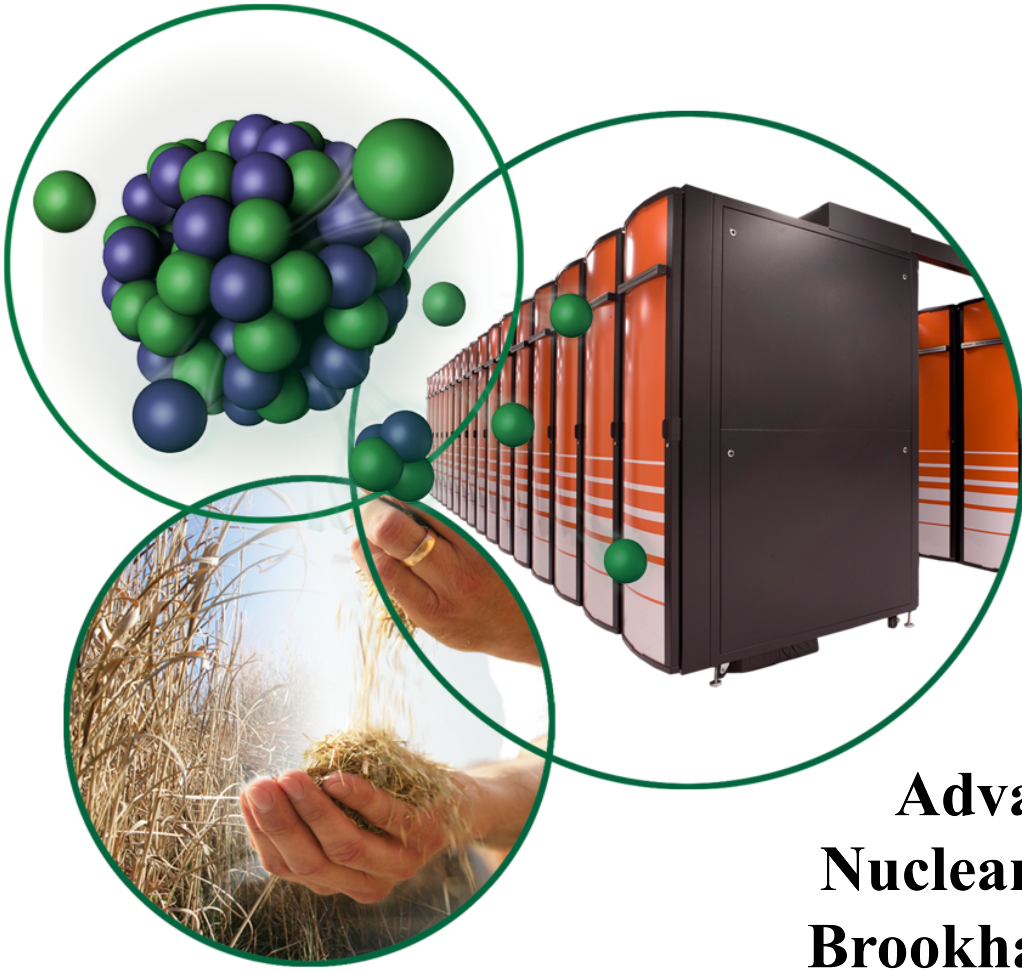
^{239}Pu Resonance Region Evaluation



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Advance Fuel Cycle R & D
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Nuclear Data Analysis and Evaluation

- **Why needed?**

  It provides directions for theoretical studies:

✓ Nuclear reaction theory is not rigorous and requires models:
Reaction theory is developed based on experimental results used in data evaluation

✓ Standard for Nuclear Data Evaluations:
Nuclear reaction theory cannot predict accurate absolute values

✓ Resonance Data Information:
Resonance properties cannot be described without experimental data and data evaluation

Nuclear Data Analysis and Evaluation

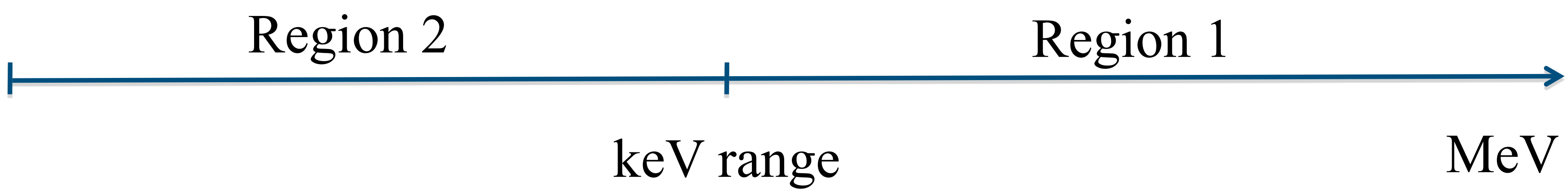
- Why needed?

✓ Provide an accurate representation of the underlying physical process in a form suitable for applications

✓ Evaluated nuclear data rather than raw experimental data are used in nuclear applications such as the design of nuclear energy systems

✓ Reduced number of information is needed to reproduce the actual data

Nuclear Data Analysis and Evaluation



- Region 1: High-energy neutrons – direct and compound nucleus formation

- Region 2: Resonance region (resolved and unresolved)

Differential and Integral Data

Differential Data:

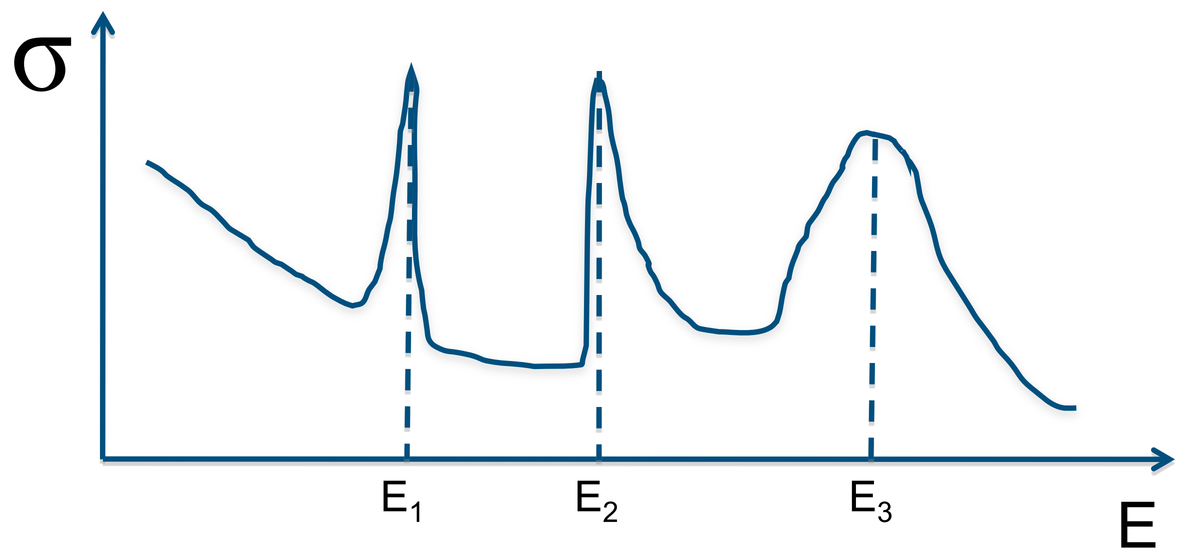
- Neutron birth is known
- Measured on Time-of-Flight (TOF) accelerators (ORELA, GELINA, RPI/Gaerttner)
- Neutron Cross Section: smoothly varying data in pointwise tabulations, angular distributions, resonance parameters and thermal scattering kernels
- Pulsed neutron source allows measurements to be made in a wide energy range: 0.001 eV to 80 MeV
- Pulsed neutron source reduces background
- TOF resolution allows to distinguish individual resonances

(a) Resolved Energy Region:

Experimental resolution is smaller than the width of the resonances; resonances can be distinguished ("seen"). Cross section representation can be made by resonance parameters.

Cross section formalisms:

General R-matrix derived formalisms such as the Single-Level Breit-Wigner, Multi-Level Breit-Wigner, Adler-Adler, Reich-More, Multipole, etc.



Derived R-Matrix Formalisms

R-Matrix

- **Single-Level Breit-Wigner** (Wigner-Eisenbud)
- **Multi-Level Breit-Wigner** (Wigner-Eisenbud)
- **Adler-Adler** (Kapur-Peierls)
- **Reich-Moore** (Wigner-Eisenbud)
- **Multipole** (Kapur-Peierls)

(b) Unresolved Energy Region:

Cross section fluctuations still exist but experimental resolution is not enough to distinguish multiplets. Cross section representation made by average resonance parameters.

Cross section formalism:

Statistical models such as the Hauser-Feshbach model combined with Optical model; level density models based on Bethe theory or Gilbert and Cameron theory, etc.; fission widths model based on Hill-Wheeler fission barrier penetration theory; giant dipole mode for gamma capture widths, etc.

(c) High Energy Region:

No cross section fluctuations exist. Cross sections are represented by smooth curves.

Cross section formalism:

Statistical models such as the Hauser-Feshbach model; intra-nuclear Cascade model; pre-equilibrium model; evaporation model, etc.

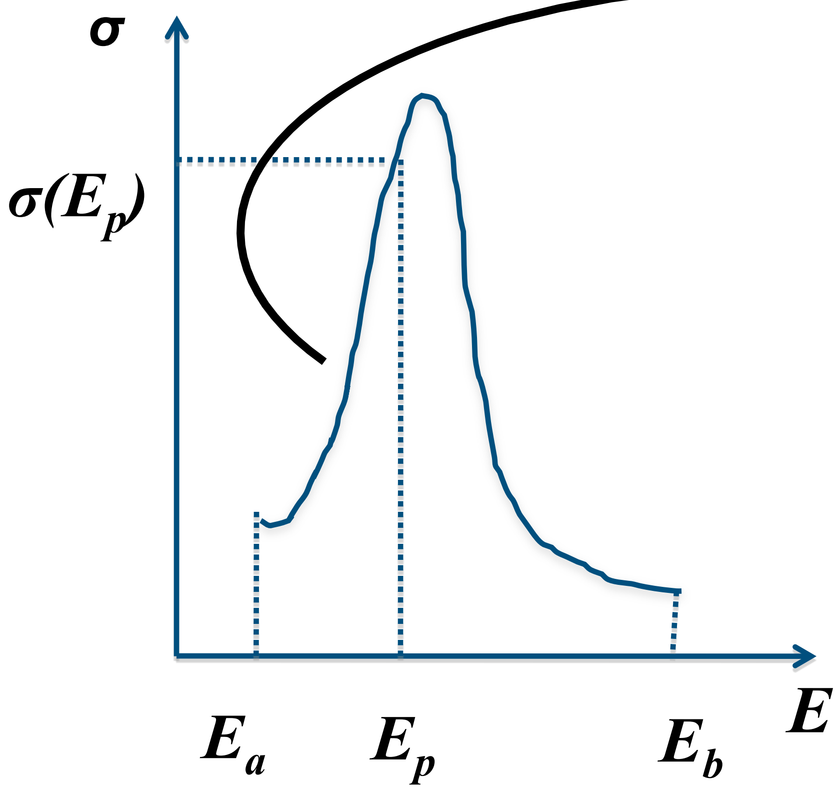
Integral Data

Ultimate Goal is to Check and Validate Evaluated Nuclear Data and Methods

- Neutron birth of neutron inducing event is unknown
- Can only obtain data integrated over neutron energy
- Sub-critical and critical assembly measurements: reaction rates, number of neutrons per fission, reactivity worth
- Decay constants for radioactive actinides and fission products for use in spent fuel reactivity analysis
- Provide excellent grounds for testing the differential data
- Integral quantities average over energy, space and angle

Simultaneous differential and integral data analysis and evaluation are necessary to remove bias on the data

Differential and Integral



σ(E) as a function of energy

Differential

$$R = \int_{E_a}^{E_b} \sigma(E)\varphi(E)\,dE$$

R **is the reaction rate (measured quantity)**

Integral

Motivations for a New ^{239}Pu Evaluation

- Existing resonance parameter (RP) representation done with three disjoint resonance parameter sets 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);

  New evaluation: single resonance parameter set covering the energy range 1.0×10^{-5} eV to 2.5 keV

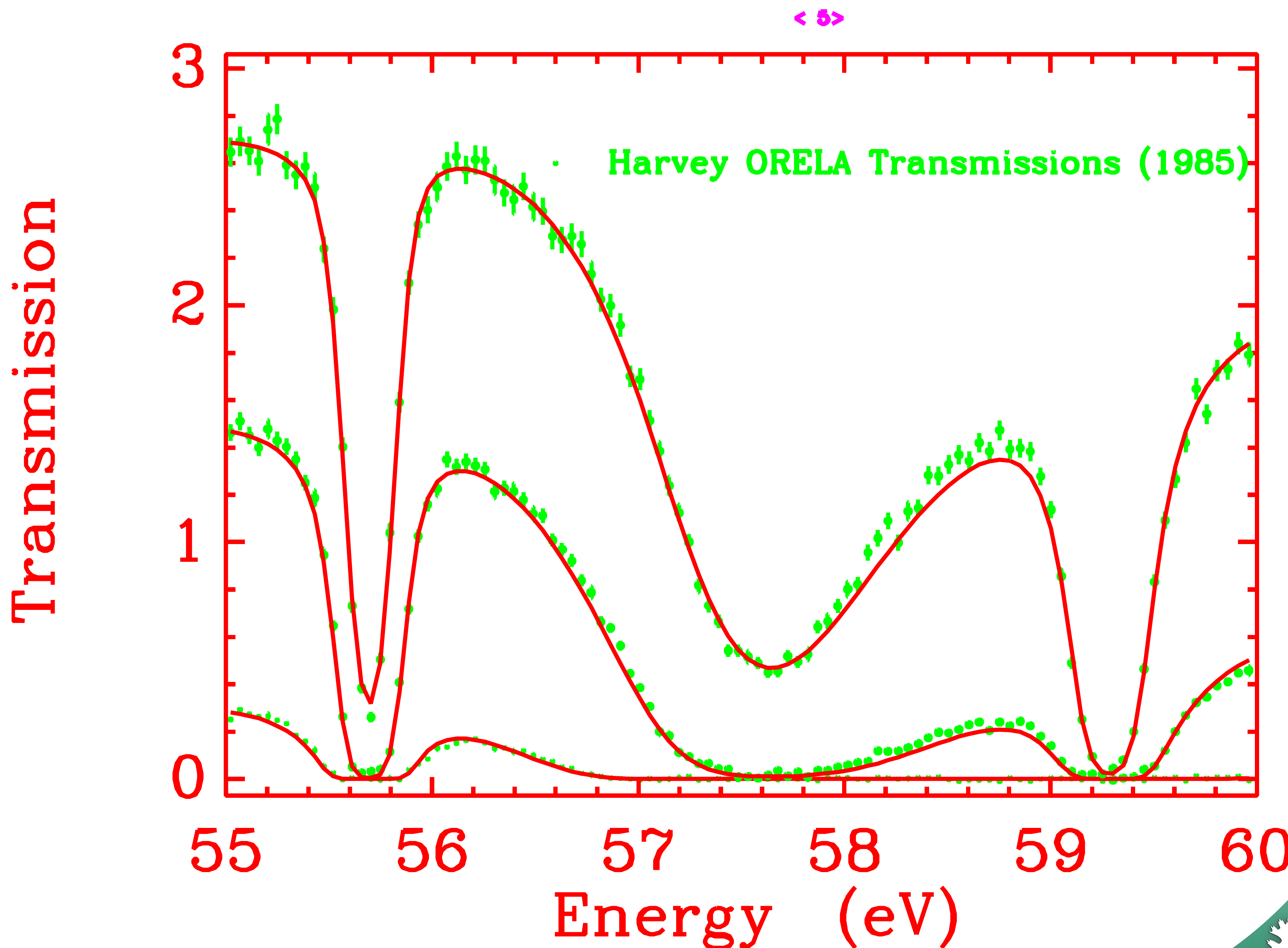
- Resonance parameter covariance generated

- Solve a long standing problem for thermal benchmark prediction;

Experimental Data Sets Used in the RR Evaluation

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

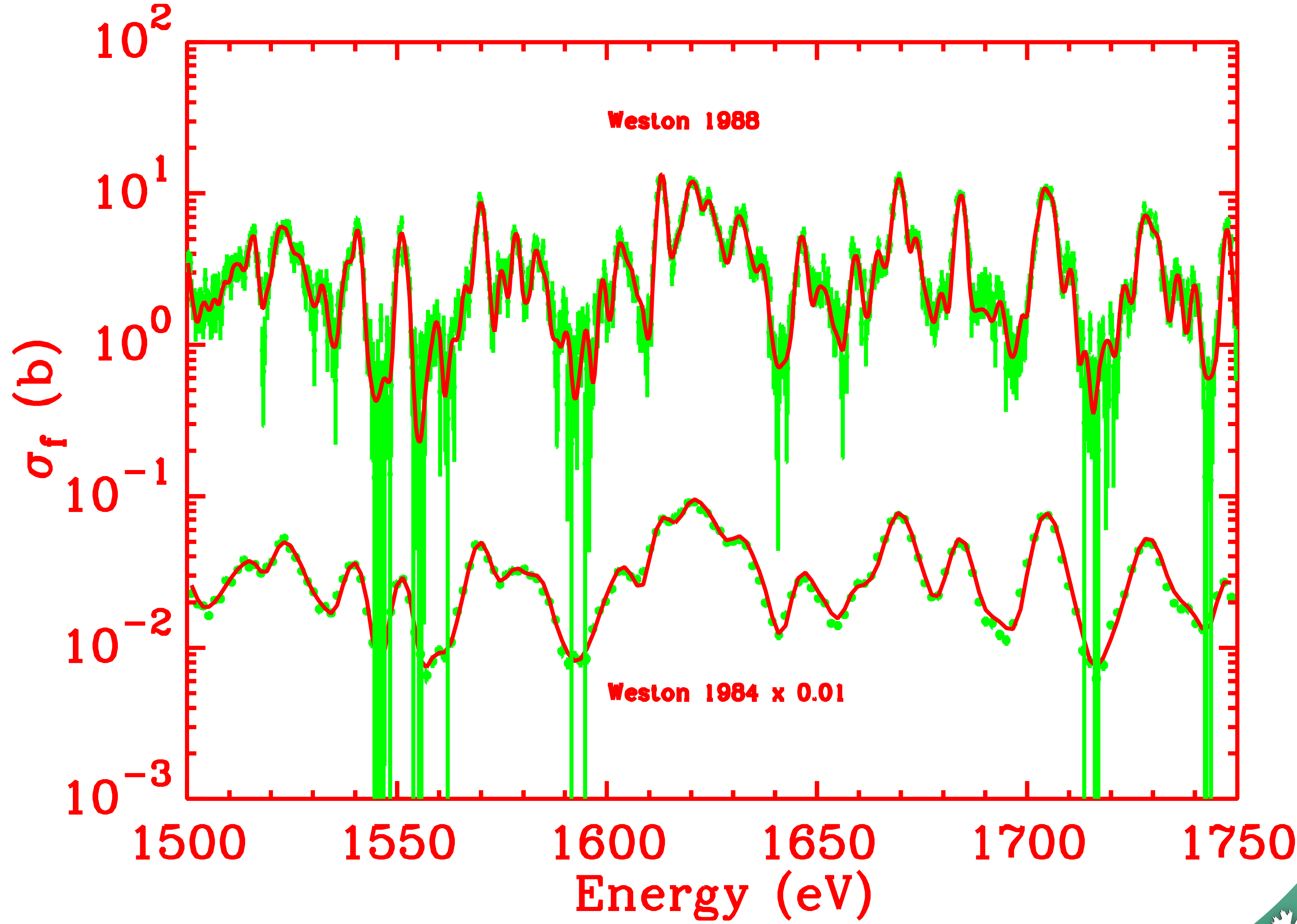
^{239}Pu Resonance Evaluation



paradigm shift

OAK RIDGE National Laboratory

^{239}Pu Resonance Evaluation



Effective System Multiplication Factor: k_{eff}

$$\frac{\mathrm{Pr}\,oduction}{Absorption + Leakage}$$

k_{eff}

$\rightarrow$ > 1 (supercritical)

$\rightarrow$ = 1 (critical)

$\rightarrow$ < 1 (subcritical)

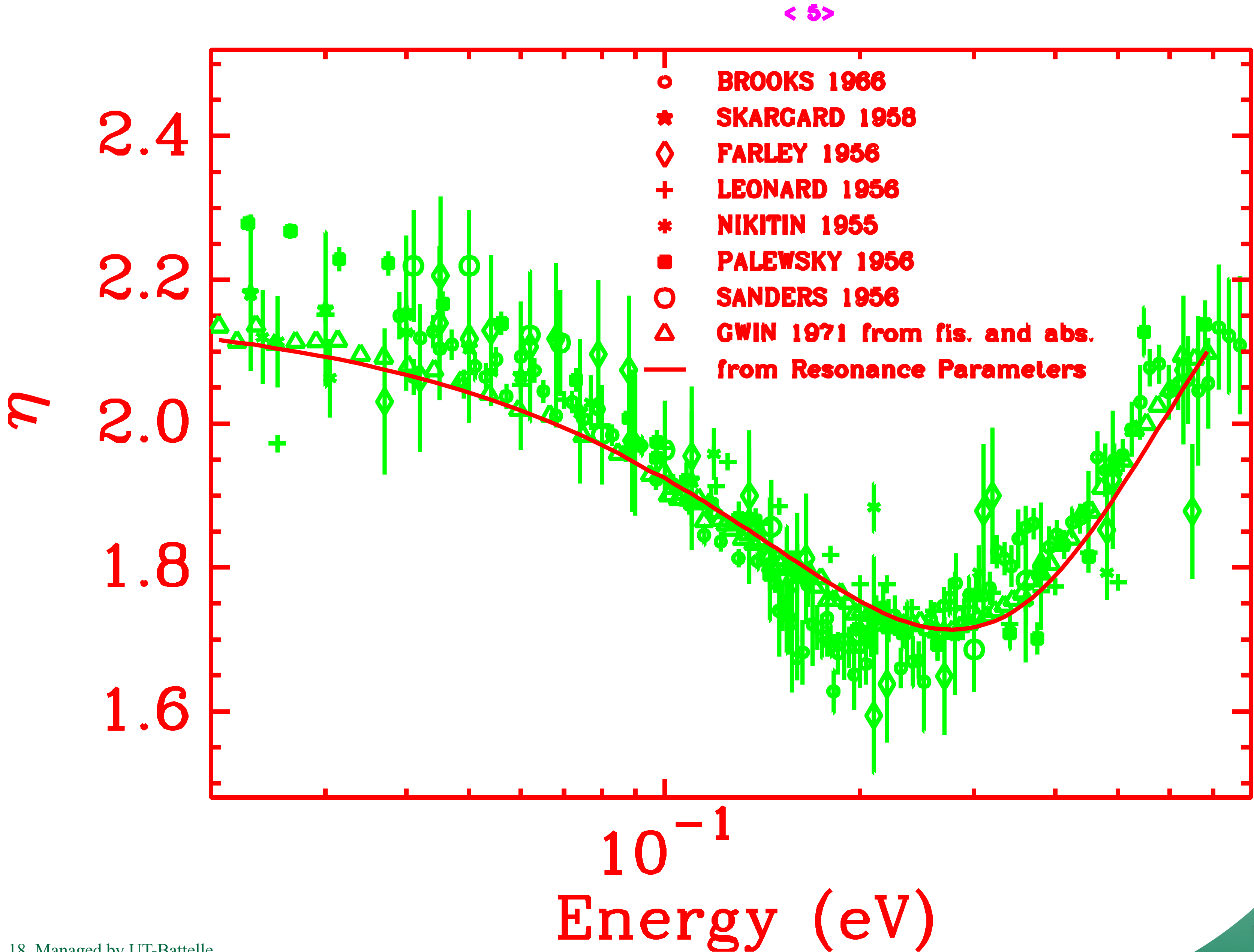
Multiplication Factor: k_∞

$$Leakage \longrightarrow 0$$

$$\frac{\mathrm{Pr}\,oduction}{Absorption}$$

$$k_\infty \propto \eta = \frac{\nu\sigma_f}{\sigma_a}$$

^{239}Pu Resonance Evaluation



paradigm shift

Issues with ORNL Evaluation

- Results of plutonium solution calculations indicate no improvement using ORNL evaluation. Longstanding problem persists!!

- Review of the ^{239}Pu is underway

- Parts involved are:

ORNL, LANL, CEA and others!!

International Community Effort:

- Working Party on International Evaluation Co-operation (WPEC) subgroup created

✓ Objective: Address issues on the discrepancies of Pu-SOL-THERMAL assemblies and Pu-INTER assemblies calculations

✓ Strategy

  – Use New Leal/Derrien ENDF resonance evaluation and covariance

  – Use sensitivity analysis tools to indentify which parameters are important on both differential and integral data adjustment

✓ Goal: obtain a ^{239}Pu resonance evaluation that :

  – Represent the differential data well,

  – leads to improvements in calculations of integral data

Effective Work

- Choice of benchmark problems :
  – Define a set of benchmarks sensitive to ^{239}Pu nuclear data from ICSBEP and IRPhEP.

    Common Benchmarks : ICSBEP ^{239}Pu benchmark systems
    Water-Reflected and bare spheres of plutonium nitrate solutions

    Intermediate and fast Benchmarks will be added

  ORNL/CEA

  – Perform calculations of these benchmarks with various evaluations (ENDF, JEFF, JENDL) using Monte-Carlo and Deterministic codes

  Skip Kahler of LANL indentified a subset of 15 Pu-Sol-Therm benchmarks in the ICSBEP that can be used to address the problem.

^{239}Pu Data Sensitivity and Adjustment at ORNL

✓Use ^{239}Pu resonance evaluation with covariance done at ORNL

✓Process the evaluation with the AMPX/PUFF code system to generate group cross sections and covariance

✓44-neutron group structure of the SCALE system was used

✓ 15 ICSBEP ^{239}Pu benchmark calculations

- Thermal water reflected benchmark experiments were used

✓ Sensitivity calculations were done with the TSUNAMI code

✓ Data adjustments were done with the TSURFER code

TSUNAMI Analysis for Cross-Section Evaluations

- TSUNAMI S/U capability invaluable tool for cross-section evaluation
  - Provides improved understanding of nuclear data physics for specific applications
  - Identify parameters and energy regions of importance

$$S = \frac{\sigma_x}{k}\frac{\partial k}{\partial \sigma_x} \quad \textbf{and} \quad V = S\,C\,S^t$$

- TSUNAMI used in support of the NCSP and DOE/RW fission program
  - Nuclear Data evaluator performs sensitivity analysis of critical experiment to understand the physics of the problem and identify energy regions that are "exercised" by the criticals

Consolidation of
Computed and Measured Responses
Using <u>Generalized Linear Least-Squares</u> (GLLS)

- GLLS consolidates calculations with measured responses
- Computes "best" data adjustments to eliminate differences
- Results in more consistent results with lower uncertainties
- Propagation of data adjustments to a proposed design system provides computational bias and uncertainty

Application of GLLS to Data Adjustment

M-dimensional discrepancy vector:

$$d(\alpha, K_m) = K_c(\alpha) - K_m$$

computed measured

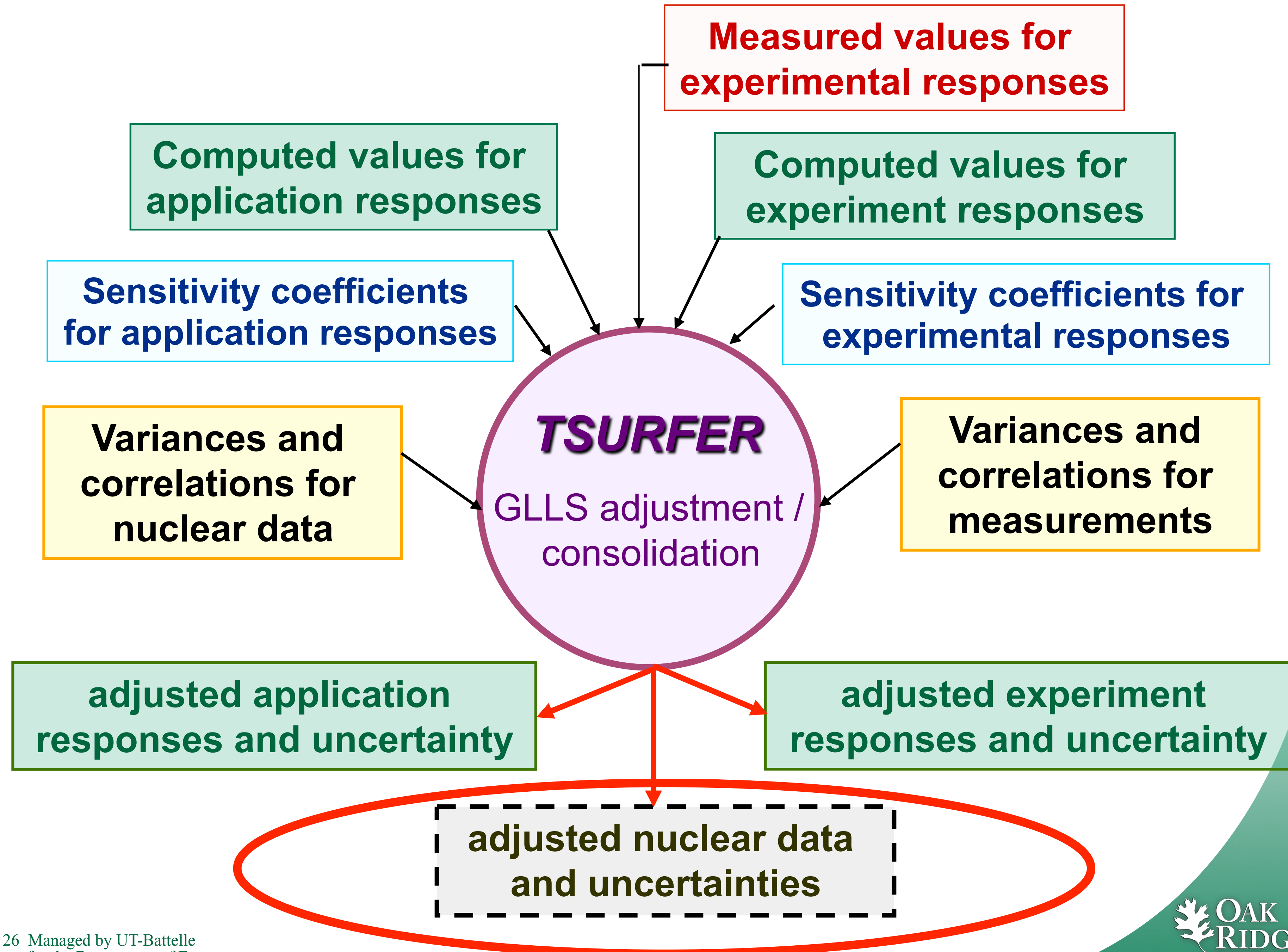
GLLS determines modified nuclear data α' and measured responses K'_m such that . . . .

- Discrepancy vector $d(\alpha', K'_m) \rightarrow 0$
- Uncertainties/correlations in α and K_m (i.e., $C_{\alpha\alpha}$ and C_{mm} respectively) are taken account
- Overall consistency maximized by minimizing chi-squared:

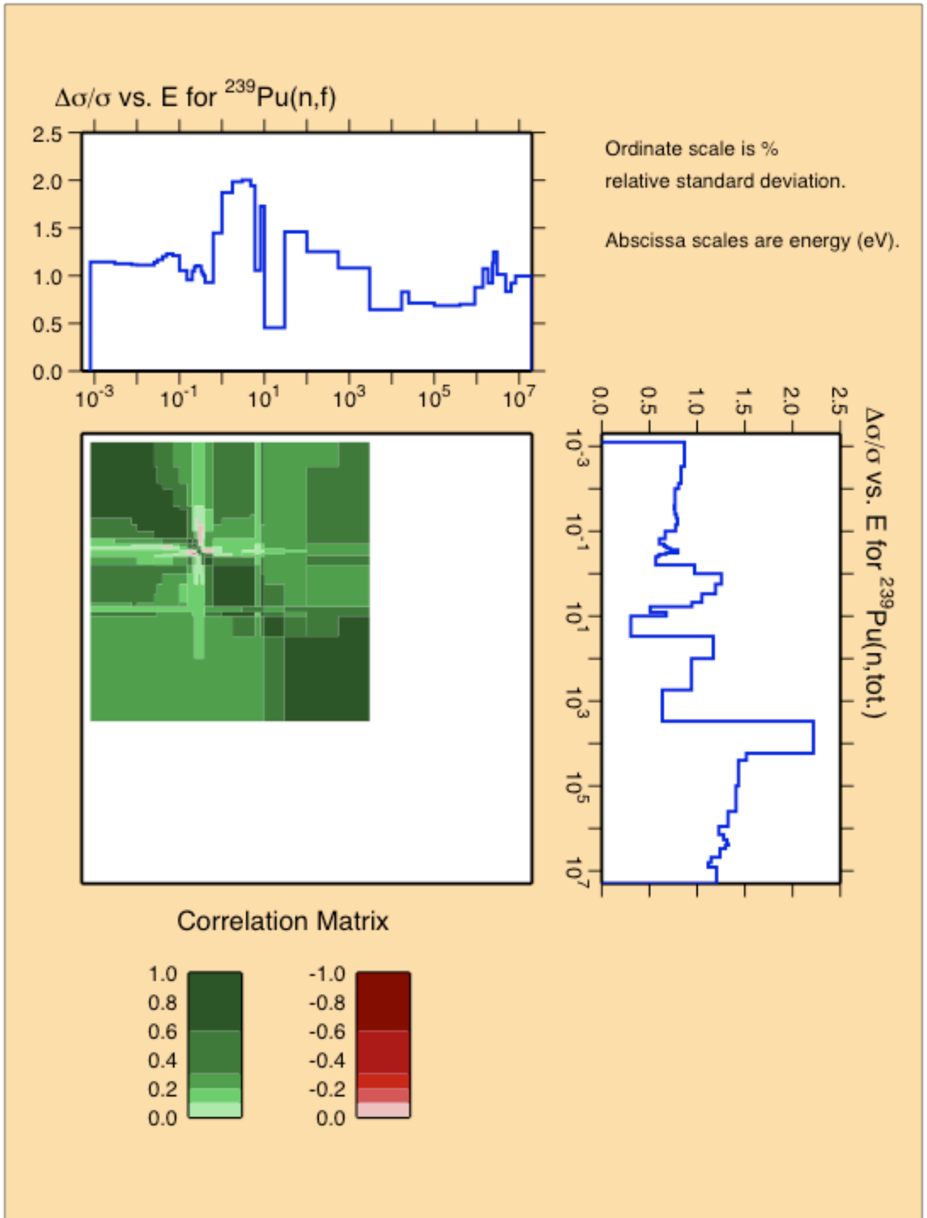
$$\chi^2 = [\alpha' - \alpha]^T [C_{\alpha\alpha}]^{-1} [\alpha' - \alpha] + [K'_m - K_m]^T [C_{mm}]^{-1} [K'_m - K_m]$$

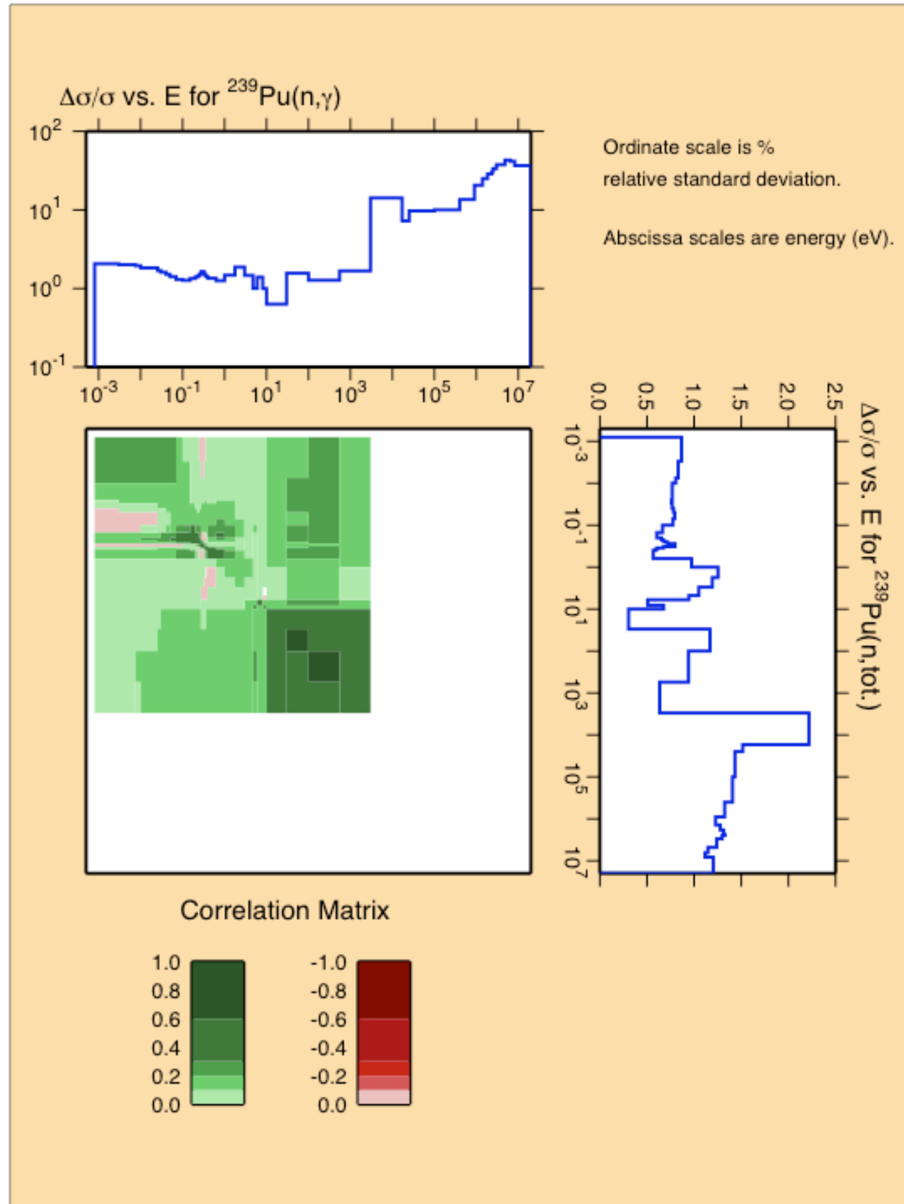
overall adjustments to data, in units of variance

overall adjustments to measurements, in units of variance

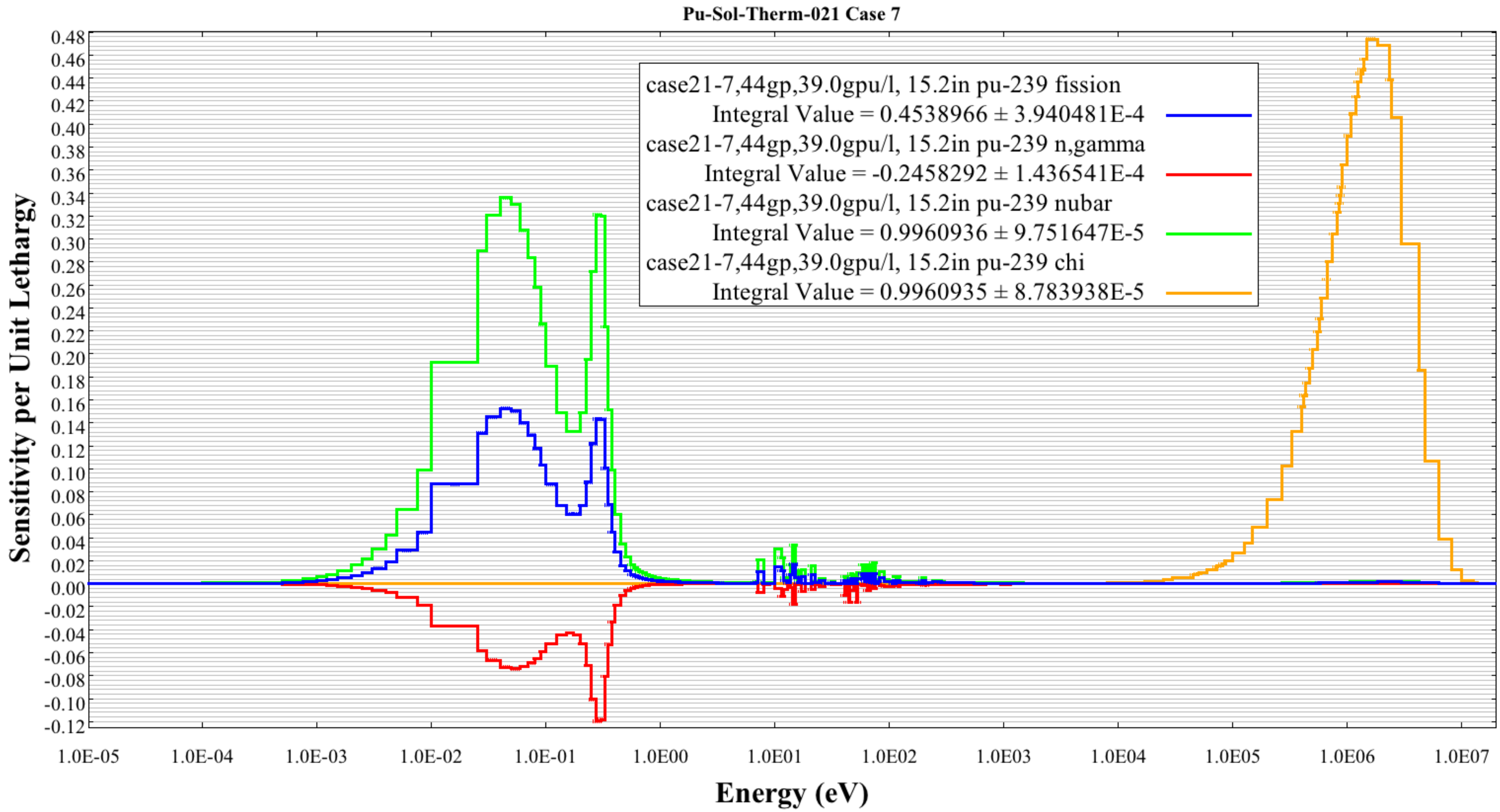

Measured values for experimental responses
Computed values for application responses
Computed values for experiment responses
Sensitivity coefficients for application responses
Sensitivity coefficients for experimental responses
TSURFER
GLLS adjustment / consolidation
Variances and correlations for nuclear data
Variances and correlations for measurements
adjusted application responses and uncertainty
adjusted experiment responses and uncertainty
adjusted nuclear data and uncertainties

Covariance Work
^{239}Pu ORNL fission/capture estimation



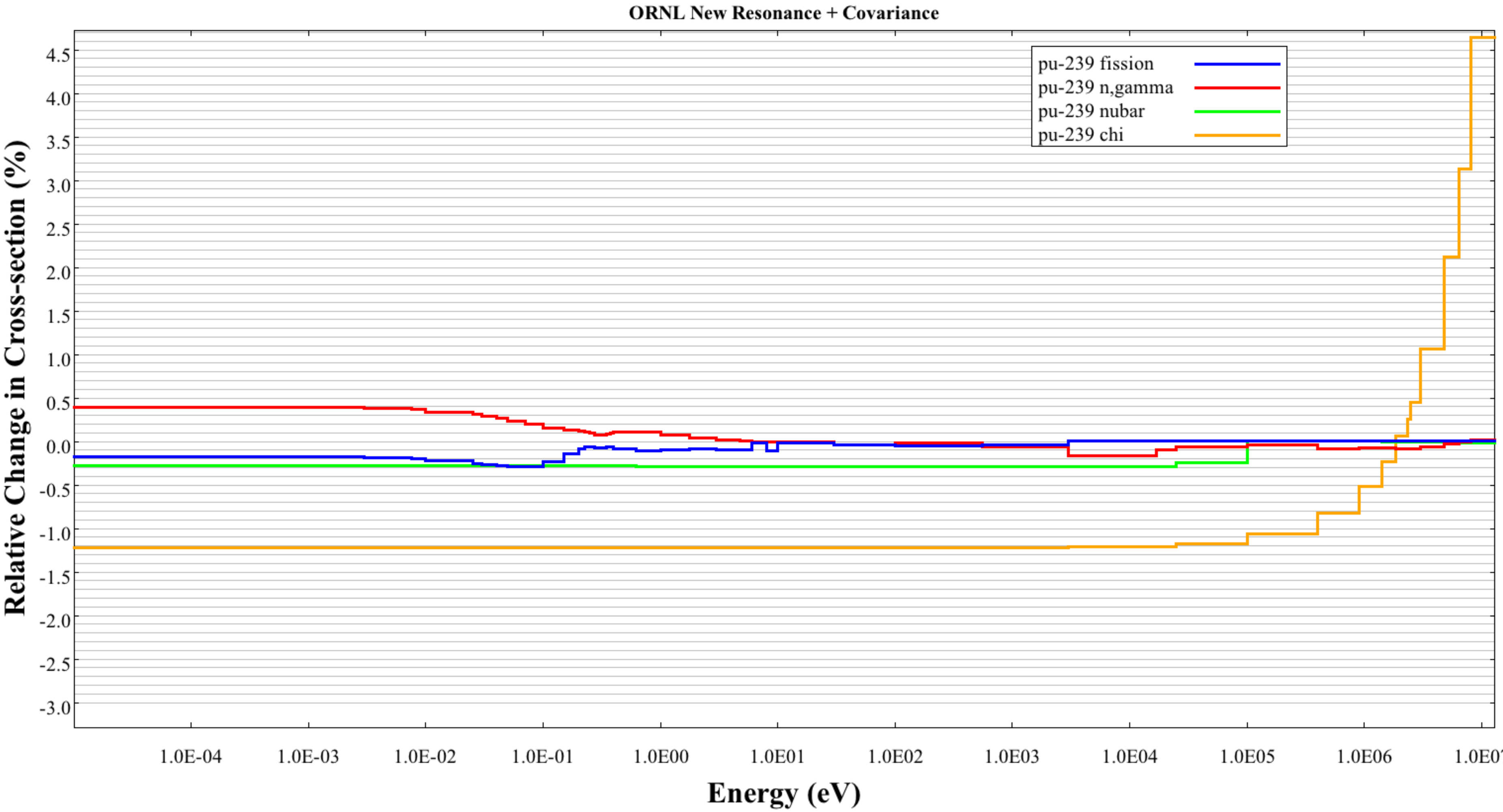


Benchmarking/Integral Data feed-back
^{239}Pu Data Sensitivity and Adjustment at ORNL



ORNL ^{239}Pu sensitivity calculations of the cross section to k_{eff} (TSUNAMI)

Benchmarking/Integral Data feed-back
^{239}Pu Data Sensitivity and Adjustment at ORNL



ORNL ^{239}Pu data adjustment for the fifteen benchmark experiments (TSURFER)

ORNL and CEA/Cadarache Work

ORNL/CEA

- Use of sensitivity analysis (combine Microscopic and Integral experiments) to help improvement of nuclear data
  - KENO/TSUNAMI/TSURFER Code at ORNL
  - ERANOS/SNATCH/CONRAD Code at CEA

ORNL/CEA

- Calculate effects of using Maslov PNFS

CEA work on the effect of ^{239}Pu PNFS on Benchmarks

- Calculations performed with TRIPOLI-4 Release 4.6
- Maslov ^{239}Pu prompt fission neutron spectra replacement in ^{239}Pu JEFF-3.1.1 evaluation file
  - Personal communication June 2009
- ICSBEP PU-SOL-THERM 001 and Pu-MET-FAST benchmarks
  - MCNP data file automatic conversion
  - TRIPOLI-4 – MCNP4C3 k_{eff} calculations checks

CEA work on the effect of ^{239}Pu PNFS on Benchmarks

PU-SOL-THERM 001

- Water reflected 11.5 inch diameter spheres of plutonium nitrate solutions

	TRIPOLI4 Result CEA2005	σ	TRIPOLI4 Result CEA2005 MASLOV	σ	Discrpancy MASLOV	σ
1.T8A	1,00252	47	1,00587	45	335	65
2.T8A	1,00374	48	1,00755	48	381	68
3.T8A	1,00631	46	1,01066	48	435	66
4.T8A	1,00137	47	1,00575	46	438	66
5.T8A	1,00446	48	1,00923	49	477	69
6.T8A	1,00779	50	1,01061	48	282	69
				MIN	282	
				MOY	391	
				MAX	477	

CEA work on the effect of ^{239}Pu PNFS on Benchmarks

PU-MET-FAST

- Bare spheres of Pu (001, 002)
- Reflected spheres of Pu (005 W, 008 Th, 009 Al, 010 U, 011 Water, 018 Be)

		TRIPOLI4 Result CEA2005	σ	TRIPOLI4 Result CEA2005 MASLOV	σ	Discrepancy MASLOV	σ
001	1	1,00002	8	0,99936	8	-66	11
002	1	1,00435	8	1,00320	8	-115	11
005	1	1,00404	9	1,00376	9	-28	13
008	1	1,00170	9	1,00108	9	-62	13
009	1	0,99936	8	0,99881	8	-55	11
010	1	1,00255	8	1,00186	8	-69	11
011	1	0,99723	11	0,99735	10	12	15
012	1 s	1,00524	10	1,00418	10	-106	14
013	1 s	1,00644	11	1,00629	11	-15	16
014	1 s	1,00185	11	1,00166	11	-19	16
015	1 s	1,00230	11	1,00147	0	-83	11
018	1	0,98385	8	0,98393	8	8	11
					MIN	-115	
					MOY	-50	
					MAX	12	

Concluding Remarks

✓ Benchmark experiments sensitive to the fission, capture cross sections, nu-bar and prompt neutron fission spectrum (PNFS)

✓ A right combination of capture-to-fission ratio (alpha) may lead to an improvement on the k_{eff};

✓Further studies are needed using new PNFS evaluations;

Scheduled Work

✓ Finalize a document related to Benchmark list and calculations

✓ Few weeks of intensive work between CEA/ ORNL in 2012 on the evaluation benchmark calculations

✓New PNFS evaluations to be tested (JEFF/ ENDF)

✓ Other Contributions from other Projects are welcomed