Los Alamos Nuclear Data Needs and Activities – From Experiment Through Application

Bob Little

Los Alamos National Laboratory

With input from: Randy Baker, Mark Chadwick, Tim Goorley, Gerry Hale, Marian Jandel, Skip Kahler, Toshihiko Kawano, Patrick Talou, Morgan White

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Presented at: RPI Nuclear Data 2011 Symposium for Criticality Safety and Reactor Applications

April 27, 2011

Abstract

- This talk is for presentation at the 2011 RPI Nuclear Data Symposium. It includes a summary of Los Alamos nuclear data priorities and capabilities in areas including experiments, theory, evaluation, processing, libraries, and applications.

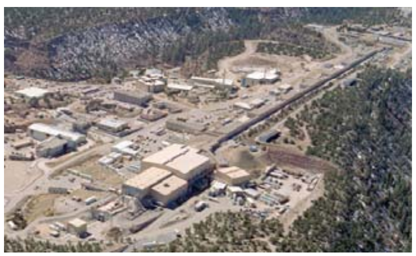
The Nuclear Data Enterprise at Los Alamos is Comprehensive, Complex, and Coordinated

Reaction and Structure theory

Fundamental experimental data

Modeling code predictions

Evaluations (ENDF/B-VII)



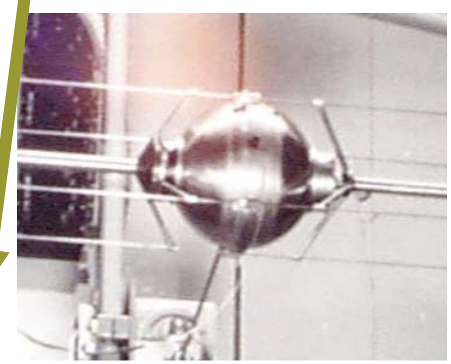
Data processing (NJOY)

Application libraries

Feedback from validation testing

Transport simulations of integral experiments

Integral experimental data



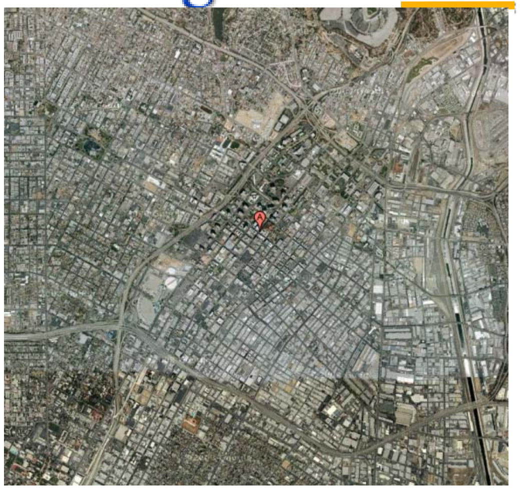
Central Mission of Los Alamos National Laboratory

Different Programs have Different Responsibilities Associated with Nuclear Weapons

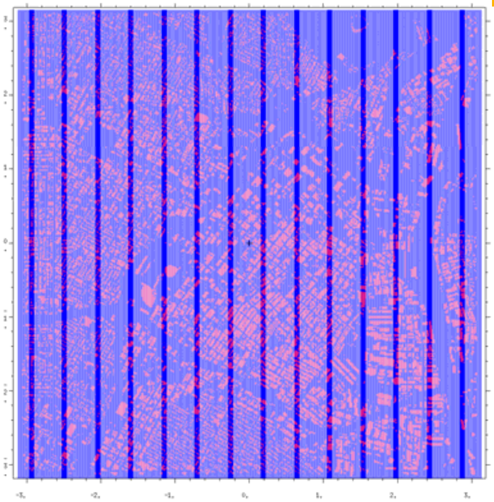
- **Stockpile Stewardship Program (SSP)**
  - responsible for maintaining the safety, security, and reliability of the nation's nuclear weapons stockpile
- **Nuclear Counter Terrorism (NCT)**
  - identifying and characterizing potential IND material and designs that pose a threat to U.S. citizens, assets, and infrastructure
- **Joint Technical Operations Team (JTOT)**
  - provides specialized technical capabilities in support of lead federal agencies to respond to weapons of mass destruction
- **National Technical Nuclear Forensics (NTNF)**
  - enable operational support for materials, pre-detonation device, and post-detonation nuclear or radiological forensics programs with the broader goal of attribution
- **Urban Consequences (UQ)**
  - Assess impacts of urban detonation of nuclear weapon to aid decision making in aftermath

Example of Urban Consequences Simulations Using MCNP (Dose contours from a 20 kT device in downtown LA)

Google maps

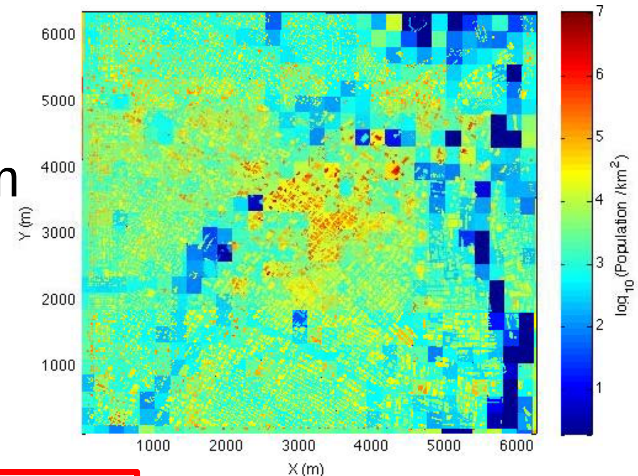


mcnp

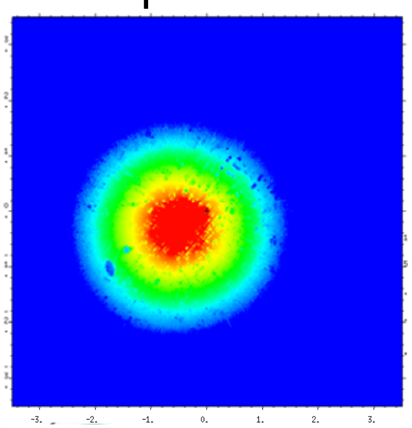


6 km

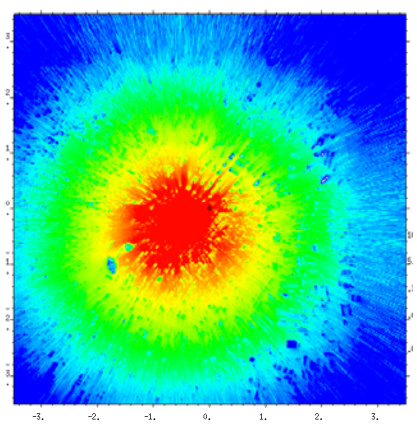
US Census Population Density



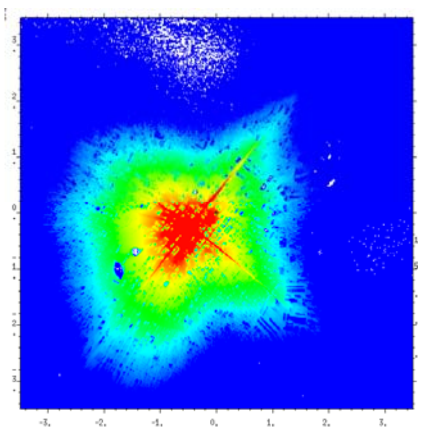
Prompt Radiation Effects - Dose



Neutron Dose (from neutron leakage)

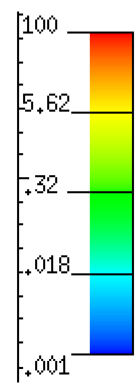


Gamma Dose (from neutron capture)

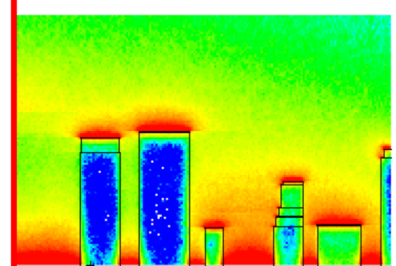


Gamma Dose (from gamma leakage)

Gy



Fallout Dose

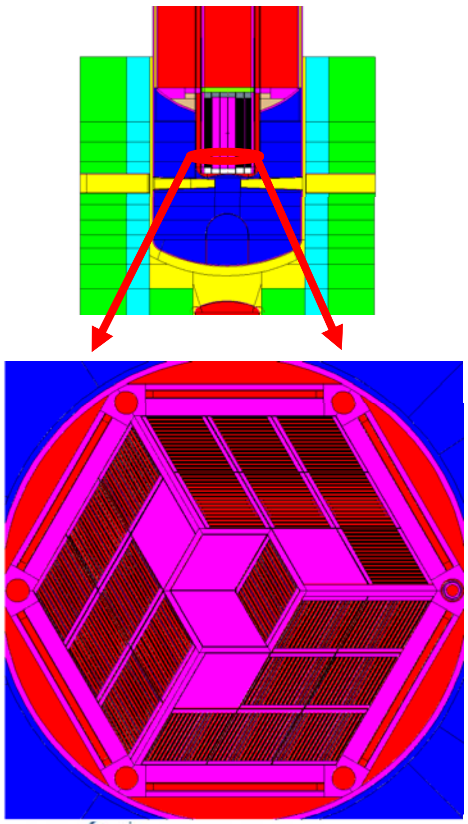


Gamma Dose

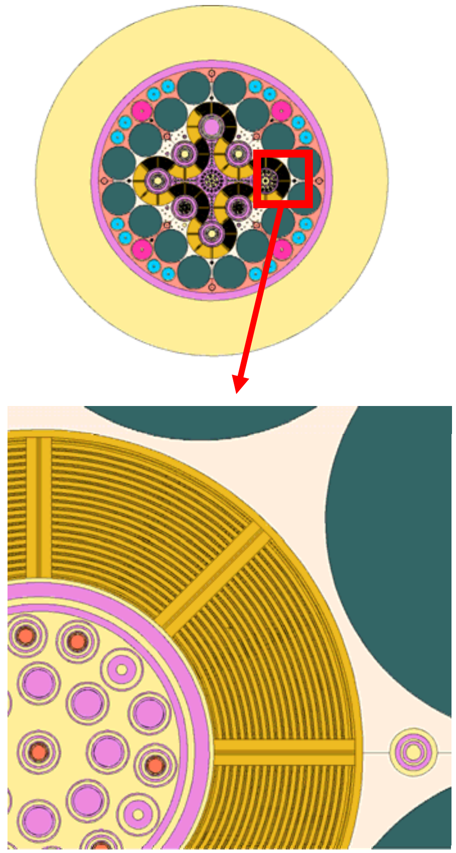
Los Alamos also Contributes to Nuclear Reactor Design (MCNP models shown here)

MIT

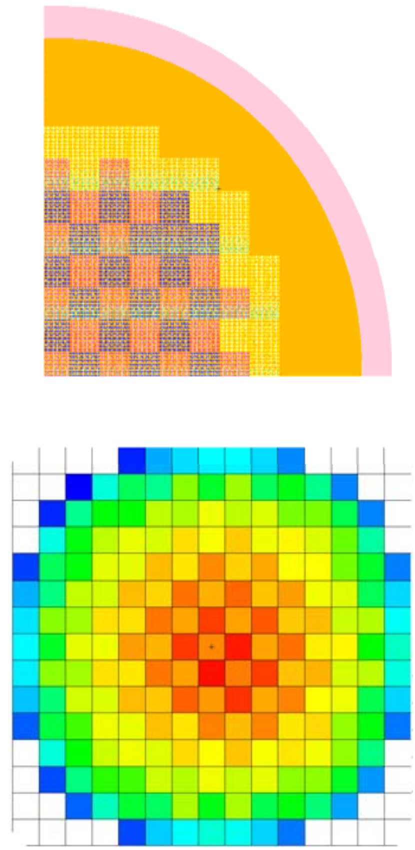
Research Reactor



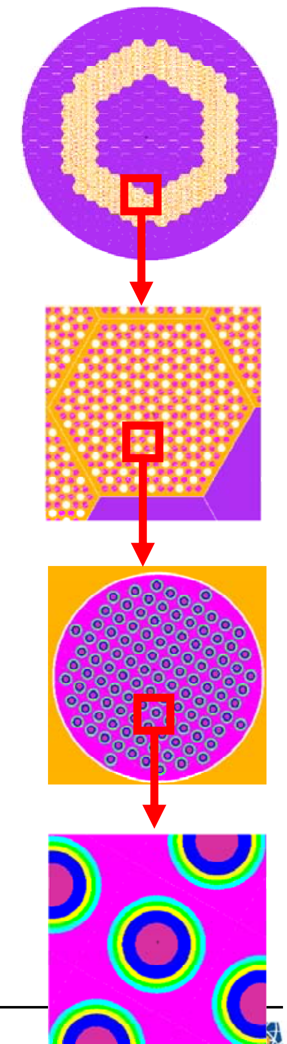
ATR



PWR

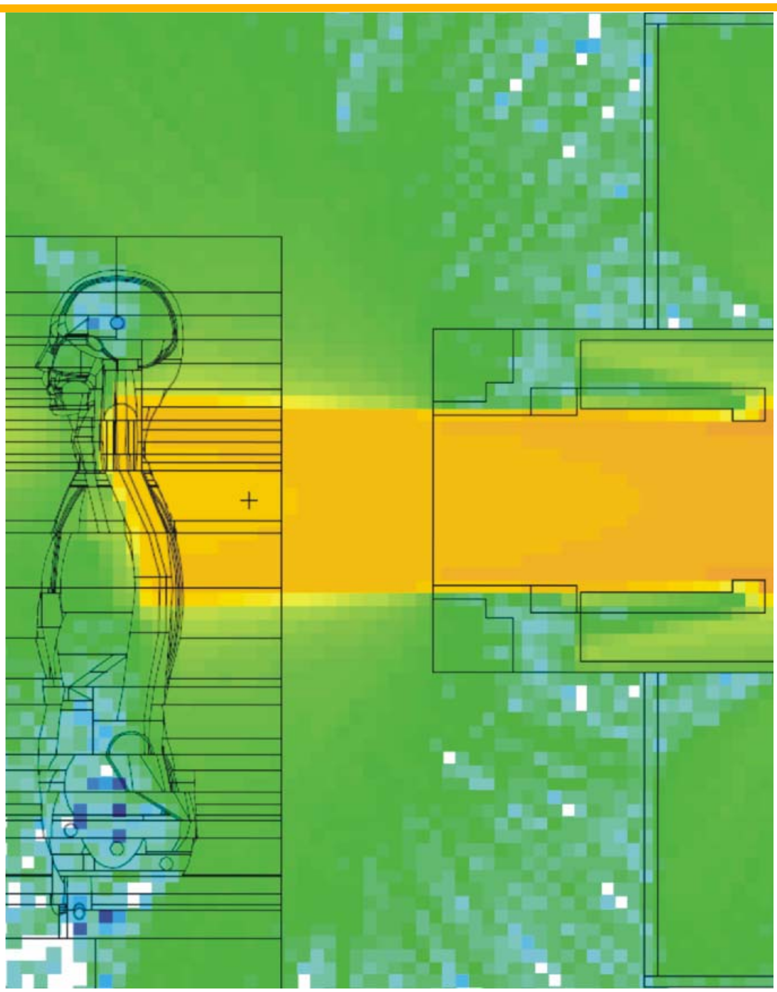


VHTR



MCNPX is the most widely used general purpose Monte Carlo code for research in radiation cancer therapy

The code is ideally suited for use in medical applications because of the accuracy of its physics models, the unique set of clinically relevant features, and the responsive support provided by the developers and the user community.



proton fluence and dose contours (arb units)

We used MCNPX to verify the Mass General Hospital Proton Center, and this information has gone into the design of the MDACC proton center and others, which are used to treat > 5K people a year.

Wayne Newhauser, Ph. D.
Dept of Radiation Physics

THE UNIVERSITY OF TEXAS
MD ANDERSON
CANCER CENTER

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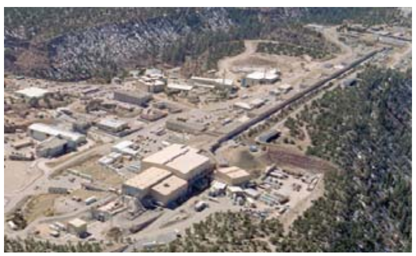

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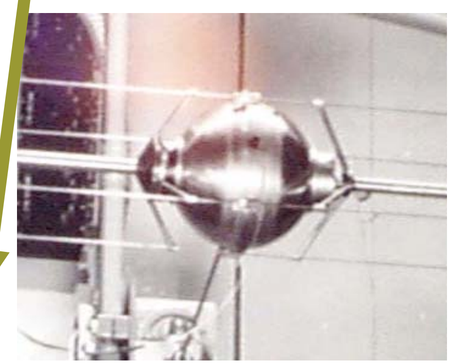
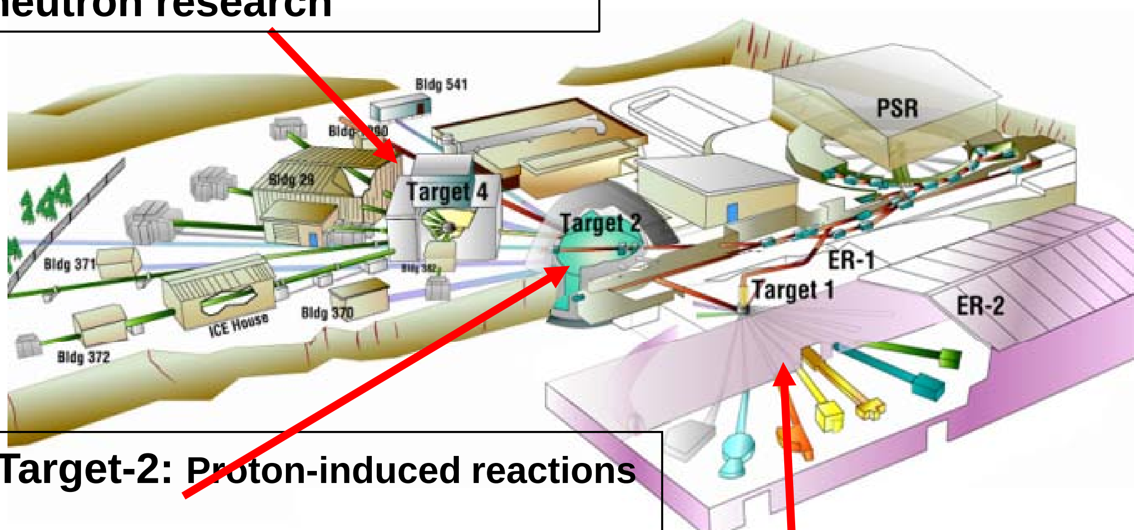


Nuclear Science research is performed at many experimental areas at LANSCE

Weapons Neutron Research Facility

Target-4: High-energy neutron research



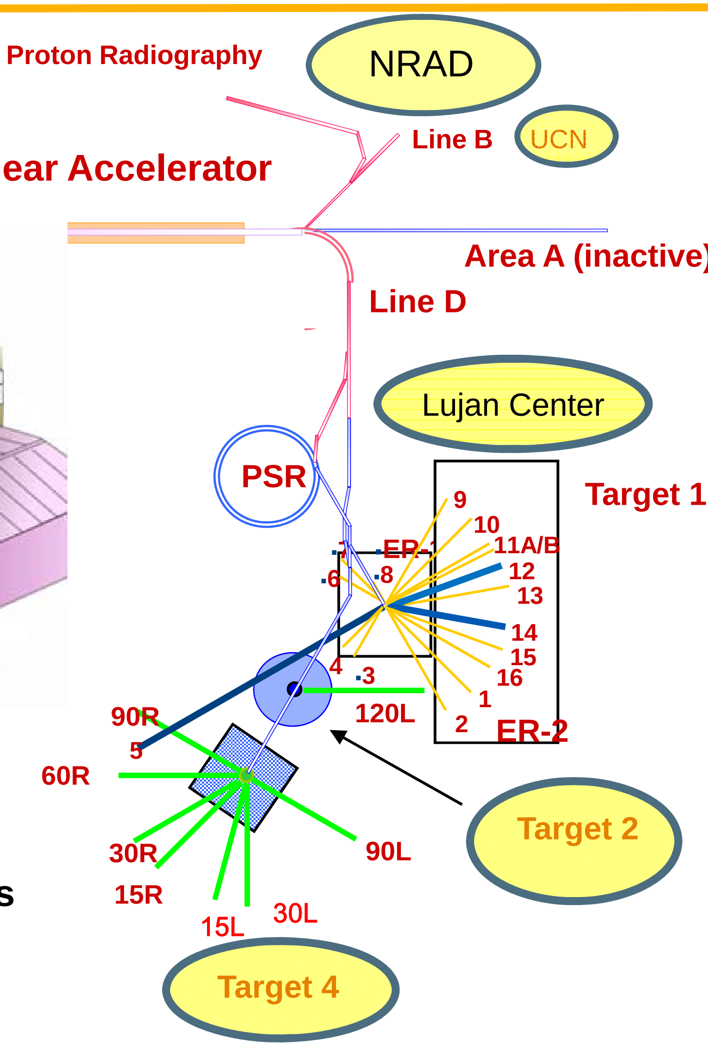
Target-2: Proton-induced reactions

- Single-pulse experiments (Sandia)
- Lead Slowing-Down Spectrometer
- SNS target testing
- Isotope production testing

Lujan Center:

Low-energy neutrons

- Material science
- Nuclear science

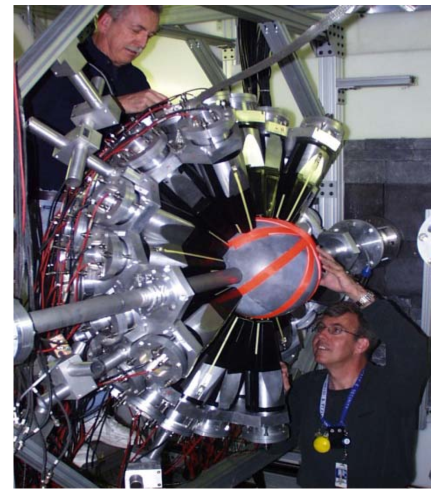


Many instruments have been developed for nuclear data measurements at LANSCE

GEANIE (n,xγ)

FIGARO (n,xn+γ) -> “Chi-Nu”

DANCE (n,γ)



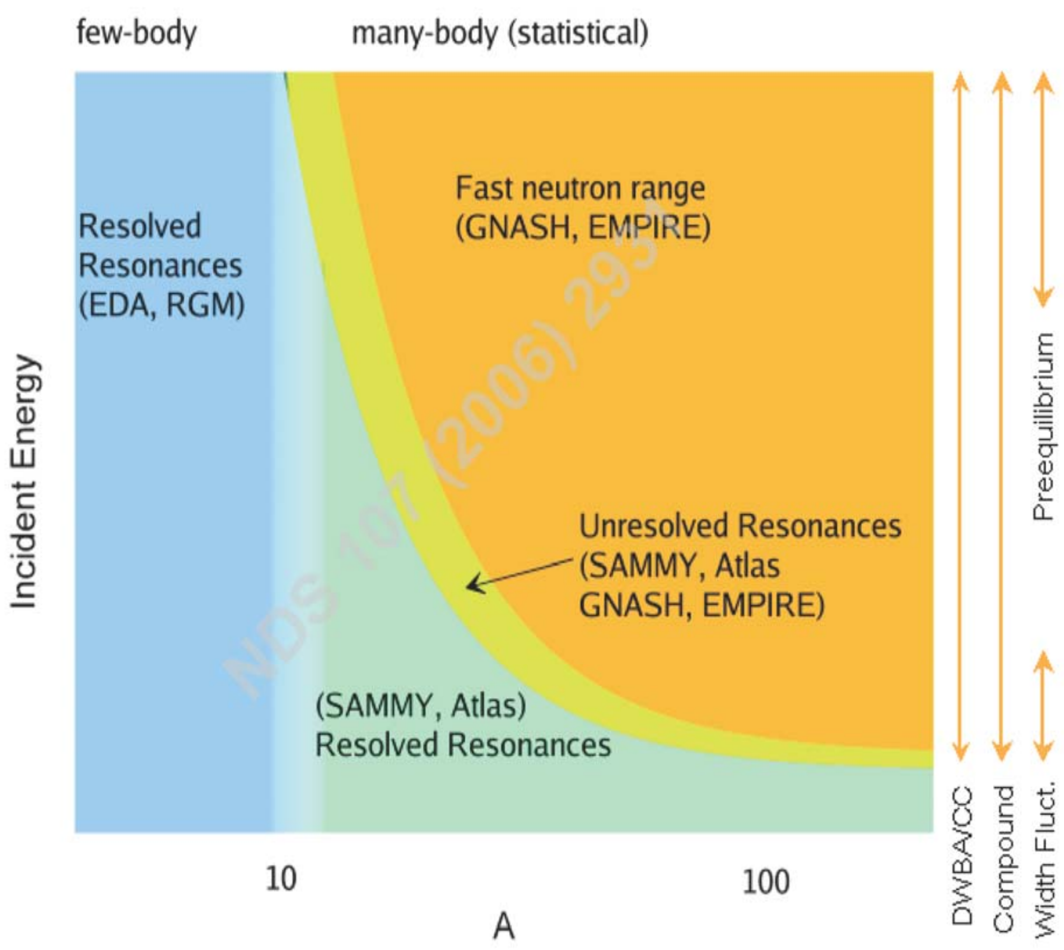
N,Z (n,charged particle)

Fission

LSDS

TPC, standard fission ion chamber

Regimes for Applying Various Models and Codes



Model codes are especially important for producing complete ENDF files:

To interpolate/ extrapolate to unmeasured regimes

For predictions where no measured data

Los Alamos Nuclear Reaction Codes Underpin our ENDF/B Evaluations

- **GNASH - reactions on actinides & medium mass nuclides**
  - Hauser-Feshbach, preequilibrium, & fission modeling
  - McGNASH = modern version

- **EDA for light nucleus reactions (R-matrix theory)**

- **CoH suite of codes**
  - Another Hauser-Feshbach code, with width fluctuation treatment, and gamma-ray capture formalism using direct-semidirect theory
  - Implements Kerman's KKM theory for deformed nuclei

- **Moller structure codes: fiss. barriers, *g.s.* masses, Q-values, & deformations.**

- **Preequilibrium codes**
  - FKK, NWY quantum treatments with RPA collectivity
  - Semiclassical HMS and exciton options

Evaluations Rely on Experimental Data, Modeling Codes, and Evaluator Expertise

- **Experimental data**
  - Key!
  - But often incomplete and discrepant
  - Uncertainties are important (both systematic and statistical)
- **Modeling codes**
  - Sophisticated physics
  - Aware of experimental data
  - Systematics can be important
  - Allow production of complete double-differential secondary spectra
- **Evaluator expertise**

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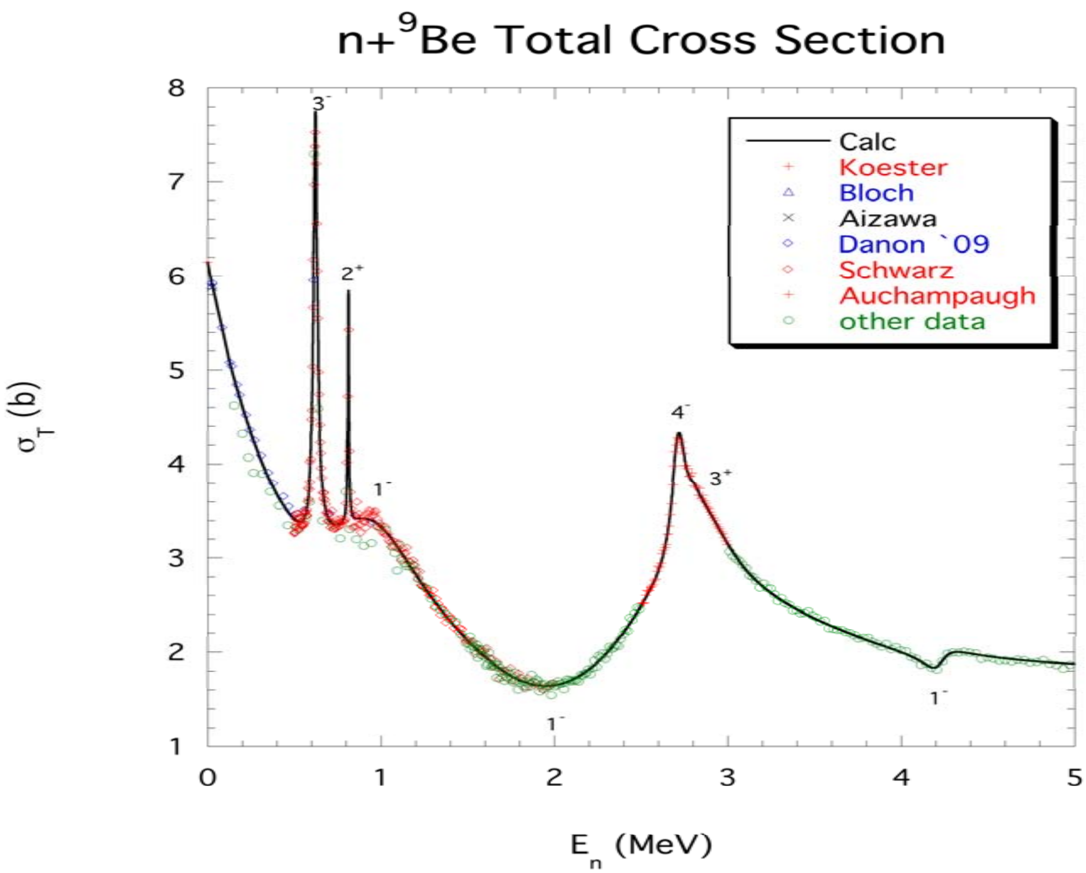
- **Evaluator expertise**
  - LANL evaluators
    - If experimental data from RPI

Example: current EDA analysis for n+^{9}Be



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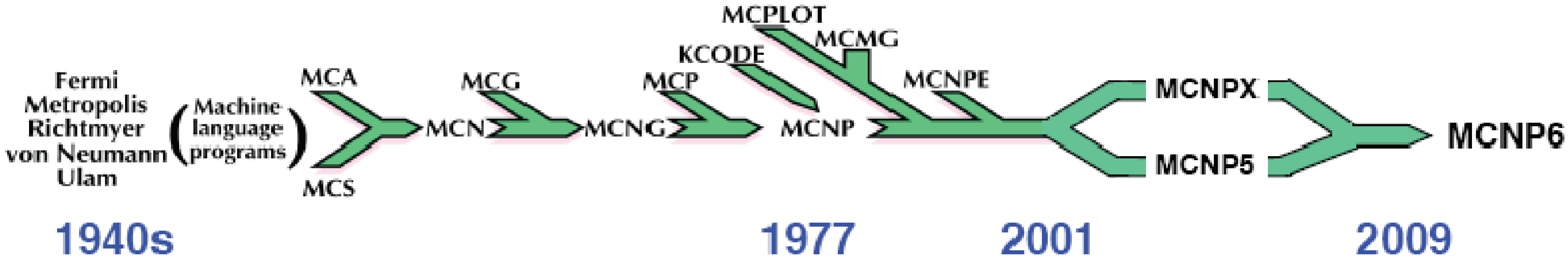
    - If experimental data from RPI *and* author list includes R.C.Little

NJOY Nuclear Data Processing Code System

- **The NJOY Nuclear Data Processing System**
  - Used to create application specific (MCNP continuous energy Monte Carlo or group-wise for Deterministic codes) nuclear data libraries from general purpose and specialized nuclear data evaluation files
    - General purpose files include
      - ENDF, United States' Evaluated Nuclear Data File
      - JEFF, Joint European Fission & Fusion File
      - JENDL, Japanese Evaluated Nuclear Data Library
      - BROND, Russian Evaluated Nuclear Data Library
      - CENDL, Chinese Evaluated Nuclear Data Library
  - Also used to process ENDF Covariance Data
  - Display cross sections, angular distributions, emission spectra, uncertainties and correlations
    - Also display ratio to easily see changes from one evaluation to another.
    - Allow overlay of continuous energy and multigroup data.

MCNP
Monte Carlo N-Particle



- 3-D generalized geometry including repeated structures and lattices
- Continuous-energy data libraries and physics
- Flexible source and tally feature
- Rich collection of variance-reduction capabilities
- Parallel; runs on PCs to Peta-Flop machines
- Over 10,000 users worldwide
- MCNP code now more than 30 years old
- MCNP6 has been beta released outside LANL

Integral Experiments: CEF (Critical Experiment Facility)

- **Historical critical assembly measurements at LANL TA-18 (such as Godiva, shown below) have been instrumental in testing and validating nuclear data and transport codes**

- **TA-18 was closed due to security concerns in the mid-2000's**
- **The capability has been largely re-constituted at CEF (located at NNSS)**
  - **Supported by Nuclear Criticality Safety Program**
- **Four general-purpose machines will be operational in next 18 months**
  - **Planet**
  - **Comet**
  - **Flattop**
  - **Godiva**
- **The broad nuclear data community at Los Alamos is in the process of prioritizing future CEF experiments**

Examples of Current Nuclear Data Priorities at Los Alamos

- **Fission cross sections**
- **Prompt fission neutron spectra**
- **Capture and (n,xn) cross sections**
- **Fission product yields, and beta-delayed emission spectra**
- **14-MeV scattering (preequilibrium emission, collective effects, MSD)**
- **Excited state fission cross sections**
- **Covariance data**
- **Validation**

- **For:**
  - Actinides
  - Light isotopes
  - Diagnostic materials

  - Including short-lived targets and excited states

Some Grand Challenges in Fission Physics

Fission neutron spectra

Large uncertainties for emitted neutrons E_n< 1 MeV & E_n > 5 MeV

Major effort underway to perform new measurements, and developed advanced theory predictions

IAEA CRP initiated

Significant impacts on criticality

Post-fission beta-delayed neutron and gamma emission

Spectra are crudely represented

Deficiencies impact various applications - incl. decay heat

Theory advances using more microscopic approaches

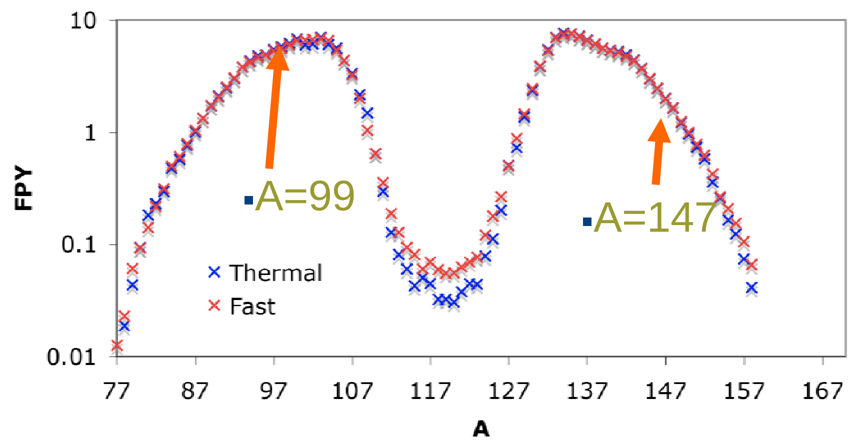
Fission cross sections

Fission cross sections for minor actinides often poorly known

Theory predictive capability is poor

Various theory and experimental programs are making progress

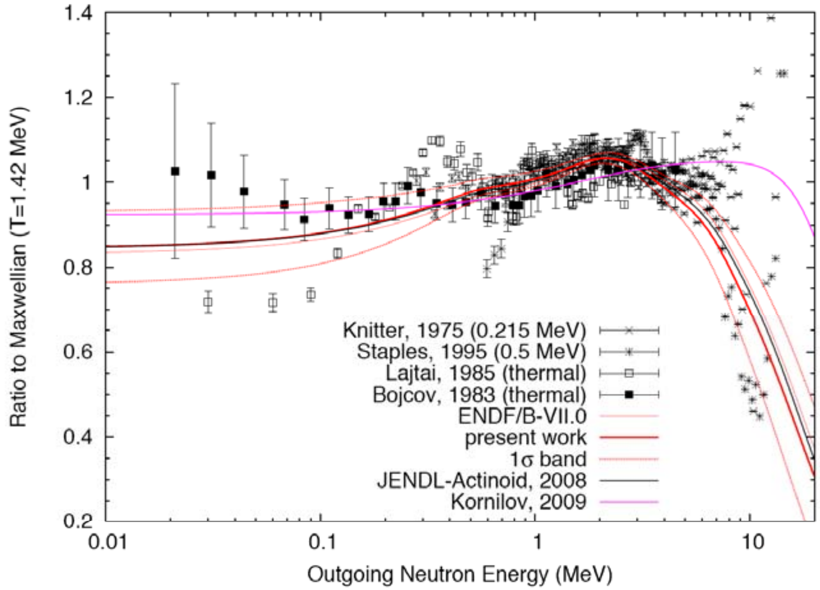
Fission product yields (FPY)



Chi-Nu (Prompt Neutron Fission Spectra)

There is a paucity of experimental data (see figure at right for Pu-239)

Both theory and experiments show at least 10% discrepancies



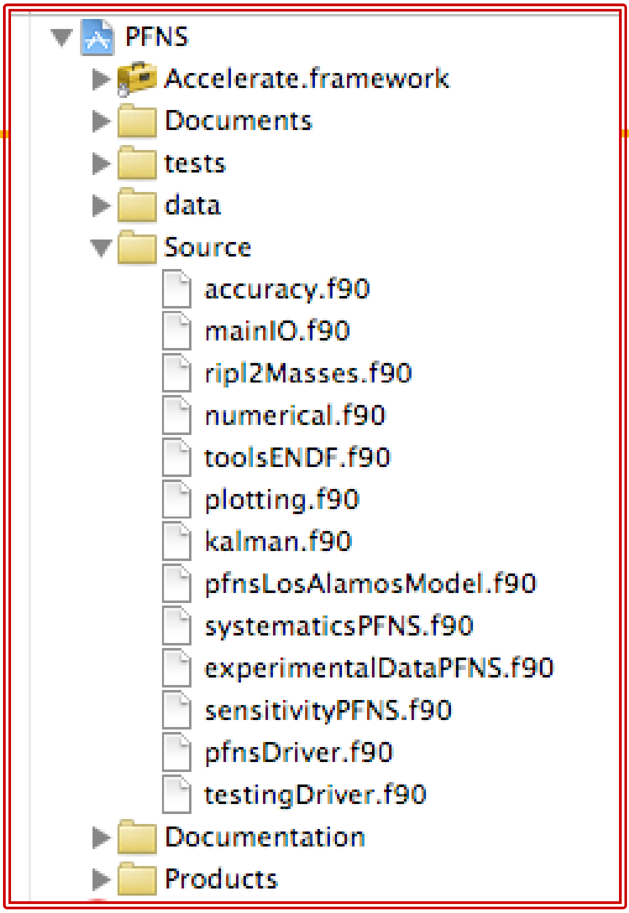
- **The goal of the Chi-Nu detector is to measure the neutron emission distribution from fission with enough fidelity to constrain theory**
- **Attempting to expand the range of emission energies**
  - Low-energy from 1 down to 0.5 MeV (Deliverable L2 June 2013)
  - High-energy from 7 up to 15 MeV (Deliverable L2 June 2015)

We are Pursuing Improved Theory and Modeling for Prompt Fission Neutron Spectra in Parallel with Chi-Nu Experiment

- **FFD code**
  - Monte Carlo code
  - Follows each step of the evaporation of excited primary fission fragments
  - Compute ***exclusive*** data on prompt fission neutrons: P(ν), n-n correlations, etc.
- **Collaboration LANL-RPI**
  - P.Talou, B.Becker, T.Kawano, M.B.Chadwick and Y.Danon, *"Advanced Monte Carlo Modeling of Prompt Fission Neutrons for Thermal and Fast Neutron-Induced Fission Reaction on Pu-239"*, submitted to Phys. Rev. C (March 2011).
- **Experimental input needed:**
  - Pre-neutron emission Fission Fragment Yields Y(A,Z,TKE)
  - Y(A,TKE) measured at RPI for $n_{th}+^{239}Pu$, $n_{th}+^{235}U$, and ^{252}Cf*(sf)*
- **In progress (with RPI):**
  - First calculation of ***prompt fission gamma spectrum and multiplicity*** using full Monte Carlo Hauser-Feshbach calculations (FFD/CGM codes)

PFNS Evaluation Code Package

- **Based on earlier UQ work for n+^{239}Pu PFNS**
  - P.Talou *et al.*, Nucl. Sci. Eng. **166**, 254 (2010)
- **Code Package**
  - Developed a code package to predict, analyze and evaluate **prompt fission neutron spectra** (PFNS) and multiplicity
  - Implements the Madland-Nix model equations
  - Model parameter systematics included
  - Experimental analysis module
  - Uncertainty Quantification using Bayesian statistics
  - ENDF formatting for easy incorporation in evaluated libraries

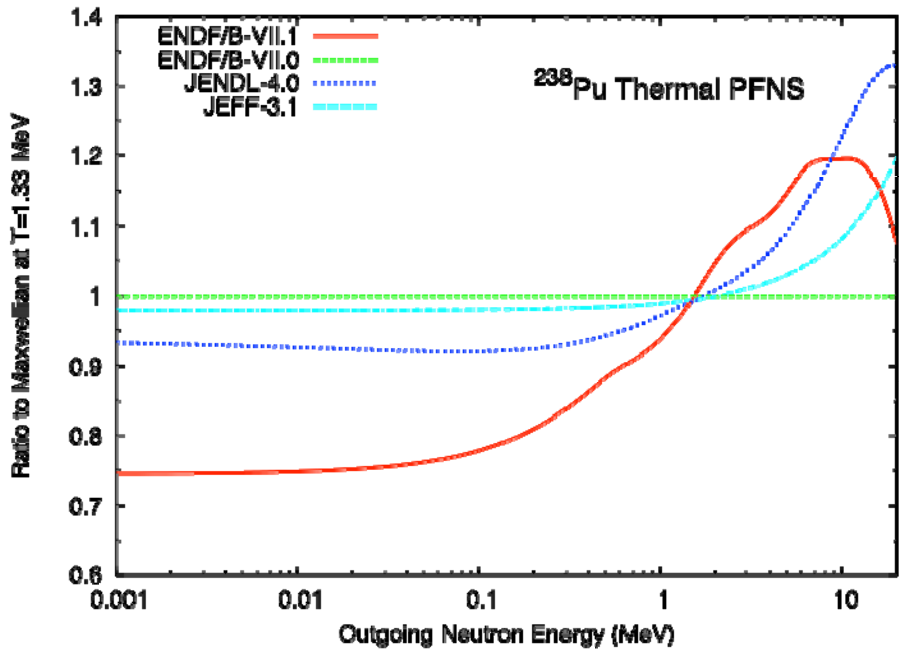


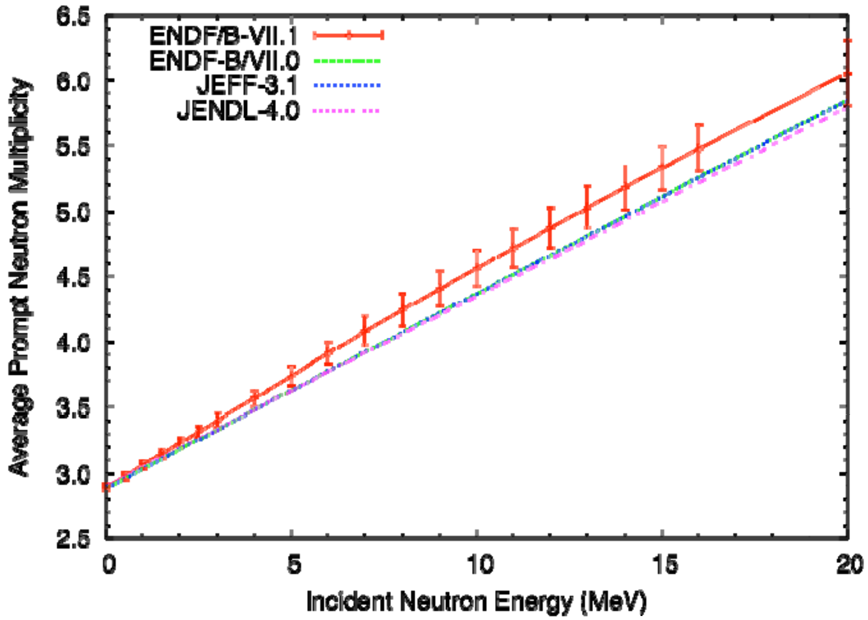
- **Already used for ^{238}Pu and ^{240}Pu evaluations**
- **In progress:** Application to suite of Minor Actinides

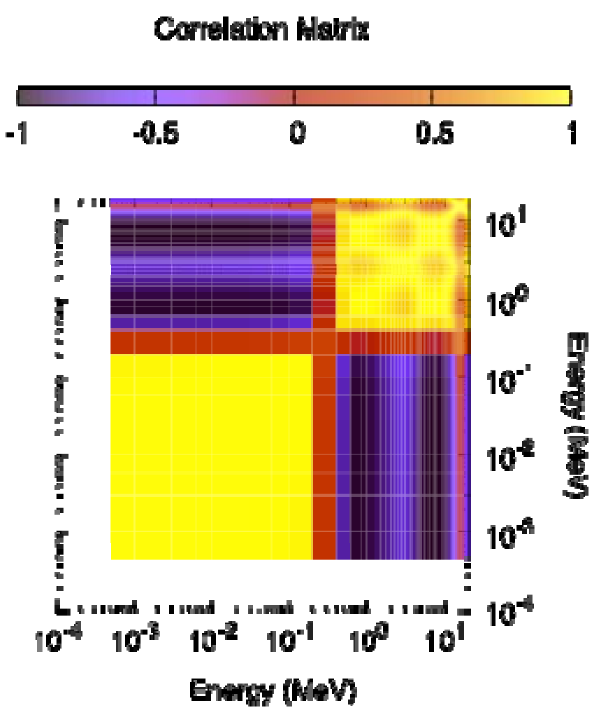
Example:

n+^{238}Pu PFNS Evaluation

Model parameter systematics used as *prior*, and modified according to thermal data for <ν>

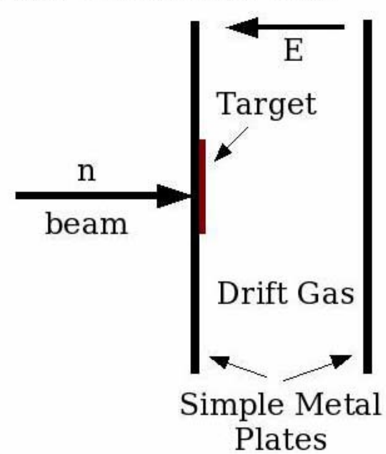






Higher precision is needed in ^{239}Pu(n,f) cross sections

- **Current uncertainties are at least 2-3% below 14 MeV and not completely understood. Goal is a 1% absolute measurement.**
- **Past fission measurements used ion chambers**
- **Ion chambers only record pulse height and time**
- **The Time Projection Chamber will not be subject to the systematic errors associated with past measurements**



The nuclear weapons programs, nuclear energy programs, and others have identified the fission cross-section uncertainties as a significant component in their applications

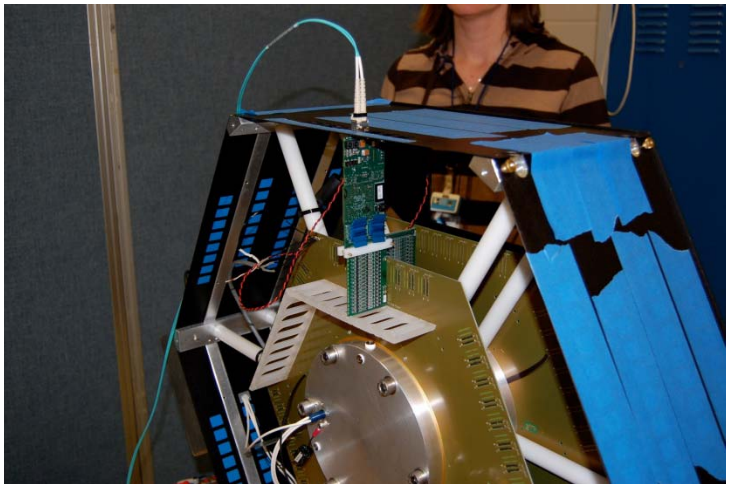
For weapons, the fission cross section affects the time evolution of neutron flux

For reactors, it is a key player in reducing safety margins

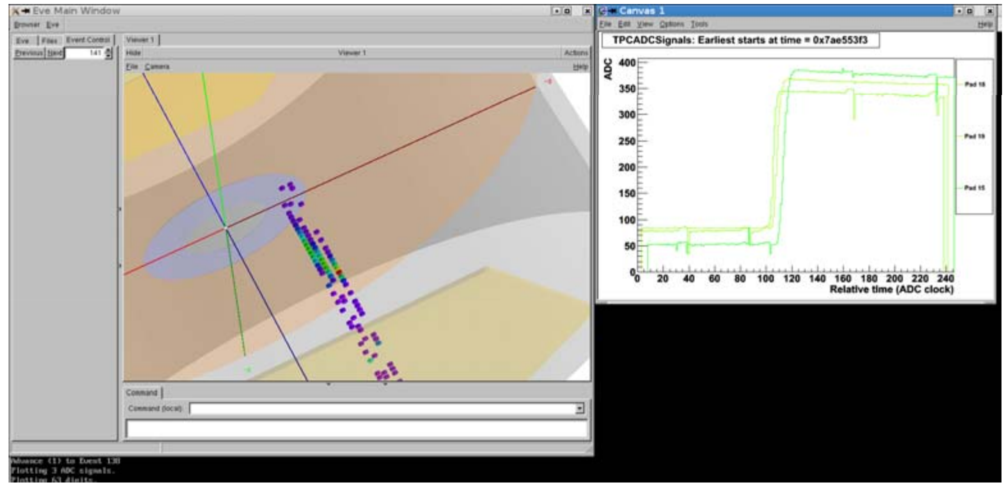
Our shared goal is to reduce fission cross-section uncertainties to below 1%

Goal is Pu239/U235 ratio data in June 2014 and Pu239/(n,p) in Dec 2015

Time-Projection Chamber is being developed for high-precision fission cross sections measurements



The fission TPC assembled with one complete electronic readout chain (32 channels). A Cm alpha source was used to produce signals in the first test.



▪Track visualization of a single alpha decay. The software used for tracking and data analysis was specifically developed for the fission TPC.

- First signals from the fission TPC were collected using an alpha source in December 2009.
- A full electronic chain was tested, corresponding to 32 channels. The complete system will have 192 sets of preamp- and digital cards (6144 channels).
- Project is on schedule with first beam data at LANSCE in the summer of 2010.

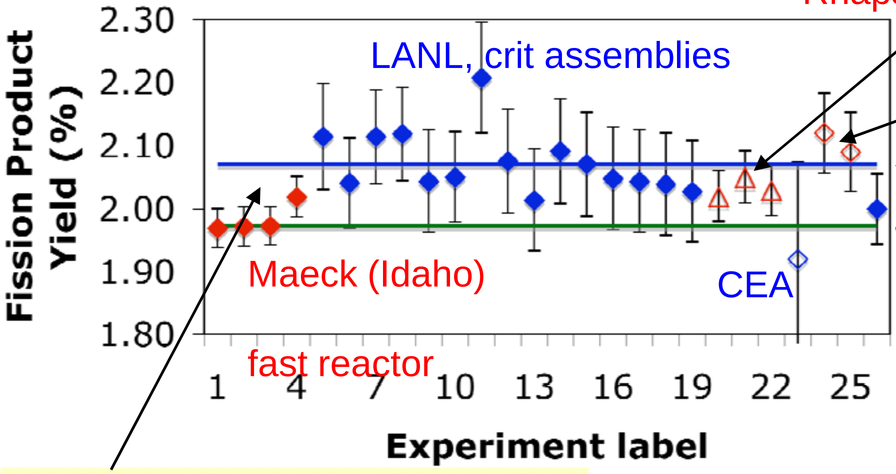
Recent FPY Emphasis at LANL has been on Incident Neutron Energy-Dependent Effects

(A=147 Fission Product Yield Measurements Appeared to be Discrepant)

Blue = LANL, fission chamber measurements in fast critical assemblies

Red = Mass spectrometry (typically accurate to 1-2%) in fast reactors

Rhapsodie (France) and BOR-60 (Russia) fast reactors



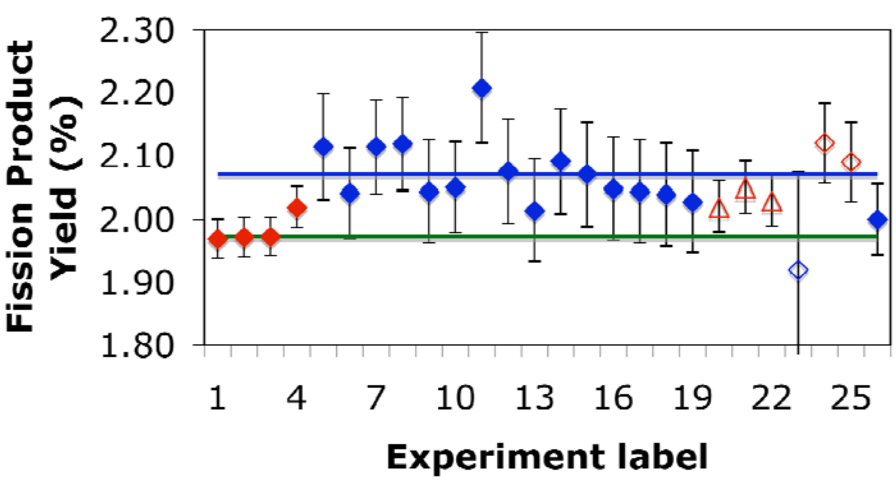
LANL evaluated value based on a fit to LANL measurements

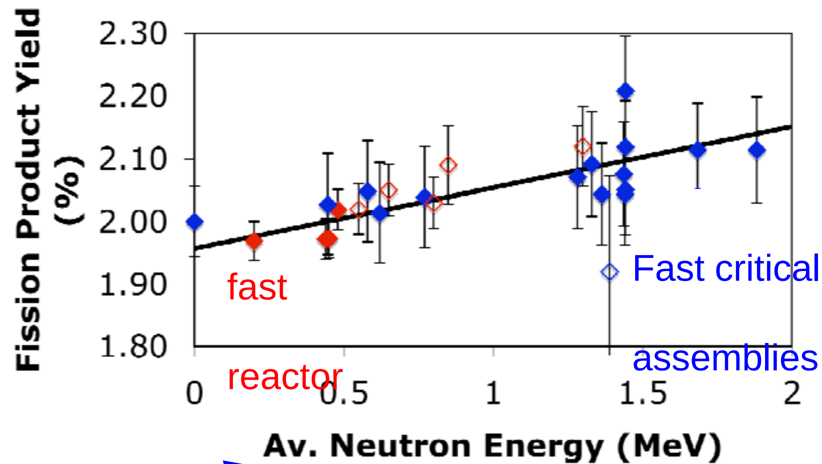
ENDF/B-VI evaluated value is 5% lower, and agrees with Maeck reactor data

This 5% discrepancy was a puzzle, since LANL and Maeck are generally consistent to <1-2%

Discrepancy Between LANL Data and the Mass-Spec Data Disappears When an Energy-Dependence is Considered

Same data plotted against average incident energy





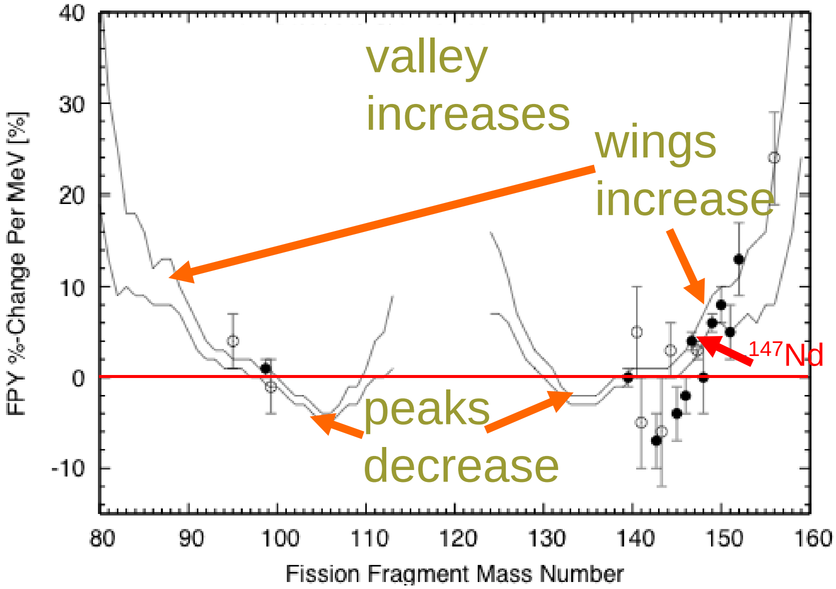
MCNP code used to determine average neutron energy

Routinely done at LANL as part of our validation testing of nuclear cross sections and codes

Discrepancy disappears. But a subtle effect – the slope (% changer per MeV) is similar to the data uncertainties

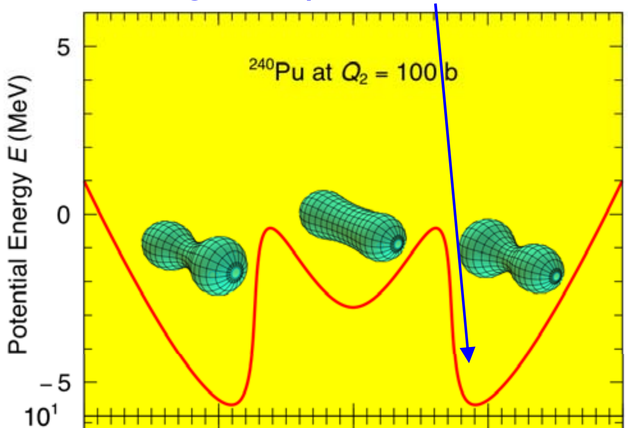
We now know the FPY to ~ <2% over this energy range

Unexpected: Even Near the Peaks, FPs Have An Energy Variation Over the 0.2-2 MeV Fast Region (ENDF Will Be Expanded)



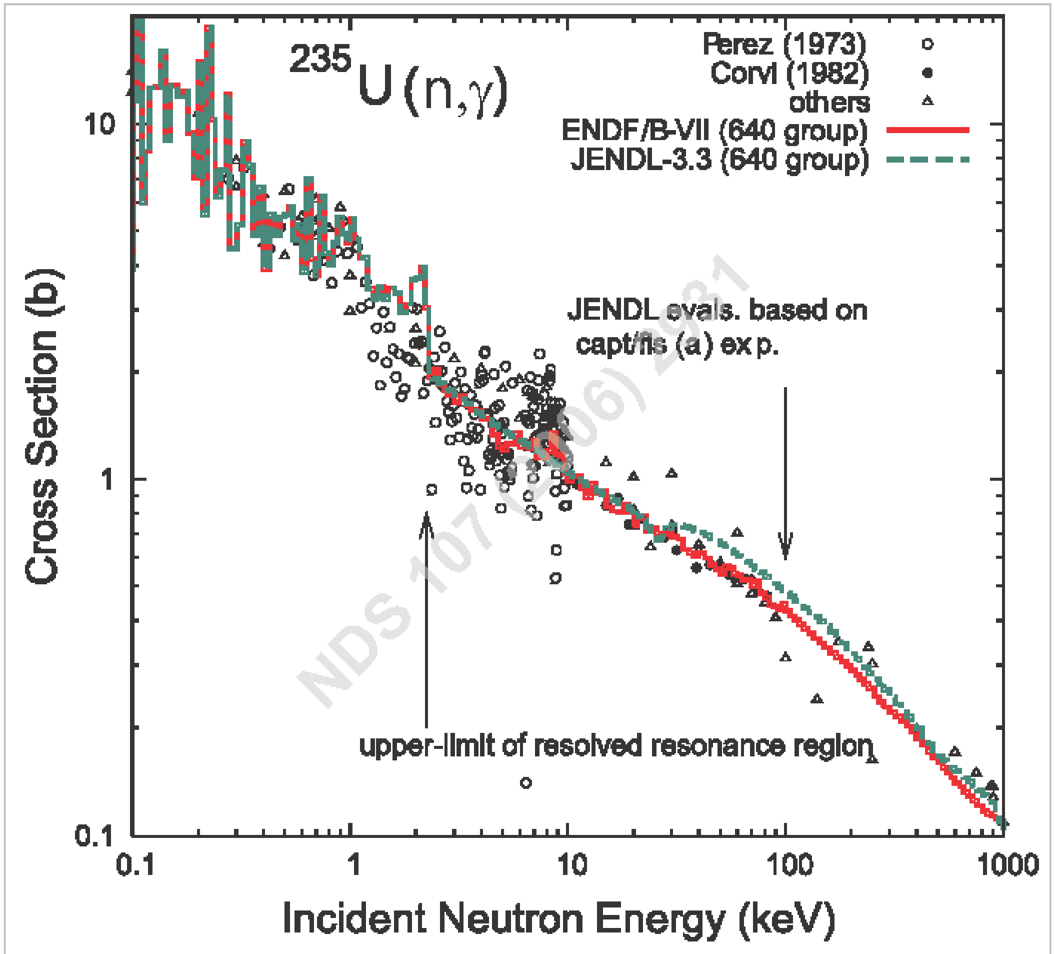
Phenomenology of en. dep. from experimental data in the 0-2 MeV range: allows us to understand the energy dependence and build this into ENDF/B-VII (John Lestone)

Theory insights for wings - Think of the fissioning system as a bobsled racing down the track - more energy allow it to move higher up the walls…..



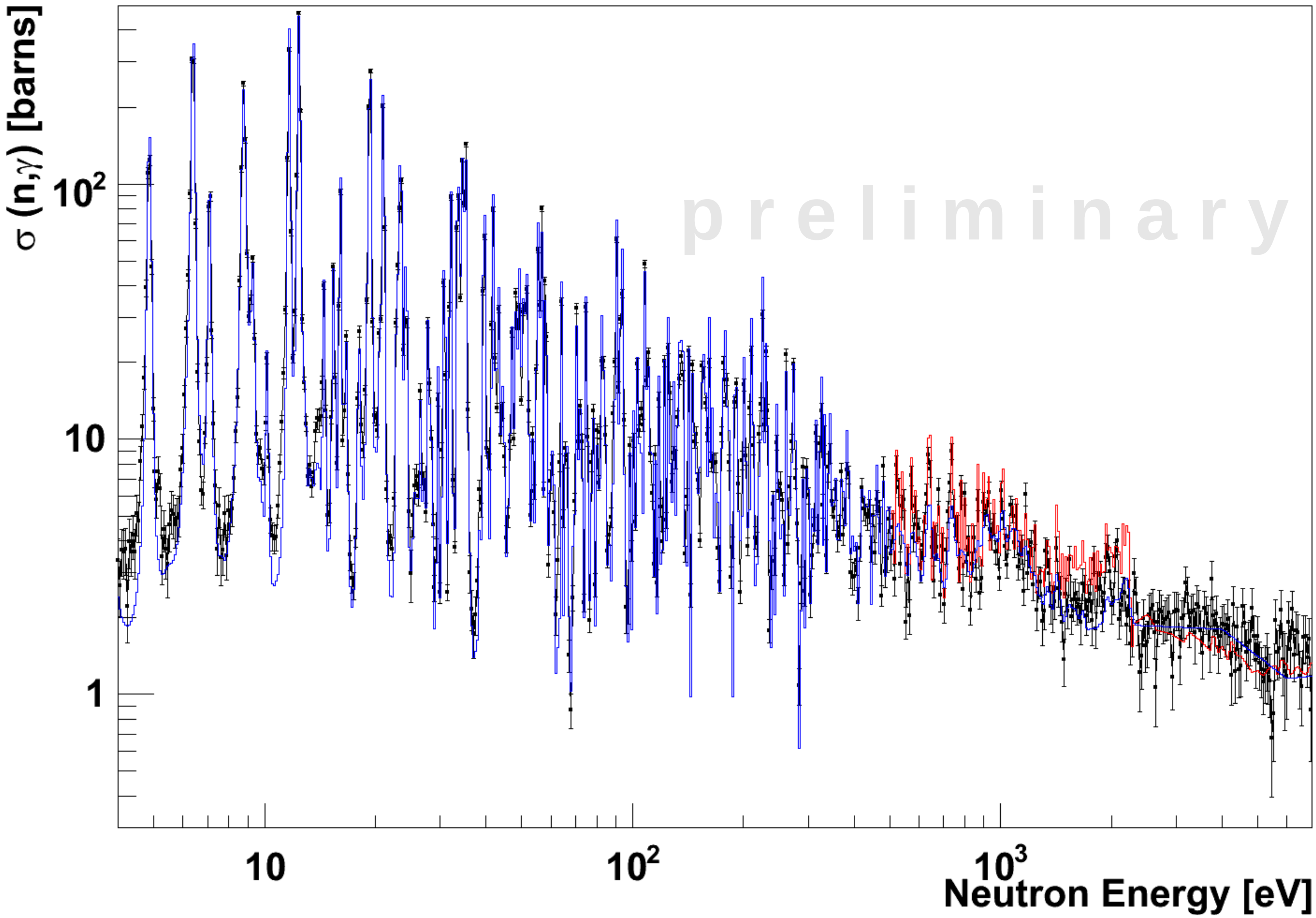
▪A, mass of product

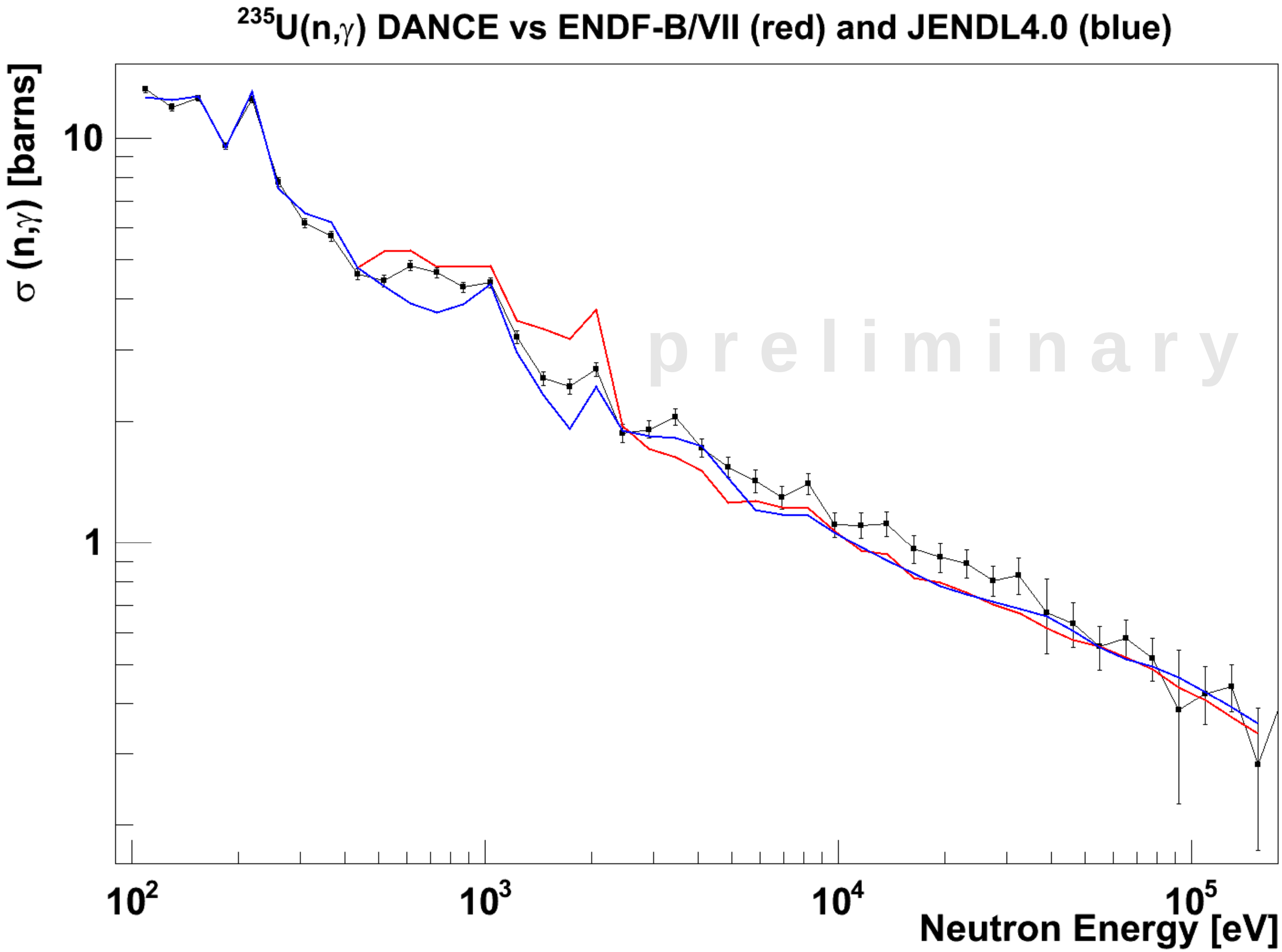
^{235}U Capture is Still Uncertain to ~ 10% for Einc= 1keV to 1 MeV: We Must Do Better



- We have preliminary data from the DANCE detector at LANSCE (see next viewgraphs) that appears to conflict with current evaluated data in few keV range.
- This is important to understand!
- We would like to compare results with RPI measurements as soon as possible (hint hint).

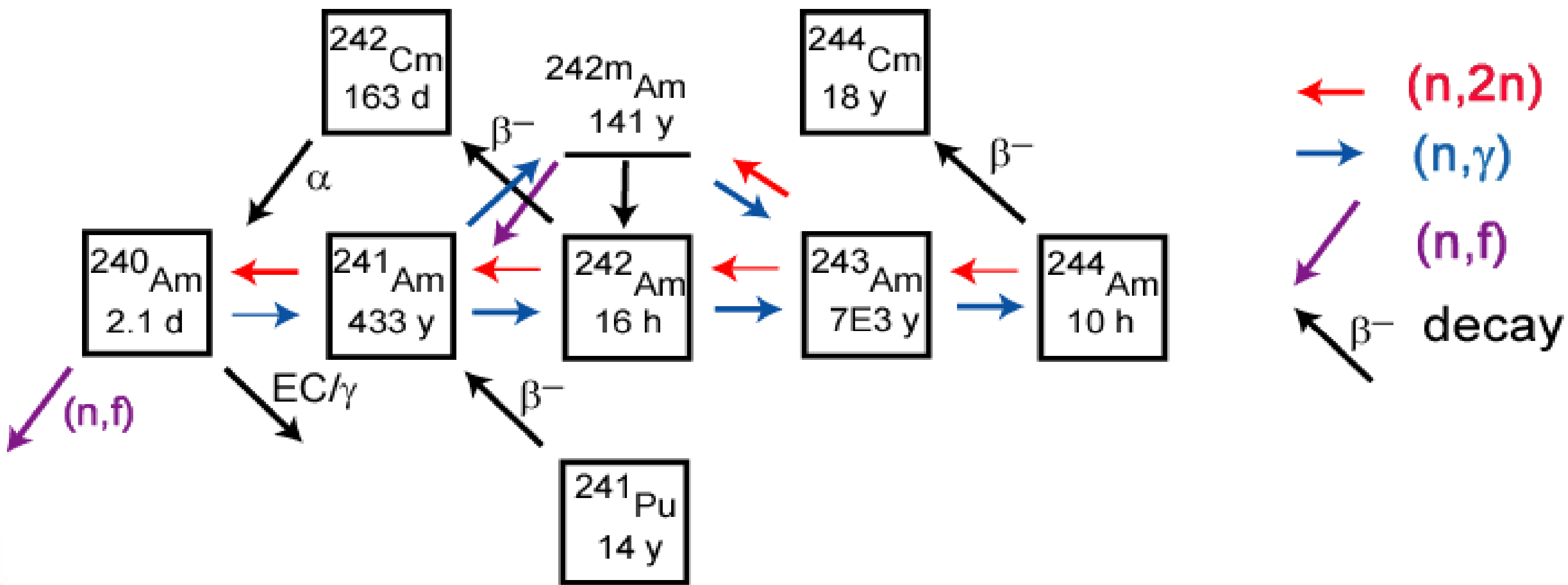
$^{235}U(n,\gamma)$ - DANCE vs ENDF-B/VII (red) and JENDL4.0(blue)



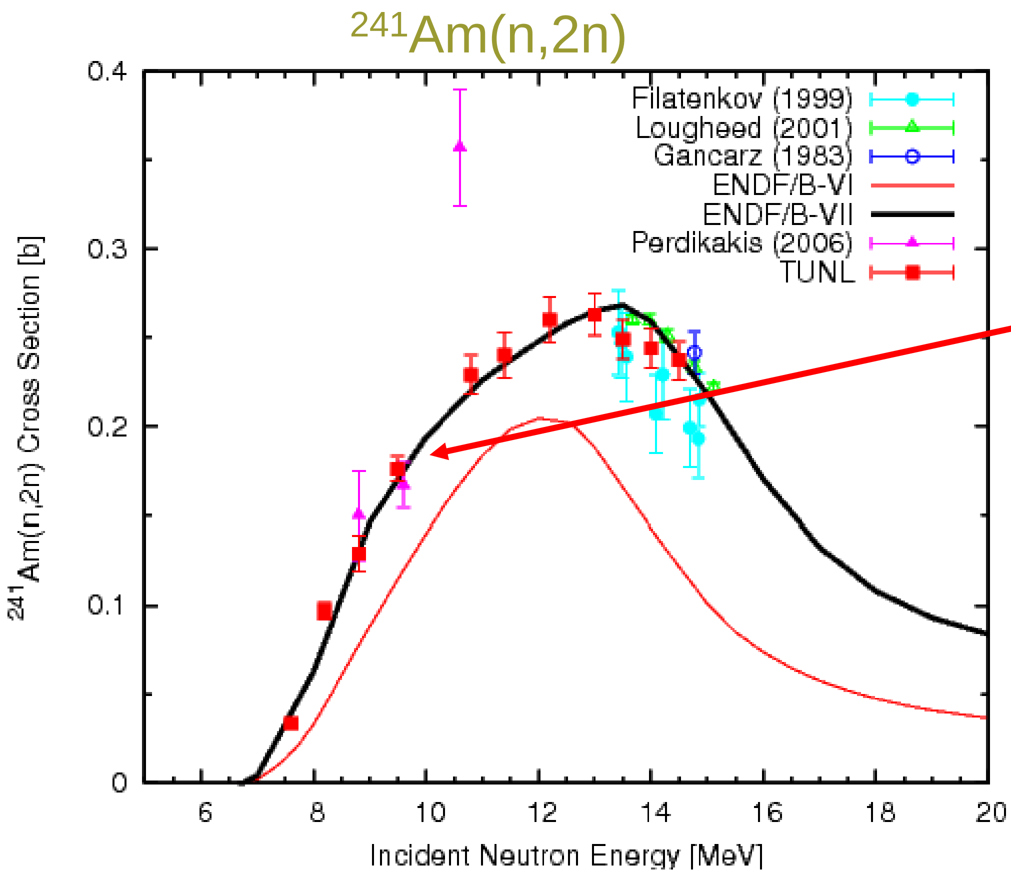

235U(n,γ) DANCE vs ENDF-B/VII (red) and JENDL4.0 (blue)
σ (n,γ) [barns]
10
1
preliminary
10^2
10^3
10^4
10^5
Neutron Energy [eV]

Capture and (n,xn) cross sections for Americium -- Important Diagnostic

- ^{241}Am(n,2n) recently measured via TUNL-LLNL-LANL collaboration
- ^{241}Am(n,γ) recently measured at DANCE….but we'd like these data to be more precise in the 100keV - ~ 1 MeV region
- ^{241}Am capture m/g ratio - much improved in ENDF/B-VII. New LANL/Karlsruhe expt. ongoing.
- ^{242m}Am fission & capture are being measured at DANCE



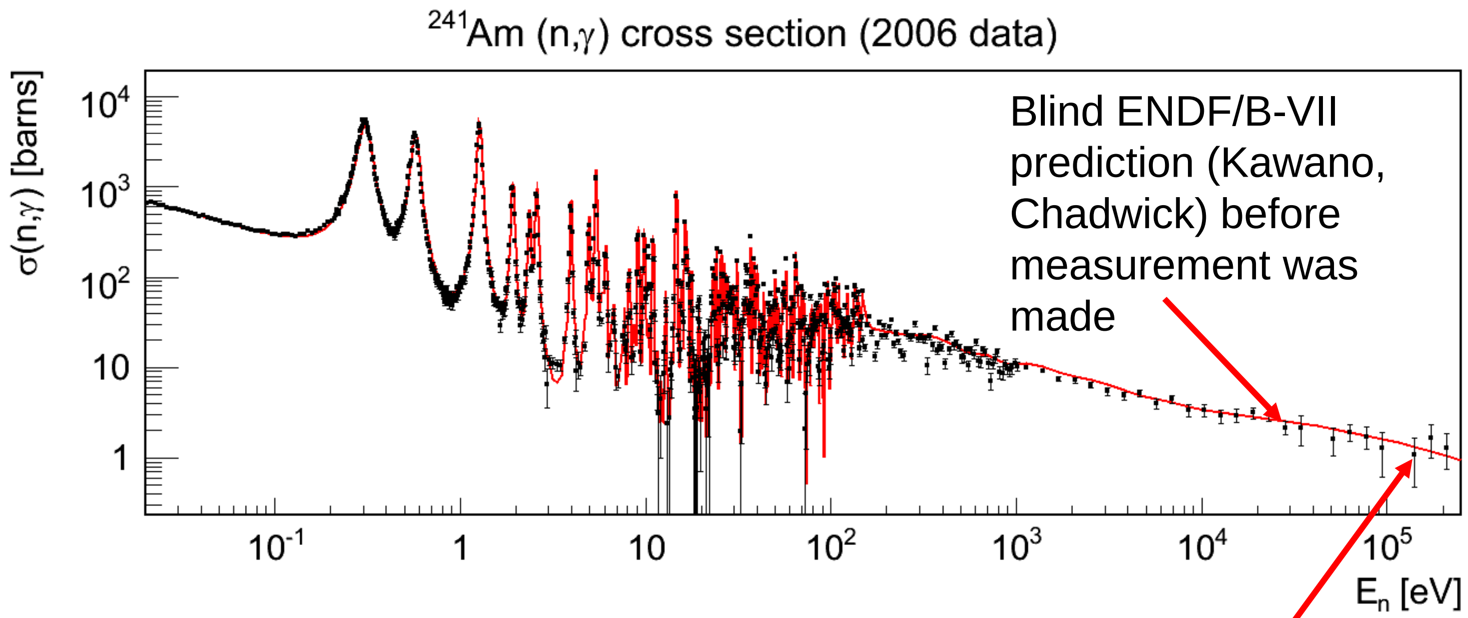
^{241}Am(n,2n) : New Results from TUNL/LLNL/LANL Collaboration Confirm ENDF/B-VII



"Blind" GNASH code prediction for ENDF/B-VII (though calibrated to data at 14 MeV), before TUNL measurement was made

Preliminary data by Plompen, from Geel, appear to confirm the TUNL expt, and extend to higher energies

^{241}Am(n,γ) capture:
Combining Experiment, Theory, and Integral Data



New data from DANCE detector - Vieira, Jandel, Rundberg, Ullmann, et al.

PRC paper accepted.

Above 100 keV, the ENDF/B-VII.0 evaluation was slightly low

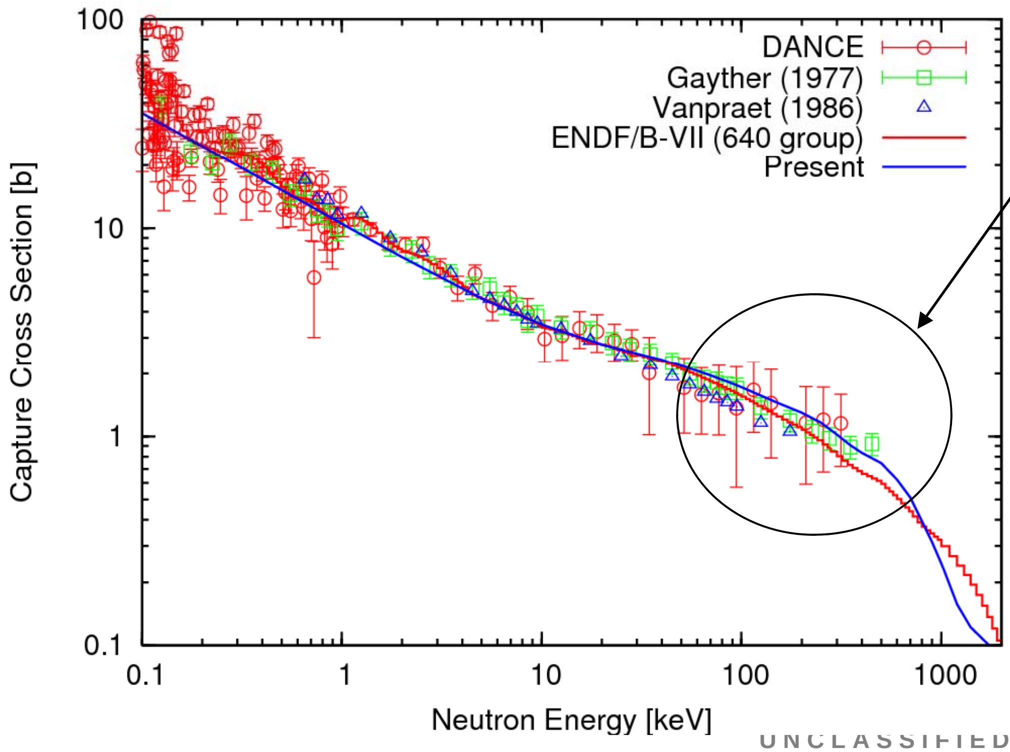
Note that the measurement uncertainties are becoming big above 100 KeV, and data end at ~ 200 keV.

We need data up to 0.5-1 MeV

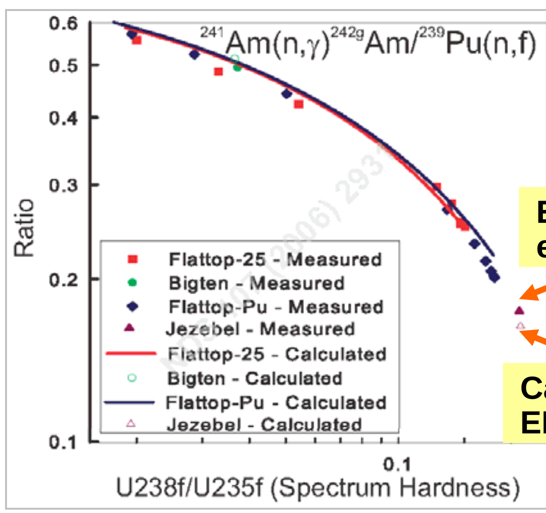
Improved Theory for Radiative Capture - Use of Formalism to Properly Calculate Inverse Coupled-Channel Process -- Example for ^{241}Am(n,γ)

- **Removes the traditionally Hauser-Feshbach assumption of using inverse channel transmission coeff. for the excited states based on the ground state**
- **Impacts neutron radiative capture channels, as it changes the inelastic scattering competition.**

Predicts ^{241}Am(n,γ) higher for E_{inc} > 50 keV, in agreement with DANCE data



Critical assembly testing: when averaged over the Jezebel spectrum, gives 5% higher rate compared to ENDF/B-VII



Expt. (Barr et al.)

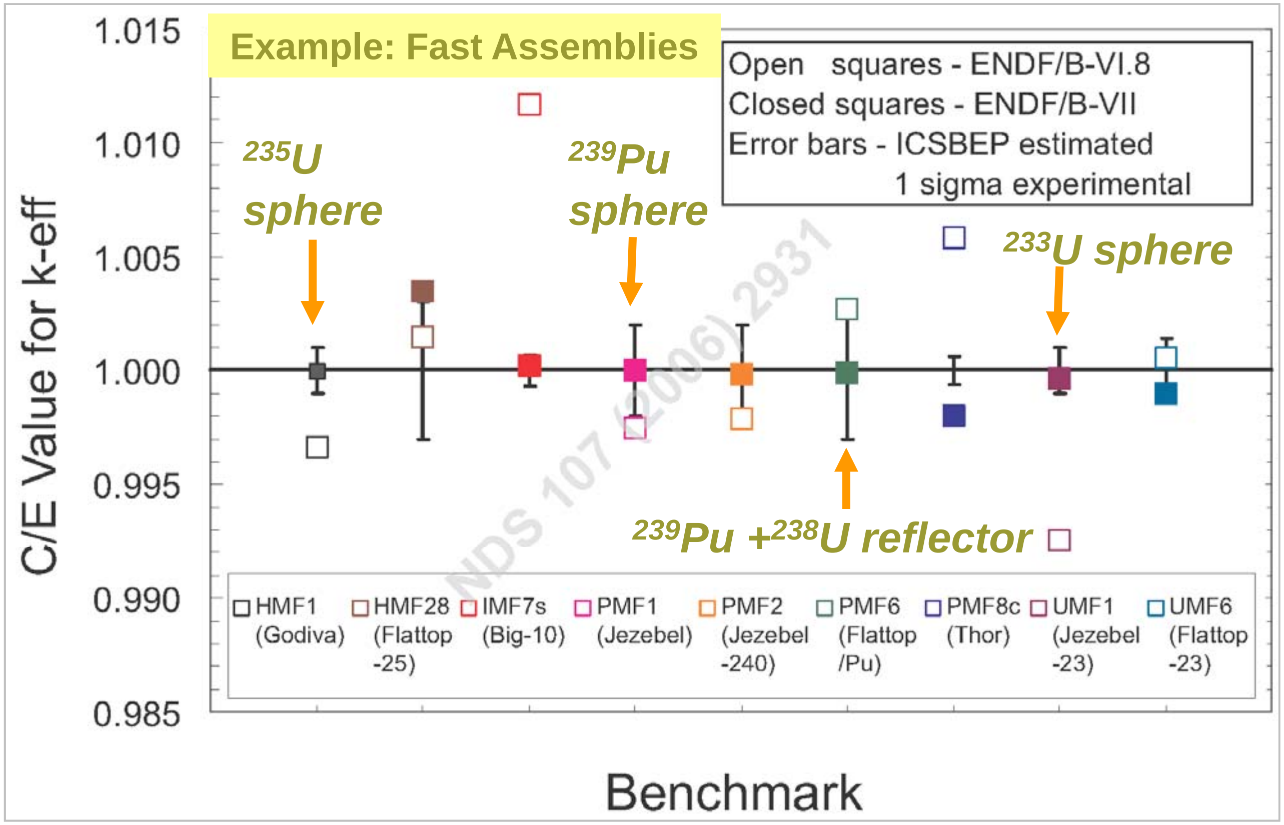
Calc. using ENDF/B-VII

We Continue to use Legacy Critical Assembly Data for Nuclear Data Testing: Excellent ENDF/B-VII Performance Shown Below

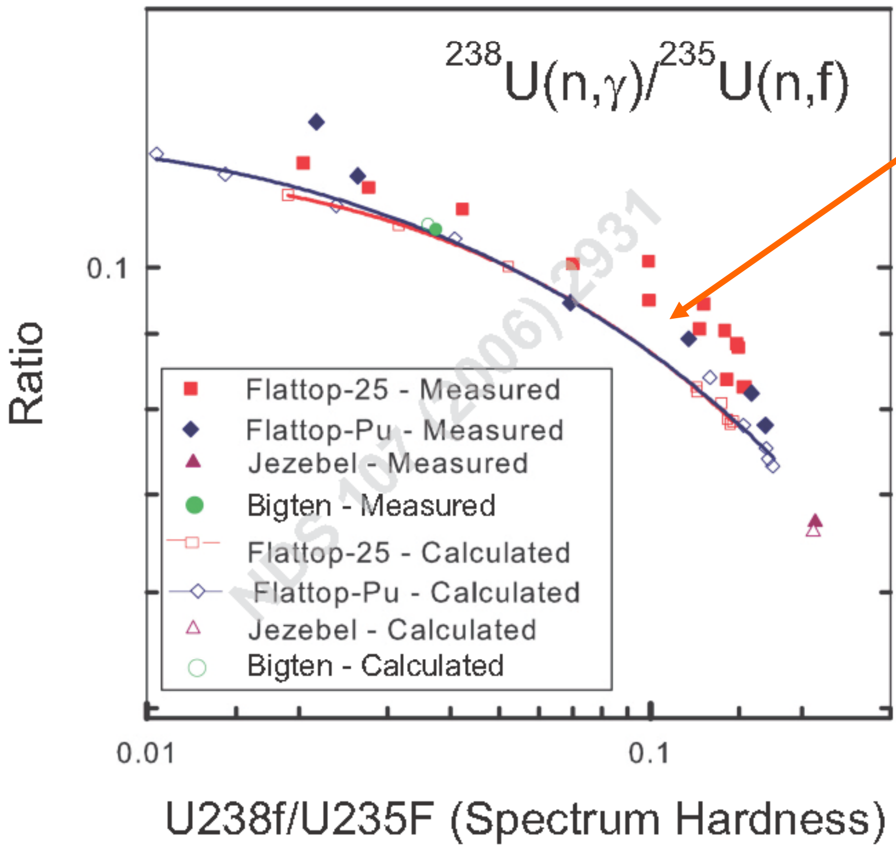
Data testing against

> 800 assemblies:

- Fast assemblies
- Reflected assemblies
- HEU
- LEU
- Pu solutions
- Np, ^{233}U
- *etc.*



Integral Information from LANL Critical Assemblies Suggests ENDF $^{238}U(n,\gamma)$ Could be Low



Integral radiochemically-measured capture rate suggests our ENDF data may be ~5% low

We hope new measurements well settle this question:

Wallner activation measurement using AMS, with quasimonoenergetic neutrons at 20 and 500 keV at FZK, with goal of 3-5% accuracy

LANSCE/DANCE measurements

As CEF Nears Fully Operation Status, we are Proposing New and Expanded Critical Experiments

- **Critical assembly experiments at NTS CEF expected to begin "soon"**
- **Experimental user facility is being run by the NCSP program**
  - http://ncsp.llnl.gov/
- **Solicitations have been made asking for highest priority from NW**
- **A number of proposals have been submitted**
  - 136 - Reaction rate and fission-product yield measurements in Pu-239 and U-238,235
  - 137 - High Precision HEU Critical Assembly Measurements To Understand Reproducibility
  - 138 - Probability of Initiation Benchmark Experiments
  - 152 - High Precision Plutonium Critical Assembly Measurements
  - 153 - Measure The Fission Neutron Spectrum Shape Using Threshold Activation Detectors
  - 163 - Reaction rate and fission-product yield measurements with the COMET assembly

Summary

- **Los Alamos has substantial interests and activities in all aspects of nuclear data**
- **Many of those interests and activities overlap with RPI capabilities**
  - This has led to various collaborations
  - We would like to strengthen and increase these collaborations as appropriate