SAMMY Workshop Part 7

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 7. Miscellaneous topics

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Auxiliary codes

- **angodf**
  - **translate differential elastic data plot file from "a function of energy for a given angle" to "a function of angle for a given energy"**
- **convrt**
  - **convert from REFIT input to SAMMY or vice versa (resonance parameters only)**
- **samamr**
  - **rearrange data-reduction parameters when analyzing data sets sequentially**
- **samamx**
  - **modify the value of one non-varied resonance parameter (to be used with extreme caution)**

Auxiliary codes, continued

- **samcpr**
  - **provide direct comparison of results of calculations from two codes**
    - **the "other" code results are used as "experimental data" for SAMMY runs, to give both calculations at the exact same energies**
- **samdis**

More on this later…

  - **calculate statistical properties after completion of an analysis**
- **samftz**
  - **adjust tzero and L for an experimental data set**

Auxiliary codes, continued

- **samort**
  - **generate plots of ORR resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samplt** More on this later…
  - **alternative method for generating plot files**
- **samqua**
  - **generate quantum numbers for spin groups (recently generalized by Olivier Bouland, Richard Babut, and Nancy Larson)**

Already discussed

Auxiliary codes, continued

- **samrpt**
  - **generate plots of RPI resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samrst**
  - **generate plots of original (RSL) resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samsmc**
  - **perform Monte Carlo simulations of multiple-scattering corrections for capture or fission, to ensure consistency with SAMMY results**
- **samsta**
  - **generate staircase plots of resonances**

Auxiliary codes, continued

- **samthn**
  - **thin dense experimental data by averaging over a specified number of points in a given energy range**
- **suggel**
  - **suggest values for l and J for a given resonance (written by S. Y. Oh and L. C. Leal, not completely portable)**
- **samrml**
  - **read ENDF file 32 LRF=7 and generate cross sections (including angular distributions) and partial derivatives**
  - **intended as prototype for processor codes**

Auxiliary codes, continued (plotting)

- **forodf**
  - **ORELA code for manipulating & plotting results**
  - **very old, not maintained, not portable**
  - **is used for this workshop**
- **rsap**
  - **more modern code for plotting results**
  - **contains helpful preprocessor features**
  - **under development (Royce Sayer at ORNL)**
  - **not yet portable, not released**

Plotting

- **What to do on your own computers if you do not have forodf or rsap?**
- **SAMMY provides two kinds of files from which plots can be made**
  - **SAMMY.ODF (ORELA Data Format; single-precision)**
  - **SAMMY.PLT (binary format; double-precision)**
- **Auxiliary program samplt was designed to read SAMMY.PLT and rewrite in other format**
  - **Users can redesign the output from samplt as needed for your own plotting package, by modifying the FORTRAN**

Program samdis

- **modified version of SAMDIST, written by Luiz Leal**
- **used to verify consistency of resonance parameter set with predicted theoretical statistical distribution.**

- **Reference**
  - **"SAMDIST: A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters", L. C. Leal & N. M. Larson, ORNL/TM-13092 (September 1995)**
  - **Also see SAMMY users' manual (pages 150z.5-6) for update**

Program samdis, continued

- **Three statistical tests (details are given in samdist manual)**
  1. **Level spacing distributions are compared with the Wigner distribution law**
  2. **Neutron, radiation, and fission width distributions are calculated and compared with the $\chi 2$ distribution with the appropriate number of degrees of freedom –**
     - **dof = 1 for the Porter-Thomas distribution of neutron widths**
     - **dof = 2 or 3 for fission**
     - **dof = ∞ for capture widths**
  3. **Long-range correlations of the energies are tested via the $\Delta 3$ statistic of Mehta and Dyson**

Other SAMMY features worth noting

- **ENDF file 2 (isotopic) can be used for initial PAR file.**
  - **LRF=1,2,3,7**
- **SAMMY can report results in ENDF file 2 format**
  - **LRF=1,2 (Breit-Wigner)**
  - **LRF=3 (so-called Reich-Moore)**
  - **LRF=7 (new R-Matrix Limited)** ← **Recommended for all future work**
- **SAMMY is not confined to ENDF File 2 RM format limitations!**
  - **Spin-group-dependent radii; channel-dependent radii**
  - **As many entrance and/or exit channels as needed for a given Jπ**
  - **Coulomb penetrabilities if needed**

Other features, continued

- **Wanted: cross section as a function of energy for a given set of resonance parameters. Unavailable: experimental data to specify the energy grid. What to do?**
  1. **Use any available energy grid, or generate a "dummy" grid, in the appropriate energy range. Run SAMMY, ignore the "data" and look only at the "theory".**
  2. **If things look odd with #1, it may be that the energy grid is inappropriate for this resonance structure. Solution: Pretend you want Doppler (and/or resolution) broadening. This will force SAMMY to generate an auxiliary grid (which *will* be appropriate for the resonance parameters you are using), which can be written to an output file using the command "plot unbroadened cross sections".**
  3. **Alternatively, use the "reconstruct cross section from resonance parameters" command. This command causes SAMMY to generate an energy grid using techniques (and programming) borrowed from NJOY.**

Other features, continued

- **Stellar (Maxwellian) averages can be generated as a function of temperature, for use in nuclear astrophysics applications.**
  - **Covariance matrix is also generated.**

- **Multigroup cross sections can be calculated with**
  - **either (1) no corrections to the theoretical values, or (2) Doppler and/or resolution broadening, multiple-scattering corrections, etc., and**
  - **either Bondarenko narrow resonance scheme or energy- or time-weighted averaging.**
  - **Covariance matrix is automatically generated**

Other features, continued

- **There is no covariance matrix in the evaluated files. What to do?**
  - **SAMMY can retroactively generate an *approximate* covariance matrix for resonance parameters, even after the evaluation is complete.**
    - **Needed – all (or most) of the data used for the original analysis.**
      - **If absolutely necessary, can use SAMMY to "invent" data, then make reasonable assumptions about the uncertainties on those data**
    - **Procedure involves simultaneous fitting (with no iteration) of the available data.**
      - **Underlying assumption is that parameter values will change very little, so covariance matrix is appropriate for the unchanged parameter values.**

Other features, continued

- **Mismatch in energy-scale between two data sets can sometimes be corrected by having SAMMY fit *t* 0 and *L*. Program samftz can then provide modified data file.**
- **Spin-group-dependent detector efficiencies can be used for analysis of capture or fission yields or self-indication data.**
- **Angle-differential reaction cross sections (as well as angle-differential elastic cross sections) can be calculated.**

Other features, continued

- **It is possible to generate a phony theoretical "cross section" which is constant, linear, delta-function, or 1/*v*. These are useful for testing resolution functions, for example.**
- **Information for resolution functions, for normalizations and backgrounds, and for "miscellaneous" parameters can now be in the INPut file instead of the PARameter file, so long as no parameters are to be varied.**
  - **CAUTION: Double-check the LPT file to be sure SAMMY is actually doing what you wanted!**

Very new, not in any released version of the code

Quality assurance

How do we know that SAMMY is doing what it's supposed to be doing?

- **SAMMY QA program involves "test cases"**
- **Each test case is designed to test a particular feature of the code**
- **A new test case is created when**
  - **a new feature is added to SAMMY**
  - **a major bug is exterminated**
- **All test cases are rerun**
  - **after major changes / additions to the code**
  - **prior to each official release**
  - **upon porting to a new computer platform**
  - **whenever the author feels the need**

Quality assurance, continued

- **Test cases (input and output) are released along with source code (from RSICC or NEA), and should be run whenever the code is ported to a new platform --**
  - **to resolve differences**
  - **to find bugs that show up on your system but not on the author's**
  - **to be sure the code you are using behaves properly**
- **NOTE: When porting SAMMY to your computer, run *all* test cases and compare your output to the author's, before beginning to run your own analyses. *At least run those cases which use the features you are using!***
  - **Be sure run the relevant test cases before you contact the author for help.**
- **Another use for test cases -- provide sample input for specific features of the code**
  - **A table in the manual provides a list of all available test cases and which features they pertain to.**

End of miscellaneous topics