UT-BATTELLE

SAMMY Workshop

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Part 2, details about use of the code SAMMY

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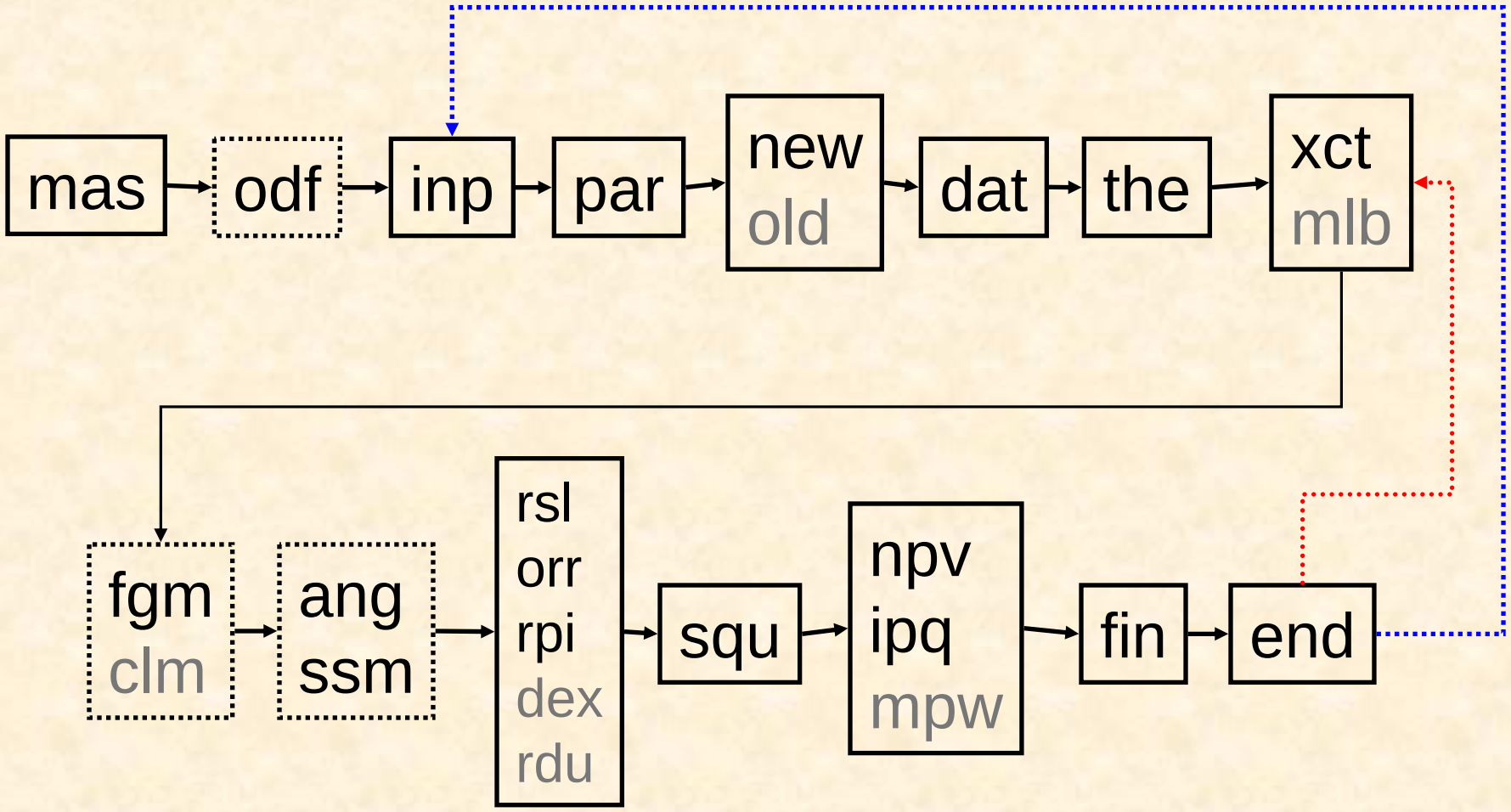
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

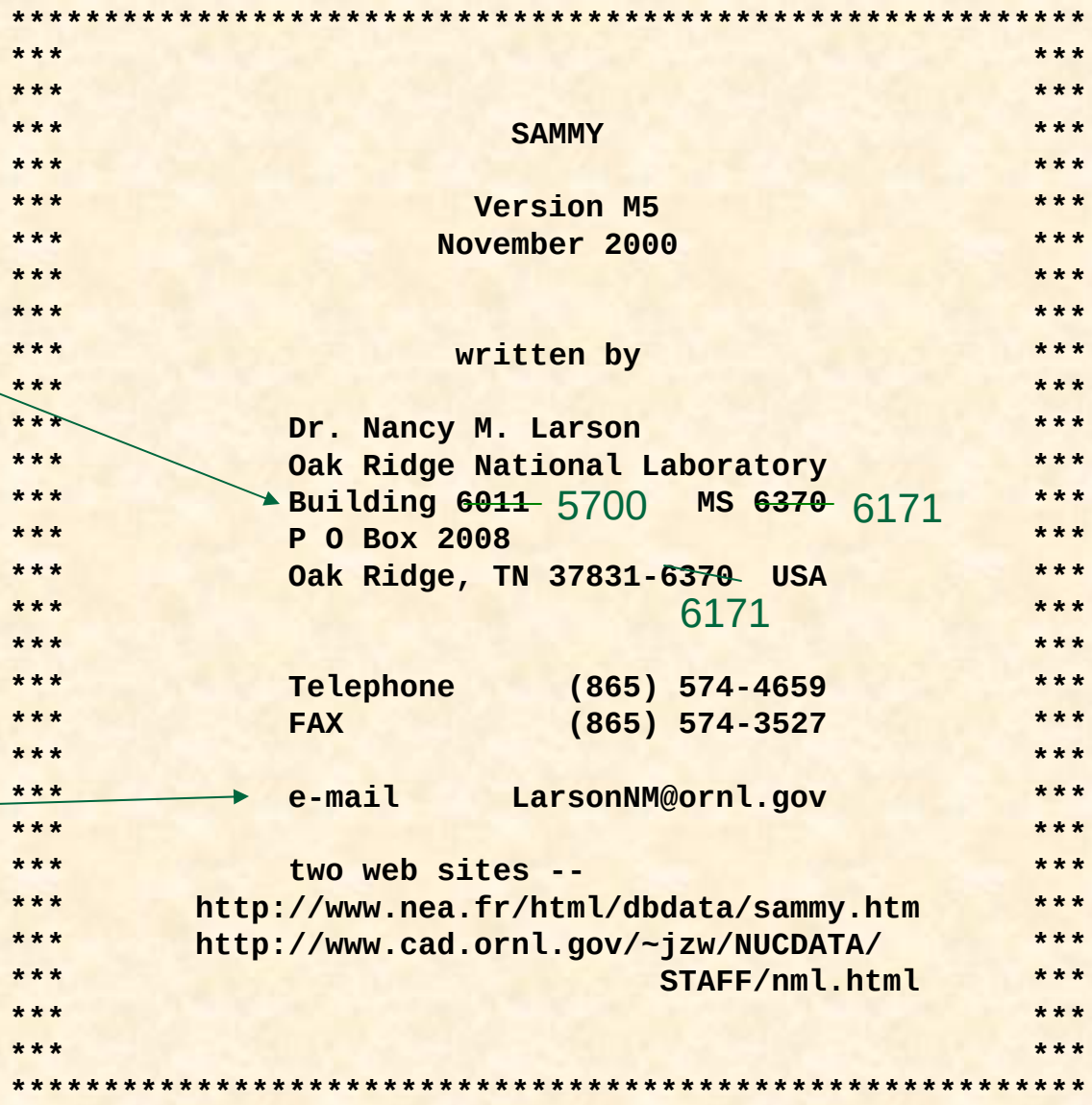
Flow chart for SAMMY



What appears on the screen as you run SAMMY

Warning – address on screen is not correct, use what was in the intro.

(e-mail address is still OK)



... the screen

```
*** M5-SAMMY       16 Feb 01 ***
 WHAT IS NAME OF INPUT FILE?
 >>> ex001a.inp                                          <<<
 WHAT IS NAME OF PARAMETER FILE?
 >>> ex001a.par                                          <<<
 WHAT IS FIRST DATA FILE NAME? EMIN? EMAX?
 >>> ex001a.dat                                          <<<
 WHAT IS NEW EMIN? EMAX? DATA SET NAME?

 *** M5-SAMMY-ODF    7 Nov 00 ***
 *** M5-SAMMY-INPUT  7 Nov 00 ***
 *** M5-SAMMY-PAR   15 Dec 00 ***
 *** M5-SAMMY-NEW    7 Nov 00 ***
 *** M5-SAMMY-DATA   7 Nov 00 ***  8.040     TO  11.96
 *** M5-SAMMY-THEOR  7 Nov 00 ***
 *** M5-SAMMY-XCT   21 Dec 00 ***
 *** M5-SAMMY-FGM    7 Nov 00 ***
 *** M5-SAMMY-INTRP  7 Nov 00 ***
 *** M5-SAMMY-(N+V)  7 Nov 00 ***
 *** M5-SAMMY-FINAL  5 Jan 01 ***
```

No iterations for this run

What appears on the screen, more typical case

```
**************************************************************
***                                                        ***
***          November 2000  Version M5 of SAMMY            ***
***                                                        ***
**************************************************************


*** M5-SAMMY       16 Feb 01 ***
WHAT IS NAME OF INPUT FILE?
>>> ex001b.inp                                            <<<
WHAT IS NAME OF PARAMETER FILE?
>>> ex001b.par                                            <<<
WHAT IS FIRST DATA FILE NAME? EMIN? EMAX?
>>> ex001a.dat                                            <<<
WHAT IS NEW EMIN? EMAX? DATA SET NAME?
...
```

... the screen, more typical case

```
*** M5-SAMMY-ODF     7 Nov 00 ***
*** M5-SAMMY-INPUT   7 Nov 00 ***
*** M5-SAMMY-PAR    15 Dec 00 ***
*** M5-SAMMY-NEW     7 Nov 00 ***
*** M5-SAMMY-DATA    7 Nov 00 ***  8.040     TO  11.96
*** M5-SAMMY-THEOR   7 Nov 00 ***
*** M5-SAMMY-XCT    21 Dec 00 ***
*** M5-SAMMY-FGM     7 Nov 00 ***
*** M5-SAMMY-INTRP   7 Nov 00 ***
*** M5-SAMMY-SQUAR   7 Nov 00 ***
*** M5-SAMMY-(I+Q)   7 Nov 00 ***
*** M5-SAMMY-FINAL   5 Jan 01 ***
*** M5-SAMMY-THEOR   7 Nov 00 ***
*** M5-SAMMY-XCT    21 Dec 00 ***
*** M5-SAMMY-FGM     7 Nov 00 ***
*** M5-SAMMY-INTRP   7 Nov 00 ***
*** M5-SAMMY-SQUAR   7 Nov 00 ***
*** M5-SAMMY-(I+Q)   7 Nov 00 ***
*** M5-SAMMY-FINAL   5 Jan 01 ***
...
```

... the screen, more typical case.

```
...
*** M5-SAMMY-INPUT   7 Nov 00 ***
*** M5-SAMMY-PAR    15 Dec 00 ***
*** M5-SAMMY-OLD     7 Nov 00 ***
Number of non-zero off-diagonal cov matrix elements is       1
*** M5-SAMMY-DATA    7 Nov 00 ***  8.040     TO  11.96
*** M5-SAMMY-THEOR   7 Nov 00 ***
*** M5-SAMMY-XCT    21 Dec 00 ***
*** M5-SAMMY-FGM     7 Nov 00 ***
*** M5-SAMMY-INTRP   7 Nov 00 ***
*** M5-SAMMY-(N+V)   7 Nov 00 ***
*** M5-SAMMY-FINAL   5 Jan 01 ***
```

Iterating to find best-fit values of the resonance parameters

Input to SAMMY

Three kinds of files are needed for (almost) every SAMMY run:

1. INPut file
- **control information**
- **quantum numbers**

2. PARameter file
- **resonance parameter values**
- **values for all variable parameters**
- **a priori uncertainties**

3. DATa file
- **energy**
- **measured value for cross section**
- **uncertainty**

We will discuss all of these in greater detail later.

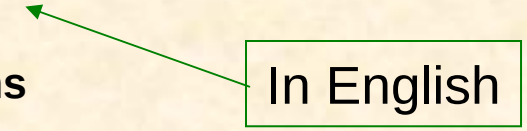
Input to SAMMY, cont.

Other files are needed for some runs:

4. **COVariance** — par covariance mtrx from previous run
5. **DCV (data cov)** — experimental covariance matrix
6. **AVG (average)** — energy ranges for averaging
7. **NDF** — to produce output ENDF/B-6 files
8. **MXW** — temperatures for Maxwellian averages
9. **SSM** — edge-effects corrections from earlier run
10. **NTG** — experimental values for integral quantities

The INPut File

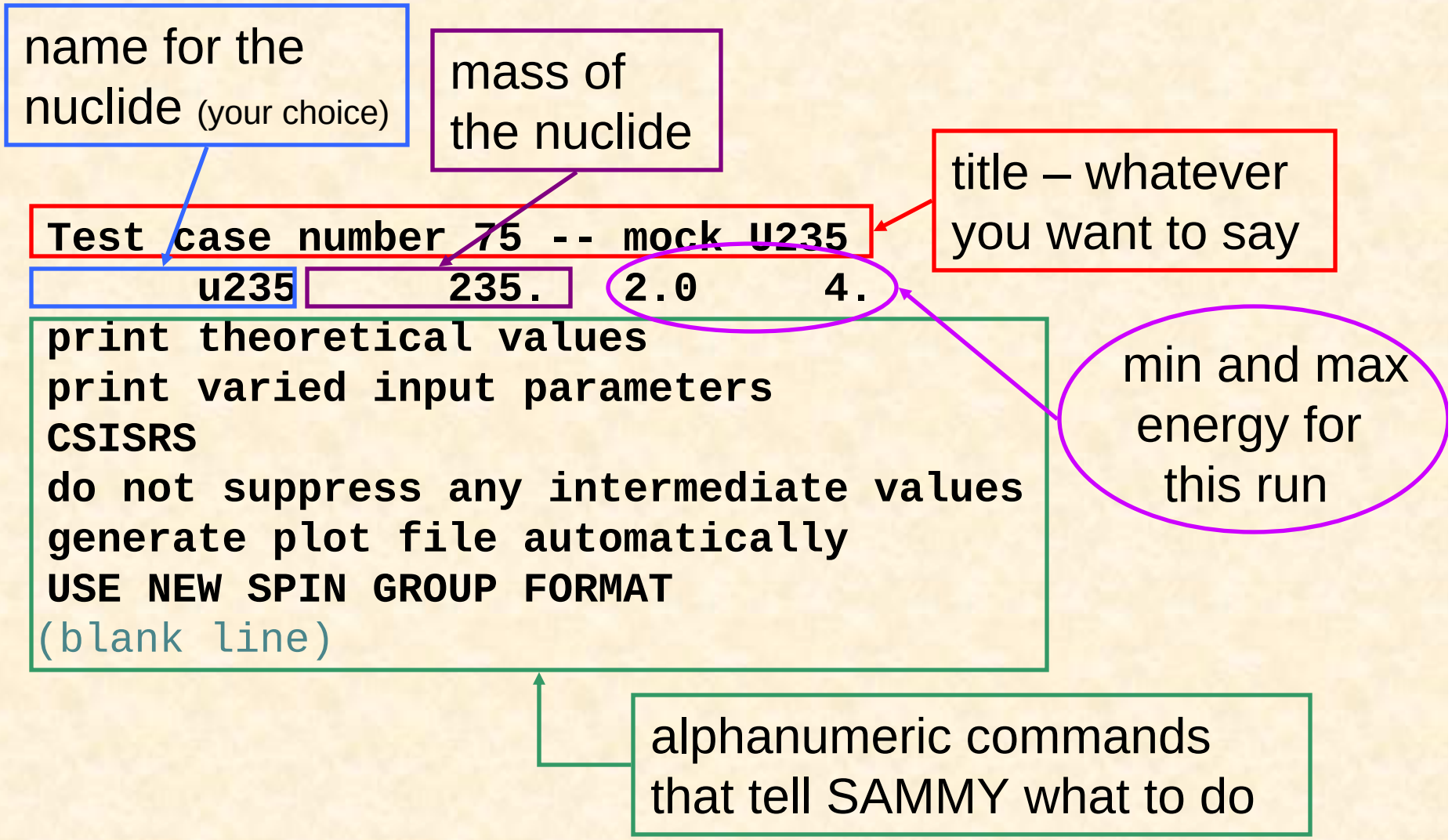
- **Title**
- **Miscellaneous information: atomic weight, Emin and Emax, density for auxiliary grid**
- **Alphanumeric control information**
  - **input / output specifics**
  - **solve / do not solve Bayes' equations**
  - **which type of R-matrix to use**
  - **which Doppler broadening**
  - **which resolution function**
  - **do not / do produce group averages**
- **Doppler- and resolution-broadening parameters (maybe)**
- **Data type**
- **Quantum numbers for the sample nuclides and for the resonances (maybe)**
- **Size information for multiple-scattering corrections**
- **Angles for detectors if angular distribution**



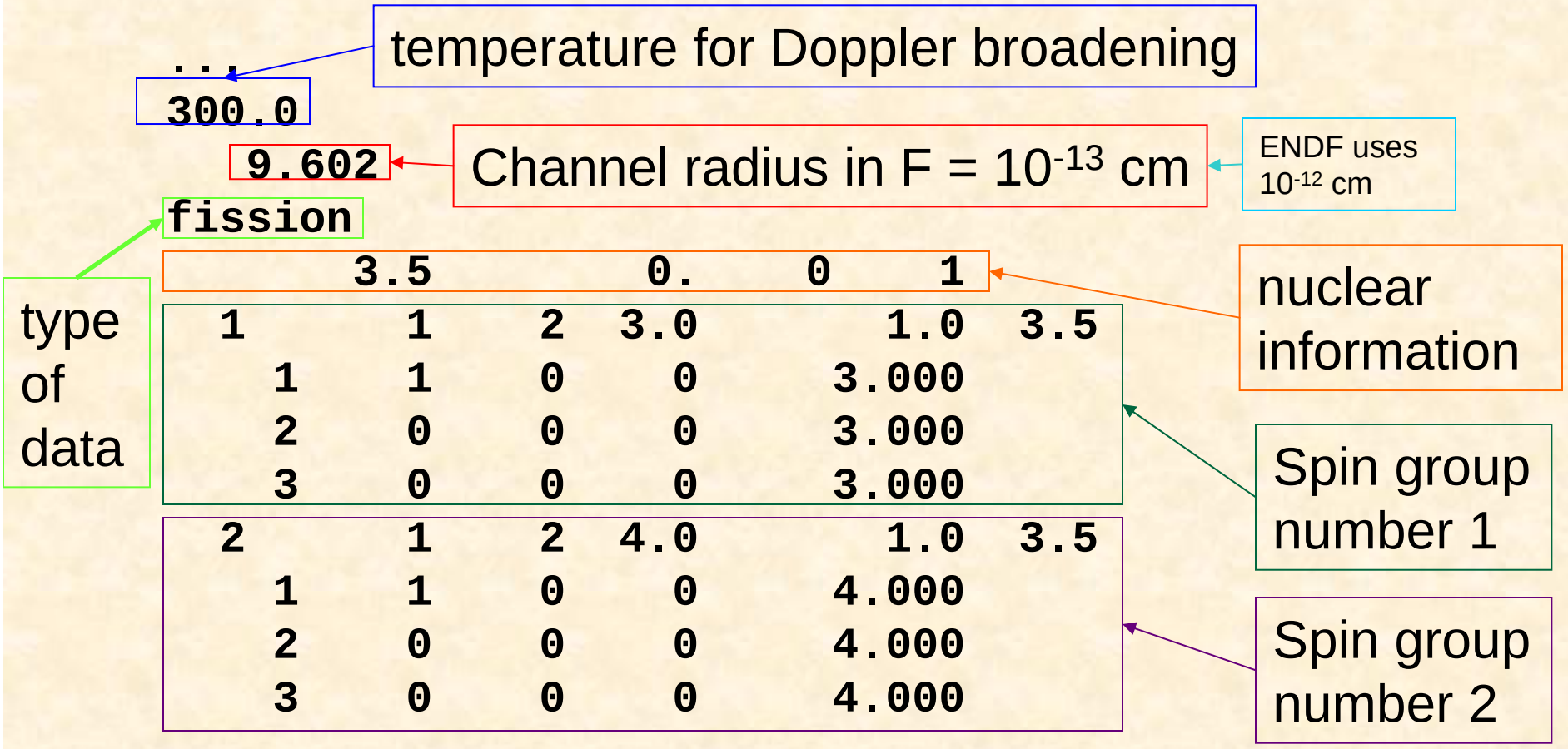
Example of INPut file

```
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
```

Example of INPut file, in more detail



INPut file detail, continued



The PARameter File

- **Values for resonance parameters:**
  - **resonance energy**
  - **capture width, neutron width(s), other widths: inelastic, fission, ...**
- **Values for other parameters:**
  - **effective temperature**
  - **resolution parameters**
  - **normalization & backgrounds**
  - **channel radii**
  - **nuclide abundances**
  - **etc.**
- **A priori uncertainties on all parameter values**
- **Flags to indicate which parameter values are to be varied and which held fixed**

Example of PARameter file (^{235}U)

(entire listing requires ~3000 lines)

Spin group number

Energy in eV	Γ_γ in meV	Γ_n in meV	Γ_{f1} in meV	Γ_{f2} 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
...						
.3018678427	4.0705E+01	4.8608E-03	1.2139E+02	1.9661E-01	1 1 1 1 1	1
1.132577300	3.1770E+01	1.4131E-02	9.8006E-02	1.2898E+02	1 1 1 1 1	2
1.308605790	4.5120E+01	1.9938E-04	-1.8055E-01	1.8730E+01	1 1 1 1 1	2
2.037662983	3.8027E+01	9.2671E-03	-9.8491E+00	9.3994E-01	1 1 1 1 1	1
...						

Example # 2 of PARameter file

(trivial case, one resonance)

```
3.000000000 5.0000E+01 3.0000E-02-4.0000E+01 6.5000E+01 1 1 1 1 1 1
(blank line)
0.50
```

Resonance parameters
plus flags & spin group number

Blank line
Indicates end of resonances

“fudge” factor
used to determine default uncertainties on resonance parameters

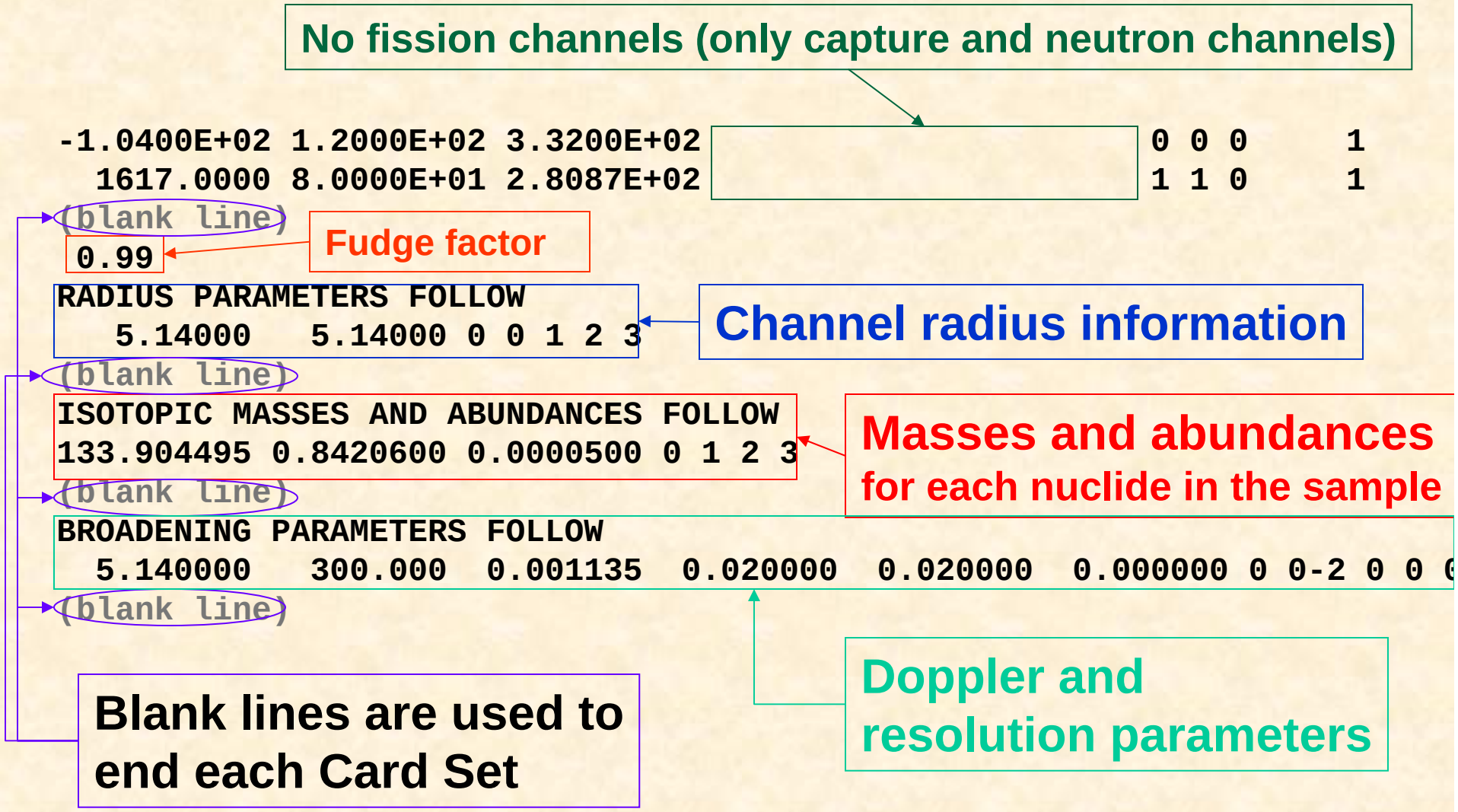
Note: default value for fudge = 0.10

Example # 3 of PARameter file
(two resonances, no fission channels, lots of other information)

```
-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 0.000E+00 0 0 0 0 0 0
```

Here's the whole thing, maybe too small to read.
Next pages: look at the pieces.

Example # 3 continued (part a)



Example # 3 continued (part b)

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

Oak Ridge Resolution function

normalization

constant background

energy-dependent background

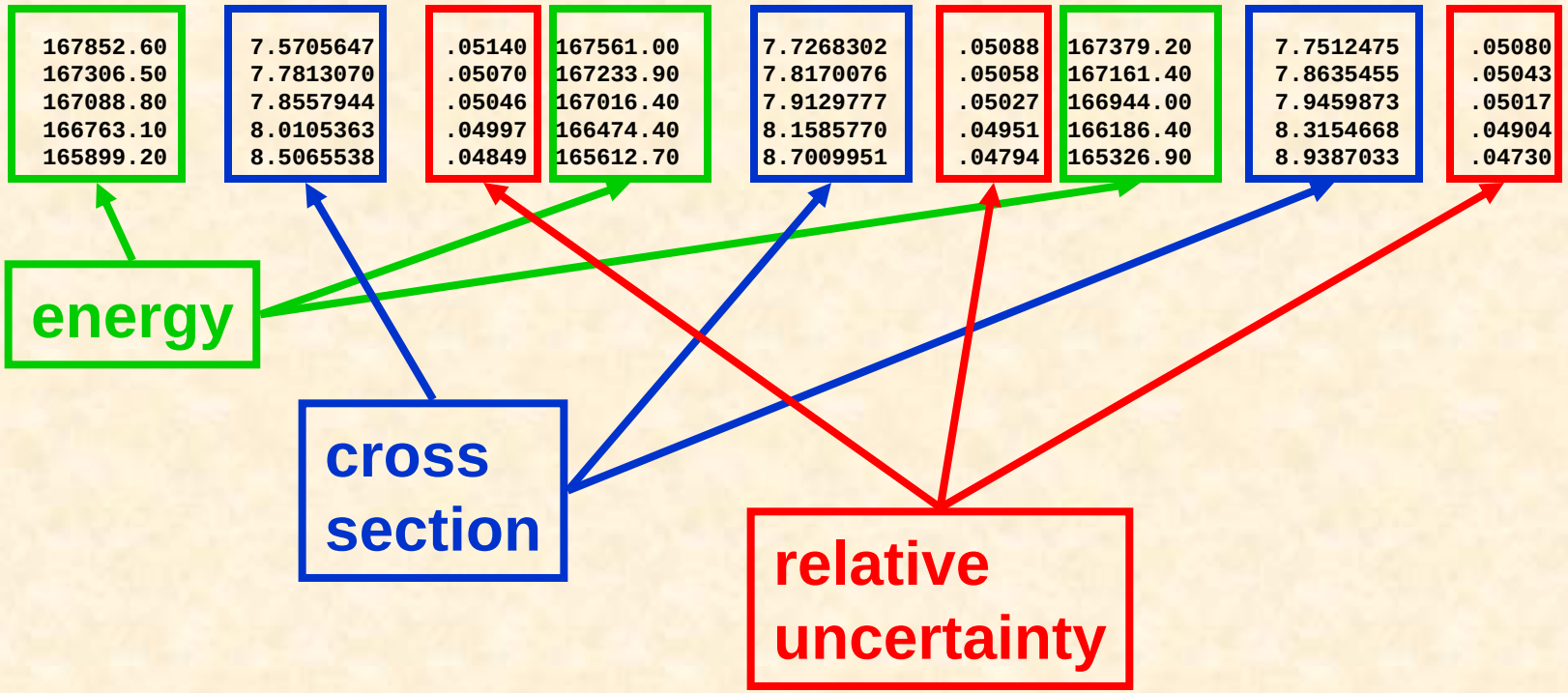
The DATa File

- **Energy**
- **Measured value of cross section (or transmission, or eta, or yield, or ...) at that energy**
- **Uncertainty on the measured value**

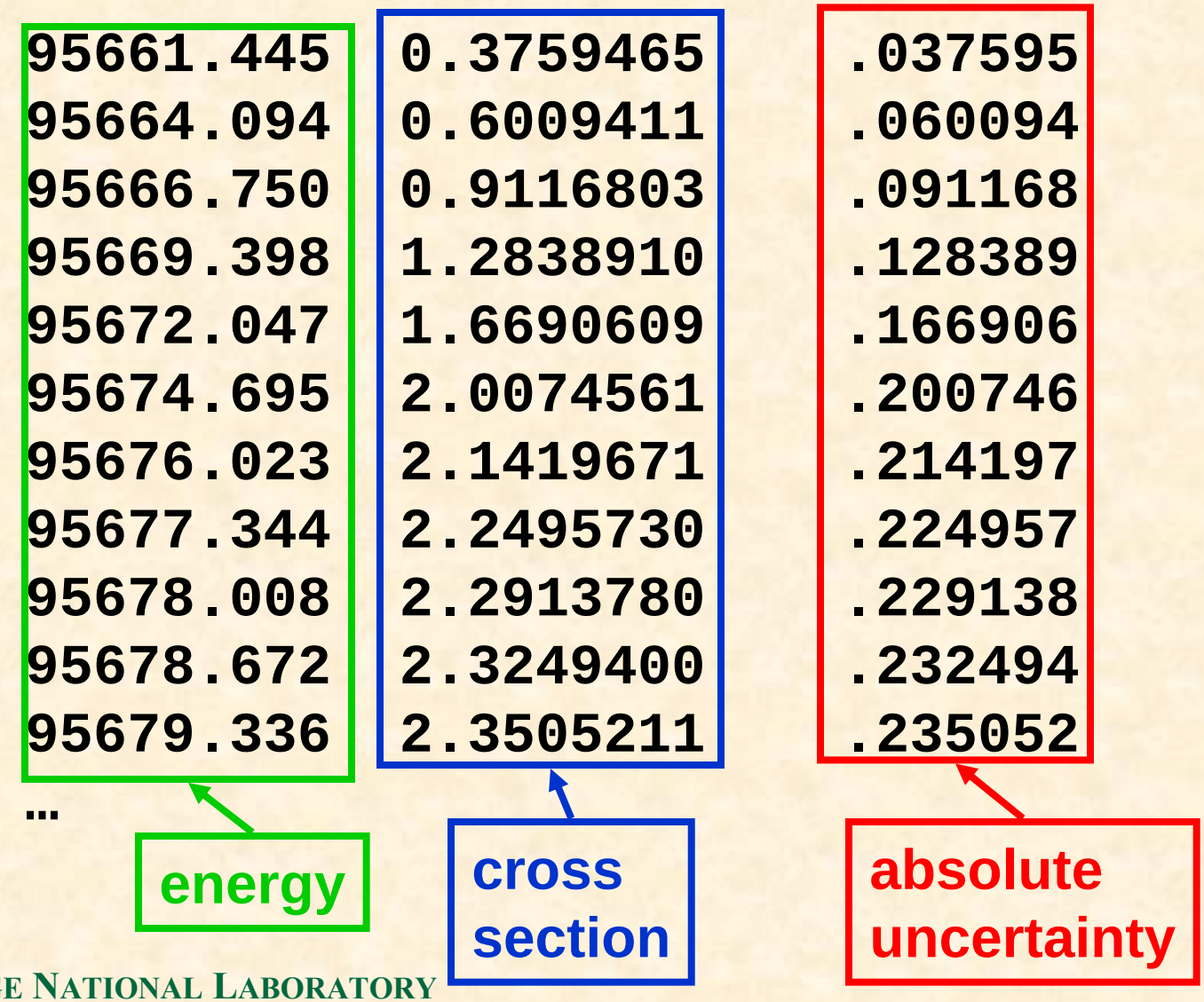
Format Options for DATa files

- **CSISRS or EXFOR, one data point per line, uncertainties are absolute, 3E11.8**
- **TWENTY significant digits**
- **PENDF files**
- **MULTI-style (the original version), three data points per line, uncertainties are relative, 3(2E14.8,F7.5)**
- **Binary ODF format (ORELA Data Format) -- not recommended**

Examples of DATa files –
Multi-style DATa file (relative uncertainties)



Examples of DATa files, continued – CSISRS DATa file (absolute uncertainties)



END of "SAMMY Input Files"

- **Note: this was only an introduction; a *lot* of information has been omitted here.**
- **There are many other input options.**
- **For complete details, see the SAMMY users' guide.**

Next: "Output files from SAMMY"

Output files from SAMMY

Files we will use in this workshop

File produced by every SAMMY run:

1. **SAMMY.LPT** — **to be (printed and) examined by the user!!**

Other output files produced by SAMMY:

2.	SAMMY.IO	Input/Output parameter values
3.	SAMMY.PAR	New values of resonance parameters and other varied parameters
4.	SAMMY.COV	Binary file with covariance matrix for varied parameters
5.	SAMMY.ODF	Binary file to be used for plotting
5a.	SAMMY.PLT	Another version of the plot file
6.	SAMMY.NDF	Resonance parameters in ENDF/B-6 format
7.	SAMMY.PDS	Partial derivatives in ascii format
8.	SAMNDF.INP	SAMMY-style INPut file, produced when ENDF/B File 2 was used instead of SAMMY-style PARameter file
9.	SAMNDF.PAR	SAMMY-style PARameter file, produced when ENDF/B File2 was used for input
10.	SAMXAC.ODF	Binary file with auxiliary grid and unbroadened cross section
11.	SAMMY.SSM	Binary file with edge-effects corrections for single-scattering correction for capture yields
12.	SAM??.DAT	Temporary files for communication between segments

To be deleted after the run concludes properly

SAMMY.LPT

- **Values for varied and fixed parameters (what you actually told SAMMY to use, not what you *intended* to tell SAMMY to use!)**
- **Verbatim alphanumeric commands (with notification if a command is unacceptable)**
- **Input file names; title for run (from INPut file)**
- **Chronological listing of modules used**

for the INPut, PARameter, and DATa files (& others)

- **Updated parameter values, uncertainties, and correlations (also intermediate values if requested)**
- **χ^2 values**

Not χ^2/(degrees of freedom) but χ^2/(number of data points)

- **Error messages (which are often repeated on-screen or in log file)**

Sample "LPT" file

version of SAMMY

Not today's date, but date at which this version was created

```
*** M5-SAMMY        16 Feb 01 ***
 Name of user's input file:
 >>> t075a.inp <<<
 Name of user's parameter file:
 >>> t075a.par <<<
 Values used for constants -- kvendf=1
   mass of neutron =   1.008664904000000 in amu
   sqrt(m/2)       =  72.298263153907186
   sqrt(2m)/hbar   =   0.000219680712129
   sqrt(Boltzman)  =   0.009282987126997
   finestructure   =   0.034447597682295 in 1/(amu*F)
  Name of user's experimental data file is:
 >>> t075a.dat <<<

 ************ READY TO RUN SAMODF *********

 ************ READY TO RUN SAMMY VERSION M5 **********
```

Names of input files

Sample "LPT" file, continued

```
### Estimated array size for SAMMY-INP is      177 ###


**************************************************************************************
*****                                                                            *****
*****  Test case number 75 -- mock U235                                          *****
*****                                                                            *****
**************************************************************************************


Input quantities from card number 2 are:
  alfnm1, alfnm2 = ##      u235##       Atomic Weight =   235.0
  energy range =       2.000           4.000
  nepnts itmax  icorr  nxtra  iptdop iptwid ixxchn
       0      0      0      0      0      0      0
  ndigit idropp matnum kkkkza
       2      2      0      0
Adjusted - itmax,icorr,nxtra,iptdop,iptwid     =      2 50  0  9  5


TARGET ELEMENT IS       u235
ATOMIC WEIGHT IS  235.000
```

Title from INPut file

Sample "LPT" file, continued

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

 PRINT THEORETICAL VALUES
 PRINT VARIED INPUT PARAMETERS
 CSISRS
 do not suppress any intermediate values
 USE NEW SPIN GROUP FORMAT
 ODF FILE IS WANTED--SAMMY.ODF ,ZERO-TH O
 PRINT BAYES CHI SQUARED
 SOLVE BAYES EQUATIONS
 CHI SQUARED IS WANTED

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

Error message would appear in here if you misspell a command

Find the best-fit parameter values.

Some of these are yours, some were added by SAMMY.

Sample "LPT" file, continued

```
 EFFECTIVE TEMPERATURE= 300.00000
   FLIGHT PATH=   0.00000 METERS +/-   0.00000/2 METERS
     DELTAE=     0.00000    DELTAG=     0.00000
     delttt=     0.00000    ELOWBR=  0.00000000

CHANNEL RADIUS=   9.602
TARGET THICKNESS=  0.0000E+00

fission
```

broadening parameters

type of data, as given in the INPut file

Sample "LPT" file, continued

```
  Spin of incident particle is  0.5
      #of  #of
group ent  exit Jspin relative  Ispin  g     chn LPNT iSHift el CHSPN  in
   #  chn  chn         abndnc                  #                      data?
   1    1    2    3.0  1.0000    3.5 0.4375
                                                1   1    0     0   3.0
                                                2   0    0     0   3.0
                                                3   0    0     0   3.0
   2    1    2    4.0  1.0000    3.5 0.5625
                                                1   1    0     0   4.0
                                                2   0    0     0   4.0
                                                3   0    0     0   4.0

### Array size used for SAMMY-INP is       178 ###
```

Spin group information from INPut file

Sample "LPT" file, continued

```
### Estimated array size for SAMMY-PAR is      252 ###

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      250 ###
### Estimated array size for SAMMY-NEW is      269 ###
```

A few details you may find useful when debugging your runs

Sample "LPT" file, continued

Resonance parameters, ordered by spin groups

```
*****INITIAL VALUES FOR PARAMETERS

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G=0.4375
                  "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= 3.0   L=0  SPIN= 3.0
      (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)
```

Numbers in parenthesis are "varied parameter number"

If you are having problems with a run, compare these values to the values you intended to use. There may be differences!

Sample "LPT" file, continued

```
 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 (SQRT 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       269 ###
```

varied parameter numbers

uncertainties on the varied parameters

Sample “LPT” file, continued

```
     Emind                Emins                Eminr                Emin
        1.8536592399         2.0000000000         2.0000000000         2.0000000000
     Emax                 Emaxr                Emaxs                Emaxd
        4.0000000000         4.0000000000         4.0000000000         4.2136676614

Doppler Width at Emin =  2.926815E-02 and at Emax =  4.273353E-02

      E(keV)    Dopp_FWHM(keV)  Gauss_FWHM(keV)  Total_FWHM(keV)
      0.002000          0.0000          0.0000          0.0000
      0.003000          0.0001          0.0000          0.0001
      0.004000          0.0001          0.0000          0.0001
```

Sample "LPT" file, continued

```
### Estimated array size for SAMMY-DAT is 41666734 ###

Energy range of data is from 2.00000E+00 to 4.00000E+00 eV.
Number of experimental data points =      41
Number of points in auxiliary grid =      49

### Array size used for SAMMY-DAT is 49999972 ###
### Array size used for SAMMY-DAT is      324 ###
### Estimated array size for SAMMY-THE is      464 ###
Number of parameters affected by this data set=    5
### Array size used for SAMMY-THE is      464 ###
### Estimated array size for SAMMY-XCT is     1358 ###
### Array size used for SAMMY-XCT is     1329 ###
### Estimated array size for SAMMY-FGM is     1094 ###
### Array size used for SAMMY-FGM is     1094 ###
### Estimated array size for SAMMY-INT is      679 ###
```

Sample "LPT" file, continued

```
***** THEORETICAL VALUES (broadnd,normed,...as required)

     ENERGY    THEORY          ENERGY    THEORY          ENERGY    THEORY
(  1)2.000000 0.367704    ( 15)2.940000  32.3681    ( 29)3.136610  12.6401
(  2)2.100000 0.442535    ( 16)2.960000  38.9885    ( 30)3.154915  10.3105
(  3)2.200000 0.546350    ( 17)2.980000  44.0630    ( 31)3.173219  8.52119
(  4)2.300000 0.696259    ( 18)3.000000  45.8657    ( 32)3.200000  6.59250
(  5)2.400000 0.924150    ( 19)3.015000  44.5803    ( 33)3.250000  4.34505
(  6)2.500000  1.29477    ( 20)3.025908  42.3619    ( 34)3.300000  3.05564
(  7)2.600000  1.95425    ( 21)3.030000  41.3055    ( 35)3.400000  1.72165
(  8)2.700000  3.33407    ( 22)3.034092  40.1510    ( 36)3.500000  1.09644
(  9)2.800000  7.03688    ( 23)3.040796  38.0915    ( 37)3.600000 0.755665
( 10)2.843390  10.6577    ( 24)3.047500  35.8868    ( 38)3.700000 0.549590
( 11)2.865085  13.4732    ( 25)3.065000  29.9244    ( 39)3.800000 0.416114
( 12)2.886780  17.3261    ( 26)3.082500  24.3524    ( 40)3.900000 0.325007
( 13)2.900000  20.3112    ( 27)3.100000  19.6277    ( 41)4.000000 0.260205
( 14)2.920000  25.8412    ( 28)3.118305  15.6837
```

Theoretical values are not usually printed in the LPT file; instead, they're in the plot file.

Sample "LPT" file, continued

```
### Array size used for SAMMY-INT is      434 ###

### Estimated array size for SAMMY-SQU is      425 ###
### Array size used for SAMMY-SQU is      425 ###

USE (I+Q) INVERSION SCHEME
### Estimated array size for SAMMY-IPQ is      943 ###

CUSTOMARY CHI SQUARED =  1.296590E+06
CUSTOMARY CHI SQUARED DIVIDED BY NDAT =   31624.2

BAYESIAN CHI SQUARED =    4749.55
BAYESIAN CHI SQUARED DIVIDED BY NDAT =   115.843
### Array size used for SAMMY-IPQ is      943 ###
### Estimated array size for SAMMY-FIN is      440 ###
```

Remember this value (initial chi-squared)

Two types of chi-squared values…
we'll talk about these later if there is time.

Sample "LPT" file, continued

```
*****INTERMEDIATE VALUES FOR RESONANCE PARAMETERS

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G=0.4375
                "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= 3.0  L=0  SPIN= 3.0
      (eV)         (MILLI-EV)      (MILLI-EV)      (MILLI-EV)      (MILLI-EV)
 3.02107E+00(  1) 5.5578E+01(  2) 2.2791E-02(  3) -3.9517E+01(  4) 6.3728E+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
```

Intermediate values

Sample “LPT” file, continued

```
### Array size used for SAMMY-FIN is      445 ###
### Estimated array size for SAMMY-THE is      464 ###
Number of parameters affected by this data set=    5
### Array size used for SAMMY-THE is      464 ###
### Estimated array size for SAMMY-XCT is     1358 ###
### Array size used for SAMMY-XCT is     1329 ###
### Estimated array size for SAMMY-FGM is     1094 ###
### Array size used for SAMMY-FGM is     1094 ###
### Estimated array size for SAMMY-INT is      679 ###
```

Sample "LPT" file, continued

***** THEORETICAL VALUES (broadnd,normed,...as required)

	ENERGY	THEORY		ENERGY	THEORY		ENERGY	THEORY
(1)	2.000000	0.262519	(15)	2.940000	18.4256	(29)	3.136610	11.8228
(2)	2.100000	0.314503	(16)	2.960000	22.9620	(30)	3.154915	9.54736
(3)	2.200000	0.386085	(17)	2.980000	27.5661	(31)	3.173219	7.79505
(4)	2.300000	0.488475	(18)	3.000000	31.1416	(32)	3.200000	5.92141
(5)	2.400000	0.642228	(19)	3.015000	32.4279	(33)	3.250000	3.78740
(6)	2.500000	0.888238	(20)	3.025908	32.3987	(34)	3.300000	2.60249
(7)	2.600000	1.31655	(21)	3.030000	32.1732	(35)	3.400000	1.41997
(8)	2.700000	2.17973	(22)	3.034092	31.8352	(36)	3.500000	0.886689
(9)	2.800000	4.34586	(23)	3.040796	31.0542	(37)	3.600000	0.603070
(10)	2.843390	6.35034	(24)	3.047500	30.0218	(38)	3.700000	0.434372
(11)	2.865085	7.86784	(25)	3.065000	26.4669	(39)	3.800000	0.326462
(12)	2.886780	9.92303	(26)	3.082500	22.3465	(40)	3.900000	0.253515
(13)	2.900000	11.5217	(27)	3.100000	18.3556	(41)	4.000000	0.202028
(14)	2.920000	14.5626	(28)	3.118305	14.7406			

generated from intermediate value of resonance parameters

Sample "LPT" file, continued

```
### Array size used for SAMMY-INT is      392 ###


USE (I+Q) INVERSION SCHEME
### Estimated array size for SAMMY-IPQ is      943 ###

CUSTOMARY CHI SQUARED =   45556.9
CUSTOMARY CHI SQUARED DIVIDED BY NDAT =   1111.14

BAYESIAN CHI SQUARED =    133.555    =    986763.    -    986629.
BAYESIAN CHI SQUARED DIVIDED BY NDAT =   3.25743
### Array size used for SAMMY-IPQ is      943 ###
### Estimated array size for SAMMY-FIN is      440 ###
```

Intermediate value for chi-squared

evaluated at the intermediate parameter values

Sample "LPT" file, continued

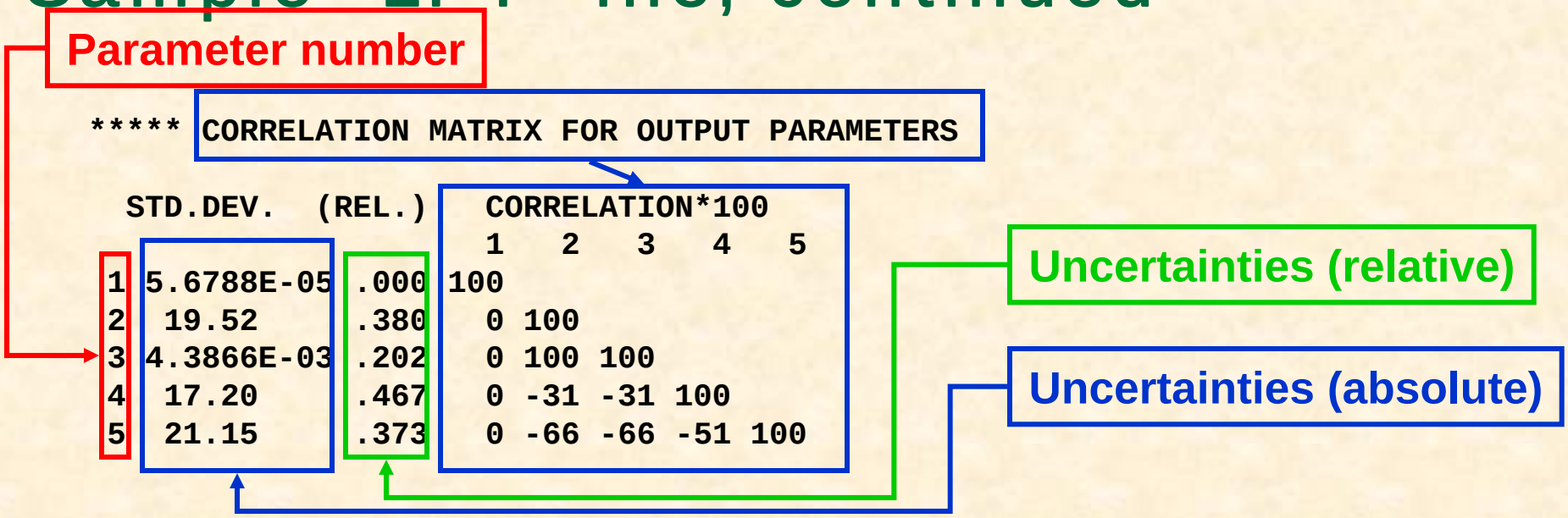
Final (best-fit) values for resonance parameters

values for resonance parameters

```
*****  NEW VALUES FOR RESONANCE PARAMETERS

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G=0.4375
                  "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= 3.0   L=0  SPIN= 3.0
      (eV)          (MILLI-EV)       (MILLI-EV)       (MILLI-EV)       (MILLI-EV)
 3.03039E+00(  1) 5.1328E+01(  2)  2.1761E-02(  3) -3.6829E+01(  4)  5.6764E+01(  5)
Expected          5.1328E+01       2.1761E-02       3.6829E+01       5.6764E+01
 Value       +/-  1.9524E+01  +/-  4.3866E-03  +/-  1.7202E+01  +/-  2.1153E+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
```

Average values

Sample "LPT" file, continued




```
***** RATIO OF UNCERTAINTIES ON VARIED PARAMETERS
        NEW/OLD                NEW/OLD                NEW/OLD                NEW/OLD
(  1)  6.5546E-04   (  2)  0.7809        (  3)  0.2924        (  4)  0.8601
(  5)  0.6509


***** RATIO OF UNCERTAINTIES ON VARIED U-PARAMETERS
        NEW/OLD                NEW/OLD                NEW/OLD                NEW/OLD
(  1)  6.5217E-04   (  2)  0.7708        (  3)  0.3425        (  4)  0.8964
(  5)  0.6965

 ### Array size used for SAMMY-FIN is      494 ###
```

Sample "LPT" file, continued

```
********** READY TO RUN SAMMY VERSION M5 **********


Name of binary parameter covariance file is:
>>> SAMMY.COV                                                    <<<
### Estimated array size for SAMMY-INP is      177 ###


*****************************************************************************
*****                                                                   *****
***** Test case number 75 -- mock U235                                  *****
*****                                                                   *****
*****************************************************************************


Input quantities from card number 2 are:
  alfnm1, alfnm2 = ##      u235##       Atomic Weight =   235.0
  energy range =       2.000           4.000
  nepnts itmax  icorr  nxtra  iptdop iptwid ixxchn
       0      0      0      0      0      0      0
  ndigit idropp matnum kkkkza
       2      2      0      0
Adjusted - itmax,icorr,nxtra,iptdop,iptwid     =      2 50  0  9  5
```

Sample "LPT" file, continued

```
TARGET ELEMENT IS       u235
ATOMIC WEIGHT IS  235.000


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

PRINT THEORETICAL VALUES
DO NOT PRINT ANY INPUT PARAMETERS
CSISRS
do not suppress any intermediate values
USE NEW 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 *********
```

This time through, calculate cross sections and determine chi-squared. Do not do any fitting.

Sample "LPT" file, continued

```
 EFFECTIVE TEMPERATURE= 300.00000
    FLIGHT PATH=   0.00000 METERS +/-   0.00000/2 METERS
      DELTAE=     0.00000    DELTAG=     0.00000
      delttt=     0.00000    ELOWBR=  0.00000000

CHANNEL RADIUS=   9.602
TARGET THICKNESS=  0.0000E+00

fission


Spin of incident particle is  0.5

### Array size used for SAMMY-INP is      178 ###
### Estimated array size for SAMMY-PAR is      252 ###

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      250 ###
### Estimated array size for SAMMY-OLD is      264 ###
Number of non-zero off-diagonal cov matrix elements is      10
```

Sample "LPT" file, continued

```
Broadening (etc.) parameters actually used for this run

            Radius (CRFN) =   9.60200       9.60200      CYCRFN =  2.100359E-03
    Effective Temperature =   300.000       300.000          DO =  1.053387E-02
         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 =  0.000000E+00
### Array size used for SAMMY-OLD is      265 ###
    Emind                Emins                Eminr                Emin
       1.8536592399         2.0000000000         2.0000000000         2.0000000000
    Emax                 Emaxr                Emaxs                Emaxd
       4.0000000000         4.0000000000         4.0000000000         4.2136676614

Doppler Width at Emin =  2.926815E-02 and at Emax =  4.273353E-02

     E(keV)    Dopp_FWHM(keV)  Gauss_FWHM(keV)  Total_FWHM(keV)
     0.002000         0.0000          0.0000          0.0000
     0.003000         0.0001          0.0000          0.0001
     0.004000         0.0001          0.0000          0.0001

### Estimated array size for SAMMY-DAT is 41666734 ###
```

Sample "LPT" file, continued

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

Number of points in auxiliary grid =      49
### Array size used for SAMMY-DAT is 49999972 ###
### Array size used for SAMMY-DAT is      324 ###
### Estimated array size for SAMMY-THE is      412 ###
### Array size used for SAMMY-THE is      412 ###
### Estimated array size for SAMMY-XCT is      935 ###
### Array size used for SAMMY-XCT is      902 ###
### Estimated array size for SAMMY-FGM is      586 ###
### Array size used for SAMMY-FGM is      586 ###
### Estimated array size for SAMMY-INT is      459 ###


***** THEORETICAL VALUES (broadnd,normed,...as required)

     ENERGY    THEORY          ENERGY    THEORY          ENERGY    THEORY
(  1)2.000000 0.223027    ( 15)2.940000  15.5835    ( 29)3.136610  12.2798
(  2)2.100000 0.266735    ( 16)2.960000  20.0658    ( 30)3.154915  9.72828
(  3)2.200000 0.326766    ( 17)2.980000  25.1774    ( 31)3.173219  7.80564
(  4)2.300000 0.412358    ( 18)3.000000  29.9294    ( 32)3.200000  5.80325
(  5)2.400000 0.540378    ( 19)3.015000  32.3720    ( 33)3.250000  3.60614
(  6)2.500000 0.744189    ( 20)3.025908  33.1636    ( 34)3.300000  2.43173
```

Sample "LPT" file, continued

```
(  7)2.600000  1.09674    ( 21)3.030000  33.2151    ( 35)3.400000  1.29678
(  8)2.700000  1.80072    ( 22)3.034092  33.1294    ( 36)3.500000 0.799861
(  9)2.800000  3.55077    ( 23)3.040796  32.6976    ( 37)3.600000 0.539828
( 10)2.843390  5.16933    ( 24)3.047500  31.9248    ( 38)3.700000 0.386703
( 11)2.865085  6.40329    ( 25)3.065000  28.6110    ( 39)3.800000 0.289469
( 12)2.886780  8.09630    ( 26)3.082500  24.2313    ( 40)3.900000 0.224098
( 13)2.900000  9.43693    ( 27)3.100000  19.7458    ( 41)4.000000 0.178153
( 14)2.920000  12.0632    ( 28)3.118305  15.6069
### Array size used for SAMMY-INT is      418 ###

### Estimated array size for SAMMY-NPV is      473 ###

CUSTOMARY CHI SQUARED =   259.957
CUSTOMARY CHI SQUARED DIVIDED BY NDAT =  6.34041
### Array size used for SAMMY-NPV is      471 ###
### Estimated array size for SAMMY-FIN is      374 ###
### Array size used for SAMMY-FIN is      232 ###
```

End of LPT file

Chi-squared started as 31,624.2
became 1,111.1
and finally 6.3

Other output files
[Rename these so you do not lose them!]

- 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
    - with or without modification
- 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

Other output files, continued

- **SAMMY.PLT and SAMMY.ODF**
  - **In "generic" binary or ODF (ORELA Data Format)**
  - **To be used for making plots of data vs theory**
  - **Contain:**

To be used for this workshop

S1 • **Energy grid**
S2 • **Experimental data**
S3 • **Absolute uncertainties for experimental data**
S4 • **Initial calculated values for cross section (or transmission, etc.)**
S5 • **Final calculated values for cross section (ditto)**

  - **May also contain**
    - **Uncertainties on calculated values**
    - **Revised energy grid**

END OF Output files

GLOSSARY (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.**

GLOSSARY continued

- **PARameter file**
  - **file containing resonance parameters and any other parameters which are to be varied**
- **DATa file**
  - **sometimes called “SAM file”; contains experimental data; formats available for this file – MULTI (original, default), CSISRS, TWENTY, ODF)**
- **ENDF file**
  - **file in the ENDF/B-VI format (often, File 2 portion only)**
- **NDF file**
  - **SAMMY input file needed to create ENDF file**
- **FGM**
  - **free gas model for Doppler broadening**
- **HEGA**
  - **high-energy Gaussian approximation to the free gas model**