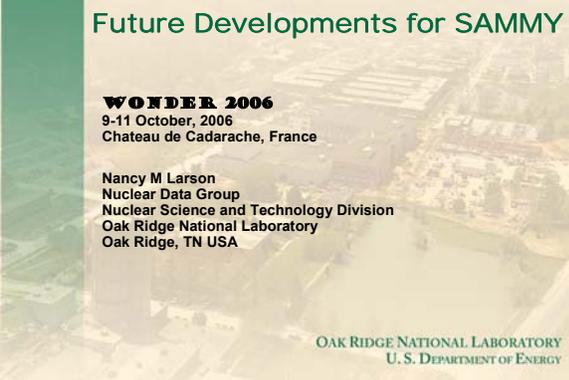




## Future Developments for SAMMY

**WONDER 2006**  
9-11 October, 2006  
Chateau de Cadarache, France

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## The SAMMY analysis code

- **Purpose –**
  - Evaluate neutron time-of-flight cross-section data such as those measured at
    - ORELA at ORNL, GELINA at IRMM, nTOF at CERN, Gaertner linac at RPI, DANCE at LANL, etc.
  - Also includes capabilities for analysis of charged-particle data

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## SAMMY, continued

- **Procedure –**
  - Calculate theoretical cross sections via R-Matrix
    - Reich Moore, Breit-Wigner
  - Modify according to experimental conditions
    - Doppler and resolution broadening, normalization, background, multiple-scattering corrections, etc.
  - Find best-fit parameter values via generalized least squares techniques
    - Include all types of uncertainties and covariances
  - Report results to evaluated nuclear data files

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## SAMMY, cont.

- **Distinctive features –**
  - Developed over three decades at ORNL
  - Portable to most modern computer platforms
  - In use around the world for neutron data; also useful for charged-particle data
  - Applications in nuclear astrophysics work, criticality safety, others
  - Extensive quality control (~170 test cases)
  - Well documented

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## Current Status

- **New SAMMY manual just released**
  - ~600 pages, interlinked pdf file
    - Printable version includes blank pages for double-sided copy
  - Contains
    - General theory
      - R-matrix, Doppler and resolution broadening, multiple-scattering corrections, etc.
    - SAMMY-specific information
      - Implementation, input, output, etc.
- **No longer “export controlled” – copies are freely available**

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## Current Status, continued

- **SAMMY code to be released by RSICC very soon**
  - Modern distribution system, easier to install
  - Version 7.0.0
  - Fully described in the manual
- **SAMMY users’ group**
  - Via NEA
  - Via ORNL

Please let me know when you find bugs in either the code or the manual.

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## New features in this release

- **Many enhancements to treatment of data and parameter covariance matrices**
  - to be discussed this afternoon
- **Option for least squares fitting**
  - Instead of generalized least squares
- **Option for simultaneous fitting**
  - Instead of sequential
- **Resolution function for GELINA and nTOF data**
  - Thanks to Frank Gunsing

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## New features, cont.

- **Strengthened ENDF connection**
  - Both input and output
  - Both parameter values and parameter covariance matrices
- **Internal coding is streamlined**
  - More to come
- **Modern distribution system**
  - Thanks to Dorothea Wiarda
- **And many more**
  - Details are available in the manual

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## Today's topic: future developments

- **Resolved resonance region**
- **Unresolved resonance region**
- **Fitting procedure**
- **Uncertainties**
- **Input reorganization**
- **Procedural changes**
- **Global improvements**

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## Resolved resonance region

Wish list for future SAMMY development

- **Inverse reactions**
  - **Wanted: to simultaneously analyze data for all reactions that use the same compound nucleus**
    - For example,  $n + {}^{16}\text{O}$  and  $\alpha + {}^{13}\text{C}$
  - **Currently, need to rewrite either resonance parameters or experimental data**
    - Awkward
    - Not all reaction data can be rewritten, so useful information is lost
    - Uncertainties do not translate nicely

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## RRR, continued

Wish list for future SAMMY development

- **Multiple-scattering corrections for capture or reaction yields**
  - **Single-scattering**
    - Available now: Circular disk with flat surface perpendicular to beam line
      - Rectangular disk description has been developed but not fully implemented
  - Improvements for inhomogeneous sample may be needed for nTOF data (other data too?)

No great incentive for improvement from evaluators – current version fits the data adequately.

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## RRR, continued

Wish list for future SAMMY development

- **Multiple-scattering, continued**
  - **Double-plus scattering**
    - Second-order effect
    - Crude approximation may not be good enough in all cases
      - Shape seems reasonable but magnitude is sometimes wrong
      - Development work is needed

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## RRR, continued

Wish list for future SAMMY development

- **Long-range interaction terms**
  - Needed to study polarizability of neutron
  - Theory under development at Technische Universität Wien
  - Will be implemented into SAMMY

Helmut Leeb

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## Unresolved resonance region

Wish list for future SAMMY development

- **Modest extensions of existing capabilities –**
  - Treat multiple nuclides in the sample
  - Calculate multigroup averages & covariance matrix
  - Include integral quantities in the fitting procedure
- **New capabilities**
  - Improved ENDF format needed to coincide with theory used in SAMMY and FITACS and elsewhere
  - Implement new formalisms when available

"Evaluation of the Unresolved Resonance Range of  $^{238}\text{U}$ ,"  
F. H. Fröhner, *Nucl. Sci. Eng.* **103**, 119–128 (1989).

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## Fitting procedure

Wish list for future SAMMY development

- **Convergence criteria when iterating for non linearity** [Section IV.A.3 of SAMMY manual](#)
  - Currently, give number of iterations
- **Simplify simultaneous fitting** [Section IV.E.1](#)
  - Currently available but awkward
  - Most analyses use sequential method
- **Simplify use of least-squares** [Section IV.E.3](#)
  - Currently available but awkward to use

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## Uncertainties

Wish list for future SAMMY development

- **Can methodology uncertainty be incorporated into the code?**
  - R-matrix treats only compound effects (not direct)
  - Multiple-scattering correction is imperfect
  - Not all experimental uncertainties are known
  - Some spin assignments are dubious
  - Small resonances are omitted
  - Integrations involve numerical computations

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## Uncertainties, continued

Wish list for future SAMMY development

- **Include information regarding relationships between measurements**
  - When two otherwise independent measurements are marginally related
    - Use same physical sample, or
    - Data were taken on same machine
  - Need options for incorporating uncertainties from that relationship into the analysis
  - Perhaps can do this with an extension of the PUP methodology

Propagated Uncertainty Parameter

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## Input reorganization

Wish list for future SAMMY development

- **R-matrix information separated from measurement-related information**
  - One PARAMeter file for each nuclide
    - Several PARAMeter files for each analysis (unless sample is isotopically pure)
  - Experiment-related information in separate file for each data set
    - Thickness, temperature, resolution function, background, normalization, etc.

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## Input reorganization, cont.

Wish list for future SAMMY development

- **Simplify input for varying measurement-related parameters**
  - Eliminate SAMAMR code

## Procedural changes

Wish list for future SAMMY development

- **SAMMY's auxiliary grid** [Section III.A](#)
  - Currently generated only once during fitting procedure
  - When resonance energies are varied, and values change significantly in early iterations, original auxiliary grid may not be adequate
  - Needed: option to regenerate this grid for each iteration
- **Treatment of angular-distribution data**
  - Corrections for experimental effects are unsophisticated [Section III.E.7](#)
  - Is improvement needed?

## Global improvements

Wish list for future SAMMY development

- **Introduce modern configuration control and archival system** [Dorothea Wiarda](#)
- **Introduce modern matrix-manipulation techniques** [Goran Arbanas](#)
  - For very large runs, preliminary studies show significant reduction in runtime
    - “Days” become “Hours”
  - No obvious improvements for small runs
    - No differences observed in SAMMY test cases

## Global improvements, cont.

Wish list for future SAMMY development

- **Graphical user interface?**
  - RSAP code? [Royce Sayer](#)
  - Other?
- **Fortran 90?**
  - Especially “allocate” and “deallocate”
    - to replace “Function Idimen” in current version

The End