Nuclear Data - Cross Section & Covariances - For GNEP and AFC

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Overview:

- **Major & Minor Actinides***
- **Nuclear Data in Neutronics Simulations**
- **Uncertainties and Covariances**

*** Minor actinide examples from Americium isotopes. Discovered in 1944 by Seaborg, named because of expected similar properties to rare earth Europium!**

US ENDF Community Provides the Link to Reactor Applications & Neutronics

Experimental
Cross sec. data

Integral data,
e.g. critical
assemblies

Nuclear models,
theory

ENDF/B-VII database

CSEWG oversees ENDF collaboration - Nat-lab /industry/universities, & NEA & IAEA collaborations

NJOY is the international standard code for processing the data for applications

Users:

Stockpile Stewardship

synergy with fast neutron systems

Advanced reactors

Accelerator technologies

Criticality safety

Medical, space, astro, RIA, …

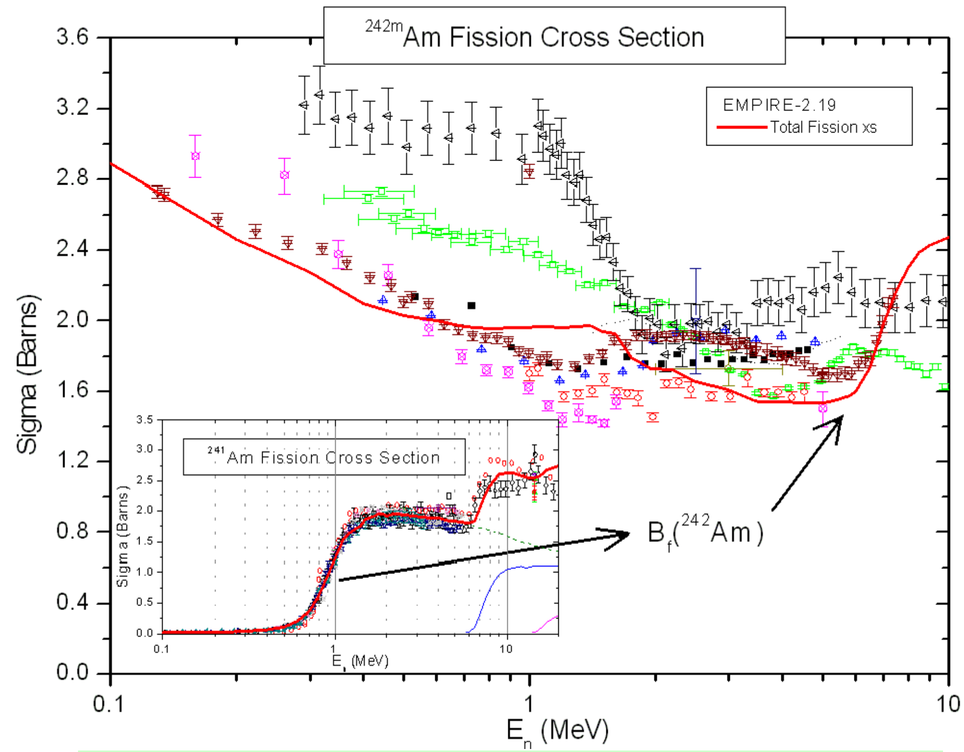
Actinide Cross Sections for Advanced Reactors

Cross sections needed for Simulations of:

- **criticality** and **transmutation**
- **radiation damage** and **heating**

Minor actinides

- **Np, Am, Cm** isotopes
- **Experiments** with extremely small radioactive targets, *e.g.* at LANSCE
- **Theory** can be used to predict unknown actinide fission and capture
- **Validation (critical assemblies)**



^{242m}Am fission cross sections (Uncertainty needs reducing <20%. LANSCE exp. Planned)

Major actinides

- **^{239}Pu, ^{235,238}U have high impact because of their abundance**
- **Significant uncertainties (> 10%) in fast neutron region for capture**

Objectives for GNEP & AFC

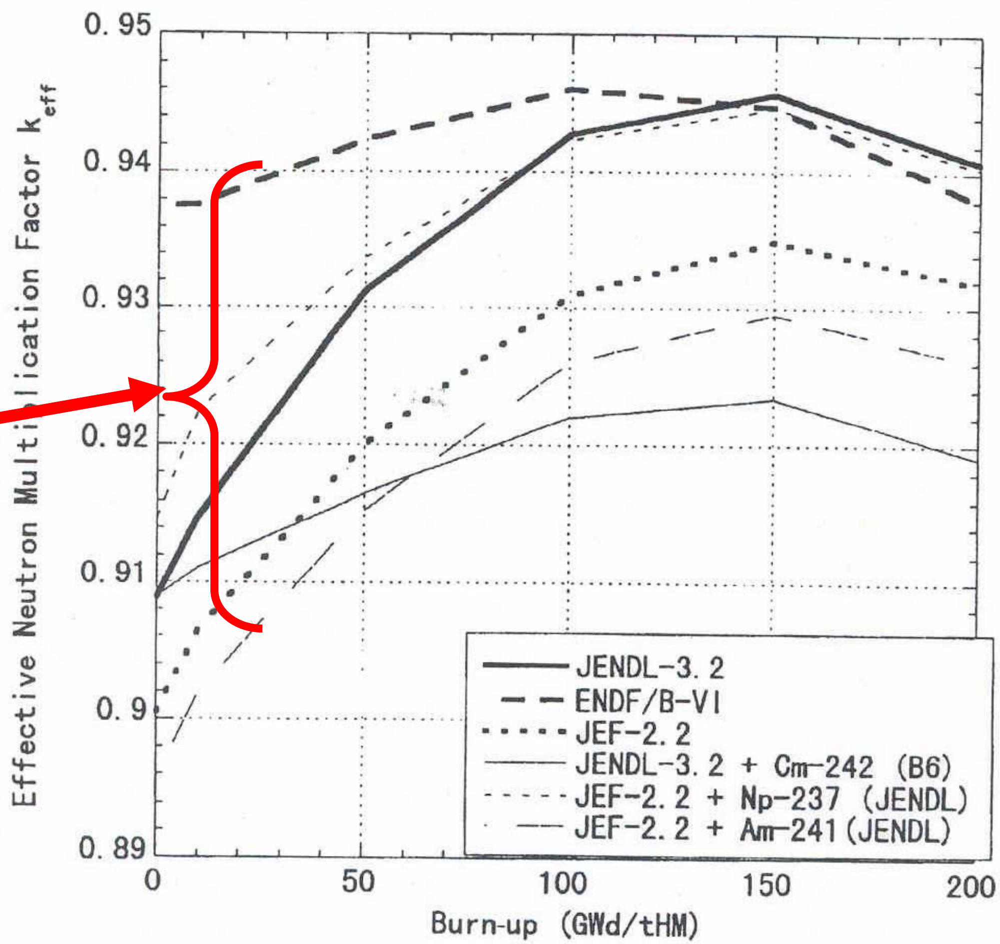
- Perform **experiments**
- Improve **theory & modeling**
- Produce precise **cross sections & covariances**

Impact of cross section uncertainties on reactor design

Example : A design involving significant quantities of minor actinides

- Uncertainties for Np, Cm, Am led to major differences in predicted criticality (Np here)
- Similar sensitivities have been determined recently by Palmiotti, Salvatores (ANL).
- Target unc. will be provided by reactor community, eg.
- ^{241}Am(n,g) < 10%, ^{242m}Am(n,f) < 10%, etc

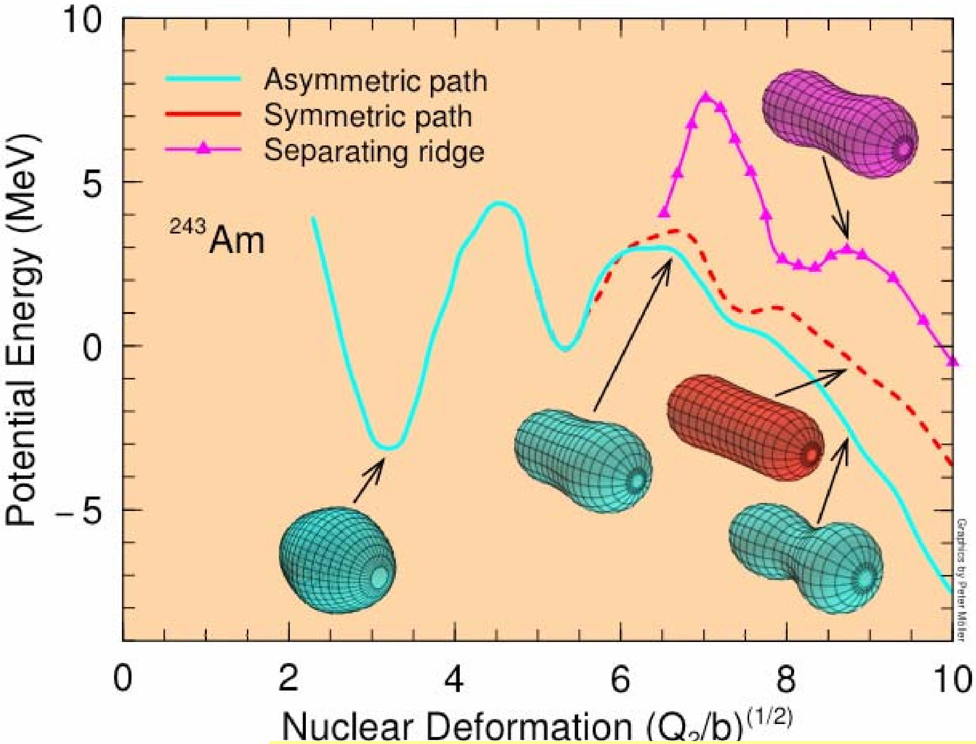
Figure 3.2. Comparison of burn-up reactivity change



Source: Nuclear Energy Agency (NEA) Working Group on Evaluation Cooperation

Fission Theory Predicts Barriers for Use in Cross Section Predictions (Americium example)

Potential energy pathways shown from 5-dimensional shape macroscopic-microscopic model of Moller et .al., Nature and PRL.



- Especially useful for minor actinides where few measurements exist (owing to short half lives), *e.g.* n+^{242g,m}Am, n+^{240}Am
- But present predictive capability insufficient for predicting data on important actinides (but can use trends from theory)
  - Current ~ 0.5 MeV unc. on barrier heights is too high
  - Dynamic effects important
  - Incorporate axial asymmetry

Challenge to theorists: ability to use nuclear structure theory predictions has not delivered to the extent we would like. Today, we rely on more phenomenological reaction model predictions.

Neutron Capture Theory: Major Increase in Predictive Capability Needed

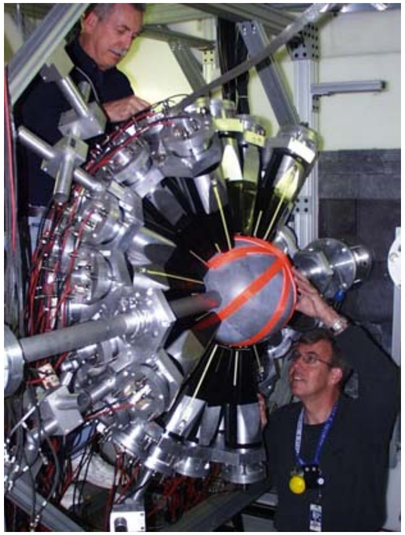
- Much research here, but present calc. unc. far exceed target requirements
  - ~ 20-30% at best for isotopes close to stability
  - >factor 2, away from stability (experience based on r-process modeling)
- Where data exist at lower energies, eg < 1keV, how well can theory be used to extrapolate to higher energies?
- Can theory support surrogate experiments to more-accurately determine capture?

Challenge to theorists: research on gamma-ray strength functions, level densities, and fission competition.

Credibility must be established via blind predictions of known capture cross sections (eg 197Au, 238U)?

Experiments (Americium example)

- Important data needed are:
  - Fission, capture, n2n, χ
  - Gas production
  - Integral criticality experiments
- The easier experiments have been done! Remaining priority is reactions on unstable isotopes:
  - LANSCE & Radiochemistry
  - Surrogate methods
  - Future exotic beam facility?



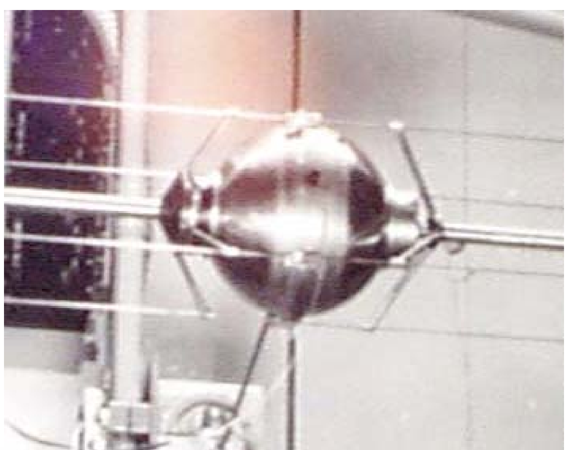
Previous ^{241}Am(n,γ) ~too unc. (> 20%); Need < 10%
Hope DANCE does better!

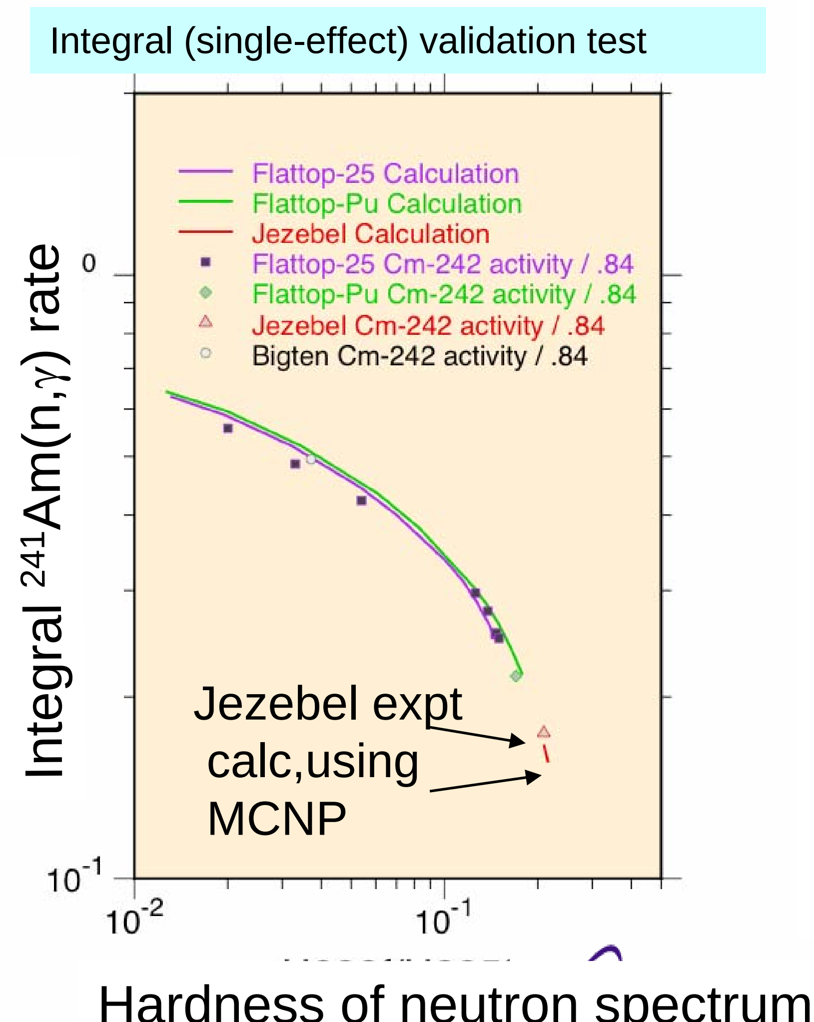
QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.

Callenge to experimentalists: capture measurements must achieve a higher level of accuracy (<10%), *extend up to 100s of keV*, **and must build confidence in their validity (validation crit assembly activation exp.; comparison with Standards values for 197Au(n,g) and 238U(n,g)**

Integral Experiments:
In Some Cases, Can Constrain & Validate Evaluations

- Reactor well-defined benchmarks will be useful (burnup rates, etc)
- Can also use historic LACEF measurements (and future ones beyond 2010 at DAF?)



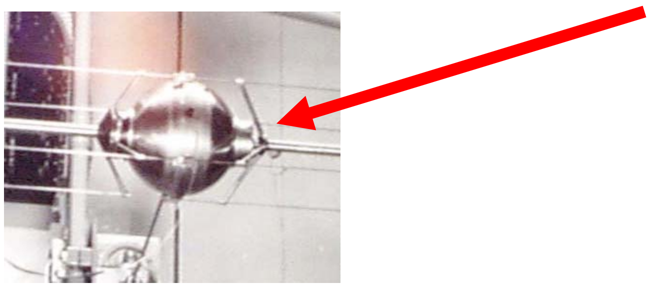


Major Actinides: Significant Advances in ENDF/B-VII

- 239Pu, 235,238U upgrades made
- 238U improvements in inelastic scattering…
  - LEU assemblies modeled well now
  - Intermediate spectrum assemblies modeled well (Big-10) - important for fast reactor design
  - Reflector properties much improved

Major Actinides: Significant Advances in ENDF/B-VII

- 239Pu, 235,238U upgrades made
- 238U improvements in inelastic scattering…
  - LEU assemblies
  - ^{235}U fission prompt neutron spectrum at thermal. Deficiencies in measurements & theory predictions
  - ^{235}U, ^{239}Pu inelastic scattering/prompt fiss spectra problem - since the neutron spectrum in fast assemblies appears to be too soft (as measured by 235Uf/238Uf spectral index)



Callenge to reaction modelers: undertake new modern (GNASH - ECIS) analysis of ^{239}Pu and ^{235}U, focused on improving inelastic scattering and prompt fission neutron χ spectra

Need Multigroup Deterministic Transport Simulations, with Accuracy & Capability of Cont. Energy Monte Carlo

- Multi-group library generation is as much art as science
  - Today, detailed knowledge of the specific application is needed to adequately perform shielding solutions to yield group constants
- Improvements can be made to our existing simulation methods
  - Using continuous-energy (e.g. MCNP) solutions to guide and inform multi-group library generation and their use
  - Using adaptive solutions that recognize that each multigroup problem is unique and interactively updating data for each simulation
  - For the next generation we must do better
    - While many separate capabilities exist and are well proven - *e.g* deterministic or MC transport codes, burnup codes, thermal hydraulic codes, transient analysis codes, etc - the ability to couple these codes in a useful manner needs significant work

Taking It To The Next Level
Uncertainty Quantification

- Important to better understand uncertainties on actinides
- Different designs have different sensitivities to nuclear cross section data
  - Reduced uncertainties will impact fuel and reactor qualification (for reactivity, transmutation) & reduce need for costly experiments in evolving design-iterations.
  - If realistic uncertainties are not used, artificially-large margins would be invoked
- We are still in the opening stages of understanding how to generate and use covariance data
  - ENDF/B-VII only has limited covariance data … more work is needed
  - Methods have been developed to apply covariance data to deterministic and Monte Carlo solutions (e.g. the TSUNAMI code), but…

    We need new and novel ways to approach or apply the use of this data to effect programs - cost, risk, reliability.

  - QMU expertise developed at NNSA labs provides important synergies

Covariance Data in ENDF/B-VII. This is a priority area for reactor design, criticality safety, and stockpile stewardship

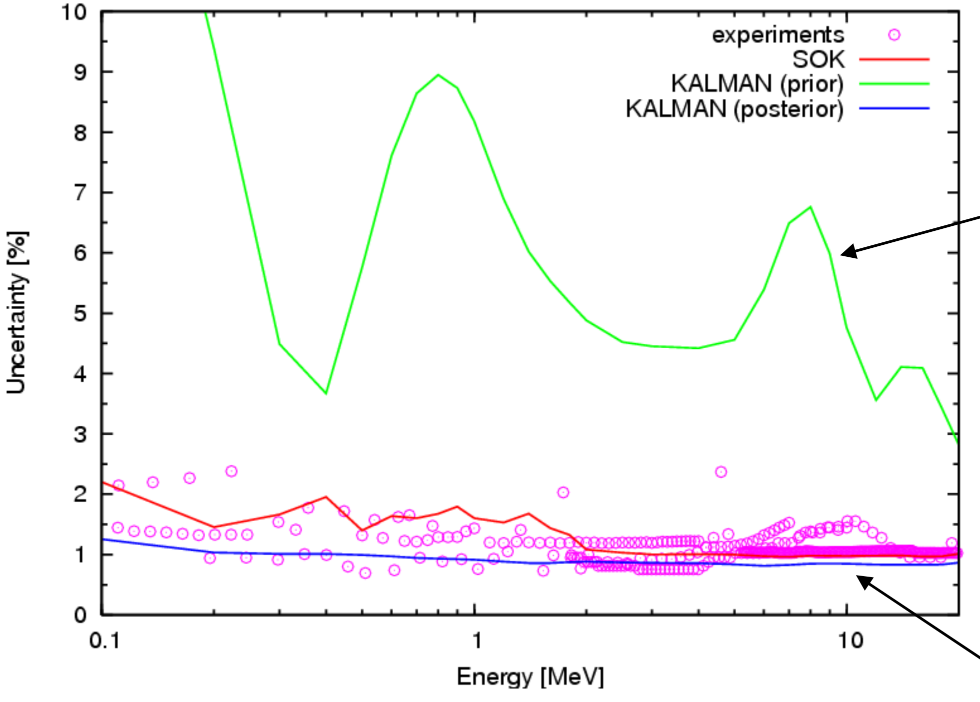
- In ENDF/B-VII only 9 materials out of 393 have full covariance data
  - Priority is fission, capture, inel., n2n for major and minor actinides

- Why so little?
  - Large multidimensional data representations needed
  - Methods to evaluate the covariances are not well established
  - Covariance data for resonance parameters need special care

- Significant progress has been made recently in the US, Europe & Japan:
  - NEA/WPEC collaboration; LANL-CEA collaboration
  - Bayesian methods combining model predictions and measured data (including integral criticality data), eg KALMAN with GNASH, EMPIRE
  - Monte Carlo methods, eg TALYS, and EMPIRE
  - Large-scale, initial, coarse method initiated for criticality safety

Example I : KALMAN Method

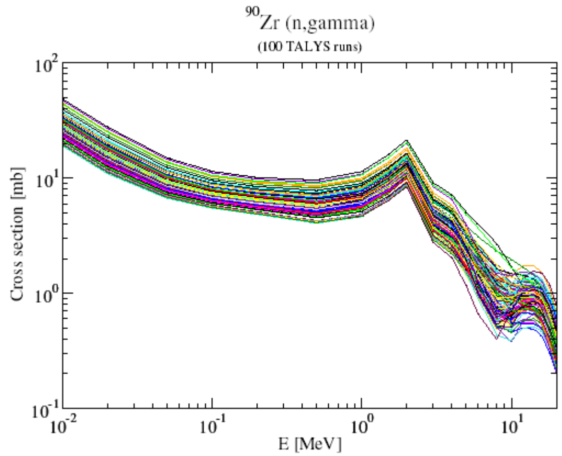
Uncertainties in the Th-232 Total Cross Sections



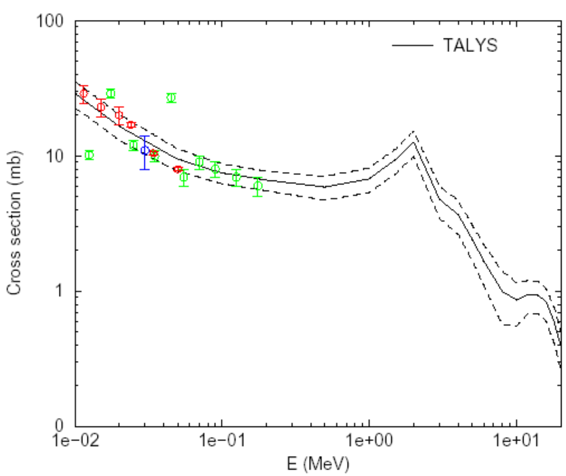
We assume that nuclear model parameters have some uncertainties. The cross section covariance is calculated by means of the error propagation from the parameter to the calculated values.

The calculated covariance is updated by including experimental information

Example II : Monte Carlo Method, that combines uncertainty in model predictions with measurements



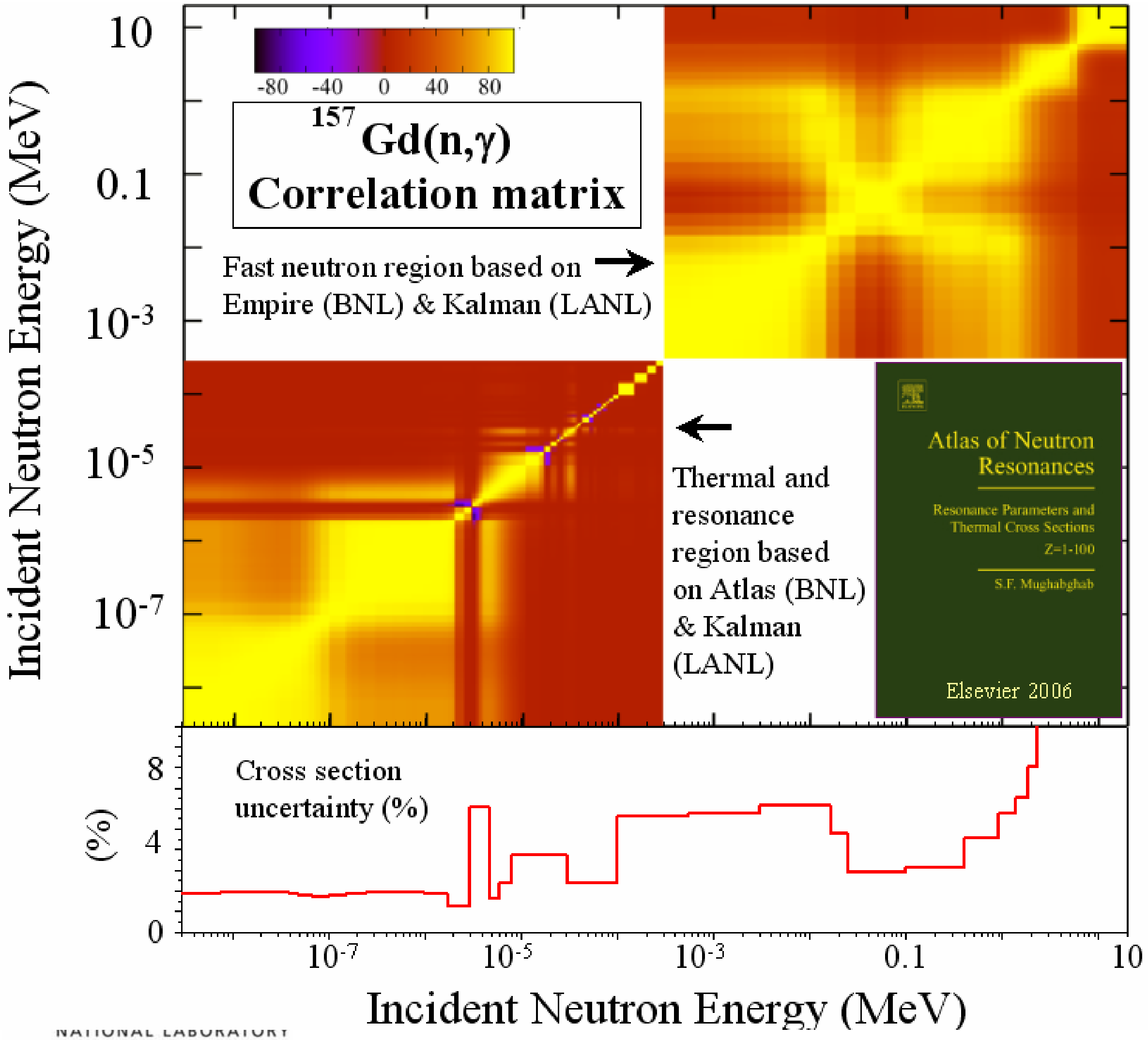
(a)^{90}Zr capture calculated with input model parameters varied within their uncertainties (over 1000 TALYS code runs)



(b) The obtained distribution is re-scaled by comparing with the experimental data – quality of fit and exp. unc. themselves.
- allows generation of covariance data

But, integral measurements not included yet in this methodology (though this has been done in NNSA applications)

Example III : New BNL-LANL Approach With Covariances for Entire Energy Range



At high energies, covariances are generated with the EMPIRE-KALMAN codes, using both theoretical and exp. uncertainties.

In the resonance region, covariances are from resonance parameters and their uncertainties compiled at BNL; KALMAN is used for error propagation to cross sections.