Upgrades to the R-Matrix Code SAMMY

N. M. Larson
Oak Ridge National Laboratory

September 30, 2004 **updated Sept 2005**
SAMMY Users' Meeting

(ND2004 Santa Fe, NM, USA, Sept. 27-Oct. 1, 2004)

TOPICS to be covered

- What is SAMMY?
- Types of data
- Theoretical cross sections
- Corrections for experimental conditions
- Fitting procedure
- Preparing SAMMY input
- Output options
- Test cases
- The ENDF Connection
- SAMMY code details
- SAMMY workshops
- Future plans

Please feel free to interrupt to ask questions.

Sometimes I'll even answer them.

What is SAMMY?

- **SAMMY is a tool for analyses of time-of-flight cross section data in the resonance region**

Information which is new after ND2001 is flagged with new

What is SAMMY, cont.

- ***Incident particles:*** **neutron, proton, alpha, …**
- ***Target:*** **one type of nuclide, or many**
  - **Multiple isotopes**
  - **Chemical compounds**
  - **Contaminants**
  - **Containers**
- ***Energy region:***
  - **Resolved resonance region (RRR)**
  - **Unresolved region (URR)**
    - **for one nuclide type, incident neutron**

Types of data

- ***In RRR:***
  - **Total, elastic, capture, fission, inelastic, other reactions**
  - **Charged-particle entrance and/or exit channels**
  - **Angular distributions**
  - **Integral data (Westcott's g-factor, resonance integral, Watt spectrum average, K1, alpha)**

- ***In URR:***
  - **Total, elastic, inelastic, capture, fission**

Theoretical cross sections

- ***In RRR:***
  - **Reich-Moore approximation to multilevel multi-channel R-matrix theory**
    - **Other options are single- or multilevel Breit Wigner**

BW is not to be used for new evaluations, please!

  - **Can mimic full (unapproximated) R-matrix with high accuracy**
  - **Direct capture component can be added** new

See paper 221 Arbanas et al

  - **Also available: fictitious "cross sections"** new
    - **For testing resolution function, for example**

Theoretical cross sections, cont.

- ***In URR:***
  - **Fritz Frőhner's FITACS code forms the basis for SAMMY's URR treatment**
  - **Uses Hauser-Feshbach theory with width fluctuations**
    - **Few changes have been made to Frőhner's version**
      - **"Cosmetic" modifications**
      - **Increased efficiency**
      - **Increased ease of input**

Corrections for experimental conditions (in RRR, mostly)

- ***Doppler broadening:***
  - **Free Gas Model (FGM)** Method of choice for most applications
  - **Leal-Hwang version of FGM** Useful if no structure in cross section
  - **High-energy approximation to FGM** Should NOT be used

  - **Crystal-lattice model (solid-state effects)** New
    - **Needed for some applications**
    - **Borrowed from Naberejnev's DOPUSH code**
    - **See paper # 215 at ND2004**
      - **A. Courcelle et al.**

      "Experimental Validation of the Crystal Lattice Model in the R-matrix code SAMMY"

Corrections in RRR, continued

- ***Resolution broadening:***
  - **Gaussian plus exponential tail (RES)**
  - **Oak Ridge Resolution function (ORR)**
  - **RPI Resolution function (RPI)**
  - **User-defined resolution function (UDR)**
  - **Straight-line energy average (DEX)**
  - **Combination of RSL plus DEX plus one of (ORR, RPI)**

A bug was corrected in calculation of partial derivatives.

Varying the parameters now works much better!

Still does not work well if combining more than one numerical function.

Corrections in RRR, continued

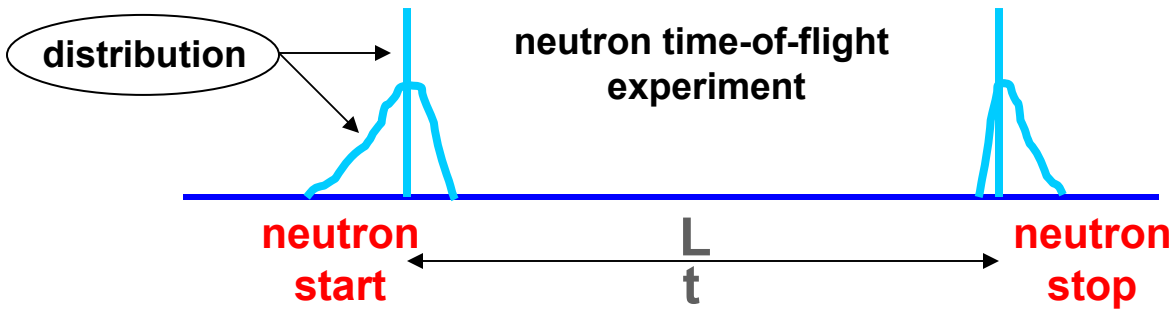
- ***Resolution broadening, continued***
  - **RPI Resolution function (RPI) extended**
    - **Extension of RPI to use with Geel & nTOF data**
      - **Details determined by Frank Gunsing**
        - **Description of energy-dependence**
      - **Implemented in SAMMY in Aug-Sept 2004**
      - **Available in the next release**

new

Analytical description in SAMMY of the resolution function of GELINA and n_TOF

Frank Gunsing
CEA/Saclay - France

What is resolution?



time-energy relation: $\sqrt{E} = \alpha \frac{L}{t}$

- **neutron time of flight:** $t + \delta t$
- **flight path length:** $L + \delta L$
- **neutron kinetic energy:** $E + \delta E$

Resolution can be expressed equivalently in time, distance or energy: $R_t(\delta t)d\delta t = R_L(\delta L)d\delta L = R_E(\delta E)d\delta E$

Resolution function of GELINA and n_TOF

- **Monte Carlo simulations of resolution function:**

GELINA (Geel):

- **Coceva et al.**
- **Flaska et al.**

n_TOF (CERN):

- **Coceva et al.**
- **Vlachoudis et al.**

- **Simulated RF available in broad energy intervals.**

$$R_{[E_1 - E_2]}(t)$$

- **Find analytical description for use in SAMMY**

$$R_E(t)$$

Resolution function of GELINA and n_TOF

- GELINA
  - **RF historically modelled in REFIT**
  - **Parametrization in SAMMY available, not satisfactory in large energy range.**

- n_TOF
  - **MC simulations have been fitted with SAMMY RPI function on specific intervals (Tain/Domingo-Pardo) or as a function of energy (Colonna/Lorusso), but necessary energy dependence is not foreseen in SAMMY.**

RPI resolution function in SAMMY

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

normalization

chi-square distribution (ν=2) of moderation distance $\Lambda = \Lambda_d$ sqrt(E)/72.3

strength of tail

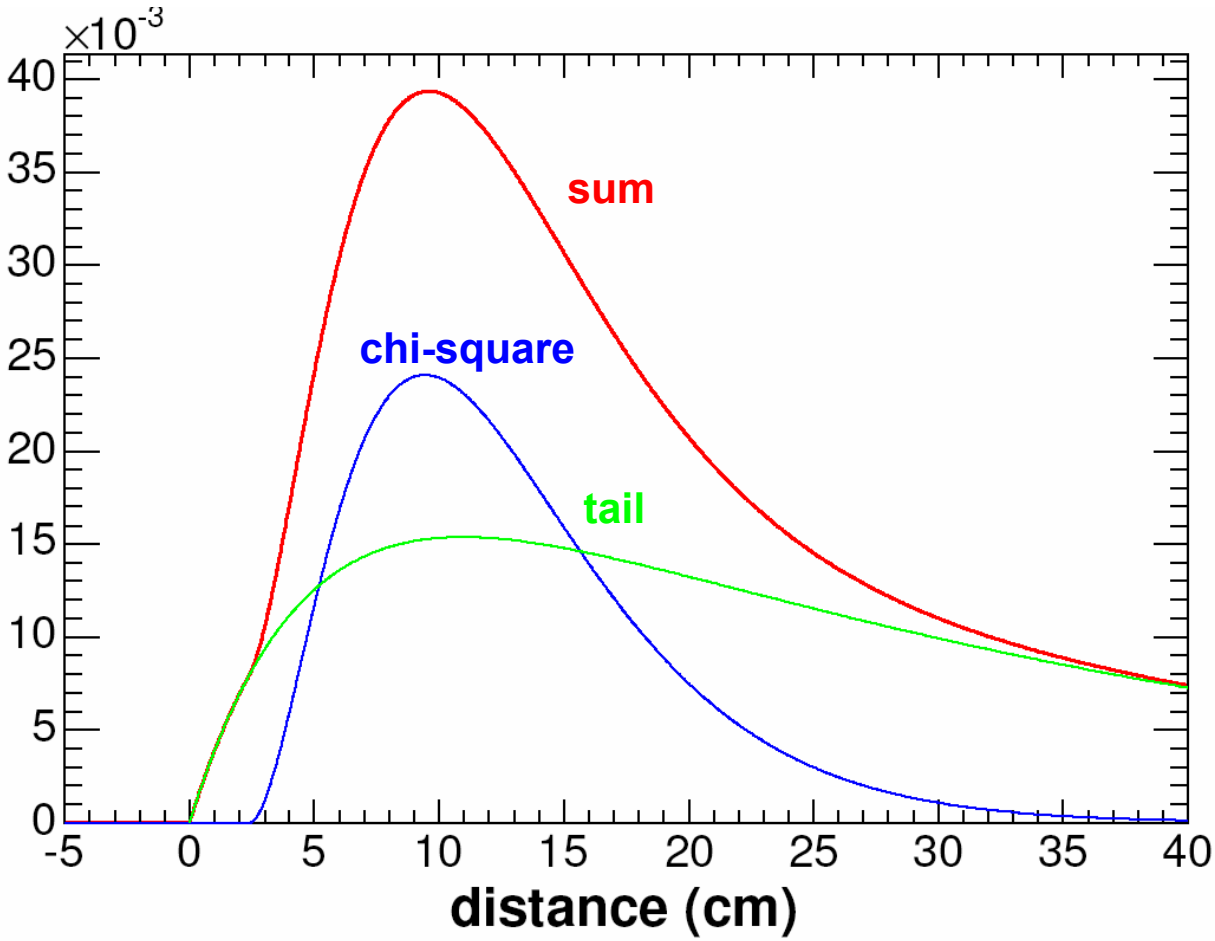
exponential tail

include tail, X(t) is 0 or 1

Energy dependent parameters:

$$\begin{cases} \Lambda = \Lambda(E) \\ \tau = \tau(E) \\ A_1 = A_1(E) \end{cases}$$

Components of RPI resolution function



Modification of exponential tail in RPI function

original:

$$\left[A_2 e^{-A_3(t+t_0)} + A_4 e^{-A_5(t+t_0)}\right]$$

from time dependent to distance dependent tail:

$$\left[A_2 e^{-A_3(d+d_0)} + A_4 e^{-A_5(d+d_0)}\right]$$

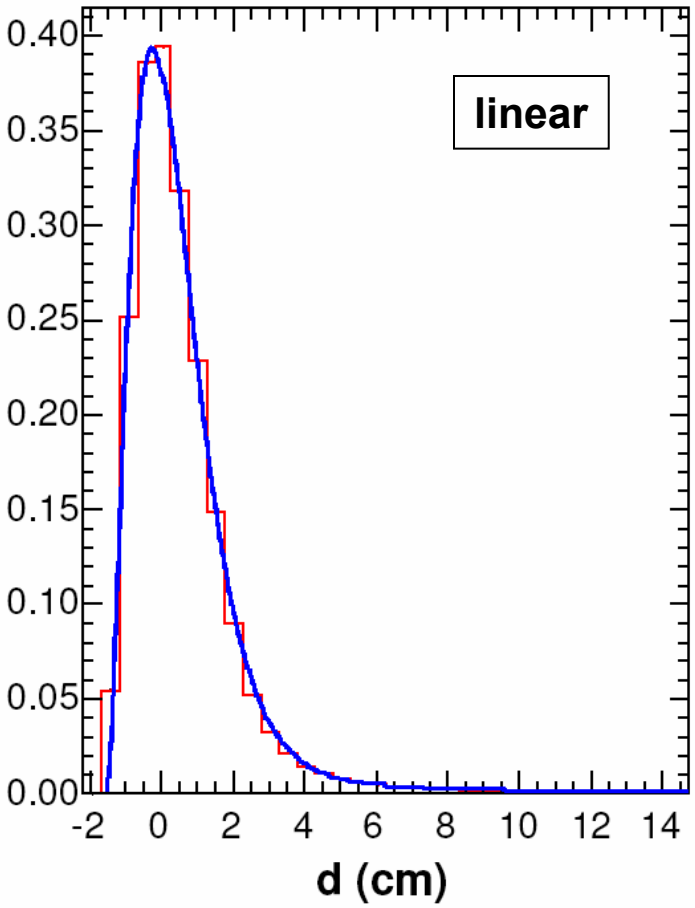
distance dependent tail keeping time representation:

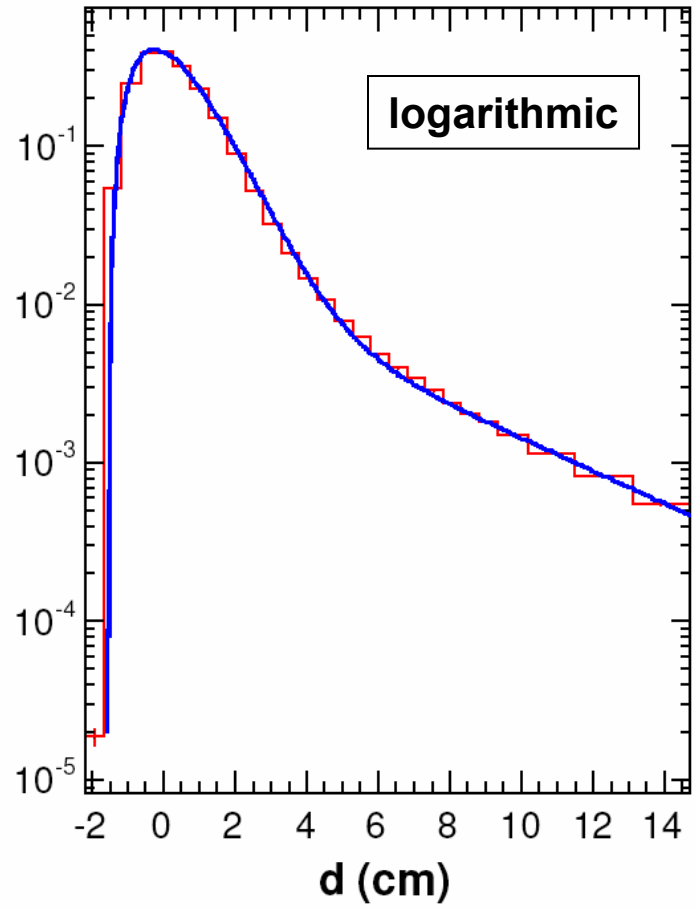
$$\left[A_2 e^{-A_3(t+t_0)\sqrt{E}} + A_4 e^{-A_5(t+t_0)\sqrt{E}}\right]$$

energy dependent "contstants":

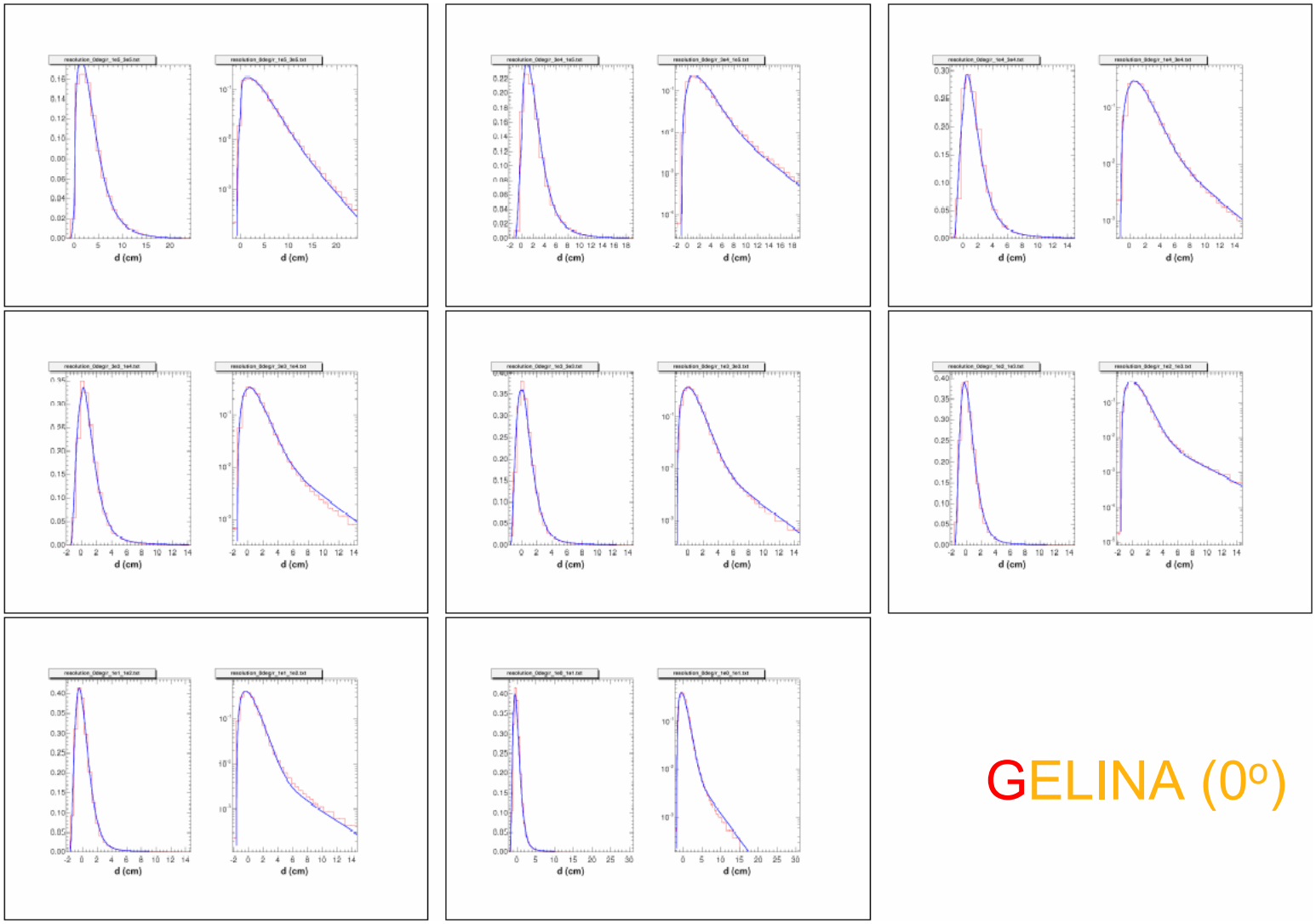
$$\left[A_2 e^{-A_3(E)(t+t_0)\sqrt{E}} + A_4 e^{-A_5(E)(t+t_0)\sqrt{E}}\right]$$

Example fit MC data with RPI function





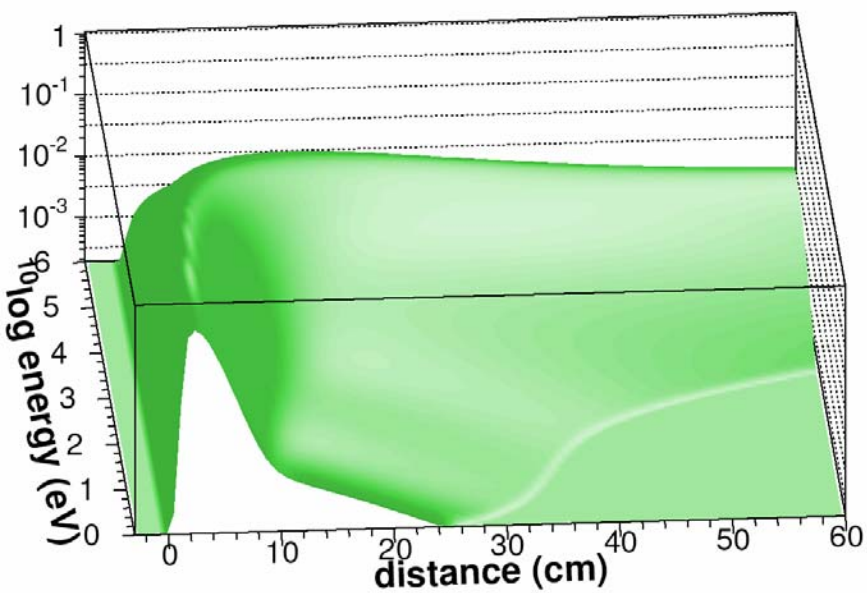
n_TOF



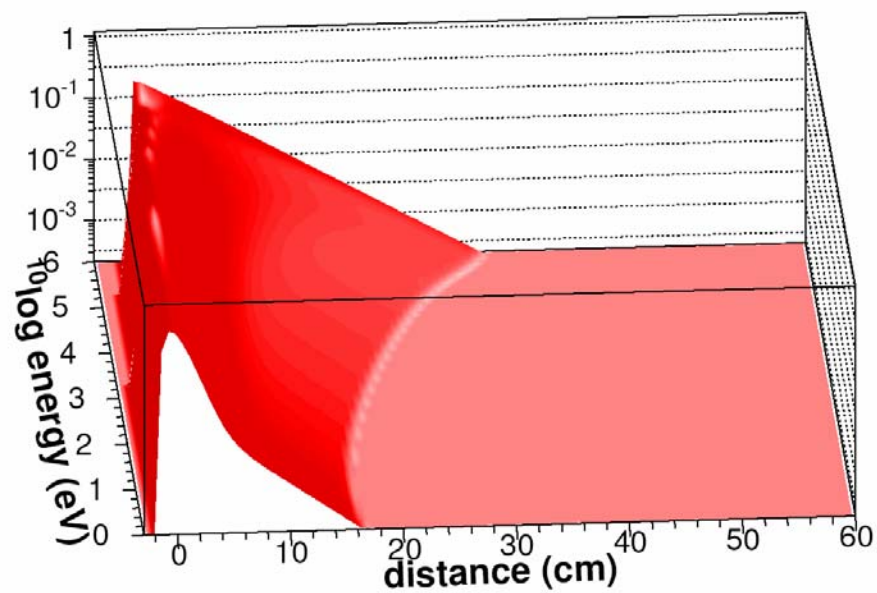
GELINA (0º)

Analytical 2D resolution function now available in SAMMY

n_TOF



GELINA (0°)



Corrections, continued

- ***Self-Shielding and Multiple-scattering:***
  - **Self-shielding: works fine**
  - **Single-scattering correction: works well**
  - **Double-plus scattering: works reasonably well**
    - **(the rest of the multiple-scattering, everything except single-scattering)**
    - **Gives the shape fairly well**
    - **Often a bit too high in magnitude**
    - **Usually not very important (~3rd-order effect)**
  - **Work in progress:**
    - **Comparison tests with Monte Carlo calculations**
      - **John Swez (Indiana State University); Sabbatical project**
      - **Roberto Capote (IAEA) improvements to Monte Carlo code**

Corrections, continued

- ***Other corrections for experimental cond in RRR:***
  - **Several types of normalization & background**
  - **Angle-average for angular distributions** new

- ***Corrections for experimental conditions in URR:***
  - **Energy-dependent normalization**
    - **May be different for each data set**

Fitting Procedure: Bayes' method

- **Iterative form of Bayes' Equations**
  - **used to determine optimal values of parameters and associated covariance matrix**

- **All covariance matrices are tested for positive-definiteness** New
  - **Implemented at Gerry Hale's suggestion**
  - **The vast majority of SAMMY- produced covariance matrices *are* positive definite**

Whew!

Fitting: Bayes' method, cont.

- **Needed –**
  - **to include all uncertainties for all parameters**
  - **to treat covariance matrices quickly, efficiently, and accurately**
- **Solution –**
  - **use PUPs**
  - **use IDC**

See paper # 119 : "Treatment of Data Uncertainties"

Fitting procedure, PUPs

- **Bayes' Equations for updating parameters *P* are**

$$P' - P = M'Y \qquad M' = \left(W + M^{-1}\right)^{-1}$$

$$Y = G^t V^{-1}(d - t) \qquad W = G^t V^{-1} G$$

$$\boxed{V = v + \boxed{g}\, m\, g^t}$$

- **where**
  - **Data can be raw or reduced**
  - **Covariance matrix for reduced data is calculated at the true values of the cross section**
    - **i.e., derivatives are calculated at true values**

"true" ➔ "theoretical"

Benefits of this definition of DCM:

- **Consistent and reasonable results are obtained**
  - **when fitting raw data**
  - **when fitting reduced data**

"results" = values and covariance matrix for varied parameters

- **"All" prior uncertainties are reflected in the final results**
  - **for varied parameters (as usual)**
  - **for unvaried parameters**
    - **experiment-related parameters**
    - **non-varied theory parameters also**

Implementation in SAMMY

- **Any parameter may be treated in this fashion**
  - **Designation: Propagated Uncertainty Parameter**
  - **Short-hand notation: PUP** **(Thanks to Royce Sayer for suggesting this name)**
- **How to use?**
  - **Simply flag with "3" rather than "1" or "0"**
  - **Provide uncertainties for PUPs in the same manner as for varied parameters**

Which parameters can be PUPs?

- tr044 (tr009) resonance parameters (res)
- tr059 (tr093,tr111) R-matrix radii (rad)
- tr040 (tr011) R-external (ext)
- tr038 (tr007) broadening etc (brd)
- tr041 (tr012,tr138) normalization and background (nbk)
- tr097 (tr056,tr121) background functions (bgf)
- tr068 (tr021,tr117) Oak Ridge resolution function (orr)
- tr096 (tr054) RPI resolution function (rpi)
- tr062 (tr029) nuclide abundance (iso)
- tr066 (many) miscellaneous parameters (msc)
- tr055 (tr055) paramagnetic cross section (pmc)

Not working yet:
- detector efficiency (det)
- user-defined resolution function (udr)

PUP test case

Related Un-PUP test case

How do we know the PUP theory and implementation are correct?

- **Use a variety of different methods, compare results**
- **Methods?**
  - **Vary the parameter**
  - **Use explicit data covariance matrix**
  - **Use as PUP with implicit data covariance matrix**
- **What is meant by "results" ?**
  - **Values for the (other) varied parameters**
  - **Associated covariance matrix**

Extensive tests have been made

All five methods give almost Identical results for the first iteration.

1. Treat as fitting parameter
2. If possible, treat as IDC (Implicit Data Covariance) parameter
   - For normalization & backgrounds, this option has been available for many years
3. Treat as user-supplied IDC
   - Derivatives were generated via a special SAMMY run
4. Treat with explicit data covariance
5. Treat as PUP parameter

Identical results

Identical for first iteration

almost identical results

Conclusions: this works!

- **Please see the various SAMMY test cases to compare results from one method to another**
- **One test that has not been done is to simultaneously use several different types of parameters as PUPs**
  - **Check your results carefully to be sure they make sense**
  - **As always, tell me if you uncover problems**
- **Also not extensively tested – PUPs in INPut file**
  - **This *should* work, but look carefully at LPT file to be sure**

PUP'd parameters are indicated by <38> instead of (38), for example.

Limitations on PUPs?

- **Not available yet:**
  - **Off-diagonal covariance matrices for PUPs**

$$P' - P = M'Y \qquad M' = \left(W + M^{-1}\right)^{-1}$$

$$Y = G^t V^{-1}(d - t) \qquad W = G^t V^{-1} G$$

$$V = v + g\,m\,g^t$$

  - **(To be implemented as the need arises)**

Fitting Procedure – IDC

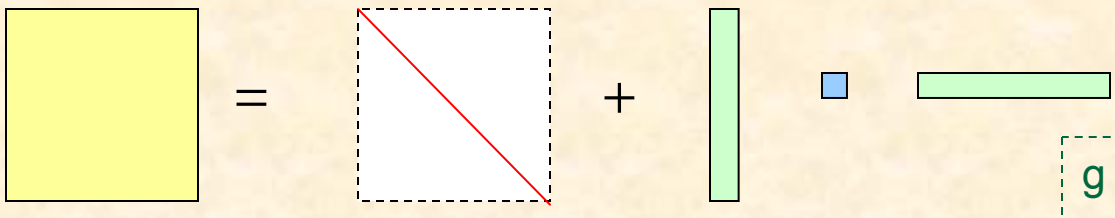
- **Inverting the data covariance matrix V**
  - **Explicitly**
    - **Large number of numbers**
      - **Takes time**
      - **Takes storage**
      - **Becomes inaccurate**
  - **Implicitly**
    - **Use matrix algebra to simplify**

Data Covariance Matrix, symbolically

Statistical part

Systematic part

$$V = v + g\ m\ g^t$$



g = sensitivity for data-reduction parameters
m = cov matrix for d-r par

where

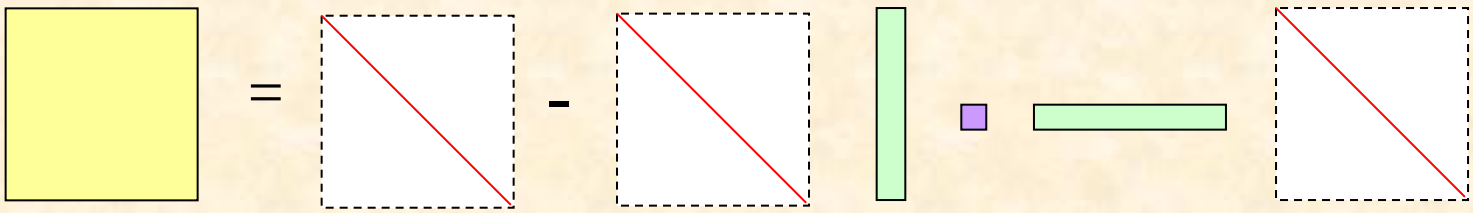
- **size of box may be considered to be logarithmic**
  - **large ~ thousands (or 10 K or 100 K)**
  - **small ~ very few (5? 10?)**
- **dashed box with diagonal line indicates diagonal matrix**
- **solid box indicates non-diagonal matrix**

Inverse of Data Covariance Matrix, symbolically

$$V^{-1} = (v + g\ m\ g^t)^{-1}$$

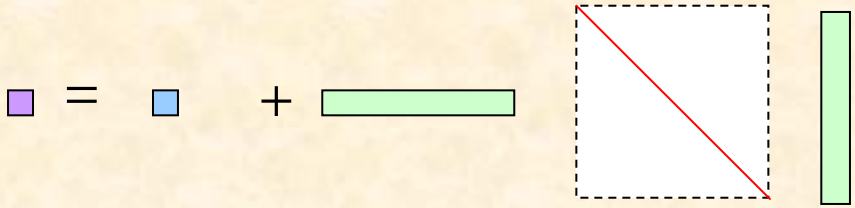
$$= v^{-1} - v^{-1} g\,(m^{-1} + g^t v^{-1} g)^{-1} g^t v^{-1}$$

$$= v^{-1} - v^{-1} g\ Z^{-1}\ g^t v^{-1}$$



where

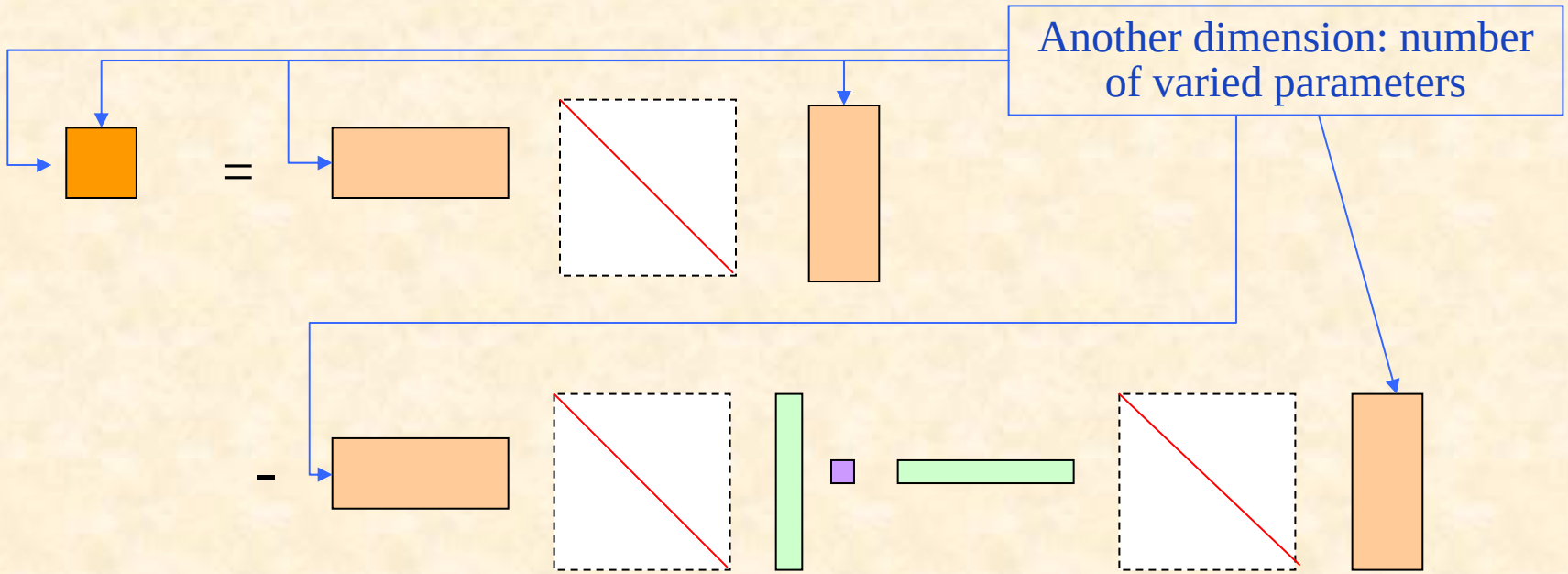
$$Z = m^{-1} + g^t v^{-1}\ g$$



Quantities needed in Bayes' equations: W

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

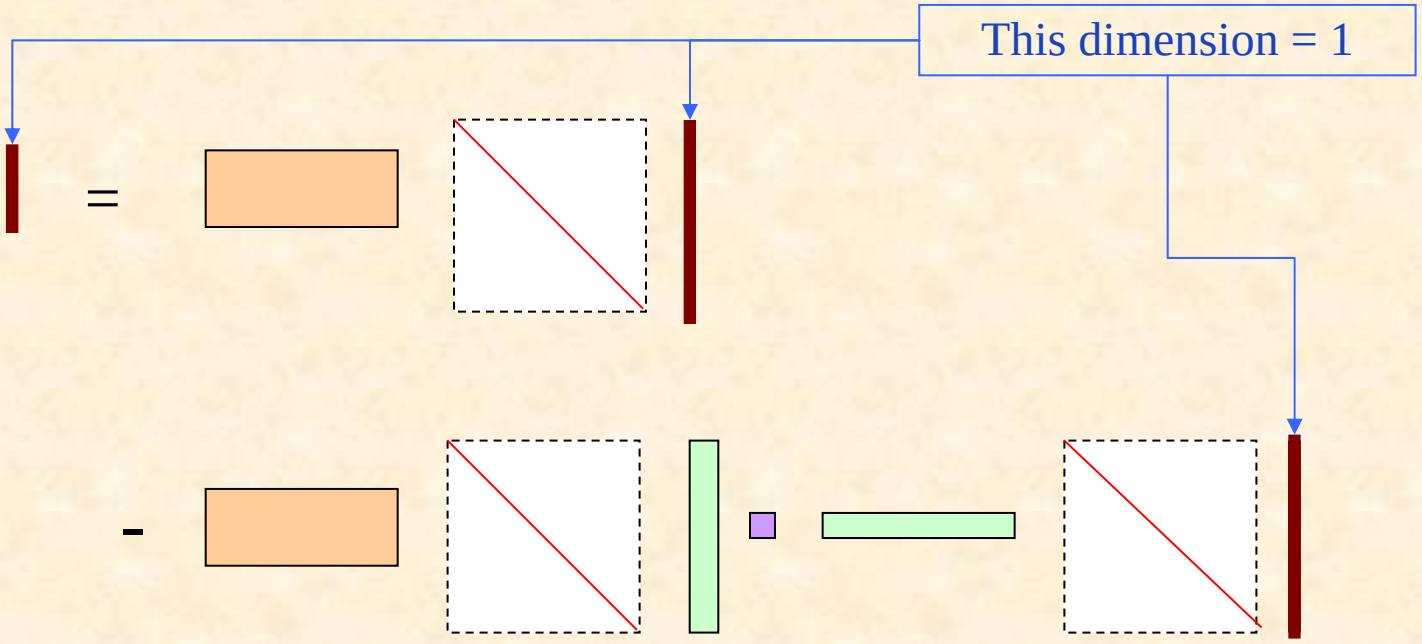
$$= G^t v^{-1} G - G^t v^{-1} g Z^{-1} g^t v^{-1} G$$



Quantities needed in Bayes' equations: Y

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

$$= G^t v^{-1} (D - T) - G^t v^{-1} g Z^{-1} g^t v^{-1} (D - T)$$



Why bother with all these arrays?

Matrices in *W* and *Y* are easier to invert than *V* –

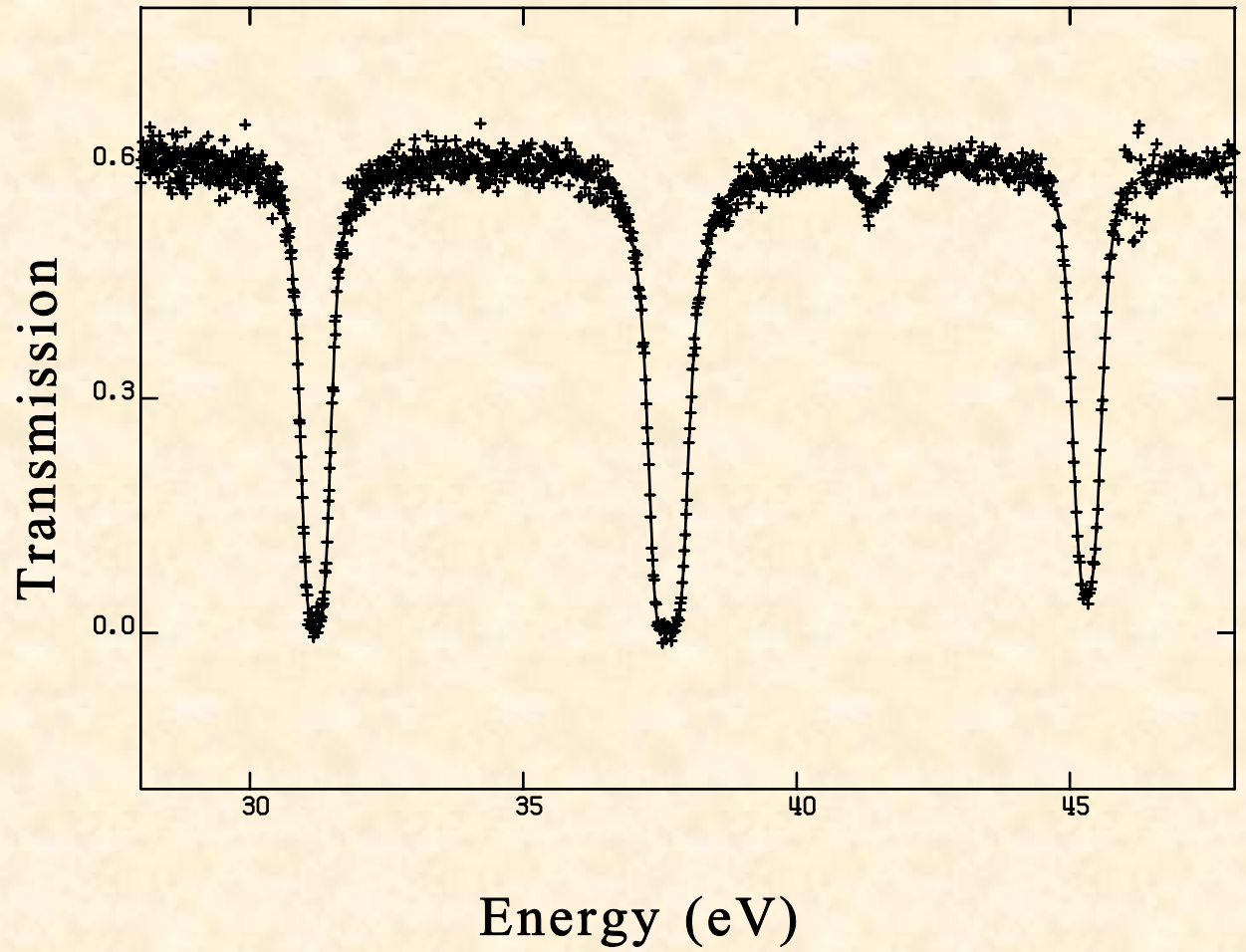
- ***v*** **is large but diagonal**
  - **(size ~ thousands of data points)**
- ***m*** **is small and often diagonal**
  - **(size ~ tens of data-reduction parameters)**
- ***Z*** **is off-diagonal but small**
  - **(size ~ tens)**

– which leads to savings in

- **computation time (never calculate *V* or V^{-1})**
- **computer memory (never store *V* or V^{-1})**
- **numerical accuracy and stability (fewer round-off problems)**

Example from SAMMY Test Case tr140: ^{129}I transmission data

Geel data provided by Gilles Noguere, Cadarache



Example, continued

1245 experimental data points;
[full data set has 32660 data points]
9 data-reduction parameters;
655 resonances; 9 varied parameters in this example

	Description of data covariance treatment for this run	Cpu time for Bayes solver (sec)	Total cpu time (sec)	Array size
a	only statistical errors	0.03	14	254 K
b	statistical plus systematic, only on diagonal	0.03	14	254 K
c	explicit data cov matrix	16.46 = x 500	59	1800 K = x 6
d	IDC matrix	0.06 = x 2	14	267 K = x 1

Note: c & d give essentially the same results provided c is done carefully

In SAMMY, **implicit data covariance (IDC) matrices** can be used for

- **normalization and background correction factors**
- **user-supplied implicit data covariance** new
  - **external code can be used to generate pieces (*g* and *m*)**
- **propagated-uncertainty parameters (PUPs)** newer

Caveat

- **Methodology described here implicitly assumes that values for data-reduction parameters are accurate**
  - **Values will not be updated**

- **Nevertheless, final results may reflect inaccuracy in input values for those parameters**
  - **as seen, for example, in studies of mistakes-in-measuring-backgrounds**

Caveat # 2

- **This methodology assumes that Bayes' Equations are correct**
  - **Bayes' Equations are based on the implicit assumption that the parameters obey Gaussian statistics**
  - **That assumption does not hold in general**
  - **Nevertheless that assumption appears to be approximately correct often enough that the equations are useful**

Preparing SAMMY input

- ***Spin-group definitions via SAMQUA*** New!
  - **Completely rewritten in collaboration with Cadarache colleagues (Bouland and Babut)**
  - **Generates quantum numbers for spin groups and associated channels**
  - **Treats all types of nuclides, charged particles, inelastic channels, reaction channels, etc.**
  - **Produces output in SAMMY input Particle-Pair format**
  - **Also provides values of penetrabilities and of hard-sphere cross sections**

For details, see paper # 309

Preparing input -- ENDF

- ***SAMMY can read ENDF files***
  - **R-matrix parameters from File 2, LRU=1 (RRR only)**
    - **Which versions?**
      - **LRF = 1 ("Single-Level Breit Wigner")**
      - **LRF = 2 ("Multilevel Breit Wigner")**
      - **LRF = 3 (so-called "Reich Moore")**
      - **LRF = 7 (new "R-Matrix Limited")**

Read these for starting parameters, but do not use Breit-Wigner for new analyses!

A highly restricted version of Reich-Moore

new

New format for ENDF/VII, fully compatible with all SAMMY conventions

Preparing input -- ENDF, cont.

- **R-matrix parameters from File 2, cont.**
  - **No longer necessary for user to edit the ENDF file to extract File 2** new
    - **SAMMY can read the entire ENDF file and search for the MAT number**
  - **SAMMY will create SAMMY-style INPut and PARameter files**
    - **User should edit these for use in future SAMMY runs**
      - **In particular, remove command to use SLBW or MLBW!**

Preparing input -- ENDF, cont.

- **Parameter covariance information from File 32**
  - **LCOMP = 1**
    - **Single "short-range" only ➔ complete covariance matrix**
  - **LCOMP = 2**
    - **New option for ENDF, compact covariance matrix**
    - **Approximate, for use when the full covariance matrix involves too many numbers for use of LCOMP = 1**

new

- **Point-wise cross sections from File 3, for use as SAMMY's DATa file**

new

Preparing input -- INPut file

- **<u>Problem</u>: formats for INPut file are becoming unwieldy due to options not originally available**
  - **outgoing channel particles have different masses and quantum numbers from incident channel particles**
  - **charge must be specified**
  - **threshold and radii must be given**
- **<u>Solution</u>: reorganize and simplify**
  - **specify the two particles (charge, spin, mass, threshold) independent of spin group definition; provide a label to pair**
  - **channel definition gives l and s plus pair-label**

Example: t100a.inp – the “old” version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17       16.99913   2000000.0 5500000.0         2  100
csisrs
spin of incident particle is +0.0
use new spin group format
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted

   5.00000   1.000
REACTION CROSS SECTION
       2.5
  1      1    1 -0.5     1.000  2.5
    1  2 1  8 0    3       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2    1    0    1       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  2      1    1  0.5     1.000  2.5
    1  2 1  8 0    2       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2    1    0    0       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  3      2    1 -1.5     1.000  2.5
    1  2 1  8 0    1       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2  2 1  8 0    3       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    3    1    0    1       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  4      2    1  1.5     1.000  2.5
    1  2 1  8 0    2       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
...
```

```
...

    2  2 1  8 0    4       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    3    1    0    2       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  5      3    1 -2.5     1.000  2.5
    1  2 1  8 0    1       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2  2 1  8 0    3       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    3  2 1  8 0    5       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    4    1    0    3       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  6      3    1  2.5     1.000  2.5
    1  2 1  8 0    0       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2  2 1  8 0    2       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    3  2 1  8 0    4       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    4    1    0    2       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649
  7      3    1 -3.5     1.000  2.5
    1  2 1  8 0    1       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    2  2 1  8 0    3       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    3  2 1  8 0    5       2.5       0.0       0.0 5.00 5.00 16.99913  4.0026
    4    1    0    3       0.5       0.0 -588708.0 3.80 3.80 19.992436 1.0086649

... [incomplete]
```

t100b.inp – the "new" version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17       16.99913   2000000.0 5500000.0         2  100
csisrs
spin of incident particle is +0.0
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted
particle-pair definitions are given
-------------------------------------------------------------------------------
a = default for incident, b = def for target
u = Lpent (1 or 0), v = Ishift (0 or 1)
name     a b  z  Zuv    i    I         m         M Threshold      Reff      Rtru
-------------------------------------------------------------------------------

alf+17O       2  810  0.0  2.5 4.0026000 16.999130          5.0000000 5.0000000
n+20Ne   n    0 1010  0.5  0.0 1.        19.992436 -588708.0 3.8000000 3.8000000

   5.00000   1.000
REACTION CROSS SECTION
       2.5
  1      1    1 -0.5  1.000   2.5
    1  alf+17O      3  2.5
    2  n+20Ne       1  0.5
  2      1    1  0.5  1.000   2.5
    1  alf+17O      2  2.5
    2  n+20Ne       0  0.5
...
```

Comments (between lines)

Information about the two particle pair sets

Spin groups then refer to particle-pair information

```
...
  3      2    1 -1.5  1.000   2.5
    1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  n+20Ne      1  0.5
  4      2    1  1.5  1.000   2.5
    1  alf+17O     2  2.5
    2  alf+17O     4  2.5
    3  n+20Ne      2  0.5
  5      3    1 -2.5  1.000   2.5
    1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  alf+17O     5  2.5
    4  n+20Ne      3  0.5
  6      3    1  2.5  1.000   2.5
    1  alf+17O     0  2.5
    2  alf+17O     2  2.5
    3  alf+17O     4  2.5
    4  n+20Ne      2  0.5
  7      3    1 -3.5  1.000   2.5
    1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  alf+17O     5  2.5
    4  n+20Ne      3  0.5

[... incomplete]
```

t100by.inp – the "newest" version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17        16.99913   2000000.0 5500000.0          2  100
csisrs
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted
key-word particle-pair definitions are given

Name = alf+17O
   Pa = alpha      Pb=17O    Zb=8   Sb=2.5        Mb=16.999130
   Mass a = 4.0026000000
Name = n+20Ne
   pa=n  particle b = 20Ne  Zb=10  Mass b = 19.992436
   Q=588708.0

   5.00000   1.000
REACTION CROSS SECTION
  1       1    1 -0.5  1.000
    1  alf+17O      3  2.5
    2  n+20Ne       1  0.5
  2       1    1  0.5  1.000
    1  alf+17O      2  2.5
    2  n+20Ne       0  0.5
  3       2    1 -1.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  n+20Ne       1  0.5 ...
```

Key word particle pair definitions

```
...
 4       2    1  1.5  1.000
    1  alf+17O      2  2.5
    2  alf+17O      4  2.5
    3  n+20Ne       2  0.5
 5       3    1 -2.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  alf+17O      5  2.5
    4  n+20Ne       3  0.5
```

```
...
 6       3    1  2.5  1.000
    1  alf+17O      0  2.5
    2  alf+17O      2  2.5
    3  alf+17O      4  2.5
    4  n+20Ne       2  0.5
 7       3    1 -3.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  alf+17O      5  2.5
    4  n+20Ne       3  0.5

[... incomplete]
```

Preparing input -- INPut file: Why bother changing what I'm doing?

- **In the past, evaluations were confined to one entrance channel per spin group in order to be publishable in ENDF**
  - **Other limitations: a maximum of two fission channels, no *l* admixture, no channel-spin admixture, no charged-particle channels, …**

- **Those limitations no longer exist**
  - **LRF=7 can accept any SAMMY evaluation**

Why do we need such generality?

- **Consider ^{27}Al, for example**
  - **In "LRF=3" conventions, there are 18 spin groups**
    - **Each has one entrance channel**
    - **The same J^{π} values apply to multiple spin groups**
  - **In a more perfect world, there are 10 spin groups**
    - **One spin group for each J^{π} value**
    - **More than one channel per spin group**

^{27}Al, “old” input file:

```
[commands, etc]

[radius etc]
[cross section type]
  1       1    0  2.0  1.000   2.5
    1     1    0    0  2.0
  2       1    0  3.0  1.000   2.5
    1     1    0    0  3.0
  3       1    0 -1.0  1.000   2.5
    1     1    0    1  2.0
...
```

```
  4       1    0 -2.0  1.000   2.5
    1     1    0    1  2.0
  5       1    0 -3.0  1.000   2.5
    1     1    0    1  2.0
  6       1    0 -2.0  1.000   2.5
    1     1    0    1  3.0
  7       1    0 -3.0  1.000   2.5
    1     1    0    1  3.0
  8       1    0 -4.0  1.000   2.5
    1     1    0    1  3.0
... plus l=2 terms
```

^{27}Al, key-word PP formulation:

```
[commands, etc]
Key-Word Particle-Pair definitions are given

PARTICLE PAIR DEFINITIONS
Name=27Al+n     Particle a=neutron  Particle b=27Al
   Sb=   2.5  Mb=    27.00000000

[radius etc]
[cross section type]
 1     1    0  2.0
   1  27Al+n      0  2.0
 2     1    0  3.0
   1  27Al+n      0  3.0
 3     1    0 -1.0
   1  27Al+n      1  2.0
. . .
```

```
 4     1    0 -2.0
   1  27Al+n      1  2.0
 5     1    0 -3.0
   1  27Al+n      1  2.0
 6     1    0 -2.0
   1  27Al+n      1  3.0
 7     1    0 -3.0
   1  27Al+n      1  3.0
 8     1    0 -4.0
   1  27Al+n      1  3.0
. . . plus l=2 terms
```

^{27}Al, PP, combining spin groups

```
[commands, etc]
Key-Word Particle-Pair definitions

PARTICLE PAIR DEFINITIONS
Name=27Al+n     Pa=neut  Pb=27Al
   Sb=   2.5  Mb=    27.00000000

[radius etc]
[cross section type]
1     3    0  2.0
  1  27Al+n     0  2.0
  2  27Al+n     2  2.0
  3  27Al+n     2  3.0
2     3    0  3.0
  1  27Al+n     0  3.0
  2  27Al+n     2  2.0
  3  27Al+n     2  3.0
```

```
3     1    0 -1.0
  1  27Al+n     1  2.0
4     2    0 -2.0
  1  27Al+n     1  2.0
  2  27Al+n     1  3.0
5     2    0 -3.0
  1  27Al+n     1  2.0
  2  27Al+n     1  3.0
6     1    0 -4.0
  1  27Al+n     1  3.0
```

```
7     1    0  0.0
  1  27Al+n     2  2.0
8     2    0  1.0
  1  27Al+n     2  2.0
  2  27Al+n     2  3.0
9     2    0  4.0
  1  27Al+n     2  2.0
  2  27Al+n     2  3.0
10    1    0  5.0
  1  27Al+n     2  3.0
```

Two channel spins s

Two values for *l*, two values for *s*

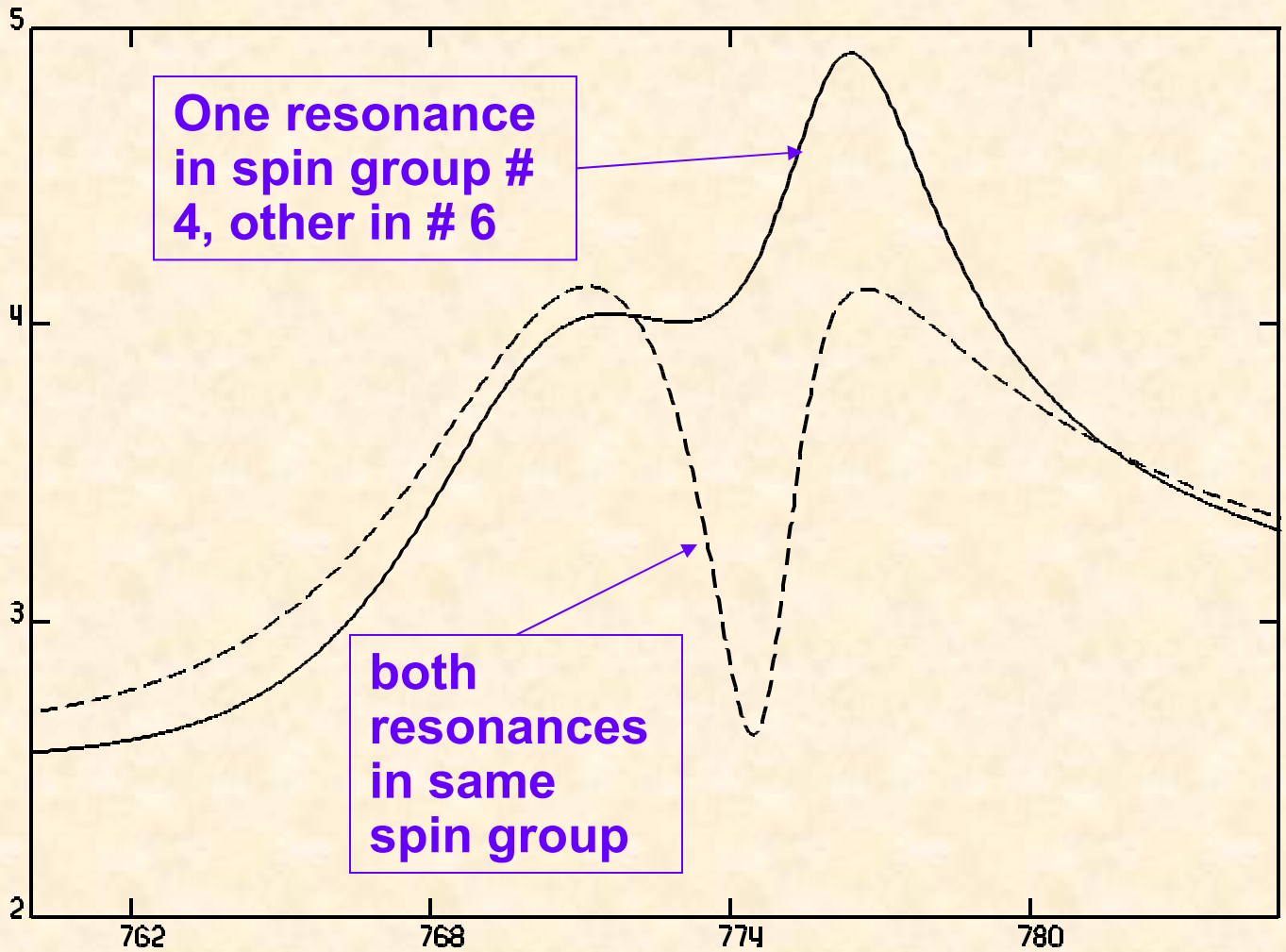
^{27}Al, combined spin groups in “old” format

```
  1       3    0  2.0  1.000   2.5
    1     1    0    0  2.0
    2     1    0    2  2.0
    3     1    0    2  3.0
  2       3    0  3.0  1.000   2.5
    1     1    0    0  3.0
    2     1    0    2  2.0
    3     1    0    2  3.0
  3       1    0 -1.0  1.000   2.5
    1     1    0    1  2.0
  4       2    0 -2.0  1.000   2.5
    1     1    0    1  2.0
    2     1    0    1  3.0
...
```

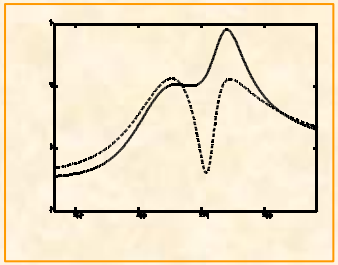
```
  5       2    0 -3.0  1.000   2.5
    1     1    0    1  2.0
    2     1    0    1  3.0
  6       1    0 -4.0  1.000   2.5
    1     1    0    1  3.0
  7       1    0  0.0  1.000   2.5
    1     1    0    2  2.0
  8       2    0  1.0  1.000   2.5
    1     1    0    2  2.0
    2     1    0    2  3.0
  9       2    0  4.0  1.000   2.5
    1     1    0    2  2.0
    2     1    0    2  3.0
 10       1    0  5.0  1.000   2.5
    1     1    0    2  3.0
```

Example: Pseudo-^{27}Al, two resonances

- **Consider two resonances, with the same J^{π} value [2^-]**
- **In the "old" formulation, each resonance was either spin group # 4 or spin group # 6, never a combination of the two**


5
4
3
2
762
768
774
780
One resonance in spin group # 4, other in # 6
both resonances in same spin group

Two resonances, cont.



- **Each channel in separate spin group: 18 groups**

```
770000.0000 2.0000E+03 9.0000E+06                    1 1 1     4
776000.0000 2.0000E+03 4.0000E+06                    1 1 1     4
```

- **Combined spin groups: 10 groups**

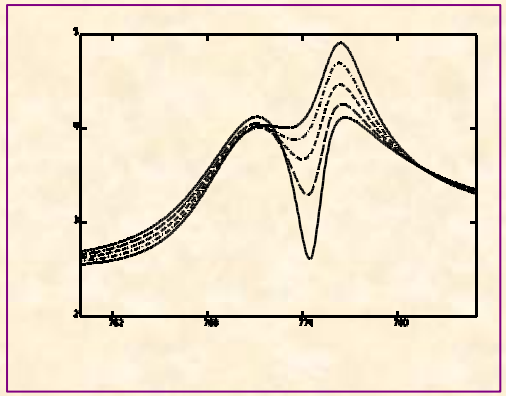
```
770000.0000 2.0000E+03 9.0000E+06 0.0                1 1 1     4
776000.0000 2.0000E+03 0.0        4.0000E+06         1 1 1     4
```

4.0000E+6

- **Both give the ~~solid~~ curve on previous slide**

dashed

Two resonances, cont.



- **Put some of the strength in the other channel**

```
770000.0000 2.0000E+03 9.0000E+06 0.0
776000.0000 2.0000E+03 1.0000E+06 3.0000E+06
```

#1

- **or**

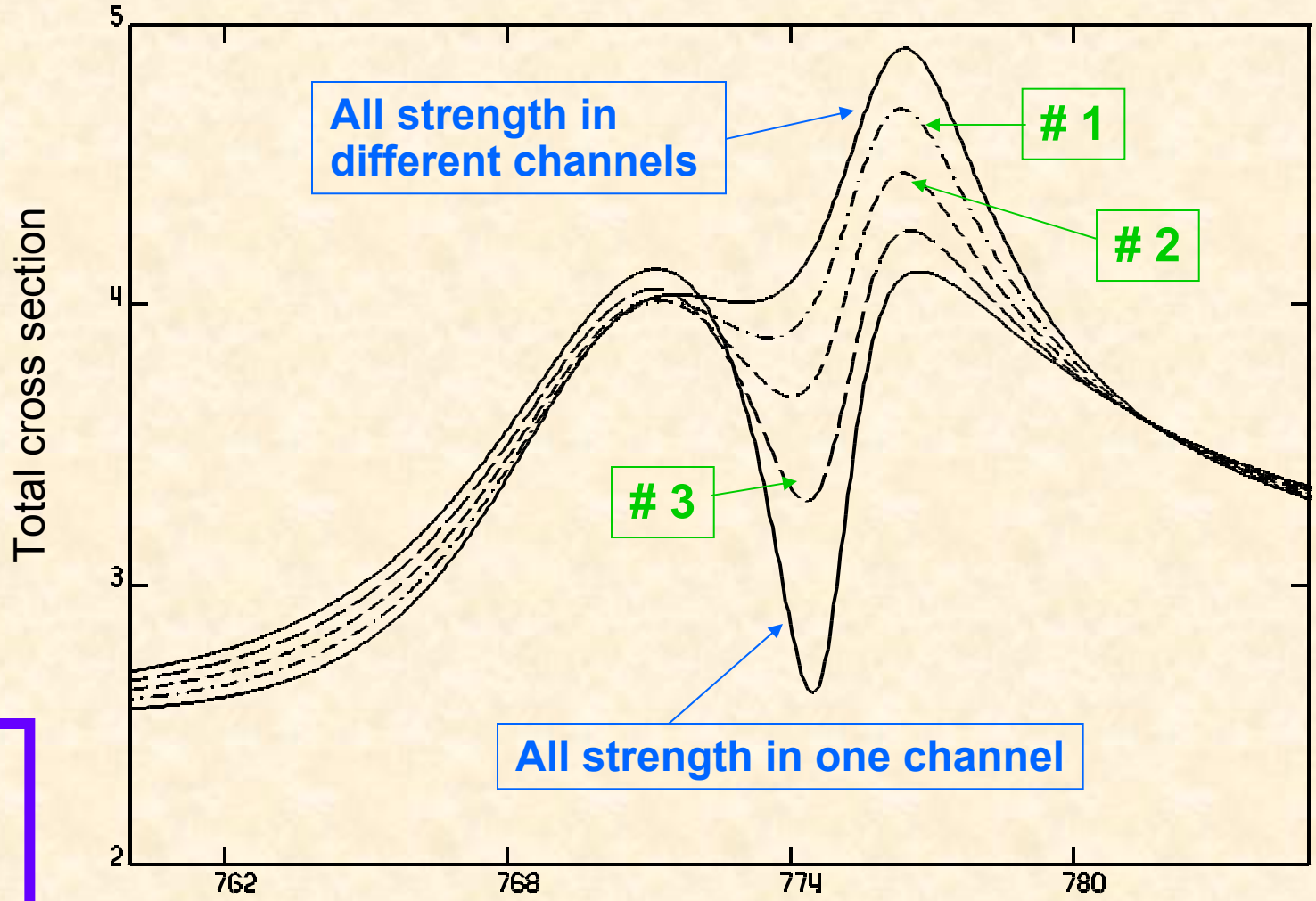
```
770000.0000 2.0000E+03 9.0000E+06 0.0
776000.0000 2.0000E+03 2.0000E+06 2.0000E+06
```

#2

- **or**

```
770000.0000 2.0000E+03 9.0000E+06 0.0
776000.0000 2.0000E+03 3.0000E+06 1.0000E+06
```

#3



See test case tr101 for this example

Preparing input -- INPut file: Conclusion

- **If data cannot be fit with all the strength in one channel or the other, maybe what is needed is some strength in each**
- **There is no physical restriction to this behavior**
  - **"Whatever is not forbidden is possible" (?)**
  - **"Whatever is not prohibited is compulsory" (?)**
- **ENDF LRF=3 restrictions no longer apply**
- **["Inertia" is the only disincentive to using this option]**

Preparing input – Misc

- **"Obsolete spin group format" is no longer supported**

new

- **Key-word input for channel radii**

new

  - **To be used in conjunction with particle-pair spin-group definitions**

Test cases 15,41,43,46,59,93,119,151,153, maybe others

Preparing input -- Misc, cont.

- **Mistakes in INPut file commands appear "on line"**
  - **No longer just in LPT file** new
- **Comments are allowed in the command section of the INPut file** new
  - **Two lines of dashes (one before, one after) are used to separate comments from commands**
  - **Lines beginning with # are ignored by the code**
    - **Commands can be turned into comments by inserting a pound sign (#) in front of the command**

Preparing input -- Misc, cont.

- **Data-related information can be given in INP file**
  - **Normalization and background**
  - **Miscellaneous parameters**
  - **ORResolution function parameters**
  - **RPI Resolution function parameters**
  - **User-defined resolution function parameters**
  - **Detector efficiencies**
  - **Data reduction parameters**

New, mostly

Preparing input – Misc, cont.

- **Data-related information in INPut file, cont.**
  - **Caveat: Parameters in INPut file can*not* be varied**
    - **(flag = 1 is ignored)**
  - **However, parameters in INPut file can be PUP'd**
    - **(flag = 3 is used)** new

- **More than 50 spin groups are allowed** new

- **More than 3 particle channels are allowed**

NOT new, but also not well known

Preparing input – Misc., cont.

- **Easier options for input of prior uncertainties on resonance parameters** new
  - **Key-word based**
  - **Give uncertainties for entire classes of resonance parameters, not only for individual parameters**
    - **Classes are defined in terms of**
      - **Energy ranges**
      - **Spin groups**
      - **Channels**
  - **Absolute or relative uncertainties**
  - **See tr151 for examples (esp. cases g, h, i)**

Preparing input – Misc., cont.

- **X-out channels for testing purposes** new
  - **These channels will be eliminated from all aspects of the calculation** See test case tr152; requires PP input
    - **(to be distinguished from "exclude from final state")**
    - **Use for testing only, not for "production" runs**

- **In URR** new
  - **"Annotated" files are now default for input and output**
    - **Descriptive information makes files easier for humans to read and amend**
    - **Comments are permitted throughout**

Output options

new

- ***SAMMY can create ENDF files***
  - **File 2, LRU=1 (RRR) [R-matrix parameters]**
    - **LRF = 1 (SLBW), 2(MLBW), 3(RM), 7(RML)**

not new

  - **File 2, LRU=2 (URR) [average resonance parameters]**
  - **File 32 [parameter covariance matrices]**
  - **File 3 [point-wise cross sections]**
  - **File 33 [covariances for cross sections]**

Use only for testing, not for submission to ENDF

Output options -- Publish, cont.

- ***Publishable tables*** new
  - **SAMMY can generate a listing of resonance parameters and uncertainties in a format suitable for porting to spread-sheet programs**
    - **(so now you have no excuses for omitting the uncertainties when you publish your results!)**

Output options – Misc.

- **User can choose energy units for plot files** new
- **Formulae for chi-squared now properly use the off-diagonal data covariance matrix** new
- **Inconsistencies have been removed from LPT file** new
  - **Please tell me if you find this task is not finished!**

Output options – Confession

new

- **<u>Confession</u>: A mistake was made in generating the output parameter covariance matrix (pcm) as reported in the LPT file**
  - **When does the mistake show up?**
    - **Only when both the resonance energy and the neutron width are simultaneously varied**
  - **What was the mistake?**
    - **The change of variable from γ to Γ must include the resonance-energy-dependence of Γ**

Reduced width amplitude, used for calculations within the code

Partial width, used for reporting the results

Output options -- Confession, cont.

new

- **Confession, cont.**
  - **How was this mistake discovered?**
    - **In the process of comparing calculations of multigroup cross sections and associated covariance matrices from SAMMY and ERRORJ**

To be discussed later

  - **What are the consequences?**
    - **Virtually none**

Is this true? If you disagree, please let me know!

    - **Until now, the output pcm has not been used for any practical purpose**
  - **When will this mistake be corrected?**
    - **In the next SAMMY release (M7, date to be determined)**

Test Cases

- **Test cases are available for two purposes:**
  - **Testing the code to be sure it is functioning properly**
    - **when changes are made in the FORTRAN**
    - **when the code is ported to a different machine**
      - **The first time you run with a particular feature, be sure to run the test case and compare results.**
  - **Guidance in preparing input for particular features**
    - **"a picture is worth a thousand words", so**
    - **"an example is better than an explanation" ?**

Test Cases, continued

- **SAMMY Test cases should NEVER be used as sources of data files for actual physics!**
  - **Experimental data files**
    - **are usually abbreviated, or may have been invented**
  - **PARameter files**
    - **are often invented or taken from preliminary analyses, and are possibly truncated**
    - **may bear no resemblance to reality**
  - **ENDF files are not necessarily official ENDF files**
    - **invented or abbreviated**

The ENDF connection

- **Two new ENDF formats have been provisionally approved for ENDF/B-VII**

#1 **File 2, LRF = 7 for resonance parameters** new

- **Fully compatible with SAMMY**
  - **Unrestricted number of spin groups**
  - **Unrestricted number and type of channels**
  - **Unrestricted channel radii values**
  - **Charged particles permitted**
- **Evaluators are no longer restricted to LRF=3 limitations**

The ENDF connection

- **Two new ENDF formats, cont.**

#1 **File 2, LRF = 7 cont.**

- **SAMRML code was developed to read this format and calculate cross sections** new
  - **SAMRML was derived from SAMMY, different from SAMMY**
  - **Calculates all types of cross sections (elastic, capture, fission, reaction, etc.) at same time, as do processor codes (NJOY, AMPX, etc)**
  - **Does no fitting, but does calculate partial derivatives**
    - **Unfortunately, the original version contained the same mistake as SAMMY! That has now been corrected, however.**
  - **Forms the basis for NJOY and AMPX implementation of LRF=7; has been used for testing PREPRO/RECENT**

The ENDF connection

- **Two new ENDF formats, cont.**

#2 **Resonance-parameter covariance matrix**

- **Existing format (LCOMP = 1) can work unless there are *many* parameters**
- **New format (LCOMP = 2) gives covariance matrix in compact, approximate form** new
- **ERRORJ code reads and uses the resonance-parameter covariance matrix (also covariance matrix for higher-energy regions) for calculating multigroup cross sections**
  - **ERRORJ is a modified version of NJOY, developed by G. Chiba, Japan**

See paper 249 Friday morning

SAMMY code details

- ***Origin:*** **~1978, ORELA extension of MULTI code**
  - **(written by G. Auchampaugh at LANL)**
- ***Language:*** **FORTRAN**
- ***Size:*** **~ 150,000 lines of code**
- ***Structure:***
  - **46 semi-autonomous segments in SAMMY itself**
    - **(stored in ~49 subdirectories)**
  - **17 auxiliary codes documented in SAMMY manual**
    - **plus plotting packages (forodf, rsap, ...)**

Code details, cont.

- ***Platforms:***
  - **UNIX (IBM, Dec, Sun, ...)**
  - **VMS (Dec)**
  - **LINUX**
  - **PC / Windows**
- ***Documentation:***
  - **419-page users' manual in pdf format**
  - **Many other publications**

430 so far in the next release

Code details, cont.

- ***Input:*** **user-friendly (hopefully!)**
- ***Quality Control:*** **> 140 test cases**
  - **Currently being reorganized to "fill in the gaps"**
  - **Altogether ~1500 sammy runs, plus auxiliary code runs**
- ***Experience:***
  - **25 years of successful analyses of many experimental data sets ranging from light to heavy nuclei**
- ***Instruction:***
  - **Tutorial exercises for novice users**
  - **Workshops**

Future plans for SAMMY

- **Simultaneous fitting of several data sets**
  - **Already available in limited fashion**
- **Input: R-matrix information to be "divorced" from measurement-related information**
  - **One PARameter file per nuclide**
    - **includes both spin-group definitions and resonance parameters**
  - **One EXPeriment file per data set**
    - **defines measurement-related quantities**

Future plans, cont.

- **GUI (Graphical user interface)**
- **More work on multiple-scattering corrections**
  - **Testing double-plus scattering**
  - **Implement a rapid-but-approximate method for multiple-scattering**
    - **Probably: after calculate it once, re-use that calculation for other runs**
- **Study propagation of uncertainties**
  - **"Why are R-matrix uncertainties so small?"**

Future plans, cont.

- **Additional studies on CLM**
  - **Are new options needed?**
- **Additional development of resolution functions**
  - **For Geel and nTOF**
  - **Others?**
- **In URR**
  - **Integral quantities**
  - **More than one nuclide**

Future plans, cont.

- **Other tasks to be completed before retirement**
  - **Release the next update of code & manual**
  - **Understand CLM**
  - **Finish detailed documentation on lots of topics**
  - **Clean-up UDR resolution function**
  - **Locate, hire, and train replacement**

ND2004 Conference papers with "SAMMY" in abstract

1. ***Hafnium Resonance Parameter Analysis Using Neutron Capture and Transmission Experiments*, Trbovich et al. (56)**
2. ***Stellar (n,γ) Cross Sections of the Stable Ne Isotopes*, Plag et al (65)**
3. ***An evaluation of the 232Th total and capture cross-section from a combined analysis of transmission and capture measurements at GELINA*, Volev et al. (97)**
4. ***Neutron Capture and Transmission Measurements on 103Rh down to Thermal Energies*, Berthoumieux et al. (99)**
5. ***Neutron Data Evaluation and Validation of Rhodium-103*, Dupont et al. (147)**
6. **Measurements of Total Cross Sections at Pohang Neutron Facility, Guinyun Kim (157)**
7. ***R-matrix Analysis for Improvement of the International Standard Cross Section*, Chen et al. (164)**

Conference papers, cont.

8. ***Direct-Semidirect Neutron Capture Calculations Applied to R-Matrix Data Evaluations in the Resolved Resonance Region*, Arbanas et al. (221)**

9. ***Revision and Application of Covariance Data Processing Code*, ERRORJ, Chiba et al. (249)**

10. ***Reich-Moore Analysis of the Iodine-127 and Iodine-129 Resolved Resonance Range*, Noguere et al. (264)**

11. ***Experimental Cross Section Data Base Selection by a SAMMY Reich-Moore Parameterisation of the Resolved Resonant Range: the Case of the 9Be(α.n) Cross Section up to 6 MeV*, Bouland et al. (314)**

12. ***New Neutron Cross Section Measurements at ORELA for Improved Nuclear Criticality Calculations*, Guber et al. (317)**

Conference papers, cont.

13. ***A New Approach for Nuclear Data Covariance Generation*, Leal et al. (55)**
14. ***ORNL Evaluation of the Resonance Parameters of ^{238}U in the Neutron Energy Range from 0 keV to 20 keV and its Impact in Reactor Calculations*, Derrien et al. (66)**
15. ***Status of the International neutron cross section Standards file, Pronyaev et al. (145)***
16. ***New Resonance Parameter Evaluation of Cl Neutron Cross Sections*, Sayer et al. (193)**
17. ***Experimental Validation of the Crystal Lattice Model in the R-Matrix Code SAMMY*, Courcelle et al. (215)**

Conference papers, cont.

18. ***SAMQUA - A Program for Generating All Possible Combinations of Quantum Numbers Leading to the Same Compound Nucleus State in the Framework of the R-Matrix Code SAMMY*, Bouland et al. (309)**

19. ***Recent Cross Section Evaluations in the Resonance Region at the Oak Ridge National Laboratory*, Leal et al. (545)**

20. ***Treatment of Data Uncertainties*, Larson (119)**

21. ***Upgrades to the R-matrix code SAMMY*, Larson (120)**

The End