

Applications of Nuclear Data in the SCALE Code System

Brad Rearden
Manager, SCALE Code System

Workshop on Nuclear Data Needs and Capabilities for Applications

May 29, 2015
Lawrence Berkeley National Laboratory

ORNL is managed by UT-Battelle
for the US Department of Energy



Outline

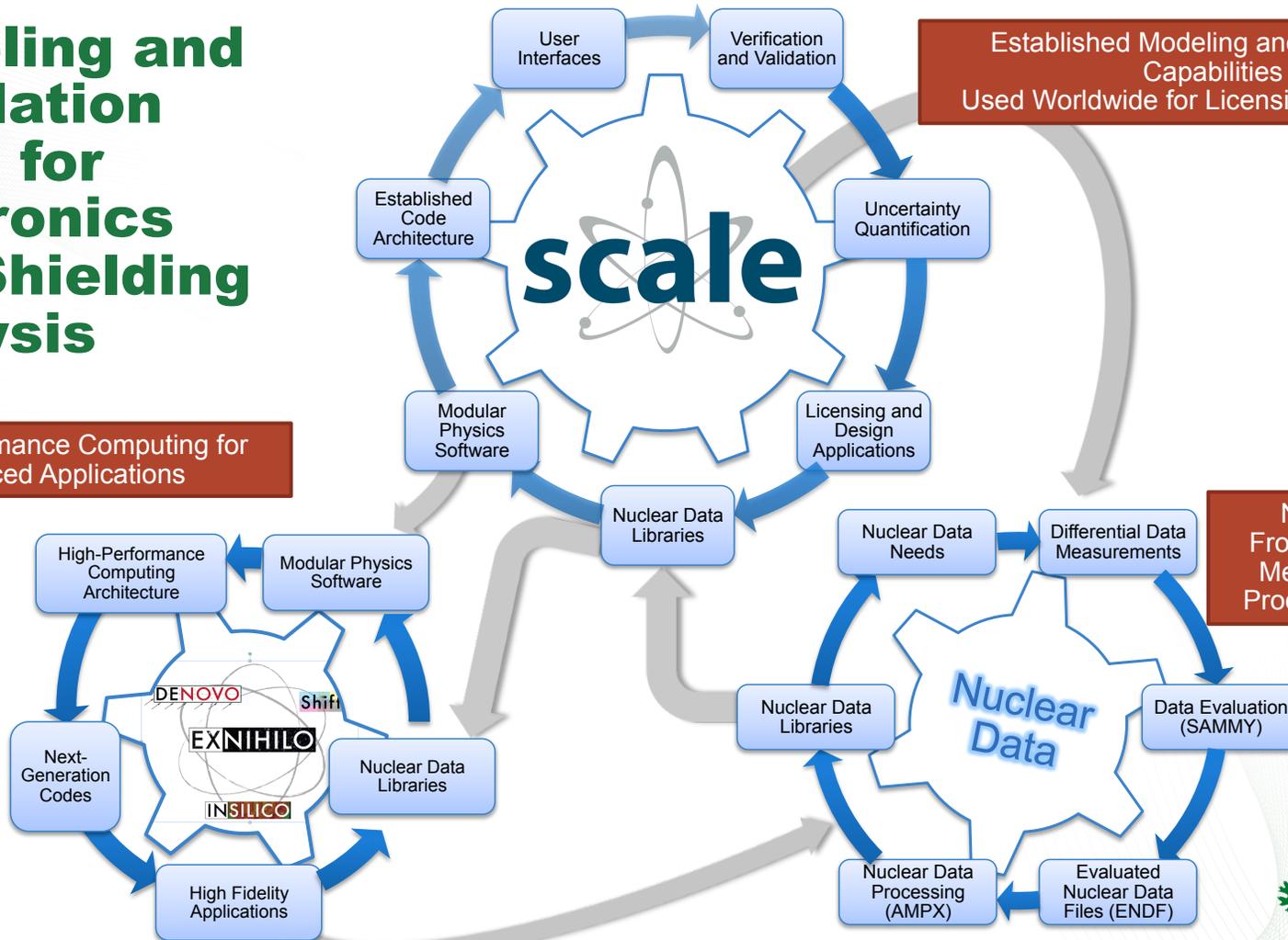
- Modeling and Simulation Tools for Neutronics and Shielding Analysis
- Sensitivity/Uncertainty Analysis
- Neutron Covariance Data
- Some recent nuclear data gaps
- Wish List

Modeling and Simulation Tools for Neutronics and Shielding Analysis

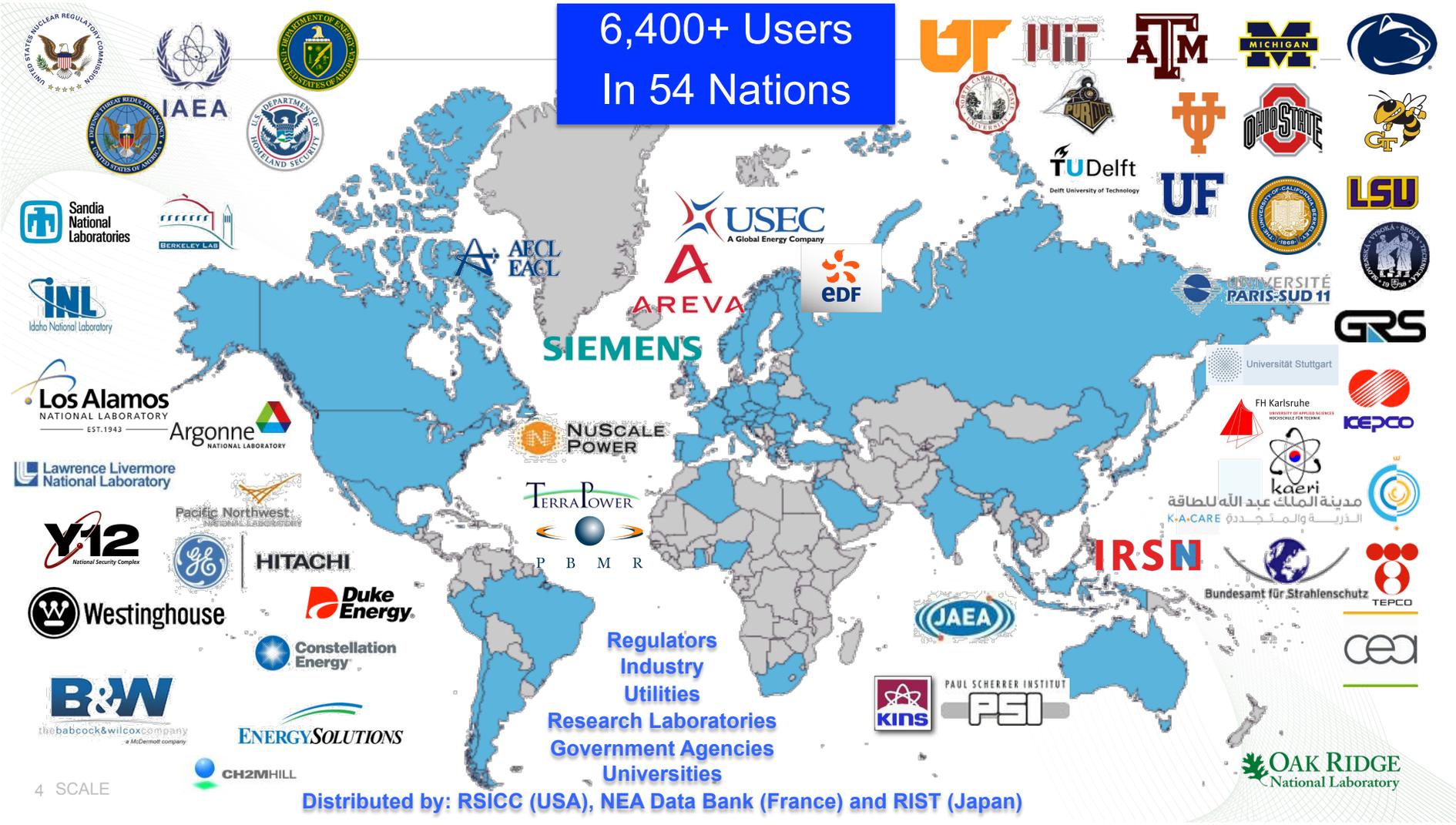
High-Performance Computing for Advanced Applications

Established Modeling and Simulation Capabilities Used Worldwide for Licensing and Design

Nuclear Data: From Fundamental Measurements to Production Libraries



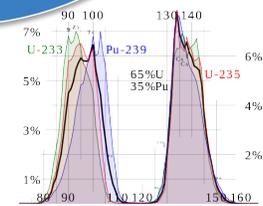
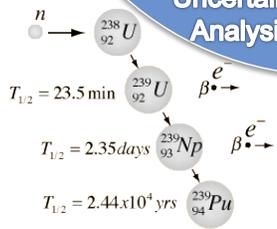
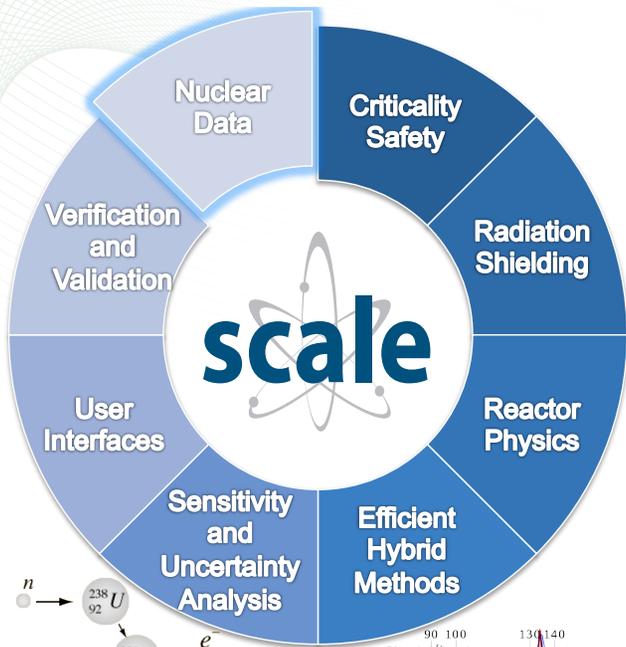
6,400+ Users
In 54 Nations



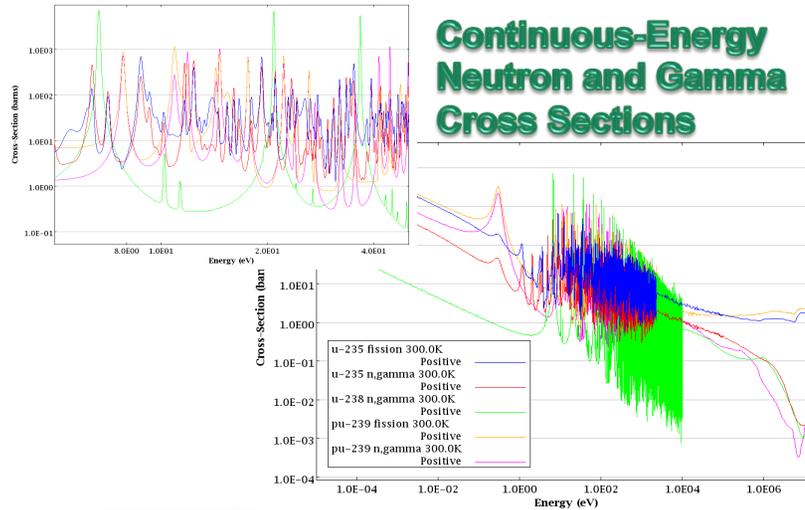
Regulators
Industry
Utilities
Research Laboratories
Government Agencies
Universities

Distributed by: RSICC (USA), NEA Data Bank (France) and RIST (Japan)

Nuclear Data from ORNL AMPX Tools



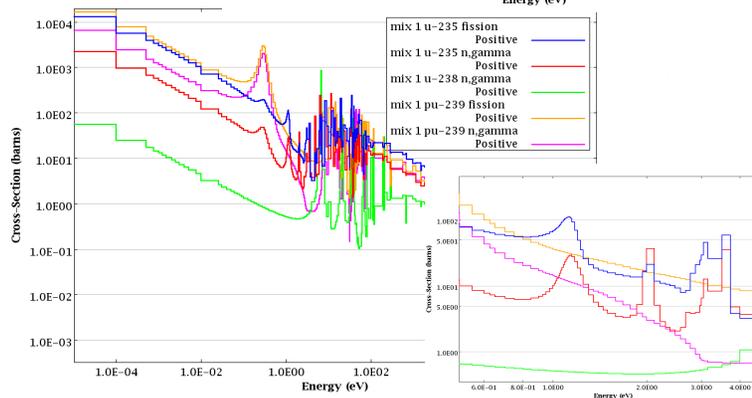
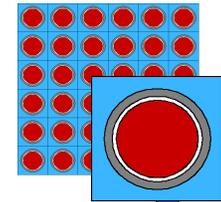
5 Depletion, Decay, and Activation Data



Problem-dependent temperature corrections

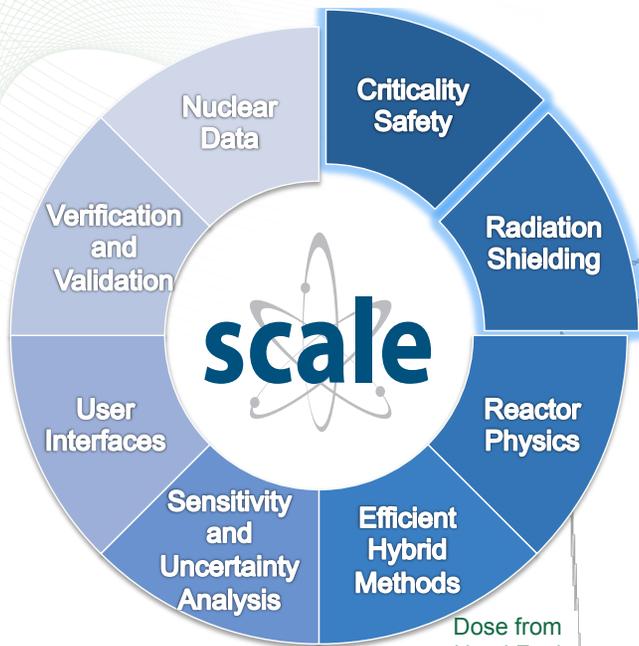


Resonance Self-Shielding

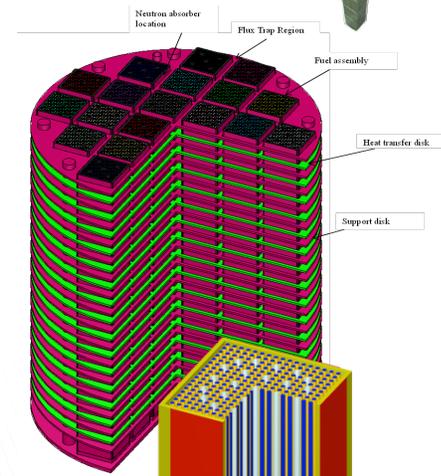
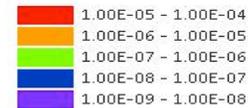
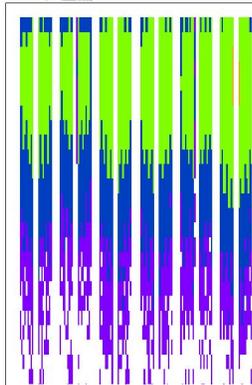
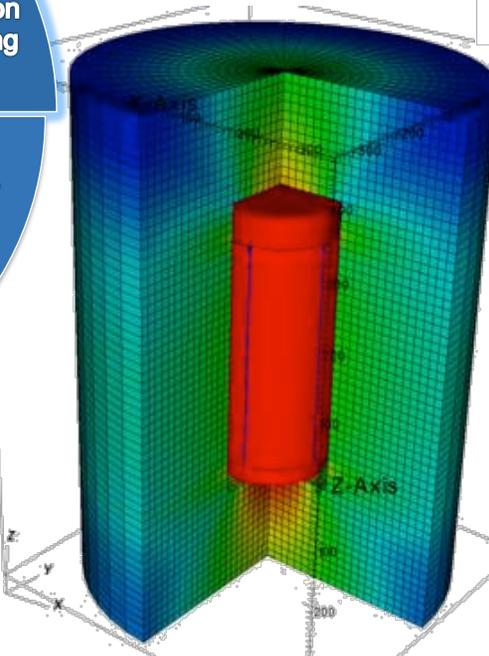
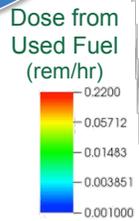
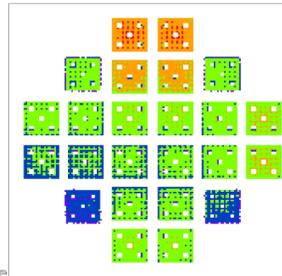


Multigroup Neutron and Gamma Cross Sections

Criticality Safety and Radiation Shielding



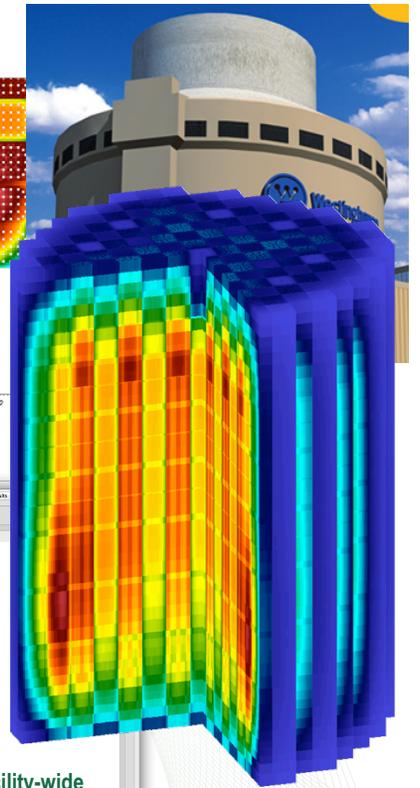
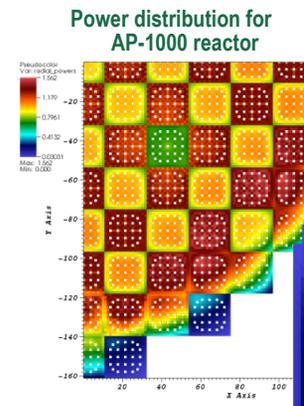
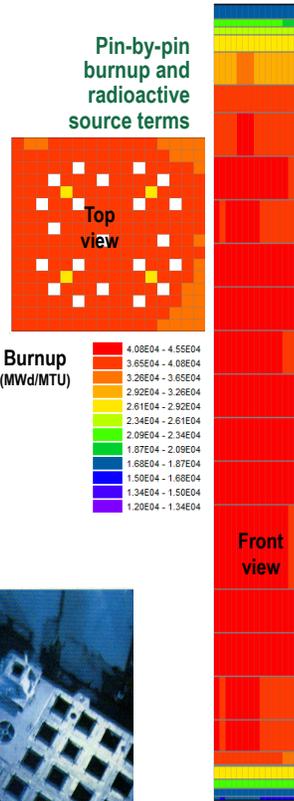
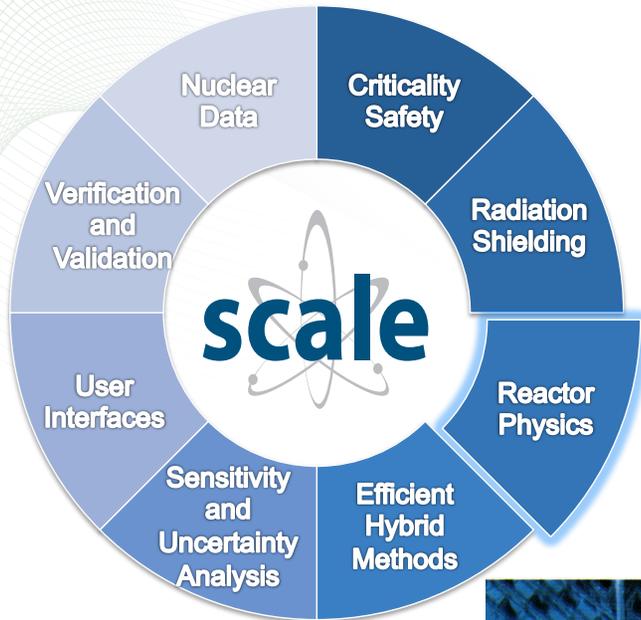
High-Fidelity Monte Carlo Methods



As-loaded used fuel cask



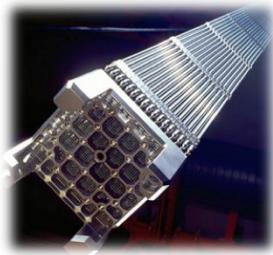
Reactor Physics and Used Fuel Characterization



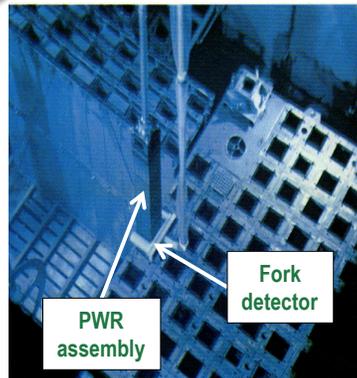
Reactor type grid plot

Column grid label	Row grid label	Assembly per row
1, A	1	7
2, P	2	13
3, M	3	13
4, W	4	13
5, L	5	13
6, K	6	13
7, J	7	13
8, H	8	13
9, C	9	13
10, F	10	13
11, E	11	13
12, D	12	13
13, C	13	13
14, B	14	13
15, A	15	7

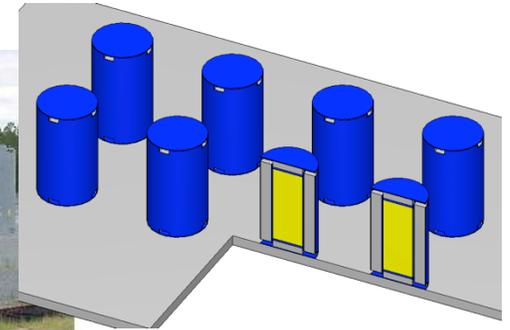
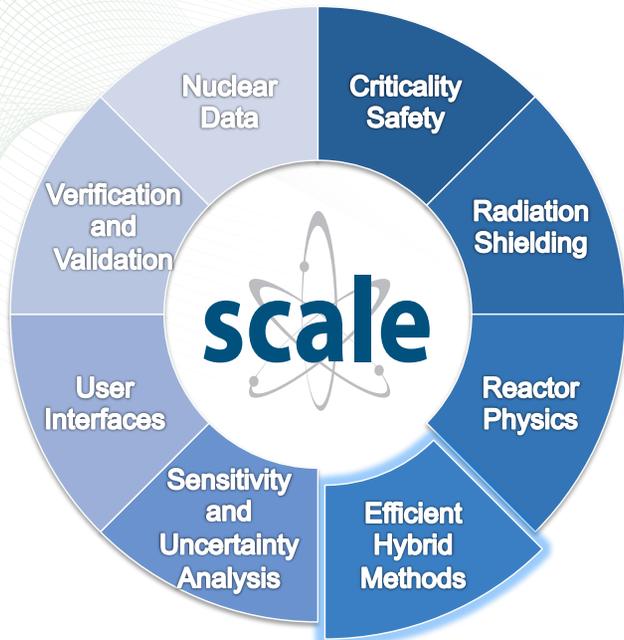
User interface for facility-wide source term characterization



7 SCALE



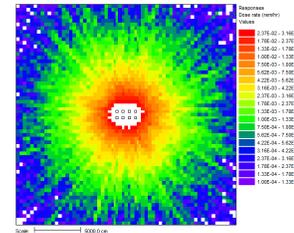
Efficient Hybrid Methods



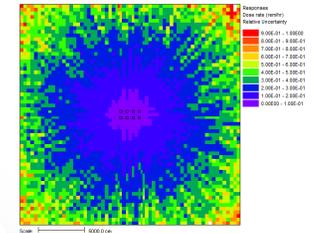
Dose analysis for used nuclear fuel storage

Analog

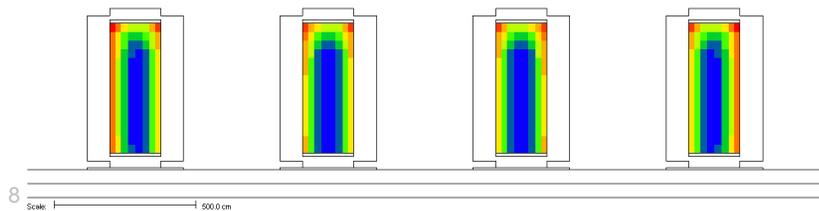
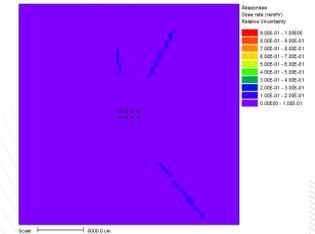
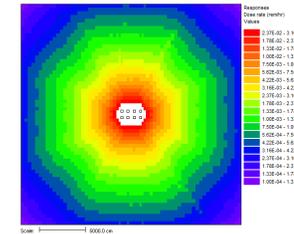
Dose Rate (rem/hr)



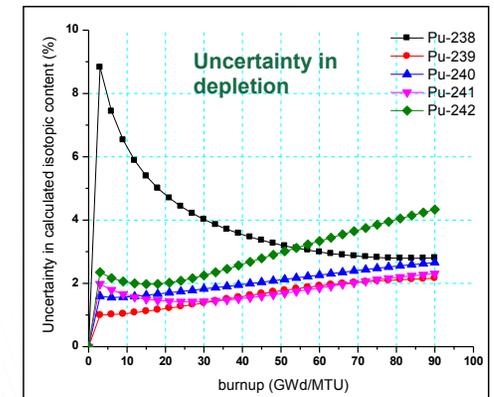
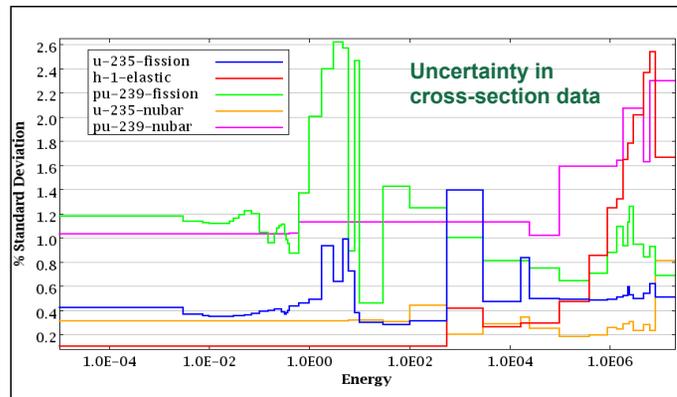
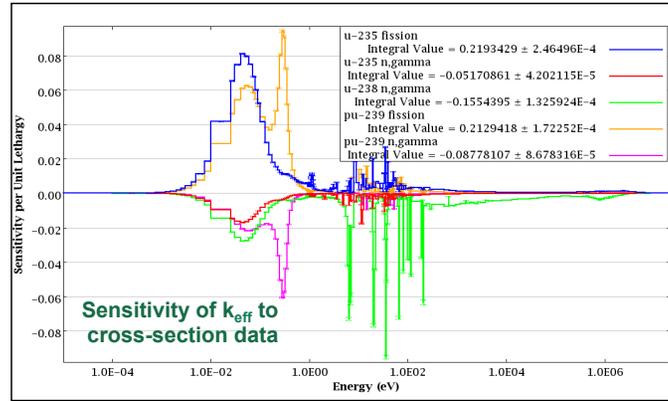
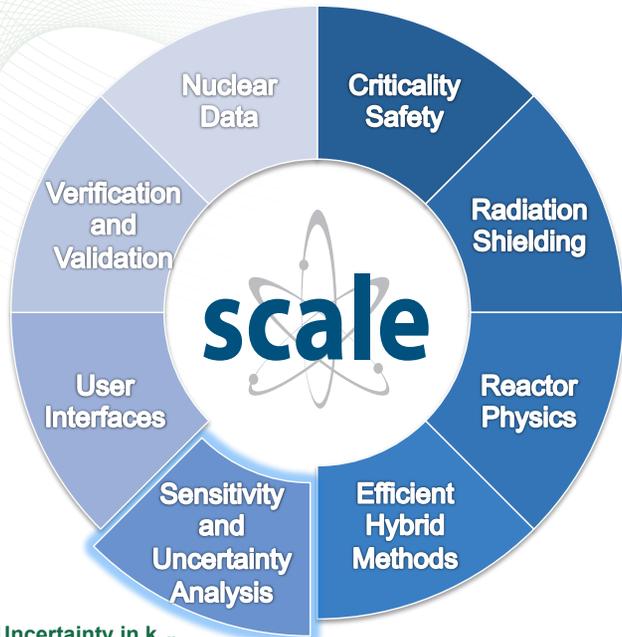
Relative Uncertainty



Hybrid (Same run time)



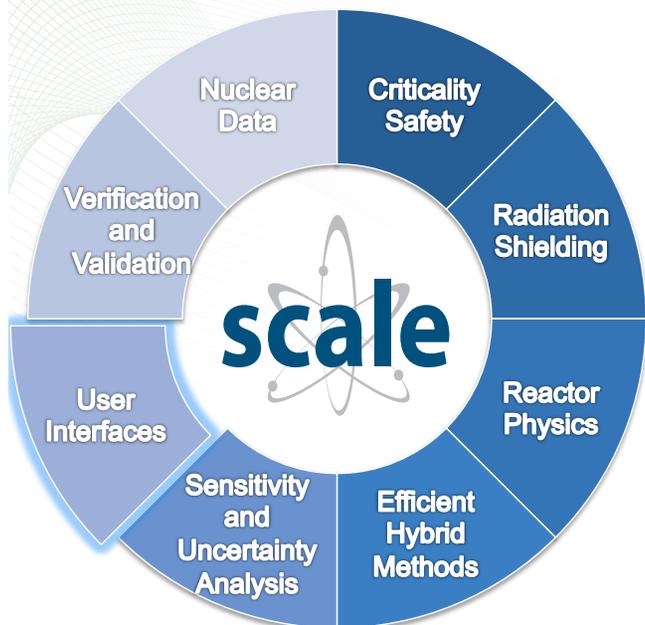
Sensitivity and Uncertainty Analysis



Uncertainty in k_{eff}

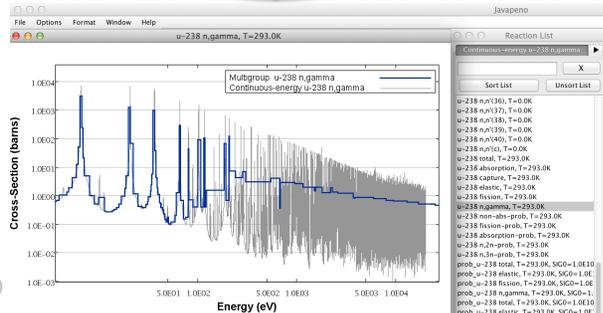
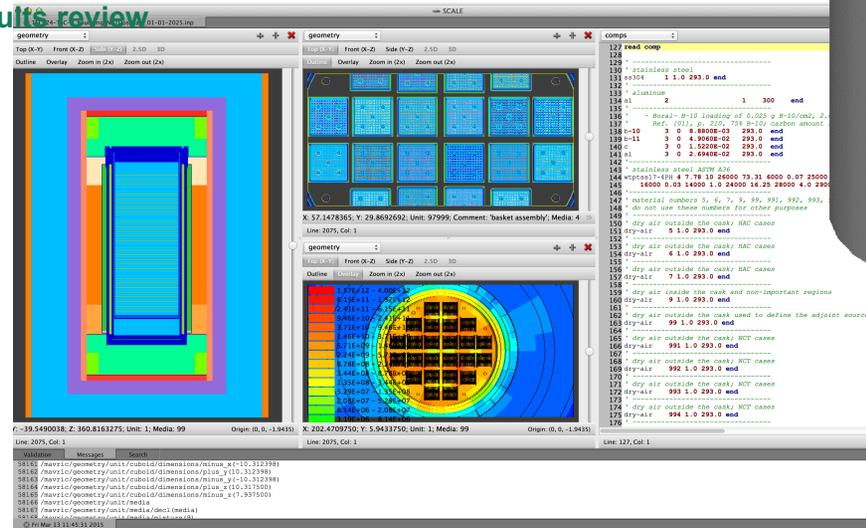
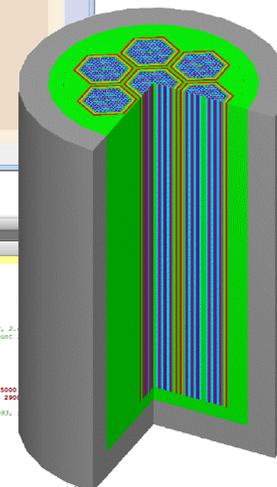
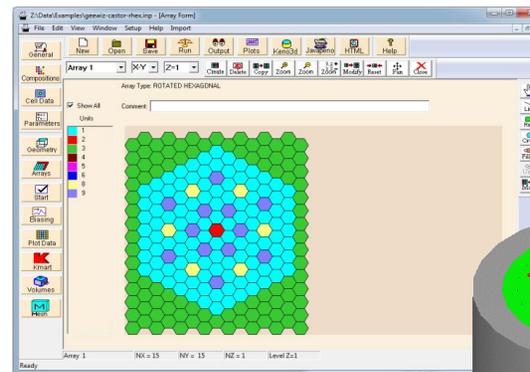
Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
²³⁹ Pu nubar	²³⁹ Pu nubar	4.0032E-01 ± 2.5625E-06
²³⁸ U n.gamma	²³⁸ U n.gamma	1.9457E-01 ± 1.2387E-05
²³⁹ Pu fission	²³⁹ Pu fission	1.5501E-01 ± 1.0838E-05
²³⁵ U nubar	²³⁵ U nubar	1.3981E-01 ± 5.0038E-07
²³⁹ Pu fission	²³⁹ Pu n.gamma	1.2261E-01 ± 4.3564E-06

User Interfaces

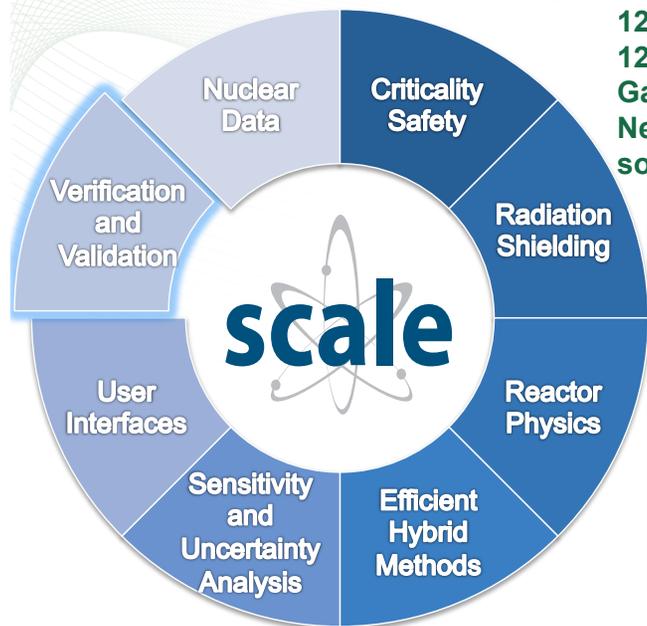


Convenient user interfaces

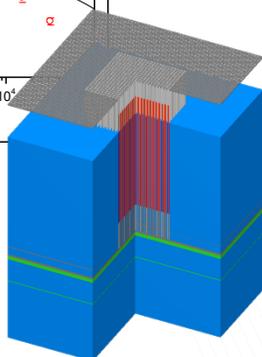
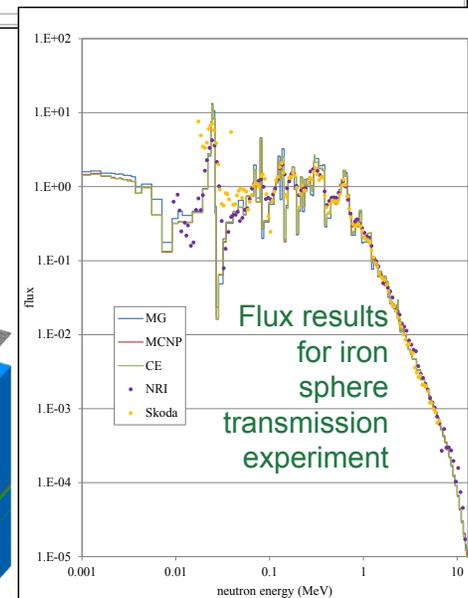
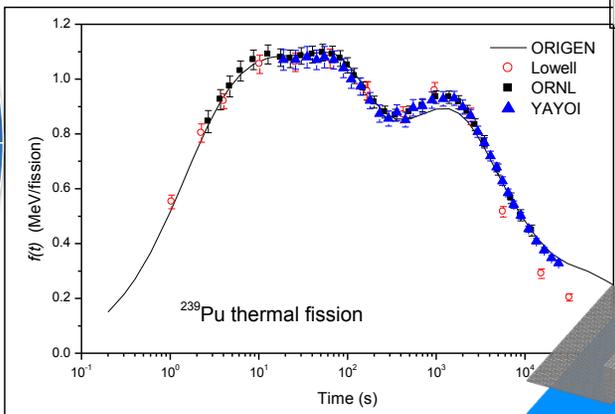
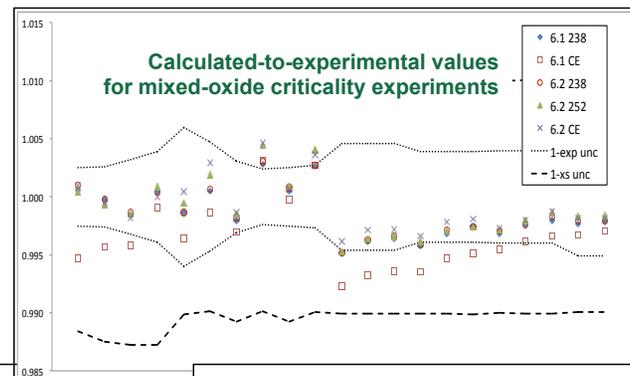
- Input generation
- Model visualization
- Nuclear data plotting
- Job execution
- Results review



Verification and Validation



Validation
 400 criticality and shielding benchmarks
 120 isotopic assays samples
 121 decay heat measurements
 Gamma spectra - burst fission
 Neutron spectra – spent fuel and (α,n) sources



MIX-COMP-THERM-004
Critical Experiment

Verification

>7000 fixed-source transmission tests for neutron/gamma spectral data
 Every nuclide/element at multiple energies
 >5000 infinite medium k_{inf} tests

Knowledge Management

There are *known knowns*; there are things we know that we know. There are *known unknowns*; that is to say, there are things that we now know we don't know. But there are also *unknown unknowns* – there are things we do not know we don't know.

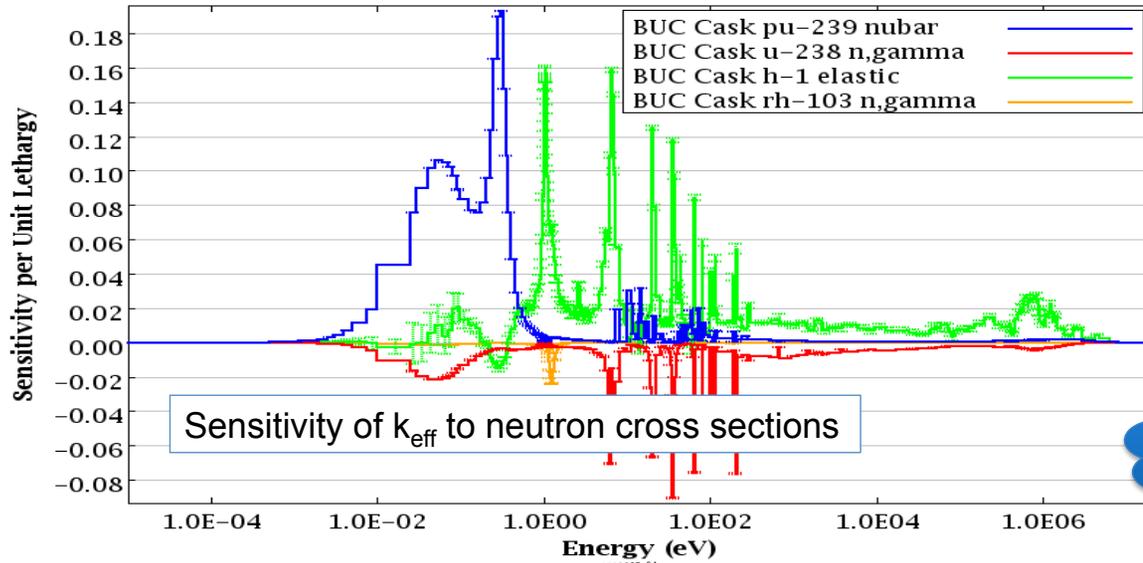
—United States Secretary of Defense, Donald Rumsfeld, 2002

KNOWN KNOWNS Measurements/ Observations	KNOWN UNKNOWNNS Uncertainty Quantification
UNKNOWN KNOWNS* Communication	UNKNOWN UNKNOWNNS Safety Margins

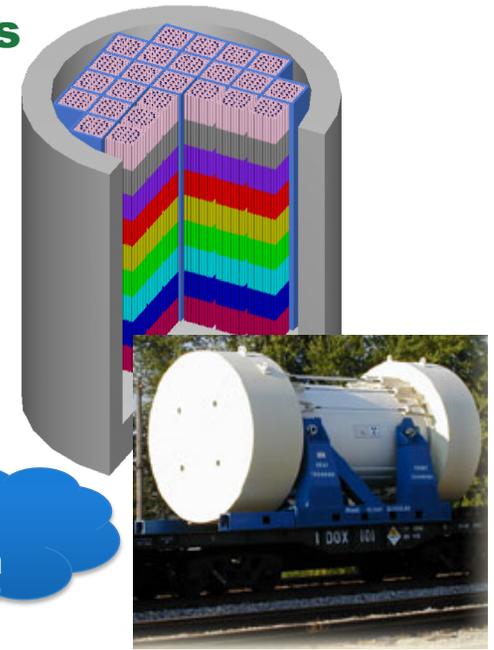
All models are wrong, some are useful.

—George E. P. Box – Statistician, Professor, Univ. of Wisconsin

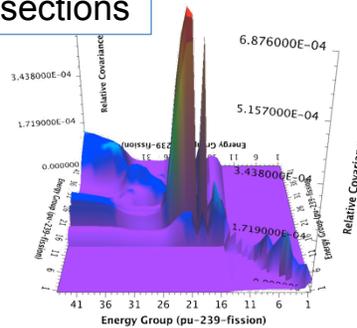
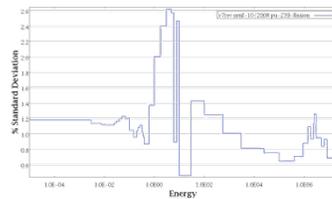
Identification of Important Processes/Uncertainties



Known
Unknown



Covariance (uncertainty) for cross sections

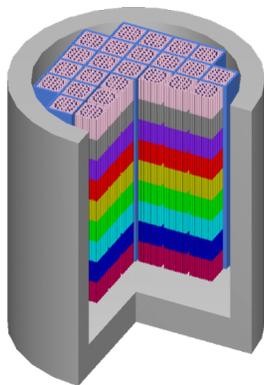


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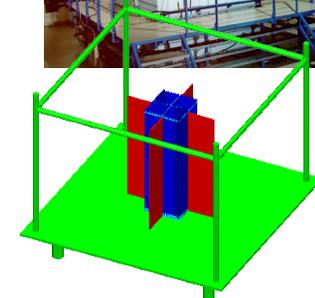
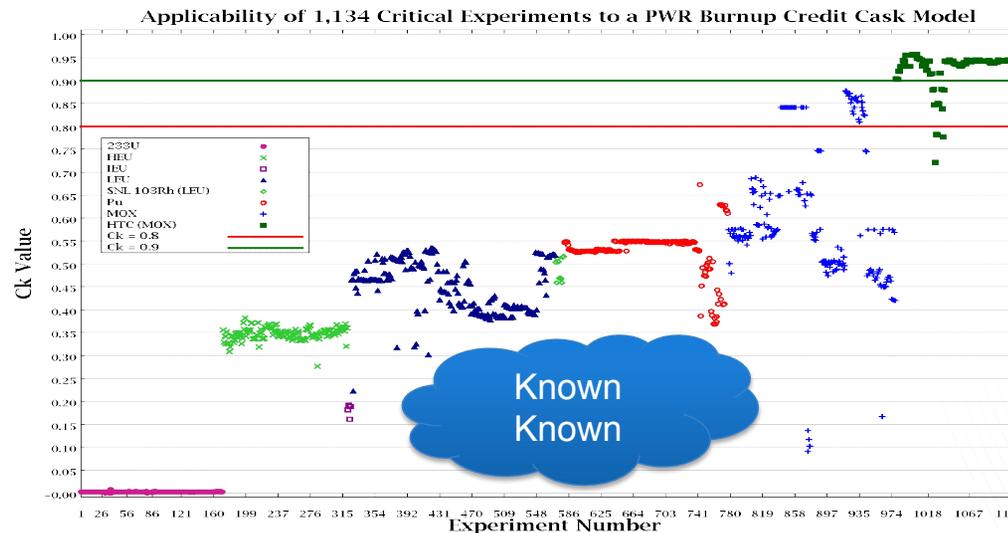
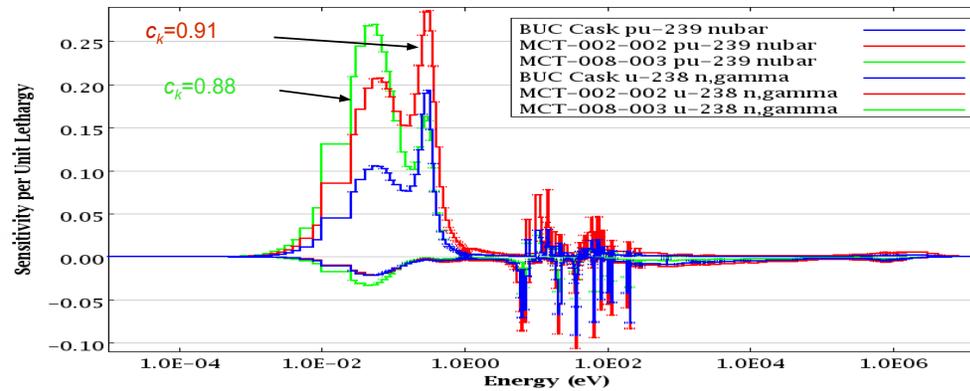
Code Validation: Identification of Laboratory Experiments that are Similar to the Targeted Application



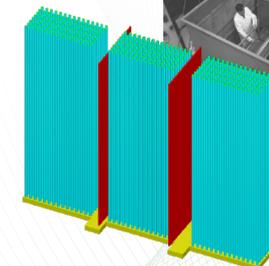
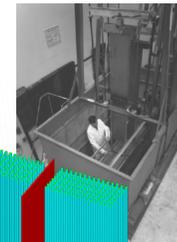
APPLICATION



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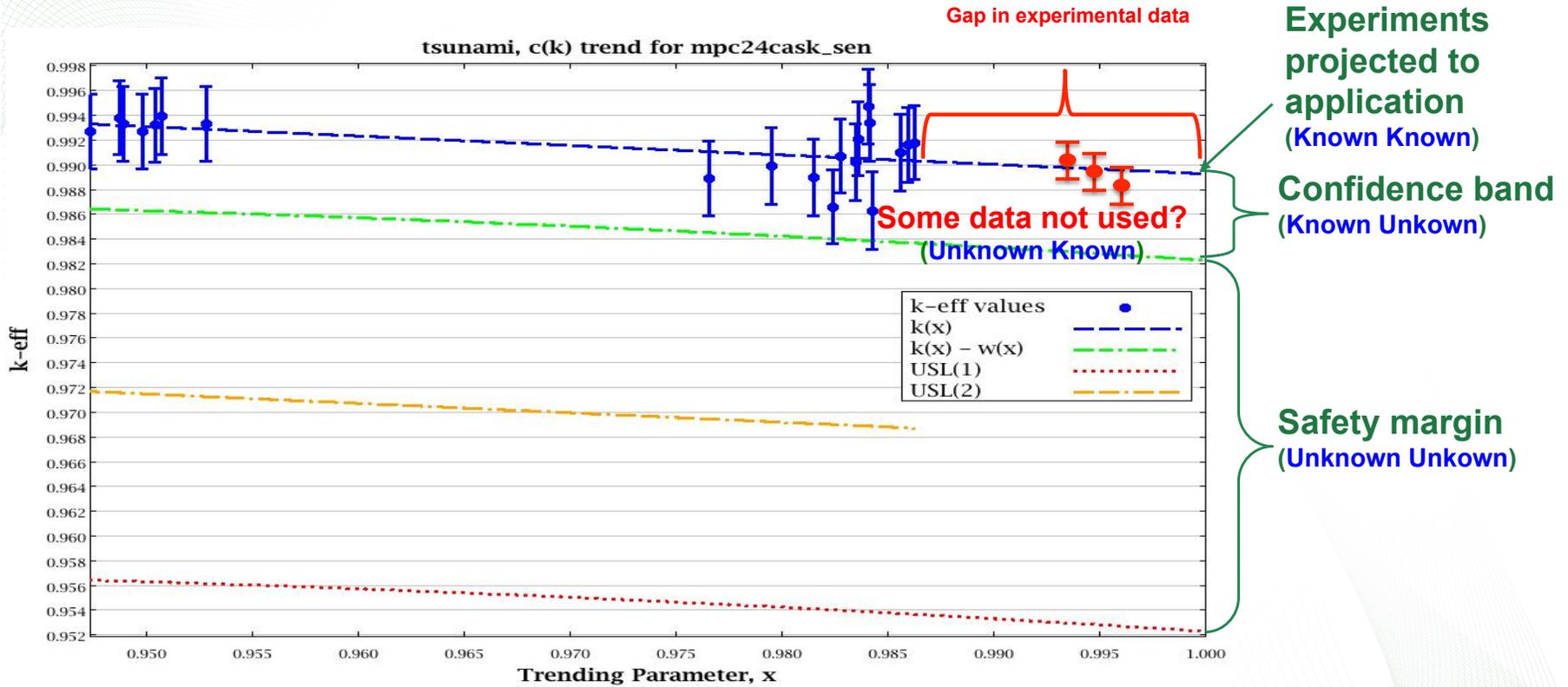


NUCLEAR CRITICALITY EXPERIMENTS



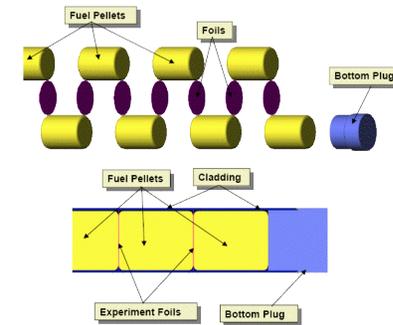
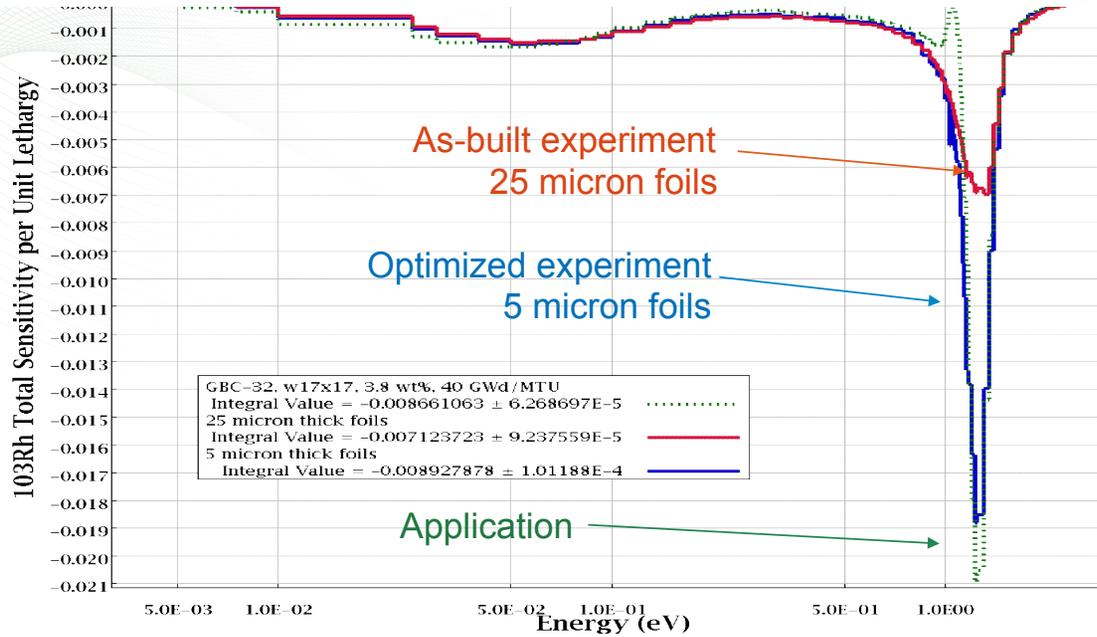
RIDGE Laboratory

Setting Safety Limits

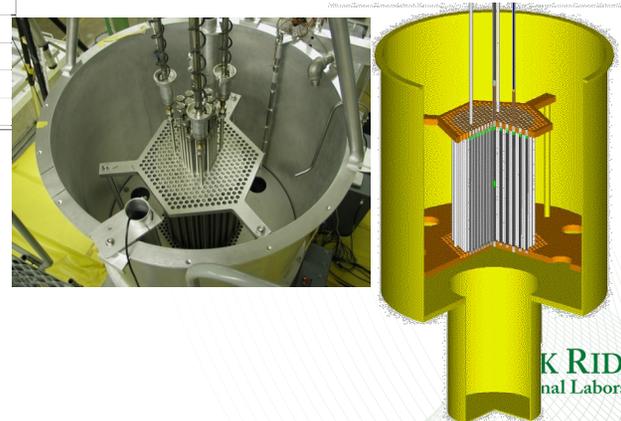


Design of Optimized Experiments in US and Abroad

- Experiment designs optimized to fill gaps not met by other experiments
- Required analysis in DOE Nuclear Criticality Safety Program $C_{E}dT$ Process



Rh-103 Critical Experiment Design for Burnup Credit



ORNL
K RIDGE
National Laboratory



UNCERTAINTY QUANTIFICATION

SCALE has two techniques for UQ:

Sensitivity Methods (*TSUNAMI*)

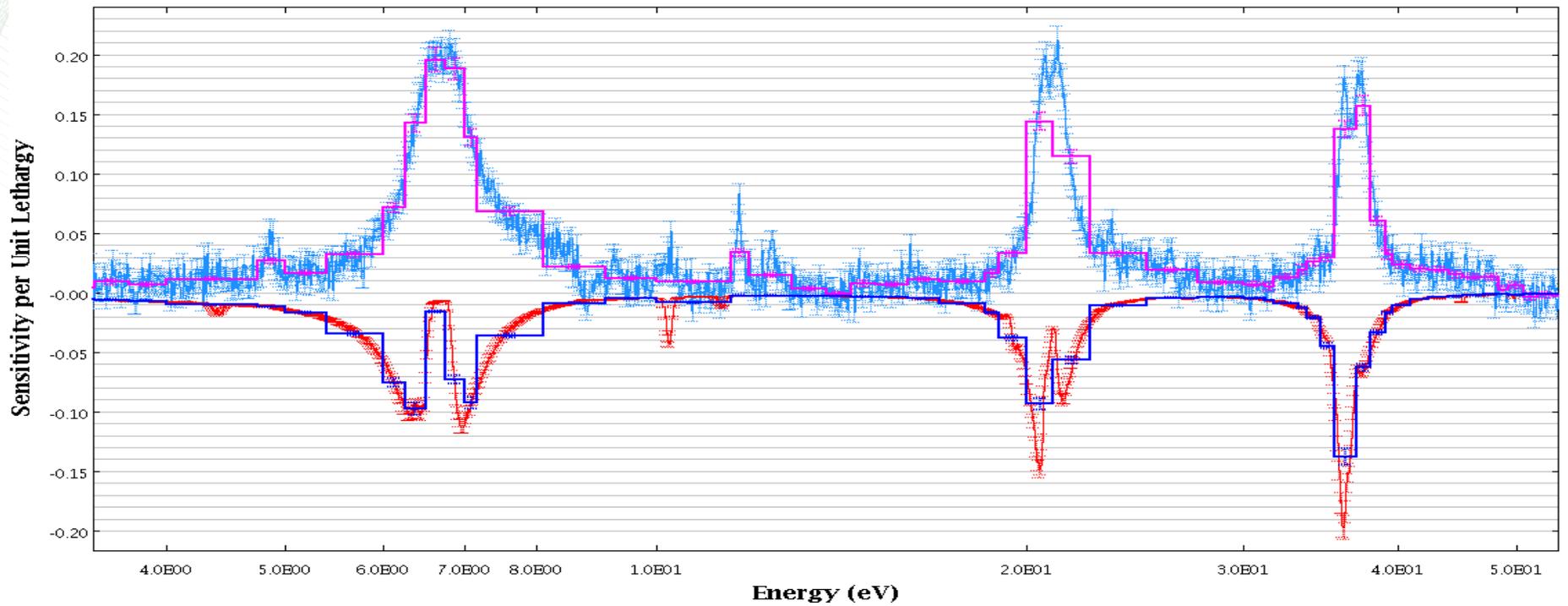
- Sensitivities are computed and combined with covariances to obtain uncertainties
- Pros
 - Quantifies uncertainty contributors
 - Obtains all data sensitivities for a single response in single calculation
- Cons
 - Requires invasive implementation of adjoint solution in simulation codes
 - Limited to radiation transport applications

Stochastic Sampling (*Sampler*)

- Covariances of input data sampled; statistical analysis of output distribution gives uncertainties
- Pros
 - Typically minimally invasive to code
 - Can address complex simulations with coupled codes
- Cons
 - Quantification of separate effects (sensitivity coefficients) is challenging

H-1 Elastic Scatter Sensitivity
238-group CLUTCH VS
Microgroup CLUTCH

U-238 Capture Sensitivity
238-group CLUTCH VS
Microgroup CLUTCH



Generalized Perturbation Theory

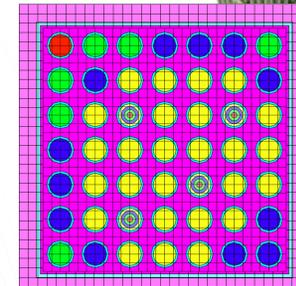
- Recent developments have enabled the calculation of generalized response sensitivity coefficients using high-fidelity, continuous-energy Monte Carlo methods.
- Generalized Perturbation Theory (GPT) calculates sensitivity coefficients for any system response that can be expressed as the ratio of reaction rates.

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

- Applications for GPT sensitivity/uncertainty analysis include:
 - Relative powers
 - Isotope Conversion Ratios
 - Multigroup Cross Sections
 - Experimental Parameters

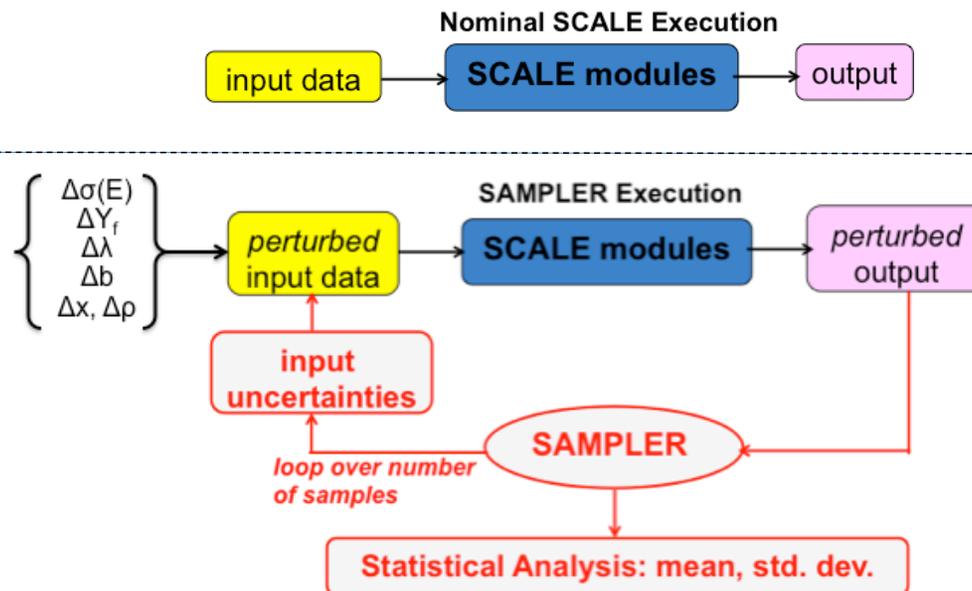
NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert
1	k_infinity	keff	Relative	1.1083E+0	4.98551E-1 % dk/k
2	fission_grp_1	gpt	Relative	1.9155E-3	6.91925E-1 % dR/R
3	fission_grp_2	gpt	Relative	2.7748E-2	3.23440E-1 % dR/R
4	absorpt_grp_1	gpt	Relative	7.1637E-3	8.36728E-1 % dR/R
5	absorpt_grp_2	gpt	Relative	5.3702E-2	2.38082E-1 % dR/R
6	comerrod_fpf	gpt	Relative	1.1458E+0	1.67147E-1 % dR/R

OECD UAM GPT Benchmark Phase 1-2 Results



UQ Analysis by Monte Carlo Sampling (*Sampler*)

- **Sampler** provides uncertainty in any computed result from any SCALE sequence due to uncertainties in:
 - neutron cross sections (σ)
 - fission product yields (Y_f), decay data (λ), and branching fractions (b)
 - Model parameters such as dimensions (x) and compositions (ρ)



PWR Assembly UNF Uncertainties

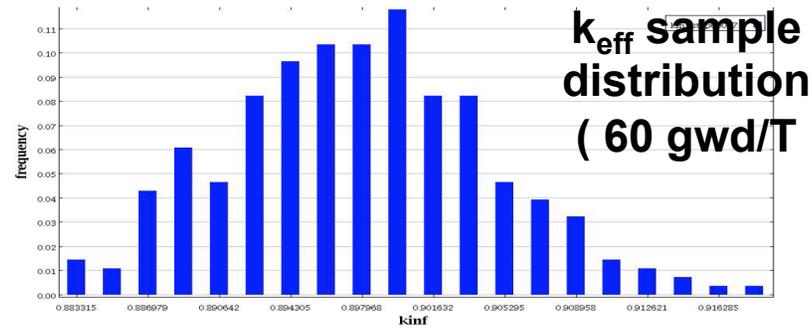
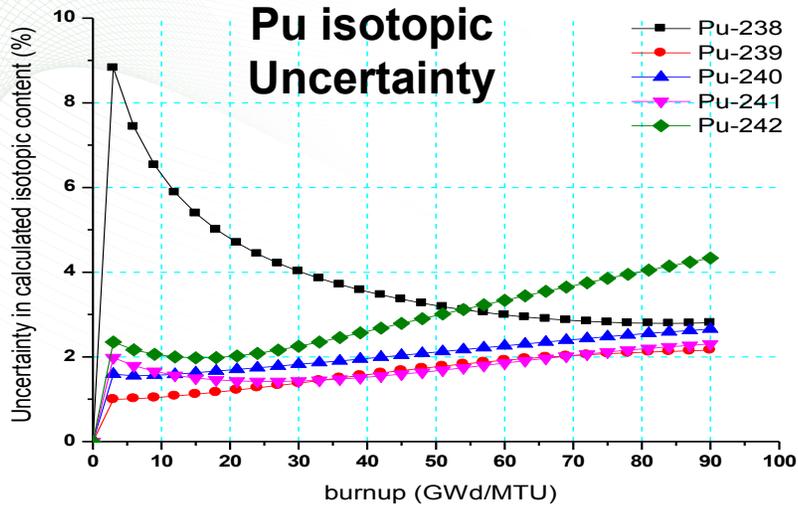
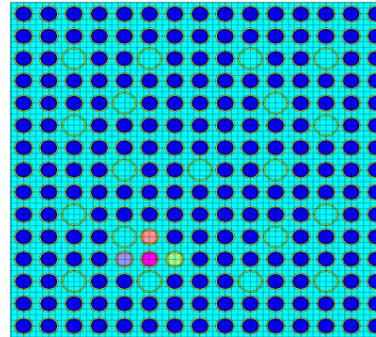
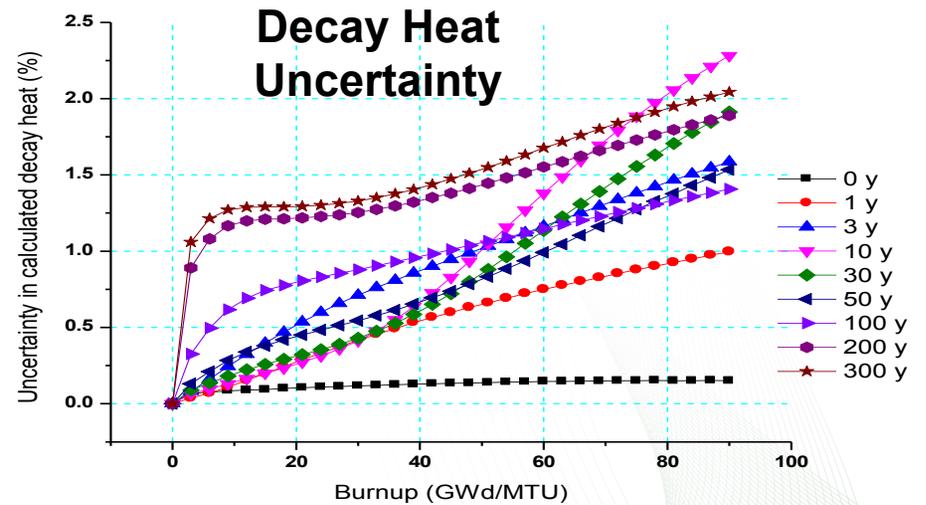


Figure 5. Distribution in sampled multiplication factors at 60 GWd/T burnup.

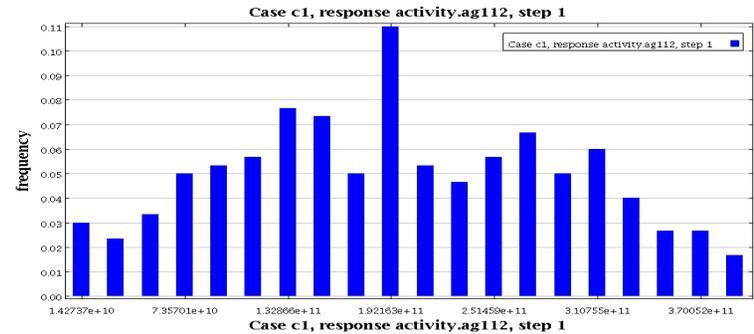
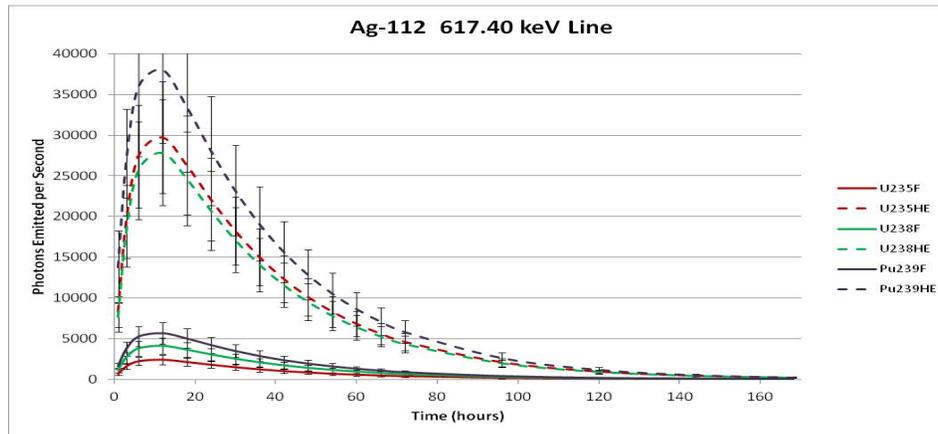
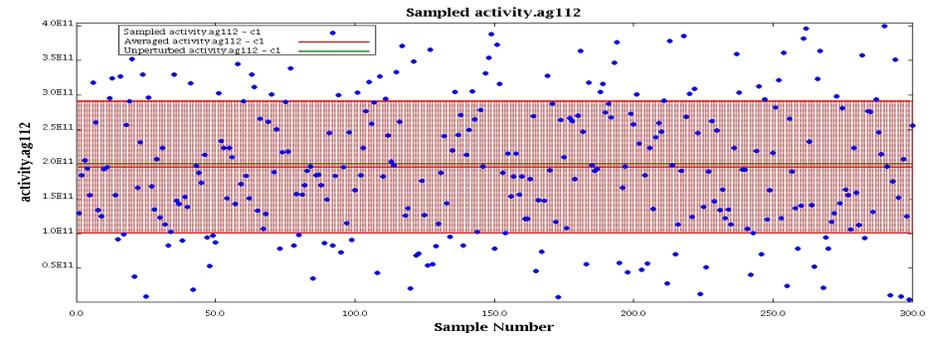
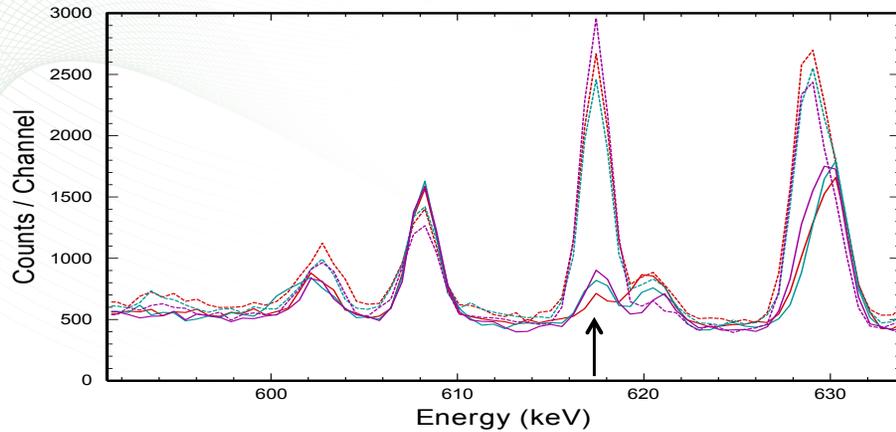


TRITON-NEWT assembly model



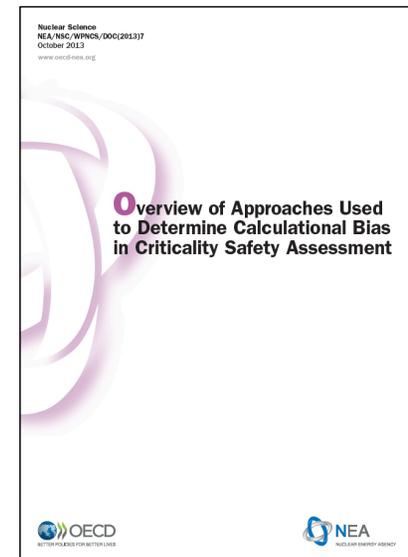
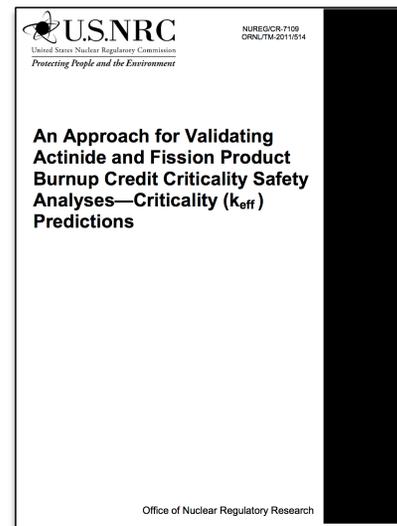
UQ for FP Gamma Spectral Analysis:

perturb XS, FP yields, decay, line intensity



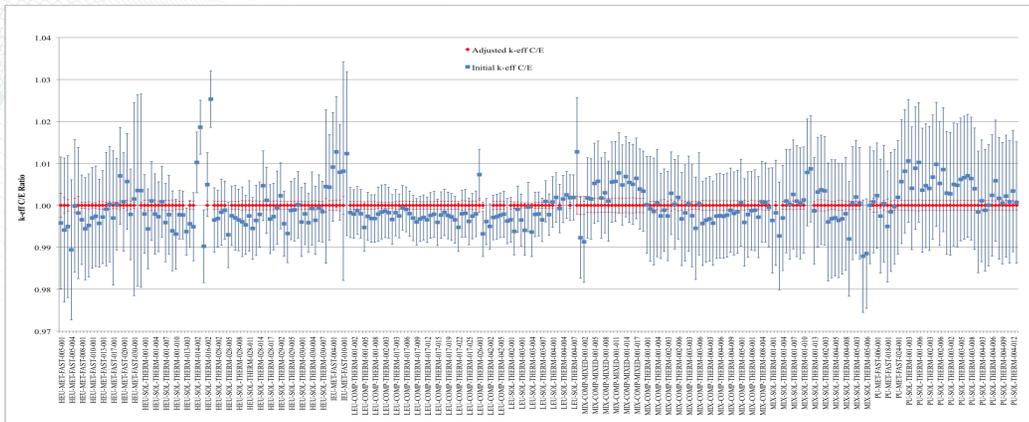
Sensitivity/Uncertainty Analysis in Practice

- ▶ U.S. Nuclear Regulatory Commission
 - ▶ Nuclear Materials Safety and Safeguards, Nuclear Reactor Regulation, Office of New Reactors
- ▶ National Nuclear Security Administration
 - ▶ Criticality safety assessment, experiment design
- ▶ U.S. DOE / Areva / Duke Energy
 - ▶ Mixed Oxide Fuel Fabrication Facility
- ▶ Candu Energy
 - ▶ ACR-1000 Design Validation
- ▶ Atomic Energy of Canada, Ltd.
 - ▶ ACR-700 NRC Review/PIRT
- ▶ U.S. DOE
 - ▶ Yucca Mountain post-closure criticality safety
- ▶ Global Nuclear Fuels
 - ▶ Transportation package licensing
- ▶ Svensk Kärnbränslehantering AB
 - ▶ Swedish used fuel repository
- ▶ Organization for Economic Cooperation and Development, Nuclear Energy Agency
 - ▶ International Expert Groups



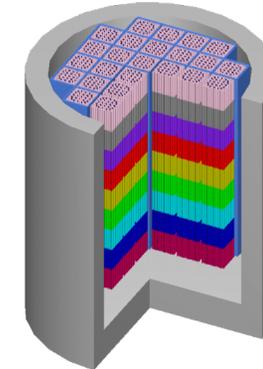
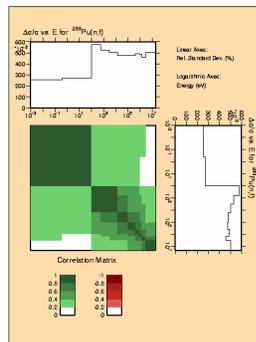
Assimilation

- Cross section adjustments to minimize bias and uncertainties in application responses

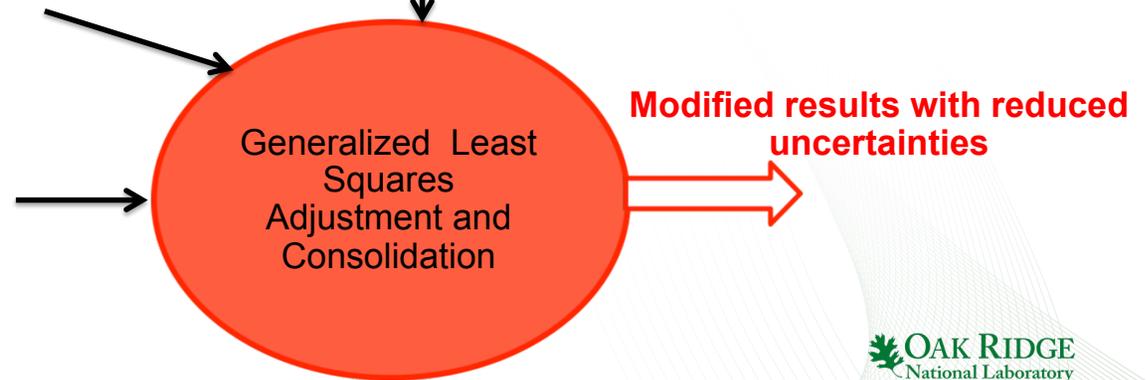


measured/computed responses and sensitivities for benchmarks; experimental uncertainties

nuclear data covariances



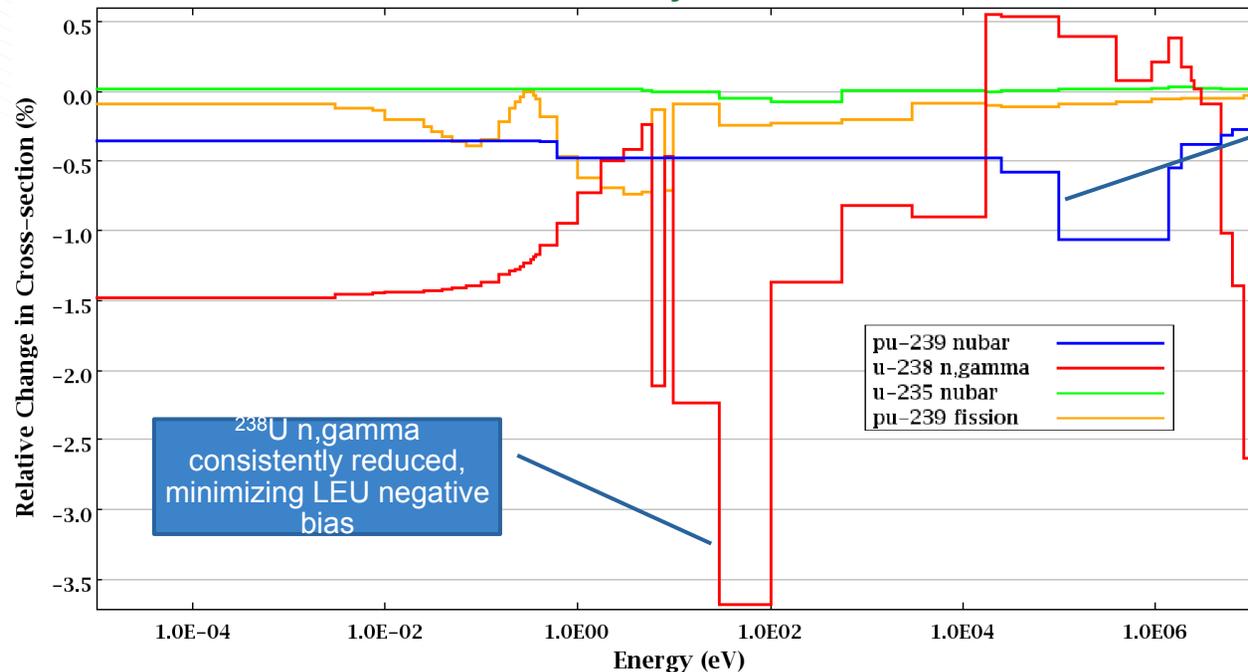
computed response and sensitivity for application response



Evaluated Differential Data Adjustment

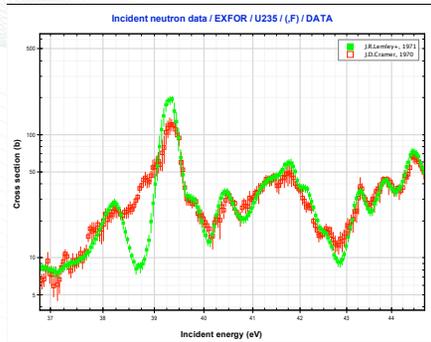
- Bayesian technique incorporates integral experiments with prior differential data to obtain adjusted differential data

Differences in Prior and Adjusted Differential Data

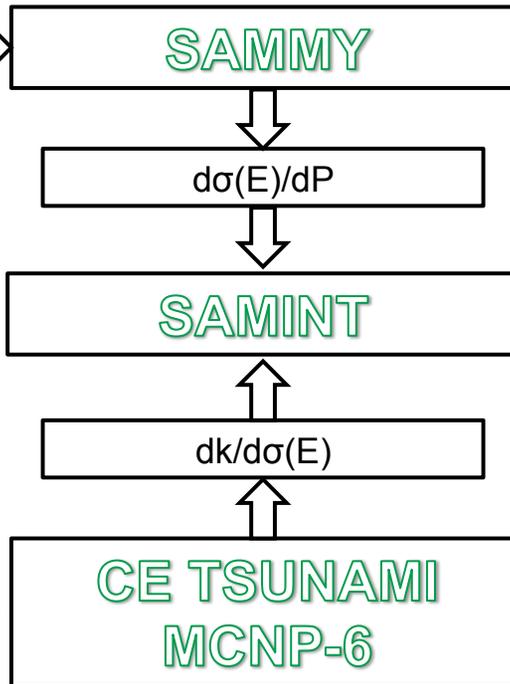


Using SAMINT with SAMMY

Differential Experimental Data



Integral Experimental Data



P stands for all resonance parameters: E_λ , Γ_γ , Γ_n , Γ_f , etc.

SCALE 6.0–6.1 Covariance Library (c. 2008) (401 materials)

Data Source	Materials
ENDF/B-VII.0	152,154-158,160Gd, 191,193Ir, 7Li, 99Tc, 232Th
ENDF/B-VII-p	197Au, 209Bi, 59Co, 23Na, 93Nb, 58Ni, 239Pu, 48Ti, 233,235,238U*, V
ENDF/B-VI	27Al, 241Am, C, C-graphite, 50,52-54Cr, 65Cu, 156Dy, 54,56-58Fe, In, 55Mn, 60-62,64Ni, 206-208Pb, 242Pu, 185,187Re, 45Sc, Si, 28-30Si, 89Y
JENDL 3.3	11B, 240,241Pu
JENDL 3.3+BLO	16O
SG-26	234,236U, 242,242mAm, 242-245Cm, 237Np, 238Pu
BLO LANL evaluation +JENDL 3.3	10B, 1H, H-ZrH, H-poly, Hfreegas
BLO LANL evaluation	6Li
BLO Approximate Data	225-227Ac, 107,109,110m,111Ag, 243,244,244mAm, 36,38,40Ar, 74-75As, 130,132,133,135-138,140Ba, 7,9Be, Bebound, 249,250Bk, 79,81Br, Ca, 40,42-44,46,48Ca, Cd, 106,108,110-114,115m,116Cd, 136,138,139-144Ce, 249-254Cf, Cl, 35,37Cl, 241,246-250Cm, 58,58mCo, 133-137Cs, 63Cu, 158,160-164Dy, 162,64,166-168,170Er, 253-255Es, 151-157Eu, 19F, 255Fm, Ga, 69,71Ga, 153Gd, 70,72-74,76Ge, 2,3H, Dfreegas, 3,4He, Hf, 174,176-180Hf, 196,198-202,204Hg, 165Ho, 127,129-131,135I, 113,115In, K, 39-41K, 78,80,82-86Kr, 138-140La, 175,176Lu, Mg, 24-26Mg, Mo, 92,97-100Mo, 14,15N, 94,95Nb, 142-148,150Nd, 59Ni, 235,236,238,239Np, 17O, 31P, 231-233Pa, 204Pb, 102,104-108,110Pd, 147,148,148m, 149,151Pm, 141-143Pr, 236,237,243,244,246Pu, 85-87Rb, 103,105Rh, 96,98-106Ru, S, 32-34,36S, 121,123-126Sb, 74,76-80,82Se, 144,147-154Sm, 112-120,122-125Sn, 84,86-90Sr, 181,182Ta, 159,160Tb, 120,122-126,127m,128,129m,130Te, 227-230,233,234Th, Ti, 46,47,49,50Ti, 232,237,239-241U, W, 182-184,186W, 123,124,126,128-136Xe, 90,91Y, Zr, 90-96Zr

ENDF/B-VII.0: evaluated covariance data released with ENDF/B-VII.0

JENDL-3.3: evaluated covariance data in JENDL-3.3

ENDF/B-VII-p: recently evaluated data proposed for future release of ENDF/B-VII.1

BLO approximate data: lo-fi covariances from BLO project (Brookhaven, Los Alamos, ORNL)

ENDF/B-VI: evaluated covariance data released with ENDF/B-VI

BLO LANL evaluation: LANL R-matrix evaluation from BLO project

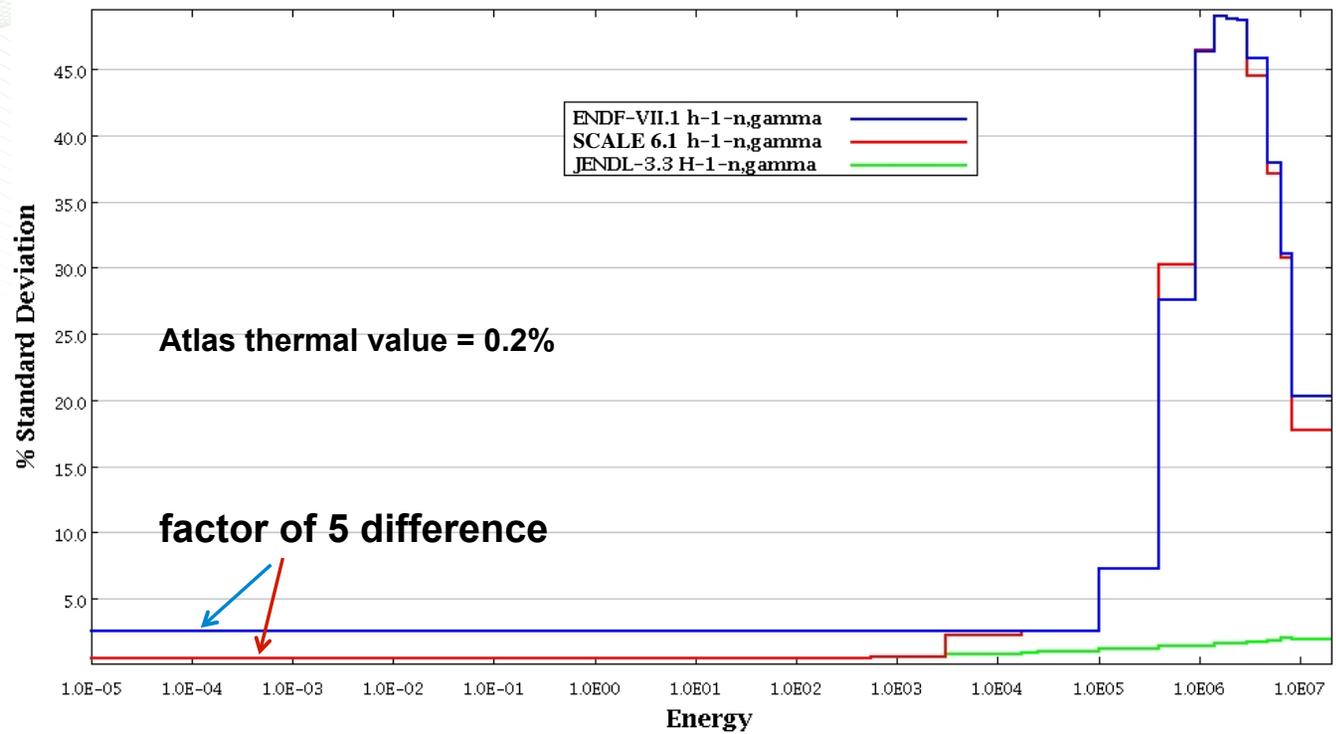
* 235U thermal nuubar data from JENDL 3.3

SG-26: approximate covariances from WPFC Subgroup-26

ENDF/B-VII.1 Covariance Nuclides

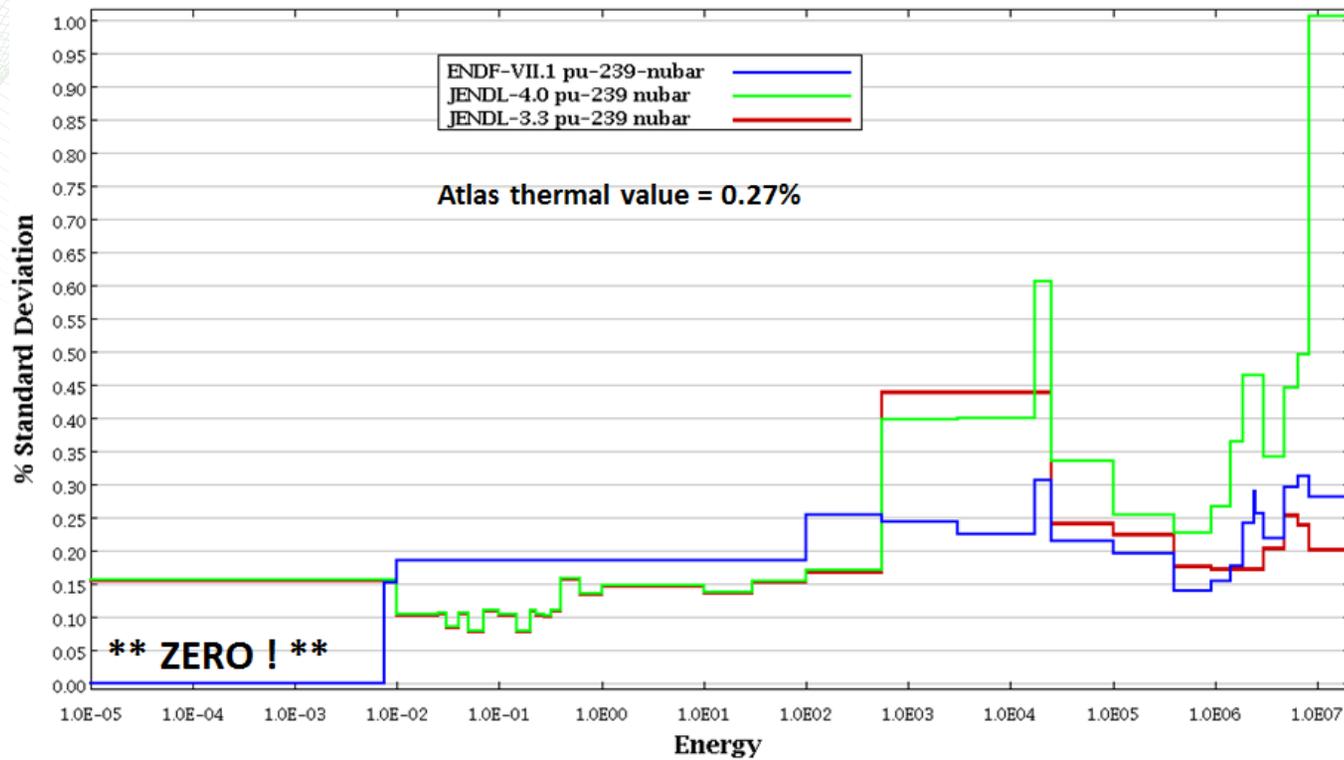
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h2	ti49	mo97	nd145	w184	u230	am243	es252
he4	ti50	mo98	nd146	w186	u231	cm240	es253
li6	cr50	mo100	nd148	ir191	u232	cm241	es254
li7	cr52	tc99	pm147	ir193	u233	cm242	es254m1
be9	cr53	ru101	sm149	au197	u234	cm243	es255
b10	cr54	ru102	sm151	tl203	u235	cm244	fm255
b11	mn55	ru103	sm152	tl205	u236	cm245	al_thermal
c	fe54	ru104	eu153	pb204	u238	cm246	fe_thermal
n15	fe56	ru106	eu155	pb206	np234	cm247	bebound
o16	fe57	rh103	gd152	pb207	np235	cm249	be-beo
f19	co59	pd105	gd153	pb208	np236	cm250	h-h2o
na23	ni58	pd106	gd154	bi209	np237	bk245	d-d20
mg24	ni60	pd107	gd155	ac225	np238	bk246	h-poly
mg25	y89	pd108	gd156	ac226	np239	bk247	h-zr2
mg26	zr90	ag109	gd157	ac227	pu236	bk248	o-beo
al27	zr91	i127	gd158	th227	pu237	bk249	o-u2o
si28	zr92	i129	gd160	th228	pu238	bk250	si28_si2o
si29	zr93	xe131	er166	th229	pu239	cf246	si29_si2o
si30	zr94	xe132	er167	th230	pu240	cf248	si30_si2o
cl35	zr95	xe134	er168	th231	pu241	cf249	u235_u2o
cl37	zr96	cs133	er170	th232	pu242	cf250	zr90_zr_zrh
k39	nb95	cs135	tm169	th233	pu244	cf251	zr91_zr_zrh
k41	mo92	la	tm170	th234	pu246	cf252	zr92_zr_zrh
ti46	mo94	ce141	w180	pa229	am240	cf253	zr93_zr_zrh
ti47	mo95	pr141	w182	pa230	am241	cf254	zr94_zr_zrh
							zr95_zr_zrh
							zr96_zr_zrh
							h-benzene
							benzene

H Capture Uncertainty



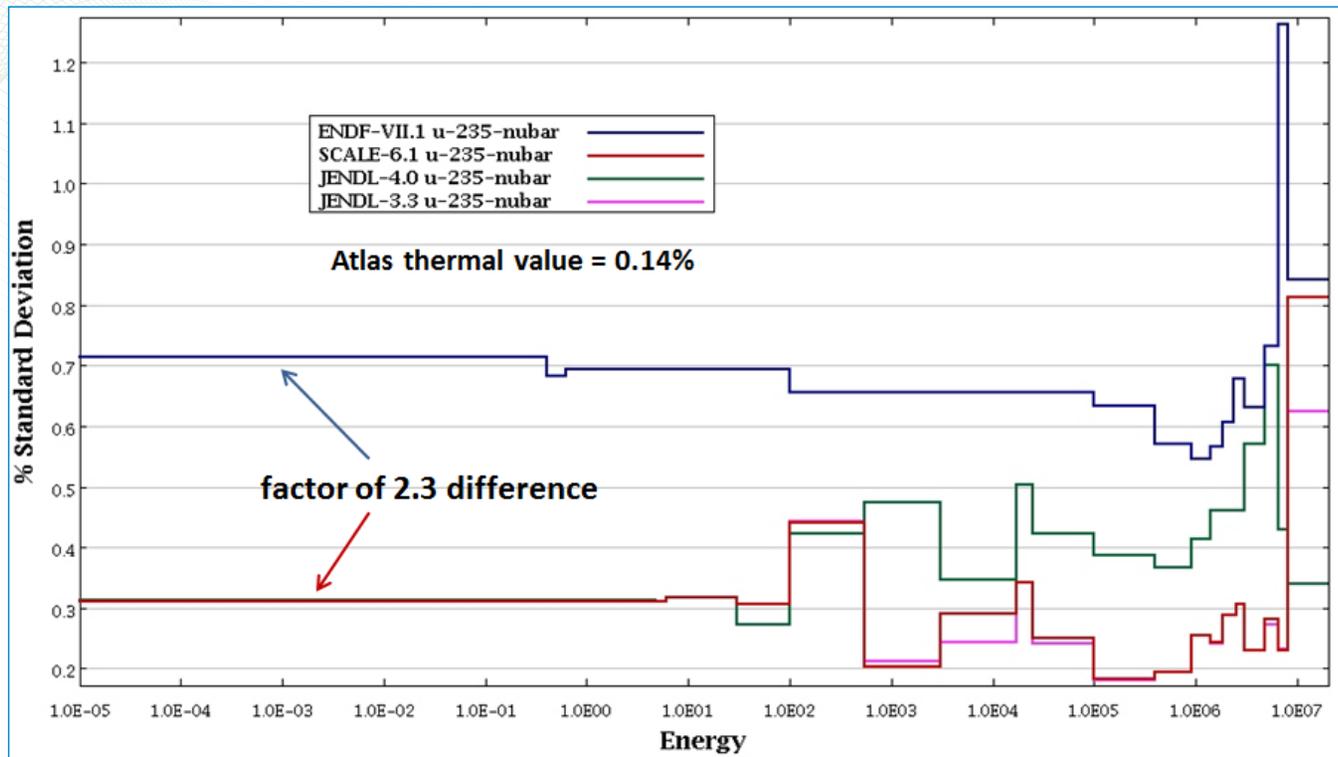
Corrected in ENDF/A

Pu-239 nubar uncertainty



Corrected in ENDF/A

U-235 nubar uncertainty

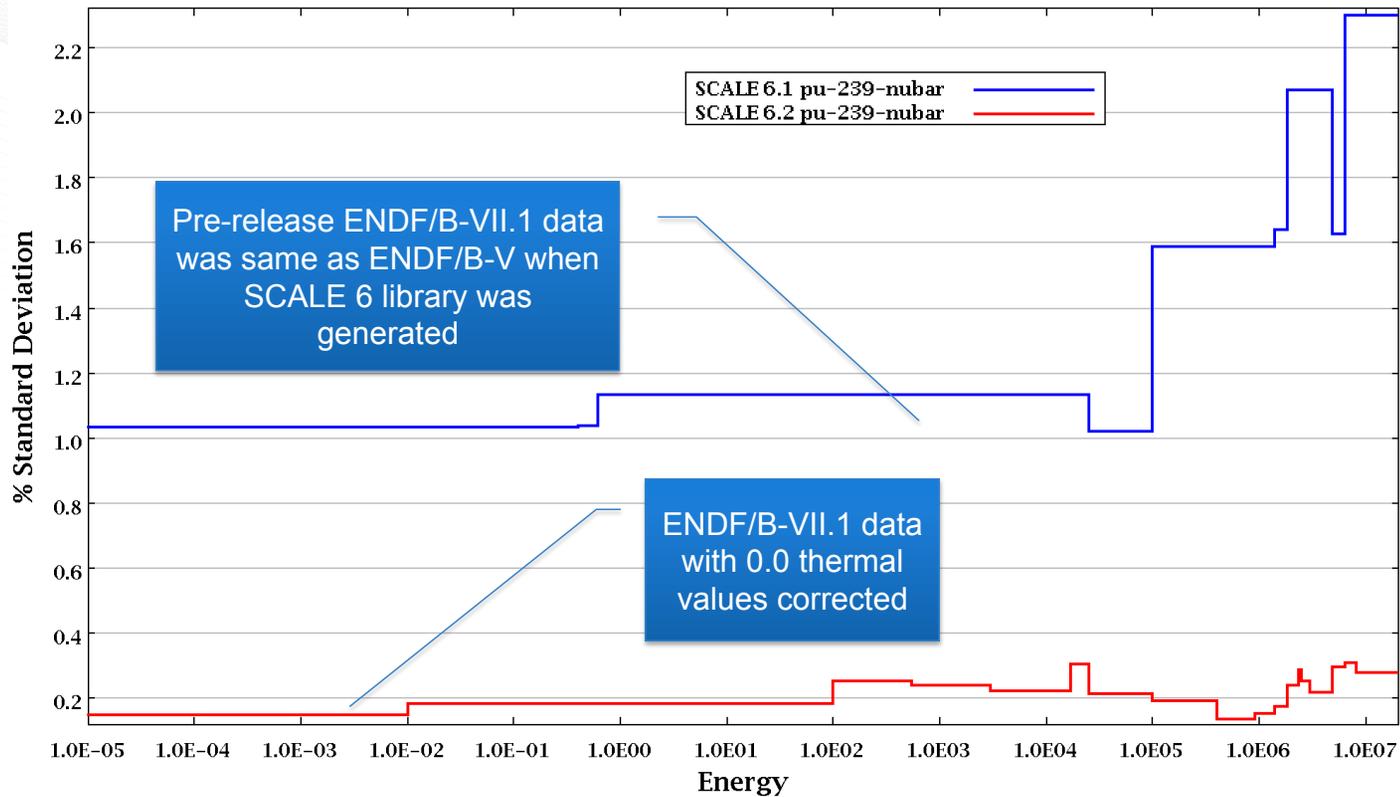


Corrected in ENDF/A

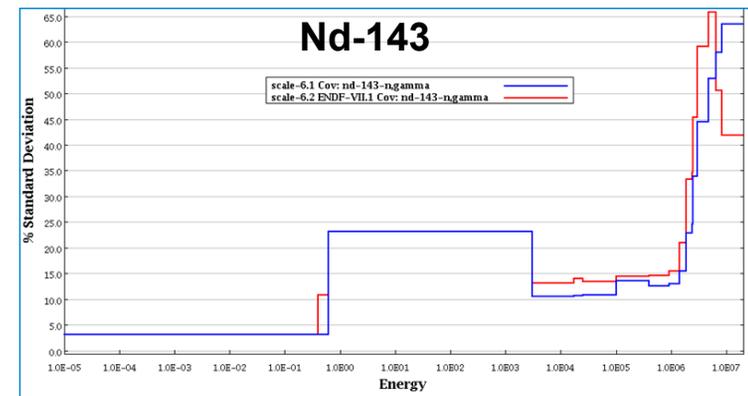
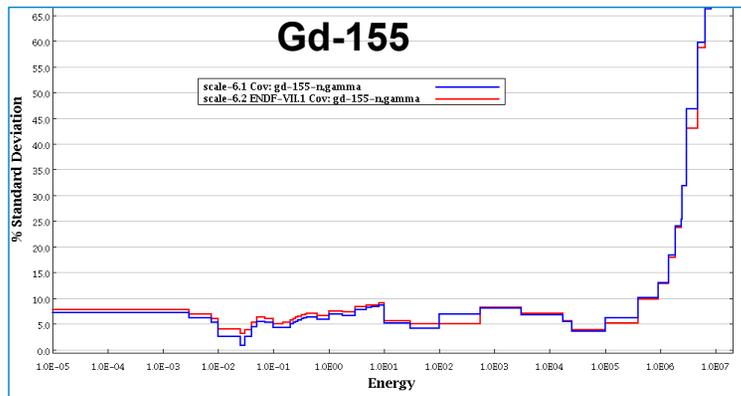
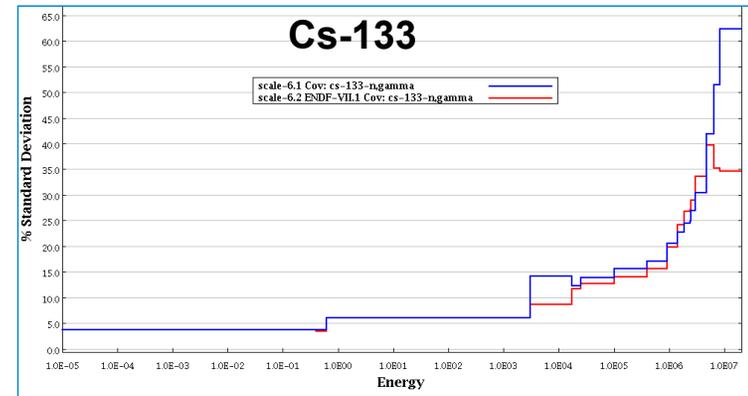
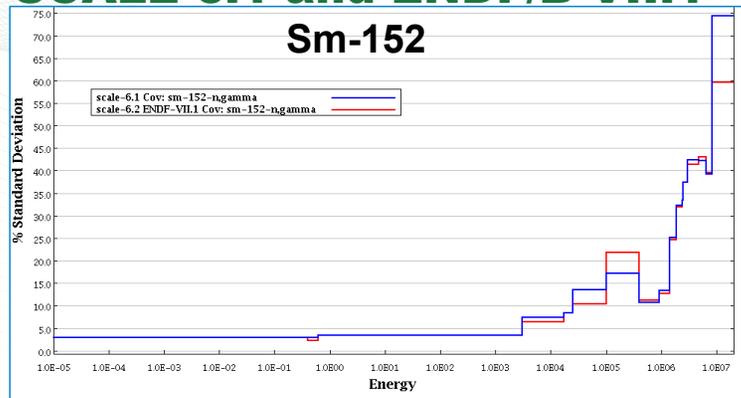
SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes;
- SCALE 6.1 data retained for ~215 missing nuclides
 - SCALE 6.1 includes covariance data from ENDF/B-VII.0, pre-released ENDF/VII.1, Lo-Fi uncertainties from BNL-LANL-ORNL, and other sources
- ENDF/A ^{235}U nubar, ^{239}Pu nubar and H capture uncertainties
- Chi uncertainties processed from new ENDF/B-VII.1 file 35
 - Many additional chi uncertainties included from JENDL
 - Previous SCALE chi uncertainties were generated from Watt spectrum data

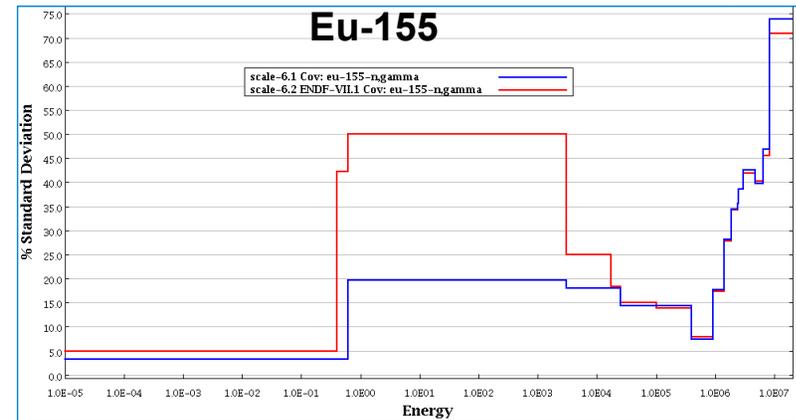
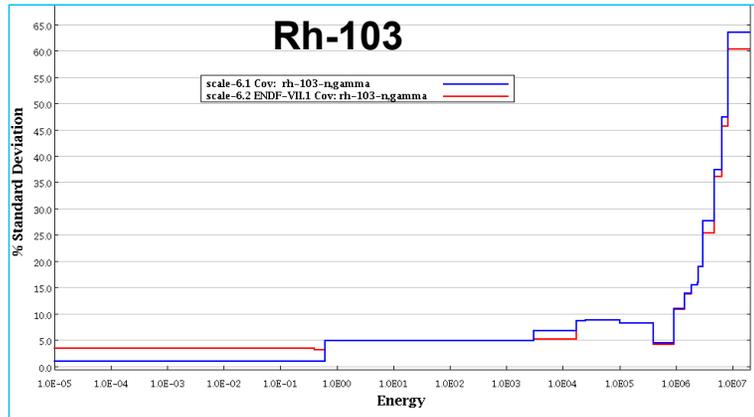
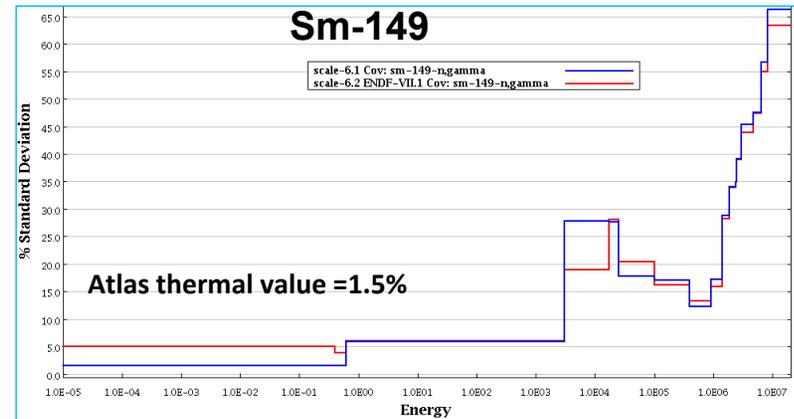
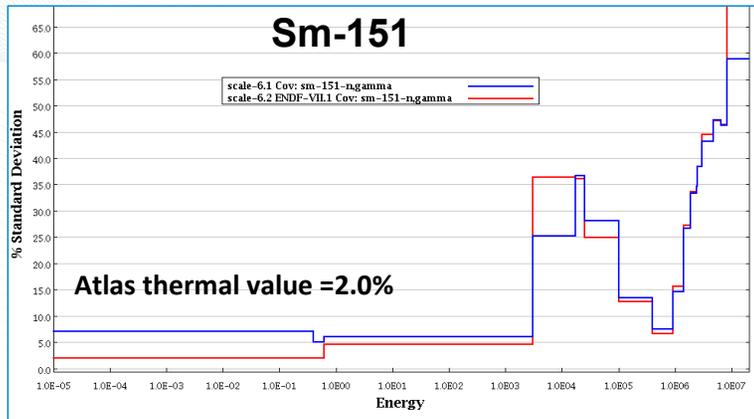
Pu-239 nubar uncertainty



Fission Product Capture Uncertainties in SCALE 6.1 and ENDF/B-VII.1

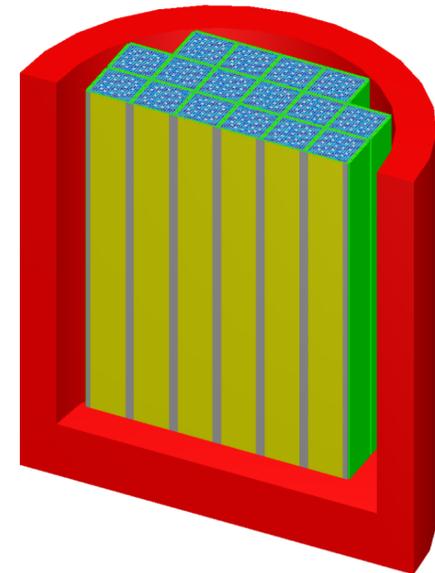


Fission Product Capture Uncertainties in SCALE 6.1 and ENDF/B-VII.1

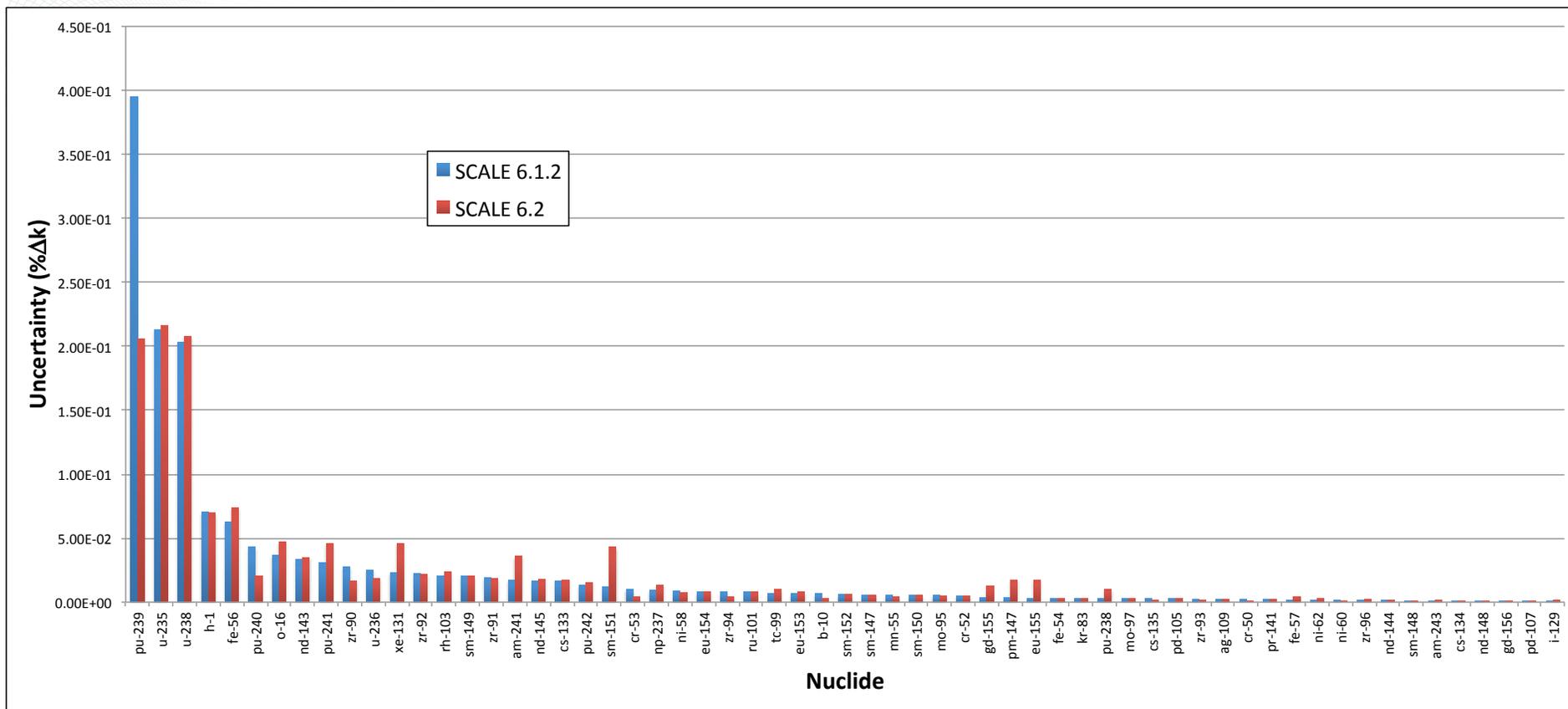


Criticality Analysis for Used Nuclear Fuel (UNF)

- UNF contains many actinides and fission products
- A limiting condition on UNF cask storage is sub-criticality margin
- NRC *Interim Staff Guidance 8 Rev. 3* allows “burnup credit” for burned fuel and certain FP nuclides
- Uncertainties are important consideration
 - SCALE 6.1 used in S/U for U.S. NRC



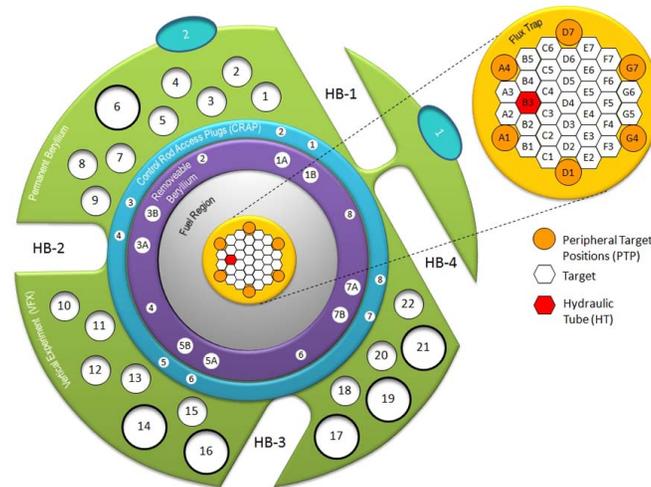
Top Contributors to Uncertainty for Spent Fuel Transportation



Motivation

- Need to Optimize Predictive Capabilities for the High Flux Isotope Reactor (HFIR)

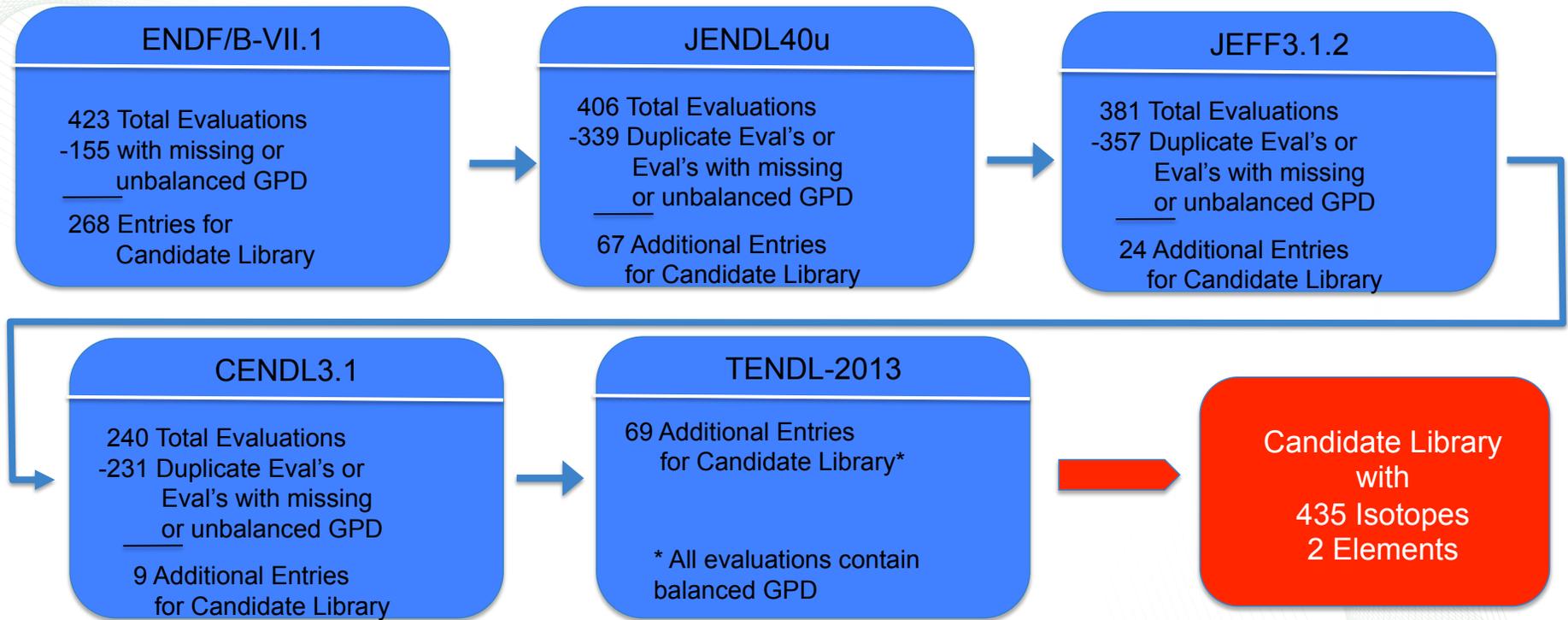
- Multiple Concurrent Missions for HFIR
 - Material irradiation experiments (MIE)
 - Isotope production (IP) campaigns
 - Four independent beam lines
- Demand is at an all-time high, and increasing
 - Reservation and advanced scheduling required for high-demand locations
- Cross section task is one part of a larger effort focused on HFIR modeling optimization



Library Definition (1/2)

- GPD (Rev. 0) Library
 - Most isotopes contain Gamma Production Data (GPD)
 - ^4He ($s_g=0$ in 16th Edition, Chart of the Nuclides) and
 - ^{22}Na (processing issues) are only exceptions
 - Evaluation is generally balanced
 - Few or no groups have non-physical (negative) KERMA
 - Multiple data repositories used to construct library
 - ENDF/B-VII.1, JENDL4.0u, JEFF3.1.2, CENDL3.1, TENDL-2013
 - Multiple formats to support various applications
 - Continuous Energy AMPX (CE Monaco, SHIFT)
 - Continuous Energy ACE (MCNP)
 - Multi-group AMPX (MG Monaco, Responses for CE Monaco/SHIFT)
 - Multi-group ANISN (ADVANTG, Denovo)

Library Definition (2/2)



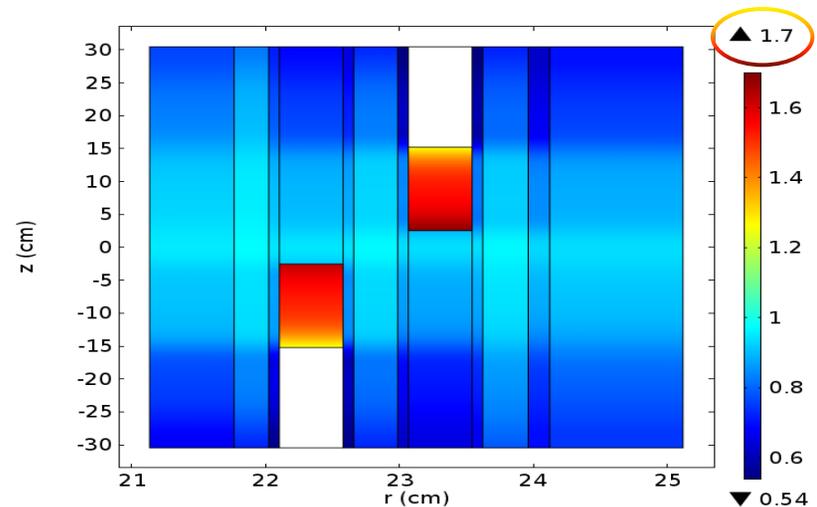
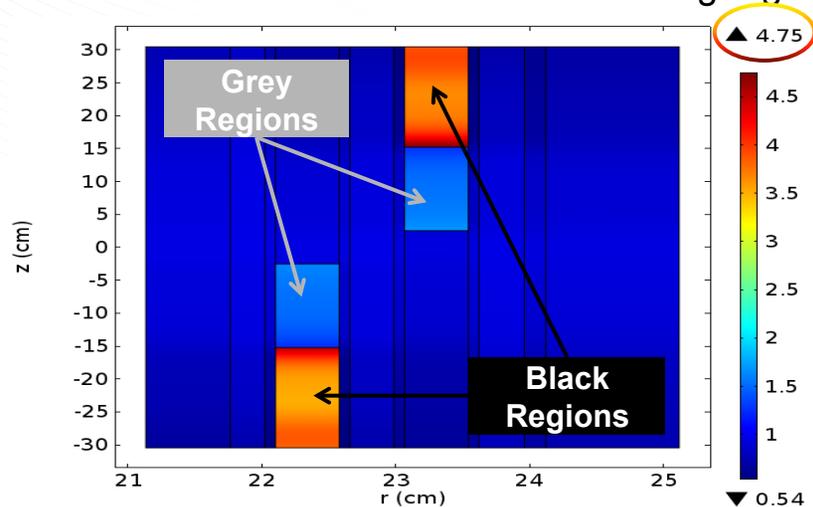
Isotopes with Negative KERMA Data

Table 2. Isotopes in ENDF/B-VII.1 That Have A Negative Neutron KERMA in at Least One Energy Group of the 200 Neutron-group Structure

Z	Isotope	Z	Isotope	Z	Isotope
16	S033	48	Cd115m	72	Hf174
16	S036	52	Te132	72	Hf176
28	Ni059	58	Ce143	72	Hf177
40	Zr092	60	Nd145	72	Hf178
40	Zr093	60	Nd147	72	Hf179
40	Zr094	62	Sm147	72	Hf180
40	Zr095	62	Sm149	79	Au197
40	Zr096	62	Sm151	80	Hg196
41	Nb093	64	Gd153	80	Hg202
42	Mo092	64	Gd155	81	Tl205
42	Mo094	68	Er166	83	Bi209
42	Mo096	69	Tm168		
42	Mo097				
42	Mo098				

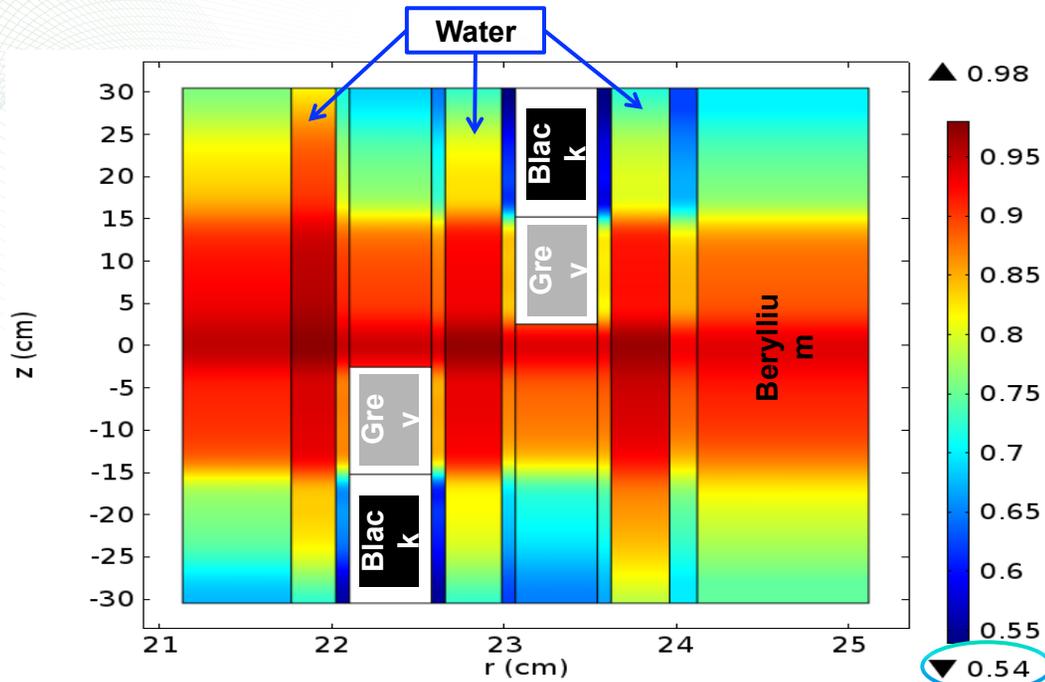
Cross-Section Development for Improved Energy Deposition Analyses - HFIR Control Elements (1/2)

- Energy deposition rates in materials composed of isotopes that lack gamma production data in evaluated nuclear data files are conservatively overpredicted.
- An initial subset of augmented cross-section libraries were used to analyze the energy deposition rates in the HFIR control elements and surrounding regions.



Ratio of energy deposition rates calculated with all ENDF/B-VII.0 cross-sections to those calculated with ENDF/B-VII.0 and a subset of augmented cross-sections.

Cross-Section Development for Improved Energy Deposition Analyses - HFIR Control Elements (2/2)



Regions not labeled are Aluminum. Ratio of energy deposition rates calculated with ENDF/B-VII.0 cross-sections to those calculated with ENDF/B-VII.0 and a subset of augmented cross-sections.

- A localized overprediction in energy deposition can lead to underpredicting the energy deposition in other regions leading to an incorrect spatial distribution of total heating rates.
- The use of the augmented cross-sections increased the predicted gamma energy deposition in the Al clad exterior to the black regions of the control elements by a factor of 1.5-2.0.
- No impacts on the effective neutron multiplicative factor, core fission densities, or neutron fluxes to the experiment facilities were observed due to the use of the augmented cross-sections.

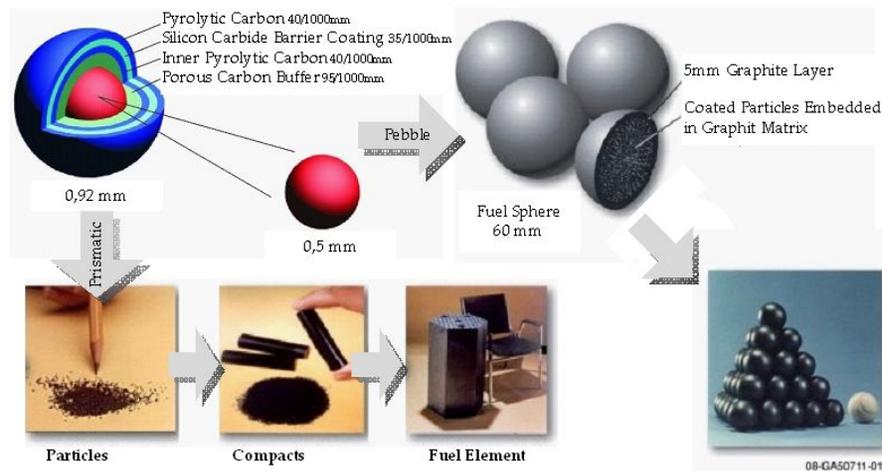
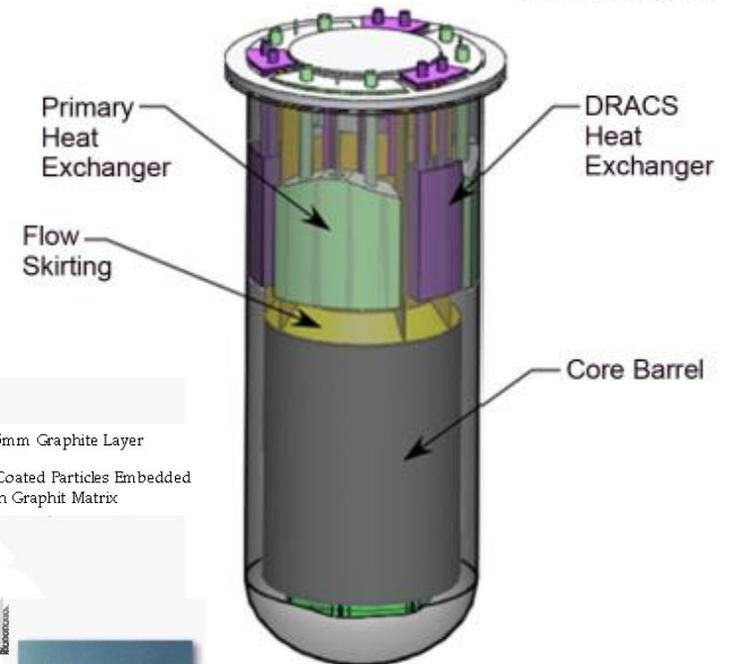
Fluoride Salt-Cooled High Temperature Reactor

Table 1. AHTR overall design values

Thermal power	3400 MW
Electrical power	1500 MW
Top plenum temperature	700 °C
Coolant return temperature	650 °C
Number of primary loops	3
Primary coolant	2^7LiF-BeF_2
Primary coolant flow rate	28,500 kg/s
Fuel type	Tri-structural isotropic particles in carbon plates
Fuel plates per assembly	18
Number of fuel assemblies	252
Uranium enrichment	9%
Refueling	2 batch, 6 month interval
Core height (fueled region)	5.5 m
Intermediate coolant salt	KF-ZrF ₄
Intermediate salt flow rate	43,200 kg/s

No S(α,β) data for FLiBe

ORNL 2011-G00112/chj



Wish List

- Apply tools to wide range of applications to identify areas for data improvement
 - Align needs with measurement and/or evaluation capabilities and capacity
- Complete set of covariance data – for everything – with high confidence
 - Neutron (all nuclides, all reactions), fission product yields, gamma production, gamma interactions, decay
 - Uncertainty on the uncertainty
- ^{239}Pu nubar investigation, ^{238}U n, gamma investigation
- Consistent fission product yield data (cumulative/independent yields)
- Complete set of gamma production and KERMA data
- $S(\alpha,\beta)$ for FLiBe