Low-fidelity Covariance Project

Bob Little

Los Alamos National Laboratory

Workshop on Neutron Cross Section Covariances

Port Jefferson, NY

June 26, 2008

LA-UR-08-4193

Co-authors (and Real Contributors!!)

- **Brookhaven National Laboratory**
  - Marco Pigni
  - Mike Herman
  - Pavel Oblozinsky
- **Oak Ridge National Laboratory**
  - Mark Williams
  - Mike Dunn
  - Goran Arbanas
  - Dorothea Wiarda
- **Los Alamos National Laboratory**
  - Toshihiko Kawano
  - Gerry Hale
- **Argonne National Laboratory**
  - Dick McKnight
- **U.S. Department of Energy**
  - Jerry McKamy
  - Jim Felty

Outline

- Motivation and Scope of Project
- Thermal and Resonance Range
- Fast Region – Structural, Fission Products, and Heavy Non-Fissile Isotopes
- Fast Region – Actinides
- Light Isotopes
- Current Status / Future Plans
- Summary

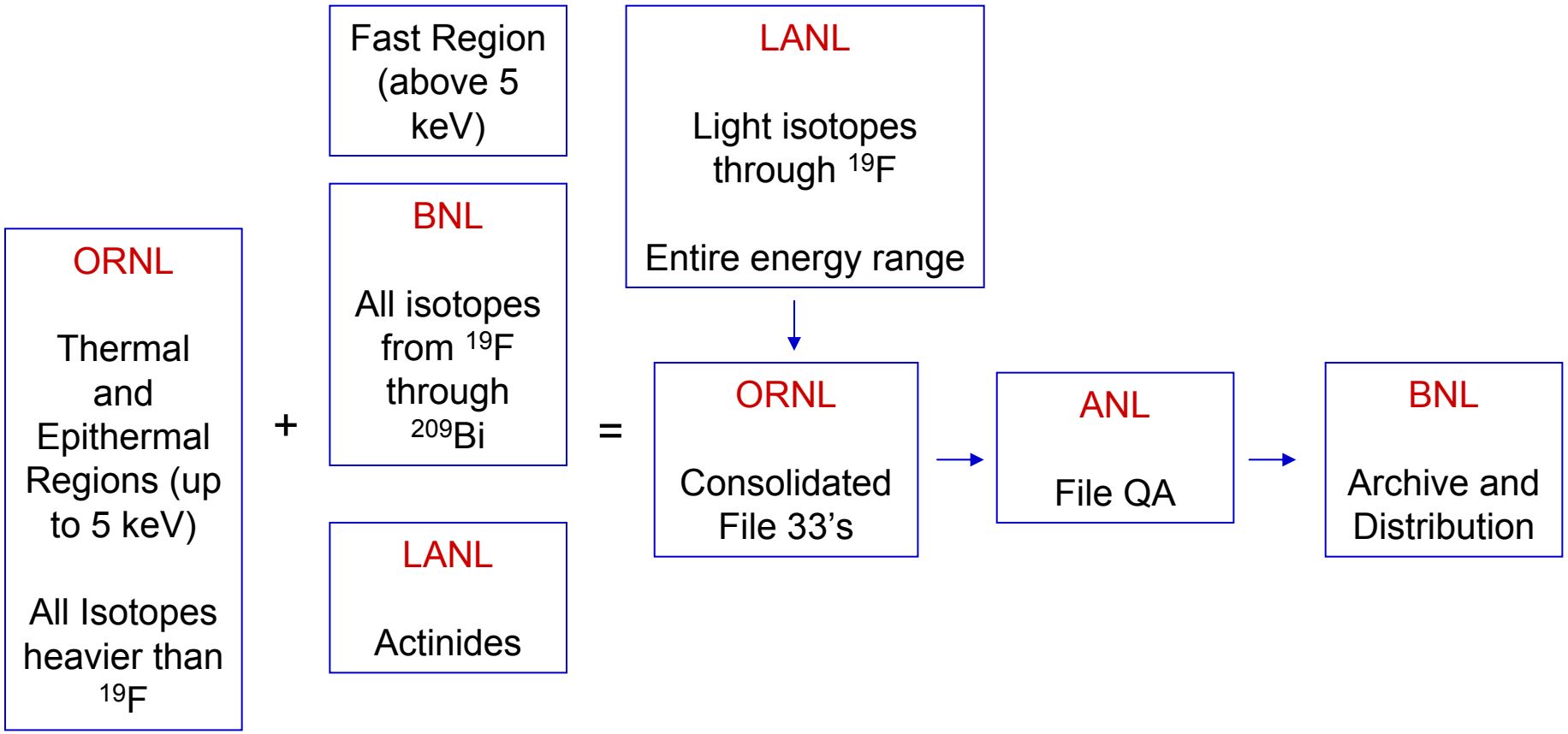
Motivation (circa June 2005)

- **Demand for Covariance Data ….**
  - Specifically for the AROBCAD Element of the USDOE Nuclear Criticality Safety Program (NCSP)
- **…. Far Exceeded the Supply**
  - ENDF/B-VII.0 included neutron evaluations for 393 materials, but covariance data (sometimes limited) for only 26 materials

Proposal Made to NCSP (McKamy / Felty)

- **Objective**
  - "Complete (in energy and reaction) set of covariance data for all ENDF/B-VII isotopes that could exercise our processing methodologies and be used by the AROBCAD Program Element."
- **Out of Scope**
  - "The goal is completeness, not high fidelity. In fact, to complete such a project in a short period requires that extremely crude approximations be made. Because of the necessarily approximate nature of the covariance data we will produce, we will not allow these data to be made available as part of a general-purpose ENDF/B release. Neither would the existence of this body of data remove at all the necessity for a more methodical and accurate evaluation of important covariance data, such as is underway at several Laboratories."

Project Work Flow



Note: "High-Fidelity" evaluations used if available

ORNL has contributed covariance data in the thermal and epithermal energy regions

- Multigroup covariance matrix is represented by three matrix partitions:
  - **Fast (F):** **E > 0.5 keV**
  - **Epithermal (H)** **0.5 eV < E < 0.5 keV**
  - **Thermal (T)** **E < 0.5 eV**
- ORNL Method – use uncertainties in measured integral data
  - **2200 m/s cross sections**
  - **Maxwell-averaged thermal cross sections**
  - **Infinitely dilute resonance integrals**
- Limited to MT's 1, 2, 18, 102

Standard deviations for epithermal and thermal data are based on uncertainty in integral parameters

- **Thermal data for 1/v cross section**
  - assume uniform relative uncertainty
  - single degree of freedom => full correlation
- **Thermal data for non-1/v cross section**
  - assume uniform relative uncertainty
  - ignore uncertainty in shape of data => full correlation
  - neglect uncertainty in g-factors
- **Most important moderator data is potential elastic which is constant over most of slowing range**
  - assume uniform relative uncertainty with full correlation
- **Resonance absorption in dilute concentrations depends mainly on *magnitude of RI***
  - ignore effects of uncertainty in shape of data
  - assume uniform relative uncertainty… initially with full correlation

Comparisons between evaluated and integral capture data are generally within the integral uncertainty

Thermal Cross Sections

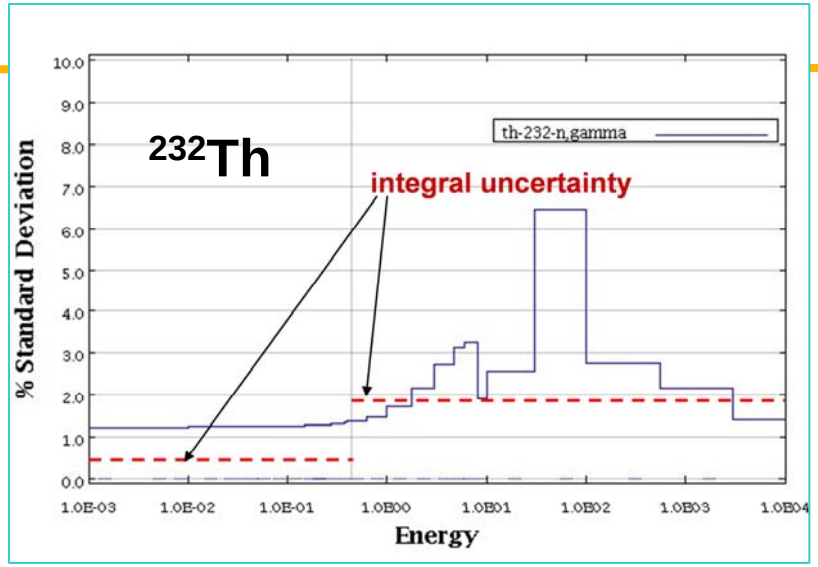
Nuclide	ENDF/B-VI	Integral(*)	difference
Cd-113	2.06E+4	2.06E+4 ± 1.9%	0%
Xe-135	2.63E+6	2.65E+6 ± 4.1%	-0.7%
Sm-149	4.02E+4	4.01E+4 ± 1.5%	0.2%
Np-237	1.81E+2	1.76E+2 ± 1.6%	-2.8%

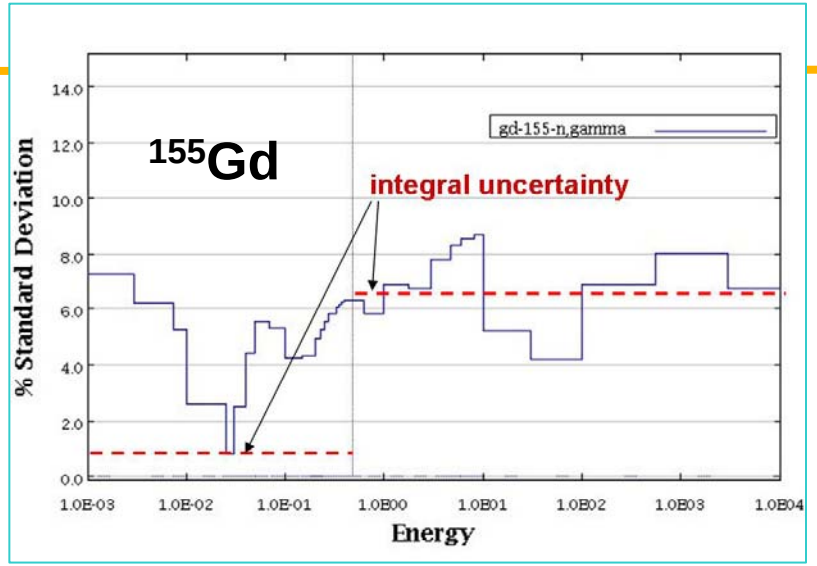
Resonance Integrals

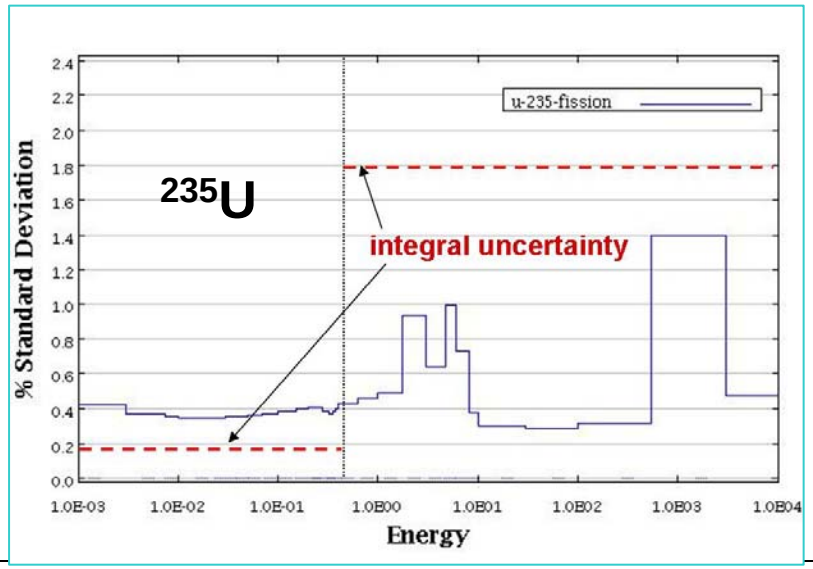
Nuclide	ENDF/B-VI	Integral(*)	difference
Cd-113	3.92E+2	3.90E+2 ± 10.3%	0.5%
Xe-135	7.65E+6	7.60E+3 ± 6.6%	0.7%
Sm-149	4.02E+4	4.01E+4 ± 5.9%	0.2%
Np-237	6.60E+2	6.40E+2 ± 7.8 %	3.0%

(*) *Atlas of Neutron Resonances*, S. F. Mughabghab

Low-Fidelity Uncertainties Compared with "High-Fidelity" Uncertainties



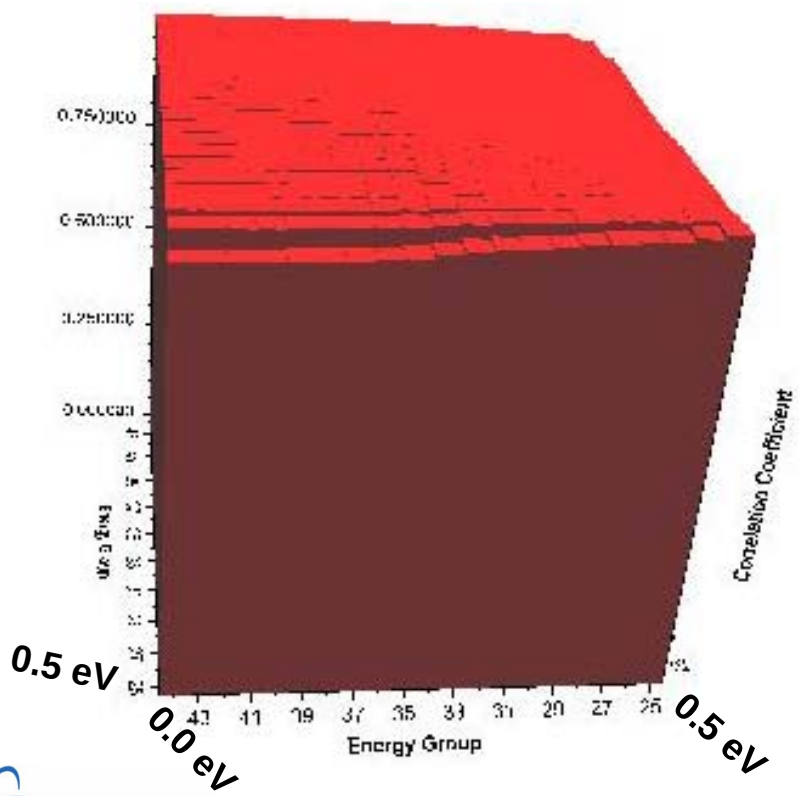




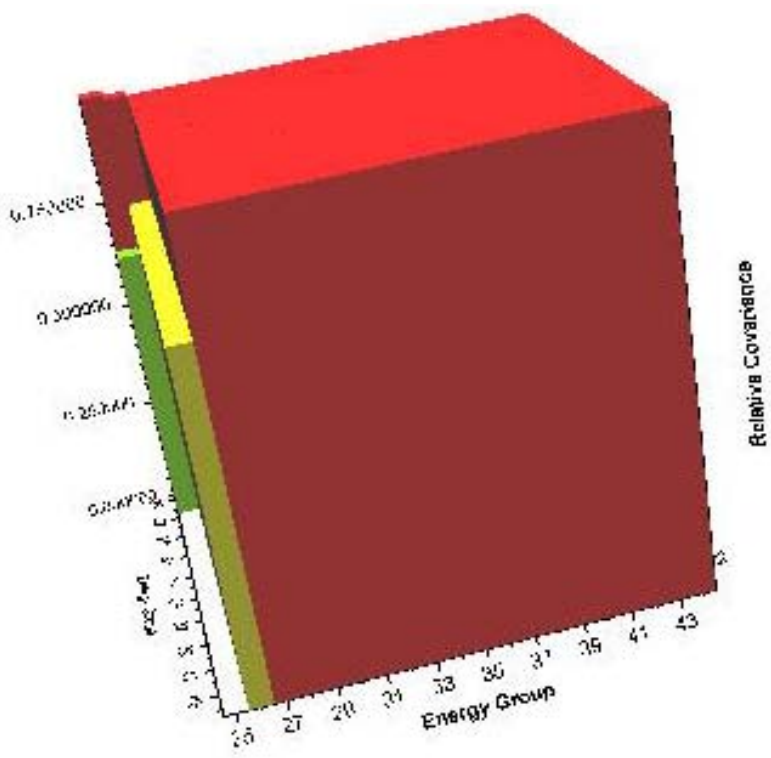
Los Alamos NATIONAL LABORATORY EST.1943

High-Fidelity versus Low-Fidelity Thermal Correlation Matrices for ^{232}Th *(1/v cross section)*

ENDF/B-VII

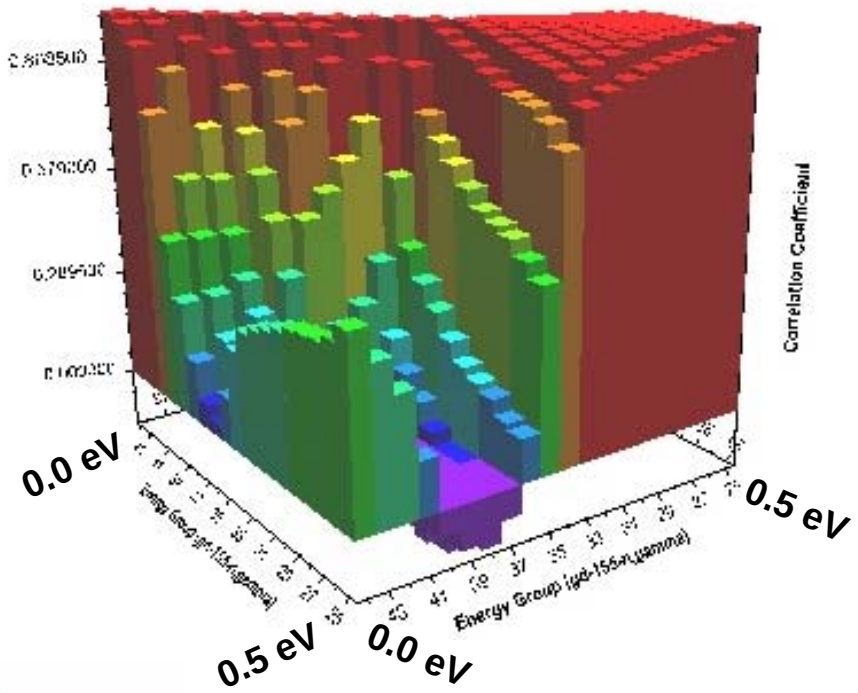


Integral Approximation

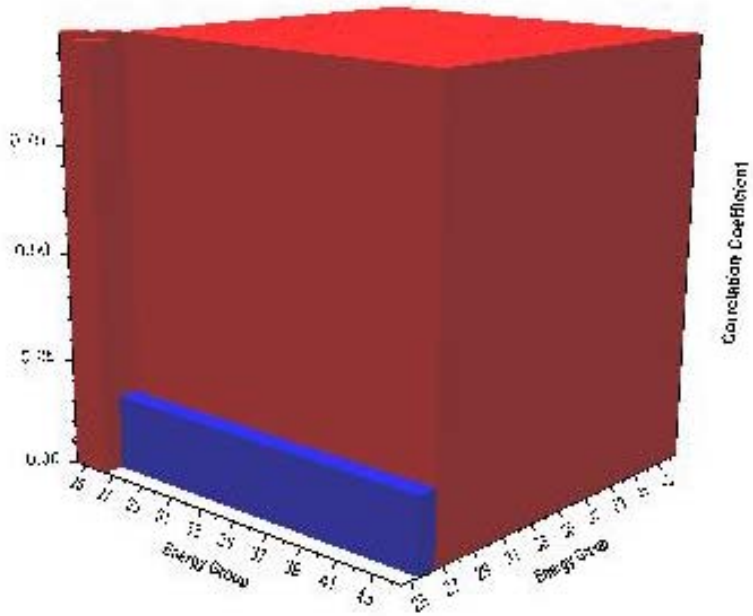


High-Fidelity versus Low-Fidelity Thermal Correlation Matrices for ^{155}Gd *(non-1/v cross section)*

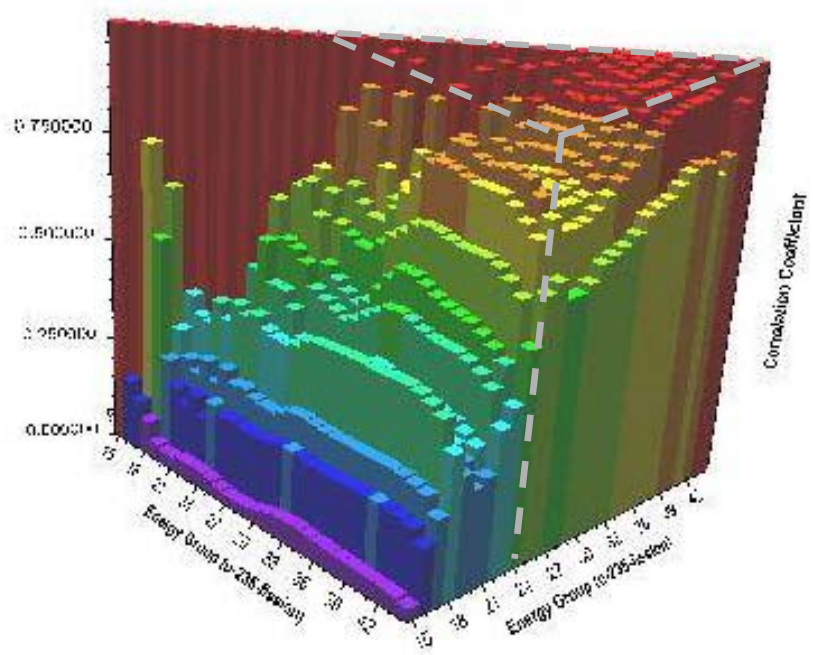
ENDF/B-VII



Integral Approximation

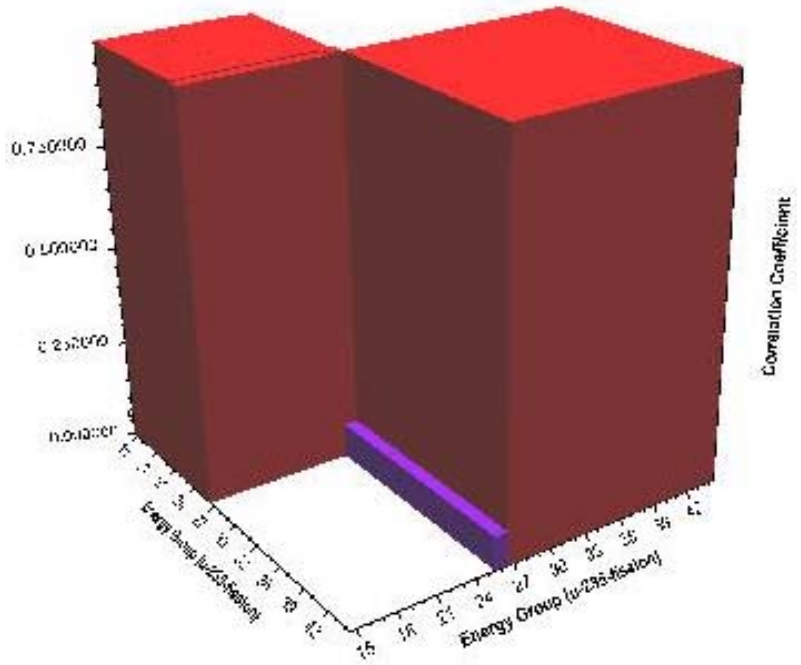


High-Fidelity versus Low-Fidelity Thermal and Epithermal Correlation Matrices for ^{235}U



proposed ENDF/B-VII

epithermal groups **thermal groups**



integral approximation (note zero correlation across thermal – epithermal)

Summary of ORNL Thermal – Epithermal Results

- Complete for all materials in ENDF/B-VII.0
- Updated to use data from 2006 Atlas
- Integral approximation provides simple method to generate low fidelity uncertainty data in thermal and epithermal ranges
- Comparisons with limited high-fidelity data indicate
  - approximation tends to underestimate thermal uncertainty
  - tends to overestimate resonance range uncertainty
  - full correlations in epithermal appear to be overly conservative
  - More testing using sensitivity analysis is being done
- See reference in AccApp07 proceedings by Williams et al.

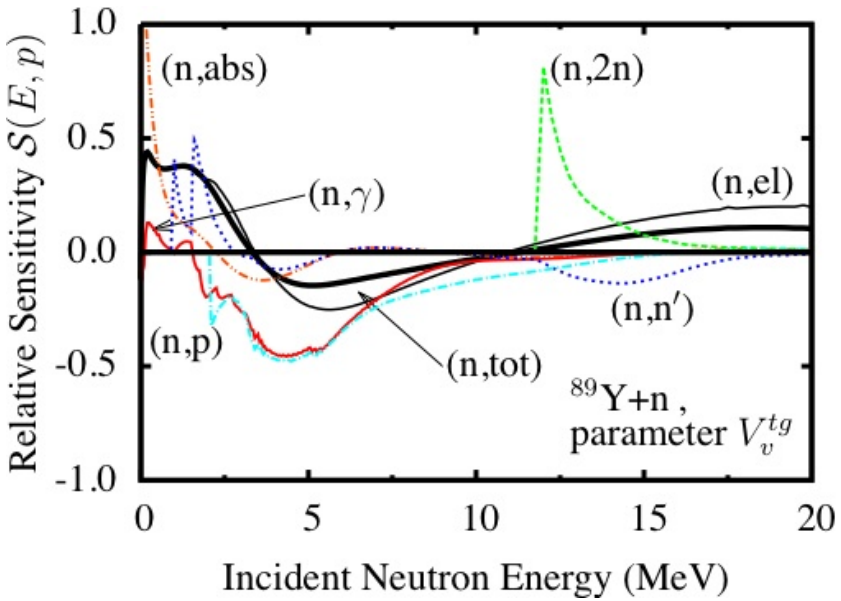
BNL Fast (> 5 keV) Low-Fidelity Methodology (1)

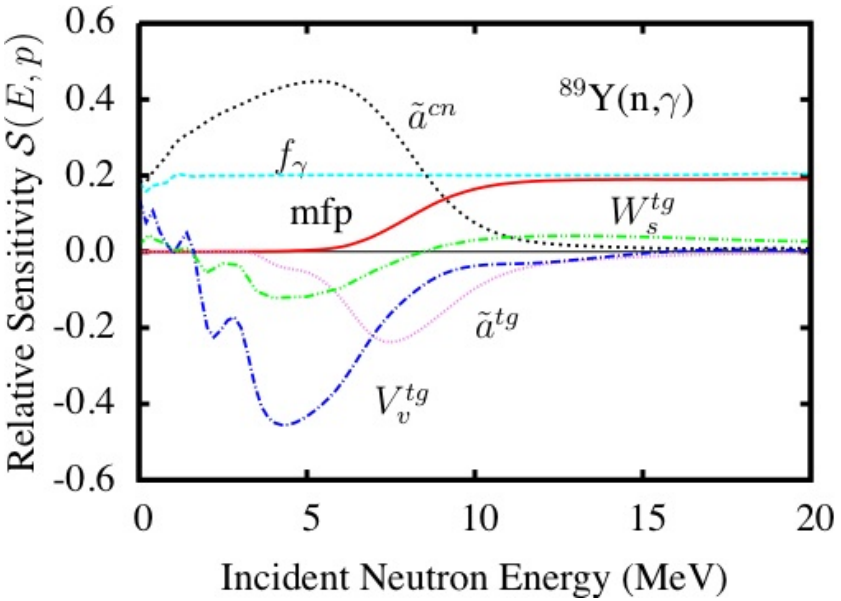
- **Relied upon**
  - EMPIRE nuclear reaction model code, and
  - KALMAN Bayesian filtering code
- **Minimal utilization of experimental data**
  - Occasionally consulted to check the quality of results
- **Nominal set of models and model parameters chosen (and used globally)**
- **Eighteen (18) model parameters that contribute most significantly to reaction cross sections were assigned uncertainties**
  - Assumed model parameters were uncorrelated

BNL Fast (> 5 keV) Low-Fidelity Methodology (2)

- Calculated sensitivities of cross sections to model parameter uncertainties
- Considered total, elastic, inelastic, capture, and (n,2n) reaction channels
- Covariance results provided at 30 incident energies between 5 keV and 20 MeV

Calculated sensitivities of ^{89}Y neutron cross sections to variations in model parameters

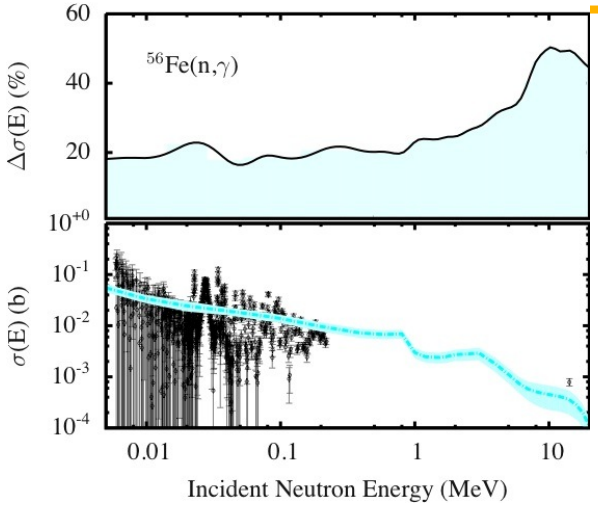


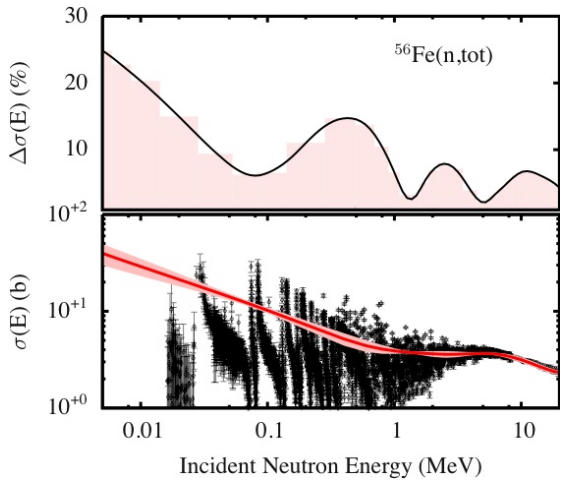


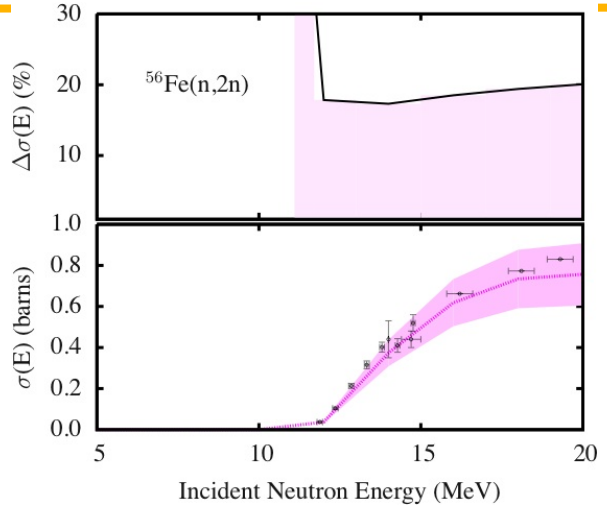
Relative sensitivity of various reaction channels to 5% perturbation of real depth optical model parameter V_v^{tg}

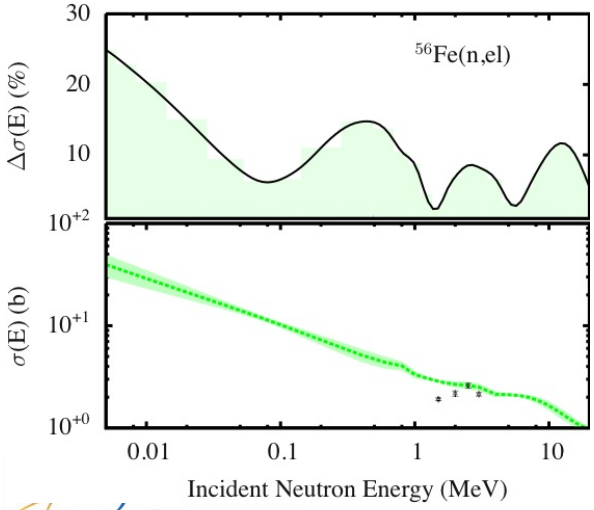
Relative sensitivity of capture cross section to perturbations of various model parameters

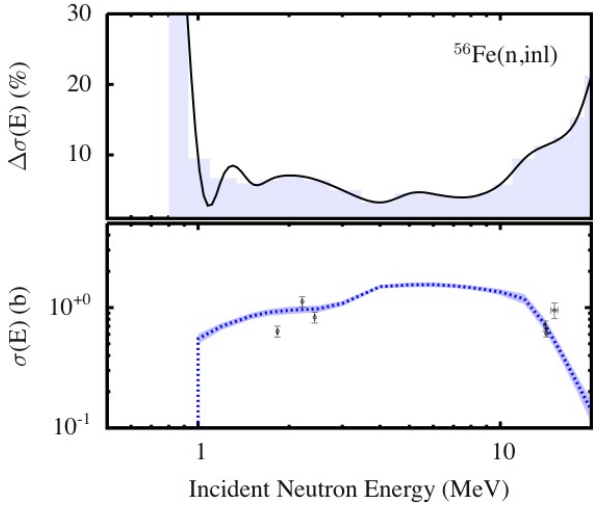
Calculated uncertainties of ^{56}Fe reactions





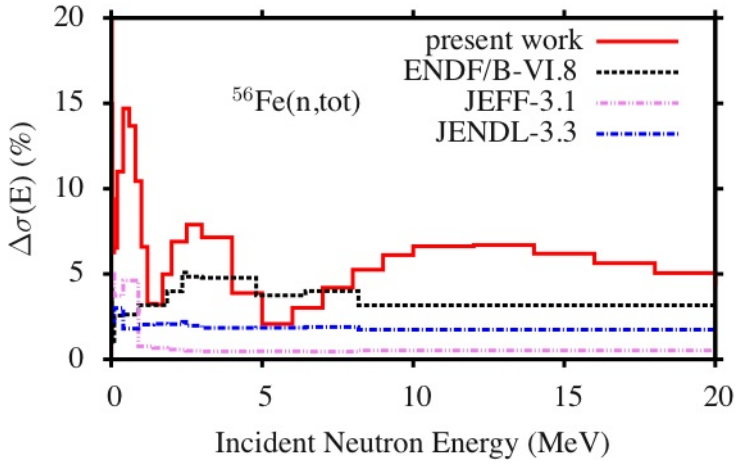


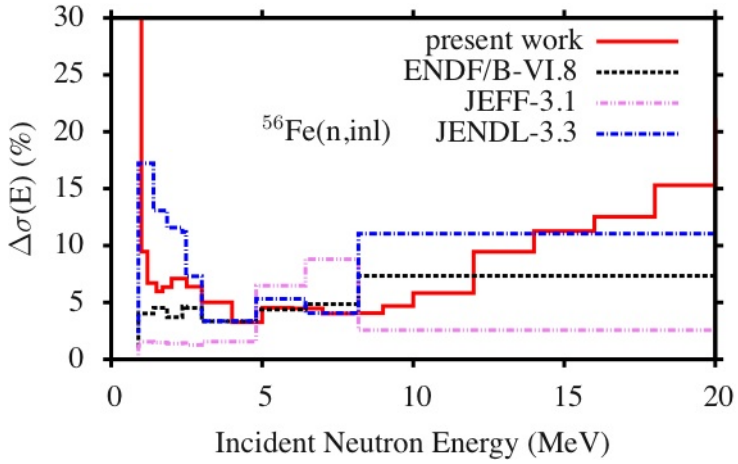


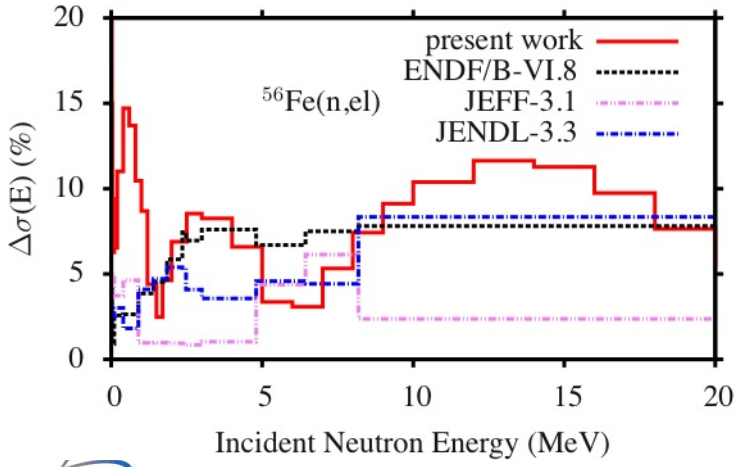


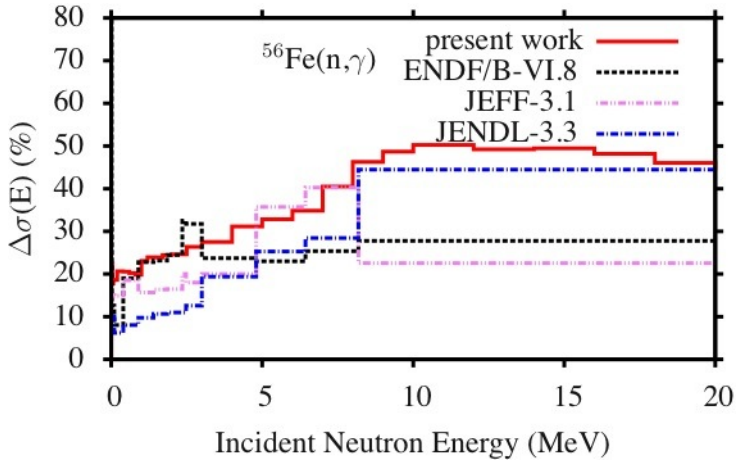
Los Alamos NATIONAL LABORATORY EST.1943

Comparison of ^{56}Fe Low-Fidelity Uncertainties to Values from Modern Evaluations



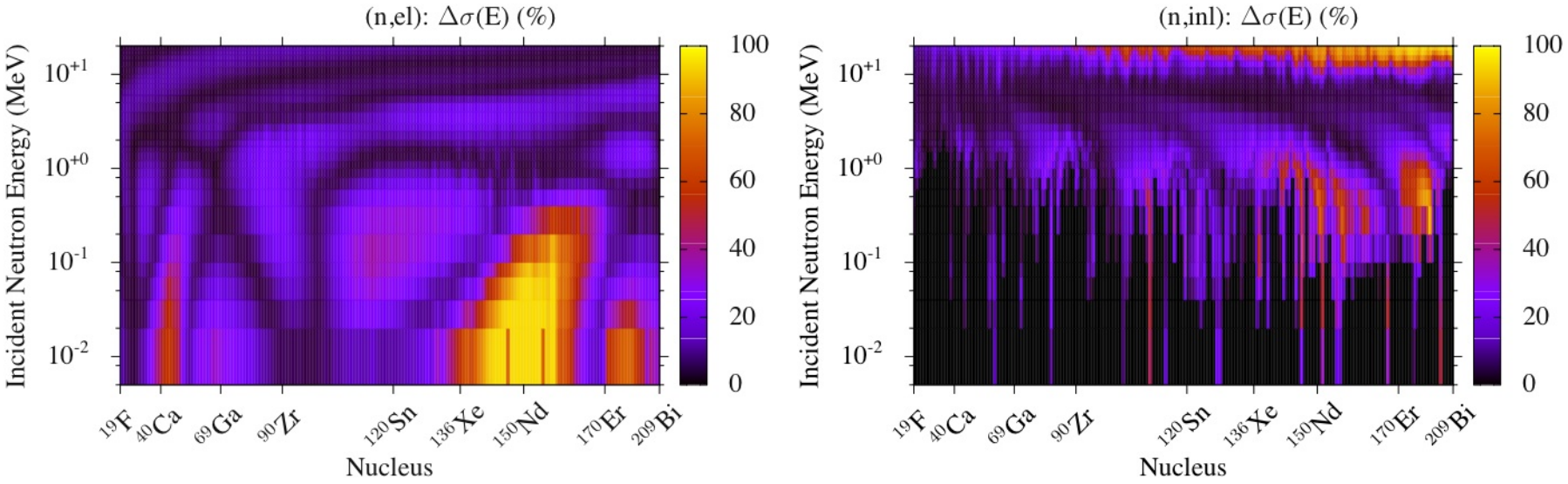




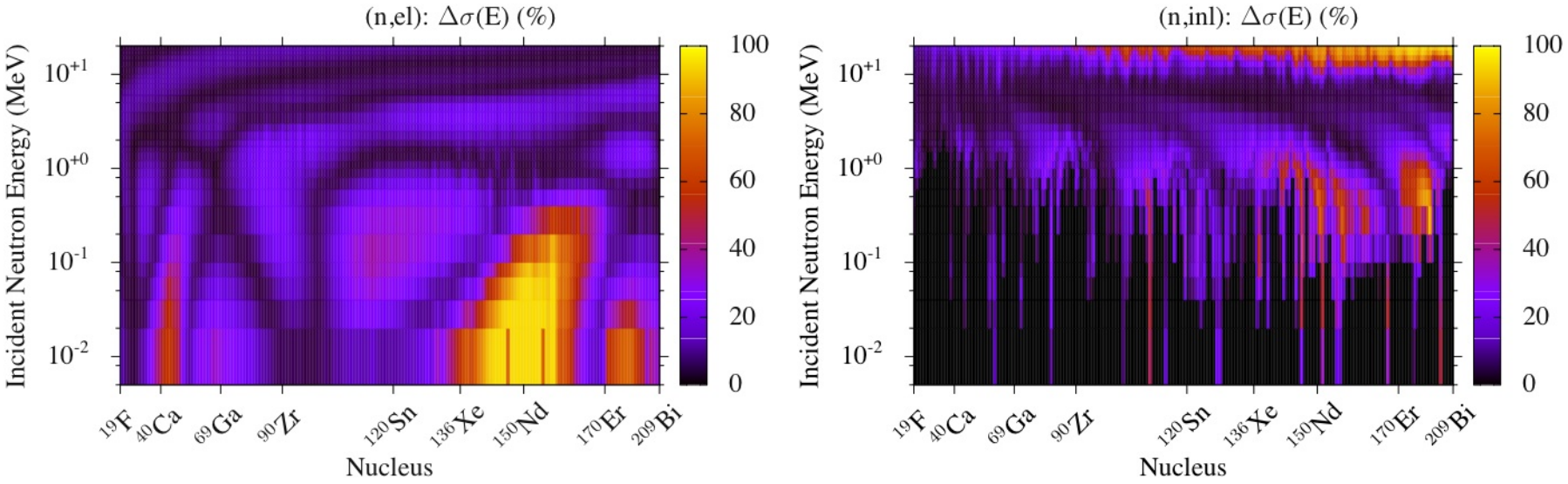


Los Alamos NATIONAL LABORATORY EST.1943

Uncertainties for 307 materials from 5 keV to 20 MeV for elastic and inelastic cross sections



Uncertainties for 307 materials from 5 keV to 20 MeV for elastic and inelastic cross sections



Available for $12.95 from www.MarcoPigni.com

Summary of BNL Fast Results

- Complete for 307 materials in ENDF/B-VII.0
  - **57 structural isotopes from ^{19}F – ^{nat}Zn**
  - **219 fission products from ^{69}Ga – ^{170}Er**
  - **31 heavy non-fissile nuclei from ^{175}Lu – ^{209}Bi**
- Results have been reviewed for physical insight
- Publication has been submitted to NSE

LANL Approach for Fast-Region (> 5 keV) Actinide Covariances

- **Use high-fidelity evaluations for ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu**
- **Adopt SG26 results (Rochman et al.) for 14 additional actinides**
- **47 actinides remaining in ENDF/B-VII.0 from ^{225}Ac through ^{255}Fm**
  - KALMAN-CoH calculations for total (MT=1) and capture (MT=102)
  - KALMAN-GNASH calculations for (n,xn) reactions (MT = 4, 16, 17, and 37)
  - Simple estimation by Kawano for fission (MT = 18) and ν
  - Elastic = Total – Sum of other reactions
  - Energy range from 5 keV to 20 MeV

Actinides: Total, Capture, and (n,xn) Cross Sections

Total Cross Section

- Simple estimates from optical model calculations
- Sensitivities calculated for 9 potential parameters (CoH code)
- Parameter uncertainties assumed
- The uncertainties are reduced, if experimental data were used, or some systematic study was made (U isotopes or Pa231, Pa233 for example)

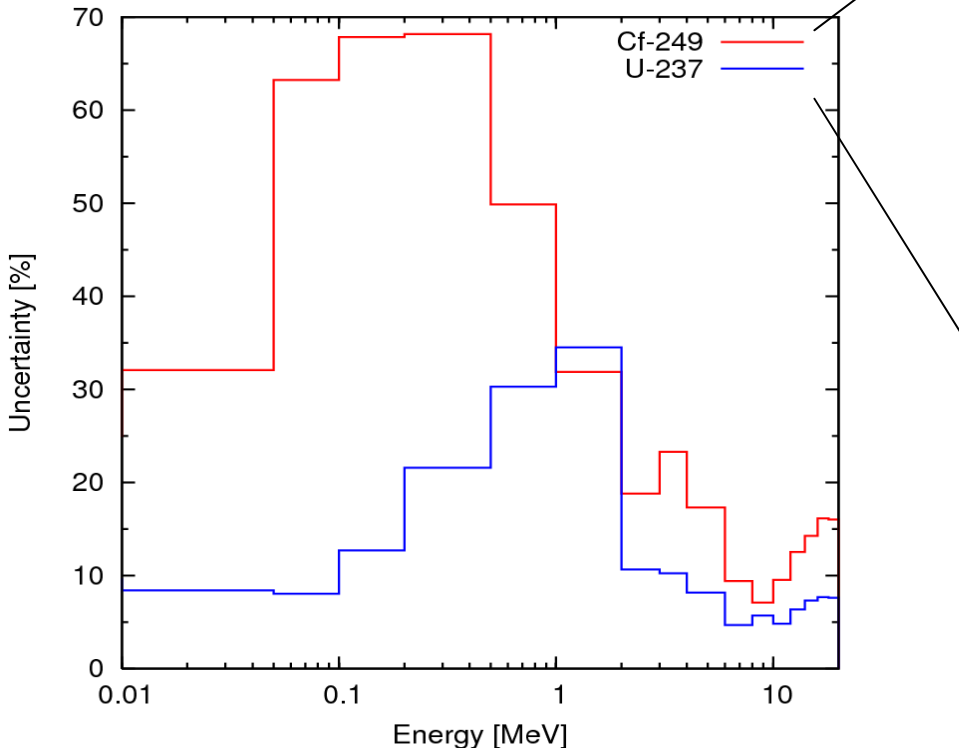
Capture Cross Section

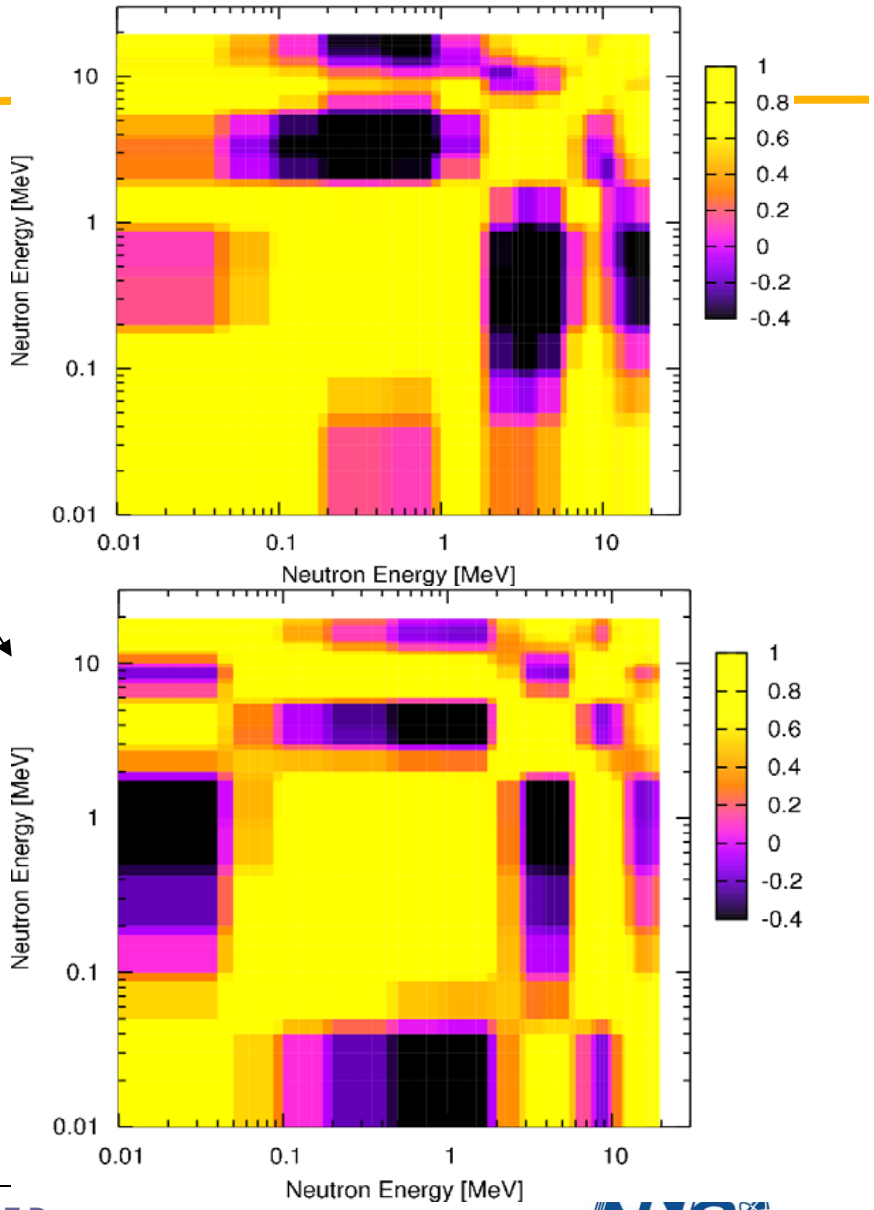
- Same procedure as the total cross section covariances
- Level densities and E1 strength function included
- Above 10 MeV, constant 80%, full correlation

(n,xn) Reactions

- GNASH-KALMAN calculations

Sample Total Cross Section Covariances





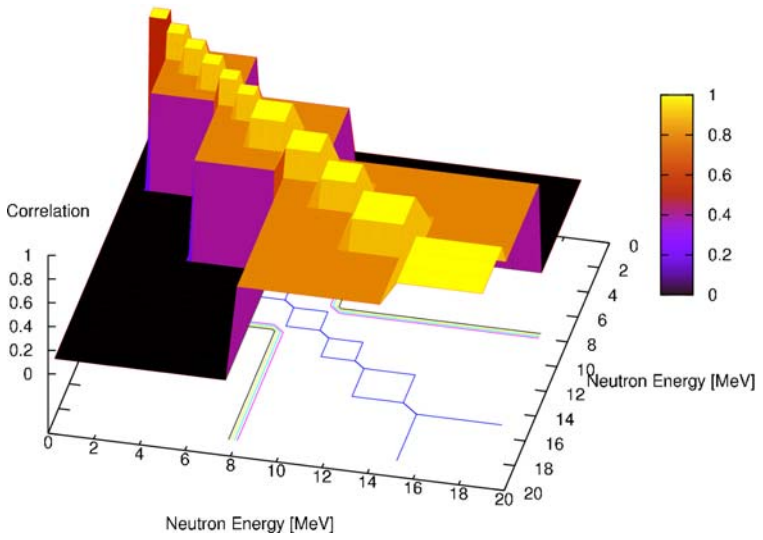
Fission Covariances

Fission Cross Section

- Estimation based on the comment section
- Estimated uncertainties, roughly 10 - 30%
- When experimental data were used, the uncertainties are reduced
- Grouped correlation matrix (80% correlation inside the group)
- Many of the minor actinide fission evaluations are in bad shape

Number of Neutrons

- ν(prompt) unc. 20%, with full correlation
- No covariance given for ν(delayed)



LANL Approach for Light Elements (Z < 10)

General Issues

- Complications in evaluation procedure
  - evaluations partly done by R-matrix,
  - or simply estimated from experimental data,
  - or just extrapolated (no information given)
- Reaction channels differ for each isotope
  - depending on Q-value, each isotope has different MT numbers
  - this makes difficult to produce the LoFi covariances in an automated manner
- **Energy range complications**
  - ^{7}Be cross section stops at 8.1MeV
  - some isotopes go up to 150 MeV
- ^{7}Li adopted from ENDF/B-VII.0

LANL Approach for Light Elements (Z < 10) (cont.)

- **Include high-fidelity R-matrix covariances (per Hale talk from yesterday)**
  - ^{1}H [el, capt], ^{10}B [el, (n,α0), (n,α1)], ^{6}Li [el, (n,t)]
    - maximum energy extended to 20 MeV
    - coarser energy grid than the original analysis
    - other channels supplied as Lo-Fi
- **For other reactions, approach is to be guided by information in MF=1**
  - Consider the evaluation method for each reaction
    - Is it an R-matrix analysis ?
    - Were experimental data used ?
    - Does the thermal value agree with Atlas ?
    - Is it just a guessed cross sections ?
    - etc
  - Assign uncertainties and correlation based on “my” expertise (“my” = Kawano)

LANL Approach for Light Elements (Z < 10) (cont.)

Thermal Region

- if R-matrix, small uncertainties and strong correlation
- 1/v capture, check the thermal value, full correlation

Fast Region

- look into the uncertainties of experimental data used
- if Hauser-Feshbach, strong correlations given

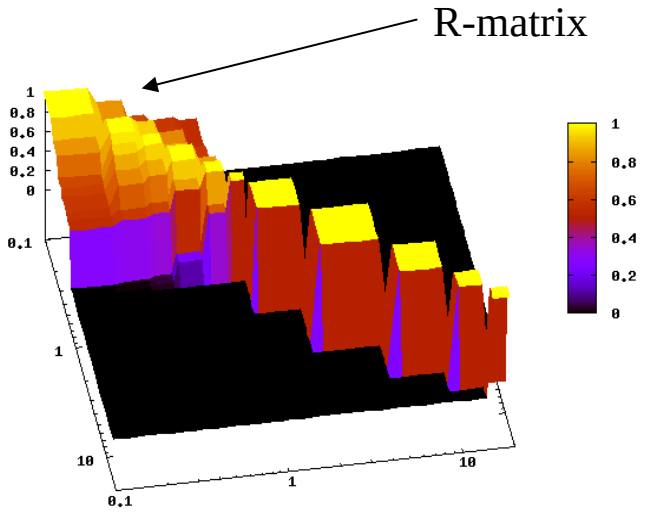
High Energy (>20MeV)

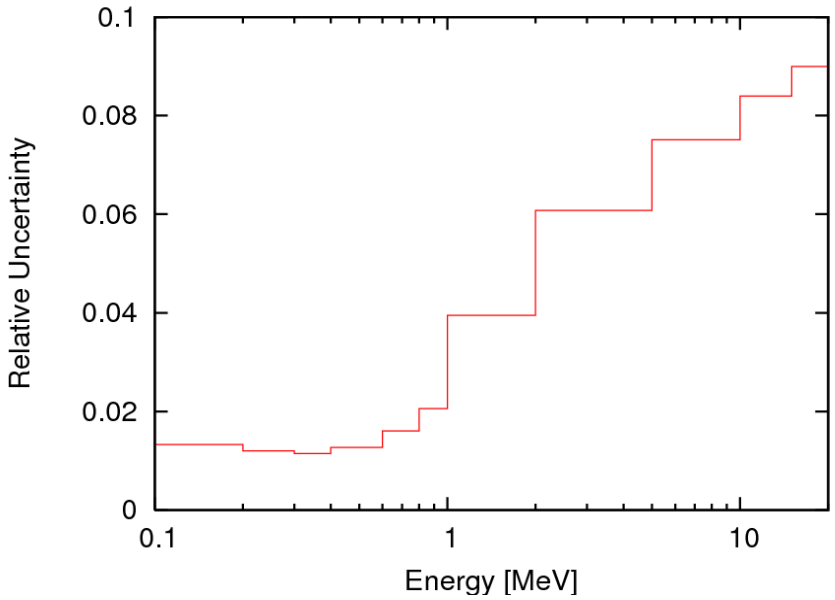
- covariances of total and non-elastic are given
- no multiplicity covariances

Derived Covariances (LTY=0)

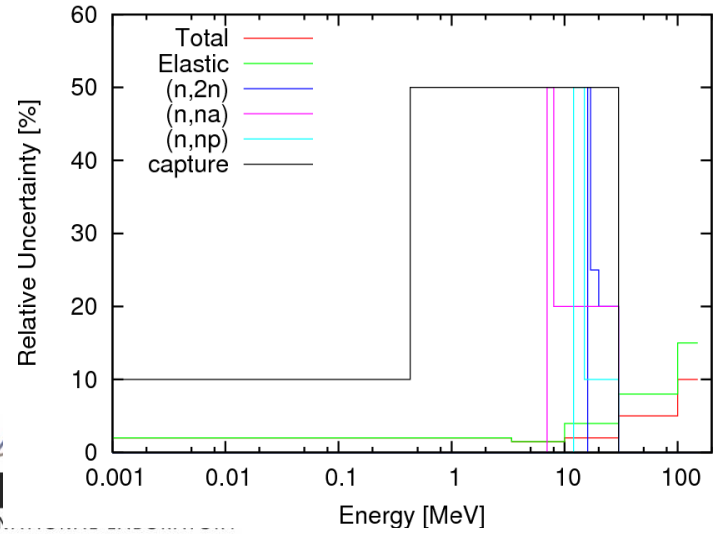
- Some channels are given as the sum of other channels
- $(n,\alpha) = (n,\alpha 0)+(n,\alpha 1)$, for example

Examples: ^{10}B Elastic Scattering and ^{16}O Reactions





Uncertainties for Reactions on O16



- Covariances are given for 42 reaction channels
- Data structure consistent with ENDF/B-VII
  - reaction threshold energies
  - derived data (MT107=MT800+801+...)

LoFi data are given for 17 materials from H to F, except for HiFi R-matrix evaluations and Li6 in ENDF/B-VI.

Summary of LANL Results

- Actinides complete for 46 isotopes
  - **Need to work to include SG26 results in Low-Fi compilation**
  - **Forgot ^{242}Am – will include soon**
  - **Covariances for ν, total, elastic, fission, inelastic, (n,xn), and capture included from 5 keV to 20 MeV**
  - **No spectra covariances included in Low-Fi**
- Light isotopes complete for 16 isotopes
  - **Results for all reactions over entire energy range**
  - **Wide variety of fidelity – from nearly full R-matrix to estimates**
  - **For the latter, much of the covariance data were simply estimated by looking into the ENDF tape comment section. These data need to be updated / replaced, depending on the importance of the covariance data for each material.**

Current Status

- **LANL and BNL provided a large number of high-energy files in File 33 format to combine with low-energy File 33 data from ORNL**
- **ORNL developed automated utility to combine low-energy and high-energy File 33 data into a single full-energy range File 33**
- **Required some resolution of minor glitches in merging files (e.g., adjusting energy boundaries of ORNL LB=1 section with BNL / LANL LB=5 section)**
- **ORNL has processed the combined files with PUFF-IV to ensure the files can be processed and conform to ENDF/B formats and procedures**
- **Combined files were distributed to ANL, BNL, and LANL in June 2008 for additional checking**
- **Initial check revealed that 20 files are missing from multi-laboratory initiative**
  - 14 missing files will be adopted from SG26
  - 4 Ra isotopes and ^{242}Am will be provided by BNL and LANL in near future
  - ^{7}Li to be used from ENDF/B-VII.0

Next Steps

- **ANL to perform QA of complete set of "merged" covariance files**
  - Work has not begun; files have only recently become available
- **At inception of the "low-fi" task this QA phase was envisaged to be principally "process, plot, and review"**
  - However, much of this has already been performed by ORNL, BNL and LANL in the process of creating these files. Note, for example, the work at BNL to facilitate visualization of the covariance data using Sigma.
- **Therefore, ANL plans to "process, plot, and review" with the expectation that these "low-fi" data are of very high quality**
  - Note: [high quality] + [low fidelity] ≠ [high fidelity]
  - To the extent possible identify and document the quality of these data
- **Ultimately, the covariance files will be archived and made available from the NNDC at BNL**

Summary

- The Nuclear Criticality Safety Program identified a shortfall and supported a multi-Laboratory project to address it
- A variety of practical methods have been pursued to develop this capability in a short period of time
- The results are possibly adequate for minor materials
- Remember, however, the original objective and scope – and particularly what was out of scope for this project
- We believe that the Low-Fi product itself has value; furthermore substantial valuable experience has been obtained that will be important for future work