ORNL Evaluations Submitted for ENDF/B-VII.1

L. Leal, H. Derrien, K. Guber, G. Arbanas, D. Wiarda, R.Q. Wright, and M. Dunn

Nuclear Data & Criticality Safety Group

Oak Ridge National Laboratory

CSEWG, Nov 1-5, 2010

Candidate Evaluations for ENDF/B-VII.1

- ^{50}Cr, ^{52}Cr ^{53}Cr, and ^{54}Cr
- ^{58}Ni and ^{60}Ni
- ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, and ^{50}Ti
- ^{239}Pu
- ^{240}Pu
- Brief comments about additional ORNL evaluations:
  - ^{55}Mn, ^{35}Cl, ^{37}Cl, ^{39}K, ^{41}K, ^{19}F, ^{180}W, ^{182}W, ^{183}W, ^{184}W, ^{186}W
  - ^{233}U, ^{235}U, ^{238}U
  - Hf-isotope evaluations (RQ Wright)
- SiO_2 thermal evaluation NCSU-ORNL—presentation by Jesse Holmes (NCSU)

^{50,52,53,54}Cr Resonance Evaluation at ORNL

Nuclear Data & Criticality Safety Group

Oak Ridge National Laboratory

CSEWG, Nov 1-5, 2010

Computer Code SAMMY

- **Used for analysis of neutron, charged-particle cross-section data.**
- **Uses Bayes' method (generalized least squares) to find parameter values.**
- **Uses R-matrix theory, Reich-Moore approximation (default) or multi- or single-level Breit-Wigner theory.**
- **Generates covariance and sensitivity parameters for resonance region.**

Cr isotope evaluation

- Transmission and capture cross section measurements done at ORELA for ^{53}Cr and natural Cr for energy below 500 keV (Guber);
- Early high resolution transmission measurements done by Harvey at ORELA above 100 keV for all Cr isotopes;
- Evaluation performed with SAMMY;
- Resolved resonance parameters determined for all Cr isotopes;

paradigm shift

Cr isotope evaluation

Energy Range for ^{50}Cr

Resolved (OLD):10^{-5} eV – 600 keV

Resolved (ORNL): 10^{-5} eV – 783 keV

Energy Range for ^{52}Cr

Resolved (OLD): 10^{-5} eV – 1.2 MeV

Resolved (ORNL): 10^{-5} eV – 1.43 MeV

Cr isotope evaluation

Energy Range for ^{53}Cr

Resolved (OLD):10^{-5} eV – 245 keV

Resolved (ORNL): 10^{-5} eV – 564 keV

Energy Range for ^{54}Cr

Resolved (OLD): 10^{-5} eV – 750 keV

Resolved (ORNL): 10^{-5} eV – 834 keV

^{52}Cr thermal cross section compared to the values listed in the Atlas of Neutron Resonances

Cross Section	ORNL		Atlas
	Resonance	Direct	
Capture	0.75+/-0.02	0.82	0.86+/-0.02
Total	3.82+/-0.01	3.93	3.82+/-0.03
Scattering	3.07+/-0.07	-	2.96+/-0.02

^{52}Cr uncertainty in the energy group 0.0253 eV - 0.3 eV calculated with covariance data

Cross Section	Average value and uncertainty
Capture	17.32+/-0.48 (2.8%)
Total	26.07+/-0.51 (2.0%)
Scattering	7.89+/-0.28 (4.7%)

^{53}Cr thermal cross section compared to the values listed in the Atlas of Neutron Resonances

Cross Section	ORNL		Atlas
	Resonance	Direct	
Capture	18.09+/-0.42	18.41	18.60+/-0.60
Total	26.07+/-0.51	26.39	26.38+/-0.62
Scattering	7.98+/-0.28	-	7.78+/-0.20

^{53}Cr uncertainty in the energy group 0.0253 eV - 0.3 eV calculated with covariance data

Cross Section	Average value and uncertainty
Capture	0.72+/-0.02 (2.8%)
Total	3.79+/-0.11 (2.9%)
Scattering	3.07+/-0.08 (2.6%)

^{58,60}Ni Resonance Evaluations at ORNL

Nuclear Data Group

Oak Ridge National Laboratory

INTRODUCTION

- **PREVIOUS EVALUATION by C. M. Perey et al., for ENDF/B-V, VI**
  - **not modified for B-VII-0**
  - **no COVARIANCE DATA available**
  - **^{58}Ni thermal to 800 keV**
  - **^{60}Ni thermal to 450 keV**
- **HIGH RESOLUTION NEUTRON TRANSMISSION at GELINA**
  - **Brusegan, 1994**
- **NEW CAPTURE CROSS SECTION MEASUREMENT at ORELA Guber, 2008**
- **RE-EVALUATION NEEDED by UPDATING THE DATA BASE**
- **RPCM and CSCM CALCULATION**

EXPERIMENTAL DATA BASE

- **OLD ORELA TRANSMISSION DATA by Harvey, Larson, Perey**
  - **^{58}Ni Flight path 78 m, Sample 0.0764 at/b Low Energy**
  - **^{58}Ni Flight path 201 m, Sample 0.172 at/b High Energy**
  - **^{60}Ni Flight path 80 m, Sample 0.029 and 0.084 at/b E < 200 keV**
  - **^{60}Ni Flight path 80 m, Sample 0.0744 at/b E > 200keV**

EXPERIMENTAL DATA BASE

- **GELINA TRANSMISSION DATA by Brusegan et al.**
  - **^{58}Ni Flight path 388 m Sample 0.044 at/b**
  - **^{60}Ni Flight path 388 m Sample 0.0744 at/b**
- **ORELA CAPTURE DATA by Guber**
  - **^{58}Ni Flight path 40 m Samples 0.360 at/b**
  - **^{60}Ni Flight path 40 m Samples 0.364 at/b**

RESULTS

- **Resonance Parameters**

	ENDF/B.VII.0 (keV)	ORNL (keV)
^{58}Ni	10^{-2} – 812.0	10^{-2} – 812.0
^{60}Ni	10^{-2} – 450.0	10^{-2} – **812.0**

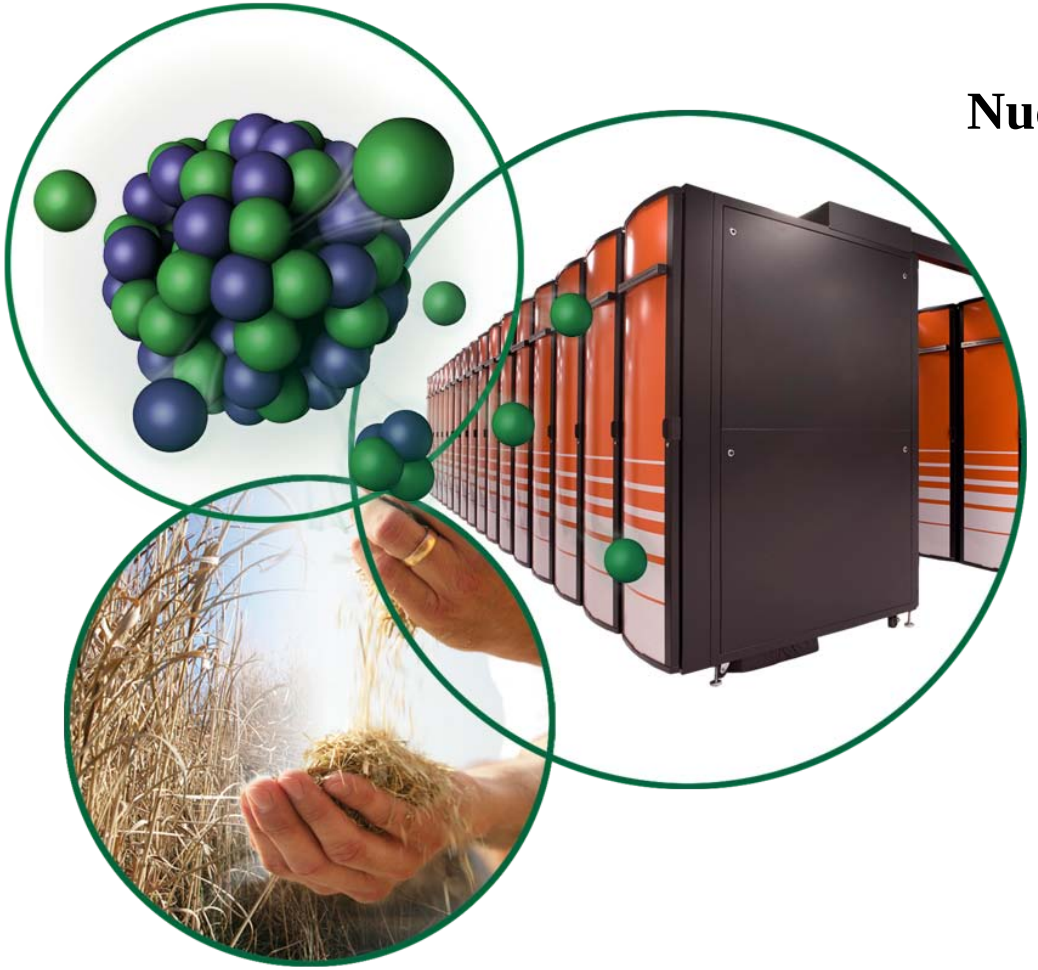
RESULTS

- **^{58}Ni Evaluation**
  - **487 resonances from thermal to 812 keV**
  - **61 s-wave; 204 p-wave; 222 d-wave**
  - **Average spacing for s-wave: $D_0 = 12.65 \pm 0.70$ keV**
  - **Neutron Strength Function from fit to PT distribution:**
  - **$S_0 = 3.38 \pm 0.61 \times 10^{-4}$**
  - **$S_1 = 0.48 \pm 0.08 \times 10^{-4}$**
  - **$S_2 = 2.27 \pm 0.30 \times 10^{-4}$**
  - **Thermal Capture : 4.27 ± 0.15 b compared to the ENDF/B-VII 4.62 b**
  - **Capture Integral: 2.095 ± 0.07 b compared to the ENDF 2.20 b**

RESULTS

- **^{60}Ni Evaluation**
  - **Extended from 450 keV (ENDF/B-VII) to 812 keV Taking advantage of Brusegan very high resolution transmission**
  - **458 resonances from thermal to 812 keV**
  - **61 s-wave; 236 p-wave; 161 d-wave**
  - **Average spacing for s-wave: $D_0 = 11.94 \pm 0.66$ keV**
  - **Neutron Strength Function from fit to PT distribution:**
  - **$S_0 = 2.64 \pm 0.64 \times 10^{-4}$**
  - **$S_1 = 0.68 \pm 0.09 \times 10^{-4}$**
  - **$S_2 = 0.83 \pm 0.20 \times 10^{-4}$**
  - **Thermal Capture : 2.40 ± 0.06 b compared to the ENDF/B-VII 2.92 b**
  - **Capture Integral: 1.259 ± 0.032 b compared to the ENDF 1.394 b**

^{46,47,48,49,50}Ti Resonance Parameters and Covariance Evaluation



Nuclear Data & Criticality Safety Group

Oak Ridge National Laboratory

Resonance Parameter and Covariance Evaluation for ^{46,47,49,50}Ti

• Resolved resonance parameters were converted from MLBW into the RM representation. The resonances were checked against the resonance parameters given in the Atlas of Neutron Resonances.

• For Ti-46 a resonance at 55.67 keV with j=1/2 (l=1) was repeated. According to the Atlas it should be at the energy 56.66 with Γ_t=0.48 eV, Γ_n=0.1 eV and Γ_γ=0.38.

• Thermal cross section and resonance integral are unchanged.

Covariance Data:

•Resolved resonance covariance data were generated with the SAMMY for ^{46,47,49,50}Ti.

•SAMMY was run with the option of generating resonance-covariance retroactively using the "propagated uncertainty parameter" option to include systematic data uncertainties.

Resonance Parameter and Covariance Evaluation for ^{48}Ti

◆ Capture (40-meter) and transmission (80-meter) measurements for enriched ^{48}Ti and natural titanium done at ORELA from 10 eV to 500 KeV;

◆ Evaluation performed with SAMMY;

◆ Resolved resonance parameters determined from 10^{-5} eV to 400 keV;

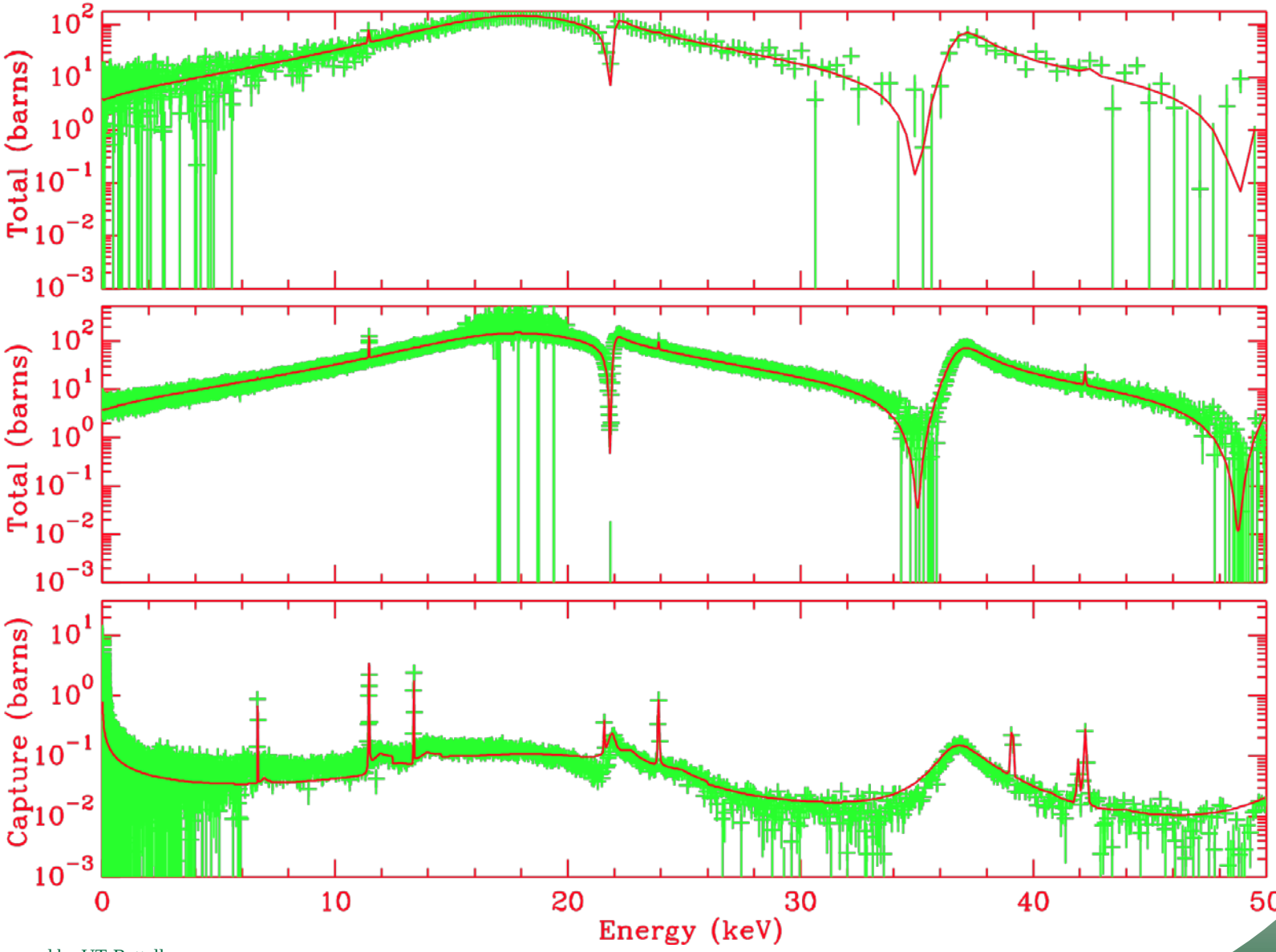
◆Evaluated Resonance parameter covariance;

◆ Thermal cross section and resonance integral and uncertainties well reproduced;

^{48}Ti thermal cross section compared to the values listed in the Atlas of Neutron Resonances

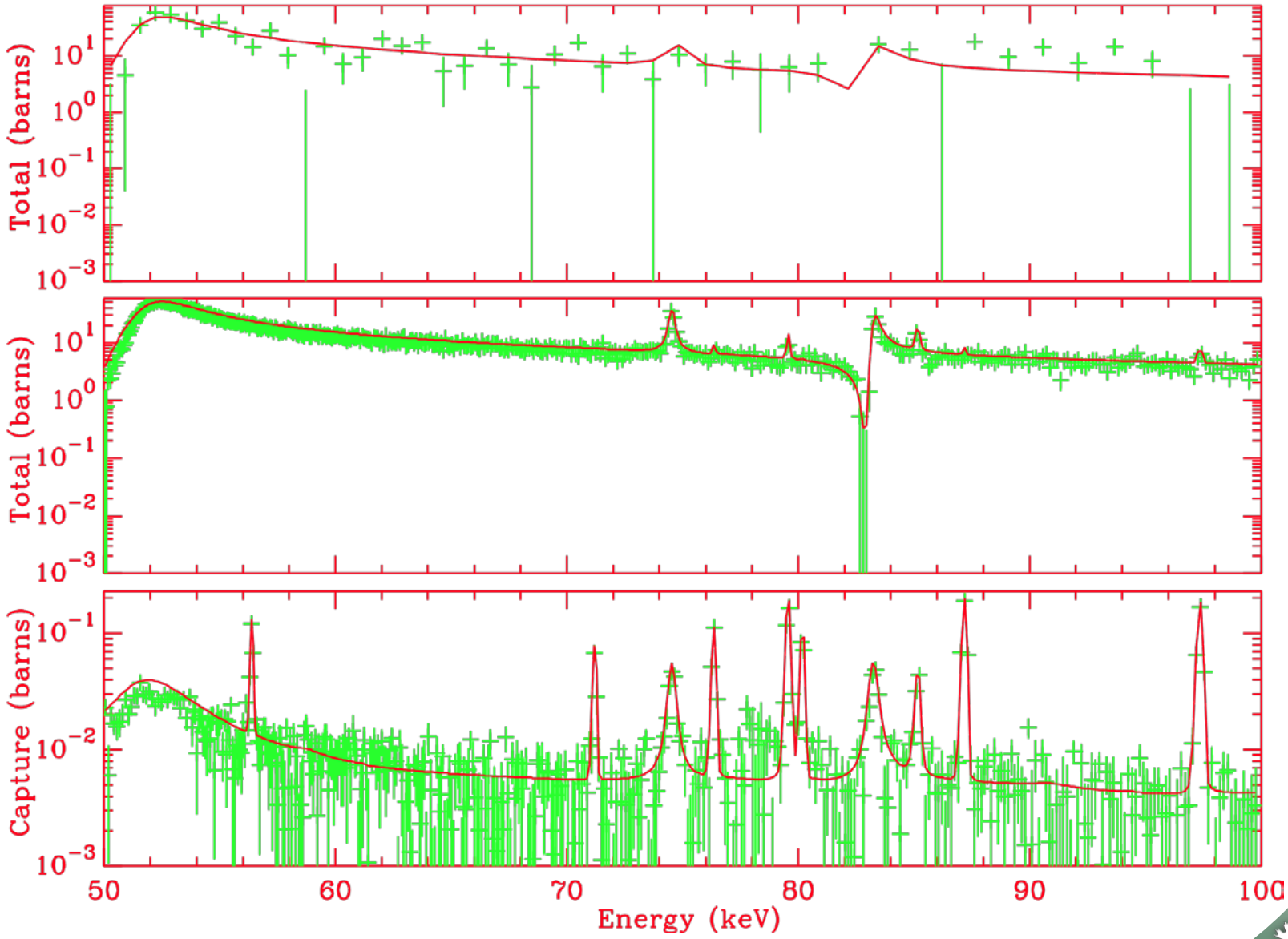
Cross Section	ORNL	Atlas
	Resonance and Direct	
Capture	8.32 +/- 0.23	8.32 +/- 0.16
Total	12.35 +/- 0.30	12.42 +/- 0.25
Scattering	4.03 +/- 0.17	4.10 +/- 0.20
RI	3.78 +/- 0.17	3.90 +/- 0.25

^{48}Ti Cross Sections Experimental and SAMMY



paradigm shift

^{48}Ti Cross Sections Experimental and SAMMY



paradigm shift

^{239}Pu Resonance Evaluation at ORNL

Nuclear Data Group

Oak Ridge National Laboratory

Motivation for a New Evaluation

- Existing resonance evaluation is divided into three disjoint resonance parameter set as 1.0×10^{-5} eV to 1 keV, 1 keV to 2 keV, 2 keV to 2.5 keV;
- Cross section mismatch at the energy boundaries;
- Not easy to generate uncertainty for the whole energy region (zero correlation);
- Solve long standing problem for thermal benchmark experiments

paradigm shift

EXPERIMENTAL DATA

Reference	Energy Range (eV)	Facility	Measurement
Bollinger et al. (1956)	0.01 – 1.0		Total Cross Section
Gwin et al. (1971)	0.01 – 0.5	ORELA	Fission and Absorption at 25.6 m
Gwin et al. (1976)	1.0 – 100.0	ORELA	Fission and Absorption at 40.0 m
Gwin et al. (1984)	0.01 – 20.0	ORELA	Fission at 8 m
Weston et al. (1984)	9.0 – 2500.0	ORELA	Fission at 18.9 m
Weston et al. (1988)	100.0 – 2500.0	ORELA	Fission at 86 m
Weston et al. (1993)	0.02 – 40.0	ORELA	Fission at 18.9 m
Wagemans et al. (1988)	0.002 – 20.0	GELINA	Fission at 8 m
Wagemans et al. (1993)	0.01 – 1000.0	GELINA	Fission at 8 m
Harvey et al. (1985)	0.7 – 30.0	ORELA	Transmission at 18 m
Harvey et al. (1985)	30.0 – 2500.0	ORELA	Transmission at 80 m

Issues with ^{239}Pu Evaluation

- Results of plutonium solution calculations indicate no improvement using ORNL evaluation. Longstanding problem persists!!
- In some case the good results from previous ^{239}Pu evaluation deteriorate
- Review of the ^{239}Pu is underway.

  ORNL, LANL and CEA

^{240}Pu Resonance Evaluation at ORNL

Nuclear Data Group

Oak Ridge National Laboratory

^{240}Pu Assessment

- Most recent resonance evaluation is by Derrien and Bouland—adopted in JEFF 3.1 and JENDL-3.3 up to 40 keV
- ENDF/B-VII.0 resonance evaluation is not latest evaluation—no covariance data in ENDF evaluation
- SAMMY re-analysis of measured data performed with “new” ORELA data—provide improved resonance analysis with covariance data to complement high-energy LANL high-energy evaluation
- Experimental data to support re-evaluation effort
  - “New” data include ORELA neutron transmission measurements by Harvey and Gwin (1988)—recently discovered in ORELA archives—sample thickness: 0.0723 at/b
  - Transmission data by Kolar et al for two different sample thicknesses: 0.00166 at/b and 0.00466 at/b
  - Experimental fission data not included—assumed fission widths (generally very small) were obtained with sufficient accuracy in previous evaluation

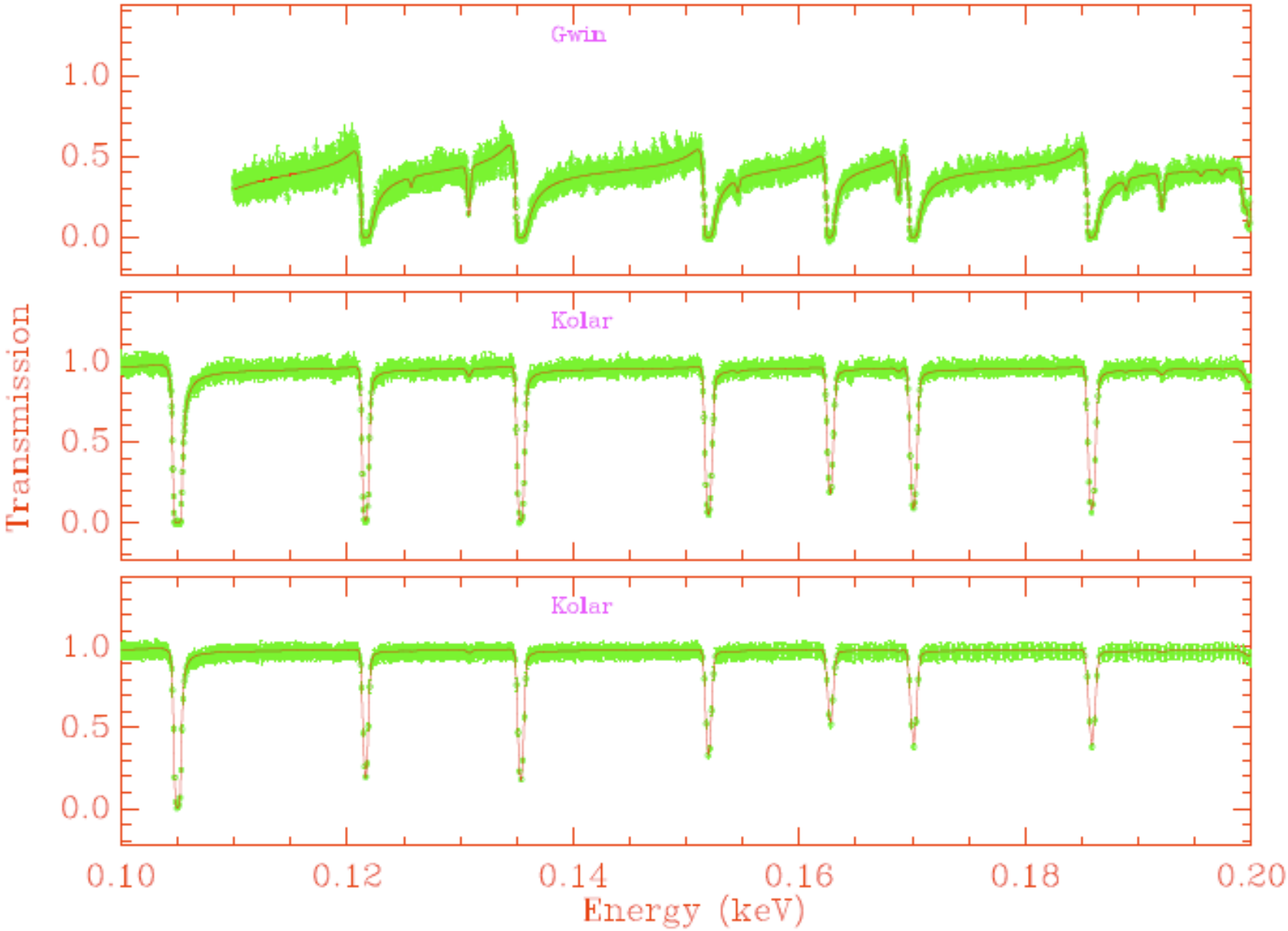
^{240}Pu Evaluation

- SAMMY analyses
  - Allowed estimation of normalization corrections and background adjustments
  - Neutron energy of all measurements aligned to ORELA data
  - Kolar et al samples too small to permit identification of small s-wave resonances and p-wave resonances (particularly above 1 keV)
  - Harvey-Gwin thick sample permitted identification of s-wave and p-wave resonances

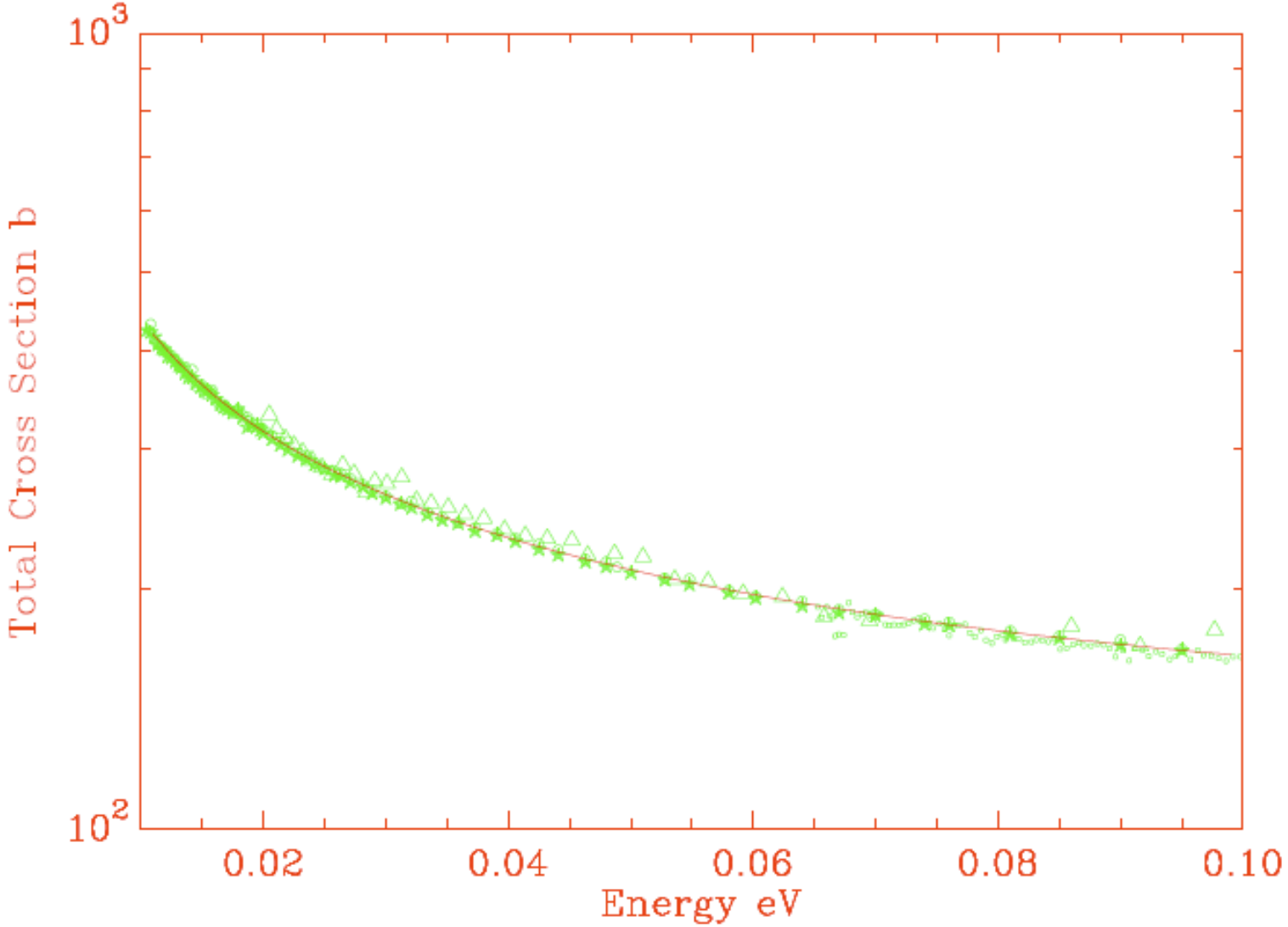
^{240}Pu Evaluation

- New evaluation compared with previous evaluation
  - Previous evaluation using Kolar data had 425-resonances (all identified as s-wave)
  - New evaluation: 428 s-wave resonances and 121 p-wave resonances
  - Values of neutron widths in new evaluation very close to previous evaluation below ~700 eV
  - Above 700 eV smaller widths obtained due to re-evaluation of experimental resolution of Kolar data
  - Total cross-section value at 0.0253 eV based on new resonance parameters: 284.05 b
    - Agrees with Spencer data
    - Significantly smaller than 289 b value recommended by Atlas of Neutron Resonance Parameters
    - Thermal capture value is also smaller
- Capture resonance integral (0.5 eV to 7.7 keV)
  - New evaluation: 8492 b
  - JEFF-3.1.1: 8479
  - ENDF/B-VII.0: 8480

SAMMY Fit ^{240}Pu Transmission

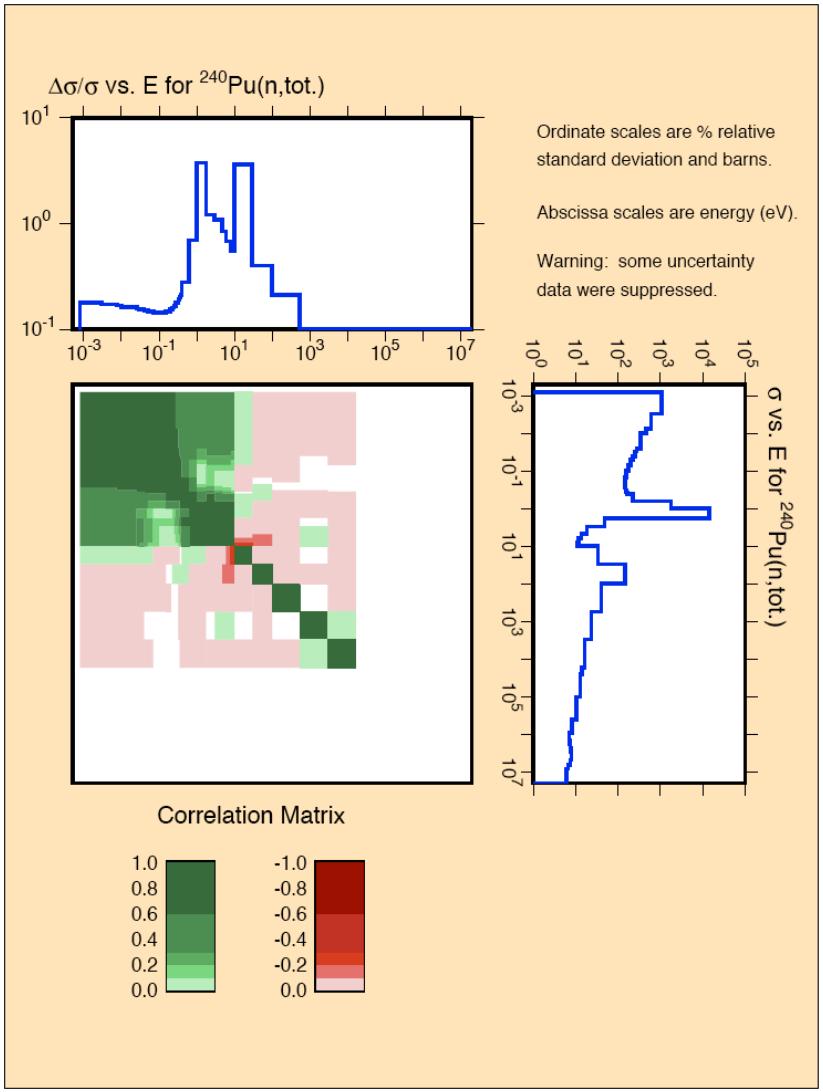


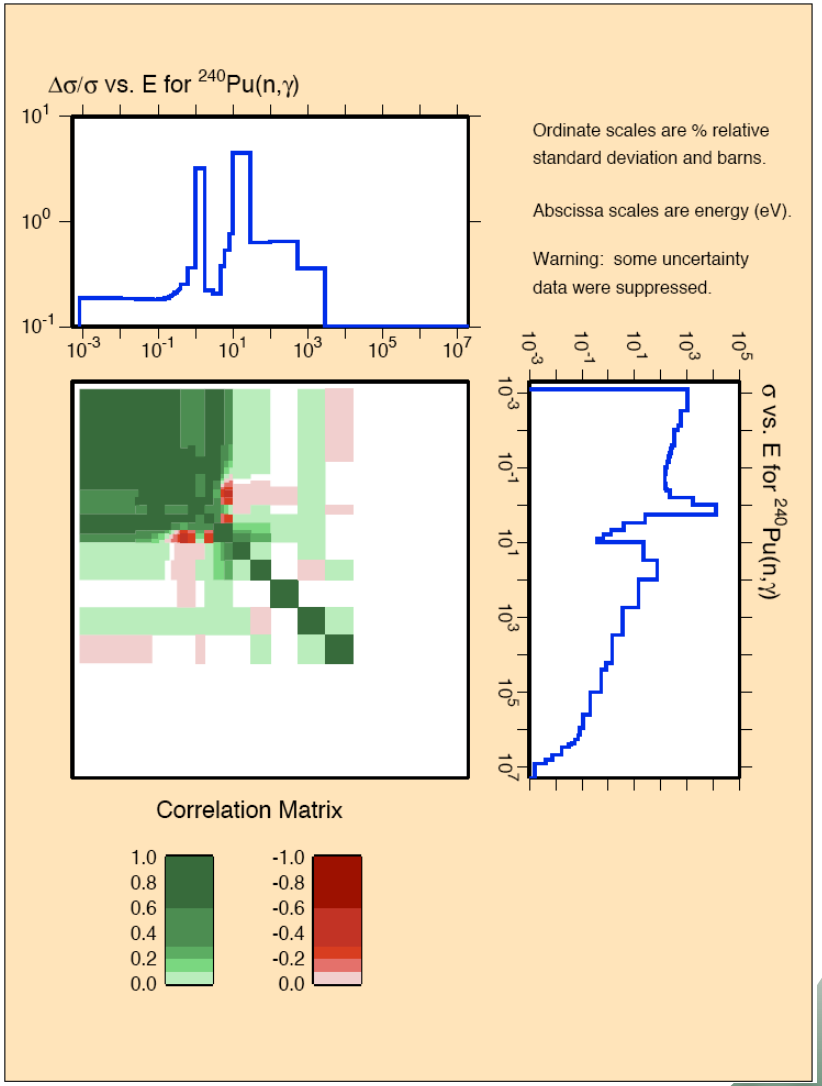
SAMMY ^{240}Pu (Thermal)



^{240}Pu Evaluation

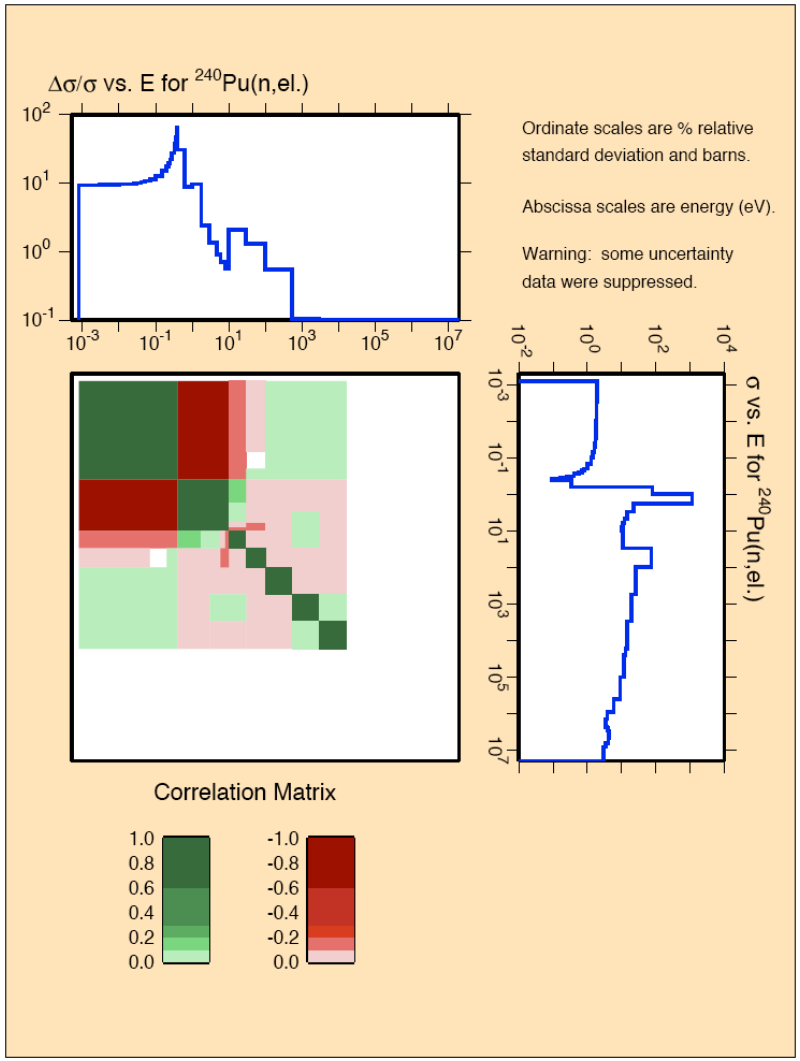
- Re-evaluation resulted in consistent set of covariance data—plots of PUFF-IV processed ^{240}Pu correlation data (total and capture shown):

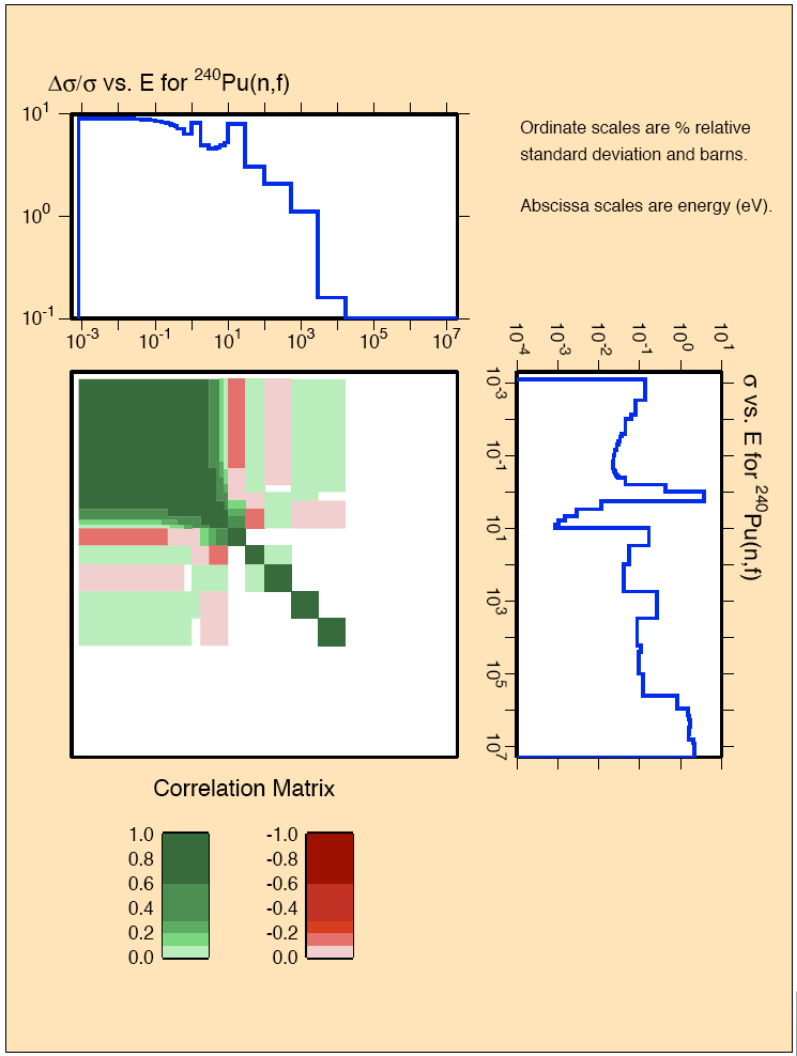




^{240}Pu Evaluation

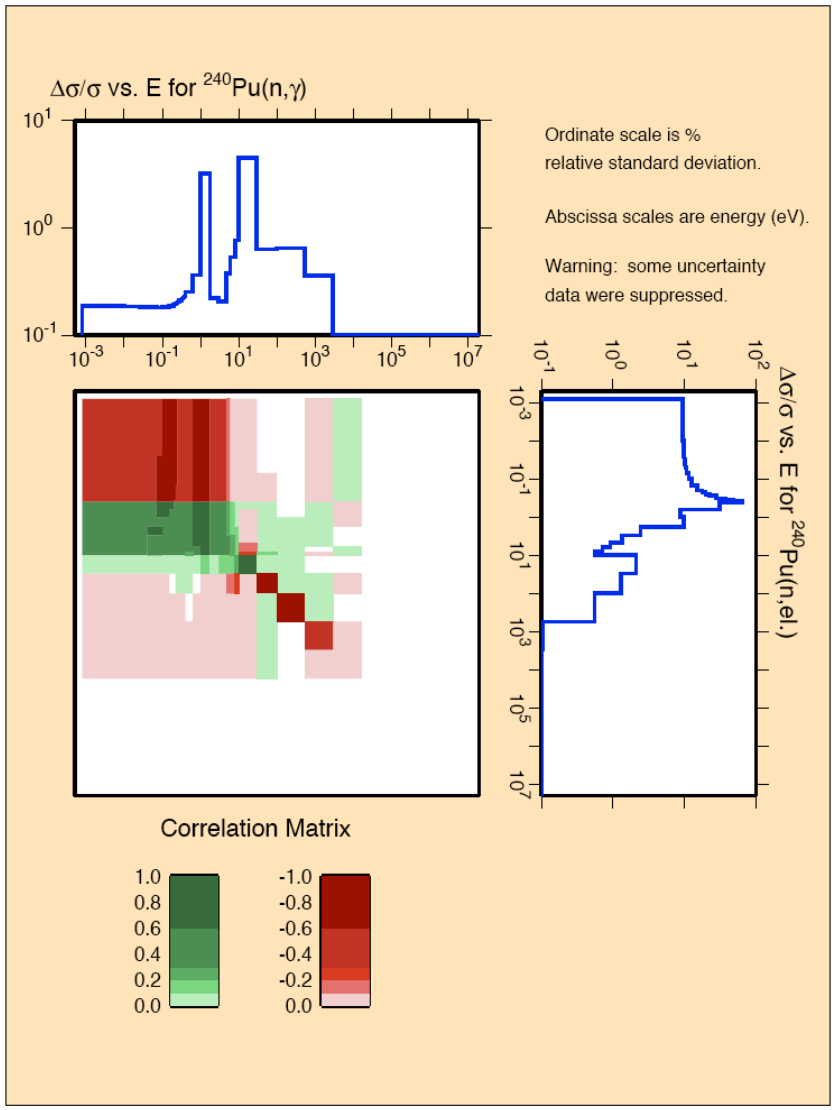
- Plots of PUFF-IV processed ^{240}Pu correlation data (elastic and fission shown):

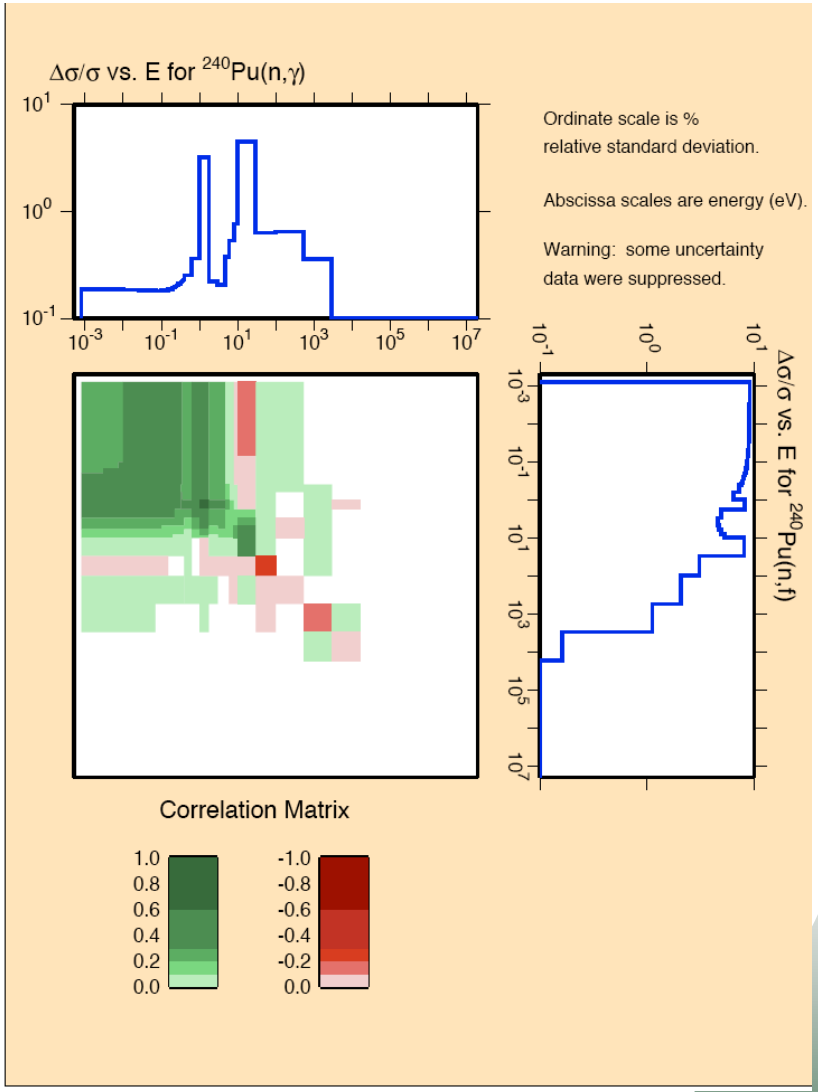




^{240}Pu Evaluation

- Plots of ^{240}Pu cross-reaction correlation data (capture-elastic and capture-fission shown):





Evaluation Summary

	Resonance Evaluation	Resonance Covariance Evaluation	High Energy Evaluation	High Energy Covariance Evaluation
^{50}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany	FZK Germany
^{52}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany	FZK Germany
^{53}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany	FZK Germany
^{54}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany	FZK Germany
^{58}Ni	ORNL (new evaluation)	ORNL (new evaluation)		
^{60}Ni	ORNL (new evaluation)	ORNL (new evaluation)		

Evaluation Summary

	Resonance Evaluation	Resonance Covariance Evaluation	High Energy Evaluation	High Energy Covariance Evaluation
W isotopes (180, 182, 183, 184, 186)	ORNL (retroactive)	ORNL (retroactive)	IAEA	IAEA
^{55}Mn	ORNL (new evaluation)	ORNL (new evaluation)	IAEA	IAEA
^{46}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{47}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{48}Ti	ORNL (new evaluation)	ORNL (retroactive)	LANL	LANL
^{49}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{50}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{240}Pu	ORNL (new evaluation)	ORNL (new evaluation)	LANL	LANL

Comments on Additional ORNL Evaluations

- ^{35}Cl and ^{37}Cl: submitted in 2007—little or no benchmark testing
  - ^{35}Cl has LRF=7 resonance format – NJOY update needed to process
- ^{39}K and ^{41}K: submitted Oct 2008—little or no benchmark testing
- ^{55}Mn:
  - Updated evaluation submitted in 2010 to add correct File 33 covariance data for resonance region
  - ORNL resonance evaluation coupled with IAEA high-energy evaluation
- ^{19}F: submitted Oct 2008
  - New LRF=7 resonance format – NJOY update needed to process
  - inelastic scattering data incorporated in resonance analysis
  - New evaluation has not improved benchmark performance—but has not made benchmark calculations worse either

Comments on Additional Evaluations

- **$^{180, 182, 183, 184, 186}$W**:
  - ORNL retroactive resonance parameter covariance evaluation in collaboration with IAEA high-energy evaluation
- **^{233}U, ^{235}U, and ^{238}U**: covariance evaluations: submitted March 2008
  - ORNL (resonance parameter covariance data) and LANL (High energy covariance data)
  - ^{233}U updated file submitted in 2010 to use LANL high-energy evaluation down to top of resolved region
  - Covariance data utilized in SG33 analyses and also distributed with SCALE 6 by ORNL
- **Hf-isotopes:** submitted by RQ Wright—testing??