual

Bayes' equations are based on Bayes' Theorem:

$$p(P|DB) \propto p(P|B)\, p(D|PB)$$

$p(a|b)$ = probability for a, given that b is true

P = parameters whose values are to be determined
D = experimental data to be analyzed
B = all other relevant information

$p(P|B)$ = prior probability density function (pd.) for the parameters

$p(P|DB)$ = posterior pd.

$p(D|PB)$ = pdf for observing data D, given that P are correct
= (maximum) likelihood function

Bayes' Theorem + three assumptions + algebra = Bayes' Equations

- Assumptions
  - Prior joint probability density function is a joint normal.
  - Likelihood function is a joint normal.
  - True value is a linear function of the parameters.
- Derivation
  - Given in the users' manual
  - Results only will be shown here

Bayes' Equations

"N+V" Version:

$$P' - P = M G^t (N+V)^{-1} (D-T)$$

$$M - M' = M G^t (N+V)^{-1} G M$$

$$N = G M G^t$$

"I+Q" Version:

$$P' - P = M(I+Q)^{-1} G^t V^{-1} (D-T)$$

$$M' = M(I+Q)^{-1}$$

$$Q = G^t V^{-1} G M$$

"M+W" Version:

$$P' - P = (M^{-1} + W)^{-1} G^t V^{-1} (D-T)$$

$$(M')^{-1} = M^{-1} + W$$

$$W = G^t V^{-1} G$$

Least-squares: Take limit as M becomes infinite.
That is, assume no prior knowledge of values of parameters.

Notation

P	=	initial (á priori) values of parameters
M	=	initial value of covariance matrix for parameters
D	=	experimental data values at energy E
V	=	covariance matrix for experimental data
T	=	theoretical calculation at energy E
G	=	partial derivatives of T with respect to P
P'	=	final (á posteriori) values of parameters
M'	=	final value of covariance matrix for parameters

Bayes' method	Least Squares
$P' - P = (M')^{-1} G' \times V^{-1} (D - T)$ $M' = (M^{-1} + W)^{-1}$ $W = G' V^{-1} G$	$P' - P = (M')^{-1} G' \times V^{-1} (D - T)$ $M' = W^{-1}$ $W = G' V^{-1} G$
M = initial covariance matrix	M = infinite, diagonal
Remembers earlier results	Forgets
OK to vary irrelevant parameters; values and uncertainties will not change	Varying irrelevant parameters will cause problems

ADVANTAGES of BAYES' METHOD

- Does not change values of irrelevant parameters
- Retains a memory of earlier results
- Can use results of one analysis as input to another
- Gives results of sequential analyses identical to those obtained from simultaneous analysis (subject to linearity restrictions)

Covariance Matrices

- Do not stand alone
- Associated with some set of measured or calculated values

Two major types:

- Covariance matrix associated with experimental data
- Covariance matrix associated with parameters of the theory

First: Why bother with them?!

Why bother with covariances?
Here's one reason:

Integral Quantities are needed for reactor applications

$$\int_{Emin}^{Emax} \sigma(E)\, \varphi(E)\, dE$$

where

- $\varphi(E)$ can be flux or any other function
- $\sigma(E)$ is cross section, calculated from resonance parameters
- *Emin* to *Emax* can be a large energy range (perhaps 0 to ∞)

Uncertainties on these integral quantities are also needed.

Calculation of uncertainties on integral quantities requires knowledge of the uncertainties on the quantities within the integrand -- and also knowledge of the covariances relating those uncertainties.

Example: Why covariances are important

Simple example: a straight line

$$\sigma(E) = a\,E + b$$

Suppose a "data fitting program" has found values, uncertainties, and correlation for a and b. That is,

$$\langle a \rangle = A \qquad \langle (\delta a)^2 \rangle = \Delta^2 A$$
$$\langle b \rangle = B \qquad \langle (\delta b)^2 \rangle = \Delta^2 B \qquad \langle \delta a\, \delta b \rangle = \Delta A\, \Delta B\, C$$

Then suppose the integral quantity of interest is

$$y = \frac{1}{Emax - Emin} \int_{Emax}^{Emax} \sigma(E)\, dE$$

$$= \frac{1}{Emax - Emin} \int_{Emin}^{Emax} (aE + b)\, dE$$

$$= \frac{1}{Emax - Emin} \left(a \frac{Emax^2 - Emin^2}{2} + b\,(Emax - Emin) \right)$$

$$= a\bar{E} + b$$

where $\bar{E}$ is the midpoint of the range.

Expected value of y is $Y = (A\bar{E} + B)$. What is uncertainty on Y?

Uncertainties are "propagated" by taking small increments, squaring, and taking expectation values.

$$\delta y = \delta a\, \bar{E} + \delta b$$

$$\langle (\delta y)^2 \rangle = \langle (\delta a\, \bar{E} + \delta b)^2 \rangle$$

$$= \langle (\delta a)^2 \rangle \bar{E}^2 + 2 \langle \delta a\, \delta b \rangle \bar{E} + \langle (\delta b)^2 \rangle$$

Rewriting this gives

$$\Delta^2 Y = \bar{E}^2\, \Delta^2 A + 2\,\bar{E}\, C\, \Delta A\, \Delta B + \Delta^2 B$$

where the range on C is -1 to +1. Usual approximation: $C \equiv 0$.

TRY SOME NUMBERS...

$A = 100 \pm 10$, $B = 40 \pm 5$, $Emin = 0.5$, $Emax = 1.5$ so $\bar{E} = 1.0$

$Y = (1)\,(100) + (40) = 140$

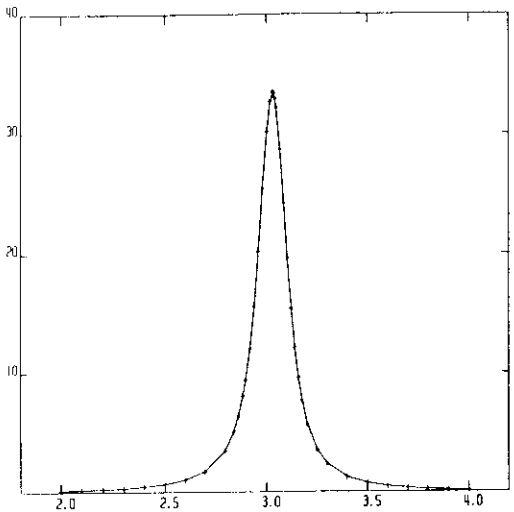
$\Delta^2 Y = (1)^2\,(10)^2 + (5)^2 + 2\,(1)\,C\,(10)\,(5) = 125 + 100\,C$

$C = 0$ implies $\Delta Y = 11.18$
$C = 1$ implies $\Delta Y = 15.00$ $C = -1$ implies $\Delta Y = 5.00$

Therefore

$$Y \pm \Delta Y = 140.00 \pm 5.00 \text{ if } C = -1$$
$$= 140.00 \pm 11.18 \text{ if } C = 0$$
$$= 140.00 \pm 15.00 \text{ if } C = 1$$

MORE REALISTIC EXAMPLE



Crosses = fission "data" for this example
Solid Curve = SAMMY fit to the data

Query: How to calculate the average cross section from 2 to 4 eV?

MORE REALISTIC EXAMPLE, continued

Uranium-like sample, fission cross section, one resonance

Values for resonance parameters

	"True" values	Fitted values	
E_0	3.0300 eV	3.03038	± 0.00006
Γ_γ	0.0402 eV	0.051323	± 0.01952
Γ_n	0.0000195 eV	0.0000218	± 0.0000044
Γ_{f1}	-0.0342 eV	-0.036825	± 0.01720
Γ_{f2}	0.0688 eV	0.056754	± 0.02115

Correlation Matrix:

E_0	100			
Γ_γ	0	100		
Γ_n	0	100	100	
Γ_{f1}	0	-31	-31	100
Γ_{f2}	0	-66	-66	-51 100

Group Cross Section (averaged from 2 to 4 eV):

With covariances:	4.028 ± 0.026 barns
Without covariances:	4.028 ± 1.061 barns
Without correct uncertainties:	4.028 ± 2.199 barns

DATA COVARIANCES

Obtaining resonance parameters is a multi-step process:

1. Data *acquisition* = experimental measurement
2. Data *reduction* = process of converting from "counts per time-channel" to "cross section"
3. Data *analysis* = process of parameterizing the cross section in terms of R-matrix theory

Generally the experimentalist who made the measurement takes care of step 2, the evaluator takes care of step 3.

However, the two processes are not nearly as independent as the definition would suggest. A simple example is Doppler-broadening, which is always (?) left for the evaluator to include.

The data covariance matrix provides the linkage between the two processes.

Experimentalists define two types of uncertainties

- Statistical (due to uncertainty in measurement of raw data, generally assumed to be Poisson statistics)
- Systematic (due to uncertainties in measurement of parameters for data-reduction process)

"Data reduction" (the process of converting "counts per channel" to something more closely related to "cross section") includes such operations as:

- corrections for detector dead time
- normalization by total run time
- conversion from time to energy scale
- subtraction of backgrounds
- dividing sample-in by sample-out counts (if transmission)
- etc.

It is the data-reduction process that leads to off-diagonal data covariance matrix elements. (Raw data are mutually independent, hence the covariance matrix is diagonal.)

Example of Data Reduction and Error Propagation

Measure "raw counts" C_i = number of times a neutron was counted in time-channel i

Uncertainty on C_i is ΔC_i

Actual "data" is $D_i = a\,C_i + b$

where a and b have also been measured, and have uncertainties Δa and Δb respectively.

What's the uncertainty on D_i? What's the correlation between D_i and D_j?

To find, consider small increments δ for each component:

$$\delta D_i = \delta a\,C_i + a\,\delta C_i + \delta b$$

Square, and take expectation values:

$$\left\langle (\delta D_i \delta D_j) \right\rangle = \left\langle (\delta a\,C_i + a\,\delta C_i + \delta b)(\delta a\,C_j + a\,\delta C_j + \delta b) \right\rangle$$

$$= \left\langle (\delta a)^2 \right\rangle C_i C_j + a^2 \left\langle (\delta C_i \delta C_j) \right\rangle + \left\langle (\delta b)^2 \right\rangle$$

$$= \Delta^2 a\,C_i C_j + a^2 \Delta^2 C_i \delta_{ij} + \Delta^2 b$$

References for Data Covariances

"User's Guide to ALEX: Uncertainty Propagation from Raw Data to Final Results for ORELA Transmissions Measurements," N. M. Larson, ORNL/TM-8676, ENDF-332 (February 1984)

"Application of New Techniques to ORELA Neutron Transmission Measurements and their Uncertainty Analysis: the Case of Natural Nickel from 2 keV to 20 MeV," D. C. Larson, N. M. Larson, J. A. Harvey, N. W. Hill, and C. H. Johnson, ORNL/TM-8203, ENDF-333 (October 1983)

"Uncertainty Propagation from Raw Data to Final Results," N. M. Larson, *Proceedings of the International Conference on Nuclear Data for Basic and Applied Science, Santa Fe, New Mexico, May 13-17, 1985*, Vol. 2, ed. Phillip G. Young, et al., Gordon and Breach Science Publishers, 1533-1536 (1986)

"Covariances as Input to and Output from Resonance Analysis," N. M. Larson, invited paper presented at the International NEANSC Specialists' Meeting on Evaluation and Processing of Covariance Data, Oct 7-9, 1992, held at ORELA in Oak Ridge National Laboratory. Published in *Proceedings of a Specialists' Meeting on Evaluation and Processing of Covariance Data*, ed. M. Wagner 221-238 (1993).

"Representation and Processing of Covariance Matrices for Resonance Parameters," N. M. Larson, *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies*, Brookhaven National Laboratory, 22-23 April 1999.

Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology, Donald L. Smith, pub. *American Nuclear Society*, 555 N. Kensington Avernue, LaGrange Park, Illinois 60525 USA (1991).

How do we find parameter values?

Five-step process:

Step 1.	Reduce the data
Step 2.	Generate covariance matrix for data
Step 3.	Choose prior values for parameters
Step 4.	Find prior covariance matrix for parameters
Step 5.	Analyze the data

Several different methods:

Method 1.	The "conventional" approach
Method 2.	A better approach
Method 3.	The "usual" approach
Method 4.	Another wrong method
Method 5.	The hybrid approach
Method 6.	Implicit data covariance method

The "conventional" approach

(Method 1)

Step 1. Reduce the data

$$r_i \rightarrow d_i$$

raw data → reduced data

counts per channel → cross section

Note that

$$d_i = D(r_i, r_{\tilde{i}}, q_1, q_2, q_3, \ldots)$$

where q are data-reduction parameters

example: See Natural-Nickel Transmission paper

Step 2. Generate the data covariance matrix

Covariance matrix for *raw* data is diagonal:

$$\begin{pmatrix} \Delta^2 r_1 & 0 & 0 & 0 \\ 0 & \Delta^2 r_2 & 0 & 0 \\ 0 & 0 & \Delta^2 r_3 & 0 \\ 0 & 0 & 0 & \Delta^2 r_4 \end{pmatrix}$$

Simple case:

$$d_i = a r_i + b$$

Covariance matrix for *reduced* data is **not** diagonal:

$$\begin{pmatrix} (a^2\Delta^2 r_1 + r_1^2\Delta^2 a + \Delta^2 b) & & & \\ (r_1 r_2 \Delta^2 a + \Delta^2 b) & (a^2\Delta^2 r_2 + r_2^2\Delta^2 a + \Delta^2 b) & & \\ (r_1 r_3 \Delta^2 a + \Delta^2 b) & (r_2 r_3 \Delta^2 a + \Delta^2 b) & (a^2\Delta^2 r_3 + r_3^2\Delta^2 a + \Delta^2 b) & \\ (r_1 r_4 \Delta^2 a + \Delta^2 b) & (r_2 r_4 \Delta^2 a + \Delta^2 b) & (r_3 r_4 \Delta^2 a + \Delta^2 b) & (a^2\Delta^2 r_4 + r_4^2\Delta^2 a + \Delta^2 b) \end{pmatrix}$$

General case:

$$d_i = D(r_i, r_{\tilde{i}}, q_1, q_2, q_3, \ldots)$$

$$\delta d_i = \frac{\partial D_i}{\partial r_i}\delta r_i + \frac{\partial D_i}{\partial r_{\tilde{i}}}\delta r_{\tilde{i}} + \sum_k \frac{\partial D_i}{\partial q_k}\delta q_k$$

$$V_{ij} = \langle \delta d_i \delta d_j \rangle$$

$$= \delta_{ij}\left[\left(\frac{\partial D_i}{\partial r_i}\right)^2 \Delta^2 r_i + \left(\frac{\partial D_i}{\partial r_{\tilde{i}}}\right)^2 \Delta^2 r_{\tilde{i}}\right]$$

$$+ \sum_k \sum_l \frac{\partial D_i}{\partial q_k}\frac{\partial D_j}{\partial q_l}\langle \delta q_k \delta q_l \rangle$$

ALEX: Computer code to do the busy-work of generating V_{ij}

Natural Nickel: 30 parameters, 60,000 data points
1,800,030,000 elements in covariance matrix

Step 3. Find "prior" values for model parameters

- from the literature
- estimate by examining the data

Step 4. Set prior parameter covariance matrix

Note that conventional least squares implicitly assumes that prior uncertainties are infinite and correlations are zero.

Bayes' method (generalized least squares) requires explicit numbers:

- When uncertainties are known, they should be used. Correlations should also be included.
- When nothing is known use "non-informative prior" (i.e. infinite uncertainty). In SAMMY use ~ 10% of the parameter value, which is effectively infinite.

Step 5. Analyze the data

I.e. find values for parameters that give "best fit" to data
I.e. run SAMMY (or REFIT, or ... ?)

Output includes parameter values and parameter covariance matrix.

The end of conventional approach.

A better approach
(Method 2)

Fit the raw data directly

Step 1. Do not reduce the data (but do figure out exactly what would need to be done to convert to cross sections)

Step 2. Do not generate data covariance matrix (raw data has diagonal covariance matrix)

Step 3. Find prior values for model parameters, *including data-reduction parameters*

Step 4. Set prior parameter covariance matrix, *including uncertainties and covariances for data-reduction parameters*

Step 5. Analyze the data
Analysis code (e.g. SAMMY) must convert from cross-section to whatever function was actually measured

The "usual" approach
(Method 3)

Just like the "conventional" approach except pretend that the covariance matrix for the reduced data is diagonal:

Simple case:

$$\begin{pmatrix} (a^2\Delta^2 r_1 + r_1^2\Delta^2 a + \Delta^2 b) & & & \\ 0 & (a^2\Delta^2 r_2 + r_2^2\Delta^2 a + \Delta^2 b) & & \\ 0 & 0 & (a^2\Delta^2 r_3 + r_3^2\Delta^2 a + \Delta^2 b) & \\ 0 & 0 & 0 & (a^2\Delta^2 r_4 + r_4^2\Delta^2 a + \Delta^2 b) \end{pmatrix}$$

General Case:

$$V_{ij} = \delta_{ij}\left[\left(\frac{\partial D_i}{\partial r_i}\right)^2\Delta^2 r_i + \left(\frac{\partial D_i}{\partial r_i}\right)^2\Delta^2 r_i + \sum_k\sum_l \frac{\partial D_i}{\partial q_k}\frac{\partial D_i}{\partial q_l}\left\langle \delta q_k \delta q_l\right\rangle\right]$$

Question: What's wrong with this?

Answer: It can

- distort results
- hide inconsistencies

Which method to use?

The data-covariance approach is OK, *but often cumbersome*:

- Experimentalists don't like to generate covariance matrices
- There are too many numbers!
- Mistakes may be hidden from evaluators

The fit-to-raw-data approach is best, *but usually neither practical nor probable*:

- Analysis codes must include all the data-reduction procedures
- Experimentalists are not happy with publishing "counts per channel" rather than "cross section"

The "drop-the-off-diagonal-elements" approach is just plain wrong!

Fortunately, there are alternatives...

Possible Analysis Methods

Method 1. Fit reduced data using true off-diagonal covariance matrix -- "the conventional approach"

Method 2. Fit to raw data, using data-reduction operations (in reverse) on the theory instead of on the data -- "a better approach"

Method 3. Fit reduced data using diagonal part of covariance matrix (both statistical and systematic errors) -- "the usual approach"

Method 4. Fit reduced data using only statistical errors (diagonal)

Method 5. Fit reduced data with pseudo data-reduction parameters included (hybrid method)

Method 6. Adjust the reduced data using parameter values obtained in Method 5, then fit using implicit data covariance

Note that method 2 is exact,
methods 1, 5, and 6 are correct,
methods 3 & 4 are wrong!

Example: ^{241}Am

(See test case tr74 and exercise ex018, neither is exactly like this example, but both are similar)

artificial data --

- Assume the "raw data" are related to the experimental fission cross section as $r_i = (1.030 \times \sigma_i + 4.970$ barns).

- Assume the uncertainty on r_i is given by

$$\Delta r_i = \sqrt{r_i}$$

- The reduced data should then be of the form

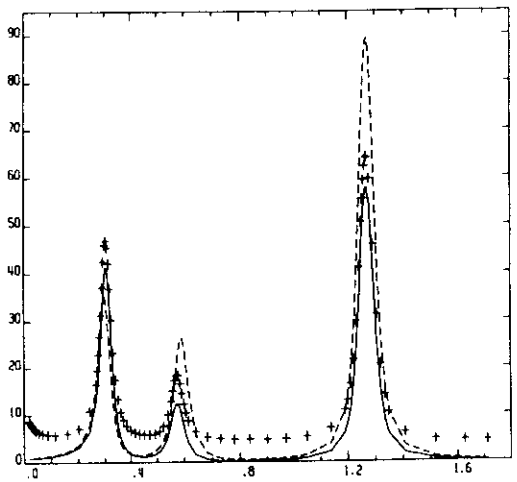
$$d_i = a r_i + b$$

where normalization a is ~ 1/1031 ≈ 0.00097
and background b is ~ - 4970/1031 ≈ - 4.82

- Assume the experimenter measured the normalization and background (erroneously) as

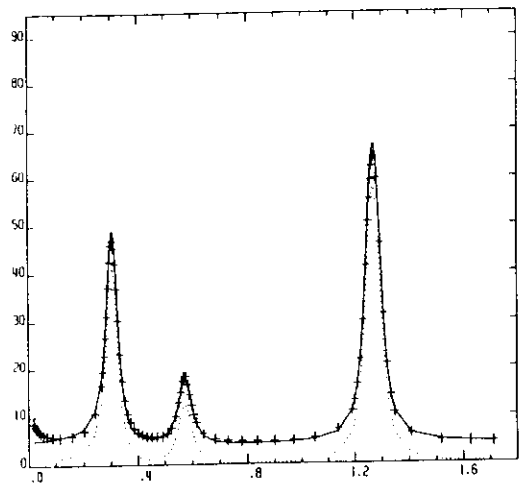
$a = 0.00105 \pm 0.00007$
$b = -1.05 \quad \pm 1.05$

Query: Can the analysis process nevertheless give the correct cross section (i.e. the correct resonance parameters) ?



Fission cross section for ^{241} Am
Using Method 1
(fit reduced data using covariance matrix)

- crosses = reduced data
- dashed curve = *a priori* parameter values
- solid curve = SAMMY fit

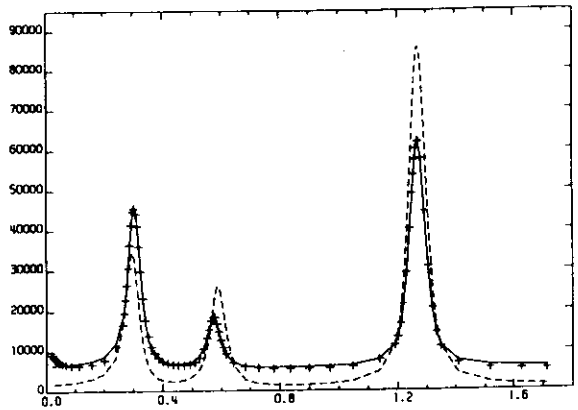


Fission cross section for ^{241} Am

Using Method 1, revised plot

(fit reduced data using covariance matrix)

- crosses = reduced data
- dotted curve = SAMMY fit (as shown in solid curve on previous plot)
- solid curve = SAMMY fit adjusted by data-reduction parameters (1.08421×dotted+4.17895)

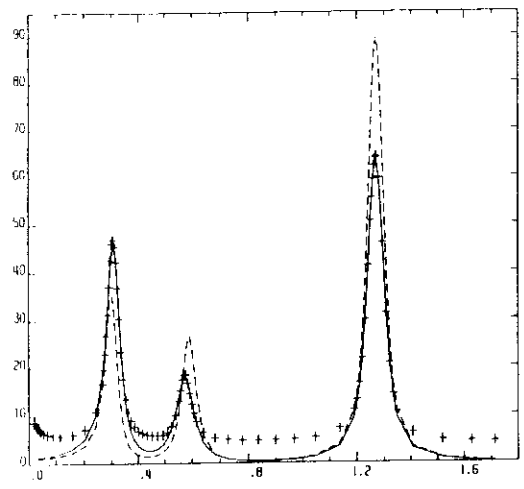


Fission cross section for ^{241} Am

Using Method 2, "a better approach"

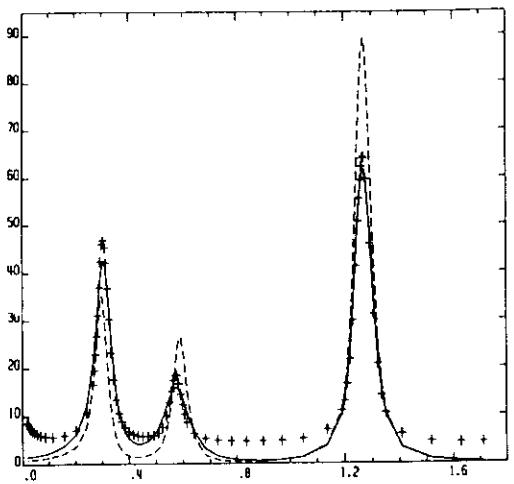
(fit raw data using data-reduction operations in reverse)

- crosses = raw data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit



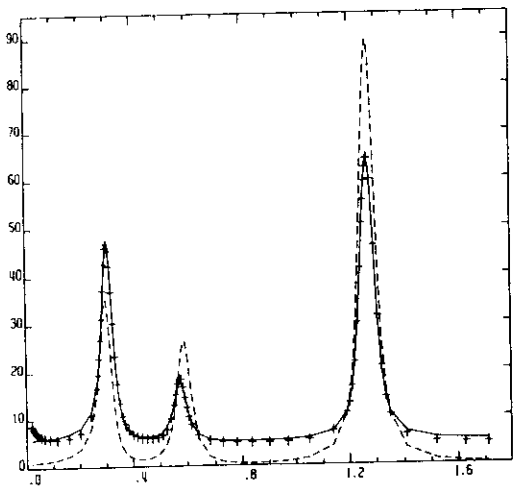
Fission cross section for ^{241} Am
Using Method 3, "the usual approach"
(fit reduced data using diagonal portion of covariance matrix)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit



Fission cross section for ^{241} Am
Using Method 4
(fit reduced data with statistical errors only)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

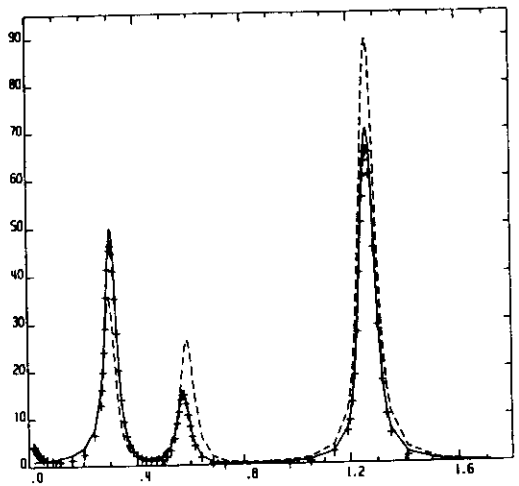


Fission cross section for ^{241} Am

Using Method 5

(fit reduced data but include data-reduction operations)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit



Fission cross section for ^{241}Am

Using Method 6, implicit data covariance

(fit *adjusted* reduced data)

- crosses = adjusted reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

Comparison of parameter values

Method 1 (full covariance matrix)
Method 2 (raw data = "truth")
Method 3 (diagonal part of covariance matrix)
Method 4 (statistical uncertainties only)
Method 5 (hybrid method)
Method 6 (implicit data covariance)

	prior	1	2	3	4	5	6
E_1	.3000	.3072	.3070	.3076	.3078	.3070	.3071
Γ_1	47.39	43.48	43.41	55.52	67.05	43.42	43.81
Γ_{1f}	.3200	.3251	.3394	.4012	.4491	.3385	.3496
E_2	.5900	.5762	.5760	.5758	.5775	.5760	.5757
Γ_2	48.15	47.58	46.80	70.20	108.5	46.85	45.66
Γ_{2f}	.6000	.4592	.4729	.6576	.8822	.4720	.4771
E_3	1.270	1.269	1.269	1.269	1.269	1.269	1.269
Γ_3	47.69	42.92	42.81	55.06	59.82	42.82	42.72
Γ_{3f}	.8001	.5897	.6267	.7571	.8033	.6243	.6478

Note that there are actually five parameters for each resonance: energy E_λ, widths Γ_γ, Γ_n, Γ_{f1}, and Γ_{f2}. However, the combinations which are relevant to fission cross sections for isolated resonances are those listed above. These are E_λ, $\Gamma_\lambda = \Gamma_{\lambda\gamma} + \Gamma_{\lambda n} + |\Gamma_{\lambda f1}| + |\Gamma_{\lambda f2}|$, and $\Gamma_{\lambda f} = |\Gamma_{\lambda f1}| + |\Gamma_{\lambda f2}|$.

Formulae for Implicit Data Covariances

Data covariance matrix has the form

$$V^{ij} = v^i \delta_{ij} + \sum_k X_k^i w_k X_k^j$$

where

V is the data covariance
v represents the statistical uncertainties
X is the sensitivity matrix (partial derivative of data with respect to data-reduction parameters)
w is the covariance matrix for the data-reduction parameters

The inverse is

$$V^{-1} = (v + X w X^t)^{-1}$$
$$= v^{-1} - v^{-1} X (w^{-1} + X^t v^{-1} X)^{-1} X^t v^{-1} \qquad *$$

Dimension of V is thousands × thousands
of v is thousands × thousands but diagonal
of X is thousands × tens (but needed anyway)
of w is tens × tens (and usually diagonal)

Use Eq. (*) for inverse of V as needed in Bayes' equations.

Parameter Covariance Matrix

- Generated automatically by SAMMY
- Printed in LPT file (as uncertainties plus correlation matrix)
- Stored in COVaraince file for use as input for subsequent SAMMY run
- Can be stored in abbreviated ASCII format

Covariance vs Correlation

$$C_{ij} = <\delta P_i \delta P_j> = \Delta P_i \, c_{ij} \, \Delta P_j$$

C_{ij} is the covariance matrix element between parameters P_i and P_j

ΔP_i is uncertainty on P_i

c_{ij} is the correlation coefficient between P_i and P_j

Note that

$$-1 \leq c_{ij} \leq +1$$

Covariances for Multigroup Cross Sections

- Used extensively for the first time by Herve Derrien et al.: *Covariance Matrices for Use in Criticality Safety Predictability Studies*; ORNL/TM-13492, September 1997

- Procedure:

  (1) fit differential & integral data => generate values and covariances for resonance parameters

  (2) calculate differential cross sections with those parameter values; integrate numerically to give group cross sections and covariance matrices

Example: ^{235}U
89 resonances in 0 to 50 eV

Parameters for first seven J=3 resonances:

*****NEW VALUES FOR RESONANCE PARAMETERS

SPIN GROUP NUMBER 1 WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G*ABNDNC= .4375

"true" radius =	9.0000E+00	9.0000E+00	9.0000E+00
effective radius =	9.6566E+00	9.6566E+00	9.6566E+00

ENERGY	GAMMA-GAMMA	GAMMA-GAMMA CHANNEL 1 L=0 SPIN= 3.0	GAMMA-GAMMA CHANNEL 2 L=0 SPIN= 0.0	GAMMA-GAMMA CHANNEL 3 L=0 SPIN= 0.0
(EV)	(MILLI-EV)	(MILLI-EV)	(MILLI-EV)	(MILLI-EV)
3.01247E-01(1)	4.0422E+01(2)	4.7777E-03(3)	1.2256E+02(4)	2.2049E-01(5)
2.03586E+00(6)	3.7310E+01(7)	9.1821E-03(8)	-1.0168E+01(9)	8.0360E-01(10)
3.14379E+00(11)	3.8108E+01(12)	2.5643E-02(13)	-2.1236E+01(14)	8.7458E+01(15)
6.18423E+00(16)	5.4780E+01(17)	7.0752E-02(18)	-4.1715E+01(19)	1.6535E+02(20)
7.65320E+00(21)	5.7182E+01(22)	3.4280E-03(23)	5.9150E+01(24)	1.0897E+02(25)
8.88961E+00(26)	4.9288E+01(27)	1.4995E-01(28)	-2.1569E+02(29)	1.3539E+02(30)
9.71692E+00(31)	4.2720E+01(32)	3.9741E-02(33)	-3.9670E+00(34)	-2.1020E+02(35)

Absolute and Relative Uncertainties and Correlation Matrix for First Seven J=3 Resonances

	Absolute Uncertainty	Relative Unc.	Correlations 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	4.6545E-04	.002	100														
2	0.8939	.022	-6	100													
3	3.6718E-05	.008	25	51	100												
4	1.255	.010	41	-57	-5	100											
5	2.0350E-02	.092	15	-4	7	-1	100										
6	1.6199E-04	.000	2	-1	0	3	1	100									
7	0.3718	.010	1	1	-3	0	-1	2	100								
8	6.1601E-05	.007	2	3	50	0	1	2	-23	100							
9	0.2398	.024	-9	-1	-1	2	3	-16	-20	-10	100						
10	5.5672E-02	.069	23	-1	0	1	-3	39	-5	3	-3	100					
11	4.1068E-04	.000	7	0	1	2	-1	-3	-3	-1	-6	3	100				
12	0.6285	.016	0	3	0	-1	-1	1	3	0	-4	2	6	100			
13	1.6094E-04	.006	1	2	51	2	2	3	-1	57	-2	2	-17	9	100		
14	0.9287	.044	-26	1	-6	-3	4	6	3	-4	11	-30	-61	-16	8	100	
15	1.175	.013	21	-2	3	5	-2	-1	-3	1	-7	26	22	-22	8	-53	100
16	1.5426E-03	.000	-2	1	-1	0	1	3	0	-2	0	-3	10	1	-2	4	-5
17	2.177	.040	-1	1	0	-1	0	0	2	1	-1	-2	2	3	1	0	-2
18	1.0838E-03	.015	-5	1	19	0	2	2	-1	22	1	-8	4	1	24	7	-7
19	2.443	.059	-26	2	-5	-5	5	1	-1	-3	8	-32	-2	2	-2	29	-26
20	3.073	.019	15	-2	0	3	-3	0	0	-1	-3	21	-1	-2	1	-15	18
21	4.8203E-03	.001	7	0	-2	2	-1	0	-2	-3	1	-3	2	-1	-4	8	-8
22	4.292	.075	1	0	-1	0	0	0	1	-1	0	-1	1	1	-1	2	-3
23	1.4500E-04	.042	-10	1	5	-3	2	1	0	5	0	-3	2	1	8	2	-1
24	5.431	.092	-3	-1	0	-2	0	-1	0	-1	-1	3	4	0	-3	-4	2
25	8.324	.076	0	0	0	0	0	2	-1	-1	0	0	-3	0	2	2	1
26	7.7058E-03	.001	13	-1	2	3	-3	-2	2	2	-2	14	-2	0	3	-9	10
27	3.446	.070	-5	1	0	-1	2	1	0	-1	0	-8	2	1	-1	5	-6
28	5.1809E-03	.035	-20	2	5	-3	6	4	-4	6	4	-25	10	1	6	20	-22
29	9.069	.042	-29	2	-1	-7	5	0	-1	2	4	-20	0	1	1	13	-13
30	7.272	.054	6	0	-4	2	0	0	-2	-4	0	-2	0	0	-4	6	-4
31	2.0991E-03	.000	0	0	-2	1	1	1	-2	-2	1	-4	4	0	-2	5	-5
32	2.413	.056	0	0	0	0	0	0	1	0	-1	0	1	2	-1	0	-1
33	8.5402E-04	.021	13	-1	15	3	-2	-1	1	16	-4	16	-7	0	19	-15	16
34	0.3810	.096	-1	0	0	0	0	1	0	0	0	-1	1	0	1	1	-1
35	5.252	.025	6	-1	1	2	-2	-1	1	0	-2	10	-9	-1	3	-9	13

			16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
17	2.177	.040	48	100													
18	1.0838E-03	.015	76	39	100												
19	2.443	.059	-24	-8	0	100											
20	3.073	.019	16	-34	24	-59	100										
21	4.8203E-03	.001	-9	0	-8	29	-26	100									
22	4.292	.075	1	0	-1	2	-2	-9	100								
23	1.4500E-04	.042	2	-2	0	-16	8	-46	22	100							
24	5.431	.092	5	-1	-5	-6	-1	14	-5	22	100						
25	8.324	.076	-12	-1	-2	5	-3	-6	-11	36	-30	100					
26	7.7058E-03	.001	2	-3	-1	-26	19	-9	-3	0	1	4	100				
27	3.446	.070	2	2	3	9	-7	2	-2	3	1	1	-19	100			
28	5.1809E-03	.035	6	3	4	31	-30	9	3	10	6	-3	-54	35	100		
29	9.069	.042	6	3	6	12	-7	-29	-1	28	7	0	-4	-1	12	100	
30	7.272	.054	-10	0	-4	18	-14	40	7	-15	-4	-2	-20	2	4	-31	100
31	2.0991E-03	.000	2	0	2	10	-7	21	4	2	-4	14	-4	5	24	-11	54
32	2.413	.056	2	1	0	-1	0	0	0	0	0	0	7	-14	-3	2	-3
33	8.5402E-04	.021	-9	-1	4	-21	17	5	-1	-9	2	-2	-10	-3	-26	-52	29
34	0.3810	.096	2	0	1	-2	1	2	1	3	0	2	5	-2	1	-15	14
35	5.252	.025	-10	-1	0	-13	15	-2	0	-8	0	-7	-13	8	-20	-30	23

			31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
32	2.413	.056	3	100													
33	8.5402E-04	.021	-17	10	100												
34	0.3810	.096	-23	-1	0	100											
35	5.252	.025	-24	-34	73	-7	100										

Group-Averaged Capture Cross Section

Table 7. The averaged capture cross sections and their uncertainties for the lowest 45 groups of the 199-group structure of the VITAMIN-B6 library. The energy boundaries of the groups are given in eV and the cross sections in barns.

	E-min	E-max	theory	uncertainty
(1)	.00001	.00050	1583.62	2.19118
(2)	.00050	.00200	581.447	.814407
(3)	.00200	.00500	332.593	.479974
(4)	.00500	.01000	217.260	.332767
(5)	.01000	.01450	160.512	.265833
(6)	.01450	.02100	126.564	.229096
(7)	.02100	.03000	99.1694	.201790
(8)	.03000	.04000	79.6855	.184531
(9)	.04000	.05000	67.0371	.175575
(10)	.05000	.07000	55.4726	.171735
(11)	.07000	.10000	44.5069	.178960
(12)	.10000	.12500	37.9880	.200970
(13)	.12500	.15000	34.9931	.235094
(14)	.15000	.18400	33.9773	.298876
(15)	.18400	.22500	36.2010	.432866
(16)	.22500	.27500	42.6642	.671274
(17)	.27500	.32500	41.2566	.722969
(18)	.32500	.36680	29.1536	.459712
(19)	.36680	.41399	20.2983	.253470
(20)	.41399	.50000	14.0817	.118298
(21)	.50000	.53158	11.2708	6.544099E-02
(22)	.53158	.62506	9.70383	4.212451E-02
(23)	.62506	.68256	8.48628	2.794191E-02
(24)	.68256	.80000	7.75934	2.375308E-02
(25)	.80000	.87643	7.55463	2.912808E-02
(26)	.87643	1.00000	8.73944	5.500305E-02
(27)	1.00000	1.04000	12.0877	.111810
(28)	1.04000	1.08000	16.3936	.180070
(29)	1.08000	1.12530	24.2145	.299789
(30)	1.12530	1.30000	20.2525	.222470
(31)	1.30000	1.44500	6.60897	8.043458E-02
(32)	1.44500	1.85540	3.84365	1.096020E-02
(33)	1.85540	2.38240	13.3112	8.596037E-02
(34)	2.38240	3.05900	3.56924	3.195349E-02
(35)	3.05900	3.92790	16.2886	.124316
(36)	3.92790	5.04350	21.0874	.123322
(37)	5.04350	6.47600	46.5651	.244552
(38)	6.47600	8.31530	16.2042	8.814033E-02
(39)	8.31530	10.67700	34.4581	.192407
(40)	10.67700	13.71000	67.3420	.253481
(41)	13.71000	17.60400	17.4441	8.699141E-02
(42)	17.60400	22.60300	43.7486	.193572
(43)	22.60300	29.02300	20.0091	.109174
(44)	29.02300	37.26600	34.8962	.157284
(45)	37.26600	47.85100	17.3388	8.418739E-02

Uncertainties and Correlations for Group-averaged Capture Cross Sections

Table 11. The correlation matrix of the capture cross sections for the lowest 45 groups of the 199- group structure of the VITAMIN-B6 library. The absolute errors are given in column 2 of the table, and the correlation coefficients (×100) follow.

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2.19118	100														
2	.814407	100	100													
3	.479974	100	100	100												
4	.332767	100	100	100	100											
5	.265833	100	100	100	100	100										
6	.229096	100	100	100	100	100	100									
7	.201790	99	99	99	100	100	100	100								
8	.184531	99	99	99	99	100	100	100	100							
9	.175575	99	99	99	99	100	100	100	100	100						
10	.171735	99	99	99	99	99	100	100	100	100	100					
11	.178960	98	98	98	99	99	99	100	100	100	100	100				
12	.200970	98	98	98	98	99	99	99	100	100	100	100	100			
13	.235094	97	97	98	98	98	99	99	99	99	100	100	100	100		
14	.298876	97	97	97	97	98	98	98	99	99	99	99	100	100	100	
15	.432866	95	95	95	95	96	96	96	97	97	97	98	98	99	99	100
16	.671274	90	90	90	91	91	91	92	92	92	93	93	94	95	96	98
17	.722969	88	88	89	89	89	89	90	90	90	90	91	91	92	93	95
18	.459712	92	92	92	92	92	93	93	93	93	93	93	93	93	93	93
19	.253470	94	94	94	94	95	95	95	95	95	95	95	95	95	94	93
20	.118298	95	95	96	96	96	96	97	97	97	97	96	96	96	95	93
21	6.544099E-02	96	96	96	96	97	97	97	97	97	97	97	96	96	95	92
22	4.212451E-02	95	95	95	96	96	96	96	96	96	96	96	95	94	93	91
23	2.794191E-02	90	90	90	90	90	91	91	91	90	90	89	89	88	86	84
24	2.375308E-02	72	72	72	73	73	73	73	72	72	72	71	70	69	68	65
25	2.912808E-02	45	45	45	45	45	45	45	45	44	44	43	42	41	40	38
26	5.500305E-02	24	24	24	24	24	24	24	24	24	23	22	21	21	20	18
27	.111810	16	16	16	16	16	16	16	16	16	15	15	14	13	12	11
28	.180070	13	13	13	13	13	13	13	13	13	13	12	12	11	10	10
29	.299789	11	11	11	11	11	11	11	12	11	11	11	10	10	9	8
30	.222470	13	13	13	13	13	13	12	12	12	11	10	10	9	8	8
31	8.043458E-02	8	8	8	7	7	7	7	6	6	6	6	6	5	5	5
32	1.096020E-02	24	24	24	24	24	24	24	23	23	22	21	20	19	18	17
33	8.596037E-02	7	7	6	6	6	6	6	6	6	6	6	5	5	5	5
34	3.195349E-02	8	8	8	8	8	8	7	7	7	7	7	6	6	6	6
35	.124316	8	8	8	8	8	8	8	8	7	7	7	7	7	7	6
36	.123322	3	3	3	3	3	3	2	2	2	2	2	2	2	2	2
37	.244552	4	4	4	4	4	4	4	4	4	4	3	3	3	3	2
38	8.814033E-02	4	4	4	4	4	4	4	4	3	3	3	3	3	2	2
39	.192407	5	5	5	5	5	5	5	4	4	4	4	3	3	3	2
40	.253481	5	5	5	5	5	5	5	5	4	4	4	4	3	3	3
41	8.699141E-02	3	3	3	3	3	3	3	3	3	3	3	2	2	2	2
42	.193572	4	4	4	4	4	4	4	4	4	4	4	3	3	3	2
43	.109174	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1
44	.157284	4	4	4	4	4	4	4	4	4	4	3	3	3	2	2
45	8.418739E-02	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1

		16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
16	.671274	100														
17	.722969	98	100													
18	.459712	94	98	100												
19	.253470	92	95	99	100											
20	.118298	90	93	98	100	100										
21	6.544099E-02	89	91	96	99	100	100									
22	4.212451E-02	87	89	94	97	98	99	100								
23	2.794191E-02	80	82	87	90	92	95	98	100							
24	2.375308E-02	62	63	68	70	74	78	85	94	100						
25	2.912808E-02	36	37	40	42	46	52	61	76	94	100					
26	5.500305E-02	17	18	20	22	25	32	41	60	83	97	100				
27	.111810	10	11	12	14	18	24	33	52	76	93	99	100			
28	.180070	9	9	10	12	15	21	30	48	71	88	96	99	100		
29	.299789	8	8	8	10	13	18	26	42	63	79	87	92	97	100	
30	.222470	7	8	8	9	12	17	24	39	57	69	71	72	73	79	100
31	8.043458E-02	4	4	5	5	7	9	12	19	26	31	33	35	36	37	15
32	1.096020E-02	16	17	18	20	23	29	37	53	71	80	79	74	70	64	64
33	8.596037E-02	5	6	6	6	7	8	9	11	13	14	13	12	11	10	10
34	3.195349E-02	5	4	4	4	5	7	9	12	16	17	16	15	15	15	13
35	.124316	6	6	6	6	7	8	10	14	17	18	16	15	15	15	14
36	.123322	1	2	2	2	2	3	4	6	8	9	8	8	8	8	7
37	.244552	2	2	3	3	4	5	7	9	12	13	12	12	12	11	11
38	8.814033E-02	2	2	2	3	3	4	6	9	11	12	11	11	11	11	11
39	.192407	2	3	3	3	4	6	8	11	15	16	15	14	14	13	13
40	.253481	3	3	3	3	4	6	8	11	15	16	15	15	15	15	14
41	8.699141E-02	2	2	2	2	3	4	6	8	11	11	11	10	10	10	9
42	.193572	2	2	3	3	4	5	7	10	14	15	14	14	14	13	13
43	.109174	1	1	2	2	2	3	4	6	8	9	8	8	8	8	8
44	.157284	2	2	2	3	3	5	6	9	12	13	13	12	12	12	11
45	8.418739E-02	1	1	1	2	2	3	4	6	8	9	8	8	8	8	8

		31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
31	8.043458E-02	100														
32	1.096020E-02	54	100													
33	8.596037E-02	6	33	100												
34	3.195349E-02	9	28	10	100											
35	.124316	8	25	11	30	100										
36	.123322	3	11	7	6	12	100									
37	.244552	5	17	9	8	15	17	100								
38	8.814033E-02	5	16	9	9	16	15	26	100							
39	.192407	6	20	11	11	20	19	28	30	100						
40	.253481	5	20	13	10	22	23	34	30	43	100					
41	8.699141E-02	4	15	9	8	16	15	23	22	30	34	100				
42	.193572	5	19	12	10	21	21	32	29	41	48	34	100			
43	.109174	3	12	8	7	15	14	21	20	28	32	25	33	100		
44	.157284	4	17	11	8	19	19	29	26	38	45	31	43	31	100	
45	8.418739E-02	3	12	8	7	16	14	22	21	30	35	27	35	28	35	100

Communicating the Resonance-Parameter Covariance Matrix

"Representation and Processing of Covariance Matrices for Resonance Parameters," N. M. Larson, Oak Ridge National Laboratory, prepared for the *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies* held at Brookhaven National Laboratory, April 22-23, 1999

Wanted: Communicate resonance-parameter covariance matrices from the originator (e.g. SAMMY) to the user (e.g. AMPX or NJOY)

Method: Store covariance matrix in ASCII file

Needed first: Abbreviate the Matrix --

- ^{235}U has 3193 resonances, five parameters per resonance => 15965 parameters total.
- Number of elements in (half of) covariance matrix = (15965×15966)/2 = 127,448,595 elements

Question:

Can an abbreviated covariance matrix contain the same information as the complete covariance matrix?

Answer:

Probably

How to test?

- Generate a realistic resonance-parameter covariance matrix
- Calculate integral quantities and associated covariance matrix using various approximations to the "true" resonance-parameter covariance matrix
- Compare results (uncertainties and covariances for the calculated multigroup cross sections)

Recommendations for ASCII storage of resonance-parameter covariance matrix (based on results of preliminary tests as described above):

- Store covariance matrix as uncertainties plus correlation matrix
- Drop correlations smaller than 1 %
- Represent correlation as n-digit integer
- $n = 2$ may be adequate
- Further study is desirable

Sensitivity Matrix

Requirements for processing code (AMPX, NJOY, ...):

- covariance matrix
- sensitivity matrix (partial derivatives of point-wise cross sections with respect to resonance parameters)

How do the codes obtain the sensitivity matrix?

- write FORTRAN to generate analytic derivatives
- make use of "automatic derivative" routines to produce line-by-line derivatives of existing code
- calculate numerical derivatives (*not* recommended!)
- read sensitivities generated by SAMMY

Alternative: Use SAMMY to generate multigroup cross sections and associated covariance matrix

- FORTRAN coding already exists

Integral Quantities in SAMMY

a "recent" addition to the code...

Cross Section Analysis: Differential Data

- Transmission
- Capture cross sections
- η
- Fission
- Absorption
- etc.

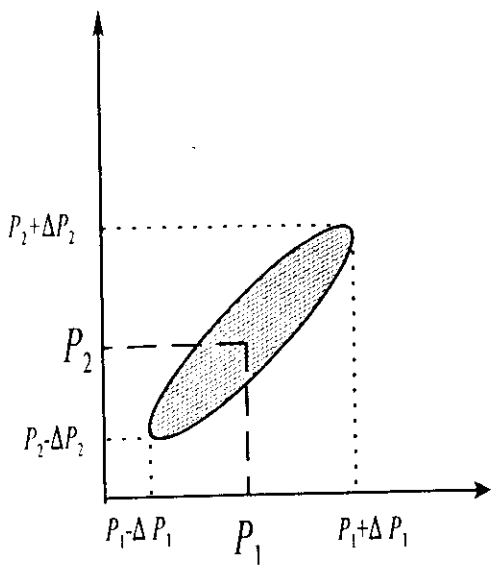
To analyze, use SAMMY:

0. Estimate values for (resonance & other) parameters
1. Generate theoretical values & partial derivatives (using appropriate theory such as Reich-Moore approx. to multilevel R-matrix)
2. Correct for "real world" effects (e.g. finite sample thickness)
3. Find "best fit" values for parameters using Bayes' method (generalized least squares)
4. Iterate steps 1-3 for nonlinearities, more data, etc.

RESULT:

A non-unique* set of resonance parameters which describe the differential data; and a covariance matrix describing the uncertainties on and interrelationships among those parameters.

* Why non-unique? Because of uncertainties and correlations...



"True" values of P_1 and P_2 are somewhere in the shaded area.

Integral Data

- Thermal cross section
- Maxwellian average
- Westcott's g-factor
- Resonance integral
- Average integral
- $K1$, K_{eff}
- α
- Reaction Rates

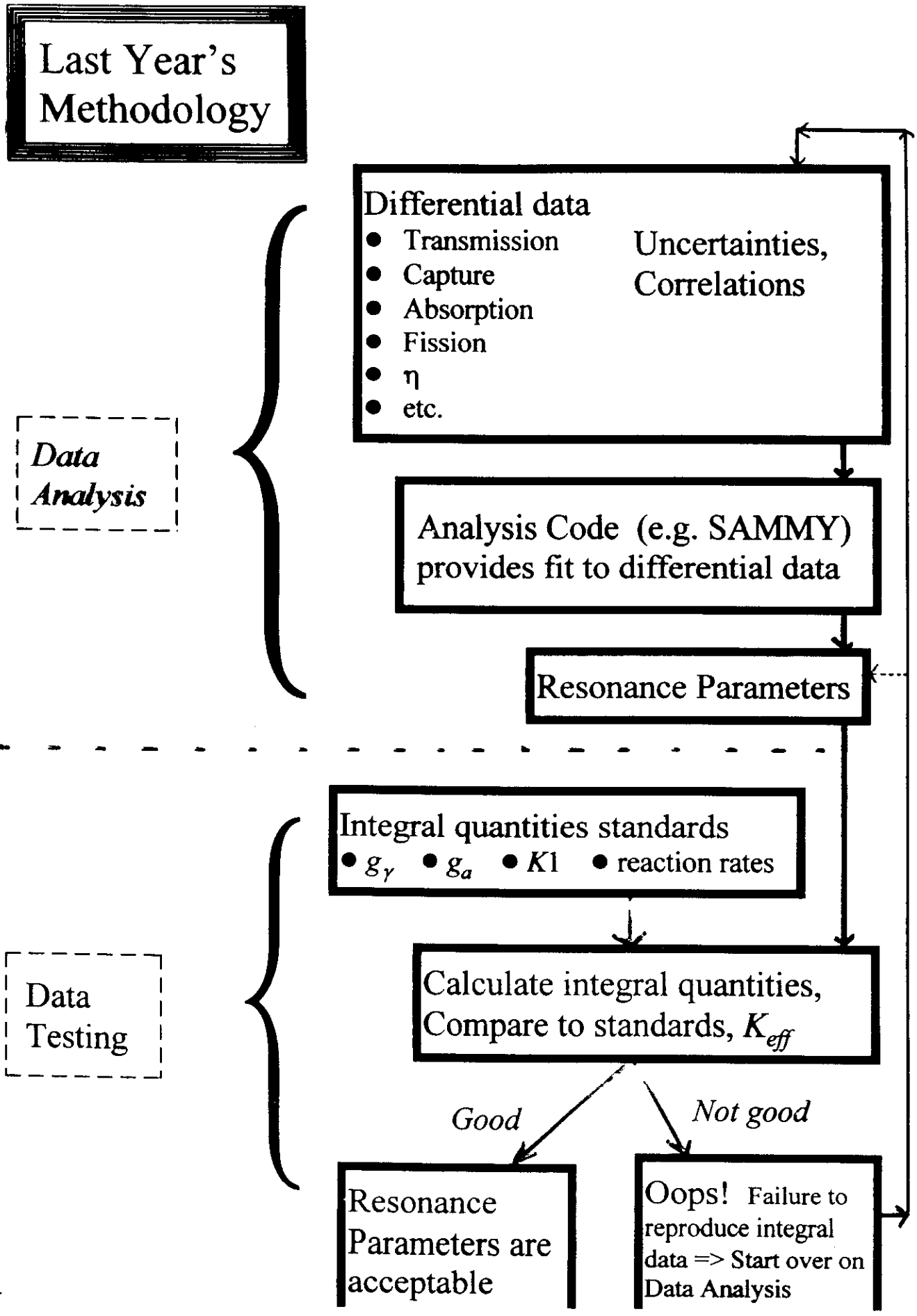
Use NJOY, AMPX, or other codes to calculate values:

0. Use resonance parameter values from differential analyses
1. Generate theoretical values
2. Correct for "real world" effects

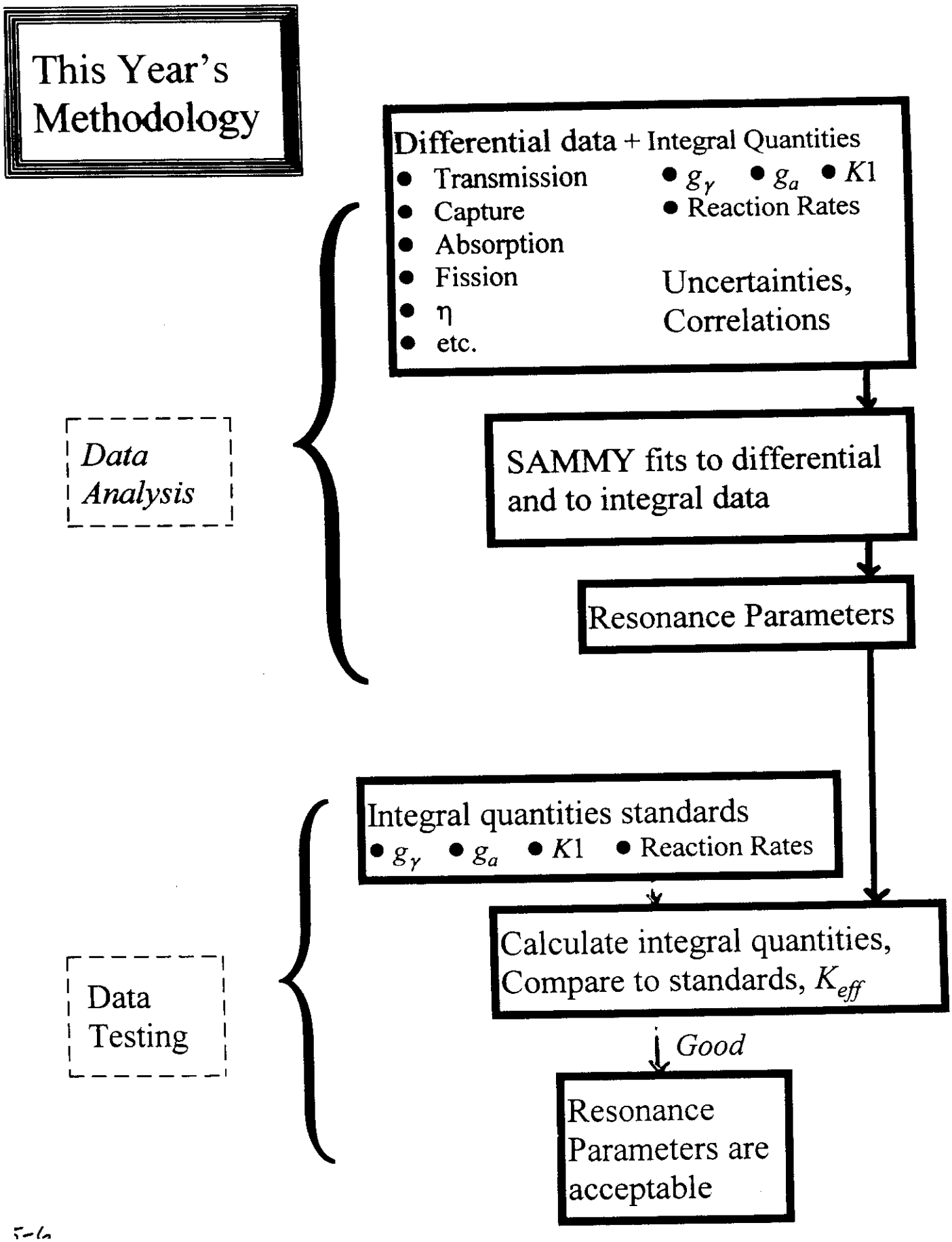
3,4. ? no options for fitting or iterating ?

RESULT:

Compare measured (or standard) values with calculation; either they agree or they don't.


Last Year's Methodology
Differential data
Transmission
Capture
Absorption
Fission
η
etc.
Uncertainties, Correlations
Data Analysis
Analysis Code (e.g. SAMMY) provides fit to differential data
Resonance Parameters
Integral quantities standards
g_γ g_a K1 reaction rates
Data Testing
Calculate integral quantities, Compare to standards, K_{eff}
Good
Not good
Resonance Parameters are acceptable
Oops! Failure to reproduce integral data => Start over on Data Analysis

This Year's Methodology



Definitions of Integral Quantities

which may be included in evaluation process in SAMMY

(1) Thermal cross section

$$\sigma_{0x} = \sigma_x(E_0) \qquad \text{for } E_0 = 0.0253\text{eV}$$

(2) Maxwellian average at thermal energy

$$\bar{\sigma}_x = \int_{E_1}^{E_2} \sigma_x(E)\ \frac{E}{E_0}\ e^{-E/E_0}\ dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0}\ e^{-E/E_0}\ dE$$

where $E_1 = 10^{-5}$ eV and $E_2 = 3$ eV

(3) Westcott's g-factor

$$g_x = \frac{2}{\sqrt{\pi}}\ \frac{\bar{\sigma}_x}{\sigma_{0x}}$$

(4) Resonance integral

$$I_x = \int_{E_3}^{E_4} \sigma_x(E)\ \frac{dE}{E} + X_{4x}$$

(5) Average integral

$$\hat{\sigma}_x = \int_{E_5}^{E_6} \sigma_x(E)\ dE \Big/ (E_6 - E_5)$$

(6) Watt spectrum average

$$\bar{\sigma}_{Wf} = \int_{E_1}^{E_7} \sigma_f(E)\ \Phi(E)\ dE \Bigg/ \int_{E_1}^{E_7} \Phi(E)\ dE$$

with $E_7 = 20$ MeV

and $\Phi(E)$ = Watt fission spectrum

$$\Phi(E) = e^{-E/a} \sinh(\sqrt{bE})$$
$$= e^{-E/a} \left(e^{\sqrt{bE}} - e^{-\sqrt{bE}}\right)/2$$

(7) $K1$ (indicative of K_{eff} for thermal benchmarks)

$$K1 = \nu\,\sigma_{0f} g_f - \sigma_{0a} g_a = (\nu\,\bar{\sigma}_f - \bar{\sigma}_a)\ \frac{2}{\sqrt{\pi}}$$

(8) Alpha

$$\alpha = I_c / I_f$$

(9) Thermal alpha integral (NJOY's α),

$$\alpha_{NJOY} = \frac{\int_{E_1}^{E_2} \frac{\sigma_c(E)}{\sigma_f(E)} \frac{E}{E_0} e^{-E/E_0} dE}{\int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE}$$

(10) Thermal eta integral (NJOY's η),

$$\eta_{NJOY} = \frac{\int_{E_1}^{E_2} \frac{\nu \sigma_f(E)}{\sigma_a(E)} \frac{E}{E_0} e^{-E/E_0} dE}{\int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE}$$

Recent Addition to SAMMY (not in M2)

Flux-weighted group cross sections:

$$\bar{\sigma}_g = \int_{E_g}^{E_{g+1}} \sigma(E)\, \Phi(E)\, dE \Big/ \int_{E_g}^{E_{g+1}} \Phi(E)\, dE$$

with several options for $\Phi(E)$ —

Option 1: Bondarenko narrow-resonance weighting scheme,

$$\Phi(E) = \frac{C(E)}{\sigma_0 + \sigma_t(E,T)}$$

where

$C(E)$ = smooth function of energy

σ_0 = dilution

$\sigma_t(E,T)$ = Doppler-broadened total cross section

Option 2: flux is given numerically on energy grid (for intermediate spectrum, useful in criticality predictability)
(not yet included in SAMMY, but "on the drawing board")

Covariances are calculated for the group cross sections.
(However, fitting is not permitted, only calculations.)

Example: ^{235}U

Differential measurements: 14 data sets analyzed via SAMMY

Details for ^{235}U can be found in

L. C. Leal, H. Derrien, N. M. Larson, and R. Q. Wright, *R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV*, to be published as ORNL/TM-13516, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (November 1997). Also *Nucl. Sci. and Eng.* **131** 230 (February 1999).

Integral Standards: six quantities have been included in analysis

Details can be found in

N. M. Larson, L. C. Leal, and H. Derrien, "Integral Data Analysis for Resonance Parameters Determination," ORNL-TM-13495, Oak Ridge National Laboratory, Lockheed Martin Energy Research, Inc. (1997). Also *Nucl. Sci. and Eng.* **131** 254 (February 1999).

References for "**Selected Measurements for ^{235}U**"

2. J. A. Harvey, N. W. Hill, F. G. Perey, G. L. Tweed, and L. C. Leal, *Proc Int. Conf. On Nuclear Data for Science and Technology*, Mito, Japan (May 30-June 3, 1988).
3. R. R. Spencer, J. A. Harvey, N. W. Hill, and L. Weston, *Nucl. Sci. Eng.* **96**, 318 (1987).
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10. G. de Saussure, R. Gwin, L. W. Weston, and R. W. Ingle, *Simultaneous Measurements of the Neutron Fission and Capture Cross Section for ^{235}U for incident neutron energy from 0.4 eV to 3 keV*, ORNL/TM-1804, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, Oak Ridge, TN (1967).
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25. H. Weigmann, P. Geltenbort, B. Keck, K. Shrenckenbach, and J. A. Wartena, *Proc. Intern. Conf. on The Physics of Reactors*, Marseille 1990, Vol. P1, p. 133 (1990).
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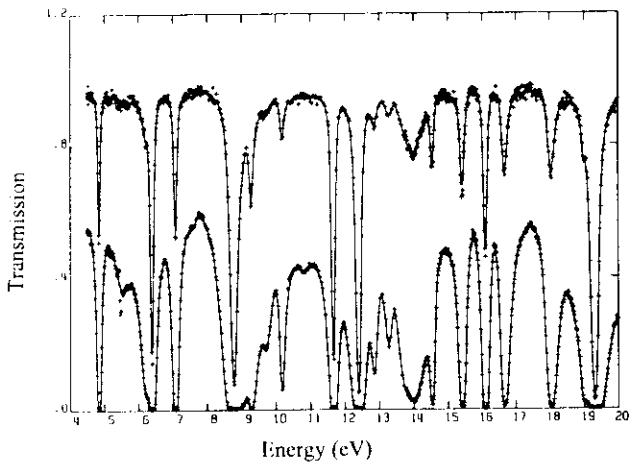
27. R. Gwin, To be published in *Nuclear Science Engineering* and as ORNL/TM (1997).
28. L. W. Weston and J. H. Todd, *Nucl. Sci. Eng.* **88**, 567 (1984).
31. C. Wagemans, P. Schillebeeckx, A. J. Deruyter, and R. Barthelemy, "Subthermal fission Cross Section measurements for ^{233}U and ^{239}Pu," *Nuclear Data for Science and Technology*, p. 91, Mito, Japan (1988).
32. R. A. Schrack, "Measurement of the $^{235}U(n,f)$ Reaction from Thermal to 1 keV," *Nuclear Data for Science and Technology*, p. 101, Mito, Japan (1988).
47. R. Gwin, R. R. Spencer, R. W. Ingle, J. H. Todd, and S. W. Scoles, *Nuc. Sci. Eng.* **88**, 37 (1984).

Selected Measurements for ^{235}U

Reference	Energy range (eV)	Data set number	Data
de Saussure (RPI/1967)[10]	0.01 - 2250.0	5,6	**Fission & capture** at 25.2 m
Perez (ORNL/1972)[11]	0.01 - 100.0	7,8	**Fission & capture** at 39.7 m
Weston (ORNL/1984)[28]	14.0 - 2250.0	14	**Fission** at 18.9 meters
Gwin (ORNL/1984)[47]	0.01 - 20.0	9	**Fission** at 25.6 meters
Spencer (ORNL/1984)[3]	0.01 - 1.0	10	**Transmission** at 18 meters and sample thickness of 0.001468 atom/barn
Harvey (ORNL/1986)[2]	0.4 - 68.0	1	**Transmission** at 18 meters. Sample thickness of 0.03269 atom/barn cooled to 77 K
Harvey (ORNL/1986)[2]	4.0 - 2250.0	2	**Transmission** at 80 meters. Sample thickness of 0.00233 atom/barn cooled to 77 K
Harvey (ORNL/1986)[2]	4.0 - 2250.0	3	**Transmission** at 80 meters. Sample thickness of 0.03269 atom/barn cooled to 77 K
Wartena (Geel/1987)[24]	0.0018 - 1.0		**Eta** at 8 meters
Wagemans (Geel/1988)[31]	0.001 - 0.4	11	**Fission** at 18 meters
Schrack (RPI/1988)[32]	0.02 - 20	4	**Fission** at 8.4 meters
Weigmann (ILL/1990)[25]	0.0015 - 0.15		**Eta** (Chopper)
Weston (ORNL/1992)[4]	100.0 - 2000.		**Fission** at 86.5 meters
Moxon (ORNL/1992)[26]	0.01 - 50.0		**Fission Yield**
Gwin (ORNL/1996)[27]	0.01 - 4.0	12,13	**Absorption and fission**



^{235}U Transmission data of Harvey et al. for two sample thicknesses (0.03269 barns and 0.00233 barns)

Comparison between experimental and calculated thermal values and integral quantities for ^{235}U

Quantity	Measured, recommended, and standard values	Fit to differential data	Fit to differential plus integral data
σ_{0f} (barn)	584.25 ± 1.11	584.28	584.88
$\sigma_{0\gamma}$ (barn)	98.96 ± 0.74	99.18	98.66
σ_{0s} (barn)	15.46 ± 1.06	15.44	15.67
$K1$ (barn)	722.7 ± 3.90	717.48	722.43
g_f	0.9771 ± 0.0008	0.9743	0.9764
g_a	0.9790 ± 0.0008	0.9774	0.9785

Higher-Energy Regions:

- Unresolved- Resonance Region
- High-Energy Region

Method: beg, borrow, steal from existing codes; incorporate into SAMMY (with the authors' blessings)

Initial modifications are for compatibility only, eventually refine and expand

Equations for Unresolved Resonance Region

SAMMY implementation based on Fritz Fröhner's FITACS program

- Hauser-Feshbach theory gives average total cross cross section

$$\langle \sigma_c \rangle = \frac{\pi g_c}{k_c^2} \left(1 - \mathrm{Re}\langle S_{cc} \rangle\right)$$

- Average scattering matrix $\langle S \rangle$ is given by

$$\langle S_{cc} \rangle = e^{-2i\phi_c} \frac{1 - \langle R_{cc} \rangle L_c^{0*}}{1 - \langle R_{cc} \rangle L_c^{0}}$$

- Average R-matrix is

$$\langle R_{cc} \rangle = R_c^{\infty} + i\pi s_c$$

with

ϕ_c	=	hard-sphere scattering phase
R_c^{∞}	=	distant-level parameter
s_c	=	pole strength, equal to $S_c \sqrt{E} / 2 k_c a$
S_c	=	strength function
a	=	R-matrix matching radius

- Moldauer's prescription gives (non-elastic) partial cross sections in terms of "transmission coefficients" T_x

$$\langle \sigma_{ab} \rangle = \frac{2\pi g_a}{k_a^2} \frac{T_a T_b}{T} \times \int_0^{\infty} dt\, e^{-tT_\gamma/T} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t\right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}}$$

where

a	=	incident channel		b =	exit channel
ν_c	=	degrees of freedom (multiplicity)			
T_c	=	transmission coefficient		γ =	photon channels
T	=	sum over all channels, $T = \sum_c T_c$			

- Transmission coefficient for neutron channels is

$$T_c = 1 - |\langle S_{cc} \rangle|^2 = \frac{4\pi P_c s_c}{1 - \langle R_{cc} \rangle L_c}$$

- Transmission coefficient for photon channel for spin J is

$$T_\gamma = 2\pi \langle \Gamma_\gamma \rangle / D_J$$

- Transmission coefficient for fission channel for spin J is

$$T_f = 2\pi \langle \Gamma_f \rangle / D_J$$

where D_J is the mean level spacing.

- Bethe formula gives J-dependence of the mean level spacing

$$\left(D_J(E)\right)^{-1} = \left(d(E)\right)^{-1} \times \left\{ \exp\left[\frac{-J^2}{2\left(\sigma(E)\right)^2}\right] - \exp\left[-\frac{(J+1)^2}{2\left(\sigma(E)\right)^2}\right] \right\}$$

where

d is independent of J
σ is the spin cutoff whose value is determined by the code.

- Gilbert-Cameron composite formula is used for energy dependence of the mean level spacing :

  - At low energy ($E_x \le E_0$) use the constant-temperature formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_0 - PE}\right)}{(E_0 - PE)^{3/2}} \times \exp\left[\frac{E_x - E_0}{2}\left(\frac{C_2}{\sqrt{E_0 - PE}} - \frac{3}{E_0 - PE}\right)\right]$$

where

E_x = excitation energy of compound nucleus
E_0 = matching energy , is given by the constant-temperature formula
PE = pairing energy
C_2 and C_3 = constants

  - At higher energies ($E_x \ge E_0$), use the Fermi-Gas formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_x - PE}\right)}{(E_x - PE)^{3/2}}$$

- Radiation widths $<\Gamma_\gamma>$ depend only on parity π and on E. Energy dependence calculated with giant dipole resonance model.

- Fission widths $<\Gamma_f>$ vary with spin as well as parity and E. Energy dependence calculated with the Hill-Wheeler fission barrier transmission coefficients.

$$\Gamma_f(E) > = <\Gamma_f(0)> \frac{1 + \exp\left(E_{HW} / W_{HW}\right)}{1 + \exp\left(-(E - E_{HW}) / W_{HW}\right.}$$

where

E_{HW} = Hill-Wheeler threshold energy

W_{HW} = Hill-Wheeler threshold width

Assumptions for derivation of Moldauer's prescription

- Single-level Breit-Wigner is an adequate description of the cross section (i.e., resonances are well separated).

- Neutron widths obey the Porter-Thomas distribution (chi-squared with one degree of freedom); averages are therefore weighted with this distribution.

- The average of products can be written as the product of averages.

- Channels with the same transmission coefficients may be combined by introducing multiplicities.

Input for Unresolved-Resonance Region

Files needed:

- INPut file with three lines; the optional fourth line may be used only for Version M5, not M2 or M2a.

  Card Set 1: This line is title only.

  Card Set 2: Nuclide name, atomic weight, energy range

  Card Set 3: UNRESOLVED RESONANCE REGION

  (optional): EXPERIMENTAL DATA ARE IN SEPARATE FILES

- ACS file (same as Fröhner's original FITACS file); see table for details (page 6-9).

- DATa files (for version M5, not M2 or M2a); see table for details.

Changes made for SAMMY-M2

- Internal changes to be consistent with SAMMY notation and to use dynamic dimensioning
- Bayes' method for fitting procedure (prototype for eventual "restructured" SAMMY fitting module)
- Extension to all l - values
- Output includes "odf" files (plotting files)
- Results are reported in same format as input ACS file, in SAMMY.PAR (as well as in more legible fashion in SAMMY.LPT)

More recent changes (available in future releases):

- As many data sets as desired (original code permitted at most one of each type)
- Separate file for each data set
- Energy-dependent normalization for each data set; normalization parameters can be varied
- Refinement (debugging) of partial derivatives for more accurate fitting
- More efficient quadrature scheme for Dresner integral

Needed Yet:

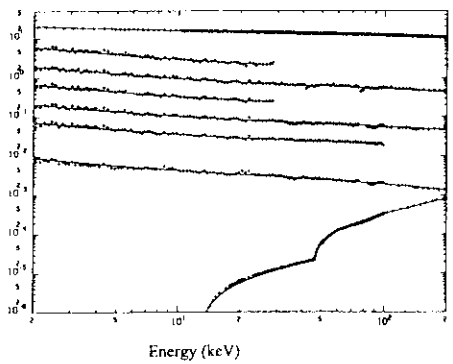
- Use results of resolved-resonance region analysis as input for analysis of unresolved region
- Experience!
- Generalize the theory as needed

Input for ACS file for treatment of the unresolved resonance region

Line No.	Description
1 - 4	First four lines are alphanumeric title
5	Number of iterations, fitting tolerance (essentially, delta chi-squared). Note that integers are to be specified as real numbers. All formats are F10
6	Mass in amu, radius in Fermi (or use default), neutron binding energy in MeV, pairing energy *PE* in MeV. Again, formats are F10
7,8,...	Center-of-mass excitation energy, spin, and parity for the *n*th target level (beginning with ground state)
9	(Blank)
10	Strength function S_c, uncertainty, distant-level parameter R_c^{∞}, uncertainty, radiation width $<\Gamma_\gamma>$ in eV, uncertainty, mean level spacing D in eV for $l = 0$
11	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
12	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
13, 14, ...	As above, for higher l values as needed
15	(Blank)
16, ...	Average fission width $<\Gamma_f>$ (eV), degree of freedom ν_f for fission width distribution, Hill-Wheeler threshold energy E_{HW}, HW threshold width W_{HW}, , uncertainty on the average fission width
17	(Blank)
(Cards 18-21 may appear in separate files, for Version M5, if the phrase EXPERIMENTAL DATA ARE IN SEPARATE FILES appears in the INPut file.)	
18	Type of cross-section data (TOTAl, CAPTure, FISSion, or INELastic)
19	Uncertainties are RELAtive or ABSOlute
20, ...	Energy, cross section, uncertainty (Note: if RELAtive then need specify only for first data point, rest are assumed to be the same)
21	(Blank)
22, ...	Repeat 18 to 21 as many times as needed, in any order
(The following cards are relevant only for version M5, not for M2 or M2a.)	
23	The single word "NORMALIZATION" in all capital letters or all lower case
24	Type of cross section, normalization parameters a, Δa, b, Δb, c, Δc, where the normalization for this data set is given by $norm = a + b\,E^{c}$
25, etc.	Repeat once for each data set. Note that normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent

Example: ^{235}U

(from current work of Herve Derrien; please note that results are preliminary and are not to be distributed)



SAMFFF fit of ^{235}U experimental data in the energy range 2 keV to 200 keV. Crosses represent the experimental data (or evaluated data); solid lines are the cross sections calculated from average resonance parameters and nuclear parameters. The upper curve is the total cross section of Harvey (ORNL). The other curves represent (from upper to lower):

- Blons (Saclay) fission cross section (not modified)
- Migneco (Geel) fission cross section (divided by 3)
- Wagemans (Geel) fission cross section (didided by 9)
- Weston (ORNL) fission cross section (divided by 27)
- Perez (ORNL) fission cross section (divided by 81)
- Capture cross section inferred from Weston fission and experimental values of alpha (divided by 243)
- Inelastic cross section from ENDF/B-VI (divided by 1000)

Experimental fission data are average values from the original values found in the EXFOR file, using the same energy grid in the averaging code. The following parameters were varied:

- neutron strength function of angular momentum $l = 0, 1, 2$
- average fission widths
- average capture widths
- effective radius
- normalization coefficient for each set of fitted data

The normalization coefficients allow us to obtain a consistent set of data, which means that the same set of nuclear and average resonance parameters could represent all data in the experimental data base (after corrections for the remaining experimental effects).

Coming Attractions

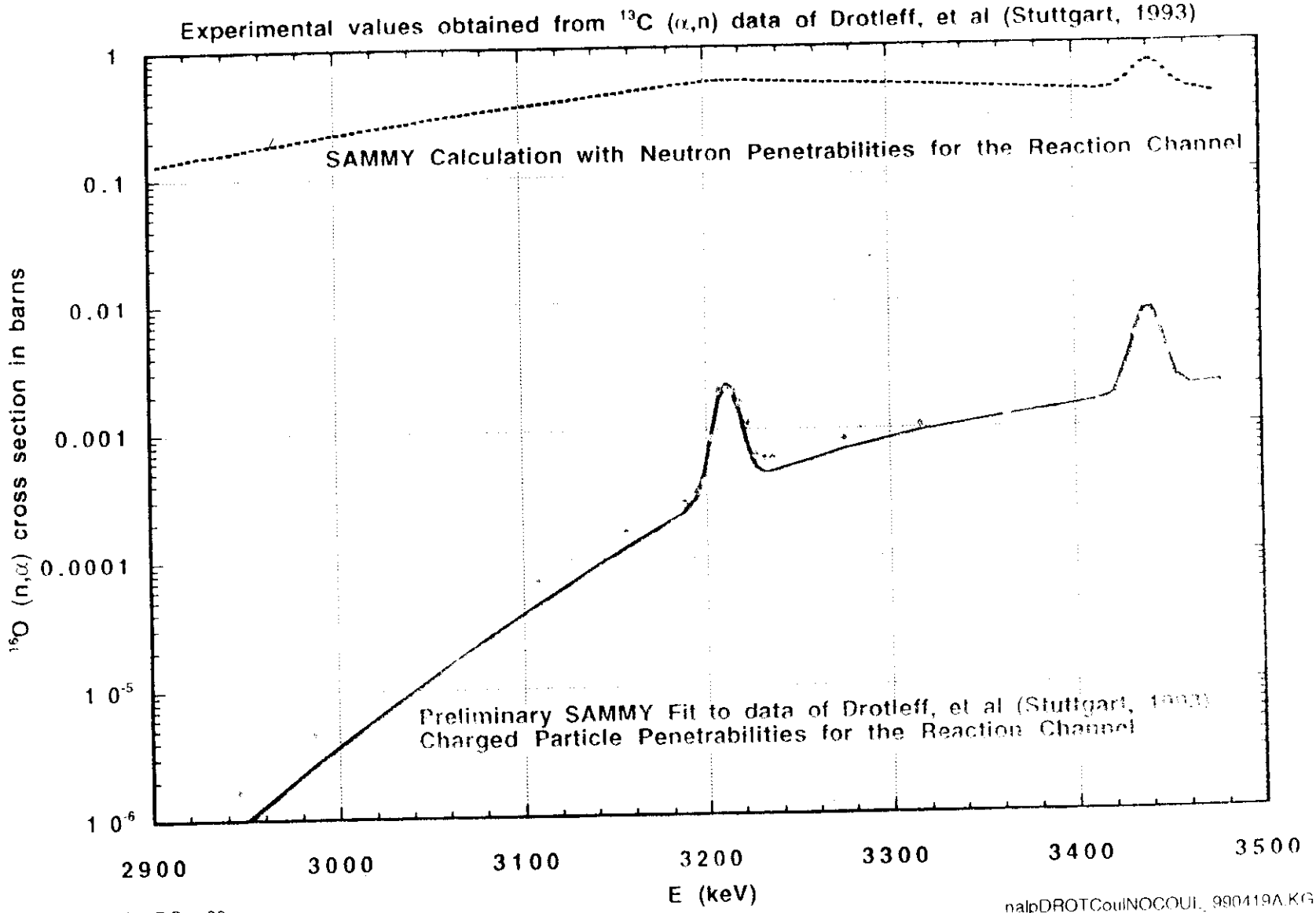
- Revision 5 of the Users' Manual, plus new RSICC release of the FORTRAN (version M5), mid 2000?
- Additional testing & improvements for multiple-scattering corrections (in M5)
- More work on unresolved-resonance and high-energy regions
- Charge-dependent penetrabilities (will be in R5 and M5)
- Restructuring to permit truly simultaneous analysis of any and all data sets
- Interface with other codes for use of covariance matrix
- More Integral Quantities (for intermediate energies)
- Full R-matrix theory (no approximation such as Reich-Moore)
- More options for resolution function
- Time-of-flight rather than energy as independent variable
- Modern Graphical User Interface (probably, extension of RSAP code)
- Separate final states (e.g. inelastic vs fission) (in M5)

Charge-Dependent

Penetrabilities, etc.

- for use with charged-particle final states
- possibly also for proton-induced reactions
- coding using charge-dependent penetrabilities, shift factors, and phase shifts has been developed by Royce Sayer, "meshed" with the author's "current working version" of SAMMY, and tested carefully
- Sayer's analysis of ^{16}O, with Coulomb, will be released soon

Predictions for $\sigma_{n,\alpha}$ using both Charged Particle and Neutron Penetrabilities for the Reaction Channel



R. O. Sayer ORNL 17 Sep 99

nalpDROTCoulNOCOUL_990419A.KG

Bayes' Equations can be rewritten as

$$P' = P + M' Y$$

$$M' = (M^{-1} + W)^{-1}$$

$$Y = G^t V^{-1} (D - T)$$

$$W = G^t V^{-1} G$$

where P represents the parameter values, M the parameter covariance matrix, D the data, V the data covariance matrix, T the theory, and G the partial derivatives of T with respect to P (i.e., the sensitivity matrix). Primes => updated values & covariance matrix.

All data-set-dependence is summarized in Y and W, which are strictly additive with respect to independent data sets:

$$Y = Y_1 + Y_2 + Y_3 + \ldots$$
$$W = W_1 + W_2 + W_3 + \ldots$$

So we can generate the pieces from each data set, add them up, and *then* solve Bayes' Equations once and for all. This simplifies current problems involving non-linearity, ordering of sequential analyses, etc.

QUESTIONNAIRE RE SAMMY RESTRUCTURING

October, 1998 (Page 243 of Users' Manual)

At some as-yet-undetermined future date, the multilevel R-matrix code SAMMY will be restructured to take full advantage of the strengths inherent in Bayes' equations, to provide the ability to perform truly simultaneous fits to multiple experimental data sets (both differential and integral). Details of this proposed restructuring are discussed elsewhere [NL98b]. The restructured code will be denoted SAMSON (SON of SAMMY).

Since major changes to input are required to accomplish this restructuring, this would seem to be a good time to make other (helpful but not necessary) changes as well. A short description of both necessary and optional changes is given here:

INPUT FILES:

Information from the SAMMY INPut file will be located more logically: A title line, and commands relevant to the complete run, will be in a new COMmand file. Spin group definitions (quantum numbers etc) will be placed in the PARameter files, along with values for any R-matrix parameters such as channel radii. Experiment-specific information (type of data, nuclear abundances, Doppler temperature, resolution parameters, etc.) will appear in a new EXPeriment file.

The SAMSON PARameter file will contain all R-matrix information, including spin group definitions (quantum numbers etc.) that had been in the SAMMY INPut file. Resonance parameters will remain in the PARameter file. No experiment-specific information (e.g. nuclear abundances) will be in the new PAR file. Although the SAMMY PARameter file often contains resonance parameters for more than one nuclide, the SAMSON PAR file will relate to one nuclide only; hence several PAR files may be needed for any given run.

The SAMSON EXPeriment file will contain all information relevant to one particular experimental data set; some of this information had been in the SAMMY INPut file, and some in the SAMMY PARameter file

The SAMSON DATa file is identical to the SAMMY DATa file.

OUTPUT FILES:

SAMMY.LPT will be similar to the SAMMY file.

An updated version of the SAMSON PARameter file will be created for each PAR file that contains flagged (varied) parameters.

An updated version of the EXPeriment file will be created for each EXP file that contains flagged (varied) parameters.

A binary COVariance file will be produced, containing essentially the same information as is now included in the SAMMY COVariance file.

SAMMY USER PREFERENCES (page 244 of Users' Manual)

Name, address, e-mail_____

1. a. Output PARameter files should be given the same name as the corresponding input PAR file, with extension _____ (please specify) to distinguish the two. YES ___ NO ___

   b. Output PAR files should be named SAM01.PAR, SAM02.PAR, ... YES ___ NO ___

   c. Output PAR file names should be specified by the user. YES ___ NO ___
   If yes, how/where?_____

2. a. Output PAR files should contain the *initial* uncertainties for flagged parameters. YES ___ NO ___

   b. Output PAR files should contain the *updated* uncertainties for flagged parameters. YES ___ NO ___

3. a. Output EXPeriment files should be given the same name as the corresponding input EXP file, with extension _____ (please specify) to distinguish the two. YES ___ NO ___

   b. Output EXP files should be named SAM01.EXP, SAM02.EXP, ... YES ___ NO ___

   c. Output EXP file names should be specified by the user. YES ___ NO ___
   If yes, how/where?_____

4. a. Output EXP files should contain the *initial* uncertainties for flagged parameters. YES ___ NO ___

   b. Output EXP files should contain the *updated* uncertainties for flagged parameters. YES ___ NO ___

5. a. Output plot files should be given the same name as the corresponding input EXPeriment file, with extension _____ (please specify) to distinguish the two. YES ___ NO ___

   b. Output plot files should be named SAM01.ODF, SAM02.ODF, ... YES ___ NO ___

   c. Output plot file names should be specified by the user. YES ___ NO ___
   If yes, how/where?_____

6. a. Default uncertainties for all parameters should be specified by the same value of FUDGE, which is given in the COM file. YES ___ NO ___

   b. A value for FUDGE should be given in each PAR and EXP file. YES ___ NO ___

7. An option should be added to provide resonance parameter uncertainties on the line following the parameter values in the SAMSON PARameter file. YES ___ NO ___

8. Please send suggestions re formatting for the input data covariance matrix. _____
   _____

9. Use this space for any other suggestions regarding SAMMY and/or SAMSON.

Please return completed questionnaire to N. M. Larson, Oak Ridge National Laboratory, Building 6011, MS 6370, Post Office Box 2008, Oak Ridge, TN 37831-6370. Or e-mail responses to nml@ornl.gov.

Feedback for SAMMY portion of
Workshop on Nuclear Reaction Data and Nuclear Reactors
March 15-20, 2000

Name (optional) _____

Favorite part of workshop _____

Least favorite part of workshop _____

What should be omitted? _____

What else should be included? _____

The lectures are too long ___ too short ___ about right ___ (Comments?) _____

Lecture content is appropriate ___ irrelevant ___ (Please provide specifics) _____

Computer sessions are too long ___ too short ___ OK ___ (Comments?) _____

Tutorial content is appropriate ___ irrelevant ___ (Specifics) _____

Time for SAMMY workshop is too short __ too long __ about right __

Would you encourage others to participate in future SAMMY workshops? Yes __ No __
Why or why not?_____

What can the lecturers do to improve their presentations? Please specify whether your comments refer to Nancy, to Luiz, or to both.

Other comments?

Many thanks for taking the time to fill out this form and help us improve the quality of the workshop! -- Nancy & Luiz