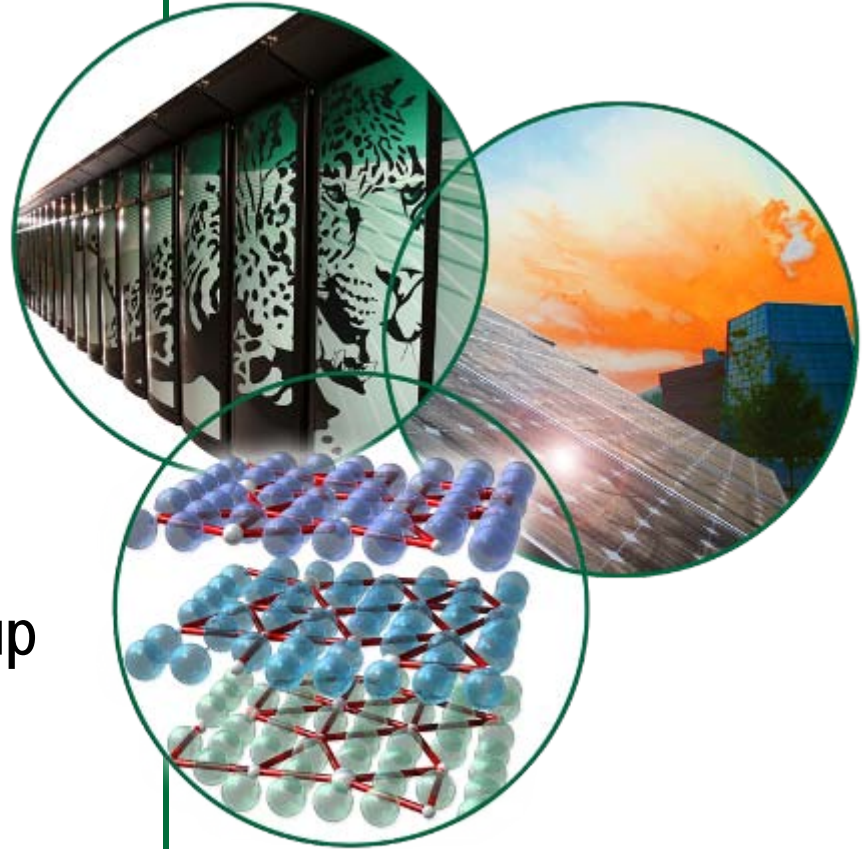


Nuclear Data Analyses to Support Nuclear Fuel Cycle Applications (US/ROK I-NERI)

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Nuclear Data and Criticality Safety Group
Reactor and Nuclear Systems Division

FCR&D Nuclear Physics Working Group
Santa Fe, NM
November 4-5, 2010



Outline

- I-NERI Project Overview
- Motivation
- FY10 Status Report
- FY11 Plans
- Summary

ORNL-KAERI I-NERI Project Overview

- ORNL and KAERI have developed a 3-year collaboration plan to investigate and address nuclear data needs for AFC and nuclear safeguards applications
- **Objective:** provide improved neutron cross-section data with covariance data for isotopes important for AFC applications
- Emphasis will be on isotopes of benefit to fuel cycle and nuclear safeguards analyses
- **NE R&D Objective 4: “Understand and minimize the risks of nuclear proliferation and terrorism”**
 - I-NERI work providing improved cross-section data with covariance (uncertainty) data needed for modeling and simulation (M&S) of detection and monitoring systems
 - Facilitates design / deployment of next-generation safeguards technologies

ORNL-KAERI I-NERI Project Overview

- Design and deployment of AFC facilities and operations will require V&V of radiation transport software and nuclear data
- Preventing proliferation of nuclear material will require state-of-the-art detection and radiation transport modeling/depletion capabilities (e.g., monitor and interrogation)
- M&S capabilities (MCNP, SCALE, etc.) are dependent upon nuclear cross-section data—ex: simulation of particle detector counters in material interrogation for nuclear safeguards applications depends on how well the basic nuclear data and their uncertainties (covariance data) are known
- Nuclear data covariance analysis determines the uncertainty in the cross section measurements and provides the user valuable information on the precision of a nuclear data measurement or simulation
 - Covariance data are essential to understand impact of data uncertainties on calculated quantities of interest—propagation of nuclear data uncertainties to calculated quantity of interest
 - Ex: SNF content determination from M&S: nuclear data are used to calculate actinide content of spent fuel from actual measurements and propagation of differential data uncertainties important to quantify uncertainties on SNF content from M&S prediction
- M&S capabilities with nuclear data uncertainties are crucial to designing new facilities with integrated safeguards capability

ORNL-KAERI I-NERI Project Overview

- International data files (ENDF, JEFF, JENDL, etc.) have limited covariance data especially for isotopes important for AFC fuel cycle and safeguards applications (^{237}Np , ^{240}Pu , ^{242}Pu , etc.)
- Concerted effort needed to produce improved nuclear data with covariance information
 - Cross-section evaluation database has little or no uncertainty data (ENDF/B-VII: 26 out of 393 evaluations have uncertainty data)
- ORNL and KAERI I-NERI collaboration:
 - Identify 2-3 isotopes important for fuel cycle and safeguards applications needing nuclear data improvements (FY09)—initial focus on neutron data
 - Generate cross-section evaluations with covariance data (FY09 and FY10)—primarily focused on neutron data but can expand to other data needs (e.g., branching ratio data)
 - Demonstrate and test the data in radiation transport and S/U analyses (FY10 and FY11)
 - Submit final files for distribution with the ENDF/B file system—would be available for ENDF/B-VII.2 (FY11)

ORNL/KAERI I-NERI Team

➤ ORNL (US)

- Project Management: Michael Dunn
- Technical Team: Luiz C. Leal, Goran Arbanas, Royce Sayer, Herve Derrien



➤ KAERI (ROK)

- Project Management: Choong-Sup Gil
- Technical Team: Do Heon Kim, Hyeong Il Kim, Young-Ouk Lee



ORNL-KAERI I-NERI Project Overview

- ORNL I-NERI Funding Request: \$300K/yr (KAERI same funding level on ROK side)
 - FY09: \$200K (NE) and \$95K (NA-242)—CR delayed ORNL start until April 2009—6 months behind KAERI
 - FY10: \$200K (NE) and \$0K (NA-242)—\$100K shortfall put US behind original work schedule with ROK
 - FY11 Projected: \$200K (NE: \$100K MPACT and \$100K Nuclear Data) and \$100K (NA-242)

Motivation for ORNL/KAERI I-NERI (U.S. Perspective)

DOE Nuclear Safeguards Vision for Advanced Fuel Cycle



- Discussion points from May 2009 Safeguards Campaign Meeting:
- Develop technologies to enable next generation safeguards for the nuclear fuel cycle of the future—reducing proliferation risks and enhancing confidence and acceptance of nuclear energy
- Science-based approach requires integration of experiment, theory, and modeling & simulation within framework of predictive capabilities
 - Instrumentation development based on fundamental knowledge of applicable physics and chemistry
 - Modeling & simulation development that enables discovery based application—significantly decreases development time and cost
 - Materials science capabilities that enable science informed design of new sensor and associated components
 - Information science applied to nuclear safeguards such that synergy is achieved from the totality of data available, full integration of information and real-time analysis

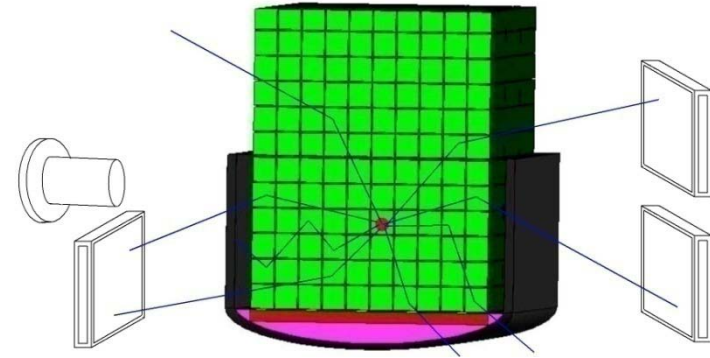
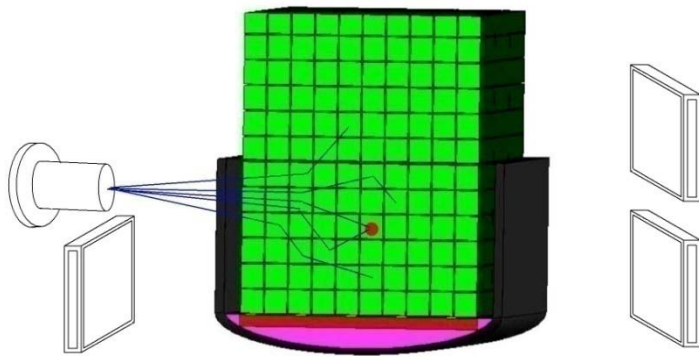


DOE Nuclear Safeguards Vision for Advanced Fuel Cycle—Grand Challenge

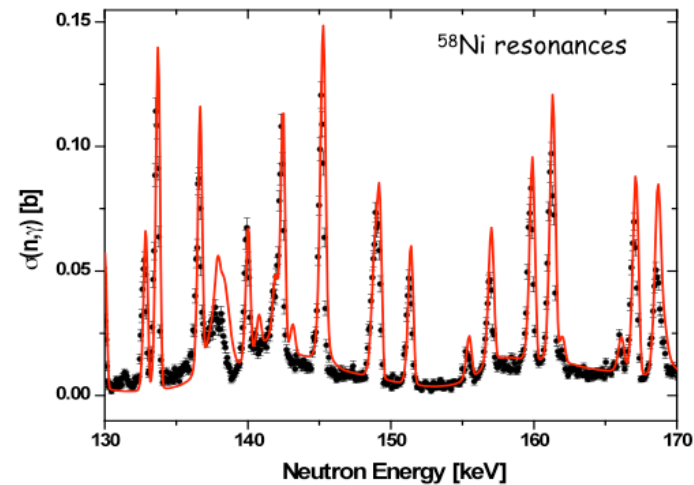


- Discussion points from May 2009 Safeguards Campaign Meeting (cont'd):
- Operator, regulator (DOE and NRC), and international verification regime (IAEA) possess real-time knowledge of nuclear material locations, quantities, forms—implemented in a cost effective manner
- Periodic inventories are no longer primary source of diversion detection but rather a mechanism to verify that the system is operating properly—continuous inventory
- Transparency in facility operation, allows for remote interaction by inspectors
- Enabling R&D required to achieve vision
 - Next generation of instrumentation more accurate, online, and in continuous operation (targeted directly at material of interest)
 - Development of 'Safeguards by Design' methodology and supporting assessments—facilities fundamentally easier to safeguard
 - Real-time knowledge extraction from disparate data—enable real-time analysis, data archiving, and remote inspection

Active Interrogation



- Possible interrogation technique: neutron resonance capture analysis coupled with prompt gamma-ray to identify trace isotope quantities nondestructively
- Resonances are isotope dependent
- Data can be used to identify isotopes present
- Work initiated at LANSCE to investigate technique



➤ Slide from presentation by Mike Miller AFCI Nuclear Physics Working Group Meeting May 12, 2009 Coronado, CA:

²⁴⁴Cm/Pu ratio
Important for
neutron multiplicity
counting



Gap and coverage analysis – in process

	U-233	U-235	U-238	Pu-238	Pu-239	Pu-241	Pu-242	Am-241	Np-237	Cm-244	
Passive Neutron											
Multiplicity	I	I			I	I		I	I		
Albedo Reactivity											
Boosted Self-Interrogation											
Active Interrogation											
Lead Slowing Down											
Nuclear Resonance Fluorescence	D			D		D	D	D	D	D	
Photon Induced Fission	D										
Ultra-High Resolution Spectroscopy											
Gamma-, X-Ray	X										
Alpha											
Neutron											
Process Monitoring											
Radiation Based											
Laser Induced Breakdown Spectroscopy	-----Elemental-----										
Other Parameters (pH, flow, temp, etc)											
Online Chemical											
		some R&D needed - low risk					I	indirect measure			
		R&D needed - medium risk					D	fundamental data needed			
		much R&D needed - high risk					X	x-ray only			

May 12, 2009

Nuclear Physics Working Group

10

➤ Physics WG expressed concern with “large” branching ratio uncertainties for isotopes needed for safeguards analyses (e.g., 11% for ²³⁷Np, 10% for ²⁴⁴Cm, etc.)



ORNL/KAERI I-NERI FY10 Status

ORNL-KAERI I-NERI FY10 Status

Task No.	Lead	ORNL Responsibilities	KAERI Responsibilities
1.0	KAERI	○ Identification of priority nuclides	○ Identification of priority nuclides
1.1	KAERI	○ Review and comments	○ Inter-comparisons of cross-section data for the priority identification
1.2	ORNL	○ Analysis of existing ^{237}Np , ^{240}Pu data	○ Review and comments
1.3	KAERI	○ Review and comments	○ Selection of ^{237}Np , ^{240}Pu , Cm-isotopes for improvements of cross-section data
1.4	KAERI	○ Review and comments	○ Uncertainty information analyses of the nuclides
1.5	KAERI	○ Review and comments	○ Testing the data for the benchmarks
2.0	ORNL	○ Improvement of Cross-Section and Covariance Data	○ Improvement of Cross-Section and Covariance Data
2.1	ORNL	○ Evaluation of cross section data for ^{237}Np , ^{240}Pu , Cm-isotopes up to resonance energies	○ Review and comments
2.2	KAERI	○ Review and comments	○ Evaluation of cross section data for ^{237}Np , ^{240}Pu , Cm-isotopes above resonance energies
2.3	ORNL	○ Production of covariance data for ^{237}Np , ^{240}Pu , Cm-isotopes up to resonance energies	○ Review and comments
2.4	KAERI	○ Review and comments	○ Production of covariance data for ^{237}Np , ^{240}Pu , Cm-isotopes above resonance energies
3.0	KAERI	○ Testing of the Improved Data	○ Testing of the Improved Data
3.1	KAERI	○ Review and comments	○ Collection and review of appropriate benchmarks for testing the improved data
3.2	KAERI	○ Review and comments	○ Analysis of benchmark results using improved and old data
4.0	SHARE	○ Documentation	○ Documentation

ORNL-KAERI I-NERI FY10 Status

- Collaboration meeting held at ORNL March 2009
 - Agreed upon collaborative data improvement efforts for ^{237}Np , ^{240}Pu , and Cm-isotopes
 - Key SNF constituents: ^{238}U , ^{235}U , ^{239}Pu , ^{240}Pu , and ^{242}Pu
- ORNL & KAERI performing detailed cross-section evaluation effort
- ORNL completed evaluation effort for ^{240}Pu —includes new covariance data
- ORNL completed preliminary testing of ^{240}Pu evaluation
- ORNL completed covariance evaluation for ^{244}Cm
- Working with KAERI to merge data with high energy evaluation work

Milestone/Deliverable Description	Planned Completion Date	Status
1.0 Identification of priority nuclides	31 January 2010	Completed
1.1 Inter-comparisons of cross-section data for the priority identification	30 April 2009	Completed
1.2 Analysis of existing ^{237}Np , ^{240}Pu data	30 April 2009	Completed
1.3 Selection of ^{237}Np , ^{240}Pu , Cm-isotopes for improvements of cross-section data	30 April 2009	Completed
1.4 Uncertainty information analyses of the nuclides	30 October 2009	Completed
1.5 Testing the data for the benchmarks	31 January 2010	Completed
2.0 Improvement of Cross-Section and Covariance Data	30 April 2011	In progress
2.1 Evaluation of cross section data for ^{237}Np , ^{240}Pu , Cm-isotopes up to resonance energies	30 April 2011	In progress ^{240}Pu completed
2.2 Evaluation of cross section data for ^{237}Np , ^{240}Pu , Cm-isotopes above resonance energies	30 April 2011	In progress
2.3 Production of covariance data for ^{237}Np , ^{240}Pu , Cm-isotopes up to resonance energies	30 April 2011	In progress ^{244}Cm completed
2.4 Production of covariance data for ^{237}Np , ^{240}Pu , Cm-isotopes above resonance energies	30 April 2011	In progress
3.0 Testing of the Improved Data	30 October 2011	In progress
3.1 Collection and review of appropriate benchmarks for testing the improved data	31 July 2010	Completed
3.2 Analysis of benchmark results using improved and old data	30 October 2011	In progress
4.0 Documentation	30 October 2009, 2010, 2011	In progress

^{237}Np Assessment

- ENDF/B-VII.0 and JENDL-3.3 evaluations in thermal and resonance range are the same
 - resonance region measurement accuracy reported to better than 5% up to 100 keV
 - Multi-level Breit Wigner (MLBW) formalism used in resonance region—not adequate to represent detailed resonance structure
- Atlas of Resonance Parameter thermal capture cross section and capture integral are 9% smaller and 5% smaller, respectively, relative to evaluated data—need to investigate difference
- Measured data status
 - Recent capture measurements performed at Lujan Center using DANCE detector—very nice work that covers several energy ranges
 - ORNL has examined data and determined resonances can be resolved up to ~20 eV
 - ORNL has previously measured data from ORELA on a cooled sample
 - Recently learned CEA has differential data that could support re-evaluation
 - **SAMMY analysis of recent DANCE data and previous ORELA data could facilitate improve resonance analysis with covariance data to complement high-energy LANL high-energy evaluation**

^{237}Np FY10 Work Effort

- Identified and gathered available measured cross-section data sets from literature and NNDC EXFOR Database
- Performed preliminary nuclear data analysis of measured data in resonance region
- Obtained recent DANCE data from LANL
- Met with staff from CERN n-TOF at ND2010 meeting and established collaboration to perform analysis of ^{237}Np data recently measured at n-TOF

^{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
- **At a minimum, Derrien-Bouland evaluation should be adopted for ENDF/B-VII.1 with retroactive resonance analysis to produce covariance matrices**
- Measured data status
 - Recent capture measurements performed at n-TOF and Lujan Center using DANCE detector
 - **SAMMY analysis of recently measured data should be performed in context with existing evaluation—provide improved resonance analysis with covariance data to complement high-energy LANL high-energy evaluation**

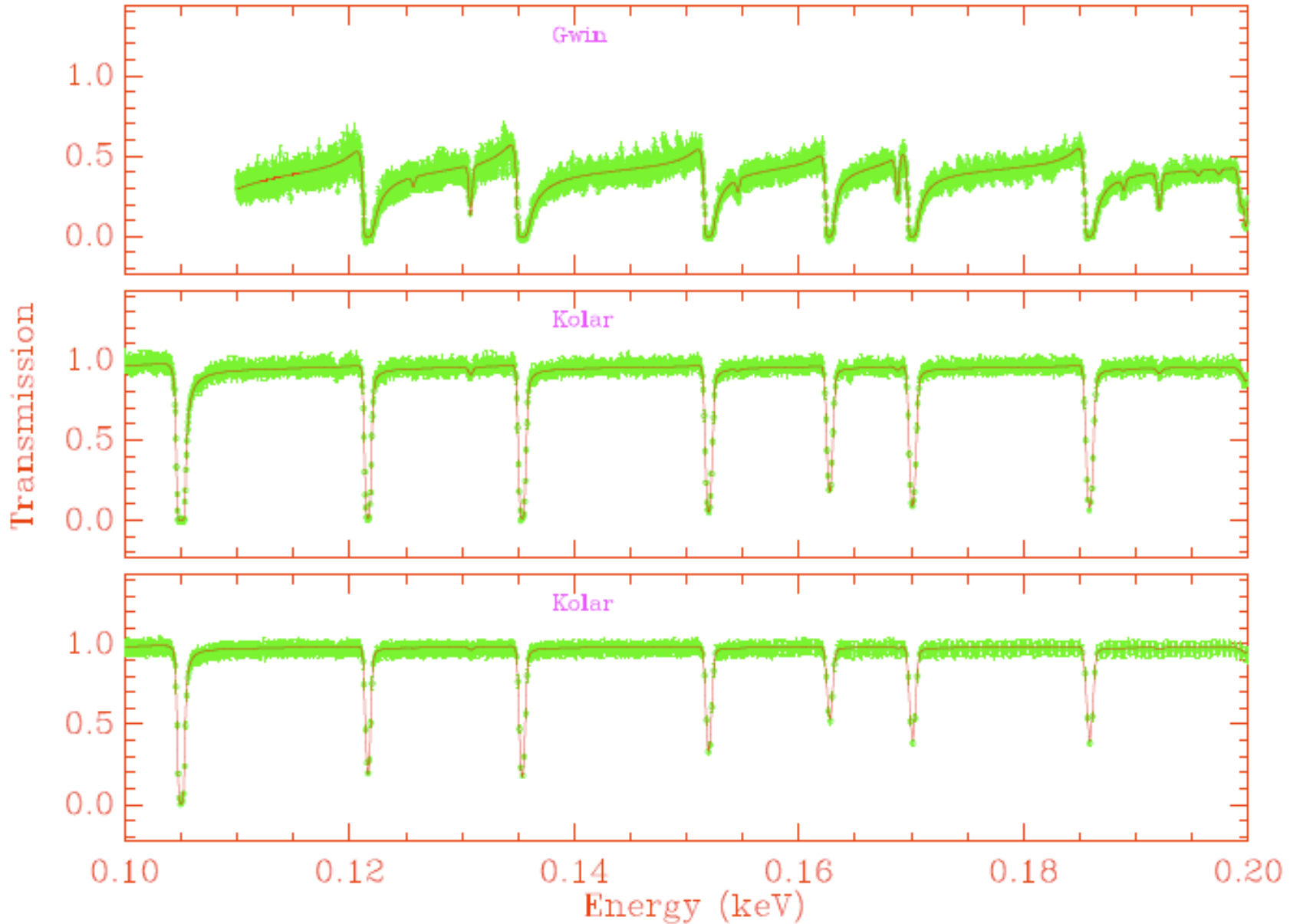
^{240}Pu Evaluation—results by H. Derrien (FY10 Work)

- 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
- 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

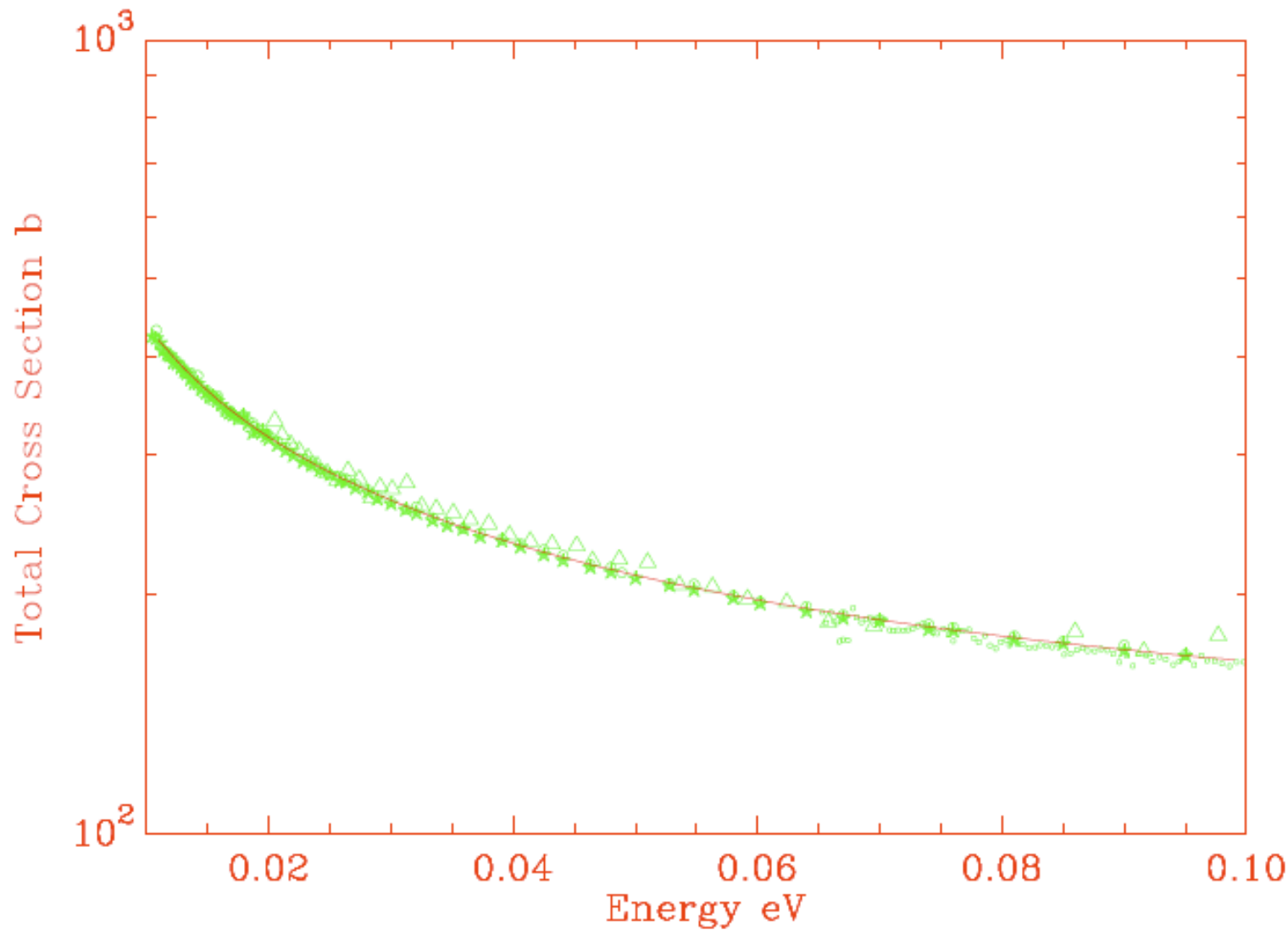
^{240}Pu Evaluation

- 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

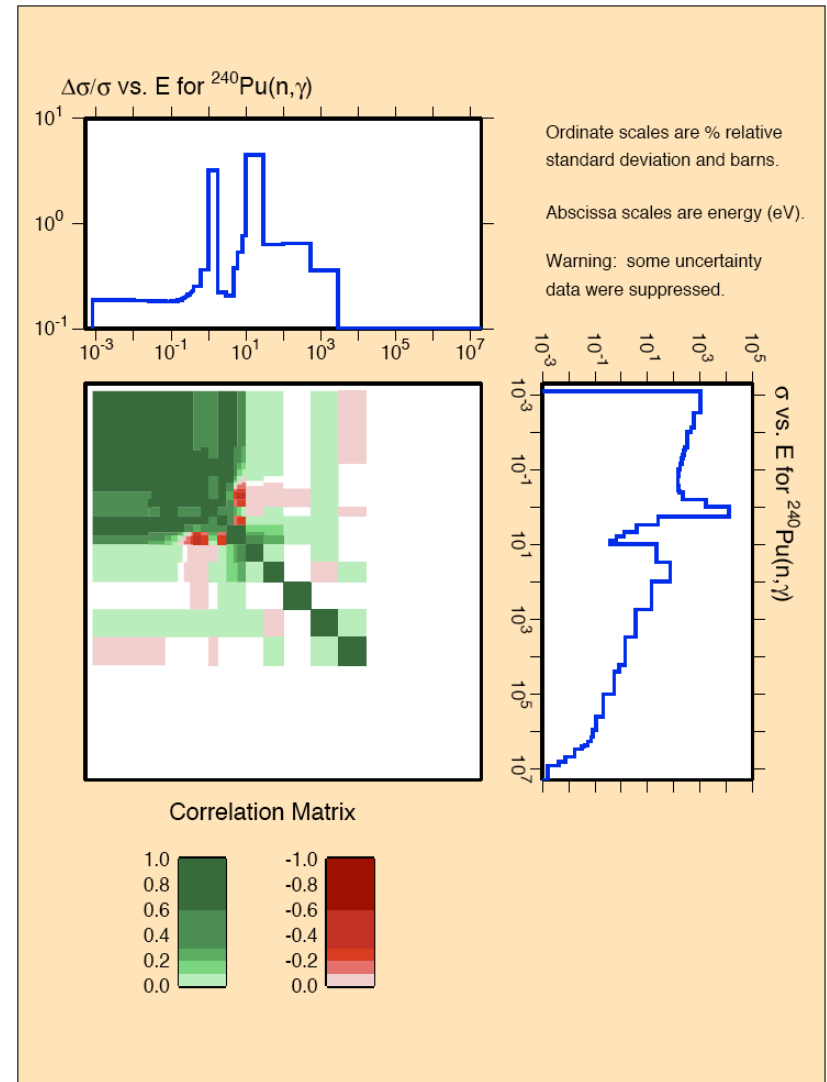
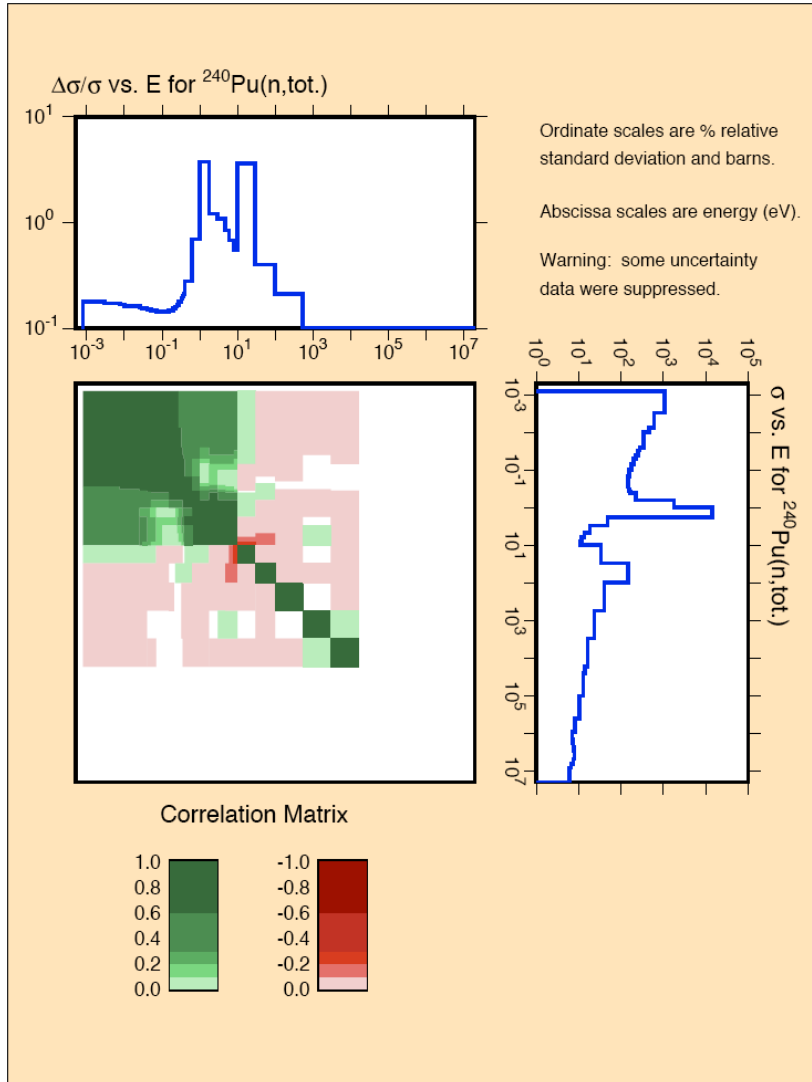


SAMMY ^{240}Pu (Thermal)



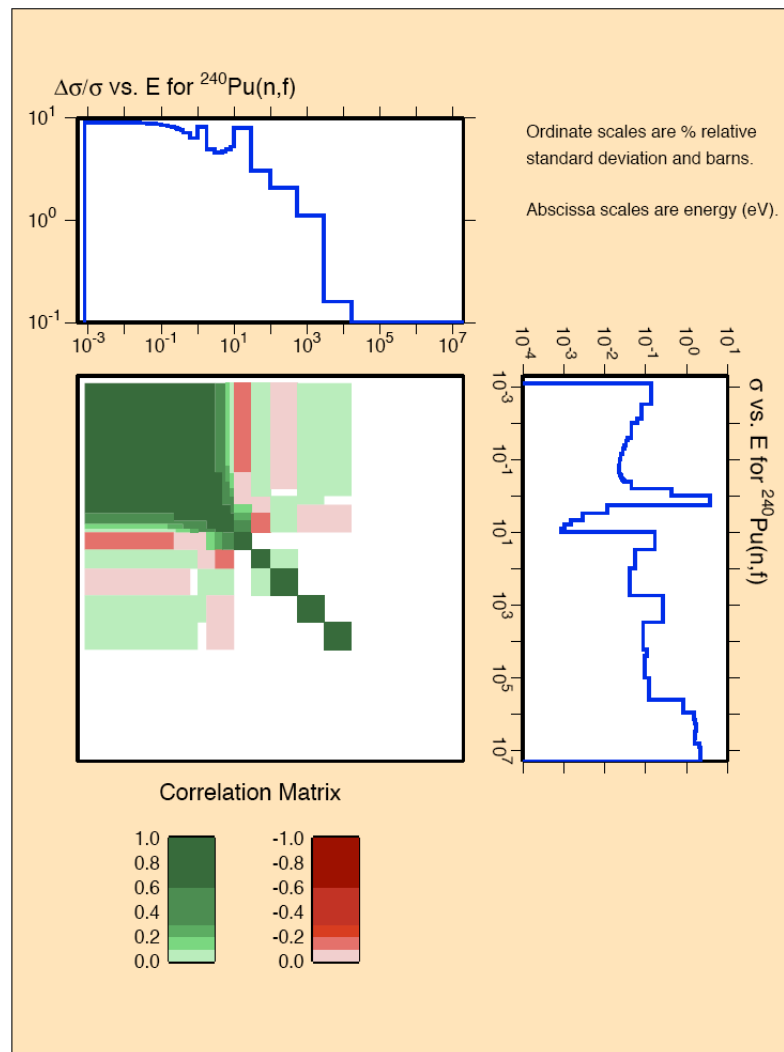
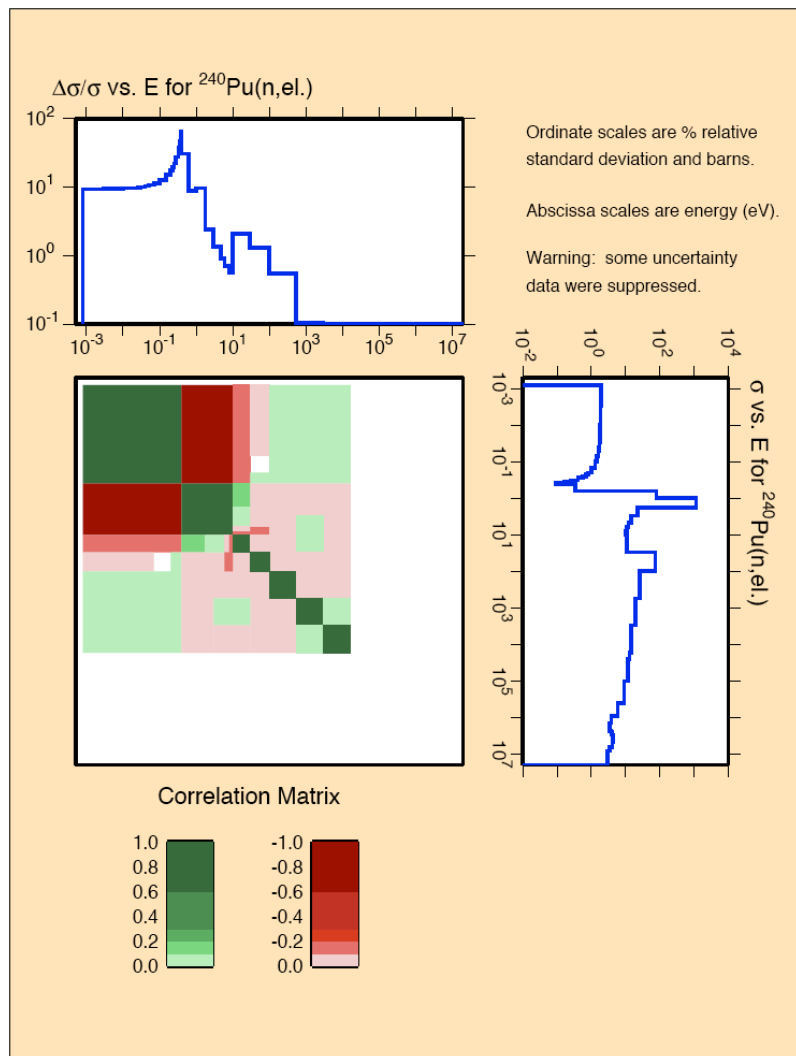
^{240}Pu Evaluation—results by H. Derrien

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



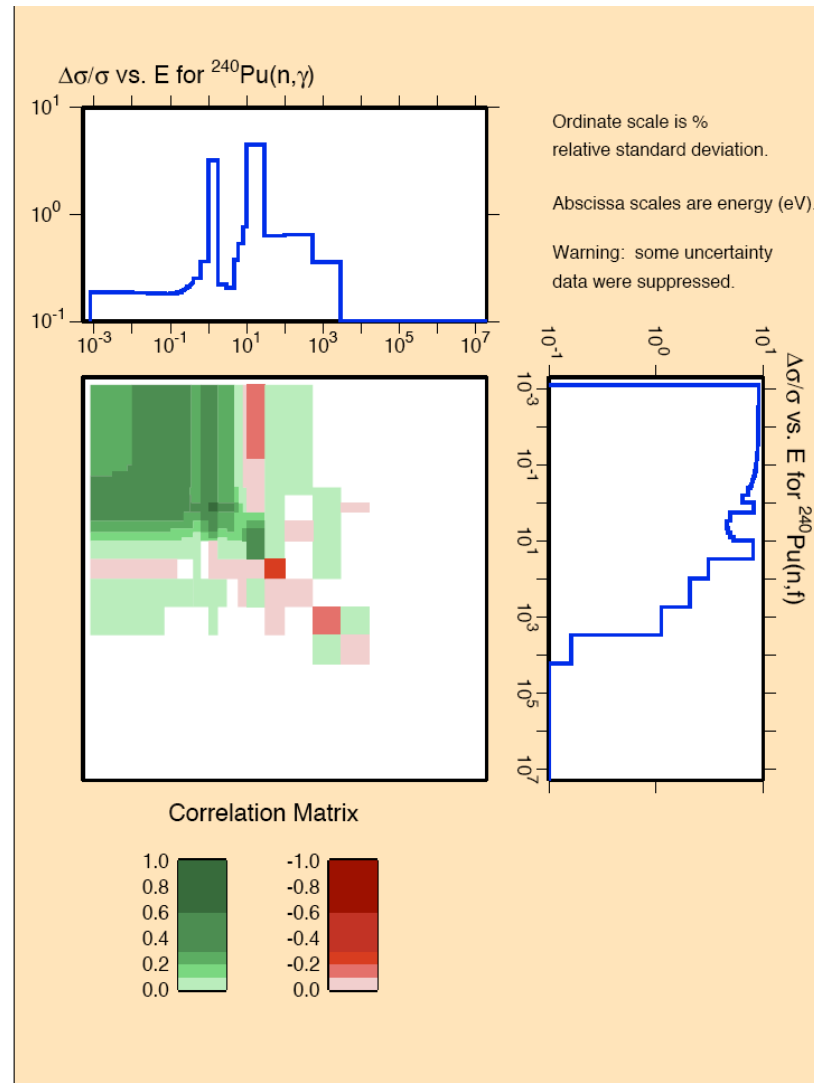
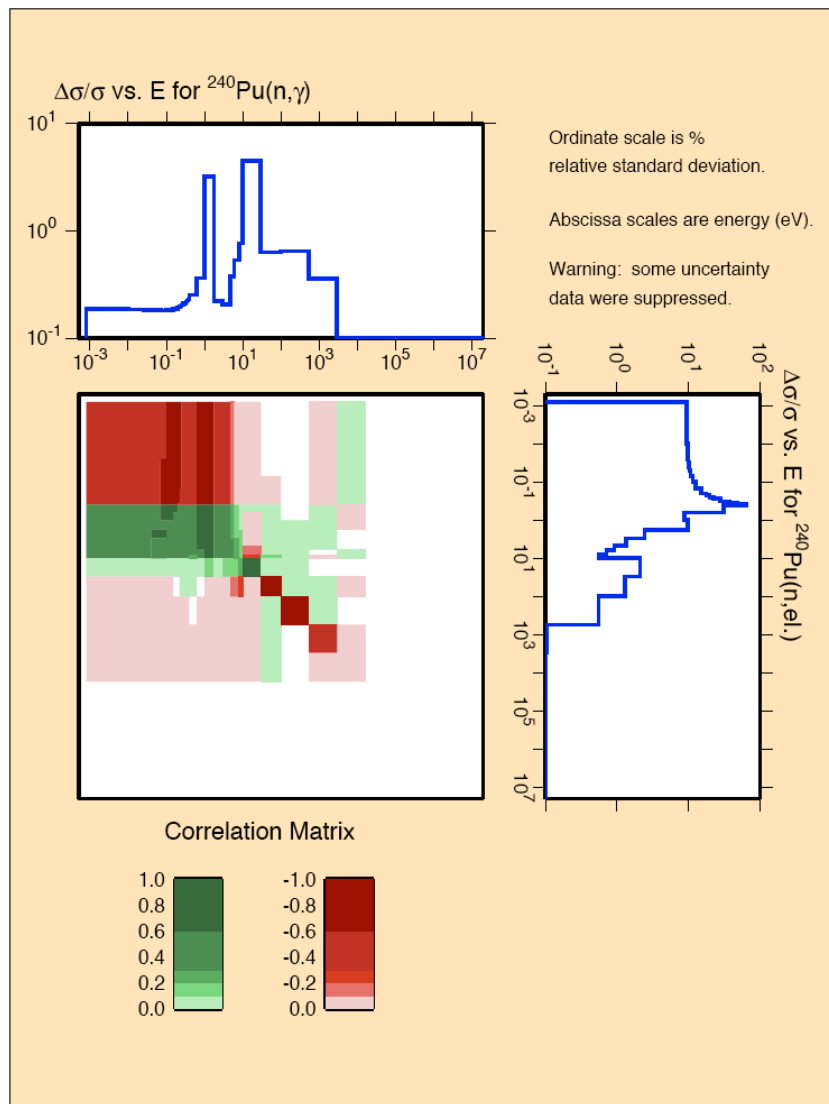
^{240}Pu Evaluation—results by H. Derrien

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



^{240}Pu Evaluation—results by H. Derrien

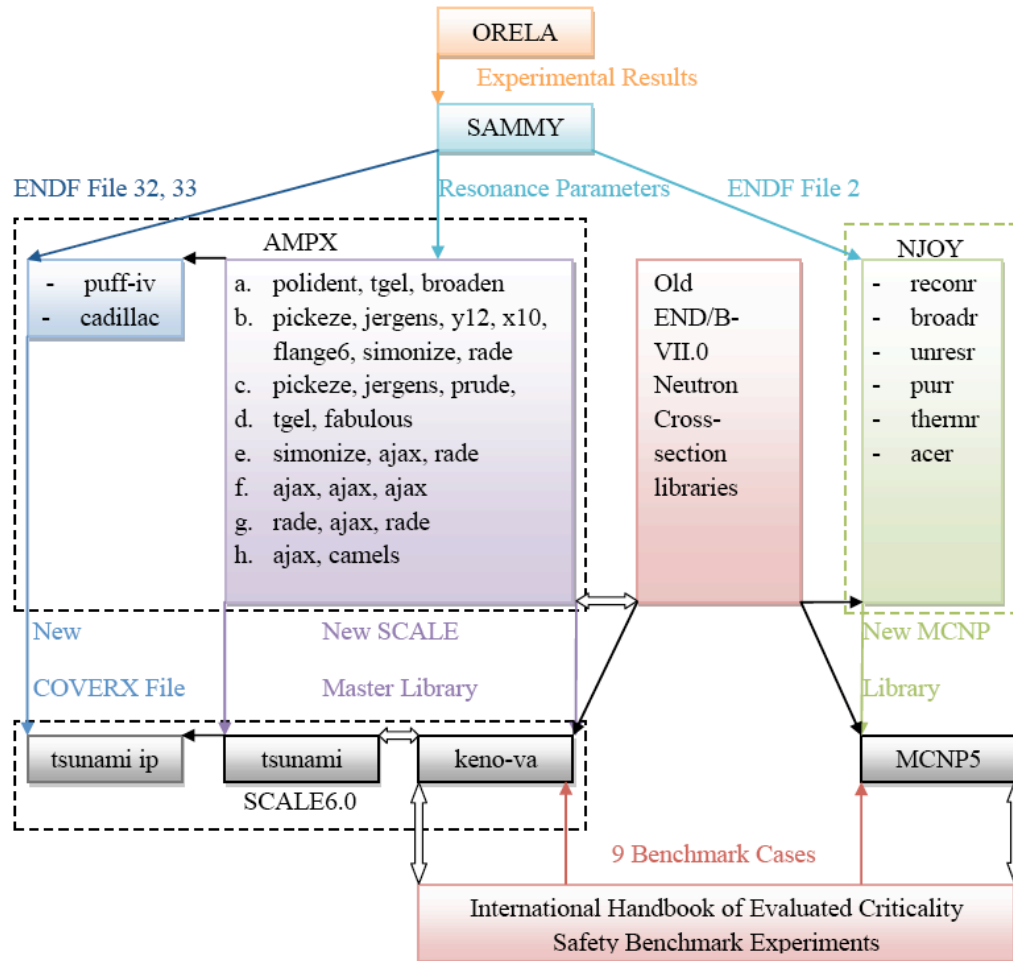
➤ Plots of ^{240}Pu cross-reaction correlation data (capture-elastic and capture-fission shown):



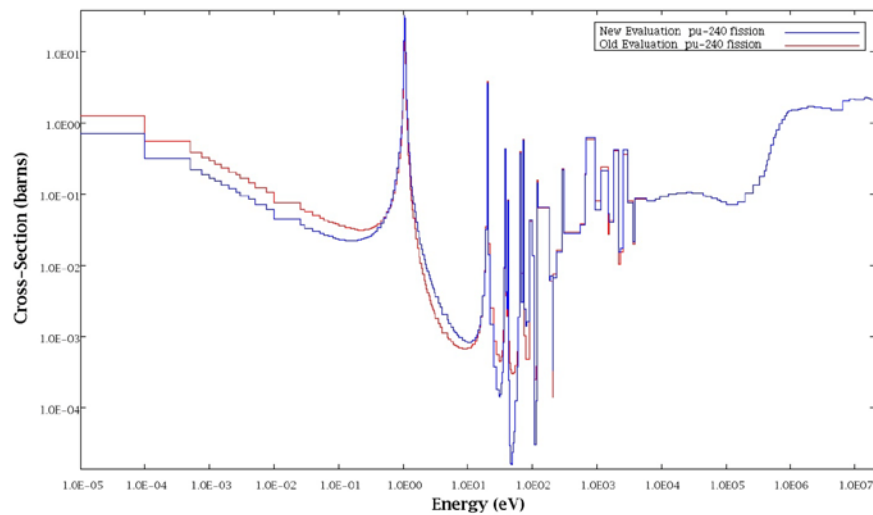
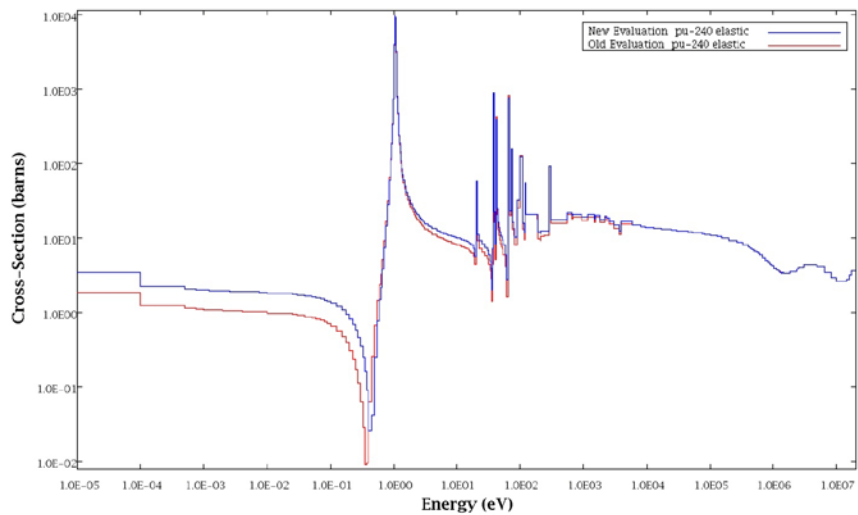
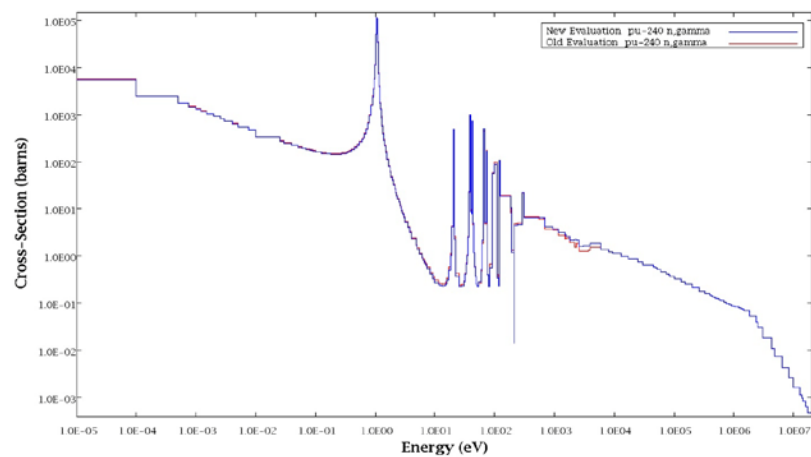
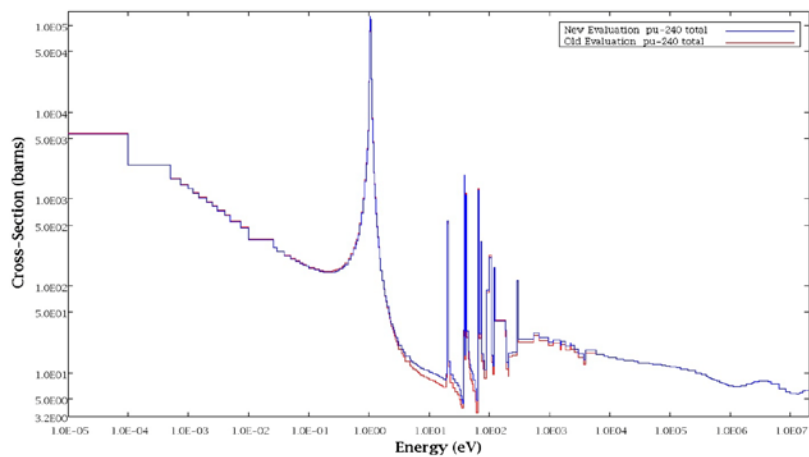
^{240}Pu Evaluation Testing—Vladimir Sobes (MIT)

➤ Testing Objectives

- Ensure new ENDF/B evaluation can be processed by AMPX (ORNL) and NJOY (LANL) cross-section processing code packages
- Generate cross-section libraries and covariance data libraries with new ^{240}Pu evaluation for use with MCNP5 and SCALE6.0
- Perform radiation transport simulation with ^{240}Pu data with emphasis on sensitivity/uncertainty analyses to assess the implications of the cross-section uncertainty data



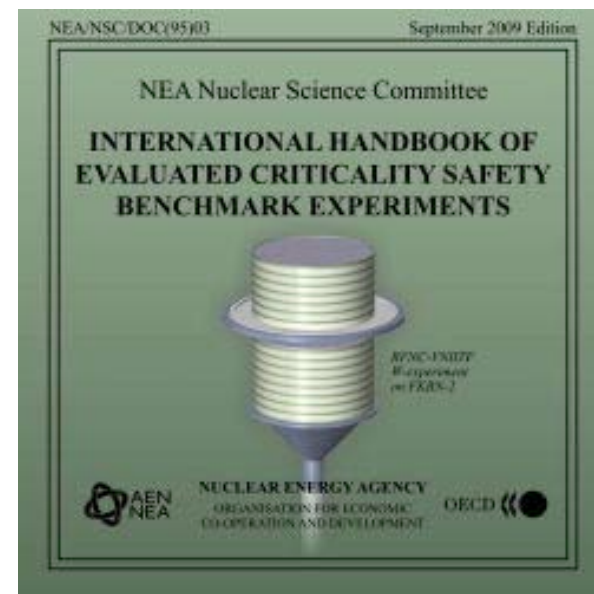
^{240}Pu Evaluation Testing—Vladimir Sobes (MIT)



^{240}Pu Evaluation Testing—Vladimir Sobes (MIT)

Name*	Abbreviated	Geometry
PU-SOL-THREM-018-001	181	Water Reflected 24-inch Diameter Cylinder of Plutonium (42.9% ^{240}Pu) Nitrate Solution
PU-SOL-THREM-001-006	106	Water Reflected 11.5" Diameter Sphere of Plutonium Nitrate Solution
PU-SOL-THREM-020-008	208	Water-Cadmium-Reflected 14" Diameter Spheres of Plutonium Nitrate Solution
PU-SOL-THREM-007-006	706	Water Reflected 11.5" Diameter Sphere of Plutonium Nitrate Solution
MIX-SOL-THERM-001-008	108	Mixed Plutonium and Uranium Nitrate Solution in Annular Geometry
MIX-SOL-THERM-007-007	707	Water-Reflected Plutonium-Uranyl Nitrate Solution Containing Gadolinium
MIX-COMP-THERM-008-001	801	Hexagonal Lattices of Mixed Oxide Fuel Pins – 2.0 Weight Percent PuO_2 , 24% ^{240}Pu , Natural Uranium
MIX-COMP-THERM-012-001	121	Polystyrene-Moderated, Mixed Oxide Slabs
MIT-MISC-THERM-004-001	401	Mixed Oxide Fuel Pin Lattices in Plutonium-Uranium Nitrate Solution

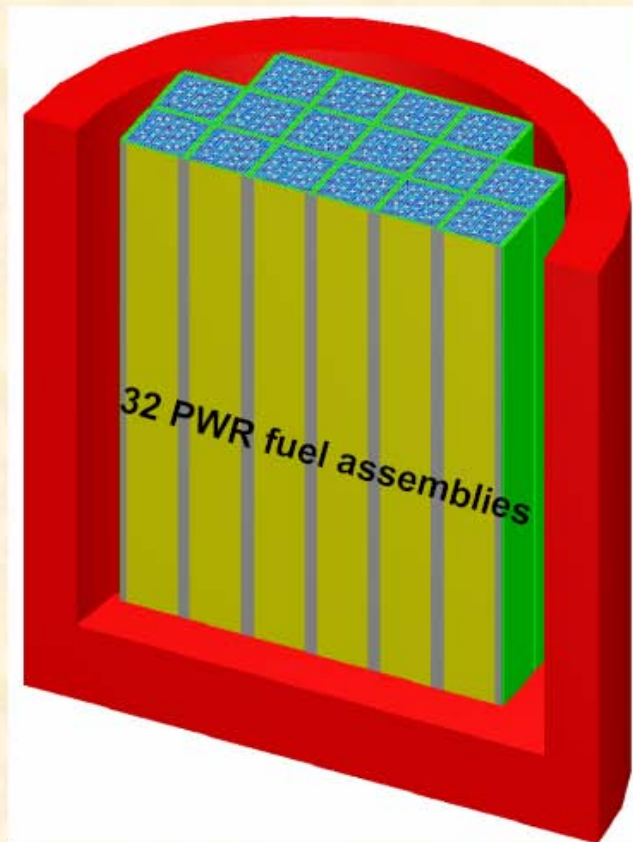
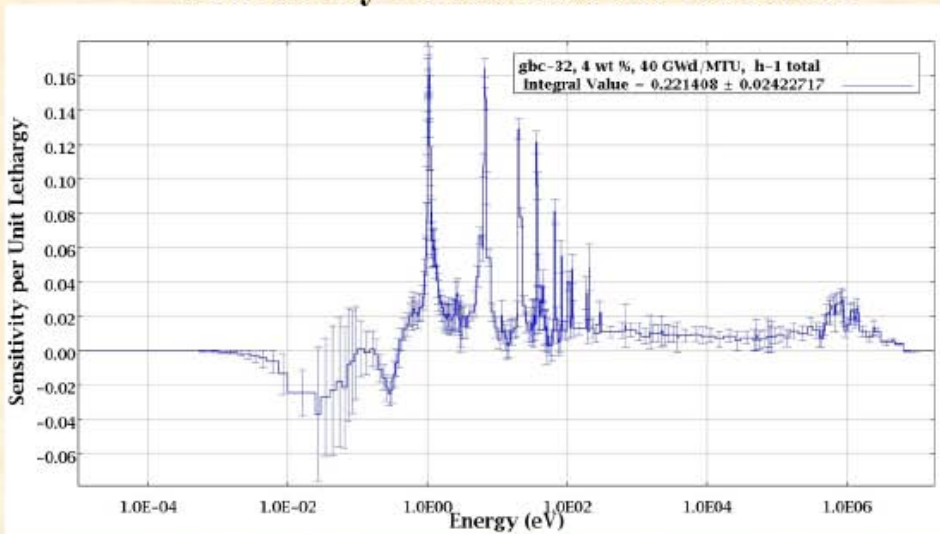
* PU=plutonium fuel, SOL=fuel is in solution, THERM=flux is thermal, COMP=fuel is in compound, MIX=mixed plutonium – uranium fuel, MISC=fuel is in miscellaneous form.



SCALE TSUNAMI Sensitivity/Uncertainty Analysis Capabilities

Monte Carlo Model for S/U Analysis of Spent-Fuel Cask

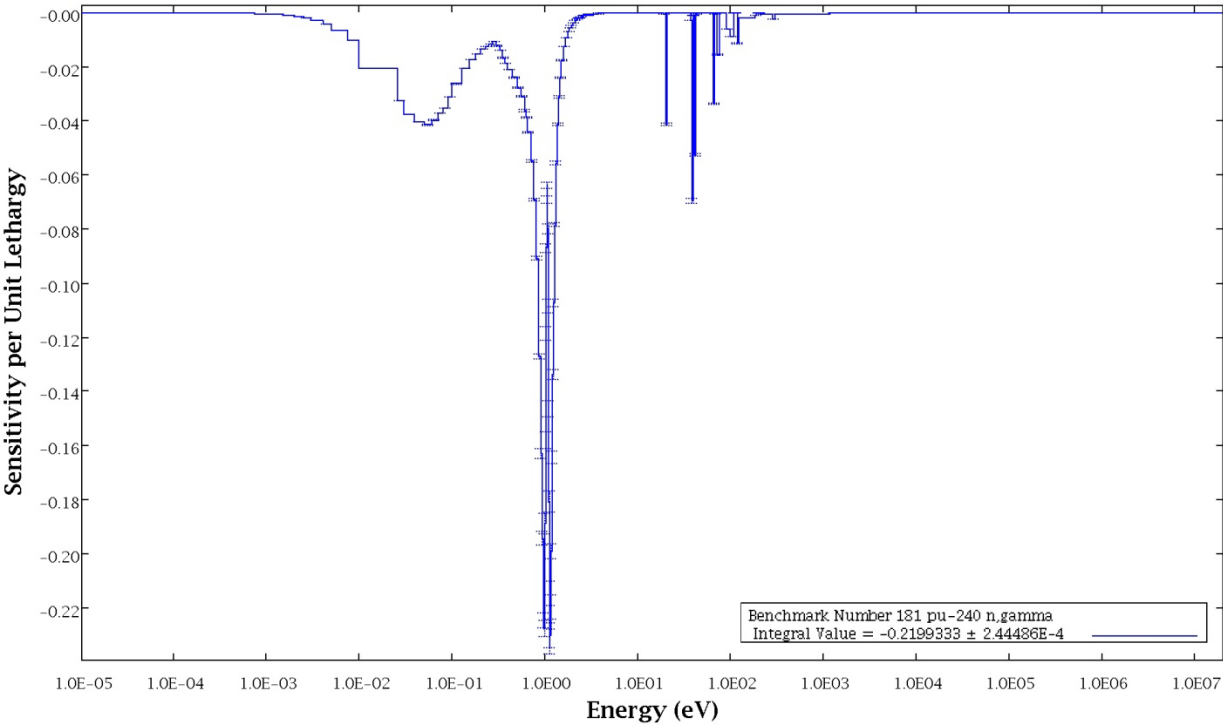
Sensitivity Coefficient for H Elastic



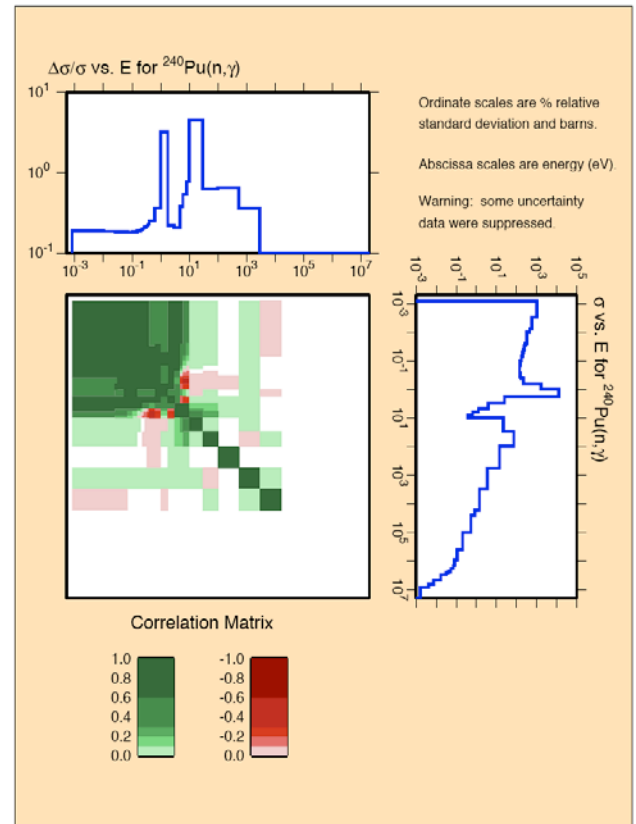
$$\text{Var}(k) \equiv \mathbf{S}^T \mathbf{C}_{\alpha\alpha} \mathbf{S}$$

complete sensitivity → \mathbf{S} $\mathbf{C}_{\alpha\alpha}$ ← *generic covariance*

^{240}Pu Evaluation Testing—Vladimir Sobes (MIT)



SCALE/TSUNAMI
Sensitivity of k_{eff} to
neutron capture as a
function of energy for
ICSBEP benchmark 181



^{240}Pu Evaluation Testing—Vladimir Sobes (MIT)

Benchmark Number	Benchmark Experiment	SCALE 6.0	
		K_{eff} with uncertainty due to all nuclear data	K_{eff} percent uncertainty due to ^{240}Pu
181	1.0000± 0.0034	1.026594± 0.009447	0.243255±6.88e-5
106	1.0000± 0.0050	1.011262± 0.012582	0.09411±2.119e-5
208	1.0000± 0.0059	0.996176± 0.014804	0.059456±9.16e-5
706	1.0000± 0.0047	1.000110± 0.013301	0.077286±1.72e-5
108	1.0000± 0.0016	0.995700± 0.014616	0.081768±2.15e-5
707	1.0000± 0.0034	0.993650± 0.011204	0.087090±3.00e-5
801	0.9997± 0.0032	0.997380± 0.012976	0.076146±1.67e-5
121	1.0052± 0.0067	0.973390± 0.013899	0.152742±4.58e-5
401	1.0000± 0.0030	1.001760± 0.009998	0.088589±2.40e-5

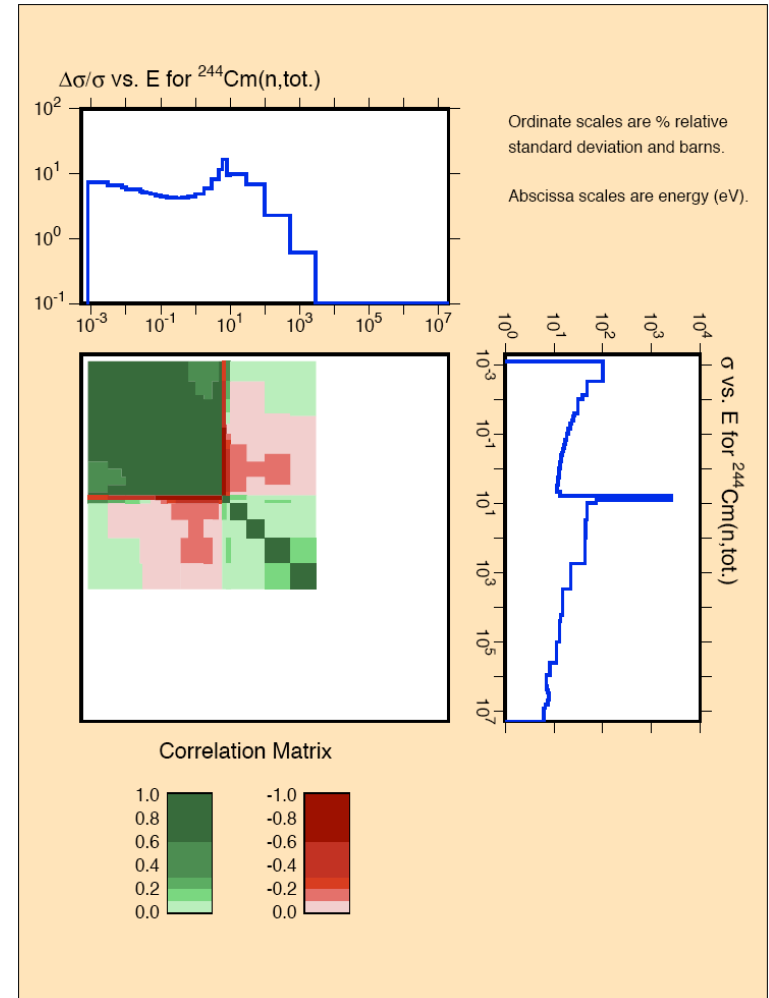
²⁴⁴Cm Assessment

		ENDF/B-VII.0	JEFF-3.1	JENDL-3.3
Evaluation		'95 T. Nakagawa and T. Liu	'78 Mann, Benjamin et al.	'95 T. Nakagawa and T. Liu
RRR		1.e-5 eV ~ 1 keV	1.0E-5 eV ~ 525 eV	1.0E-5 eV ~ 1 keV
URR		1 keV ~ 40 keV	525 eV ~ 10 keV	1 keV ~ 40 keV
Cross sections at 0.0253 eV (barn)	Total	27.23	17.97	27.23
	Elastic	11.09	7.0	11.09
	Fission	1.04	0.6	1.04
	Capture	15.10	10.37	15.10
Resonance Integrals (barn) (Spectrum : 1/E) (0.5 eV ~ 100 keV)	Total	1025.47	922.87	1025.47
	Elastic	359.78	318.90	359.78
	Fission	5.97	10.83	5.97
	Capture	659.47	592.90	659.47

- Most recent resonance evaluation is by Nakagawa and Liu (1995)—adopted in ENDF/B-VII.0 and JENDL-3.3
- JEFF 3.1 evaluation by Mann (1978)
 - Thermal cross-section data ~30% smaller than JENDL 3.3
 - Elastic and capture resonance integrals ~10% smaller than JENDL 3.3
 - Fission resonance integral is ~30% larger than JENDL 3.3

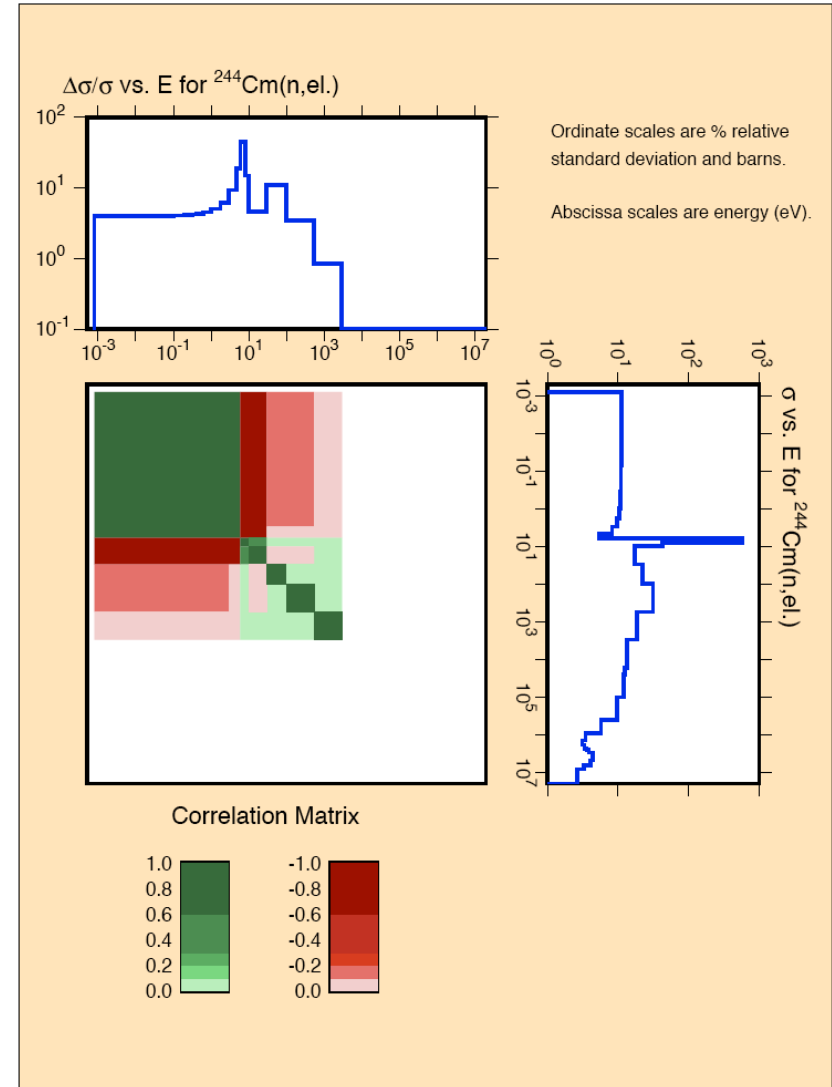
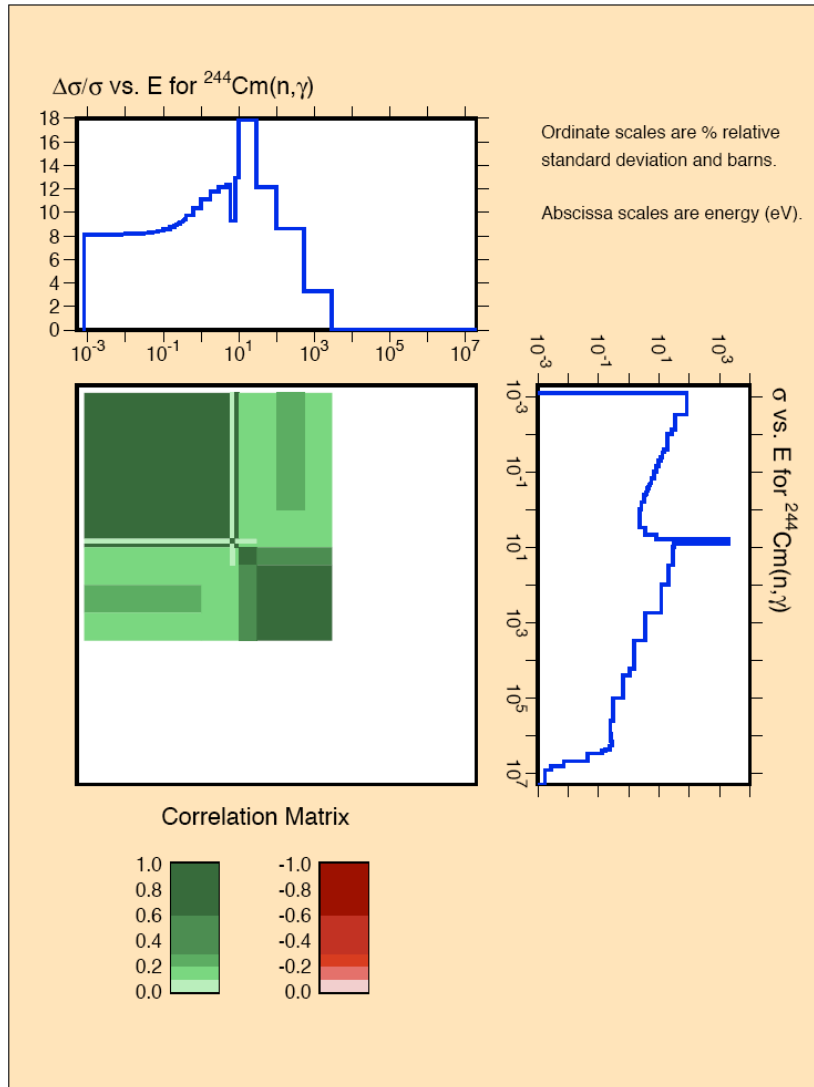
^{244}Cm Evaluation—work L. Leal

- Objective: provide resonance parameter covariance matrices while preserving existing resonance parameters in File 2
- “Retroactive” methodology used in SAMMY software to generate RPCMs in energy range 10^{-5} eV to 1 keV
- Current work JENDL 3.3 resonance parameters used in re-evaluation
- Atlas of Neutron Resonance Parameters used to provide uncertainties on thermal cross-section value and capture resonance integral
- Combined resonance evaluation work with high-energy evaluation work by KAERI



^{244}Cm Evaluation—work L. Leal

➤ Plots of PUFF-IV processed ^{244}Cm correlation data (capture and elastic shown):



ORNL-KAERI FY10 Highlights/Accomplishments

- Developed new ^{240}Pu cross-section evaluation
- MIT summer student completed preliminary testing with detailed report and paper for November ANS Meeting
- Plan to submit ^{240}Pu evaluation to NNDC in FY11 for release with ENDF/B-VII.1
- Completed covariance data evaluation for ^{244}Cm
- Published full paper on ORNL-KAERI collaboration at ND-2010 conference in Jeju, Korea (May 2010)
- ORNL-KAERI collaboration meeting at KAERI in May 2010



ORNL-KAERI FY10-11 Summary

- ORNL Milestones (September 30, 2010)
 - Complete preliminary nuclear data evaluations
 - Status report on cross-section evaluation effort
- Combine ORNL evaluation work with KAERI high-energy evaluation data
- Perform testing of preliminary evaluation files
- FY2011 Plan (Assumes full funding)
 - Complete evaluation effort and testing of new ORNL/KAERI evaluations
 - Deliver ^{237}Np , ^{240}Pu , ^{244}Cm to U.S. National Nuclear Data Center (NNDC) for release as ENDF/B files

Summary

- ORNL and KAERI initiated 3-year collaboration to provide improved nuclear data for AFC and nuclear safeguards applications
- Emphasis is on isotopes of benefit to fuel cycle and nuclear safeguards analyses
- ORNL/KAERI have been performing work to provide new cross-section evaluations with covariance data for ^{237}Np , ^{240}Pu , and Cm isotopes (i.e., including ^{244}Cm)
- On pace to deliver ^{240}Pu and ^{244}Cm evaluations to NNDC in FY11
- Final data product will greatly facilitate radiation transport modeling and simulation effort that will benefit nuclear safeguards R&D efforts