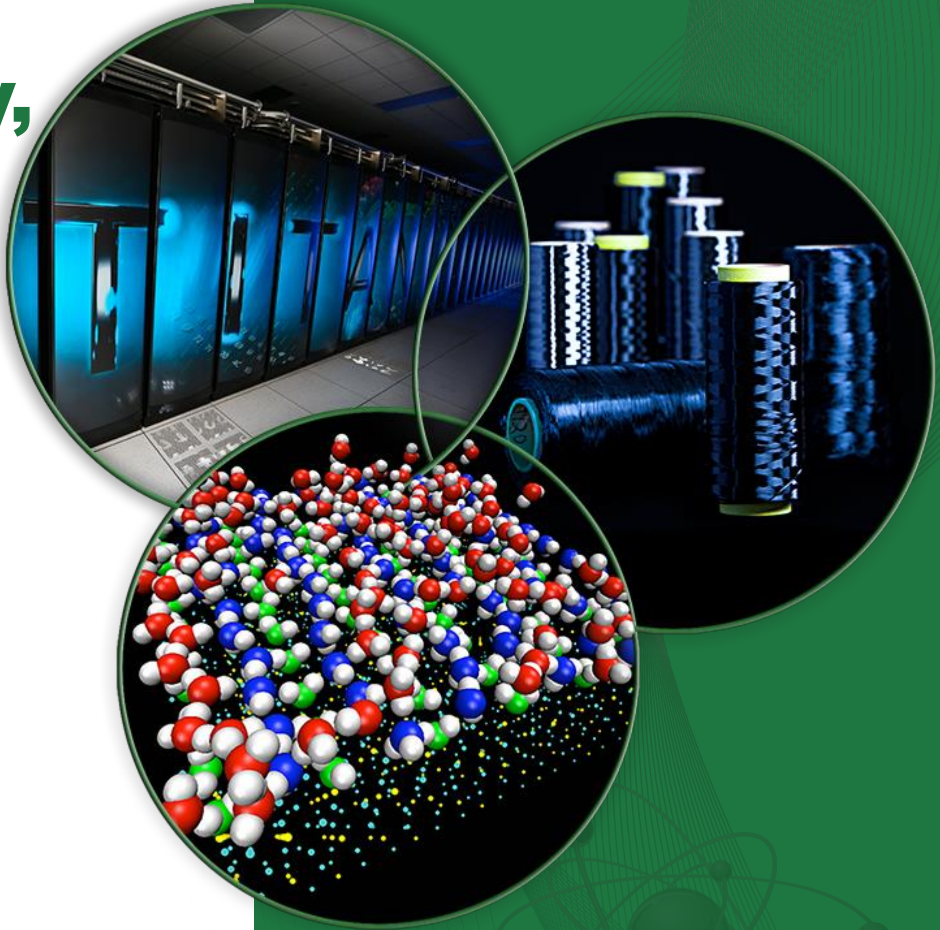
Nuclear Data Uncertainty Quantification for Applications in Energy, Security, and Isotope Production



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Workshop on Nuclear Data Needs and Capabilities for Applications
Berkeley | 27-29 May 2015

Outline

- Data needs in nuclear energy, with cross cutting applications to safeguards and isotope production
- Spent fuel safeguards nuclear data roadmap project
- Quantitative approaches to data evaluation
- Tools for uncertainty analysis
- Covariance data
- Experimental benchmarks
- Examples of data needs

Applications and Data

Applications

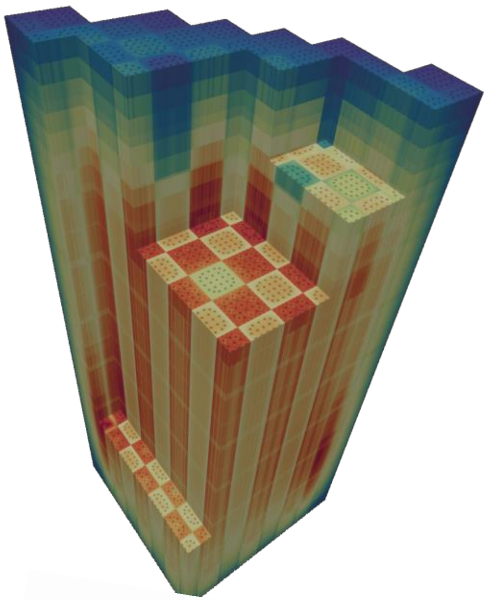
- Nuclear energy (safety)
- Safeguards and security
- Isotope production
- Non proliferation
- Nuclear forensics

Nuclear Data

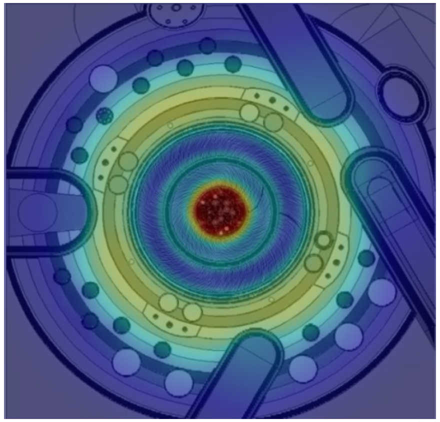
- Cross sections
- Nuclear decay data
- Fission product yields
- Neutron emission
- Gamma emission
- Multiplication and multiplicity
- Covariance information

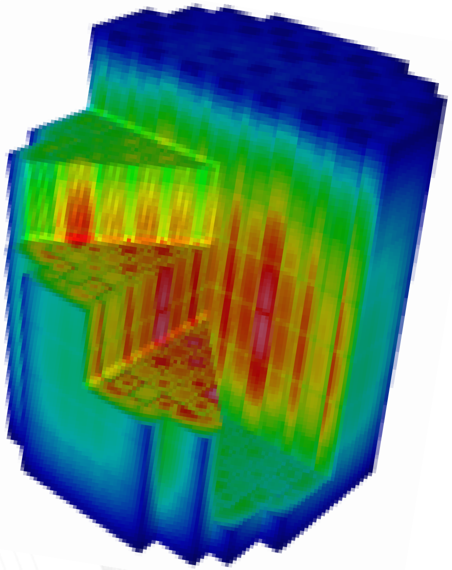
Nuclear data are common to all applications – importance dependents on the end use

We are becoming data limited



- R&D focus has been more on transport methods
- Advanced 3-D geometries and continuous energy methods enable very detailed analysis
- Accuracy is increasingly limited by data

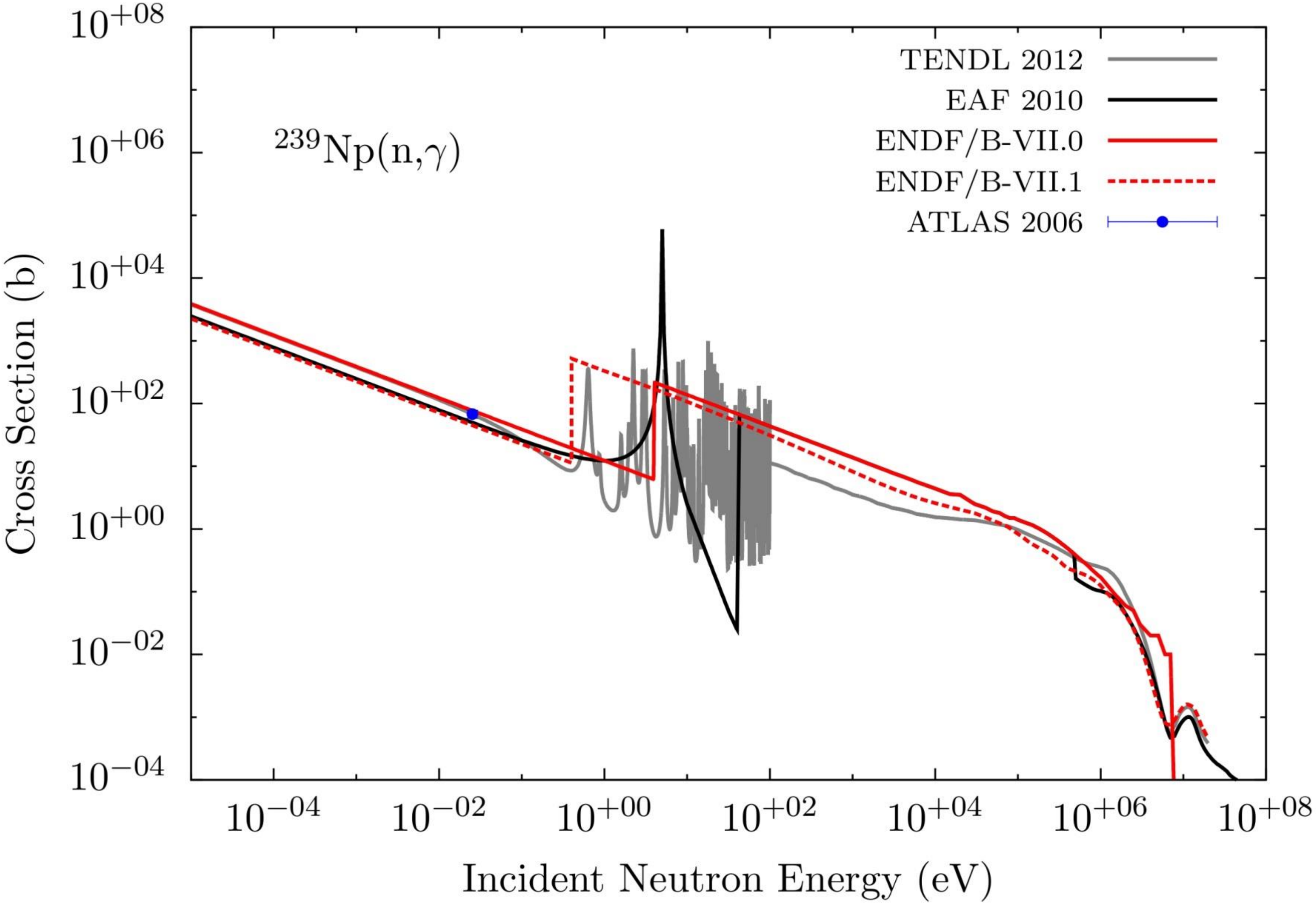




HFIR central target region and surrounding core (L), and detailed HFIR core model (R).

Watts Bar reactor modeling performed under the CASL project.

Example – ^{239}Np capture cross section



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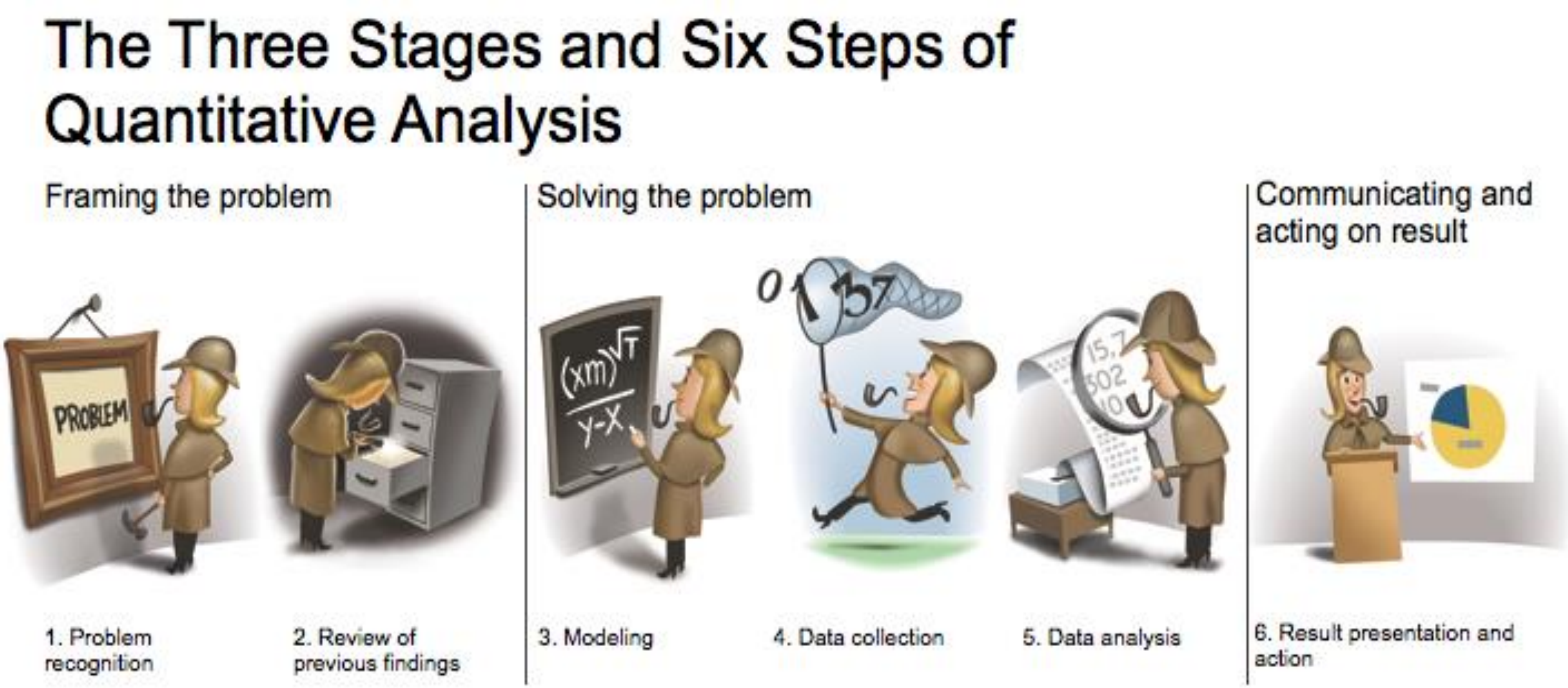
From qualitative to quantitative analysis

Experience-based needs assessments

- Expert opinions
- More subjective
- Aging experts
- We rely increasingly on analysis tools

Quantitative data UQ framework for decision making

Towards systematic data uncertainty analysis



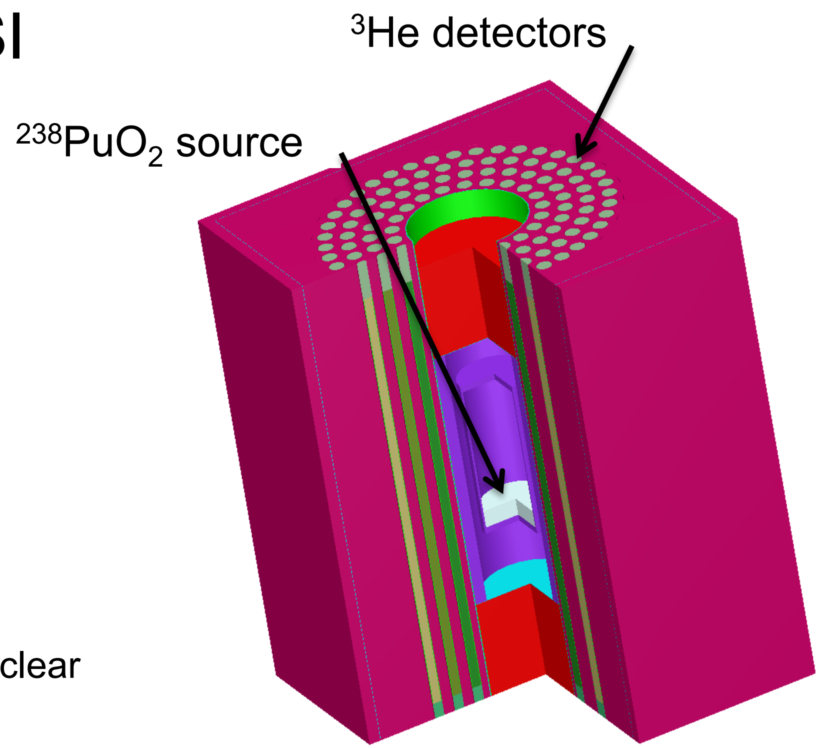
Used with permission from T. Davenport, *Keeping Up with the Quants: Your Guide to Understanding and Using Analytics* (Harvard Business Review Press)

Nuclear energy applications – Defining the problem

- Conventional reactors
- Advanced reactors
- Spent nuclear fuel data
  - Decay heat (reactor, pool storage, dry storage, repositories)
  - Nuclear criticality safety (spent fuel burnup credit for transportation, interim pool and dry storage, and repositories)
  - Safety analysis – releases and off-site dose consequence
  - Repository safety analysis
  - Dose assessment
  - Spent fuel verification for safeguards (neutron and gamma sources for NDA, multiplication)

Spent Nuclear Fuel Data UQ Project* (Roadmap of priority data needs)

- ORNL/LLNL/LANL collaboration
- Methods and data development
- Benchmarks - Advanced instruments being tested in Sweden
- Methods: PG, PN, DDA, DDSI
- Nuclear data
  - Fuel compositions
  - Gamma emission
  - Neutron emission
  - Neutron multiplication
  - Detector models

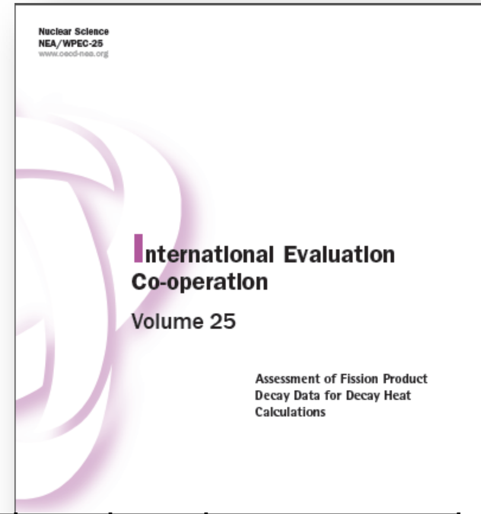


ENMC125 detection system model

*U.S. Department of Energy, Office of Defense Nuclear Nonproliferation R&D

Nuclear data reviews

- OECD/NEA WPEC Subgroup 25 on decay heat data needs*
- OECD/NEA WPEC Nuclear Data High Priority Request List (HPRL)
- IAEA Report on Long-term Needs for Nuclear Data Development, INDC(NDS)-0601
- IAEA Intermediate-term Nuclear Data Needs for Medical Applications INDC(NDS)-0596
- A Survey of Nuclear Data Deficiencies Affecting Nuclear Non-Proliferation, LA-UR-14-26531


Nuclear Science
NEA/WPEC-25
www.oecd-nea.org

International Evaluation Co-operation

Volume 25

Assessment of Fission Product Decay Data for Decay Heat Calculations

Radionuclide	Priority	Q_{β}-value (keV)	Half-life	Comments
35-Br-86	1	7626(11)	55.1 s	
35-Br-87	1	6852(18)	55.65 s	Extremely complex decay scheme with substantial gamma component; large uncertainties in the mean gamma energy arises from significant disagreements between the various discrete gamma-ray measurements. Also (β^-,n) branch.
35-Br-88	1	8960(40)	16.36 s	(β^-,n) branch.
36-Kr-89	1	4990(50)	3.15 min	Incomplete decay scheme.
36-Kr-90	1	4392(17)	32.32 s	Incomplete decay scheme.
37-Rb-90m	2	6690(15)	258 s	Repeat of INL TAGS measurement; data check.
37-Rb-92	2	8096(6)	4.49 s	Small (β^-,n) branch.
38-Sr-89	2	1493(3)	50.53 d	
38-Sr-97	2	7470(16)	0.429 s	Extremely short half-life (0.429 s), and possible (β^-,n) branch.
39-Y-96	2	7096(23)	5.34 s	
40-Zr-99	3	4558(15)	2.1 s	
40-Zr-100	2	3335(25)	7.1 s	
41-Nb-98	1	4583(5)	2.86 s	

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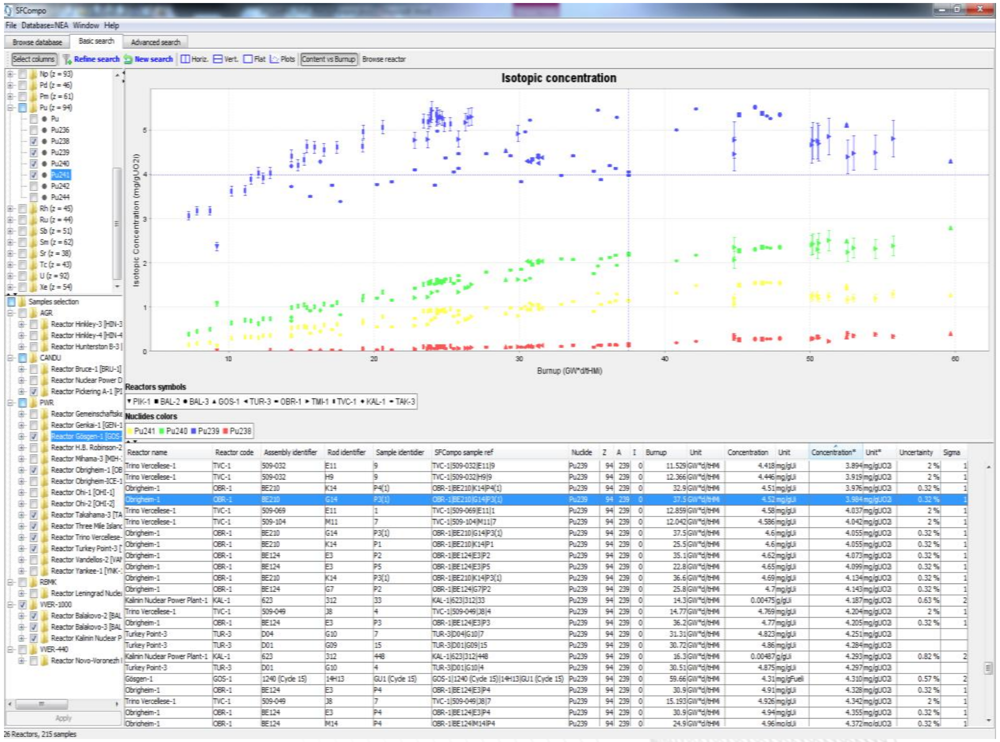
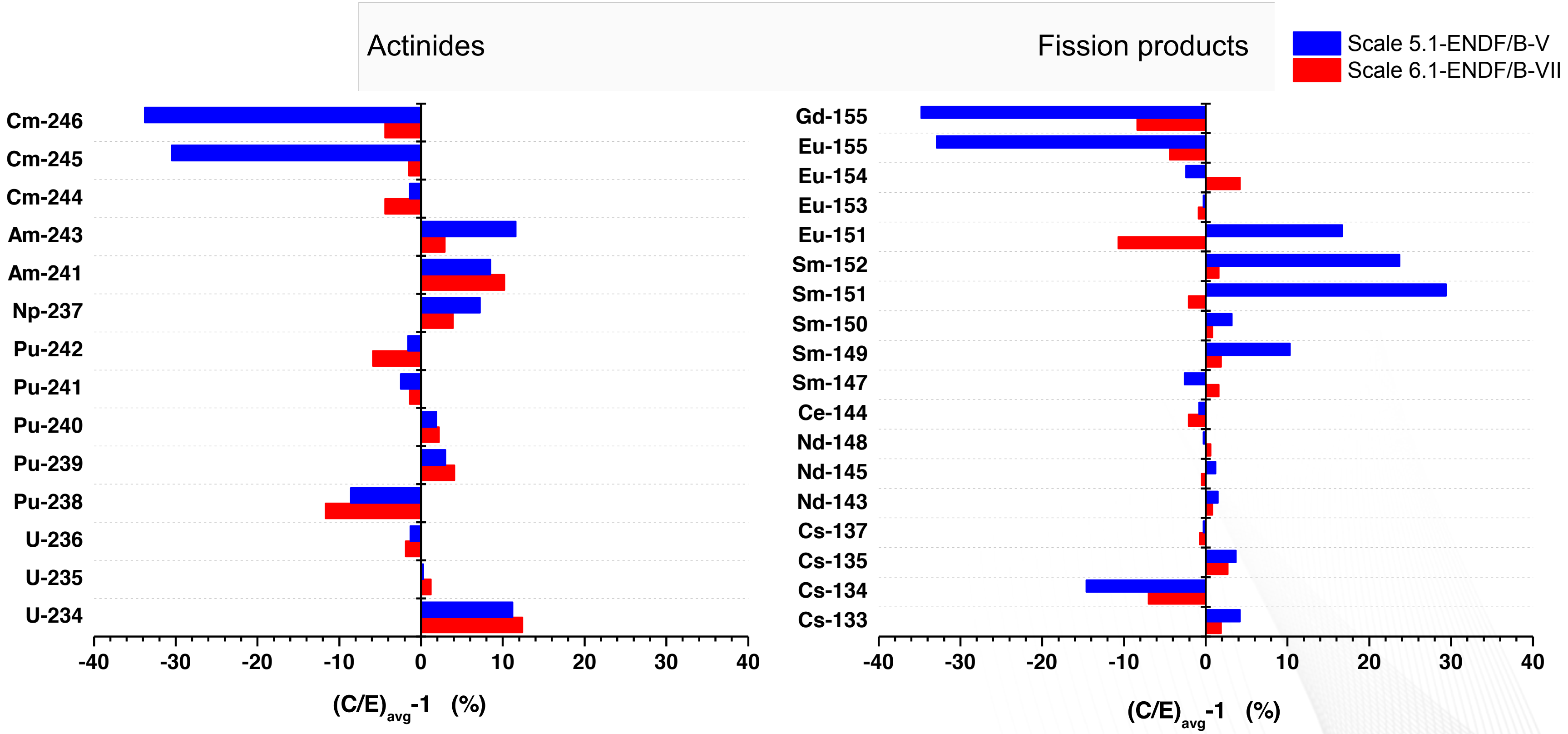
Spent Fuel Assay Data Benchmarks

- SFCOMPO 2.0 database developed through the international OECD/NEA Expert Group on Assay Data now contains >600 fuel samples with destructive analysis measurements
- Experimental uncertainties are included
- https://www.oecd-nea.org/science/wpncs/ADSNF/index.html

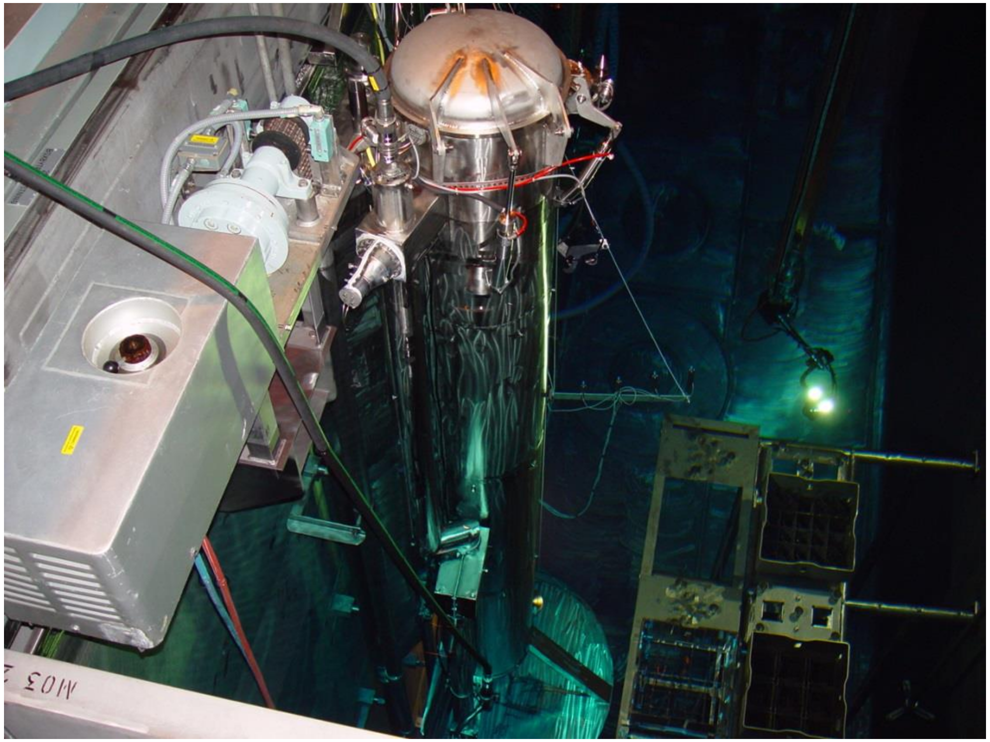
- SFCOMPO expanded for world reactor data
  - Commercial PWR and BWR designs
  - VVER-440 and VVER-1000
  - Russian RBMK graphite
  - AGR and MAGNOX graphite
  - CANDU heavy water
  - Recent data from Hanford B production reactors, Magnox and CANDU fuel



Isotopic validation (ENDF/B-V and ENDF/B-VII.0)



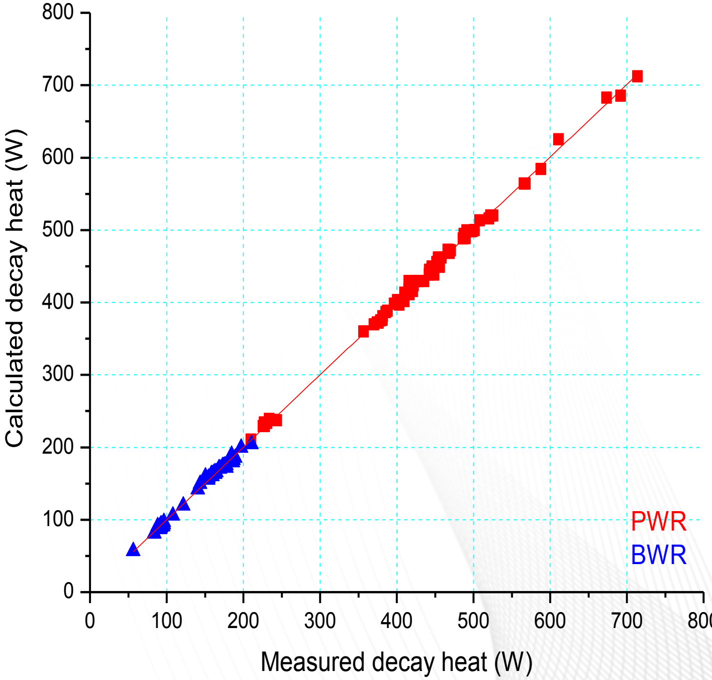
Benchmarks – calorimeter measurements



Spent fuel assembly calorimeter at the SKB CLAB facility Sweden

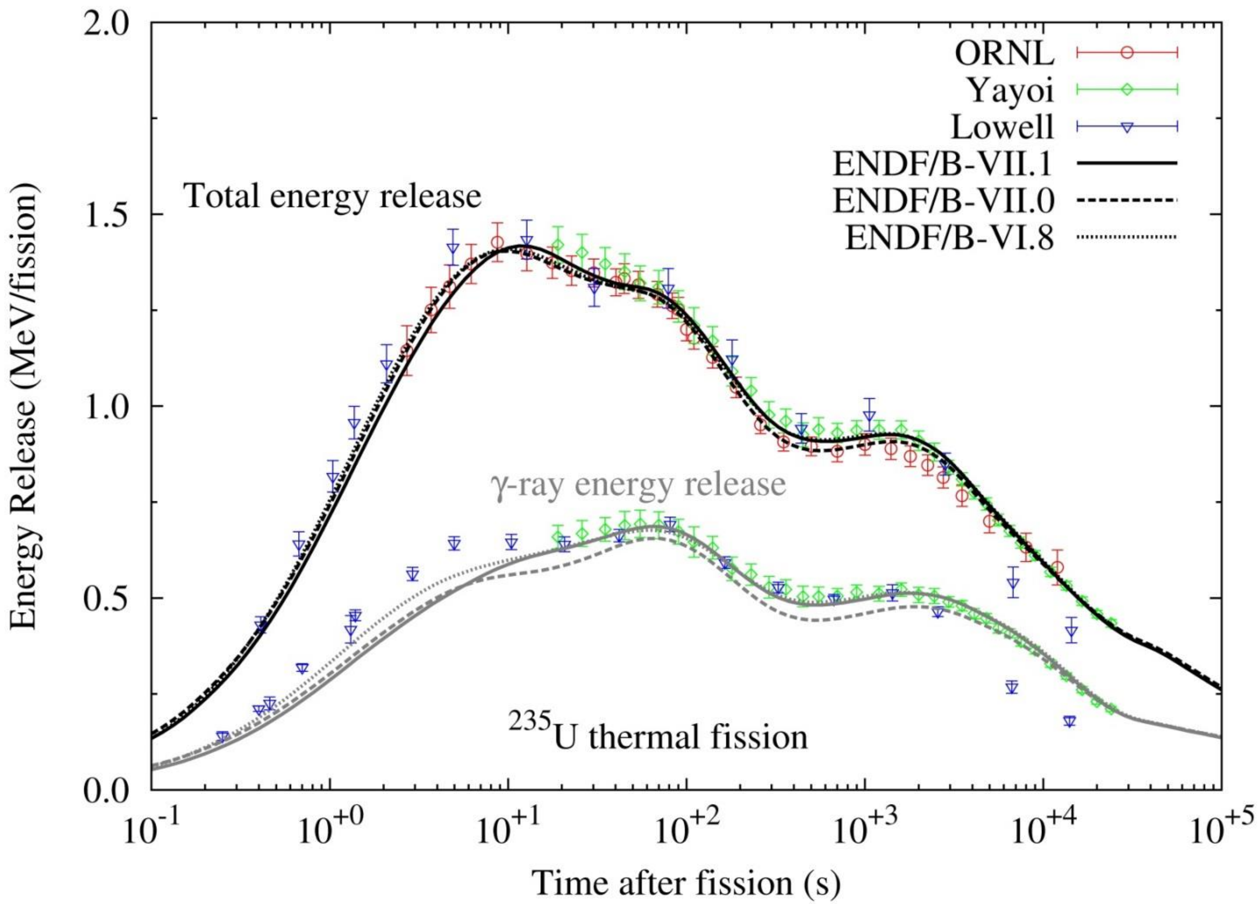
Comparison calculation – experiment *

- Cooling times 12 – 30 years
- BWR assemblies
  number of measurements = 45
  average C/E = 1.003 ± 0.025
  average residual = -0.2 ± 3.4 W
- PWR assemblies
  number of measurements = 38
  average C/E = 1.011 ± 0.012
  average residual = 4.7 ± 5.0 W



* Germina Ilas, Ian C. Gauld, Henrik Liljenfeldt, "Validation of ORIGEN for LWR used fuel decay heat analysis with SCALE," *Nuclear Engineering and Design* **273** (2014) 58–67

Benchmarks – decay heat at short times after fission (^{235}U)



* I. C. Gauld, M. Pigni, G. Ilas, "Validation and Testing of ENDF/B-VII Decay Data," *Nuclear Data Sheets* **120** (2014), pp. 33-36.

Modeling Methods for Nuclear Data UQ

Total Monte Carlo Method
Stochastic Sampling

- *Covariances of input data sampled; statistical analysis of output distribution gives uncertainties*
- Pros
  - Can be used with existing codes
  - Obtains uncertainties for all responses at once
- Cons
  - Cannot quantify individual contributors to uncertainty
  - Requires many calculations

Sensitivity Analysis
Adjoint method

- *Sensitivities are computed; combined with covariances to obtain uncertainties*
- Pros
  - Quantifies individual uncertainty contributors
  - Obtains sensitivities for all data and single response at once
- Cons
  - Requires implementation of adjoint solution
  - Adjoint calculation for each response.

Sources of covariance data

- Cross section covariances

ENDF-VII.1 supplemented by other sources (SCALE cov library) – 423 nuclides, 190 with cov data

- Fission product yield

No covariance data. Retroactive generation by combining independent and cumulative yield uncertainties

- Decay data

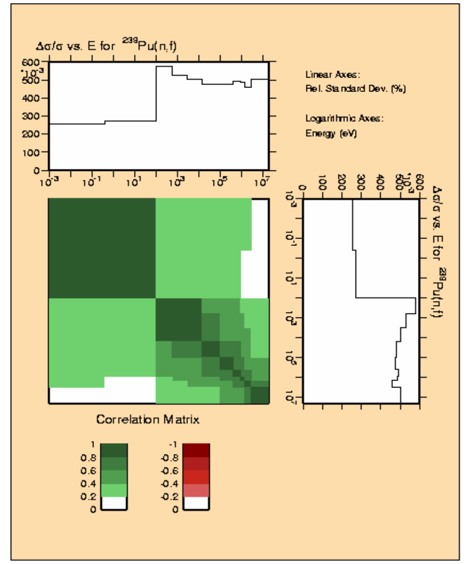
ENDF-VII.1 modified to include branching correlations

- Gamma emissions

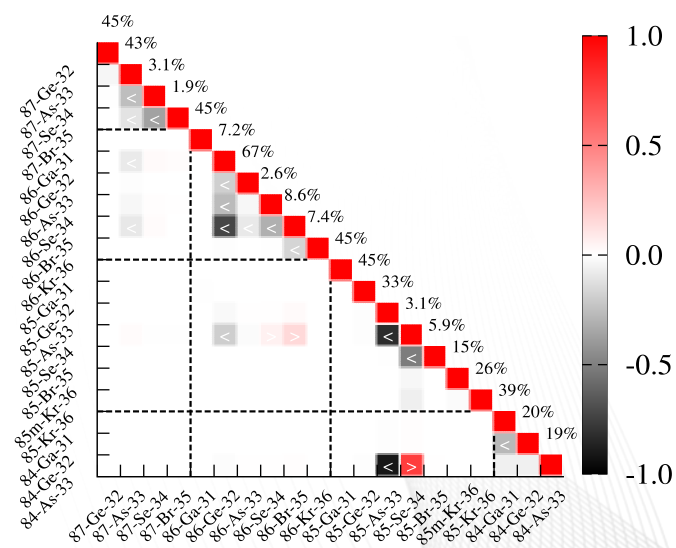
ENDF-VII.1, no covariance data

- Neutron emissions

ENDF-VII.1, except ^{252}Cf, no covariance



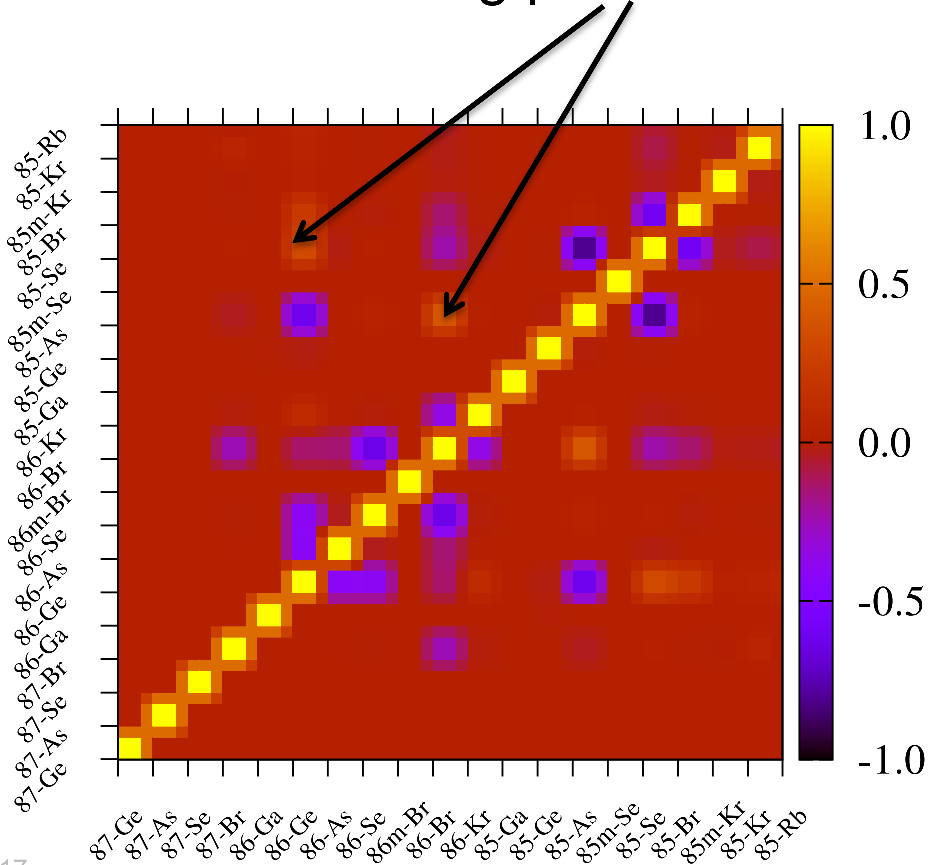
Pu-239 fission covariance



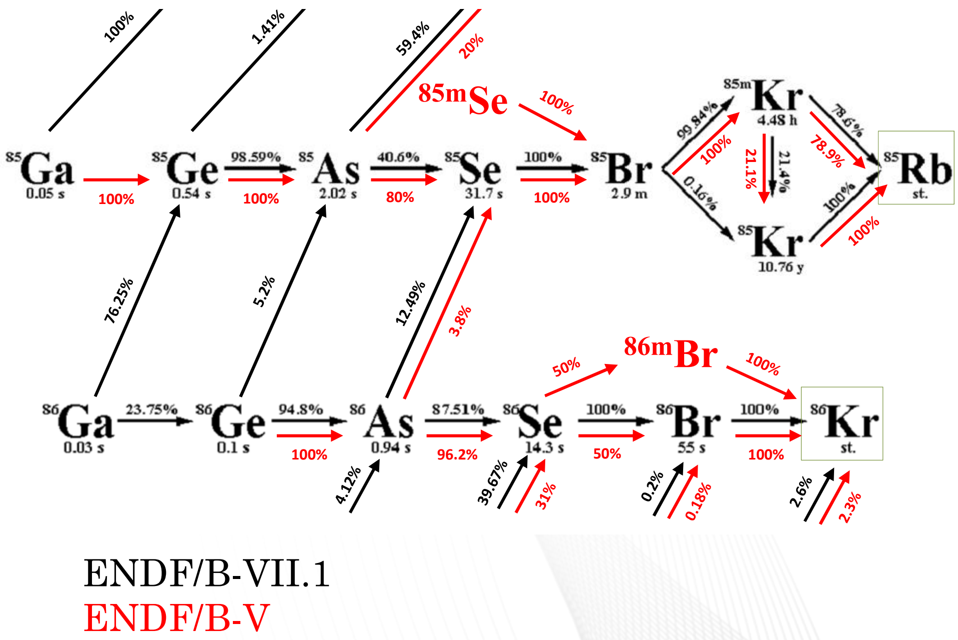
Yield covariance

Fission yield covariance data

- Retroactive covariance data generated using a Bayesian approach by Lack of covariance data –
- Strong negative correlations exist within chains
- Relative strong positive correlations (delayed-neutrons)



Decay scheme



Fission yield data

- Fission yield and decay data in ENDF/B-VII.1 are inconsistent
- Yields are largely from England and Rider (1994)
- Decay data revised in ENDF/B-VII.1 (2011)
- Direct and cumulative yields are highly correlated
- Krypton noble gases have 5-8% error

Cumulative yields   Independent FPY   Branching ratios

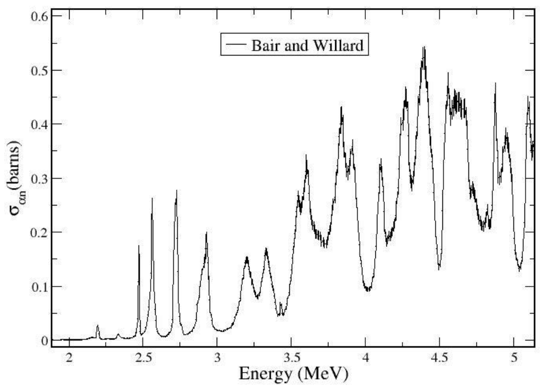
$$C_i(\mathbf{I}) = I_i + \sum_{j \in \mathbf{k}^i} C_j(\mathbf{I})\; b_{i,j}$$

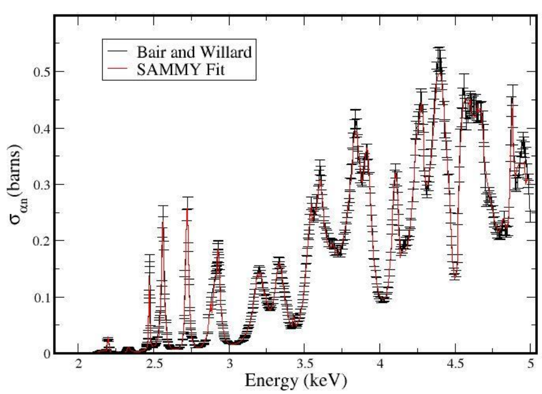
- Decay data and fission yields should not be developed independently

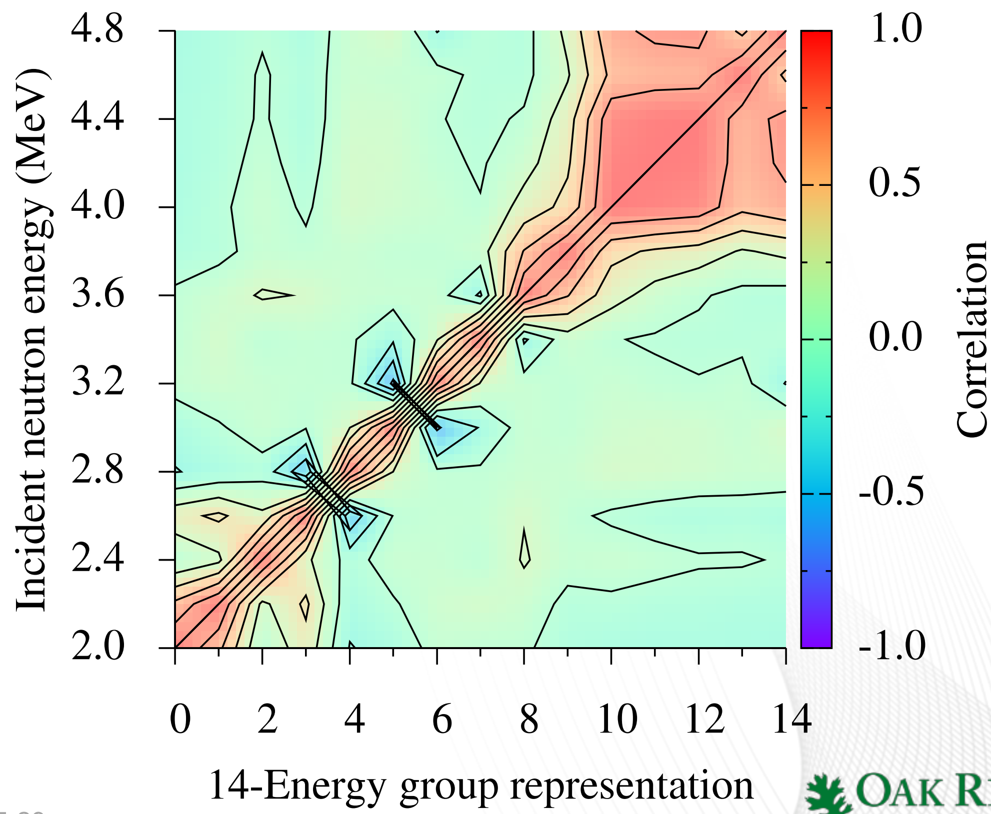
M. Pigni, M. W. Francis, I. C. Gauld, "Investigation of Inconsistent ENDF/B-VII.1 Independent and Cumulative Fission Product Yields with Proposed Revisions," *Nuclear Data Sheets* **1** (2015), p. 123.

Neutron source covariance data

- SOURCES code used for spontaneous fission and (α,n) has no uncertainties
- ENDF/B-VII.1 only contains SF covariance data for ^{252}Cf
- A retroactive covariance data generation performed using the SAMMY code with R-Matrix evaluation for alpha cross sections







(α,n) covariance matrix (L. Leal)

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Summary/Recommendations

- Sponsors need unbiased information on data needs and priorities
- Require a structured quantitative process to evaluate uncertainties – cannot rely entirely on judgement
  - Rigorous sensitivity/uncertainty analysis tools
  - More complete covariance information for all nuclear data
  - Better covariance data
  - Experimental benchmarks for diverse applications
  - A prioritized data roadmap with acquisition paths and costs
  - A coordinated and clear message to funding organizations and measurement institutes
- Tools and data for the Safeguards UQ project will be applicable to many different applications