Tungsten "Resonance Evaluation"

Luiz Leal
Herve Derrien
Roberto Capote
Ivo Kodeli
Andre Trkov

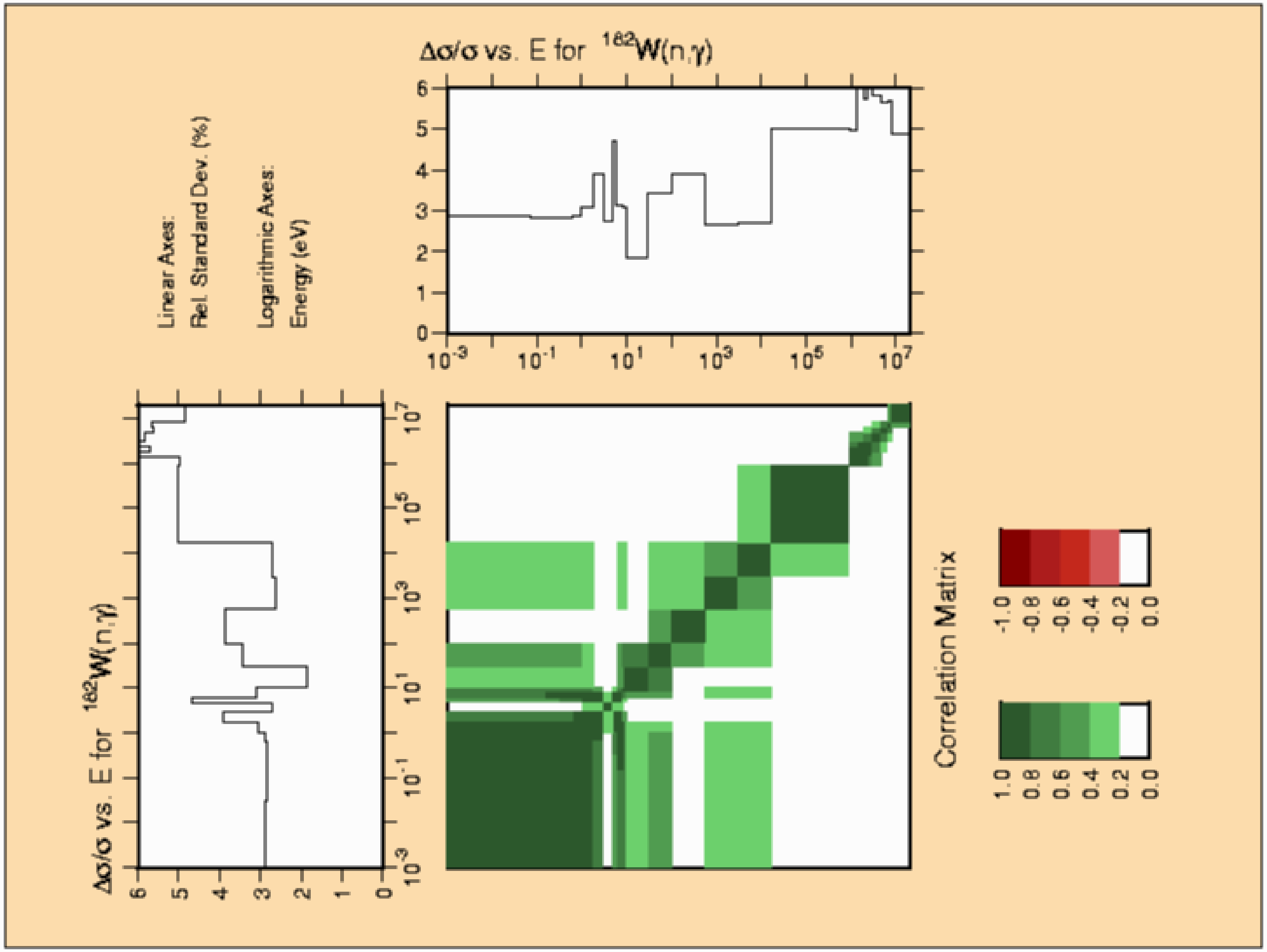
Oak Ridge National Laboratory

CSEWG
Nov 6-8, 2007

^{182}W

	ENDF	NEW	Mughabghab
RRR	$10^{-5} – 4.5 \times 10^{3}$ (MLBW)	$10^{-5} – 1.2 \times 10^{4}$ (RM)	-
σ_0	20.55	20.71	19.9 ± 0.3
I_γ	597.16	628.33	600 ± 60

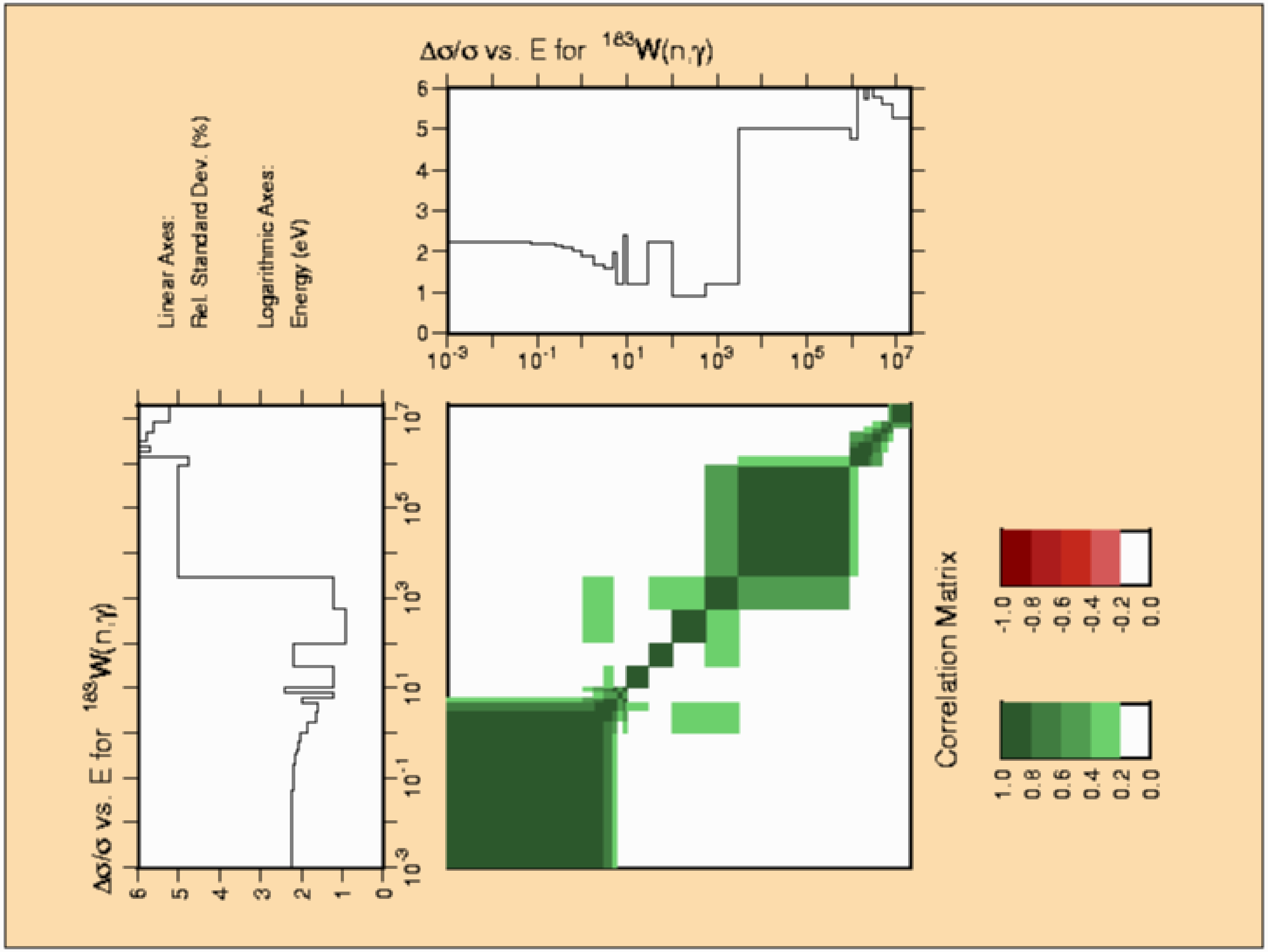
^{182}W Covariance



^{183}W

	ENDF	NEW	Mughabghab
RRR	$10^{-5} – 7.65 \times 10^{2}$ (MLBW)	$10^{-5} – 2.2 \times 10^{3}$ (RM)	-
σ_0	10.01	10.11	10.4 ± 0.2
I_γ	356.32	334.73	355 ± 30

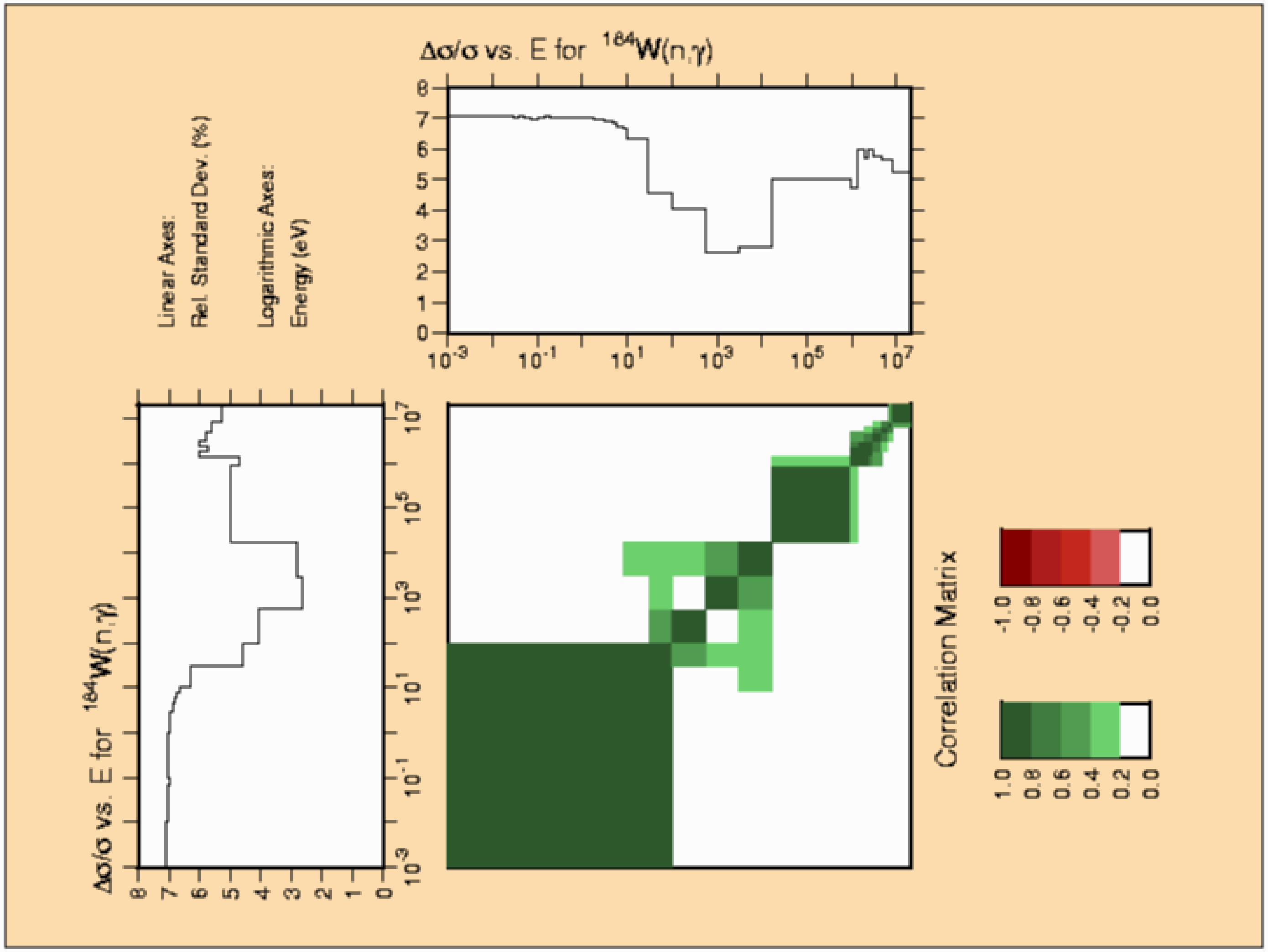
^{183}W Covariance



^{184}W

	ENDF	NEW	Mughabghab
RRR	$10^{-5} – 2.65 \times 10^{3}$ (MLBW)	$10^{-5} – 1.5 \times 10^{4}$ (RM)	-
σ_0	1.75	1.70	1.7 ± 0.1
I_γ	16.56	16.22	14.7 ± 1.5

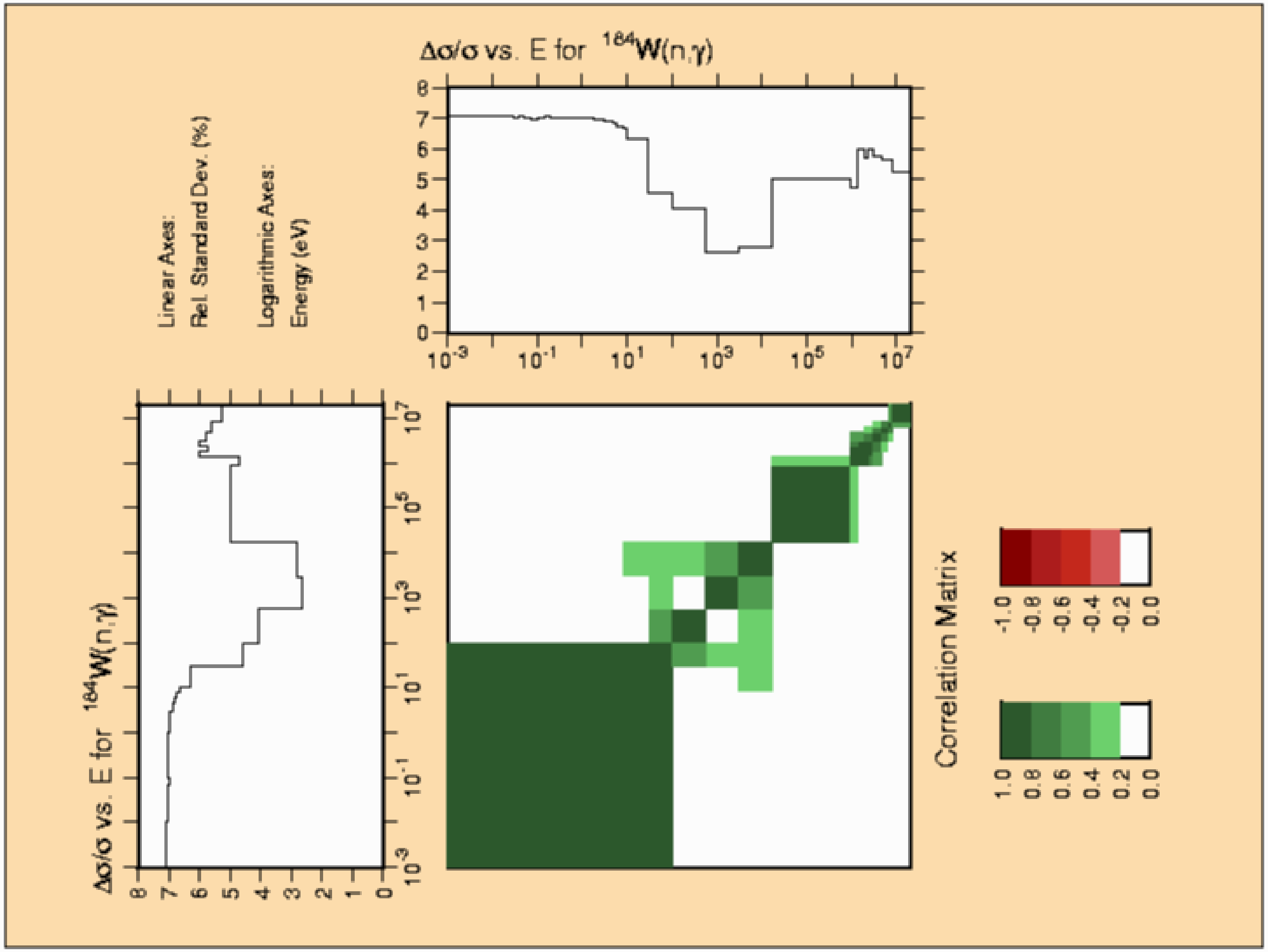
^{184}W Covariance



^{186}W

	ENDF	NEW	Mughabghab
RRR	$10^{-5} – 3.2 \times 10^{3}$ (MLBW)	$10^{-5} – 1.5 \times 10^{4}$ (RM)	-
σ_0	38.1	38.06	38.1 ± 0.5
I_γ	518.92	481.74	480 ± 15
$K_0 = I_\gamma / \sigma_0$ (measurements) 12.59 ± 0.23			

^{186}W Covariance



^{55}Mn Resonance Evaluation
Status of the analysis of recent neutron transmission and capture cross sections in the energy range below 120 keV (H. Derrien)

- **Experimental data base**

New Data:

ORELA neutron transmission, Harvey et al. 1988

GELINA neutron capture, Shillebeeckx et al. 2006

ORELA neutron capture, Guber et al. 2007

Old data for evaluation in thermal range:

Total cross section, Rainwater et al. 1947

Total cross sections, Cote et al. 1964

Capture cross section, Widder et al. 1975

Correction applied to the data from preliminary SAMMY analysis:

Residual background between resonances in ORELA and GELINA capture data

Part could be due to d-wave contribution and to direct capture

Under investigation

Results

- **Cross section at 0.0253 eV close to Mughabghab values and Tkrov evaluation. Capture cross section adjustable by small variation of the capture width of a bound level at -243.10 eV**

- **Average value of Harvey transmission systematically lower by about 0.8% than the values calculated from the resonance parameters, within the experimental errors**

- **Average effective cross sections in good agreement with values calculated from the resonance parameters, both GELINA and ORELA.**

Resonance parameters

- **Energy range 0 to 120 keV**

  44 s-wave resonances

  116 p-wave resonances distributed in 6 non interfering groups with spin assignment at random according to Bethe level density relation;

  about 30 of these resonances could be d-wave resonances

- **Average Spacing and Neutron Strength Function**

  From reduced neutron width distribution:

  $<D>_{l=0} = 2.40 \pm 0.20$ keV **$S0 = 3.83 \pm 0.78$ 10-4**

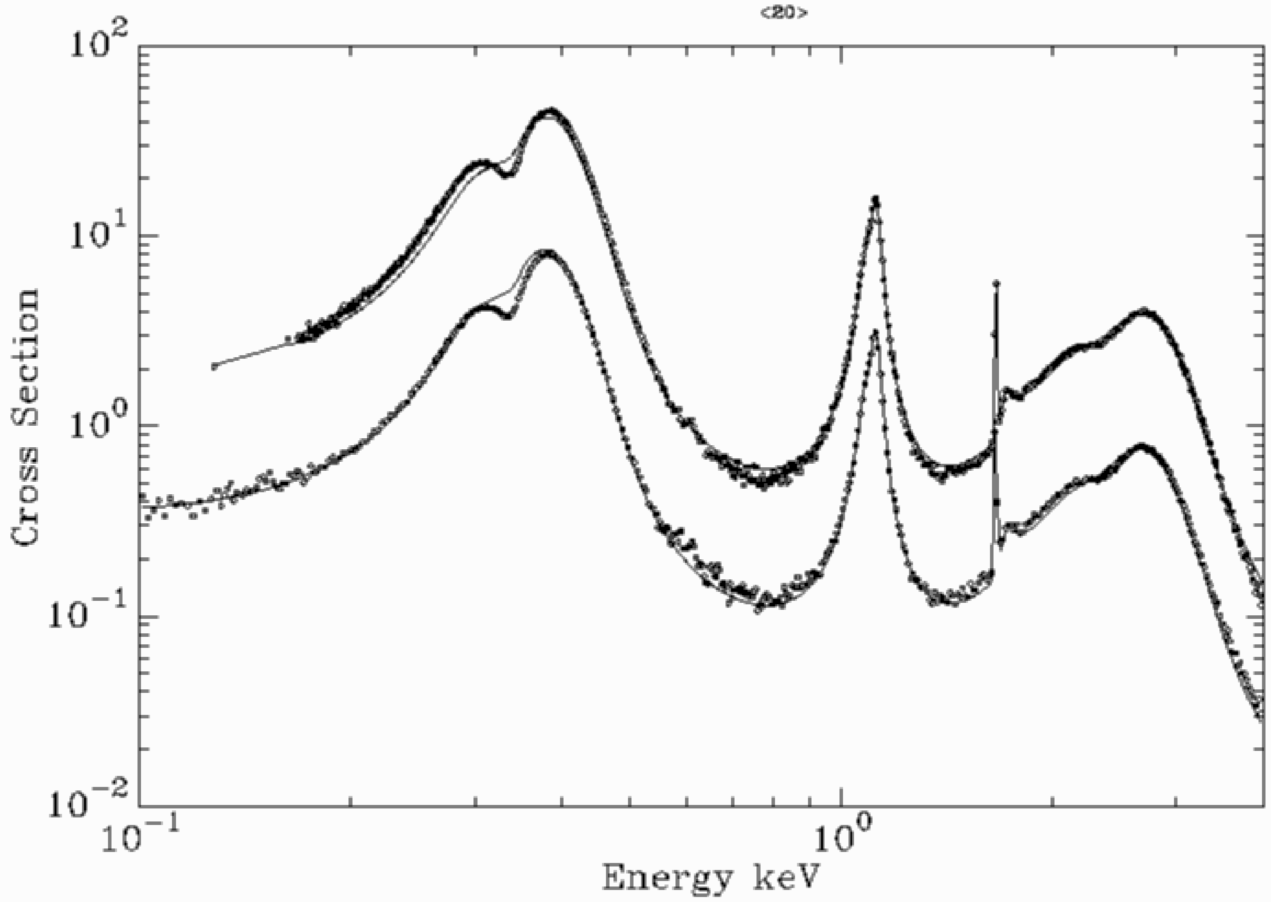
  $<D>_{l=1} = 1.41 \pm 0.28$ keV **$S1 = 0.52 \pm 0.08$ 10-4**

- **Neutron Width of the s-wave resonance in agreement with Garg et al.**

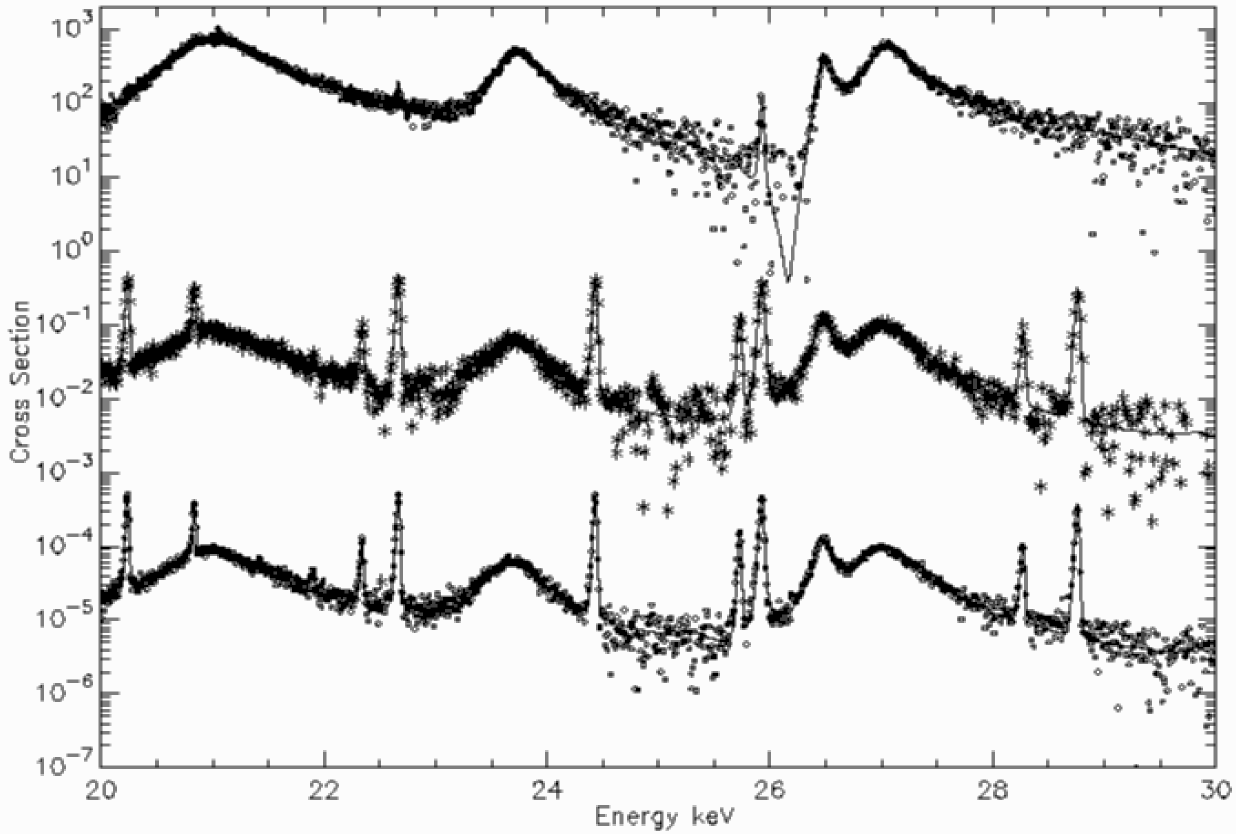
Resonance parameters

- **Capture Widths of the three first s-wave resonances much larger than Macklin 1984 values, 50% to 70% differences**
- **GELINA and ORELA capture with thick samples; difficulties of correcting strong multiple scattering effects, mainly in the first resonance**
- **Effect on the accuracy of the capture widths needs to be checked**
- **Above 5 keV, the capture widths of the s-wave resonances agree reasonably well with the results of Garg-Macklin**
- **In the 5 to 60 keV energy range Garg-Macklin capture area of the p-wave resonances are, on average, 5% larger than in the present evaluation**

SAMMY fit of GELINA (upper) and ORELA(lower) capture data from 0.1 keV to 5 keV



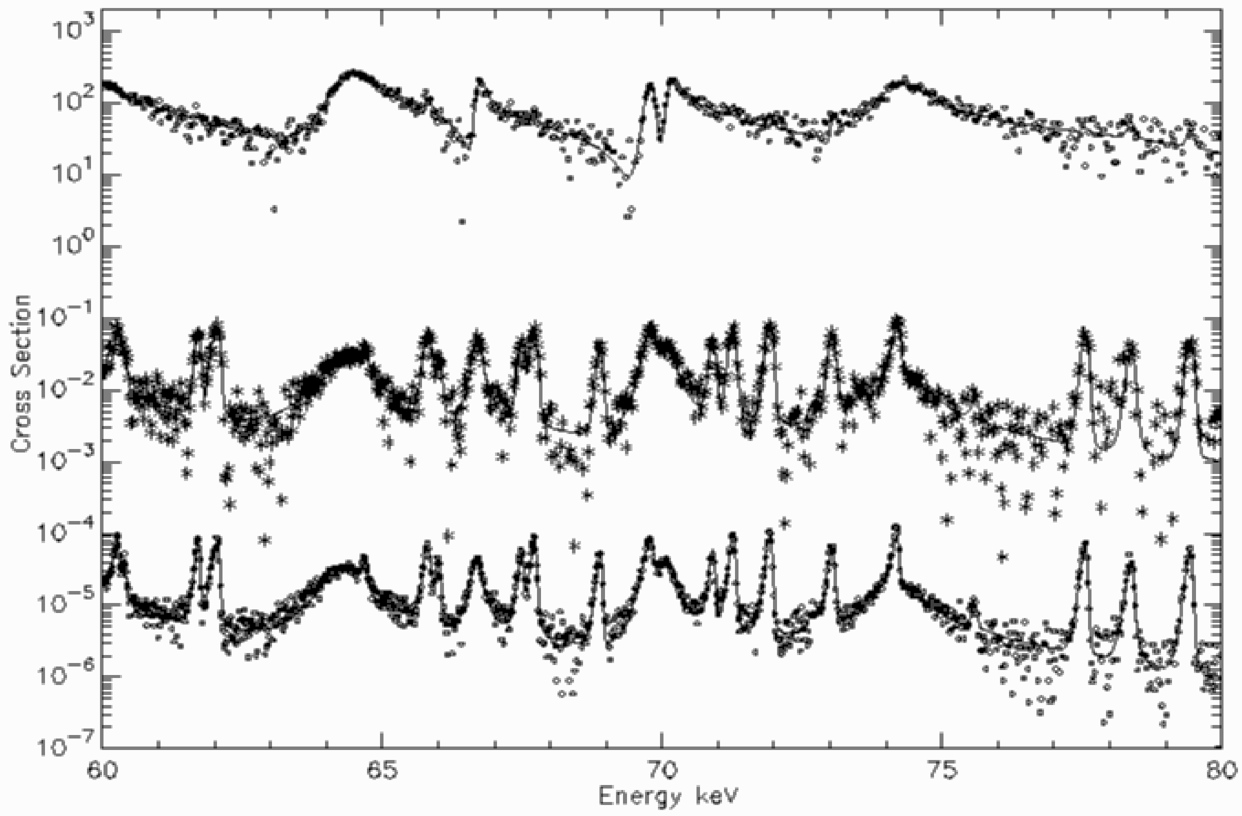
SAMMY fit of ORELA total (upper), ORELA capture (middle) and GELINA capture (lower) cross section from



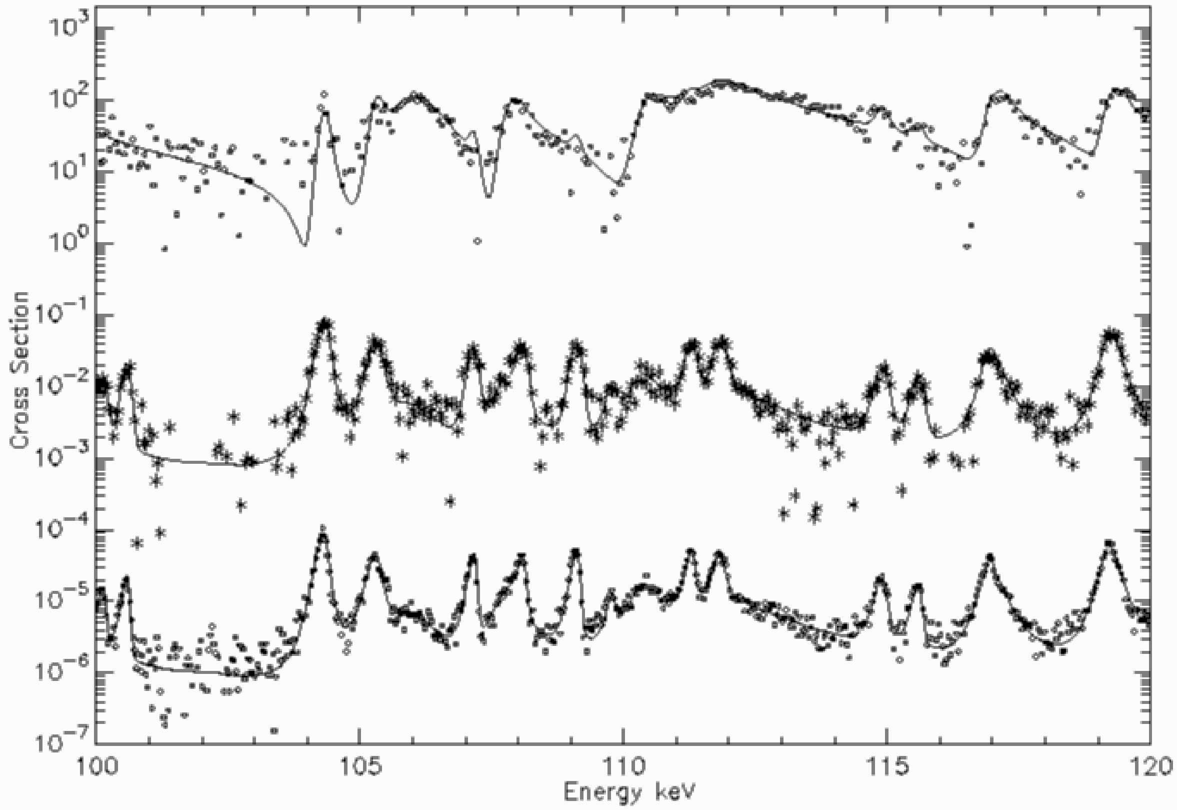
paradigm shift

OAK RIDGE National Laboratory

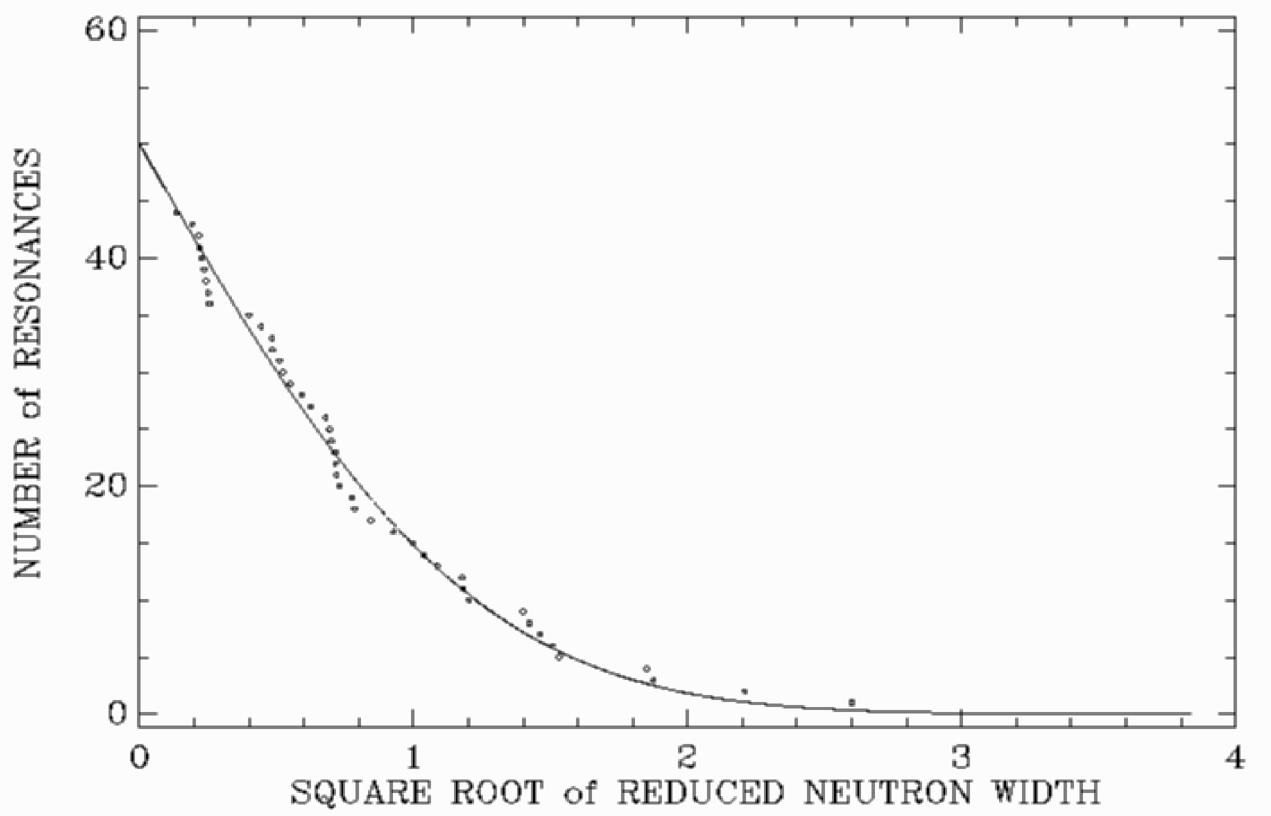
SAMMY fit of ORELA total (upper), ORELA capture (middle) and GELINA capture (lower) cross section from 60 keV to 80 keV



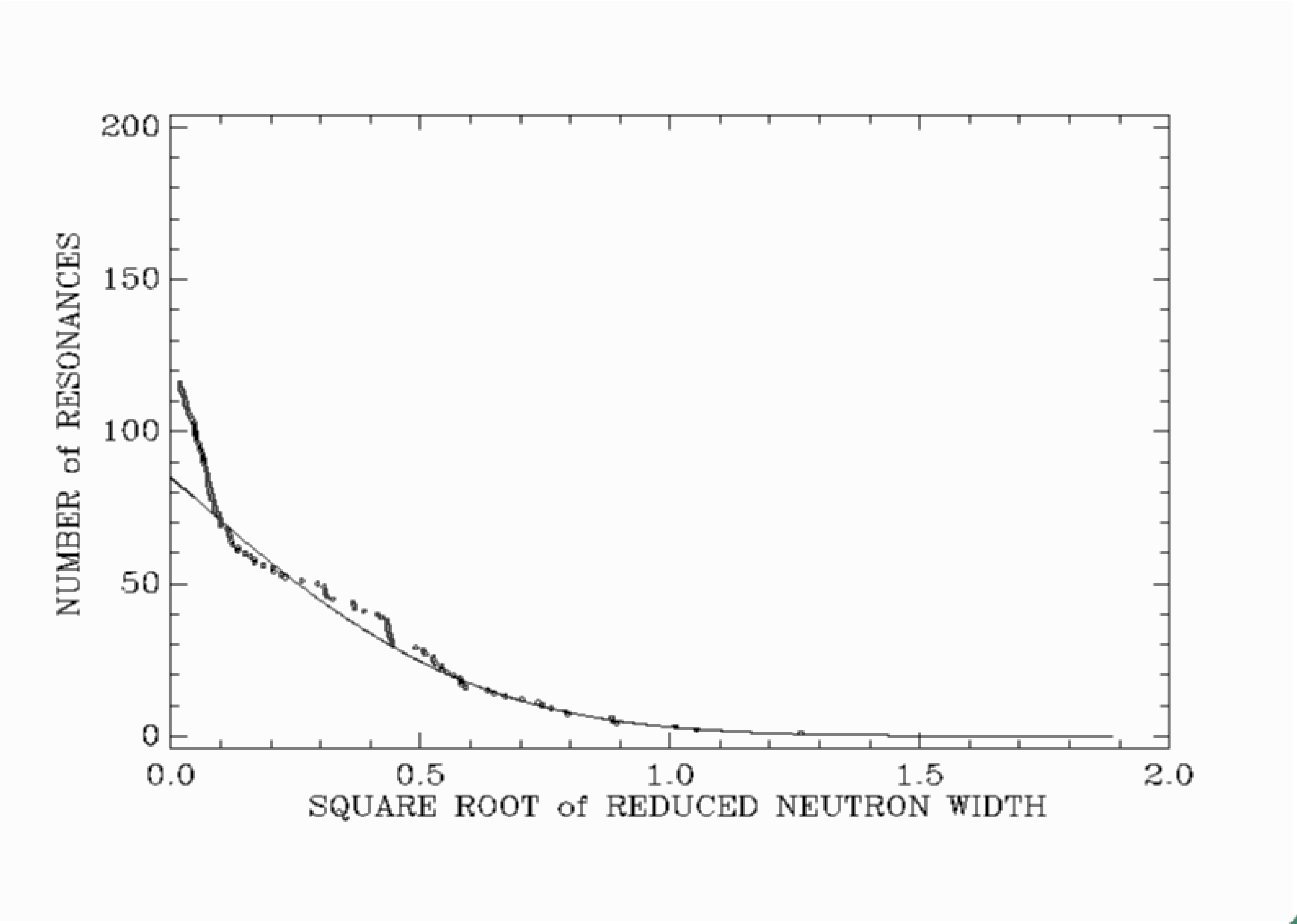
SAMMY fit of ORELA total (upper), ORELA capture (middle) and GELINA capture (lower) cross section from 100 keV to 120 keV



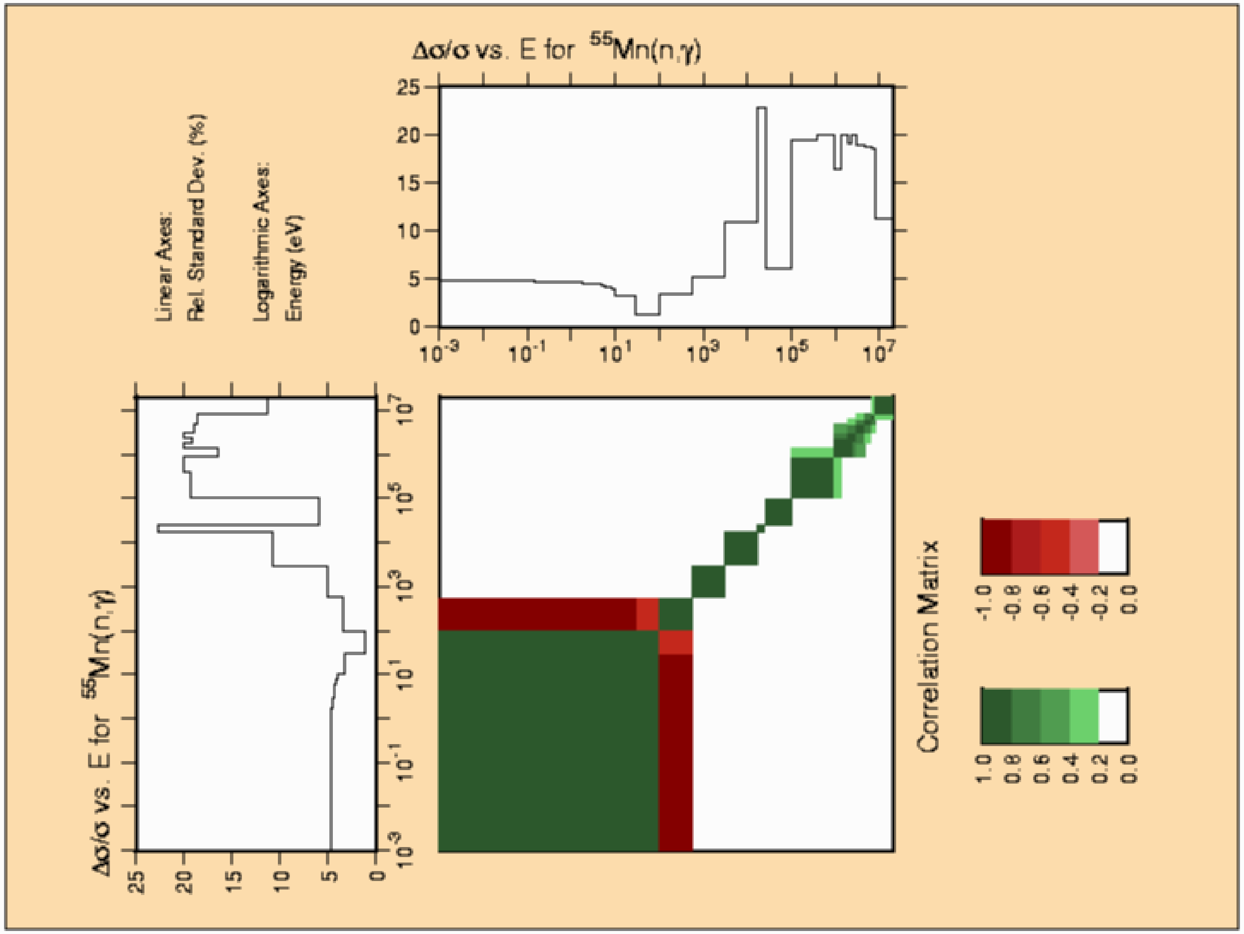
Porter-Thomas Distribution of s-wave reduced neutron widths in the energy range from 0 to 120 keV



Porter-Thomas Distribution of p-wave reduced neutron widths in the energy range from 0 to 120 keV

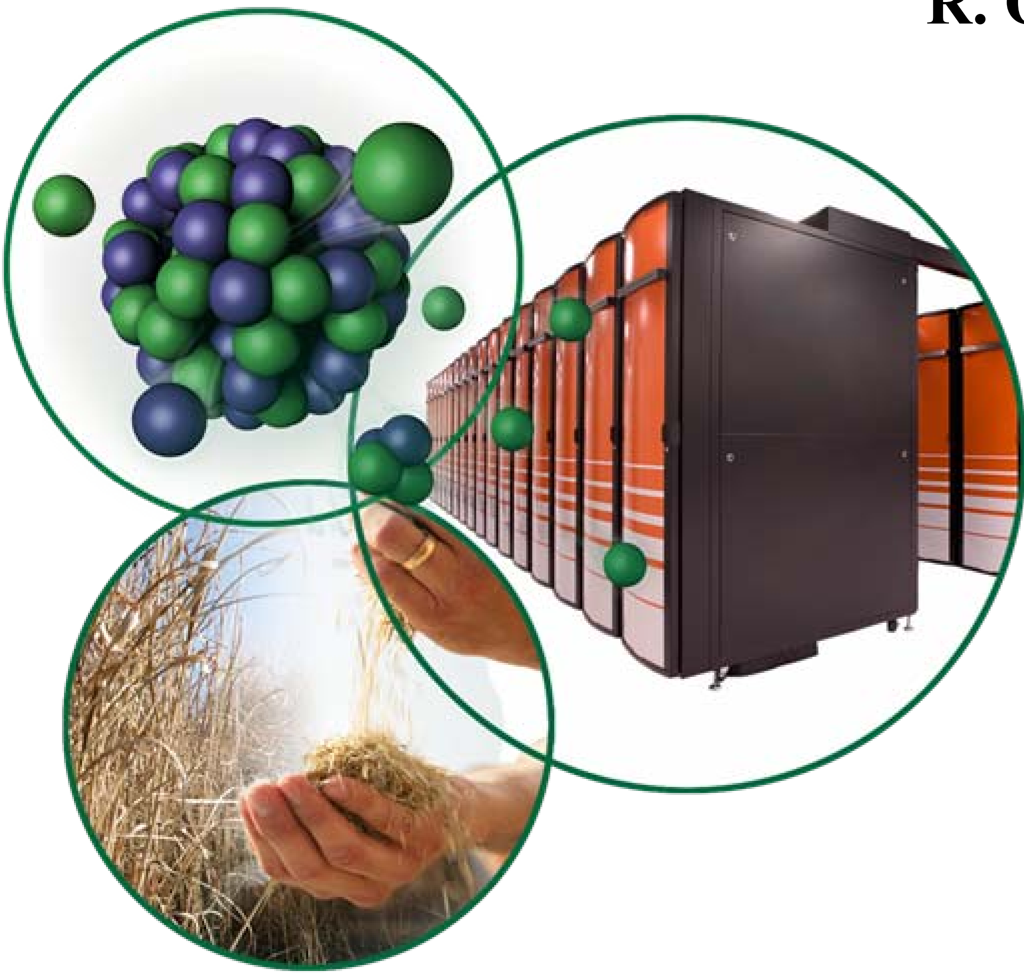


44-group covariance processed with PUFF-IV for the capture cross section



^{35,37}Cl Resonance Parameter Covariances

R. O. Sayer, K. H. Guber, L. C. Leal, and N. M. Larson



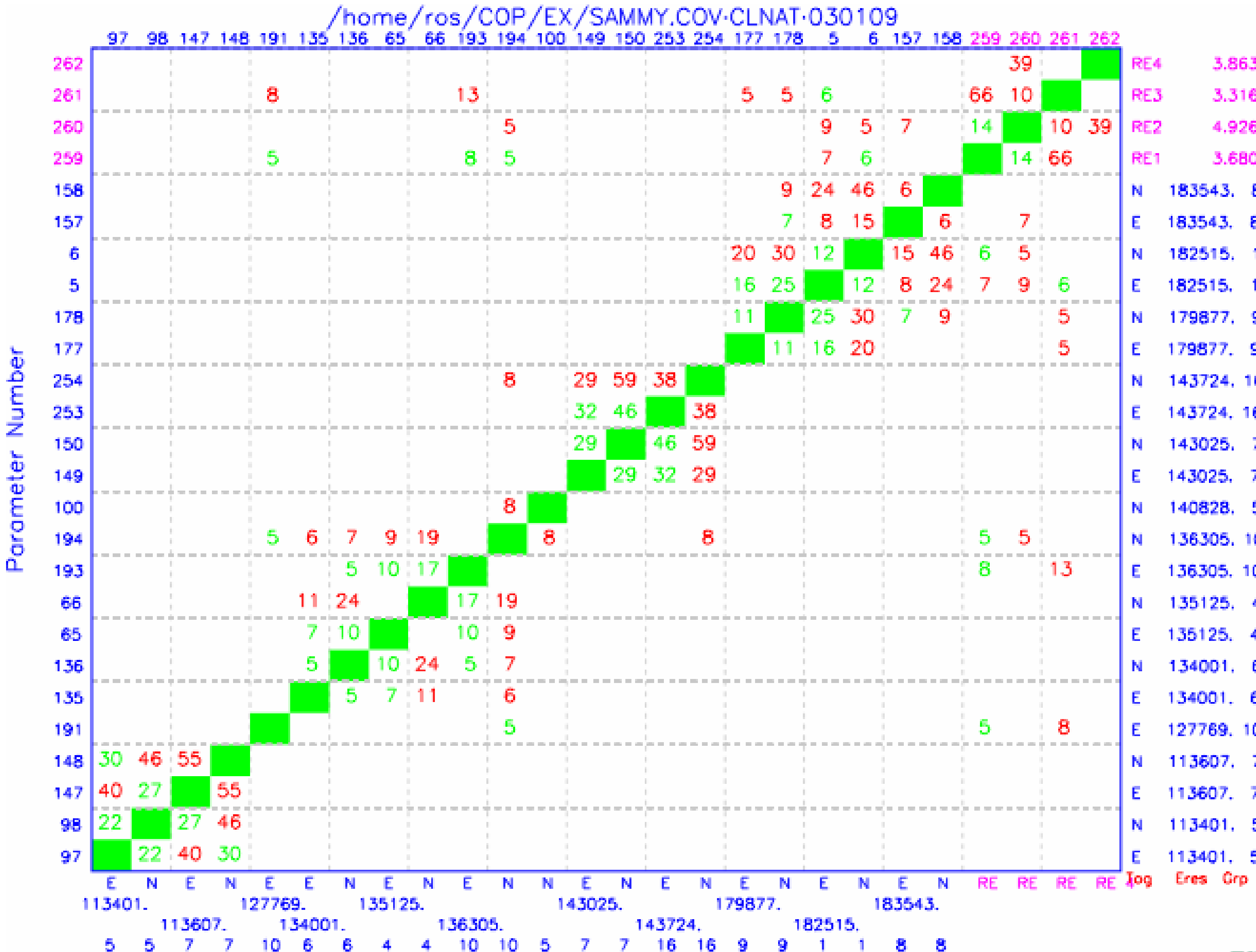
Managed by UT-Battelle
for the Department of Energy

Oak Ridge National Laboratory

^{35,37}Cl Resonance Parameter Covariances

- File 32 generated for 10^{-5} eV to 1.2 MeV. (RADCOP code)
- ^{35}Cl : Proton exit channel taken into account: LRF = 7, LCOMP = 2
    - First use of the Reich-Moore Limited Compact Format. File size = 384 kB
- ^{37}Cl : LRF = 3, LCOMP = 1 (expanded format). File size = 2.5 MB
- Uncertainties and correlations verified against master SAMMY covariance (binary) file.
- 44- and 238-group uncertainties from PUFF-IV and SAMMY agree.
- Complete ENDF files submitted to NNDC.

RADCOP Plot of Cl Covariances for 113 keV < E < 184 keV

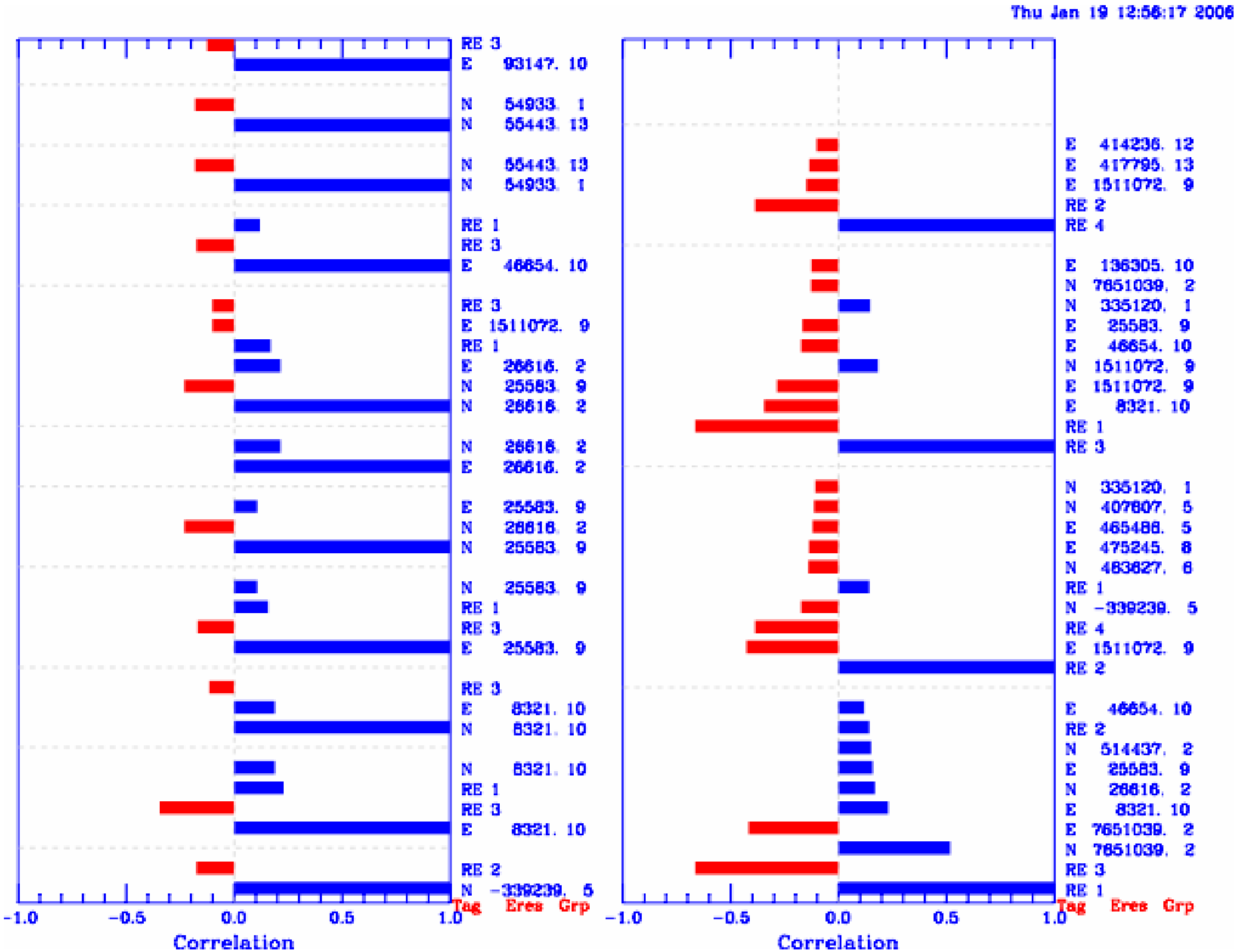


 Managed by UT-Battelle
for the Department of Energy

paradigm shift

OAK RIDGE National Laboratory

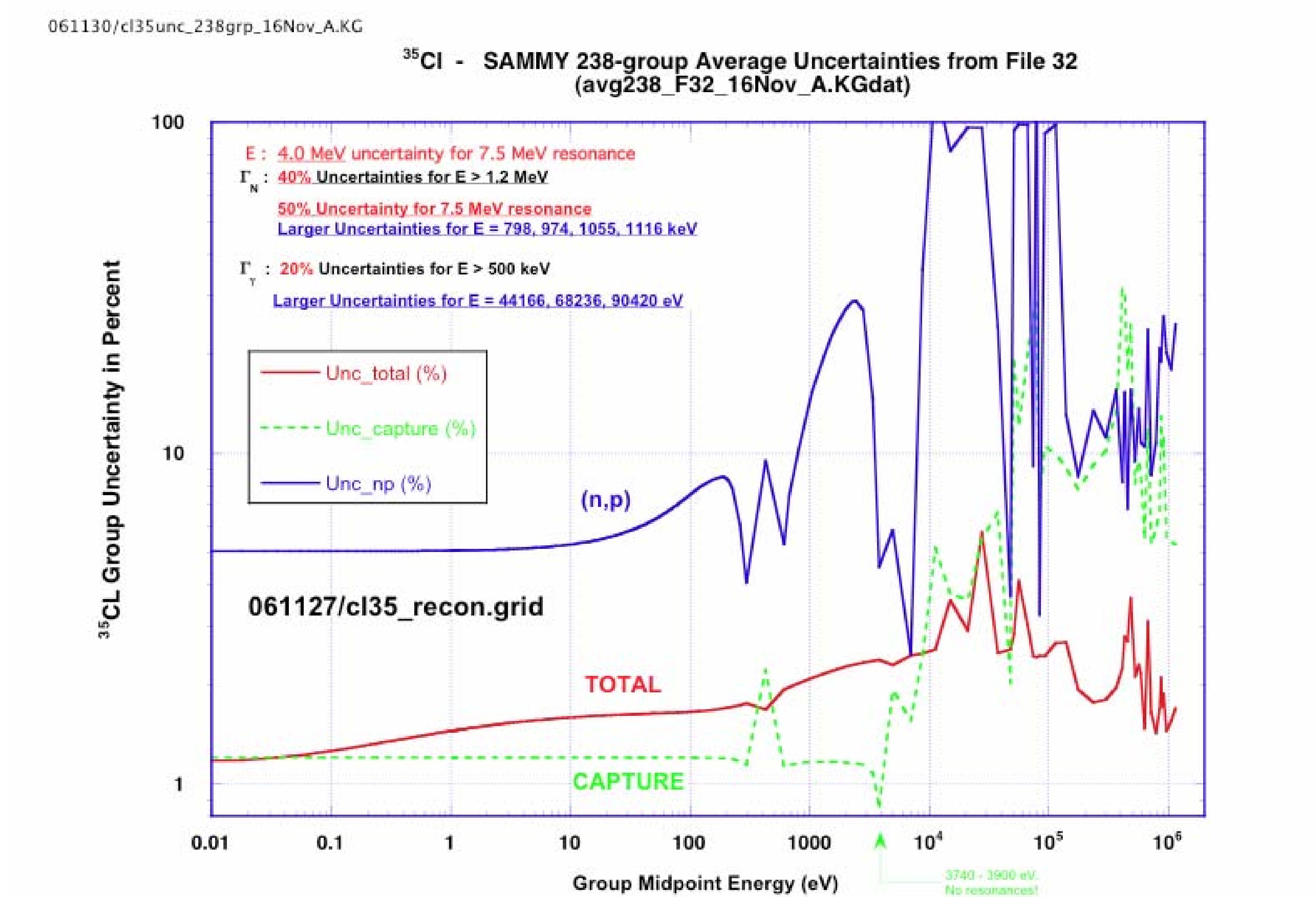
Example RADCOP 1D Plot showing extreme off-diagonal correlations for Cl. **Blue** (red) bars indicate **positive** (negative) correlations. Tags E, N, and RE, denote resonance energy, neutron width, and effective radius. respectively.



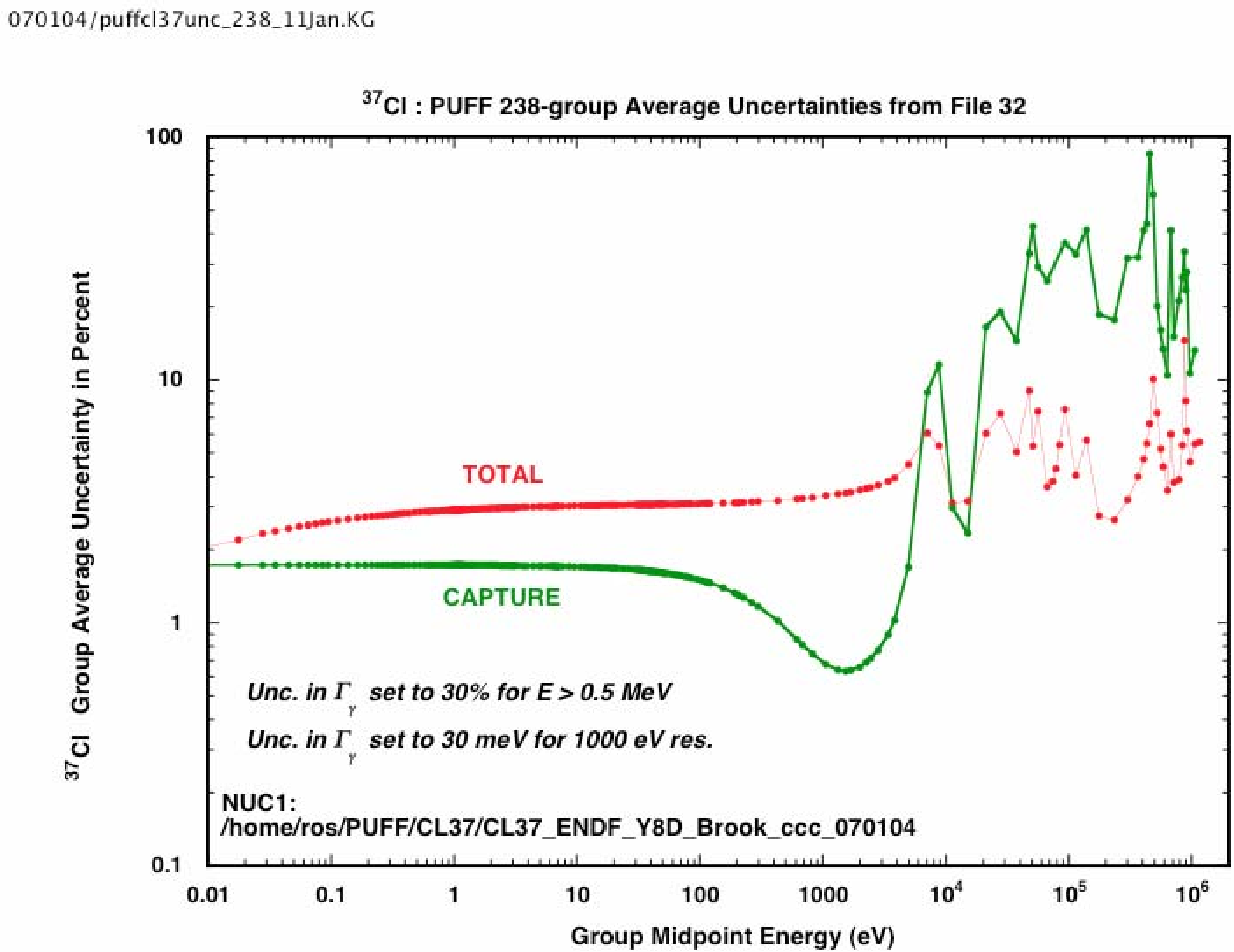
RADCOP Capabilities

- 1D and 2D parameter correlation plots for specified energy range.
- Plot formats facilitate rapid identification of important off-diagonal correlations.
- Output of ENDF File 2 and 32 files for Reich-Moore representation for the resolved resonance region (LRU = 1).
  - LRF = 3 and LRF = 7 (compact format) supported.
  - ENDF File 32 covariance files have been generated for $^{35,37}Cl$:
    - ^{37}Cl : LRF = 3, LCOMP = 1 (expanded format)
    - ^{35}Cl : LRF = 7, LCOMP = 2 (compact format). Proton exit channel included.

^{35}Cl Group Average Uncertainty vs. Energy



^{37}Cl Group Average Uncertainty vs. Energy



R-Matrix Evaluation ^{19}F Neutron Cross Sections up to 1 MeV

Luiz Leal and Herve Derrien

Nuclear Science and Technology Division

^{19}F Evaluation

Features:

Three transmissions, one capture cross section data, and one inelastic cross section data were used in the evaluation.

- **Evaluation performed up to 1 MeV with 2 s-wave, 5 p-wave, 17 d-wave, and 7 f-wave resonance for a total of 31 resonance.**
- **Inelastic Channels: 109.9 ($1/2^-$) keV and 197.2 ($5/2^{+)}$ keV**
- **Reich-Moore formalism was used.**
- **LRF=7 ENDF format used for resonance parameters representation**
- **AMPX (POLIDENT) version used to process RM with inelastic channels (Doro Wiarda changes to POLIDENT)**
- **Resonance Parameter Covariance generated**

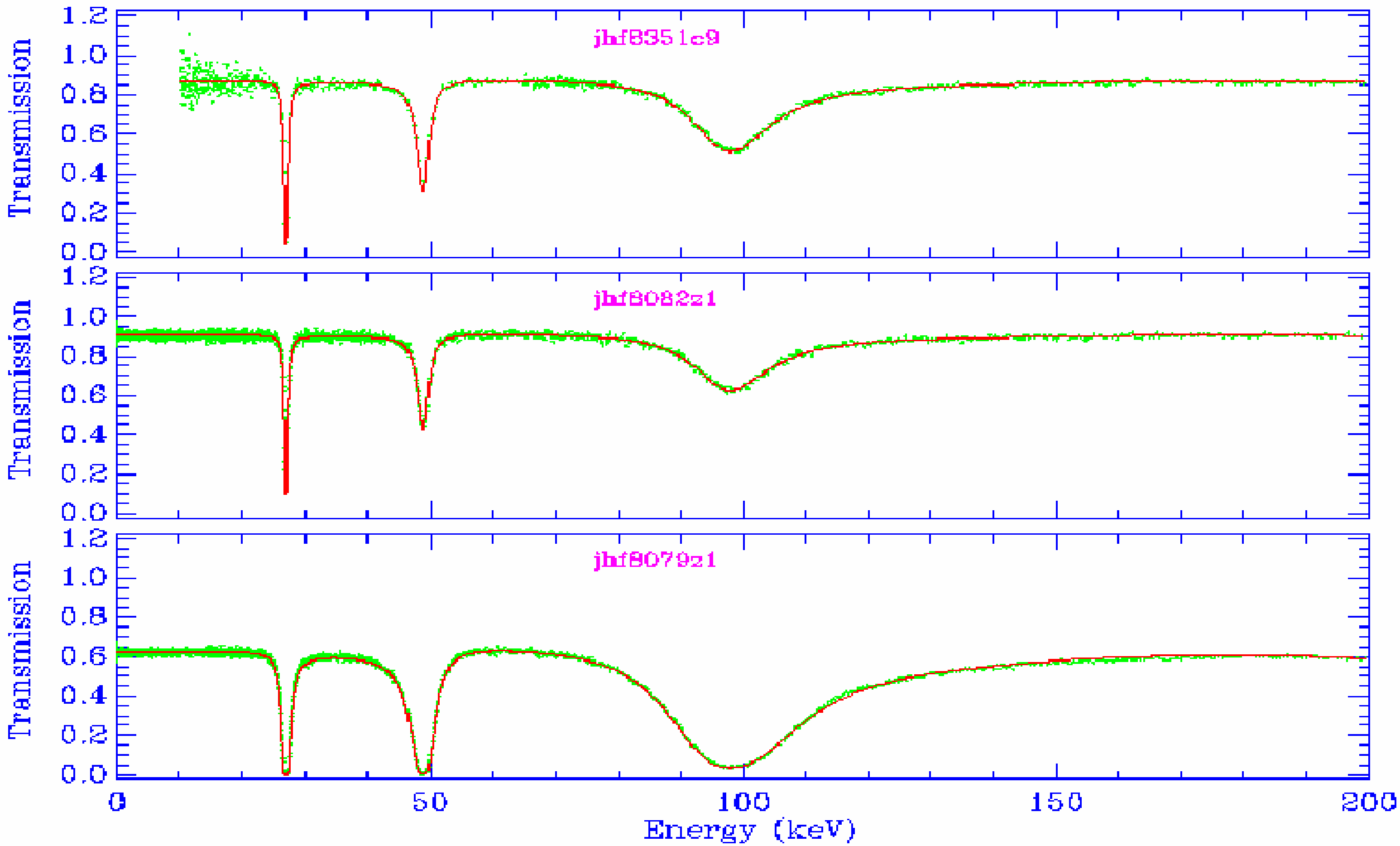
Experimental Data Bank

- **Three Transmission Data Measurements of Larson *et al.* made at ORELA 80 meters flight path with sample thicknesses 0.13093 at/b, 0.016886 at/b, and 0.024184 at/b, respectively in the energy range 5 ev to 20 MeV**

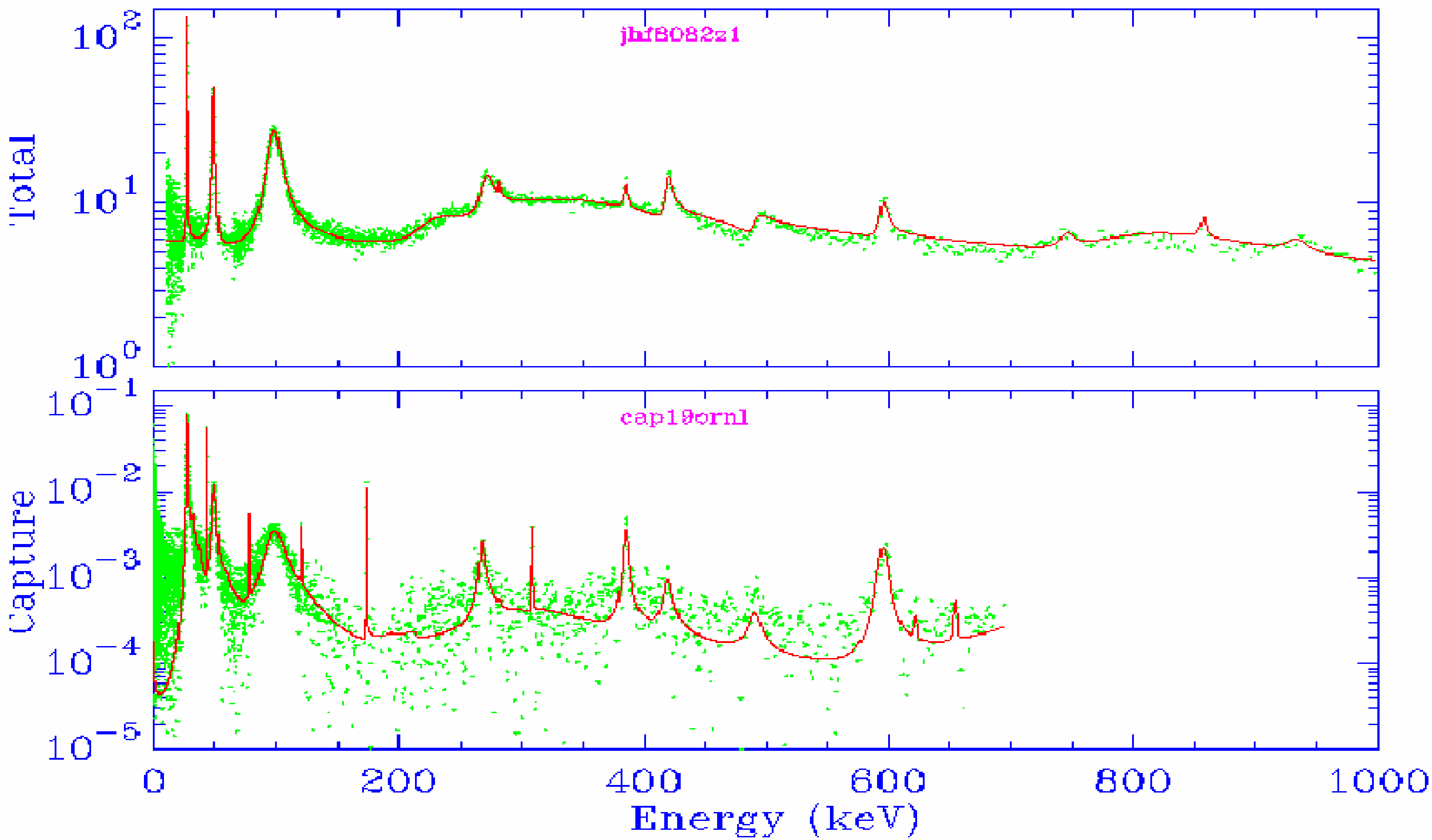
- **One Capture measurement done at ORELA 40 meters flight path performed by Guber *et al.* up to 700 KeV**

- **Inelastic Cross Section Measurements Performed by Broder *et al.* at Obninsk up to 1 MeV**

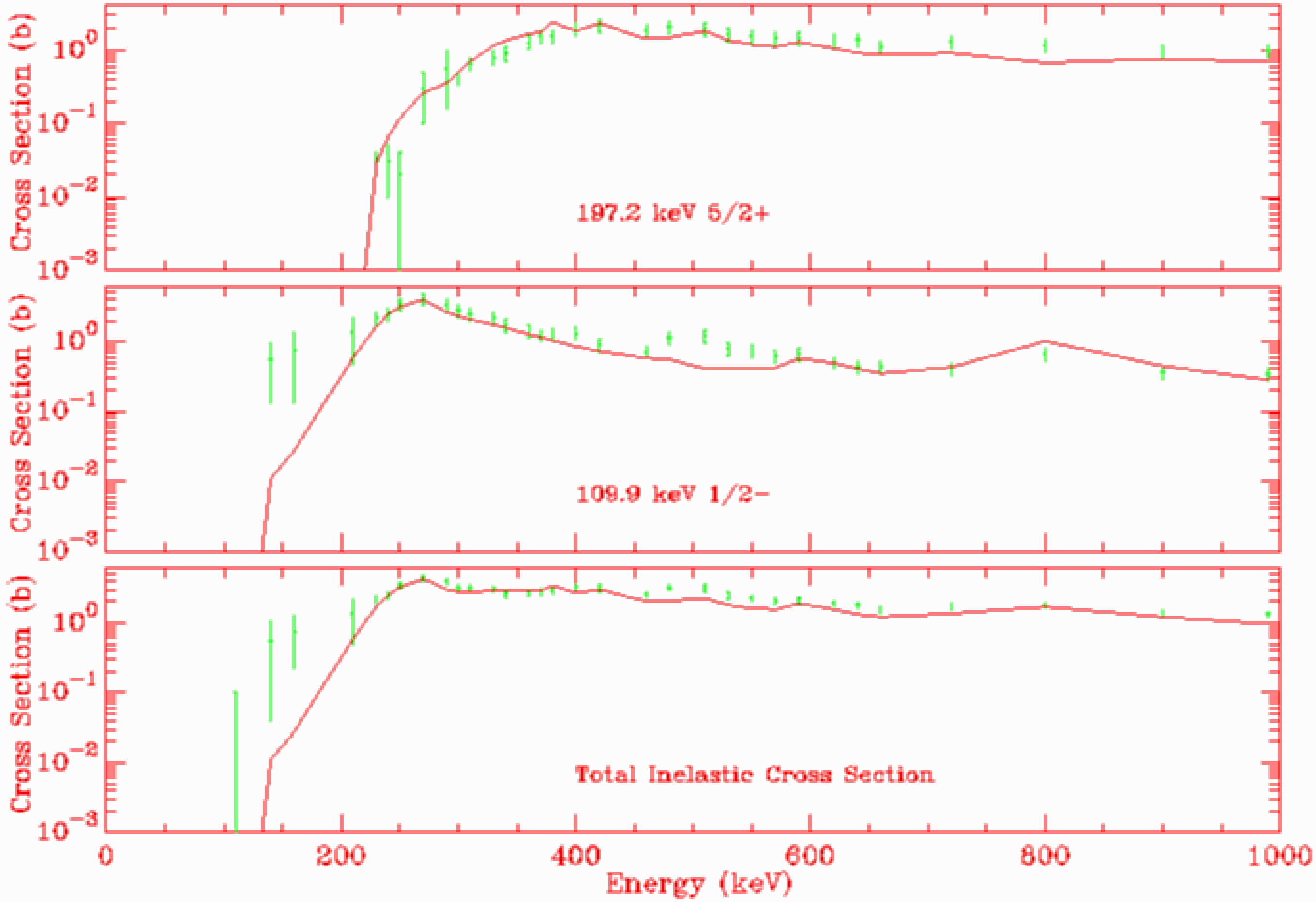
Transmission



Total and Capture Cross Sections



Inelastic Cross Sections



ASSESMENT OF TITANIUM CROSS SECTIONS AND UNCERTAINTIES FOR APPLICATION IN CRITICALITY SAFETY

L. LEAL and R. Westfall
Nuclear Data Group
Nuclear Science and Technology Division
Oak Ridge National Laboratory

D. Eghbali and F. Trumble
Washington Safety Management Systems
Savannah River Site

MOTIVATION

- Address criticality safety of the Actinide Removal Process (ARP) facility at the Savannah River Site
- Monosodium Titanate (MST, $NaHTi_2O_2$) is added to the diluted salt solution to adsorb soluble radionuclides including uranium and plutonium
- Existing ENDF/B-VII.0 Titanium cross sections and uncertainties used in the ARP criticality calculations were investigated
- New uncertainty evaluations were done for Titanium using the ORNL computer code SAMMY

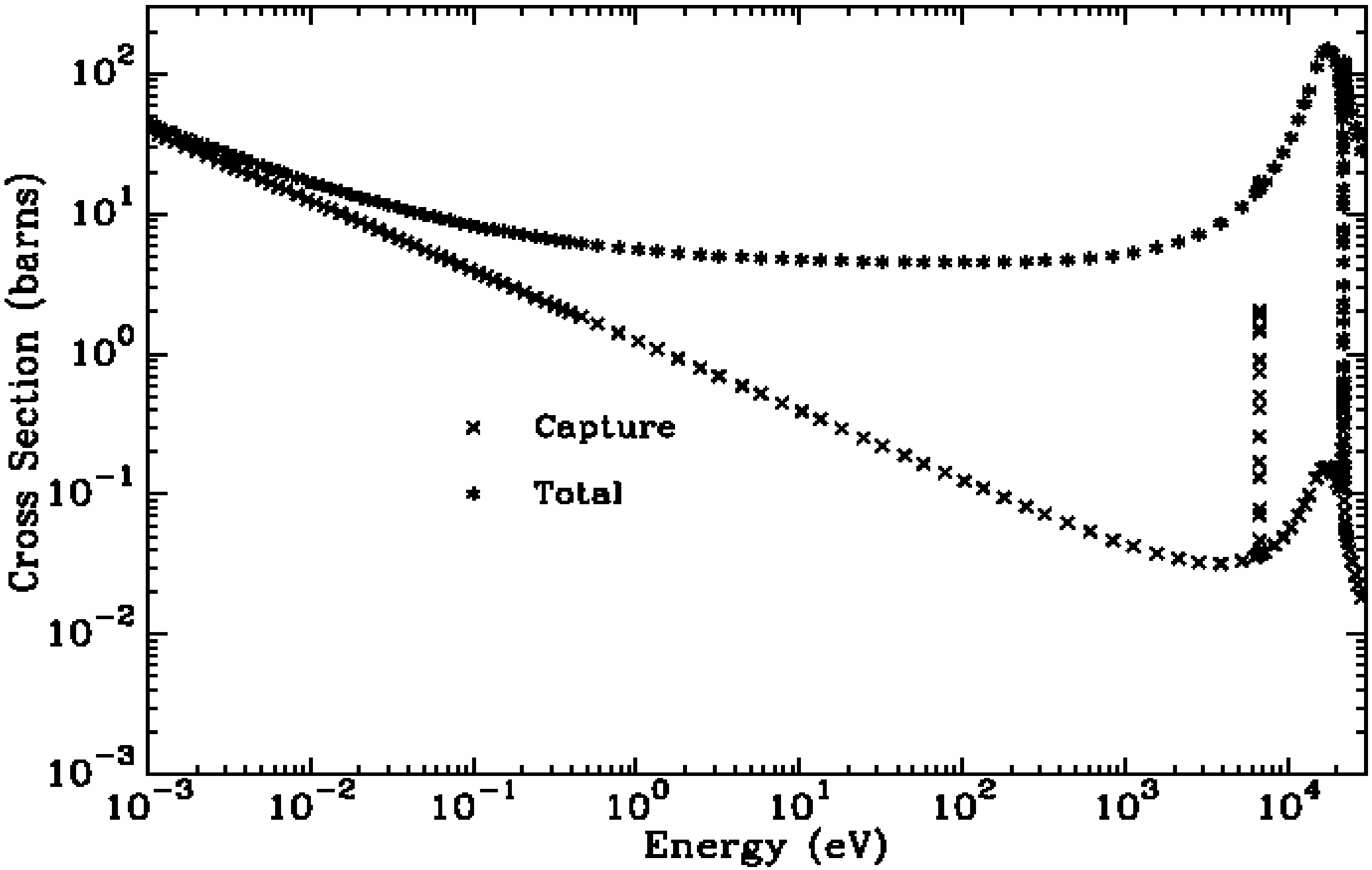
^{48}Ti data and uncertainty processing

- ENDF/B-VII.0 ^{48}Ti evaluation investigated. This evaluation includes data covariance
- NJOY and AMPX codes used to process cross sections
- ERRORJ and PUFF-IV used to process covariance data
- Group cross sections and covariance generated in the SCALE 238- and 44-neutron energy groups structures

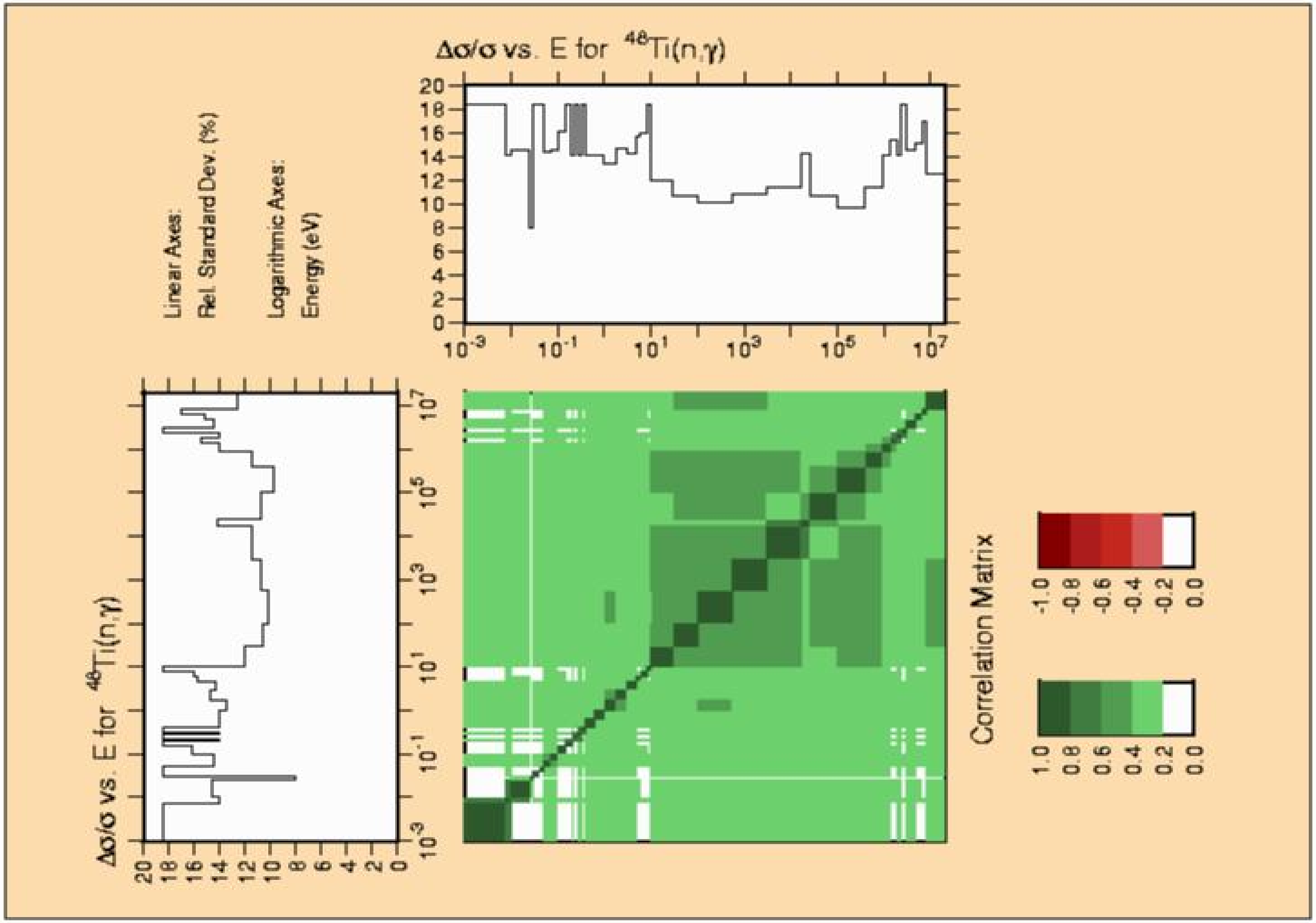
Titanium Data

Isotope Name	Abundance (%)	σ_γ (thermal)	$\delta\sigma_\gamma / \sigma_\gamma$ (%)
^{46}Ti	8.25	0.59 ± 0.18	30.5
^{47}Ti	7.44	1.63 ± 0.04	2.4
^{48}Ti	73.72	8.32 ± 0.16	1.9
^{49}Ti	5.41	1.87 ± 0.04	2.2
^{50}Ti	5.18	0.18 ± 0.03	16.7

ENDF/B-VII ^{48}Ti Capture cross section processed with NJOY (10^{-3} eV to 30 keV)



ENDF/B-VII capture covariance data processed with ERRORJ



Titanium Data

Isotope Name	Abundance (%)	σ_γ (thermal)	$\delta\sigma_\gamma / \sigma_\gamma$ (%)
^{46}Ti	8.25	0.59 ± 0.18	30.5
^{47}Ti	7.44	1.63 ± 0.04	2.4
^{48}Ti	73.72	8.32 ± 0.16	1.9
^{49}Ti	5.41	1.87 ± 0.04	2.2
^{50}Ti	5.18	0.18 ± 0.03	16.7

Concerns with ^{48}Ti ENDF uncertainty evaluation

- ENDF/B-VII average capture cross section uncertainty is ~16 %
- Experimental thermal capture cross section uncertainty is ~ 2 %
- First resonance in the capture cross section occurs at 8 keV; One expects that the uncertainty in the cross section be 2 % up to 8 keV;
- Structure in the capture cross section uncertainty below 8 keV may not be right
- New covariance evaluation needed for ^{48}Ti in the resonance region

Retroactive covariance scheme

1. **Pick representative data sets covering the energy range of the R-matrix evaluation**
2. **Do simultaneous fit to all those data sets**
   - **Take ENDF resonance parameters for initial values**
   - **Flag all resonance parameters so that they are treated as variables in the fitting procedure**

Retroactive covariance scheme, cont.

3. **Check whether output parameter values are very different from input**
   – **Hopefully there are not significant changes**
4. **Assume that the output parameter covariance matrix is a reasonable approximation to use in conjunction with the original (input) parameter values**
5. **Write the output parameter covariance matrix into the ENDF format**

Details, cont.

1. **Do simultaneous fit to all those data sets**
   - **Start from Bayes' Equations (generalized least-squares)**

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

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

Notation: (primes indicate updated values)

P = parameters
M = covariance matrix for parameters
D = experimental data
T = theoretical calculation
G = partial derivatives (sensitivity matrix)
V = covariance matrix for experimental data

Details, cont.

- **Bayes' Equations** in a slightly different form

$P' = P + M' Y$ where $Y = \Sigma_i Y_i$

with $Y_i = G_i^t V_i^{-1} (D_i - T_i)$ for data set i

$M' = (M^{-1} + W)^{-1}$ where $W = \Sigma_i W_i$

with $W_i = (G_i^t V_i^{-1} G_i)$ for data set i

- **Treat individual data sets separately, calculating Y_i and W_i using ENDF values for resonance parameters**
- **Add Y_i's and W_i's to obtain Y and W**
- **Solve Bayes' equations once to fit all data sets**

Details, cont.

2. **Check whether output parameter values = input values**

   ***Question:* Is it true that $P' \approx P$?**

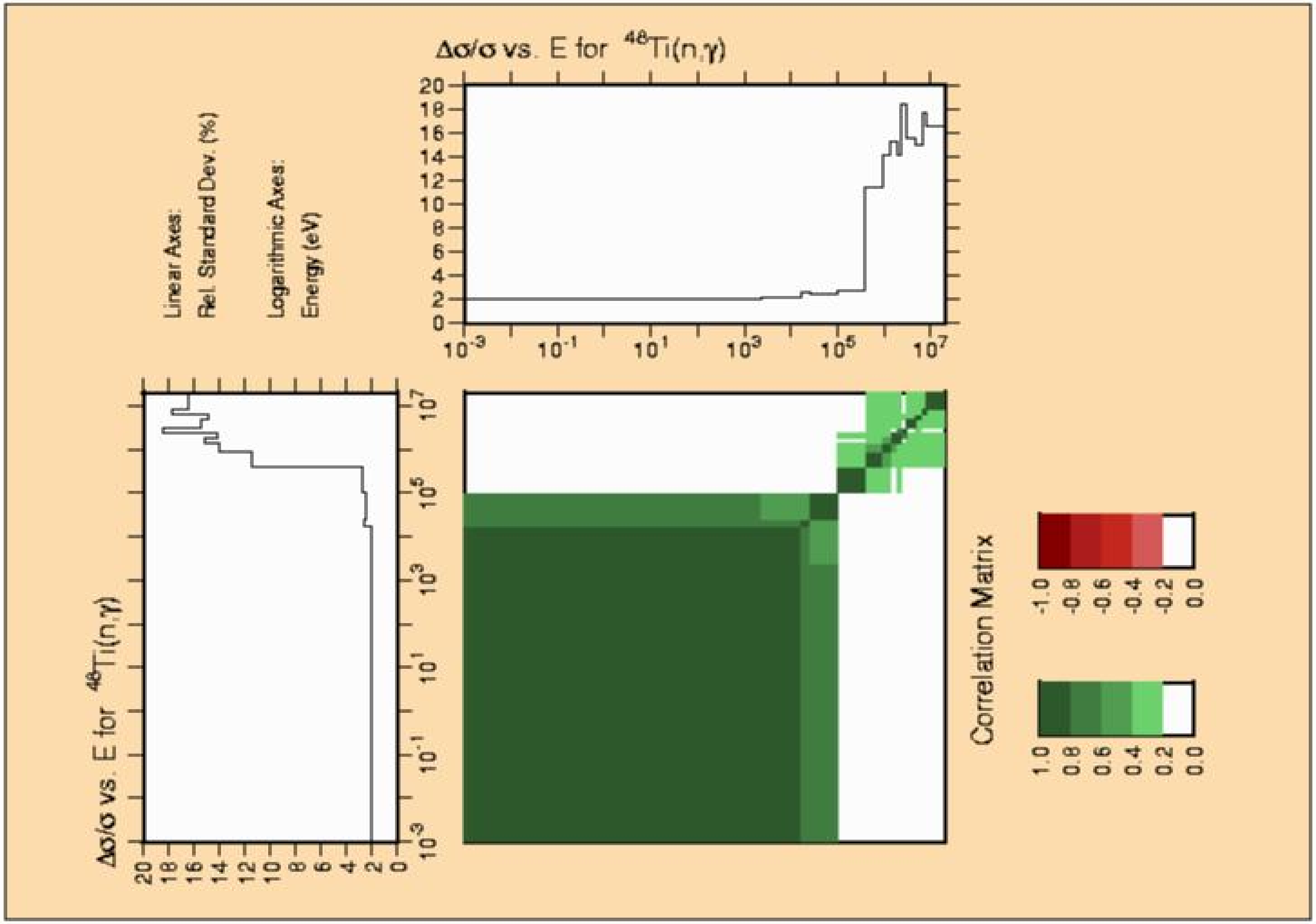
   ***Answer:* Probably, because $Y = G^t V^{-1} (D - T) \approx 0$**

   because D was chosen $\approx T$

3. **Assume *M'* is appropriate for *P***

4. **Write *M'* in ENDF format**

^{48}Ti Covariance Matrix Generated with SAMMY Processed with ERRORJ



Impact of the revised ^{48}Ti Cross Section Uncertainties in Benchmark Calculations

- **Analysis of the Actinide Removal Process Facility (ARP) at the Savannah River Site (SRS)**
- **SCALE sensitivity sequence TSUNAMI used;**
- **238-neutron energy group structure for cross section was used**
- **44-netutron energy group structure for covariance was used**

FLOW DIAGRAM

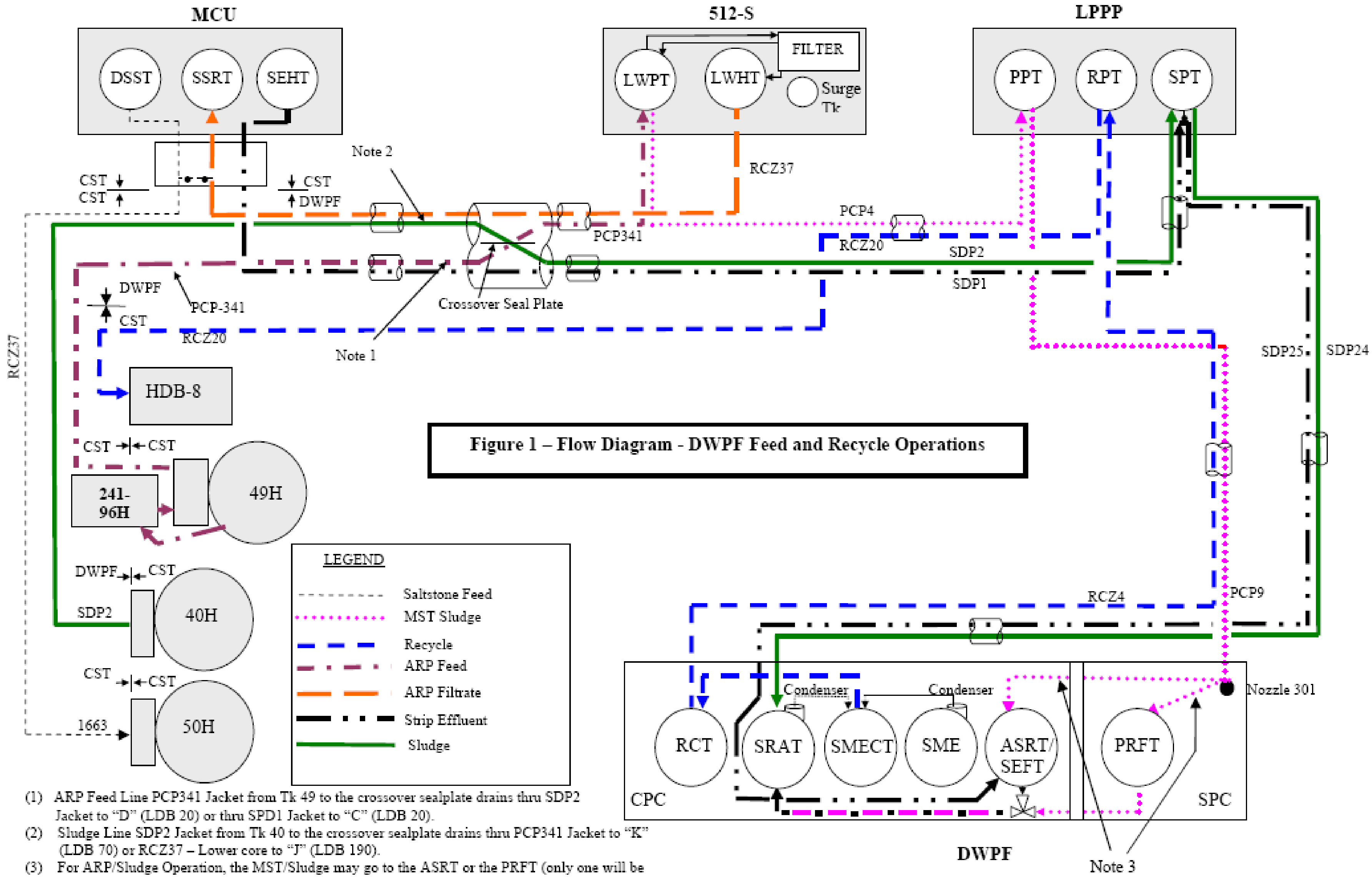


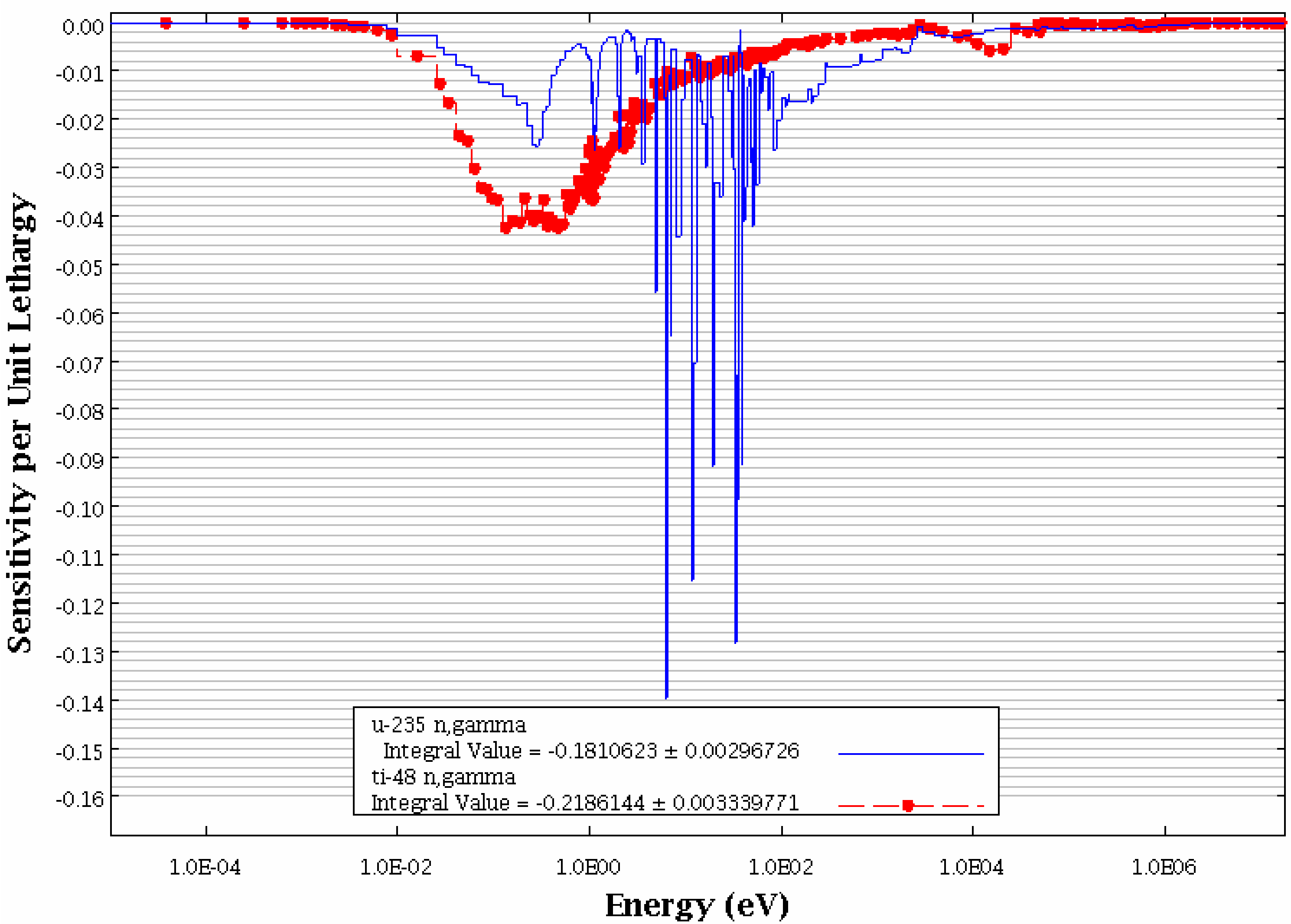
Figure 1 – Flow Diagram - DWPF Feed and Recycle Operations

(1) ARP Feed Line PCP341 Jacket from Tk 49 to the crossover sealplate drains thru SDP2 Jacket to "D" (LDB 20) or thru SPD1 Jacket to "C" (LDB 20).
(2) Sludge Line SDP2 Jacket from Tk 40 to the crossover sealplate drains thru PCP341 Jacket to "K" (LDB 70) or RCZ37 – Lower core to "J" (LDB 190).
(3) For ARP/Sludge Operation, the MST/Sludge may go to the ASRT or the PRFT (only one will be jumpered at a time). For ARP & MCU Operation the flow will go to the PRFT.

paradigm shift

OAK RIDGE National Laboratory

Sensitivity of the system multiplication factor to the ^{48}Ti and ^{235}U capture cross sections



Relative standard deviation of k_{eff} due to ^{48}Ti uncertainty data in ENDF/B-VII

	(n,γ)	(n,n)	(n,n')	(n,2n)	(n,p)	(n,α)
(n,γ)	1.7474 ± 1.4397×10^{-2}					
(n,n)						
(n,n')			3.6275×10^{-2} ± 1.9952×10^{-2}			
(n,2n)				7.1547×10^{-5} ± 2.6364×10^{-5}		
(n,p)					6.5078×10^{-5} ± 1.0821×10^{-5}	
(n,α)					5.6918×10^{-6} ± 7.5055×10^{-9}	
Relative standard deviation in k_{eff} computed from individual values by adding the square of the values and taking the square root.						
1.7478 ± 0.0503						

paradigm shift

OAK RIDGE National Laboratory

Relative standard deviation of k_{eff} due to ^{48}Ti uncertainty data with a revised covariance

	(n,γ)	(n,n)	(n,n')	(n,2n)	(n,p)	(n,α)
(n,γ)	0.445440 ± 3.5007×10^{-3}					
(n,n)	-4.5693×10^{-2} ± 2.2033×10^{-2}	2.2027×10^{-2} ± 3.9200×10^{-2}				
(n,n')			3.6275×10^{-2} ± 1.9952×10^{-2}			
(n,2n)				7.1547×10^{-5} ± 2.6364×10^{-5}		
(n,p)					6.5078×10^{-5} ± 1.0821×10^{-5}	
(n,α)					5.6918×10^{-6} ± 7.5055×10^{-9}	
Relative standard deviation in k_{eff} computed from individual values by adding the square of the values and taking the square root.						
0.4451 ± 0.0043						

paradigm shift

Concluding Remarks

- **Resonance covariance data were generated for ^{48}Ti using SAMMY using the retroactive scheme**
- **Data uncertainty processed with PUFF-IV and ERRORJ codes**
- **Benchmark calculations were done with the SCALE sensitivity sequence TSUNAMI**
- **Revised ^{48}Ti covariance leads to smaller uncertainty in the k_{eff} compared with ENDF results**