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*ICTP 40th Anniversary*

SMR.1555 - 27

**Workshop on  
Nuclear Reaction Data and Nuclear Reactors:  
Physics, Design and Safety**

**16 February - 12 March 2004**

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**Resonance Theory**

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These are preliminary lecture notes, intended only for distribution to participants



# SAMMY Workshop

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

(16 February - 12 March 2004)

Dr. Nancy M. Larson  
Oak Ridge National Laboratory

Part 1, Introduction

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# How-to's

- **obtain the SAMMY code and/or manual**
- **join the SAMMY users' group**
- **add your name to SAMMY distribution list**



# How to obtain the SAMMY code and/or manual (USA) --

- Contact RSICC
  - Radiation Safety Information Computational Center (RSICC)
  - P.O. Box 2008, Oak Ridge, TN 37831-6362 USA
- on the web at <http://www-rsicc.ornl.gov/rsic.html>
- or telephone at 865-574-6176
- Note:
  - “package name” = “SAMMY”
  - “ID number” = “PSR-158”

# How to obtain the SAMMY code and/or manual (outside the USA) --

- Contact the NEA
  - OECD Nuclear Energy Agency
  - Le Seine-St Germain
  - 12, Boulevard des Îles
  - F-92130 Issy-les-Moulineaux, France
- Telephone: (33) 1 45 24 10 10
- Fax: (33) 1 45 24 11 10
- on the web as: <http://www.nea.fr/html/dbprog>

# How to join the SAMMY users' group

- Log on to the SAMMY web site  
<http://www.nea.fr/html/dbdata/sammy.htm>
- Fill out the registration form there

# How to add your name to our distribution list

- for ORNL/TM and other reports from the
  - Nuclear Data Group (Mike Dunn, Group Leader), Nuclear Science and Technology Division,
  - Oak Ridge National Laboratory :
- Send e-mail to **LarsonNM@ornl.gov** with your return address; include both e-mail and regular mail addresses
- Or, write to me at  
Dr. Nancy M. Larson  
Oak Ridge National Laboratory  
Building 5700, MS 6171  
P O Box 2008, Oak Ridge, TN 37831-6171  
USA

# SAMMY References

- Users' Guide (Manual) :
  - N. M. Larson, *Updated Users' Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-9179, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (August 1984)
- Revisions
  - 1 ORNL/TM-9179/R1 (July 1985)
  - 2 ORNL/TM-9179/R2 (June 1989)
  - 3 ORNL/TM-9179/R3 (September 1996)
  - 4 ORNL/TM-9179/R4 (December 1998)
  - 5 ORNL/TM-9179/R5 (November 2000)
- Current Version
  - ORNL/TM-9179/R6 (May 2003) pdf , interlinked
  - Revision 7 is under development

## Other documents:

- “Introduction to the Theory and Analysis of Resolved (and Unresolved) Neutron Resonances via SAMMY”
  - N. M. Larson, Proceedings of the UNESCO/IAEA Workshop “Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety” held at the International Centre for Theoretical Physics, Trieste, Italy, 23 February - 27 March 1998, pub. World Scientific 1999.
  - Also published as ORNL/M-6576, July, 1998 and revised March 2000.

## Other documents, continued:

- “Covariance Matrices for Use in Criticality Safety Predictability Studies”
  - H. Derrien, N. M. Larson, L. C. Leal, ORNL/TM-13492 (September 1997)
- “Integral Data Analysis for Resonance Parameters Determination”
  - N. M. Larson, L. C. Leal, H. Derrien, ORNL/TM-13495 (September 1997).
  - Also *Nucl. Sci. and Eng.* **131** 254 (February 1999).

## Other documents, continued:

- “SAMDIST: A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters”
  - L. C. Leal & N. M. Larson, ORNL/TM-13092 (September 1995)
- “Doppler Broadening Revisited”
  - N. M. Larson, M. C. Moxon, L. C. Leal, H. Derrien, ORNL/TM-13525 (January 1998)
- “Derivation and Implementation of Multiple-Scattering Corrections for Capture and Fission Yields”
  - N. M. Larson, in preparation



## Other documents, continued:

- ““Merger of Nuclear Data with Criticality Safety Calculations”
  - N. M. Larson, L. C. Leal, H. Derrien, *Sixth International Conference on Nuclear Criticality Safety*, September 20-24, 1999, Versailles, France
- “Representation and Processing of Covariance Matrices for Resonance Parameters”
  - N. M. Larson, *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies*, Brookhaven National Laboratory, 22-23 April 1999
- etcetera

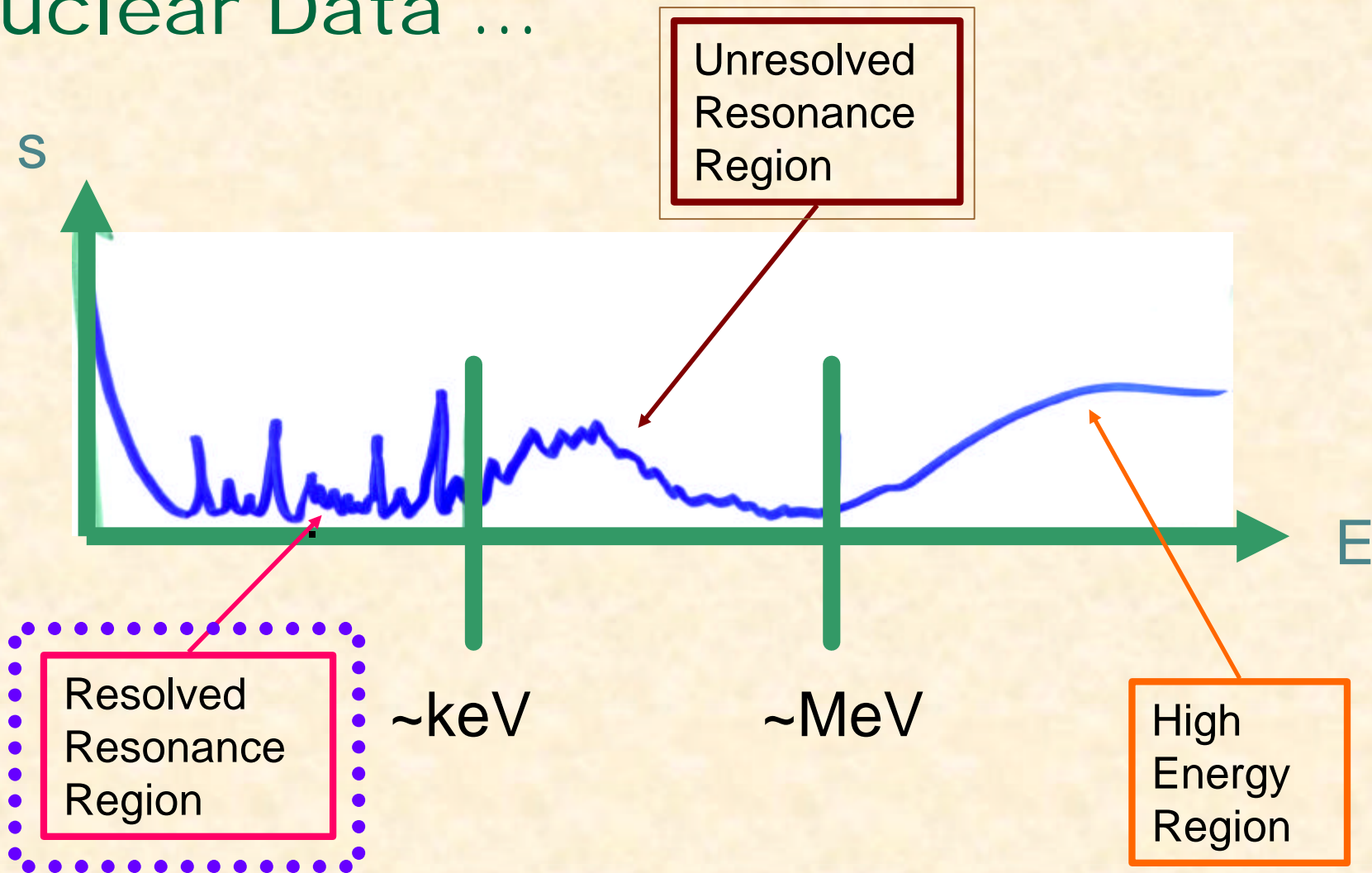
# Biographical Information

- For Nancy Larson, author of SAMMY code
- PhD, Michigan State University, 1972 (three-body problem)
- Senior Research Staff Member at Oak Ridge National Laboratory (ORNL), 1972-present (part time from 1976 to 1996, currently full time)
- Working on SAMMY since ~1977
- (Husband Duane Larson is retired as director of ORELA)
- For additional information, visit the web site [when we get it back up]

Important !

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

# Nuclear Data ...



# Description of the problem to be solved

- What do we have?
  - Raw data as counts per time-channel
  - Many thousands of pairs of numbers
- What do we want?
  - Cross sections as a function of energy
  - Parameterized in terms of resonance energies, widths, and quantum numbers

# How do we accomplish this?

- Perform the experiment
- Reduce the data
  - (counts => cross section, time-of-flight => energy)
- Generate covariance matrix for data
- Estimate prior values for parameters
- Estimate prior covariance matrix for parameters
- Analyze the data using multilevel multi-channel R-matrix code (e.g. SAMMY)

In this workshop we concentrate on the analysis, but will also talk about the other steps.

# SAMMY Overview

- Purpose: analyze time-of-flight cross-section data in the resonance region
  - resolved
  - unresolved
- (Other codes are used to analyze experimental data in high-energy region)

# SAMMY Overview, continued:

## I. Physics for Resolved-Resonance Region

- *Incident particles:* neutron, proton, alpha, ...
- *Target:* one type of nuclide, or many (multiple isotopes, chemical compounds, contaminants)
- *Types of data:*
  - total, elastic, capture, fission, inelastic, other reactions
    - Coulomb or not
  - angular distributions for elastic cross sections
  - certain types of integral data



# I. Physics for Resolved-Resonance Region, continued

- *Theoretical cross sections:* Reich-Moore approximation to multilevel multichannel R-matrix theory
- *Corrections for experimental effects:*
  - Four versions of Doppler broadening
  - six types of resolution broadening
  - self-shielding and multiple scattering
  - several types of normalization & broadening
  - etc.
- *Fitting procedure:* Bayes' method

# SAMMY Overview, continued:

## II. Pre- & Post- Processors (RRR)

- ***Prepare input “from scratch”:***
  1. Determine appropriate quantum numbers using SAMQUA
    - Written by O. Bouland, R. Babut, and N.M. Larson
  2. Estimate resonance parameter values (energies and widths) from experimental data via code RSAP
    - Written by R. O. Sayer
  3. Use program SUGGEL to suggest appropriate quantum numbers for a resonance
    - Written by S. Y. Oh and L.C. Leal
- ***Start from existing resonance parameters:***
  1. Use values from Evaluated Nuclear Data Files
    - SAMMY reads ENDF File 2 format

## II. Pre- & Post- Processors (RRR) continued

- **ENDF Format:** report results in ENDF File-2,3,32,33 formats
- **Statistics:** statistical properties for resonance parameters
- **Averaging:** two methods to calculate multigroup cross sections (including associated covariances)
- **Astrophysics:** stellar averages as a function of temperature

# SAMMY Overview, continued:

## III. Physics for Unresolved-Resonance Region

- *Incident particles:* neutron
- *Target:* one type of nuclide
- *Types of data:* total, capture, fission, inelastic
- *Theoretical cross sections:* Hauser-Feshbach for total, Moldauer's prescription for partial cross sections
- *Corrections for experimental effects:* energy-dependent normalization
- *Fitting procedure:* Bayes' method

SAMMY's treatment is based on Fritz Froehner's FITACS code

# SAMMY Overview, continued:

## IV. Code Details

- *Origin:* ~1978, ORELA extension of MULTI code
  - (written by G. Auchampaugh at LANL)
- *Language:* FORTRAN 77 (moving towards FORTRAN 90)
- *Size:* ~ 130,000 lines of code
- *Structure:*
  - 42 semi-autonomous segments
  - 16 auxiliary codes
  - plotting packages (forodf, rsap, ...)
- *Platforms:*
  - Unix (IBM, Dec, Sun, ...)
  - VMS (DEC)
  - Linux
  - PC Windows

## IV. Code Details, continued

- *Input:* User-friendly (gradually becoming friendlier)
- *Documentation:*
  - 411-page users' manual, pdf
  - many other publications
  - web sites
- *Quality Control:* 152 test cases [~1000 individual SAMMY runs]
- *Experience:* two decades of successful analyses of a large number of experimental data sets ranging from light to heavy nuclei
- *Instruction:* tutorial exercises for novice users; workshops

End of Introduction