Nuclear Data Accomplishments for FY 2010

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Nuclear Engineering Division
Argonne National Laboratory

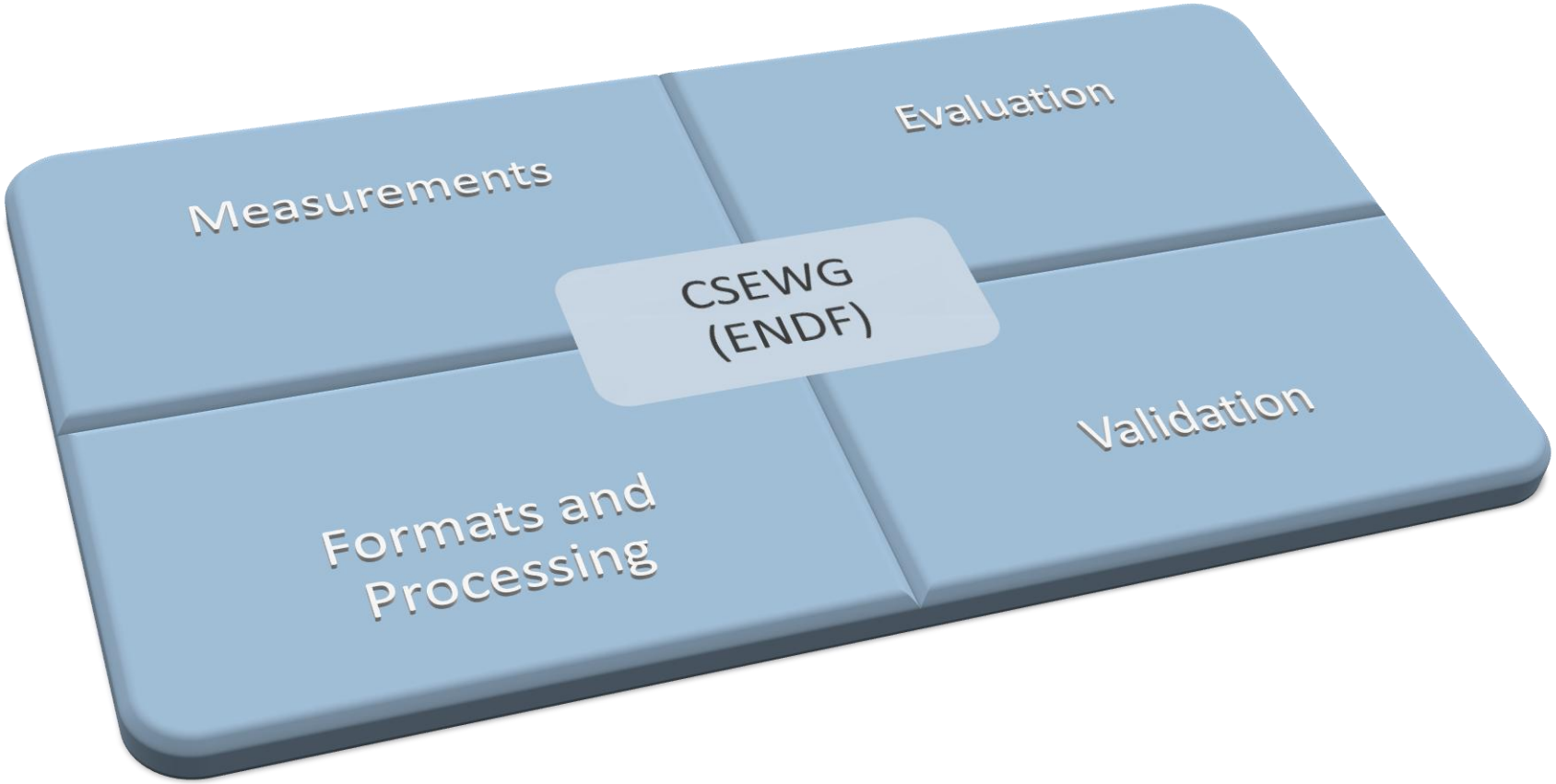
DOE Workshop: "NCSP Accomplishments"

Friday, July 1, 2011
ANS 2011 Annual Meeting
Hollywood, FL

Overview

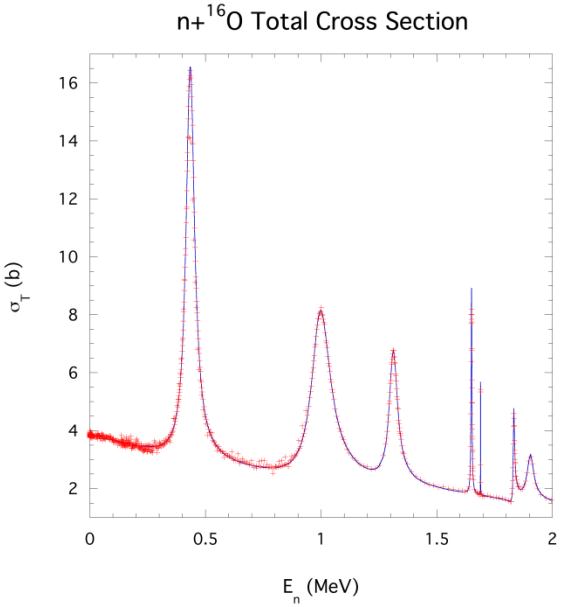
- High-level Overview of the “Evolution” of Nuclear Data for Criticality Safety (~5 min.)
- Snapshot of the Recent Nuclear Data Advances in Support of Criticality Safety (~10 min.)
- Questions and Answers (~5 min.)

“Evolution” of Nuclear Data for Criticality Safety



Measurements and Evaluation

- Modern Nuclear Data Files are Evaluated using Measured (Experimental) Data and Nuclear Reaction Theory Models
  - Evaluated files can be produced solely using Nuclear Reaction Codes (such as McGNASH, EMPIRE, SAMMY, …)
  - However, uncertainties are ALWAYS reduced if experimental data are included in the evaluation

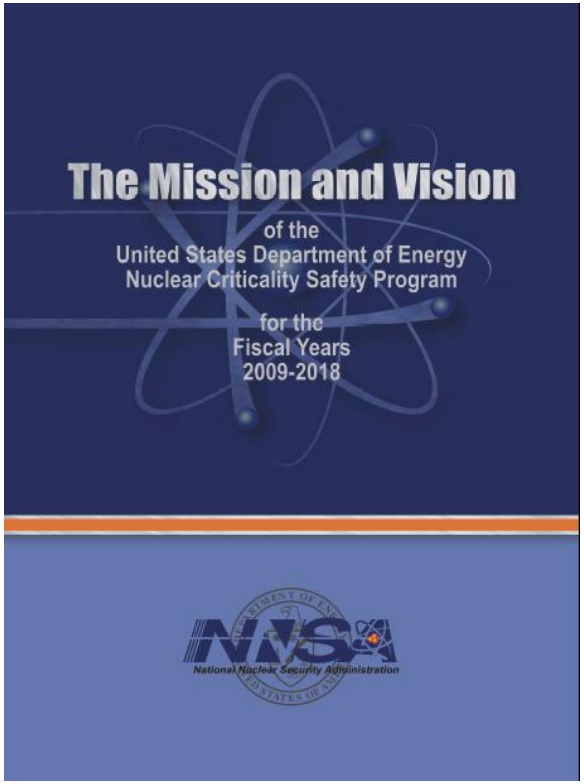


Processing and Validation

- New Evaluations are Accepted in ENDF only after
  - Phase I testing (checking codes, peer review, …) and
  - Phase II testing (validation calculations)
- Validation can only occur after Processing
  - Formats are (slowly but) continually CHANGING
  - Therefore Processing Codes, such as NJOY, AMPX, PREPRO, …, must (slowly but) continually CHANGE
- Validation requires the availability of Integral Measurements

The NCSP Nuclear Data Mission and Vision

- **MISSION**
  - The Nuclear Data (ND) program element includes the measurement, evaluation, testing, and publication of neutron cross-section data for nuclides of high importance to nuclear criticality safety analyses. The NCSP continues to improve coordination of nuclear data activities by fostering a strong collaborative effort among all of our national and international resources in this highly technical area. The objective is to solve the highest priority nuclear data problems relevant to criticality safety in a timely manner. This program element is essential for the NCSP because it provides the nuclear cross-section data required by the AM program element.
- **ND Vision**
  - The ND element will **sustain** world-class **expertise** and capabilities to **continually improve** and disseminate measured and evaluated differential cross-section and covariance data in a manner that is **responsive** to the needs of those responsible for developing, implementing, and maintaining criticality safety.



Nuclear Data Accomplishments

- NCSP supported Nuclear Data Activities at
  - ANL, BNL, LANL, LLNL, ORNL and RPI

- Principal support and major accomplishments in Measurements and Evaluation made by **ORNL** and **LANL**

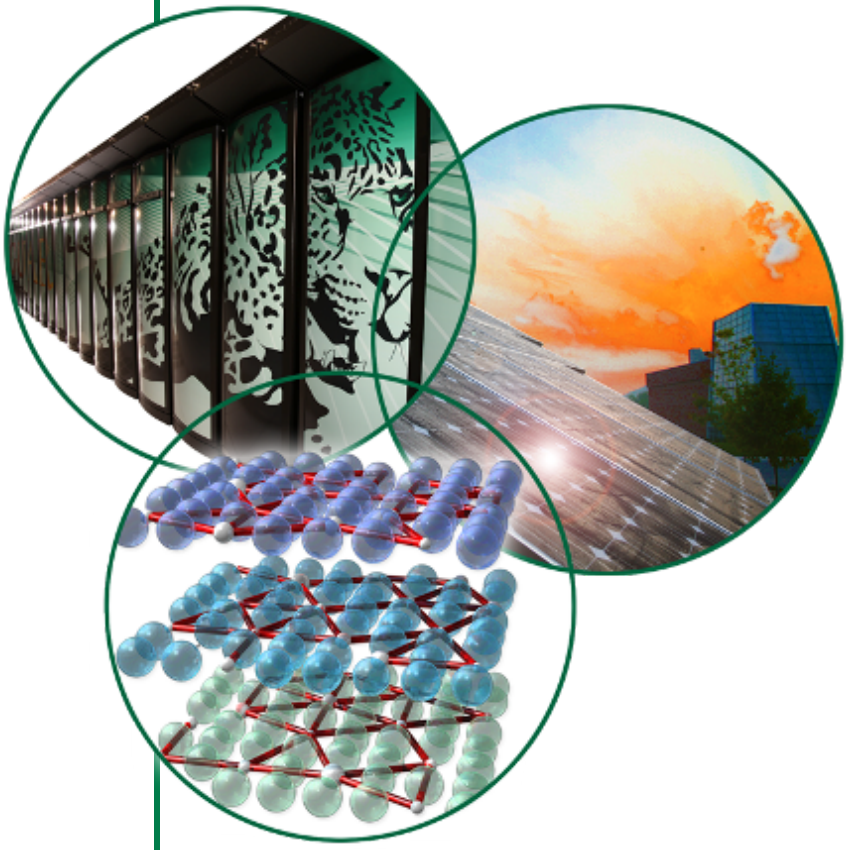
- However, all of these organizations tend to contribute (through CSEWG) in most areas:
  - Measurement
  - Evaluation
  - Formats and Processing
  - Validation

Nuclear Data Accomplishments for FY 2010

- The following 59 slides (#9-67) are excerpted from presentations given at the DOE NCSP Technical Seminar March 1-2, 2011 Oak Ridge National Laboratory
  - They are only a representative portion of these activities
  - See http://ncsp.llnl.gov/accomplishmentsMain.html for the full presentations

- They are followed by two summary slides

ORNL Nuclear Data Accomplishments for FY 2010



Mike Dunn, Luiz Leal, Klaus Guber, Doro Wiarda and Goran Arbanas

Reactor and Nuclear Systems Division

US DOE Technical Seminar
Oak Ridge National Laboratory March 1 – 2, 2011

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

- ORNL NCSP Nuclear Data Program
- Measurements and Evaluations
- Status of Evaluations submitted to NNDC
- Summary

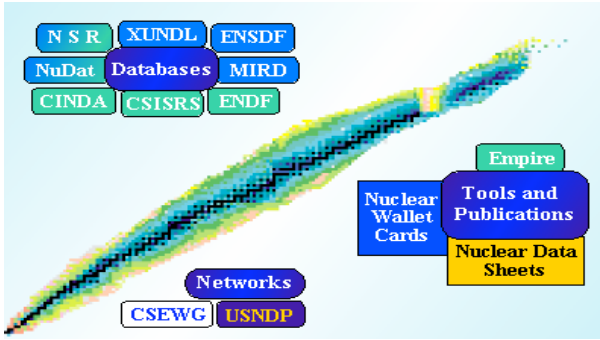
Nuclear Data Work for Criticality Safety

- ORNL Nuclear Data and Criticality Safety (NDCS) group provides technical support to NCSP working to develop and maintain state-of-the-art radiation transport (**SCALE**) and **nuclear data capabilities** for criticality safety applications
- ORNL **nuclear data contribution** to NCSP mission
  - Cross-section measurements for resonance region (Data from facilities: IRMM, RPI, and ORELA)
  - Nuclear modeling methods development (SAMMY)
  - Cross-section evaluation and preparation of ENDF/B nuclear data files
  - ORNL participation in international nuclear data activities:
    - OECD/NEA Working Party on International Nuclear Data Evaluation Cooperation (WPEC)
    - IAEA/CRP (Coordinated Research Projects)
  - Cross-section processing methods development for generating nuclear data libraries (AMPX)
  - Support radiation transport methods development and application

ORNL Measurement and Evaluations

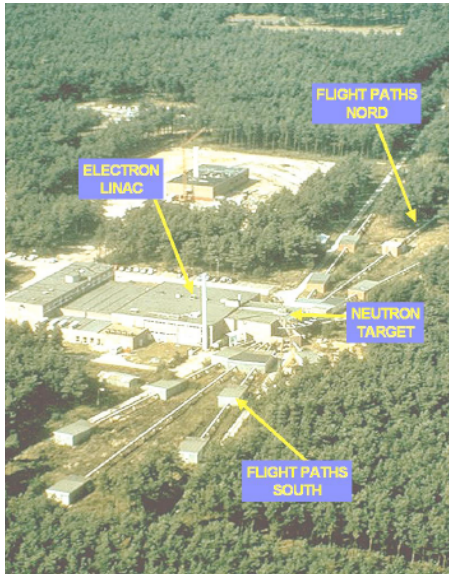
- ORNL Evaluation Contributions to ENDF/B during past 5 Years
  - ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{237}Np, ^{232}Th,
  - ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd
  - ^{35}Cl, ^{37}Cl, ^{231}Pa, ^{239}Pa,
  - ^{39}K, ^{40}K, ^{41}K, ^{19}F
  - ^{55}Mn, ^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr
  - ^{58}Ni, ^{60}Ni
  - ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, ^{50}Ti
  - SiO_2

NNDC



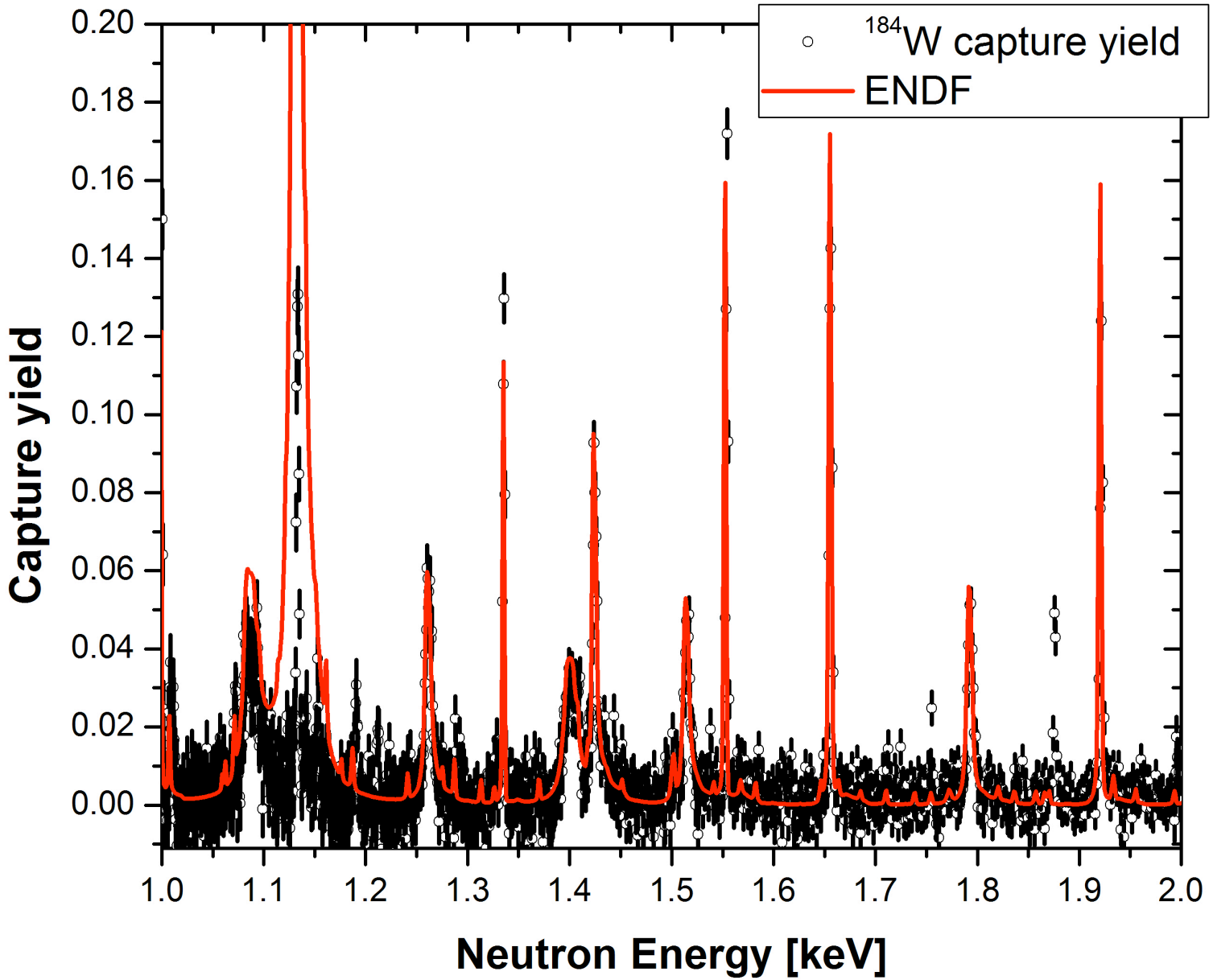
- FY10 Resonance Region Measurements
  - ^{182}W, ^{183}W, ^{184}W and ^{186}W (IRMM)
  - ^{63}Cu and ^{65}Cu (IRMM)
- FY10 Resonance Region Evaluation Tasks
  - ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, and ^{50}Ti
  - SiO_2 thermal evaluation NCSU-ORNL

IRMM



ORNL Measurement Activities in FY10: I

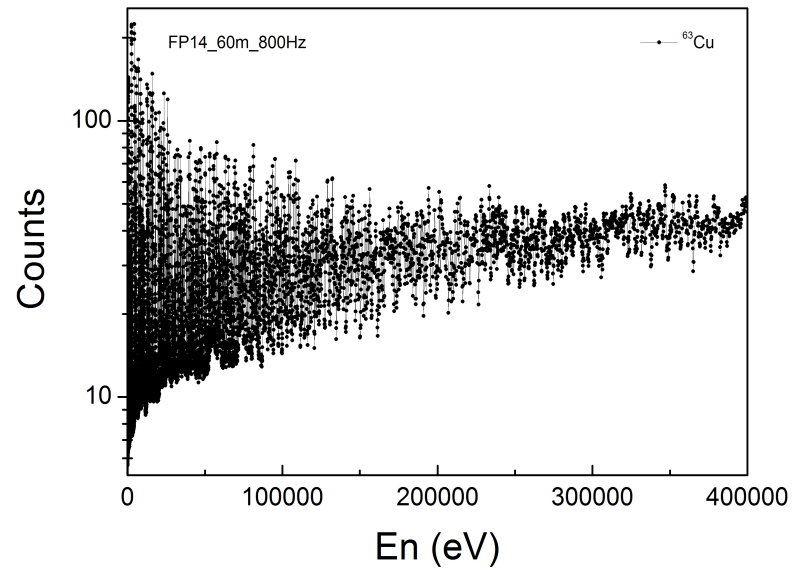
- Completed measurements for stable tungsten isotopes —enriched samples for $^{182,183,184,186}W$.
- Data now covers complete resolved resonance region as well as part of the unresolved region.
- Normalization of the capture data finalized.
- Capture Data for $^{182,183,184,186}W$ from the high repetition run available to analyze.
- Transmission data for $^{184,186}W$ with different sample thickness available.


^{184}W capture yield
ENDF
Capture yield
Neutron Energy [keV]
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0

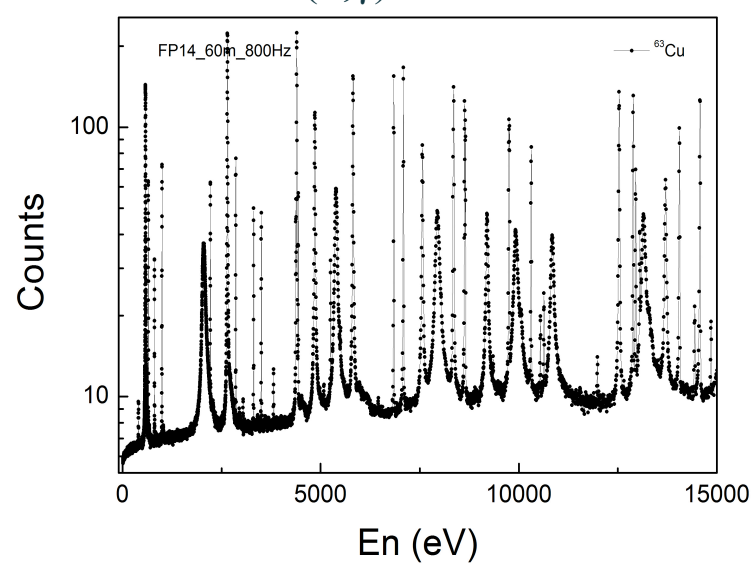
ORNL Measurement Activities in FY10: II

- **Neutron Capture measurements for ^{63,65}Cu at GELINA using set up at FP14, 60m station**
- **Neutron transmission on natural Cu using GELINA FP4, 50m station**
- **Use of metallic samples, >99% isotopic enrichments; 8cm diameter disks with 1mm thickness.**
- **Will include old ORELA transmission data in evaluation**

^{63}Cu (n,γ) Data



^{63}Cu (n,γ) Data - detail



ORNL FY10 Evaluation Accomplishments
^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, ^{50}Ti and SiO_2

ORNL SAMMY R-Matrix Resonance Region Analysis Software Used to Prepare Evaluations

- Used for time-of-flight cross-section data in resonance region—analysis of neutron, charged-particle cross-section data.
- Uses Bayes' method (generalized least squares) to find parameter values.
- Uses R-matrix theory, Reich-Moore approximation (default) or multi- or single-level Breit-Wigner theory.
- Generates covariance and sensitivity parameters for resonance region

Incident particles: neutron, proton, alpha, …

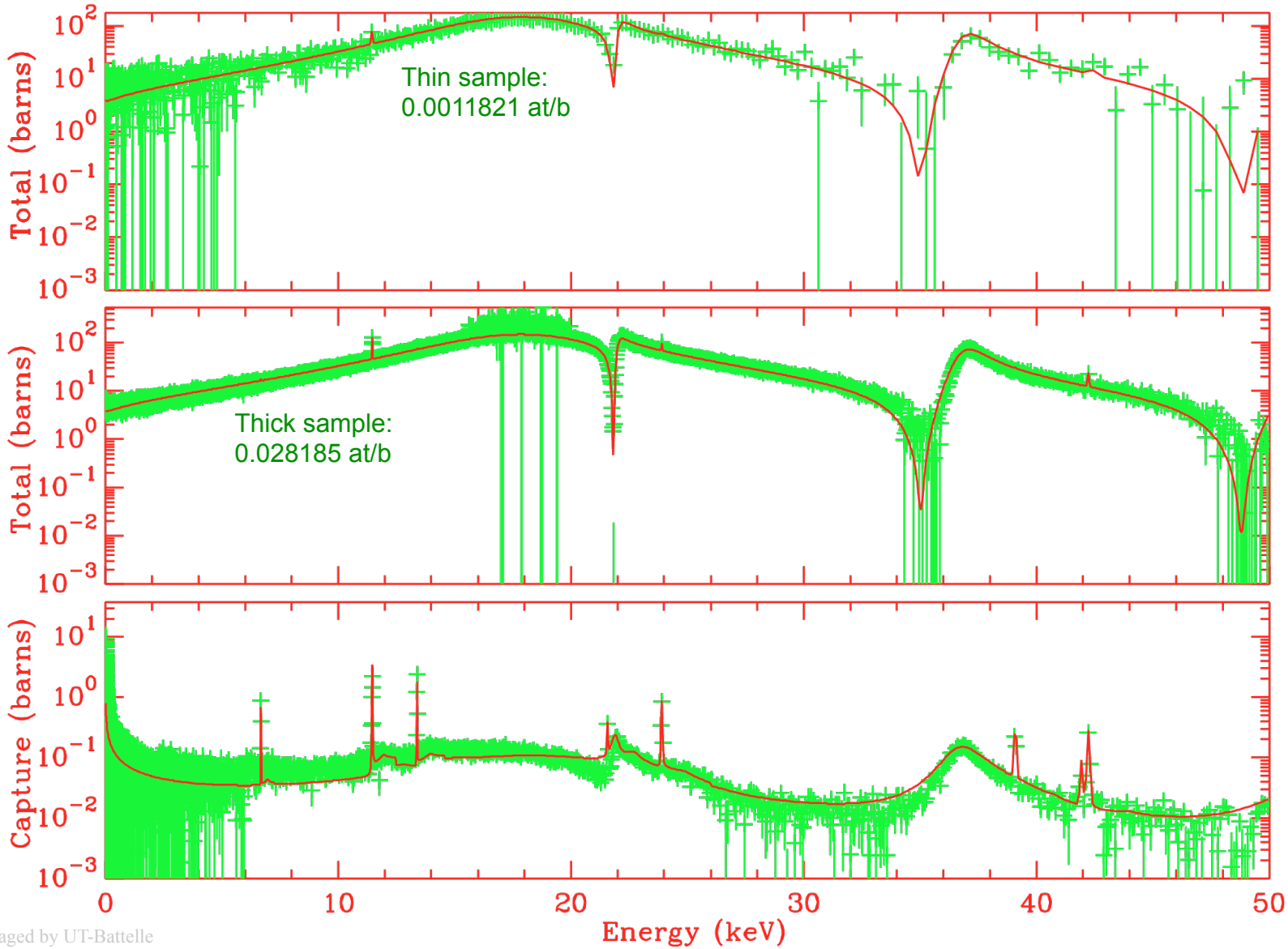
Target: one type of nuclide, or many

- Multiple isotopes
- Chemical compounds
- Contaminants

Energy region:

- Resolved resonance region (RRR)
  - Total, elastic, capture, fission, inelastic, other reactions
  - Charged-particle entrance and/or exit channels
  - Angular distributions
  - Integral data (Westcott's g-factor, resonance integral, Watt spectrum average, K1, alpha)
- Unresolved region (URR)
  - Total, elastic, inelastic, capture, fission

^{48}Ti Cross Sections: Experimental and SAMMY



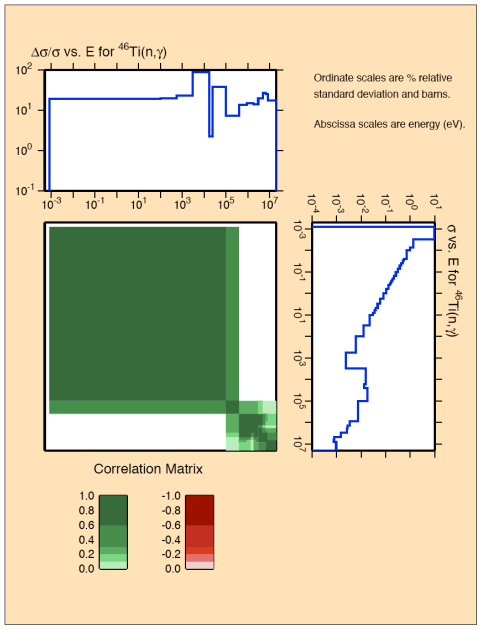
Resonance Parameter and Covariance Evaluation for ^{46,47,49,50}Ti

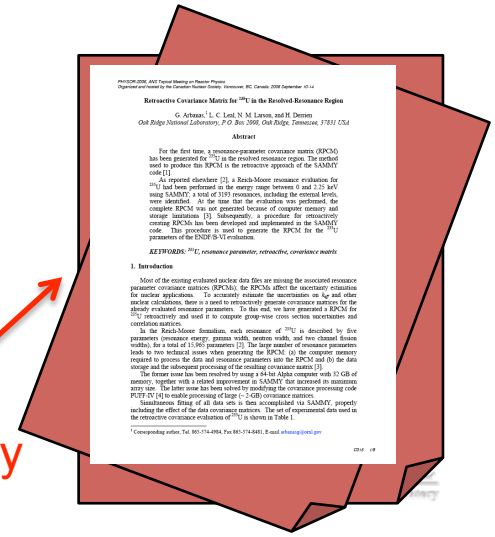
- Resolved resonance parameters were converted from MLBW into the RM representation. The resonances were checked against the resonance parameters given in the Atlas of Neutron Resonances

- For ^{46}Ti a resonance at 55.67 keV with j=1/2 (l=1) was repeated. According to the Atlas of Neutron Resonance Parameters—should be at the energy 56.66 with Γ_t=0.48 eV, Γ_n=0.1 eV and Γ_γ=0.38

- Thermal cross section and resonance integral are unchanged

- Covariance Data:
  - Resolved resonance covariance data were generated with the SAMMY for ^{46,47,49,50}Ti
  - SAMMY used with option to generating resonance-covariance retroactively using the "propagated uncertainty parameter" option to include systematic data uncertainties





PHYSOR-2006, ANS Topical Meeting on Reactor Physics
Organized and Hosted by the Canadian Nuclear Society, Vancouver, BC, Canada, 2006 September 10-14

Retroactive Covariance Matrix for ^{235}U in the Resolved-Resonance Region

G. Arbanas,[1] L. C. Leal, N. M. Larson, and H. Derrien
Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee, 37831 USA

Abstract

For the first time, a resonance-parameter covariance matrix (RPCM) has been generated for ^{235}U in the resolved resonance region. The method used to produce this RPCM is the retroactive approach of the SAMMY code [1].

As reported elsewhere [2], a Reich-Moore resonance evaluation for ^{235}U had been performed in the energy range between 0 and 2.25 keV using SAMMY; a total of 3193 resonances, including the external levels, were identified. At the time that the evaluation was performed, the complete RPCM was not generated because of computer memory and storage limitations [3]. Subsequently, a procedure for retroactively creating RPCMs has been developed and implemented in the SAMMY code. This procedure is used to generate the RPCM for the ^{235}U parameters of the ENDF/B-VI evaluation.

KEYWORDS: ^{235}U, resonance parameter, retroactive, covariance matrix

1. Introduction

Most of the existing evaluated nuclear data files are missing the associated resonance parameter covariance matrices (RPCMs); the RPCMs affect the uncertainty estimation for nuclear applications. To accurately estimate the uncertainties on k_{eff} and other nuclear calculations, there is a need to retroactively generate covariance matrices for the already evaluated resonance parameters. To this end, we have generated a RPCM for ^{235}U retroactively and used it to compute group-wise cross section uncertainties and correlation matrices.

In the Reich-Moore formalism, each resonance of ^{235}U is described by five parameters (resonance energy, gamma width, neutron width, and two channel fission widths), for a total of 15,965 parameters [2]. The large number of resonance parameters leads to two technical issues when generating the RPCM: (a) the computer memory required to process the data and resonance parameters into the RPCM and (b) the data storage and the subsequent processing of the resulting covariance matrix [3].

The former issue has been resolved by using a 64-bit Alpha computer with 32 GB of memory, together with a related improvement in SAMMY that increased its maximum array size. The latter issue has been solved by modifying the covariance processing code PUFF-IV [4] to enable processing of large (~ 2-GB) covariance matrices.

Simultaneous fitting of all data sets is then accomplished via SAMMY, properly including the effect of the data covariance matrices. The set of experimental data used in the retroactive covariance evaluation of ^{235}U is shown in Table 1.

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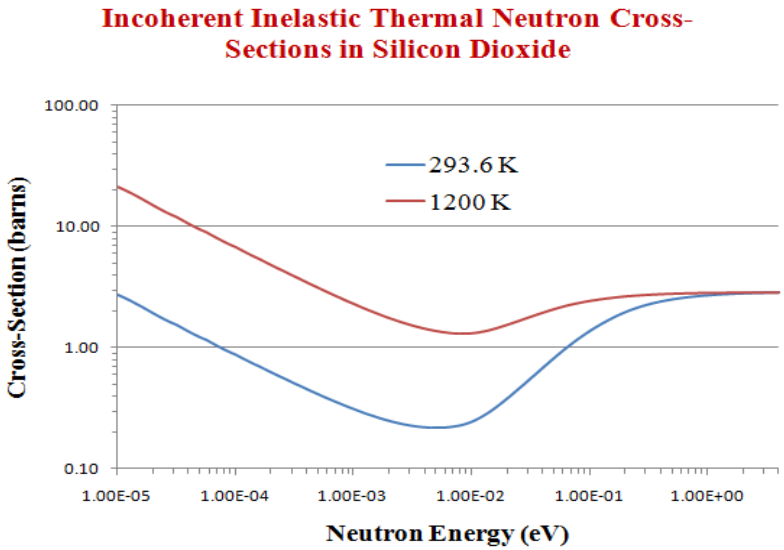
CD-id v.0

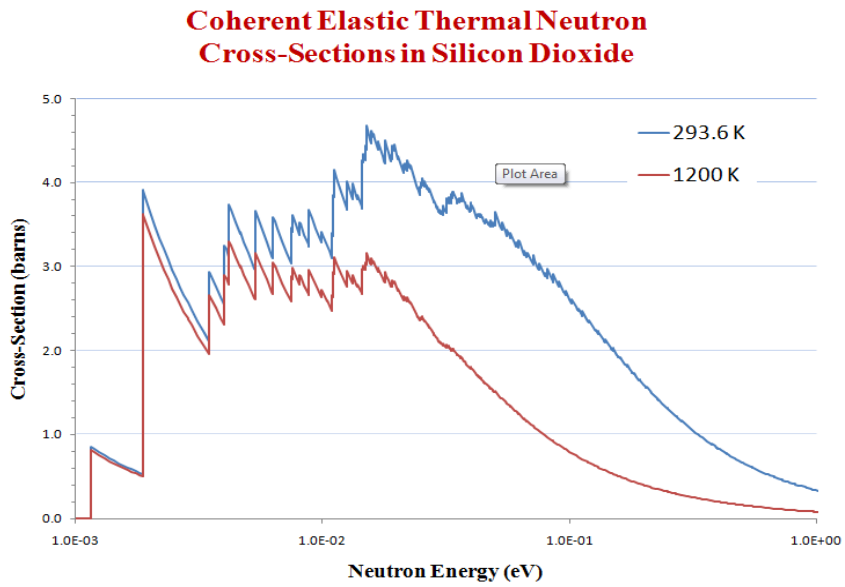
Retroactive Covariance Analysis Methodology
PHYSOR-2006 PAPER

NCSP Work to address Thermal Scattering Data Needs

- Evaluated nuclear data libraries have limited S(α,β) or thermal scattering law data for moderators important for nuclear applications (~20 moderators in ENDF/B-VII.0)
- Example NCSP thermal data needs: SiO_2, HF, D_2O, CH_2, C_2F_4, etc.
- Also, no covariance data available for S(α,β) data files currently in ENDF/B
- ORNL has been performing work with NCSU to provide thermal scattering data for moderators important for criticality safety applications
- ORNL-NCSU planning to provide S(α,β) covariance data for future thermal evaluations

ORNL work with NCSU produced new SiO_2 Evaluation in FY2010





Evaluation Status for ENDF/B-VII.1

- **^{46,47,48,49,50}Tl (5 isotope evaluations):** submitted to NNDC—ORNL (Resonance Evaluation) combined with LANL (High Energy Evaluation)—criticality benchmark testing shows improved performance
- **SiO_2**: evaluation submitted to NNDC—CSEWG testing in progress
- **^{180,182,183,184,186}W (5 isotope evaluations):**
  - ORNL (Retroactive Covariance Evaluation—not new resonance evaluation) combined with IAEA (High Energy Evaluation)
  - Current ORNL measurement and evaluation work expected to improve resonance evaluation
- **^{50,52,53,54}Cr (4 isotope evaluations):**
  - Updated evaluations submitted in 2010 (work based on new measurements and evaluation)
  - ORNL resonance evaluation coupled with FZK High Energy Evaluation
- **^{58}Ni and ^{60}Ni (2 isotope evaluations):**
  - Updated evaluation submitted in 2010 (based on new measurements and evaluation
  - ORNL resonance evaluation coupled with ENDF/B-VII.0 high energy evaluation

Evaluation Status for ENDF/B-VII.1

- **^{240}Pu:** submitted to NNDC October 2010—CSEWG testing in progress
  - ORNL resonance evaluation (re-evaluation of existing measured data) coupled with LANL high-energy evaluation
- **^{55}Mn:**
  - Updated evaluation submitted in 2010 to add correct File 33 covariance data for resonance region
  - ORNL resonance evaluation coupled with IAEA high-energy evaluation
- **^{35}Cl and ^{37}Cl:** submitted in 2007
  - ^{35}Cl has LRF=7 resonance format – NJOY update needed to process
- **^{39}K and ^{41}K:** submitted Oct 2008—little or no benchmark testing
- **^{19}F:** submitted Oct 2008
  - New LRF=7 resonance format – NJOY update needed to process
  - inelastic scattering data incorporated in resonance analysis
  - New evaluation has not improved benchmark performance—but has not made benchmark calculations worse either

Evaluation Status for ENDF/B-VII.1

- **^{233}U, ^{235}U, and ^{238}U**: covariance evaluations submitted March 2008
  - ORNL (resonance parameter covariance data) and LANL (High energy covariance data)
  - ^{233}U updated file submitted in 2010 to use LANL high-energy evaluation down to top of resolved region
  - Covariance data utilized in WPEC SG33 analyses and also distributed with SCALE 6 by ORNL

Summary

- ORNL nuclear data contribution to NCSP mission:
  - Cross-section measurements for resonance region
  - Nuclear modeling methods development (SAMMY)
  - Cross-section evaluation and preparation of ENDF/B nuclear data files
- Completed multiple resonance region nuclear data measurements and corresponding nuclear data evaluations of direct importance to NCS applications
- ORNL FY10 Evaluation Accomplishments include new evaluations for ^{46,47,48,49,50}TI and SiO_2—submitted to NNDC
- Within the NCSP, ORNL sustained efforts working with ANL, BNL, and LANL to provide improved nuclear data evaluations for dissemination as new ENDF/B data libraries

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NJOY & Data Evaluation Status

Presented at the NCSP FY10 Technical Symposium
held at Oak Ridge National Laboratory
March 1 – 2, 2011

A. C. (Skip) Kahler, R. E. MacFarlane,
G. M. Hale, S. T. Holloway, T. Kawano & P. Talou
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This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

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LANL T2 NCSP Summary

- **Program Elements**
  - **Analytical Methods**
    - NJOY Developments
  - **Nuclear Data**
    - Data Evaluations
      - Data Testing
        - Criticality calculations (primarily with ICSBEP benchmarks)
        - Reaction rate ratios (primarily historical LANL measurements)

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Analytical Methods – NJOY Developments

- During FY10 two concurrent versions of NJOY were under development
  - NJOY99.xxx
    - Base Version Released through RSICC and the NEA Databank
      - Update files released via a local (t2.lanl.gov) web site
      - Has worldwide user community

        Local control of updates allows this community to have access to the latest version.

    - Several dozen code patches are typically released each year.
      - NJOY99.304 at the beginning of FY2010
      - NJOY99.336 at the end of FY2010 (plus NJOY99.347 and later have been shared with selected users during the Fall 2010 and Winter 2011 to support ENDF/B-VII.1 development)

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Analytical Methods – NJOY Developments

- NJOY99 enhancements
  - Improved R-M processing in ERRORJ (consistent with RECONR);
  - Refined beta mesh in THERMR for free gas scattering;
  - More robust processing of IRDF (MF10) sections in RECONR, GROUPR & ACER;
  - More efficient processing & error detection in PURR;
  - Improved processing in RECONR, BROADR & ACER for (TENDL-2009) photonuclear and charged particle files;
  - Scattering radius uncertainty processing in ERRORR (via User input or from November, 2009 format revision);
  - MF=40 processing in ERRORR & COVR;
  - Miscellaneous upgrades in RECONR, GROUPR, ACER & ERRORR for JENDL-4 processing;
  - More scratch space in various modules.

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Analytical Methods – NJOY Developments

- NJOY2010
  - F90/F95 based coding
    - Includes LRF=7 (Limited Reich-Moore resonance format)
      - Appearing in ENDF/A ^{19}F & ^{35}Cl files developed at ORNL and expected to be included in ENDF/B-VII.1
    - "smarter" interpolation for emission spectra (available in NJOY99 but turned off by default)
      - Sqrt(E') rather than histogram at low energy
      - Denser energy grid at high energy
  - Retain all NJOY99 capabilities
  - Internal LA-CC and LA-CP computer code and document numbers have been obtained.
    - Final release to RSICC has been delayed so that last minute upgrades needed for ENDF/B-VII.1 beta processing are incorporated.

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Analytical Methods – NJOY Developments

- "Methods for Processing ENDF/B-VII with NJOY"
- Published in the December 2010 Special Issue on Nuclear Reaction Data of the Nuclear Data Sheets

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Nuclear Data Sheets 111 (2010) 2739–2890

Nuclear Data Sheets

www.elsevier.com/locate/nds

Methods for Processing ENDF/B-VII with NJOY

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(Received 2 July 2010; revised received 16 September 2010; accepted 1 October 2010)

The NJOY Nuclear Data Processing System is widely used to convert evaluations in the Evaluated Nuclear Data Files (ENDF) format into forms useful for practical applications such as fission and fusion reactor analysis, stockpile stewardship calculations, criticality safety, radiation shielding, nuclear waste management, nuclear medicine procedures, and more. This paper provides a description of the system's capabilities, summary descriptions of the methods used, and information on how to use the code to process the modern evaluated nuclear data files from ENDF/B-VII. It begins with the generation of pointwise libraries, including reaction and resonance reconstruction, Doppler broadening, radiation heating and damage, thermal scattering data, unresolved resonance data, and gas production. It then reviews the production of libraries for the continuous-energy Monte Carlo code MCNP, multigroup neutron, photon, and particle cross sections and matrices, and photon interaction data. The generation of uncertainty information for ENDF data is discussed, including new capabilities for calculating covariances of resonance data, angular distributions, energy distributions, and radioactive nuclide production. NJOY's ability to prepare thermal scattering data evaluations for bound moderators (which was used during the preparation of the ENDF/B-VII library) is described. The strong plotting capabilities of NJOY are summarized. Many examples of black&white and color Postscript plots are included throughout the paper. The capabilities of NJOY to output multigroup data in several different formats to suit various applications is reviewed. Finally, a section is included that summarizes the history of the development of the NJOY system over the last 37 years.

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Nuclear Data – Evaluations

- ^{4}He, ^{9}Be, ^{16}O – Gerry Hale
- ^{50,51}V – Toshihiko Kawano
- ^{237}Np – Shannon Holloway
- Fission Spectra – Patrick Talou
  - Data Testing – Skip Kahler & Bob MacFarlane

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Nuclear Data – Evaluations – ^{4}He

- Update of 1973 Evaluation.
- New multi-channel R-Matrix Analysis Includes Data from (n + ^{4}He) and (d + t) Systems.
- Includes Covariance Data for Total and Elastic Scattering Cross Sections.

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Nuclear Data – Evaluations – ^{9}Be

- Single-channel fit to the total cross section (including new RPI data) at energies up to 14 MeV.
- Preliminary criticality testing indicates k_{calc} values for Be reflected assemblies have moved back toward ENDF/B-VI levels.
- Full multi-channel R-matrix analysis of reactions in the ^{10}Be system continues.
  - Changes in the elastic scattering angular distributions may affect integral data testing.
  - Covariances for all cross sections will be obtained.

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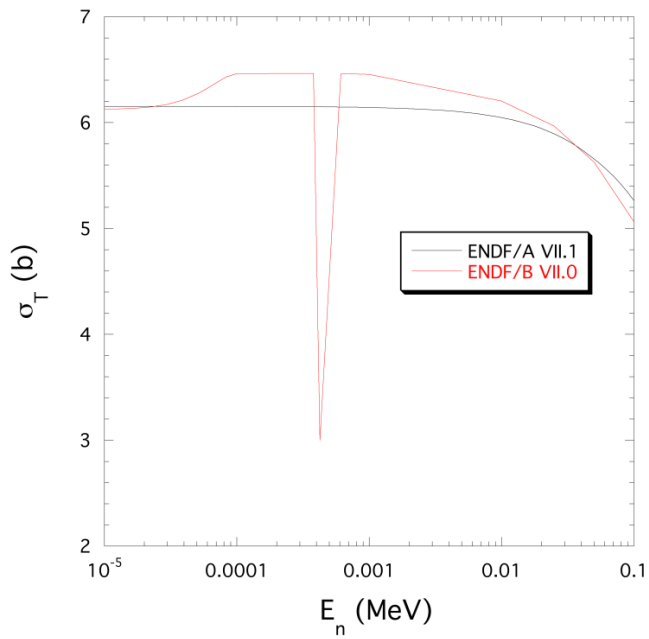
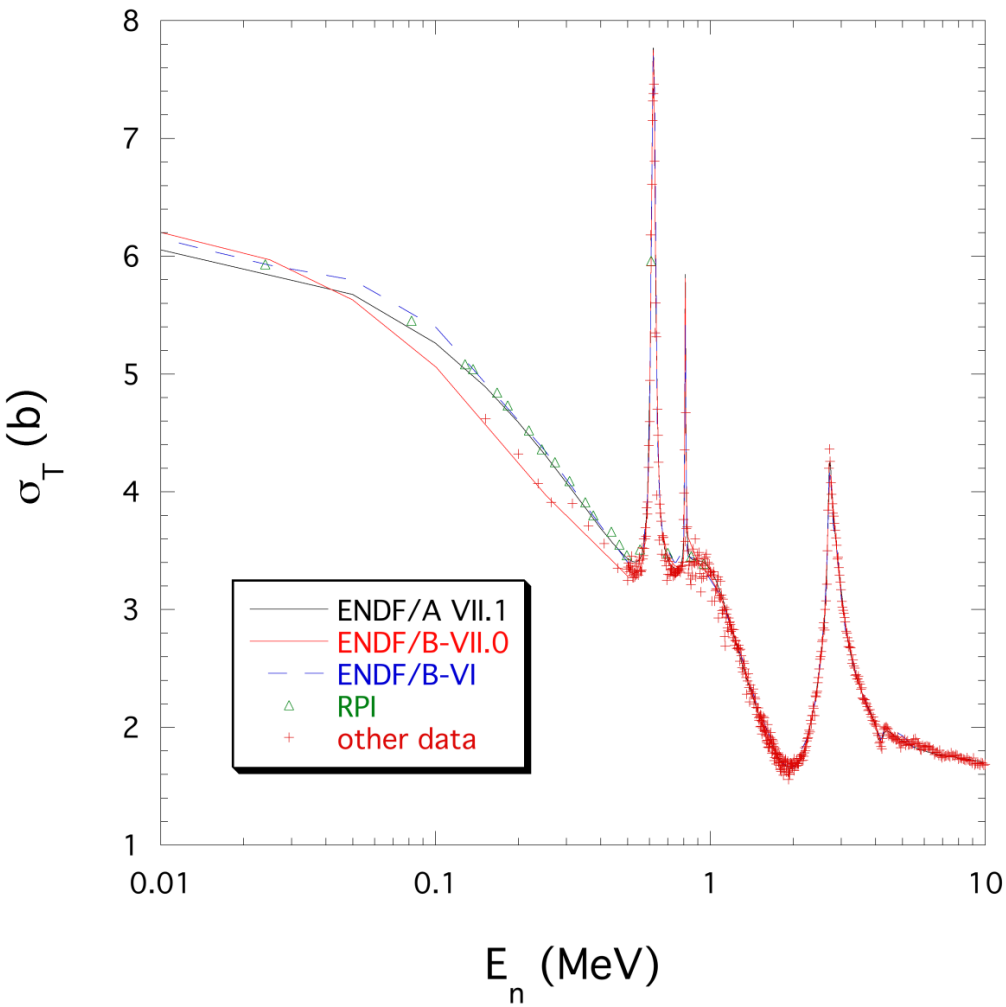
Nuclear Data – Evaluations – ^{9}Be





ENDF/A:

- "Glitch" in σ_{tot} removed
- Better fit to RPI data below 500 keV

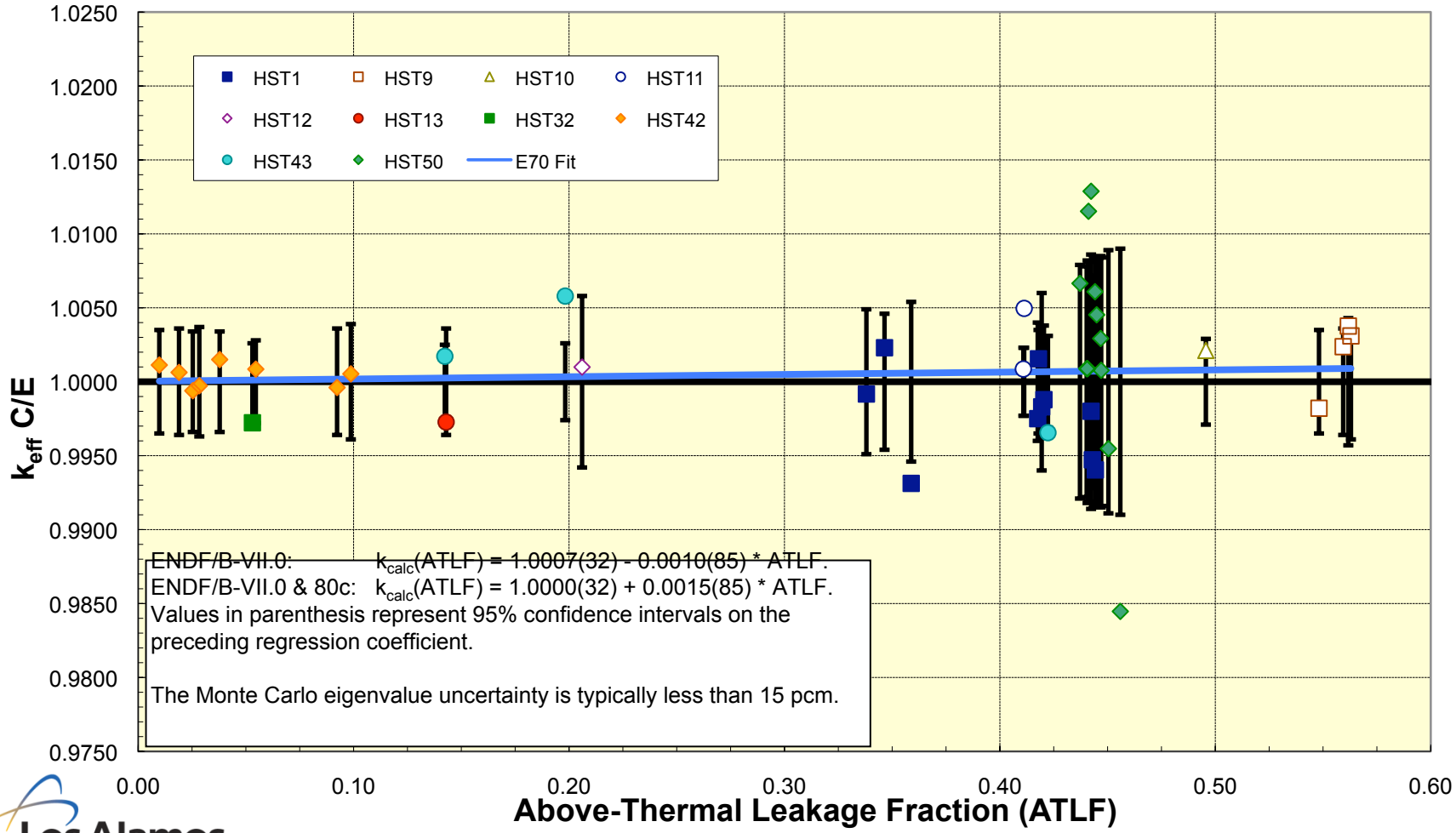
LA-UR-11-10053

Nuclear Data – Evaluations – ^{16}O

- Small changes in σ_{el} and σ_{tot} at energies below 7.5 MeV.
- Scale of $\sigma_{n\alpha}$ cross section increased about 35% below 9 MeV, putting it back about where it was before the previous change.
- All cross sections above 9 MeV are unchanged.
- Little change in already good k_{calc}; calculations of the "broomstick" transmission measurement are underway (but this is a low-resolution experiment).
- Covariances are given for the major cross sections, and for the first elastic scattering Legendre coefficient.

LA-UR-11-10053

Nuclear Data – Evaluations – ^{16}O



ENDF/B-VII.0: k_{calc}(ATLF) = 1.0007(32) - 0.0010(85) * ATLF.
ENDF/B-VII.0 & 80c: k_{calc}(ATLF) = 1.0000(32) + 0.0015(85) * ATLF.
Values in parenthesis represent 95% confidence intervals on the preceding regression coefficient.

The Monte Carlo eigenvalue uncertainty is typically less than 15 pcm.

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Nuclear Data – Evaluations – Vanadium

- $^{50,51}V$
  - Elemental ENDF/B-VII.0 evaluation will be replaced by isotopic evaluations; adopt JENDL-4 for ^{50}V; new evaluation for ^{51}V.
- For ^{51}V:
  - Total Cross Section
    - 100 keV - 5 MeV adopt JENDL-4; above 5 MeV, optical model calculations using a modified Koning-Delaroche potential.
  - Reaction Cross Sections
    - all cross sections above 100 keV were evaluated consistently with the Hauser-Feshbach code CoH.
  - Scattering Angular Distributions
    - Retain elemental ENDF/B-VII.0 elastic scattering data
    - Use COH calculated results for inelastic levels.

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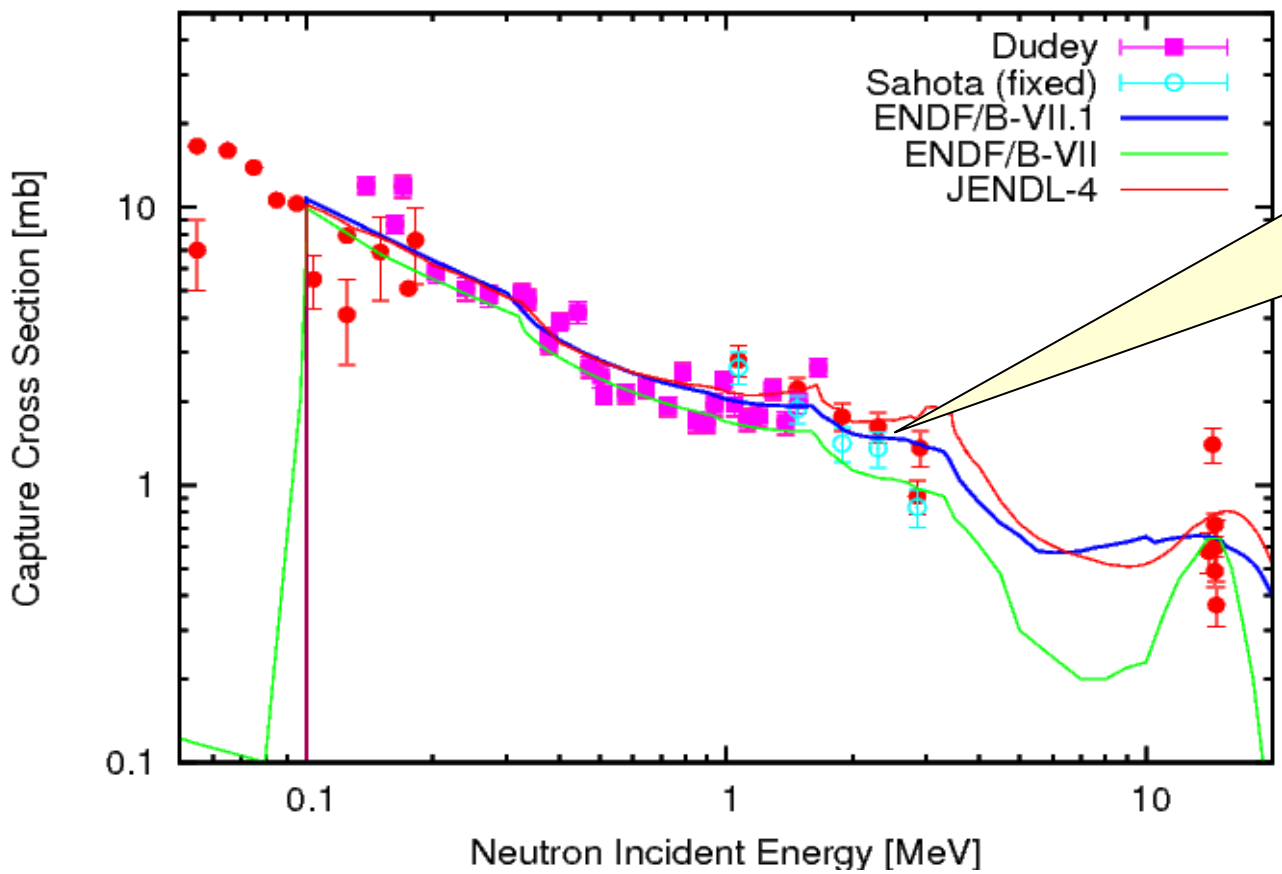
Nuclear Data – Evaluations – Vanadium (^{51}V)



Exp. data of Sahota et al. corrected by using updated reference cross section

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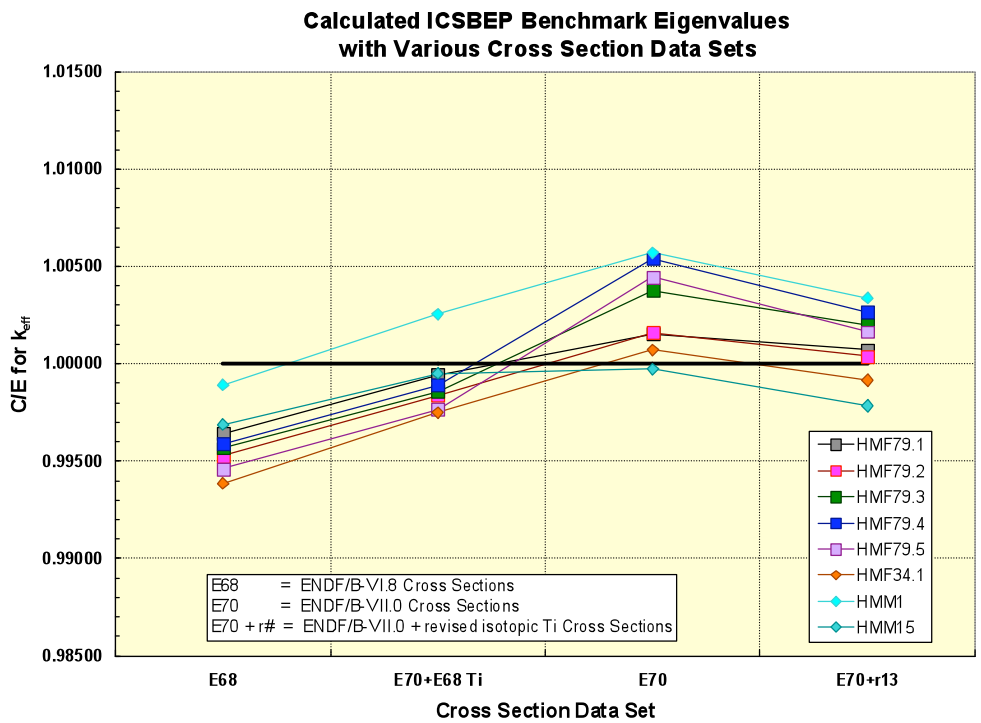
Data Testing: Ti Benchmarks



- ENDF/B-VII.0 based eigenvalues are less accurate than those obtained with ENDF/B-VI.8.
- Revised LANL Ti isotopic data sets eliminate much of this deficiency.
  - Average calculated eigenvalues are still biased high.

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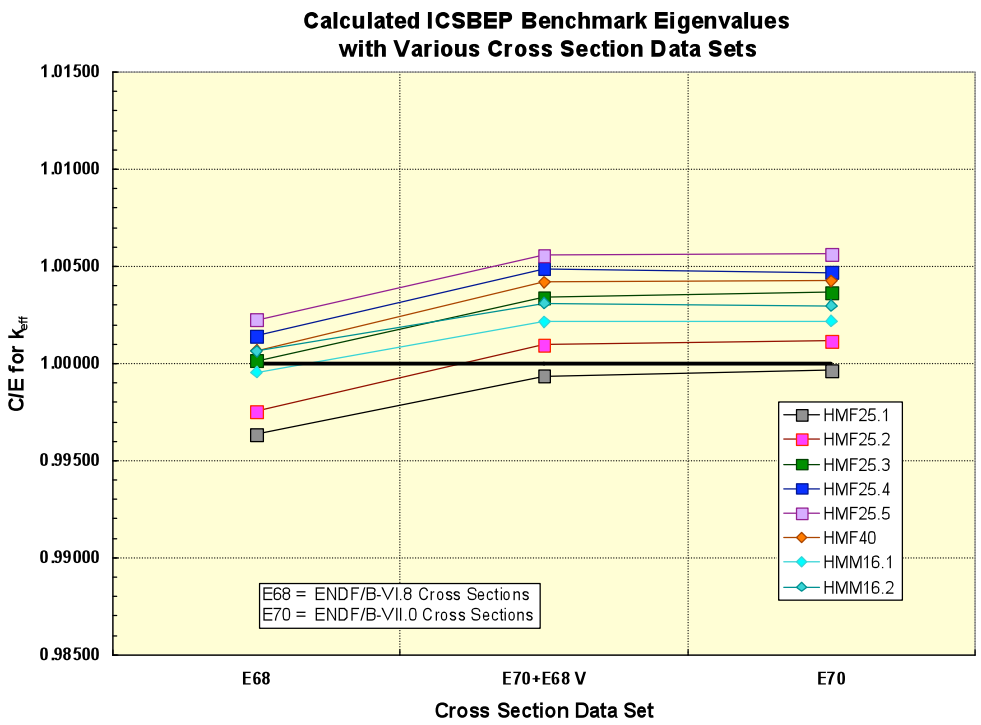
Data Testing: V Benchmarks



- Average calculated eigenvalue is too high.
- HMF25.x exhibits increasing calculated eigenvalue trend with increasing axial reflector thickness.

LA-UR-11-10053

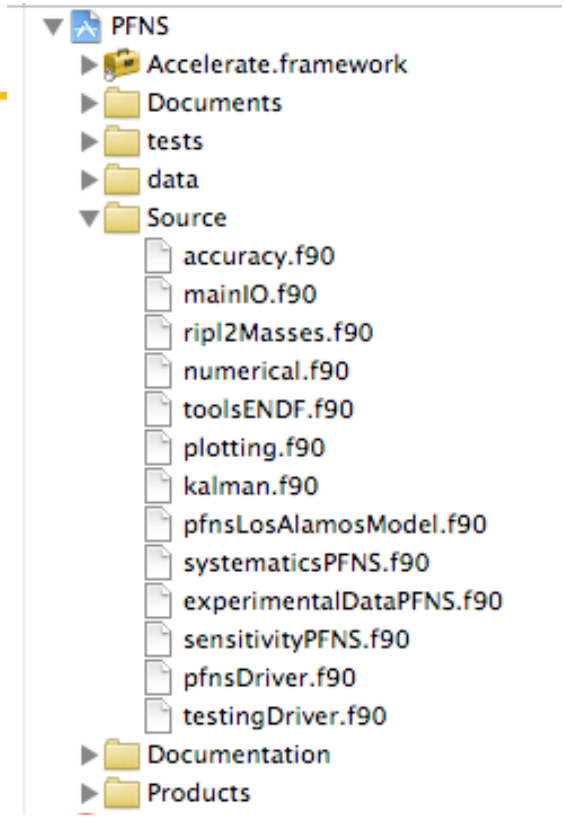
Data Testing: Ti and V Benchmarks

- Conclusions
  - Eigenvalues for Ti bearing benchmarks are calculated more accurately with the latest LANL generated isotopic Ti data files.
    - The increasing calculated eigenvalue trend introduced with the current ENDF/B-VII.0 isotopic Ti data sets has been significantly reduced.
  - ENDF/B-VII.0 V is a carryover from ENDF/B-VI, evaluated by ANL in the late 1980's, with minor revisions by BNL. These integral data testing results suggest there may be deficiencies in either the elastic scattering angular distributions and the secondary energy distributions.

LA-UR-11-10053

PFNS Evaluation Package

- Complete code package to analyze, compute and evaluate prompt fission neutron spectrum and multiplicity
  - Implementation of the Madland-Nix model
  - Model input parameter systematics included
  - Complete module to analyze various experimental data sets
  - Search for optimal model parameters
  - Uncertainty Quantification of spectrum and multiplicity
  - ENDF formatting for easy incorporation in evaluated libraries
- Version 1.0 released (internally)
- AFCI-NEUP collaboration with A.Prinja, M.Rising, UNM
- First application to suite of plutonium isotopes
- Ongoing:
  large suite of actinides studied to replace values in ENDF/B-VII.0



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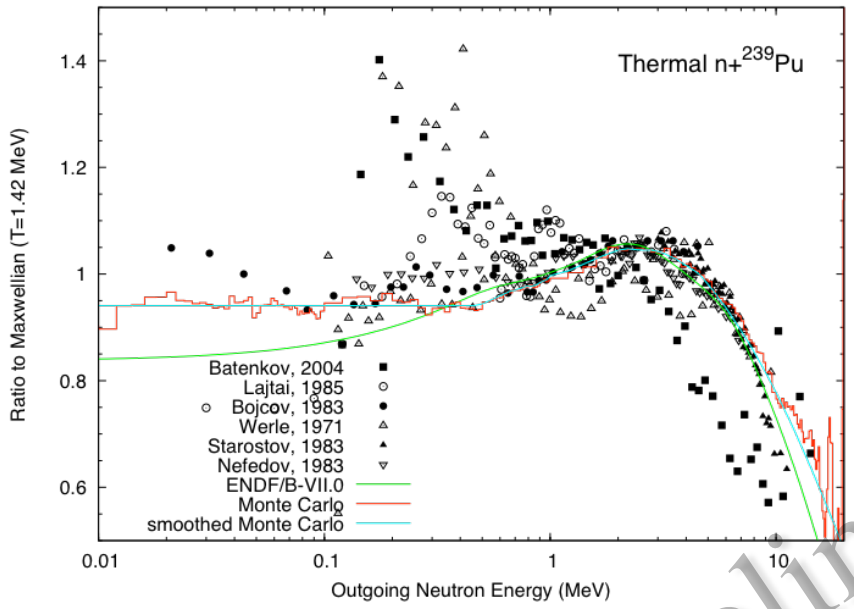
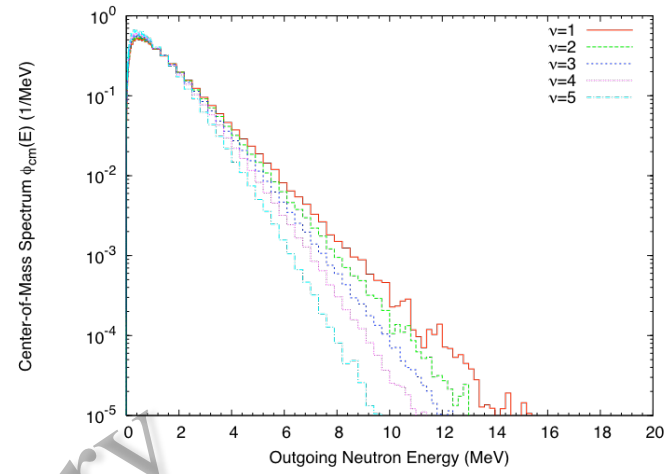
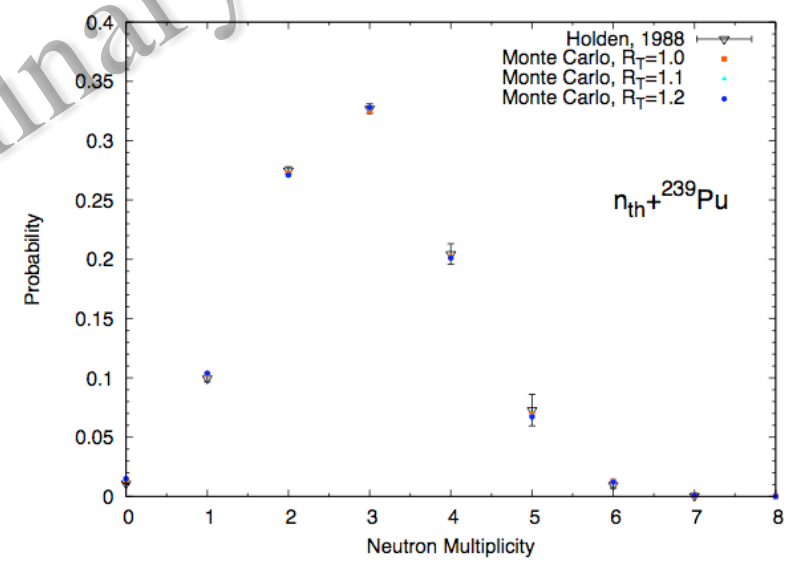
PFNS Evaluation Package







Preliminary

LA-UR-11-10053

Nuclear Data – Evaluations – ^{237}Np

- Revised (n,2n) and (n,3n) cross sections
  - Include ^{236,236m}Np production based upon Maslov evaluation.
  - MT=1 & MT=3 adjusted to remain consistent with these revisions.

- C/E for ^{237}Np(n,2n)/^{235}U(n,f) in Godiva, Flattop-25 and Big-10 remain high, but are closer to unity.

LA-UR-11-xxxxx

Initial ICSBEP Criticality Calculations with ENDF/B-VII.1β3 Cross Sections

Summer CSEWG Meeting
Brookhaven National Laboratory
June, 2011

A. C. (Skip) Kahler, R. E. MacFarlane
Los Alamos National Laboratory

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

E71β3 File & NJOY Summary

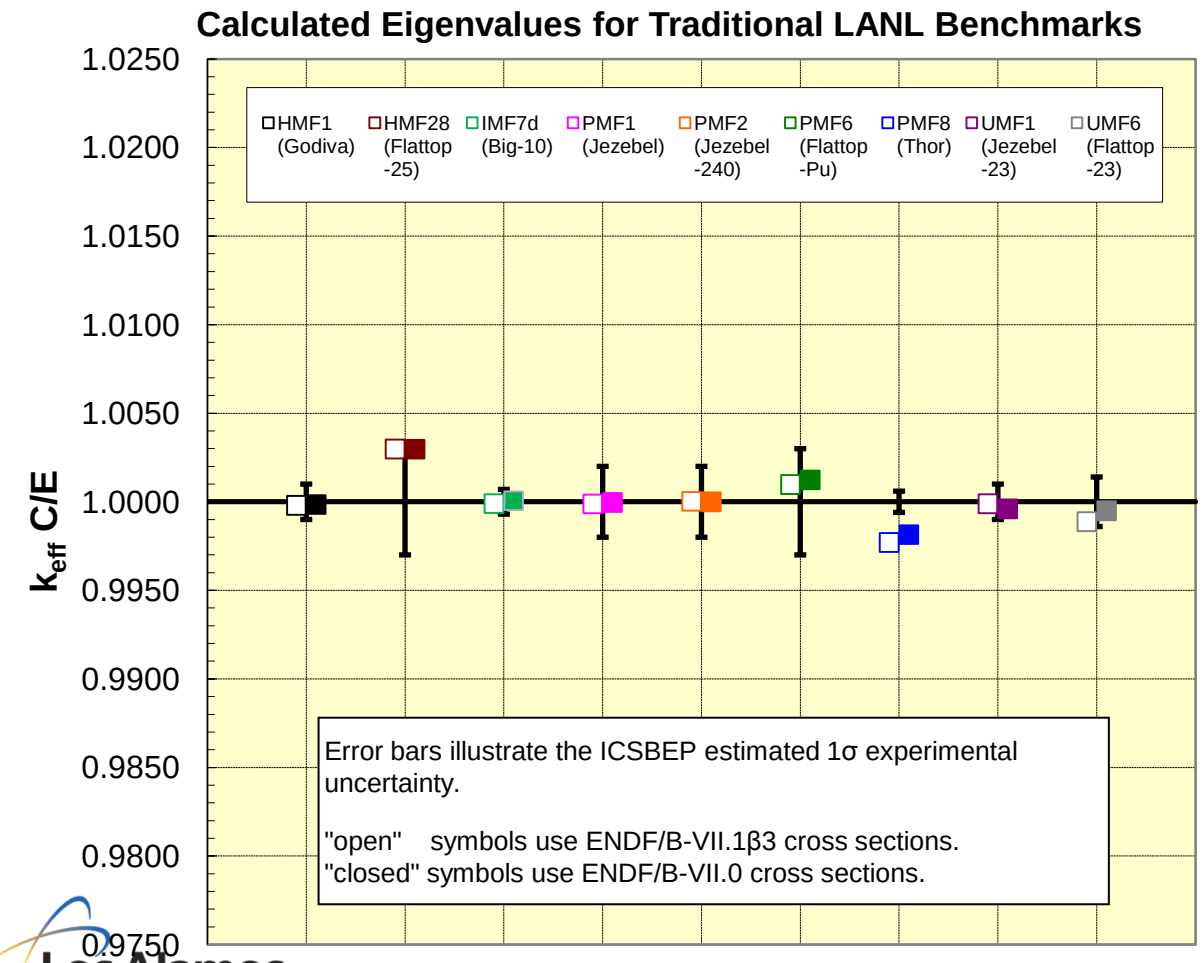
- 418 evaluations in the ENDF/B-VII.1β3 file.
- Previous processing issues from the β2 file are now resolved
  - … but several evaluations need an ad-hoc patch in ACER to avoid plotting issues, ☹.
- All files processed to create MCNP ACE files with NJOY2010.
  - Still much data checking and comparing tbd.
  - NJOY sequence was MODER/RECONR/BROADR/UNRESR/HEATR(2)/THERMR/GASPR/PURR/ACER(2).
  - Independent files created by REM for his calculations.

LA-UR-11-xxxxx

E71β3 File & NJOY Summary

- Significant changes from ENDF/B-VII.0 to VII.1:
  - ^{9}Be, ^{16}O, ^{50,51}V, ^{46,47,48,49,50}Ti, ^{113}Cd, ^{155,157}Gd, ^{174,176,177,178,179,180}Hf, ^{180,182,183,184,186}W, ^{185,187}Re
    - ENDF/B-VII.0 has ^{nat}V.
    - ENDF/B-VII.0 omits ^{180}W.
    - Others discussed earlier yesterday and/or today.
    - Also show some ^{233}U results
      - Was the subject of an IAEA Consultants Meeting late last year.
      - Clear deficiencies exist in calculated eigenvalues for solution systems.

Traditional LANL Critical Assemblies



- Traditional LANL Assemblies
  - HEU, bare and reflected
  - Pu, bare and reflected
  - Heterogeneous uranium
  - ^{233}U, bare and reflected

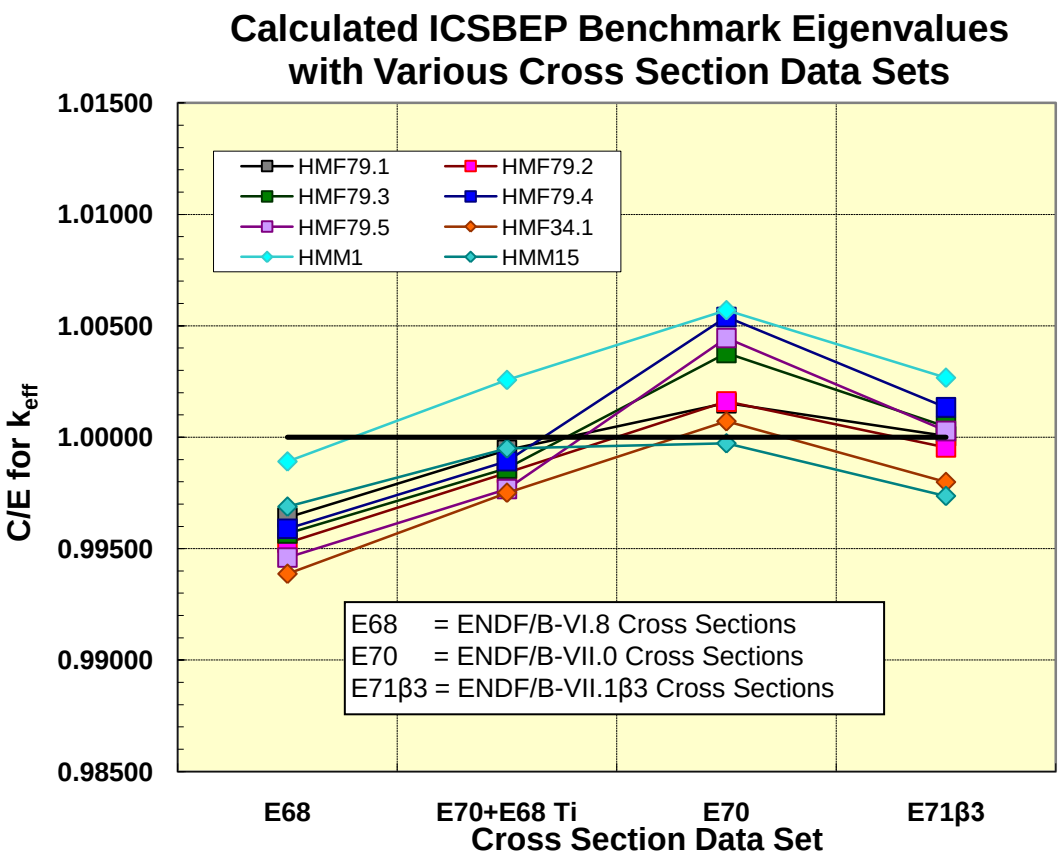
^{9}Be

- Latest revision to the ^{9}Be file is believed to be fundamentally more correct.
- Impact of revised angular distributions remains to be assessed.
  - But an ad hoc change indicates that k_{calc} can vary significantly due to these data.
- Apparent discrepant critical experimental data are puzzling; a proposal for additional measurements at the Critical Experiments Facility (CEF) at NTSS has been accepted by the NCSP, but probably won't occur for a couple of years, ☹.

^{16}O

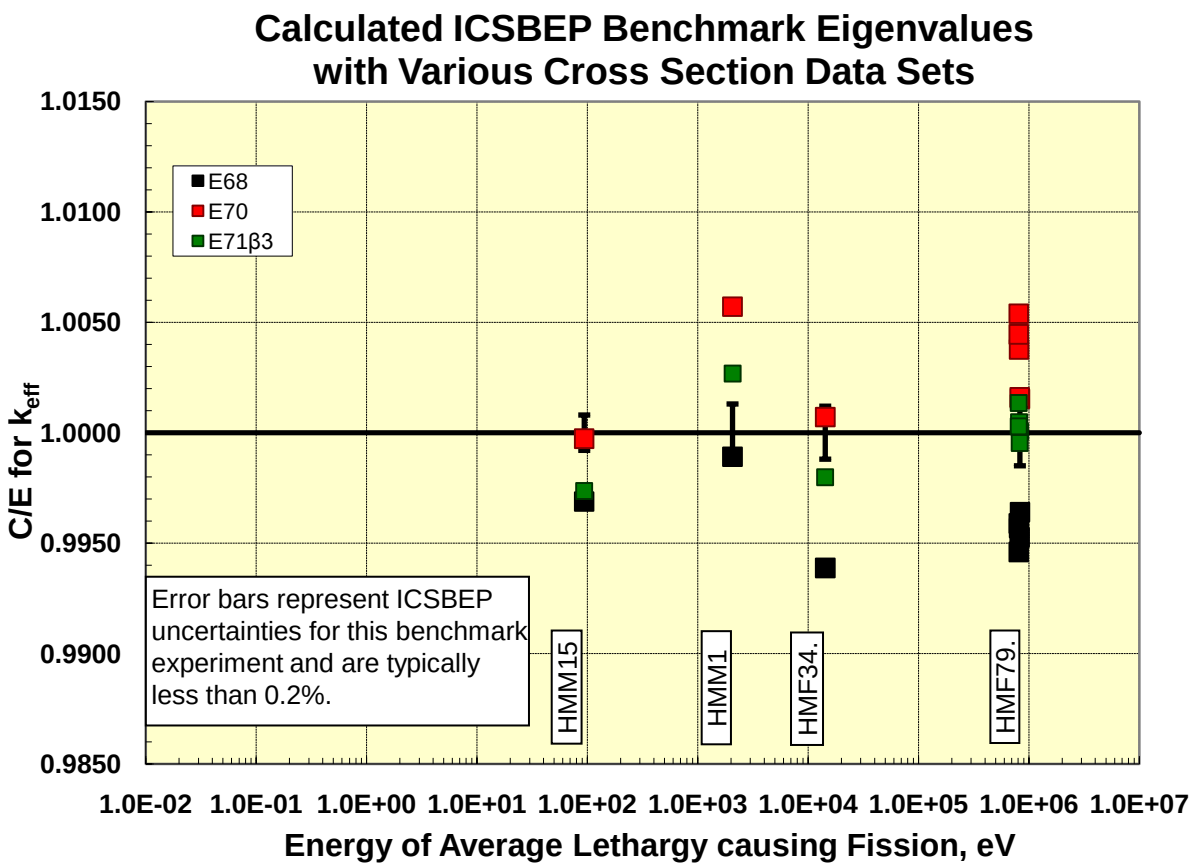
- Impact of revised ^{16}O evaluations are small
  - HST regression retains excellent near unity intercept and statistically insignificant slope with ATLF
    - β3 is slightly "better", but when values are statistically indistinguishable "better" may be in the eye of the beholder!
  - PST regression retains intercept bias, but near zero slope with various experimental and calculated parameters.
  - LCT eigenvalues typically change by less than ± 100 pcm
    - Change is often less than 25 pcm
    - ~ -80pcm for LCT8; ~ +80 pcm for LCT25 for b2
    - β3 differences are even smaller (as expected).
  - Seems like criticality testing can support either β2 or β3; knowing that further "Kadonis" tweaks remain to be added.
    - **NOTE: b3 may be e70, but different NJOY processing for (n,α) – mt107 versus sum of mt800 + mt801 now versus 2006.**

^{46,47,48,49,50}Ti



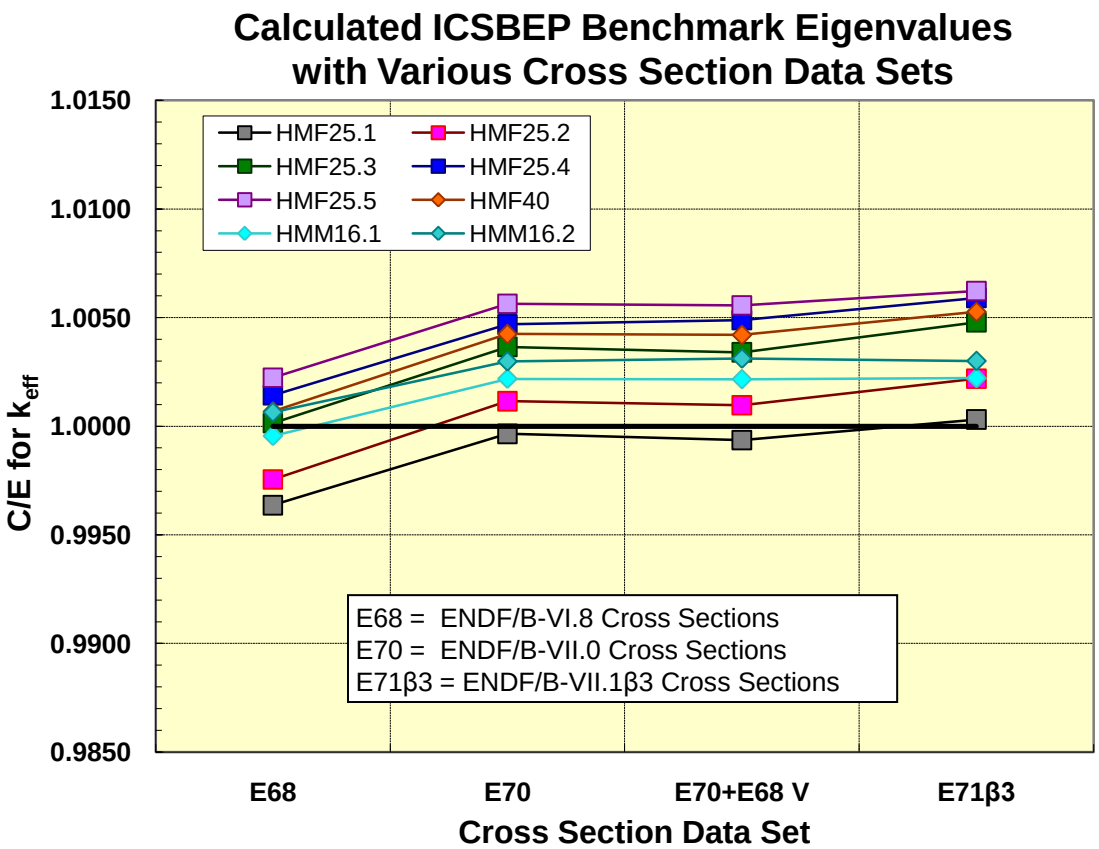
- E68 is too cool.
- E70 is too hot.
- E71β3 is just right.

^{46,47,48,49,50}Ti



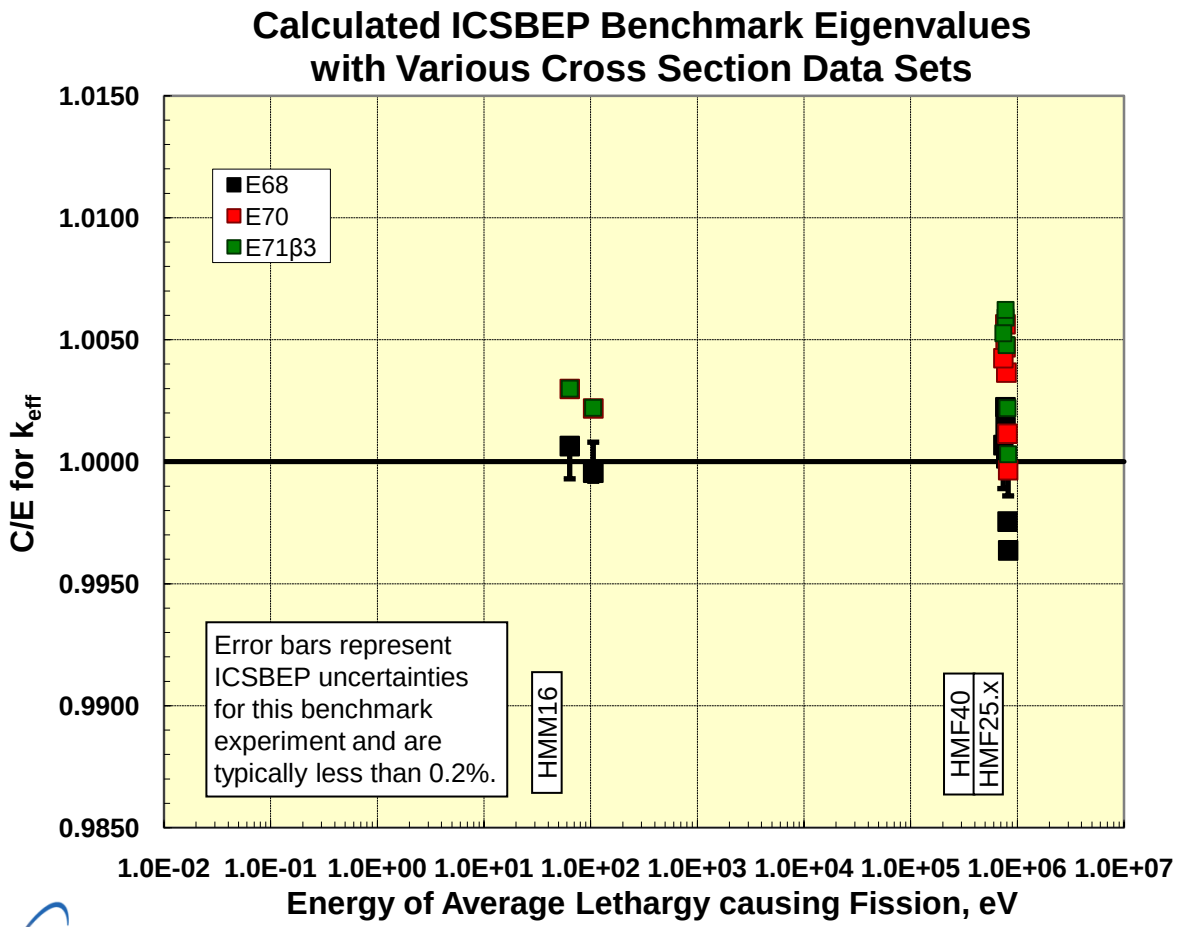
- No trend in calculated eigenvalues versus average fission energy.

$^{50,51}V$



- ENDF/B-VI.8 average is close to unity
- ENDF/B-VII.0 is biased high by several tenths of a percent
- Little change in k_{calc} with the latest ^{iso}V evaluated files.

$^{50,51}V$



- HMF25 results suggest trend with increasing axial reflector thickness.
- No trend in calculated eigenvalues with average fission energy, but data are limited.

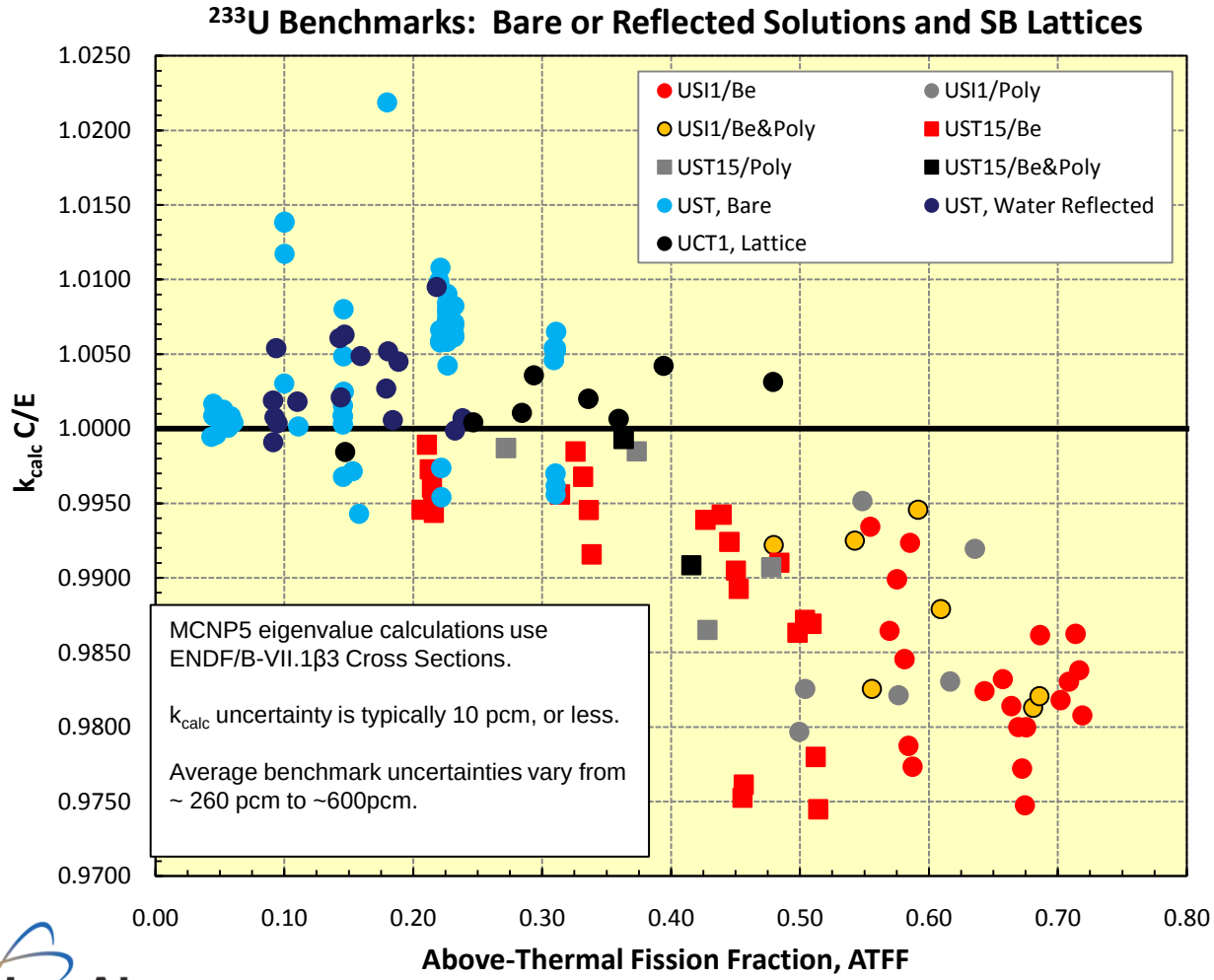
Data Testing: Ti and V Benchmarks

- Conclusions
  - Eigenvalues for Ti bearing benchmarks are calculated more accurately with the latest LANL generated isotopic Ti data files.
    - The increasing calculated eigenvalue trend introduced with the current ENDF/B-VII.0 isotopic Ti data sets has been significantly reduced.
  - ENDF/B-VII.0 V is a carryover from ENDF/B-VI, evaluated by ANL in the late 1980's, with minor revisions by BNL. These integral data testing results indicate that LANL's latest revisions have not eliminated the existing k_{calc} bias.

^{180,182,183,184,186}W

- Isotopic W Evaluations from the IAEA
  - Criticality testing to date
    - HMF3.8 to 3.11: 1.9” to 6.5” thick spherical reflector
    - HMF49.1 to 49.3: cylindrical geometry with 1 cm, 3 cm and 8 cm axial reflector
    - PMF5: 1.85” thick spherical reflector
    - UMF4.1, 4.2: 0.96” & 2.28” thick spherical reflector
- ENDF/B-VII.0 Calculated Eigenvalues are Too High
  - HMF3.8 - 3.11 = 1.00838(11), 1.00919(11), 1.01283(11) and 1.01685(10)
  - HMF49.1 – 49.3 = 1.0009(9), 1.0042(9), 1.0048(9)
  - PMF5 = 1.00947(10)
  - UMF4.1 – 4.2 = 1.00483(11), 1.00508(11)
- ENDF/B-VII.1β3 Calculated Eigenvalues are ~750 pcm Lower, but the Increasing Trend of k_{calc} with Increased Quantity of W Remains.
  - HMF3.8 – 3.11 = 1.00134(10), 1.00161(10), 1.00525(11) and 1.01000(11)
  - HMF49.1 – 49.3: 0.99799(9), 0.99961(9), 0.99844(16)
  - PMF5 = 1.00067(10)
  - UMF4.1 – 4.2 = 0.99890(11), 0.99603(11)
    - These new evaluations represent a significant improvement over ENDF/B-VII.0.

^{233}U Solutions



- H_2O, CH_2 and Be reflectors
- Results in a large ATFF interval.
- Mostly small (< 20pcm) increase compared to E70.
- β2 yields a further small k_{calc} increase.
- Not news, but something isn't right!

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CSEWG 2010 Annual Meeting - Nov. 1-3, 2010

- **Argonne Data Testing of New Evaluations for ENDF/B**
  - Revised evaluations were downloaded about 3 weeks ago from NNDC for:
    - ^{239}Pu
    - ^{240}Pu
    - ^{55}Mn
    - ^{52,53}Cr
    - ^{58,60}Ni
    - Minor Cr and Ni isotopes were not tested
  - A set of benchmarks were selected which might test ^{240}Pu and the structural materials

Summary

- **^{239}Pu** – generally small changes on THERM, INTER and FAST systems.

- **^{240}Pu** – Generally increases the over-prediction of the THERM systems; no effect in the FAST systems.

- **^{55}Mn** – Nice improvement in FAST systems; little effect in THERMAL systems.

- **^{52,53}Cr** – Increased the under-prediction of the THERM systems and mixed performance in the INTER and FAST systems.

- **^{58,60}Ni** – Most of these systems are insensitive to Ni; the only two systems with significant changes are improved.

ANL Data Validation Results Test Beta-Versions of ENDF/B-VII.1

Cross Section Evaluation Working Group Meeting

Montauk, NY

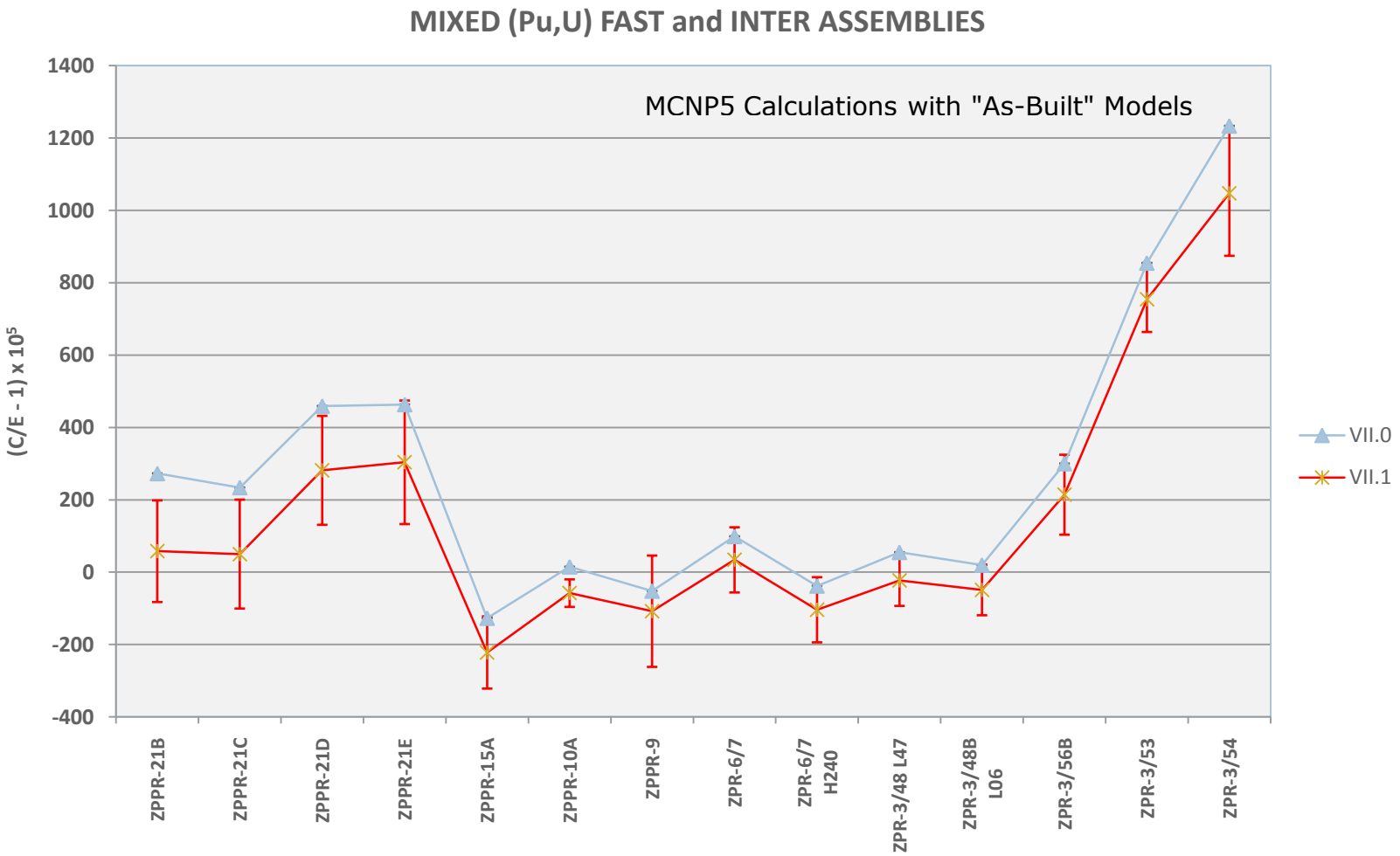
June 22, 2011

R. M. Lell and R. D. McKnight

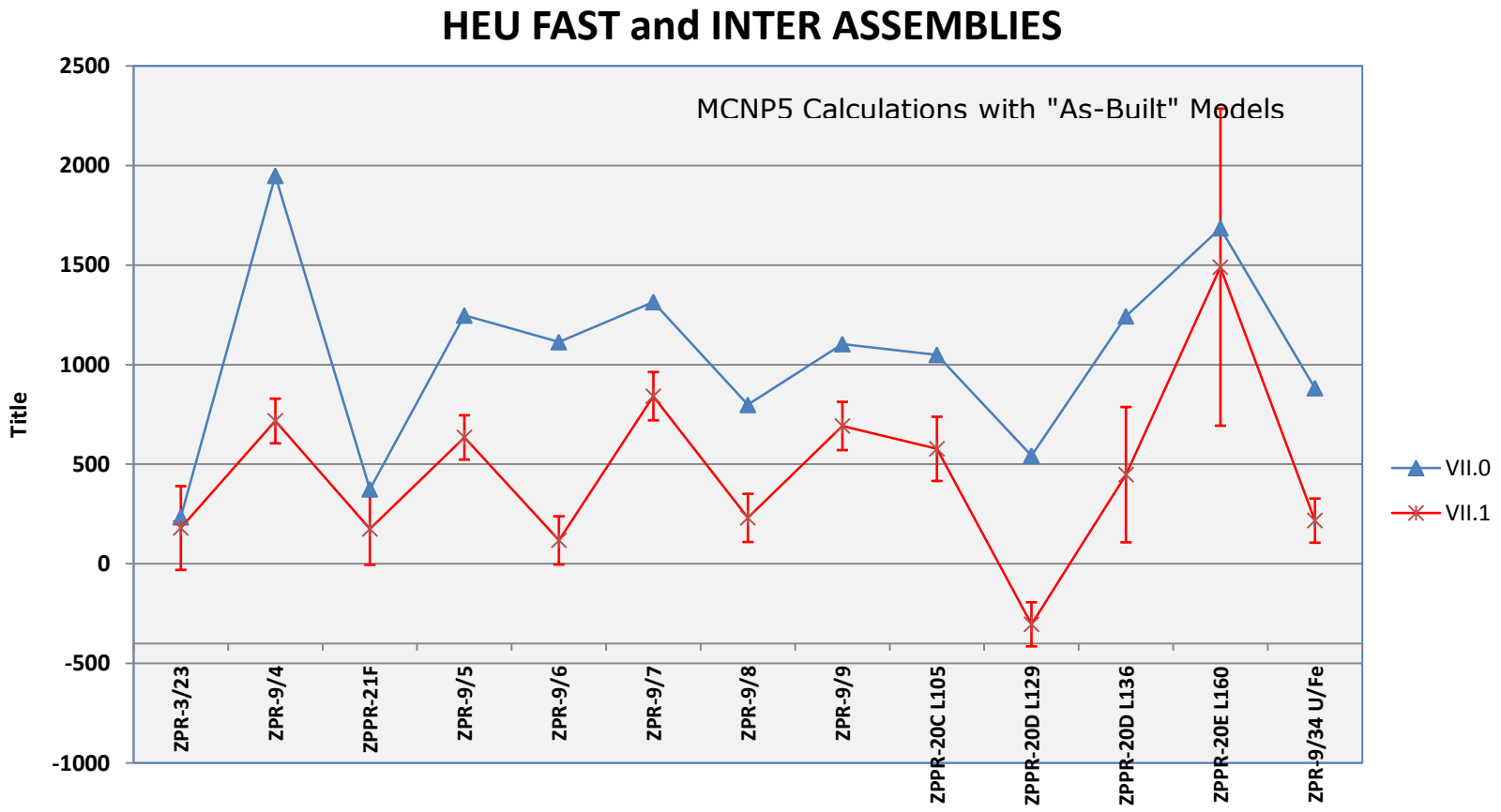
Nuclear Engineering Division

Argonne National Laboratory

ZPR/ZPPR MCNP5 Calculations with "As-Built Models MIXED (Pu,U) FAST and INTER ASSEMBLIES



ZPR/ZPPR MCNP5 Calculations with "As-Built Models HEU FAST and INTER ASSEMBLIES



ENDF/B-VII.1 status beta3 release

Assembling, Verification, Further steps

M. Herman
National Nuclear Data Center
Brookhaven National Laboratory

Mini-CSEWG Meeting, Montauk, New York, June 21-23, 2011

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ENDF/B-VII.1b3 release

- Release May 26, 2011 (neutron sublibrary)
- 418 materials (the same as in beta2)
- GForge revision 319 (71 commits since beta2)
- 28 materials modified
- 186 materials with covariance data (111 in beta2, COMMARA-2.0 covariances migrated)
- ACE files available to GForge registered users
- NJOY covariance plots by MacFarlane
- NJOY energy-balance plots by MacFarlane
- POINT2011 by Red Cullen

Covariances in ENDF/B-VII.1-β3

- Total materials with covariance data : 186
- (see talk by S. Hoblit)

Covariance	# materials
MF31	72
MF32	54
MF33	180
MF34	67
MF35	62

Status of ENDF/B-VII.1 papers

Pavel Oblozinsky

Ex National Nuclear Data Center, BNL
Currently Bratislava, Slovakia

Status of ENDF/B-VII.1 papers (*Nuclear Data Sheets*)

10 papers = 2 on library, 6 on covariances, 2 on FPY; 260 pages

Library	*Lead author, lab*	*Pp.*
1. Evaluations	Chadwick, LANL	95
2. Validation	Kahler, LANL	30
Covariances		
3. Overview	D. Smith, ANL	15
4. Light nuclei	Hale, LANL	15
5. Actinides	Talou, LANL	20
6. Struct+FPs	Herman, BNL	25
7. Resonances	Leal, ORNL	15
8. Other	Capote, IAEA	15
FPY		
9. Theory	Lestone, LANL	15
10. 14 MeV	MacInnes, LANL	15

Summary for ND Accomplishments for FY 2010

- NCSP activities have been focused on **priority data needs for criticality safety**.
  - FY10 Resonance Region Measurements
    - ^{182}W, ^{183}W, ^{184}W and ^{186}W (IRMM)
    - ^{63}Cu and ^{65}Cu (IRMM)
  - FY10 Resonance Region Evaluation Tasks
    - ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, and ^{50}Ti
    - SiO_2 thermal evaluation NCSU-ORNL
  - FY10 Fast Energy Region Evaluation Tasks
    - ^{4}He, ^{9}Be, ^{16}O, $^{50,51}V$, ^{237}Np
    - Preliminary Evaluation of Prompt Fission Neutron Spectra
  - Improved Covariance Data (in Quantity and Quality)
  - Preparation for release of ENDF/B-VII.1 in December, 2011

Summary for ND Accomplishments for FY 2010 (Continued)

- In addition to the new measurements and evaluations submitted to ENDF/B (CSEWG), there have been a number of necessary adjunct accomplishments .
  - Creation of new ENDF formats to handle new data types
  - Modification of processing codes to handle new formats and data types
  - Considerable progress on the evaluation methodologies for covariance data
  - Considerable progress on the quality assurance procedures for new covariance data
  - Continual effort to test the performance of the new evaluations
- These adjunct accomplishments are supported by NCSP and are necessary activities for the criticality safety community to actually benefit from the new advances in nuclear data measurement and evaluation