

ENDF Project Report to WPEC 2014

M. Herman for CSEWG



ENDF Project Pages

D. Brown
BNL

- **Reorganized the set of ENDF web pages:**
<http://www.nndc.bnl.gov/endl/project.html>
- **Compiling ENDF history back to ENDF/B-I**
 - Data files
 - Lab reports (BNL & others)
 - Formats
- **Links to ENDF development pages**
- **ENDF QA Page:** <http://www.nndc.bnl.gov/endl/b7.dev/qa.html>
 - Includes ADVANCE requirements document
 - Various ENDF QA requirements documents

Post ENDF/B-VII.1 activities



- 2 new thermals scattering law evaluations for SiO₂
- New evaluation for ^{236m}1Np
- New RR evaluations for ^{63,65}Cu, ⁵⁶Fe and ²³⁵U
- Numerous but minor fixes to VII.1
- ENDF/B-VII.1 validation
- Modernizing infrastructure
 - Evaluation methodology (reaction codes, PFNS, inelastic scattering, assimilation)
 - Continuous verification and validation
 - New XML format
 - CIELO

Priorities for the next ENDF/B

Highest Priority

- 239-Pu
- 235-U
- 238-U
- 56-Fe
- 16-O
- Standards
- Update covariances

Lower Priority

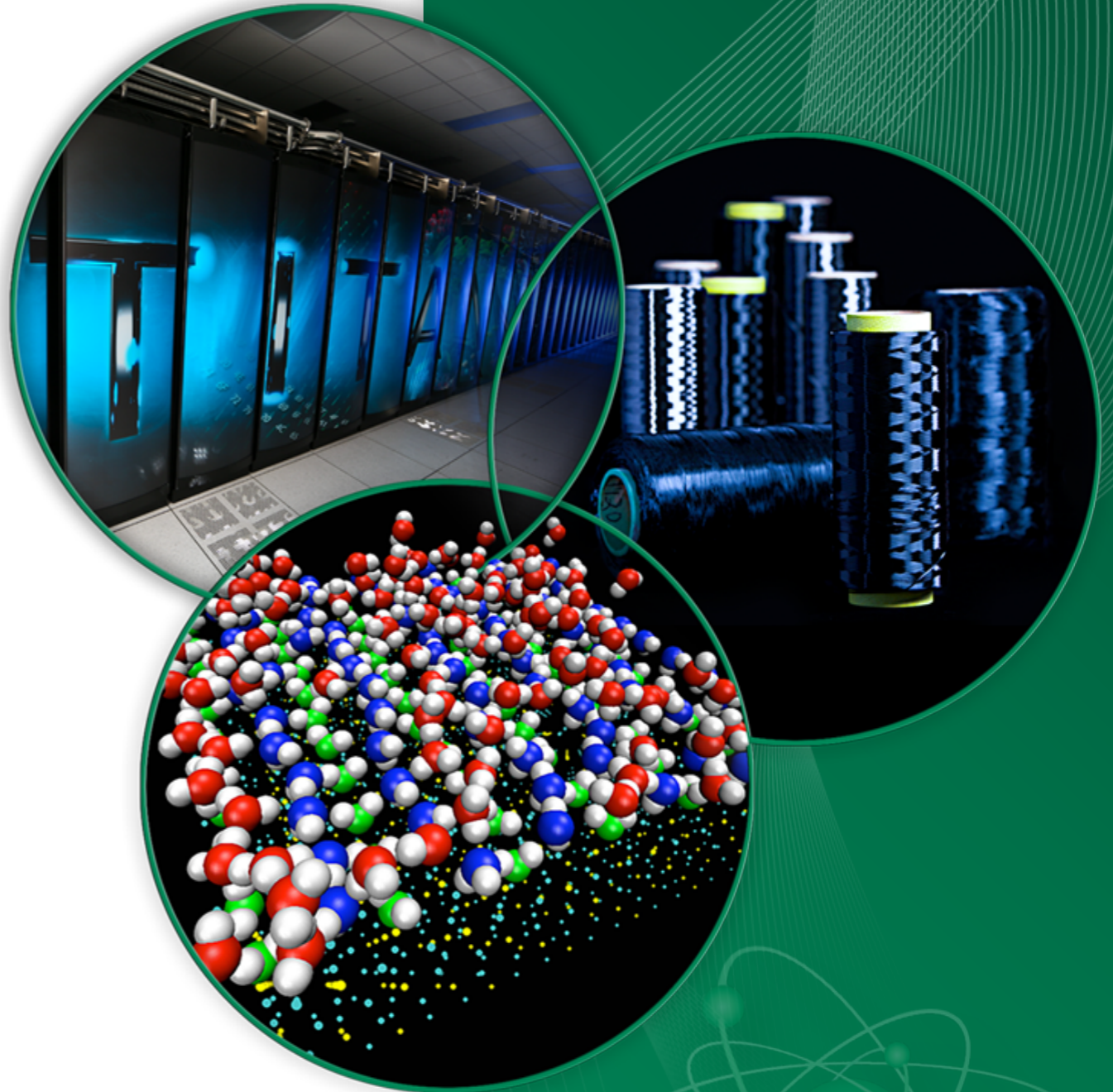
- CP reactions
- Be
- 12,natC
- 23-Na
- Ca
- V
- Ti?
- Cr
- Ni
- Cu
- Zr
- Mo?
- Ta
- Gd
- Dy

New ENDF/B evaluations

Status Report on ORNL Nuclear Data Evaluations

Luiz Leal, Marco Pigni, Vladimir Sobes, Doro Wiarda, Klaus Guber, Royce Sayer, Goran Arbanas, RQ Wright, and Mike Dunn

Nuclear Data & Criticality Safety Group



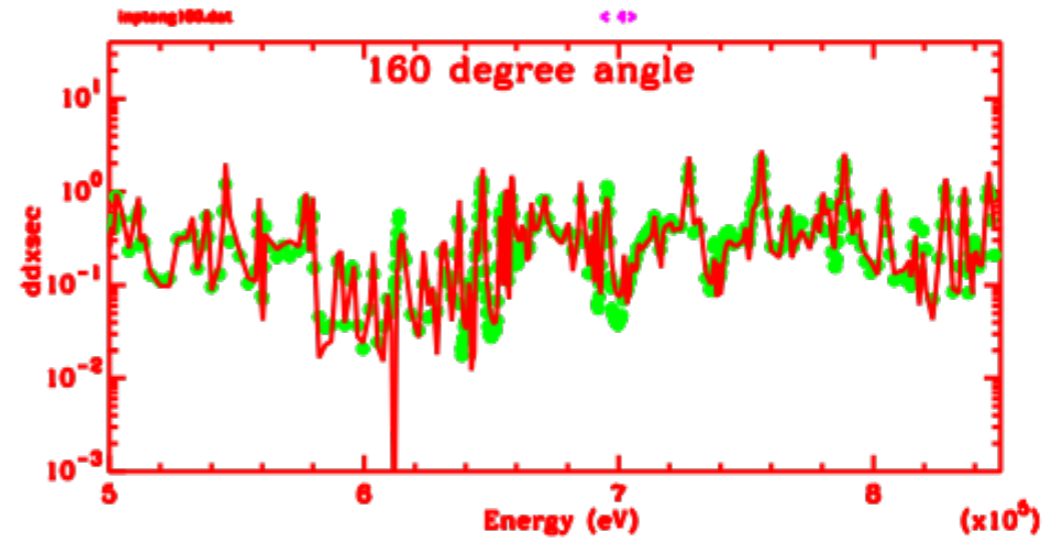
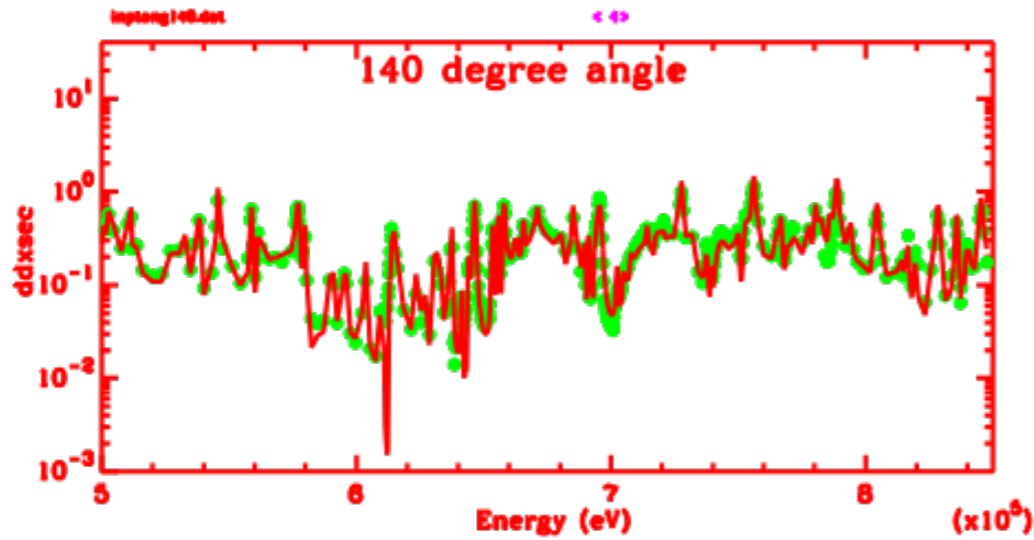
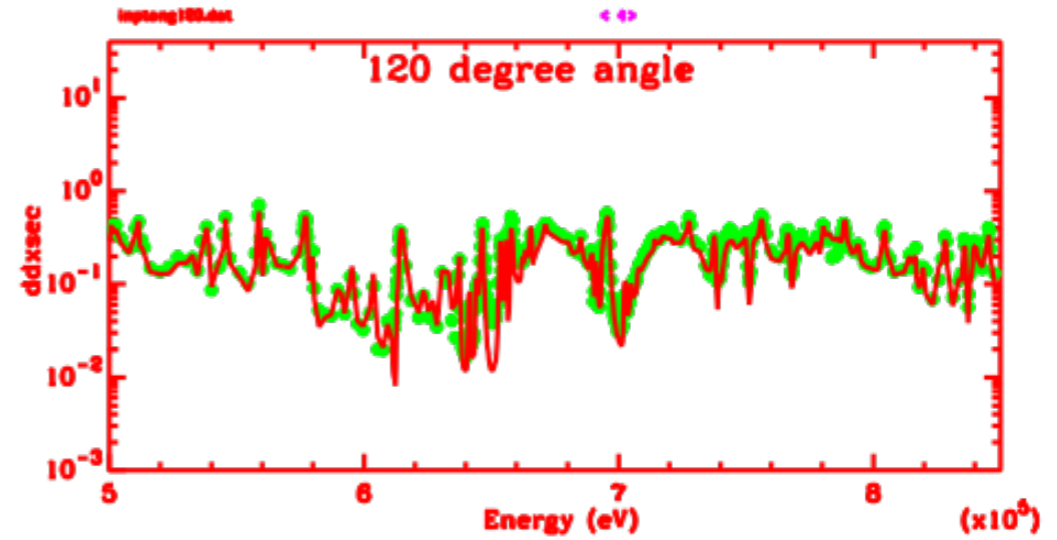
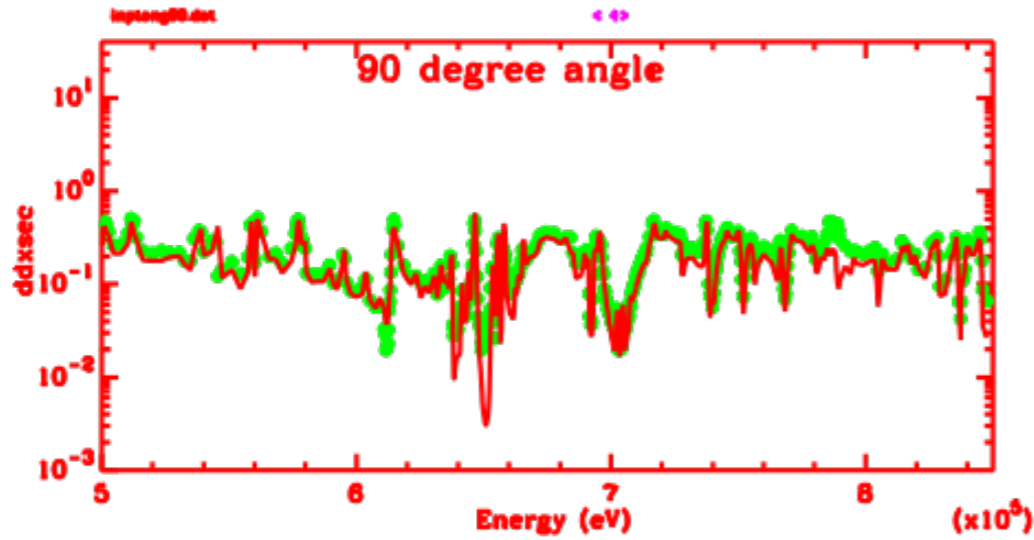
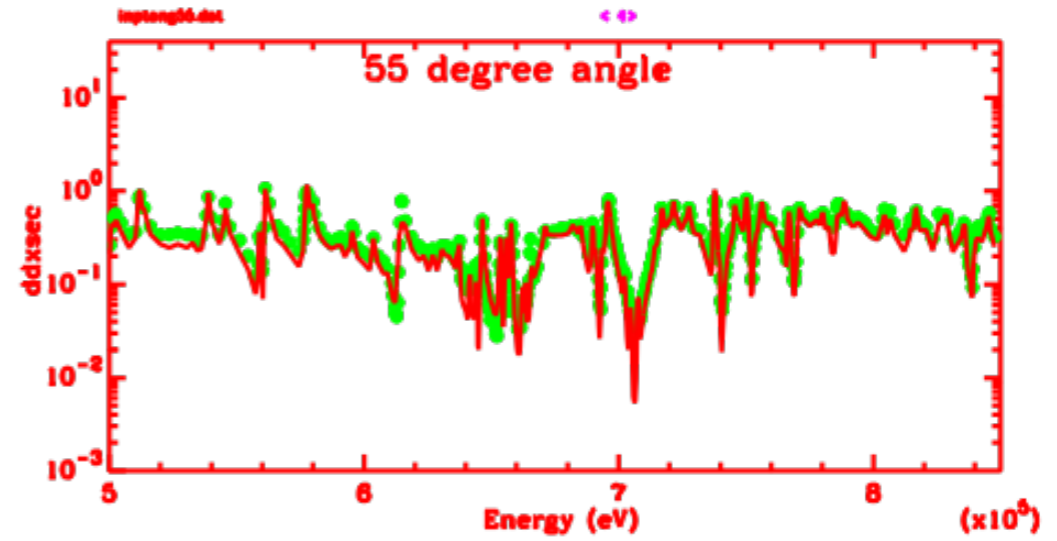
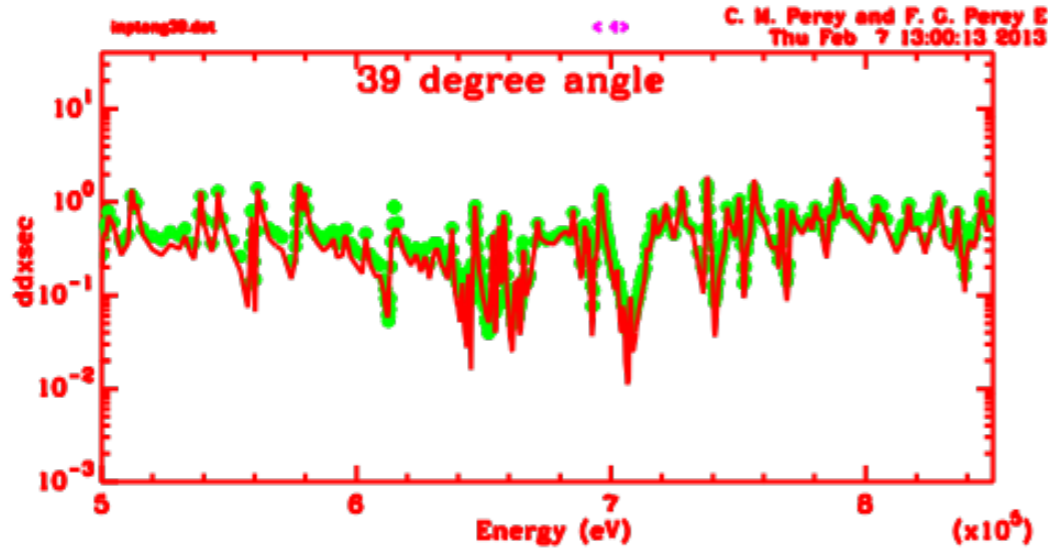
ORNL Resonance Evaluations and deliverables

	Energy Range	Resonance Covariance Evaluation	Target date for delivery the evaluation
63,65	Thermal to 300 keV	Yes	Completed
182	Thermal to 10 keV	Yes	FY2014
183	Thermal to 5 keV	Yes	FY2014
184	Thermal to 10 keV	Yes	FY2014
186	Thermal to 10 keV	Yes	FY2014
56	Thermal to 2 MeV	Yes	CIELO
16	Thermal to 6.3 MeV LRF=7; includes (n, α)	Yes	CIELO
239	Thermal to 2.5 keV	Use ENDF/B-VII.1 (FILE33)	Completed
235	Thermal to 2.25 keV	Use ENDF/B-VII.1 (FILE33)	CIELO

^{56}Fe Resolved Resonance Region Evaluation

- New high resolution transmission measurements at RPI extending the resonance region up to 5 MeV
- New inelastic cross-section measurements done at GEEL
- Extend the resolved resonance region from 850 keV to 2.0 MeV
- Include new transmission measurements and inelastic cross section data
- Use the extended (RML=7) R-matrix formalism in the SAMMY code for fitting the experimental data

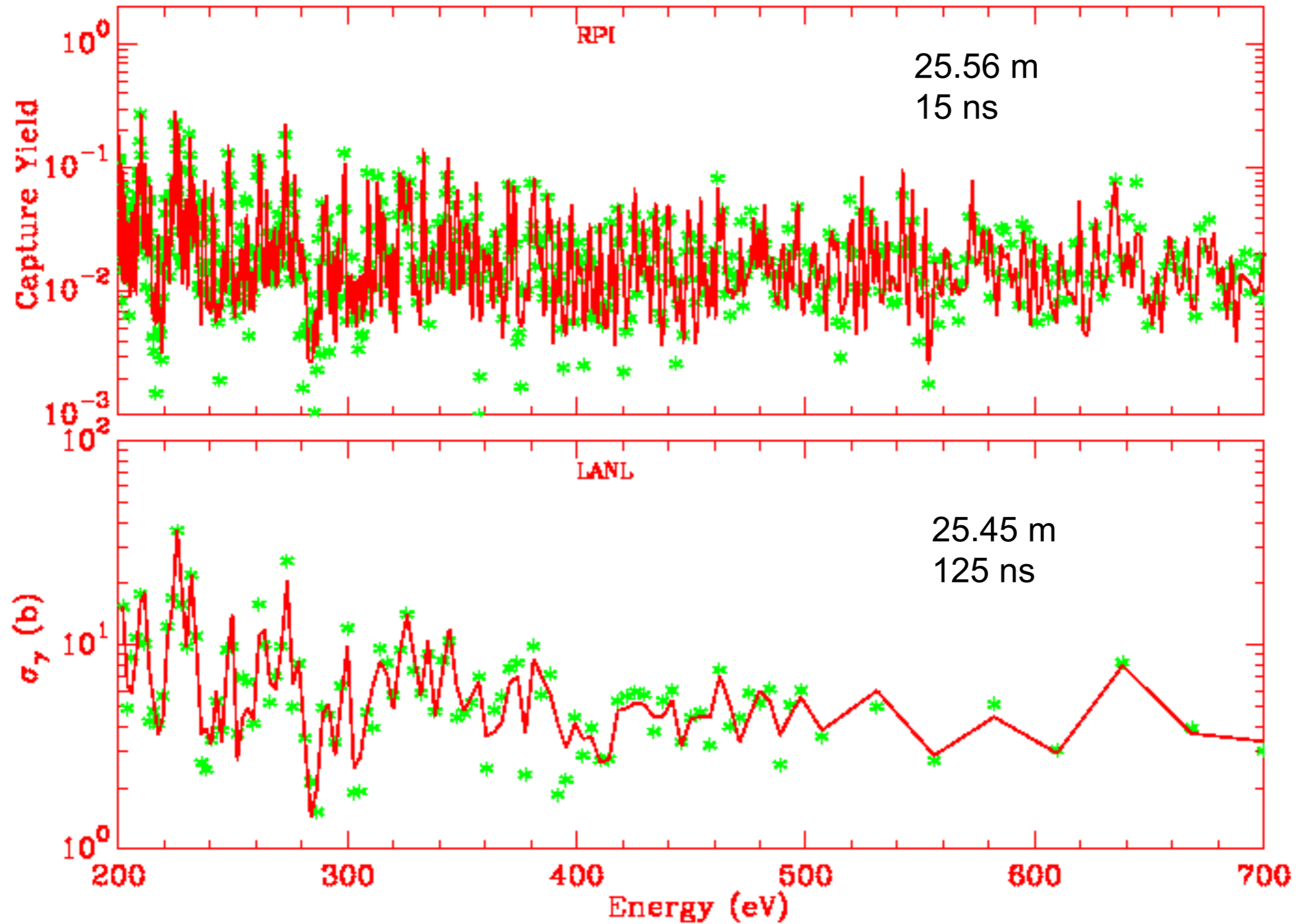
Comparison of SAMMY predictions to differential elastic data of Perey.



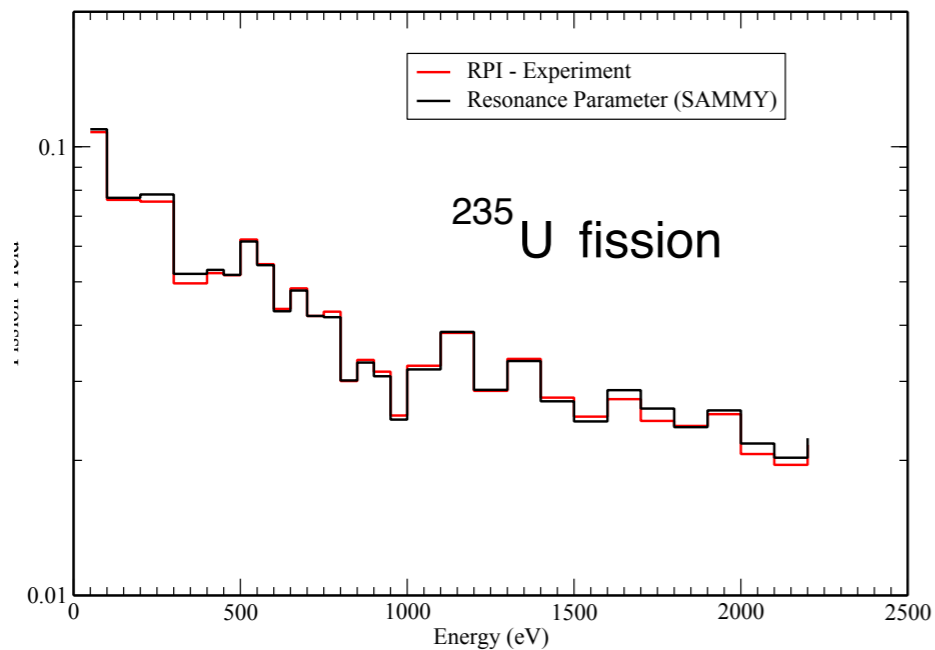
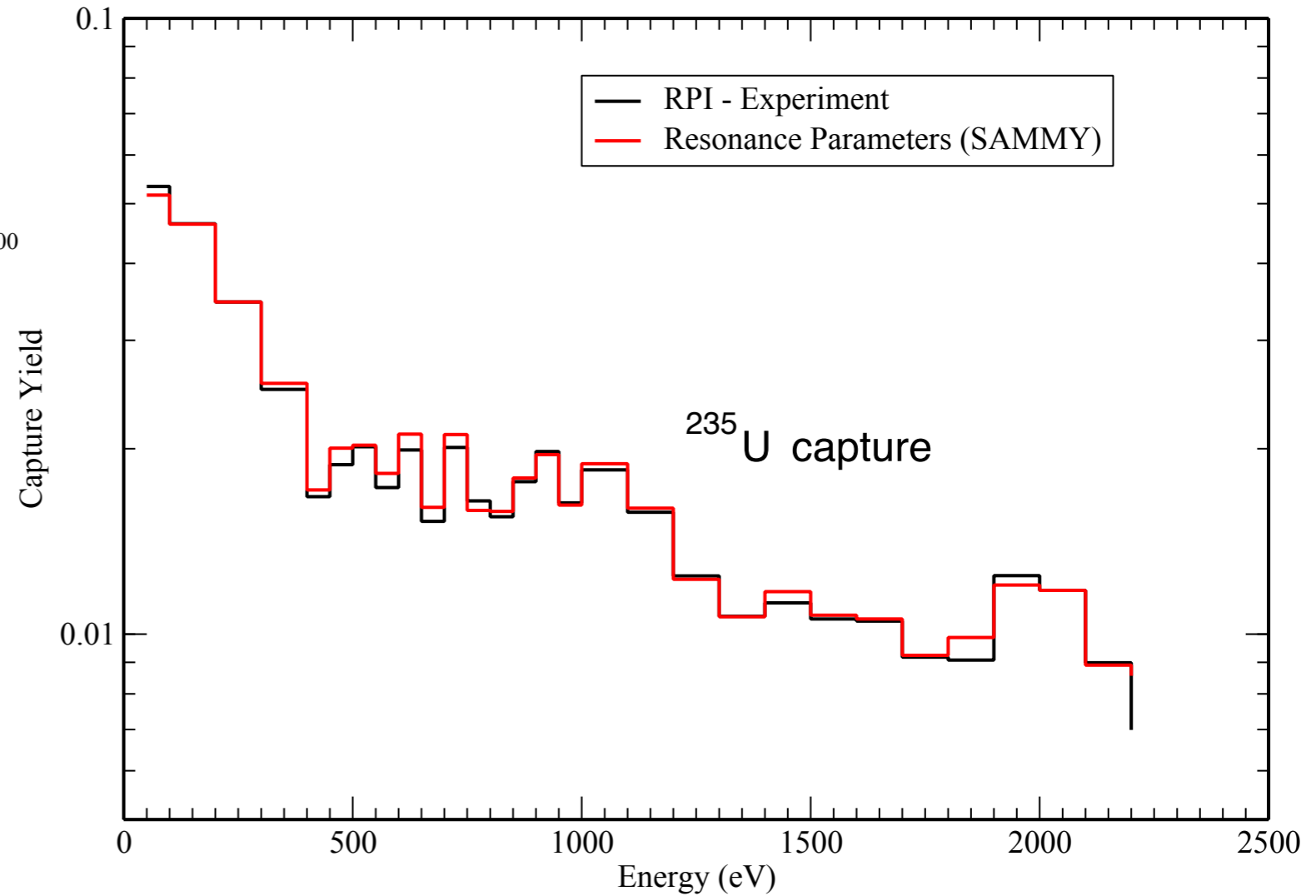
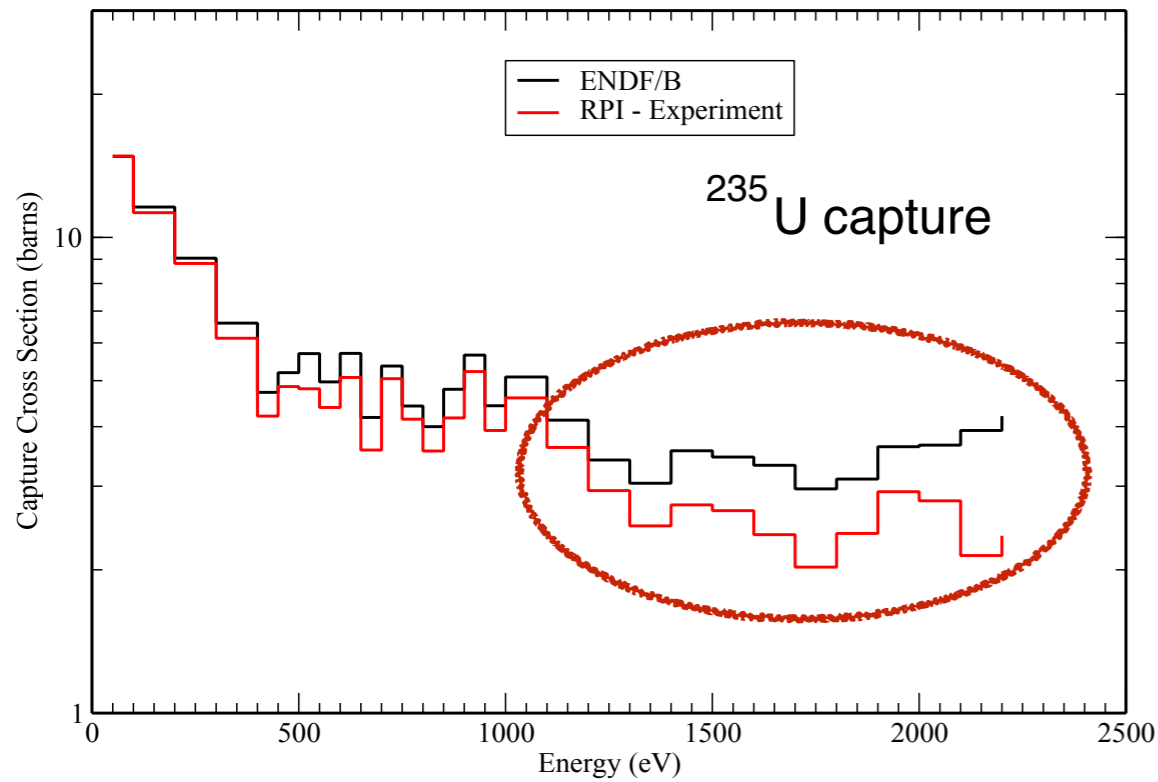
^{235}U Resonance Region Evaluation

- ✓ New data measurements from RPI (capture and fission yields) (kind of alpha measurements)
- ✓ New capture data from LANL
- ✓ Use SAMMY code for fitting the new data
- ✓ Test the new evaluation in benchmark calculations: ZEUS benchmarks (**FCA not available**)
- ✓ Use JENDL4 as the template
- ✓ Benchmark Calculations done with MCNP with everything else from ENDF/B-VII.0

RPI and LANL Capture Data



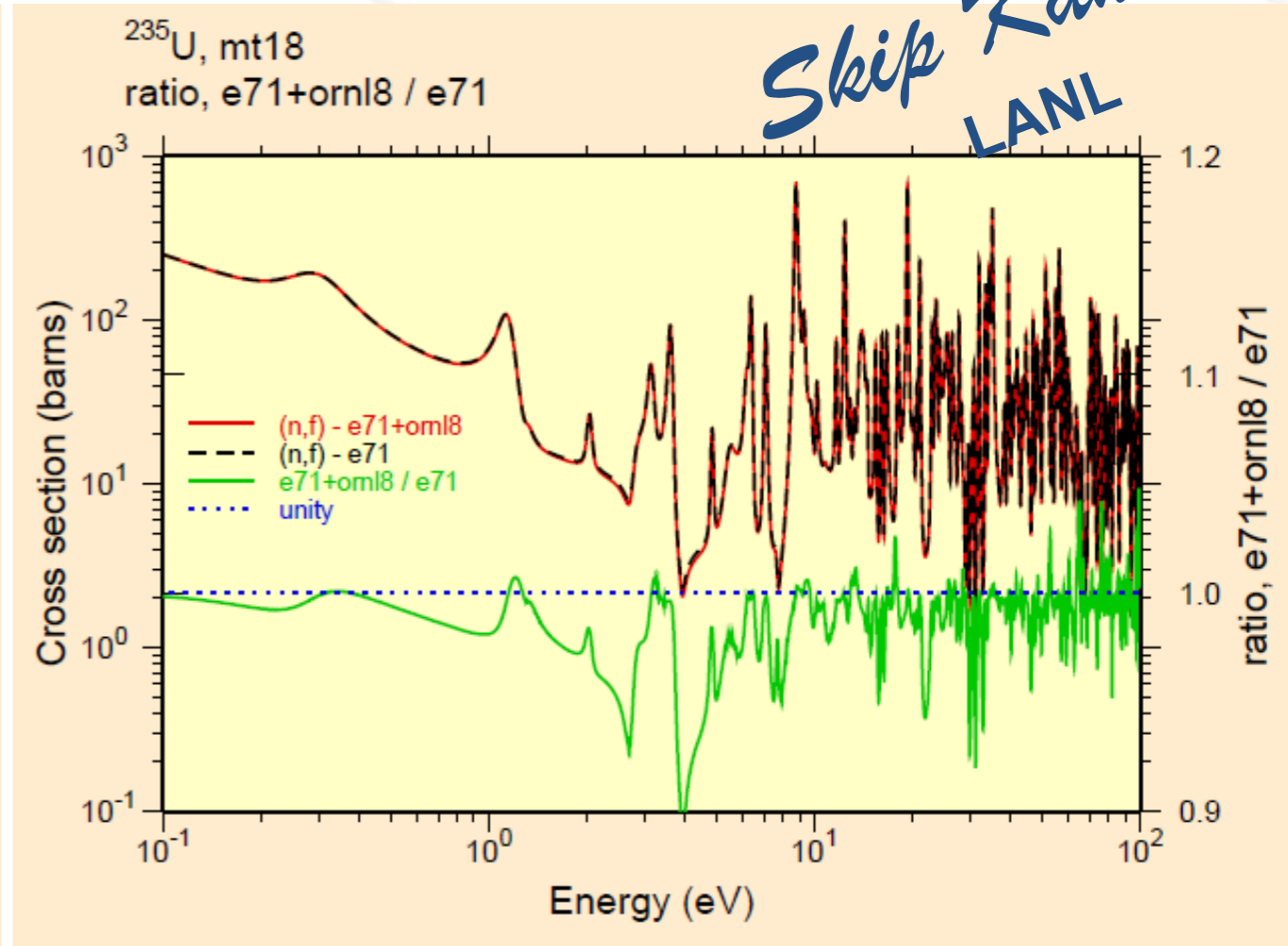
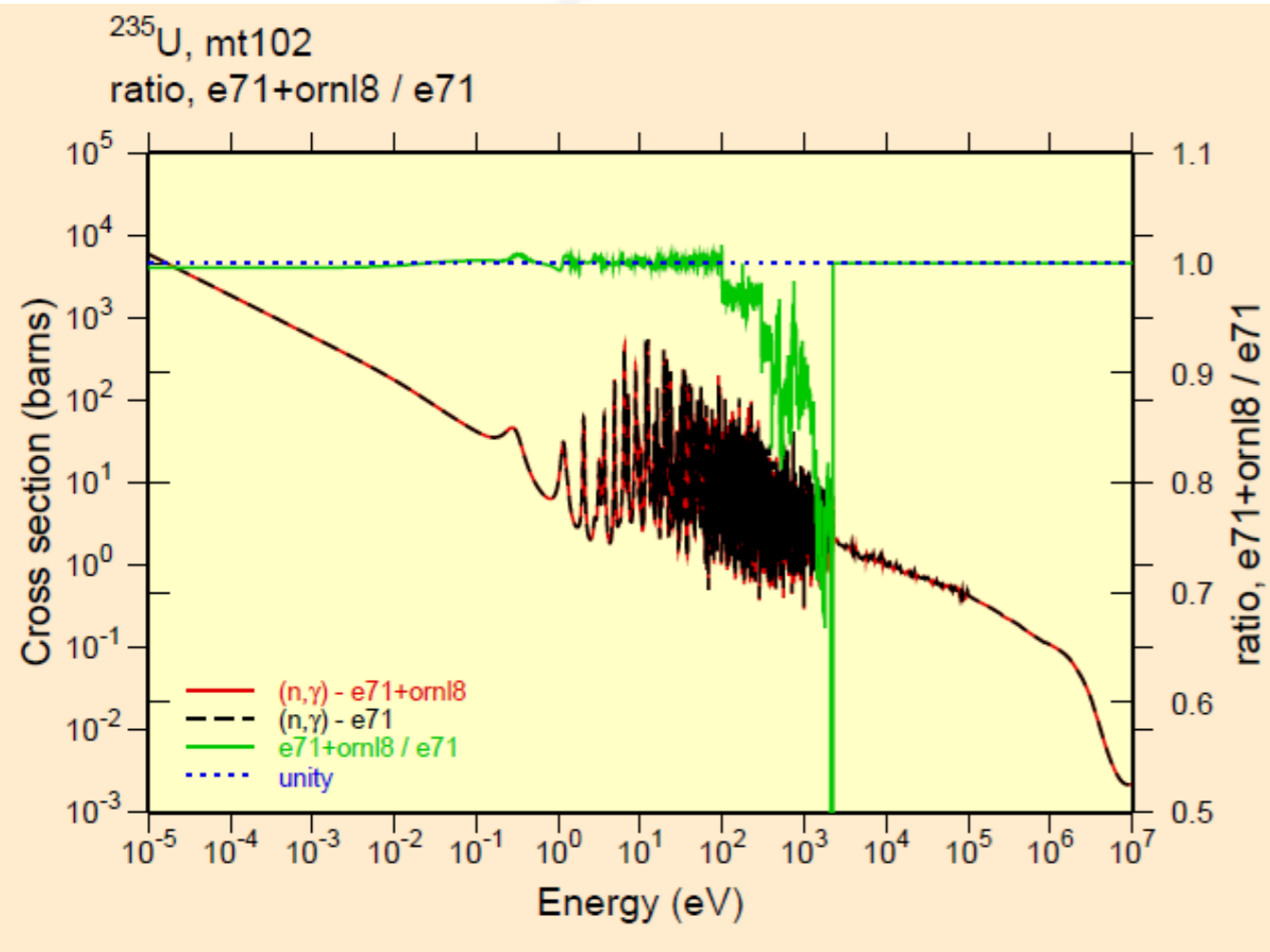
Fit of the RPI ^{235}U Data





^{235}U – Primarily Revised Capture

Skip Kahler
LANL



Comparison of $^{235}\text{U}(n,\gamma)$ and $^{235}\text{U}(n,f)$ cross sections ... recent ORNL re-evaluation, designated ORNL8, based upon new LANL and RPI data versus the current (ENDF/B-VII.1) evaluation ... “a work in progress” per Luiz Leal.

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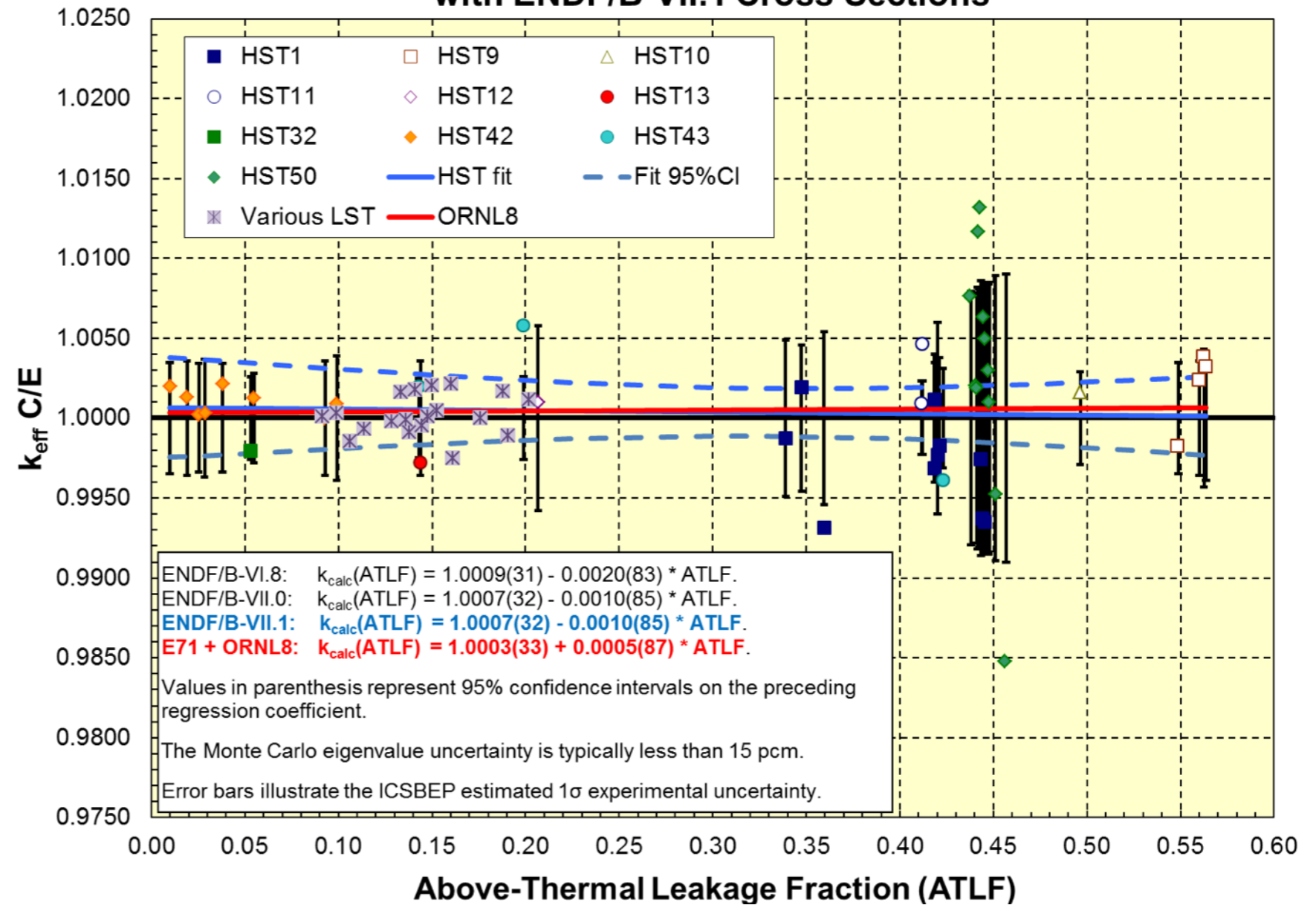


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LANL

HST Benchmarks

- Regression fit to HST benchmarks versus ATLF has been excellent since ENDF/B-VI.3 (Lubitz).
- This excellent fit is retained with the latest (**ORNL8**) ²³⁵U resolved resonance file.

Calculated xxx-SOL-THERM Eigenvalues with ENDF/B-VII.1 Cross Sections



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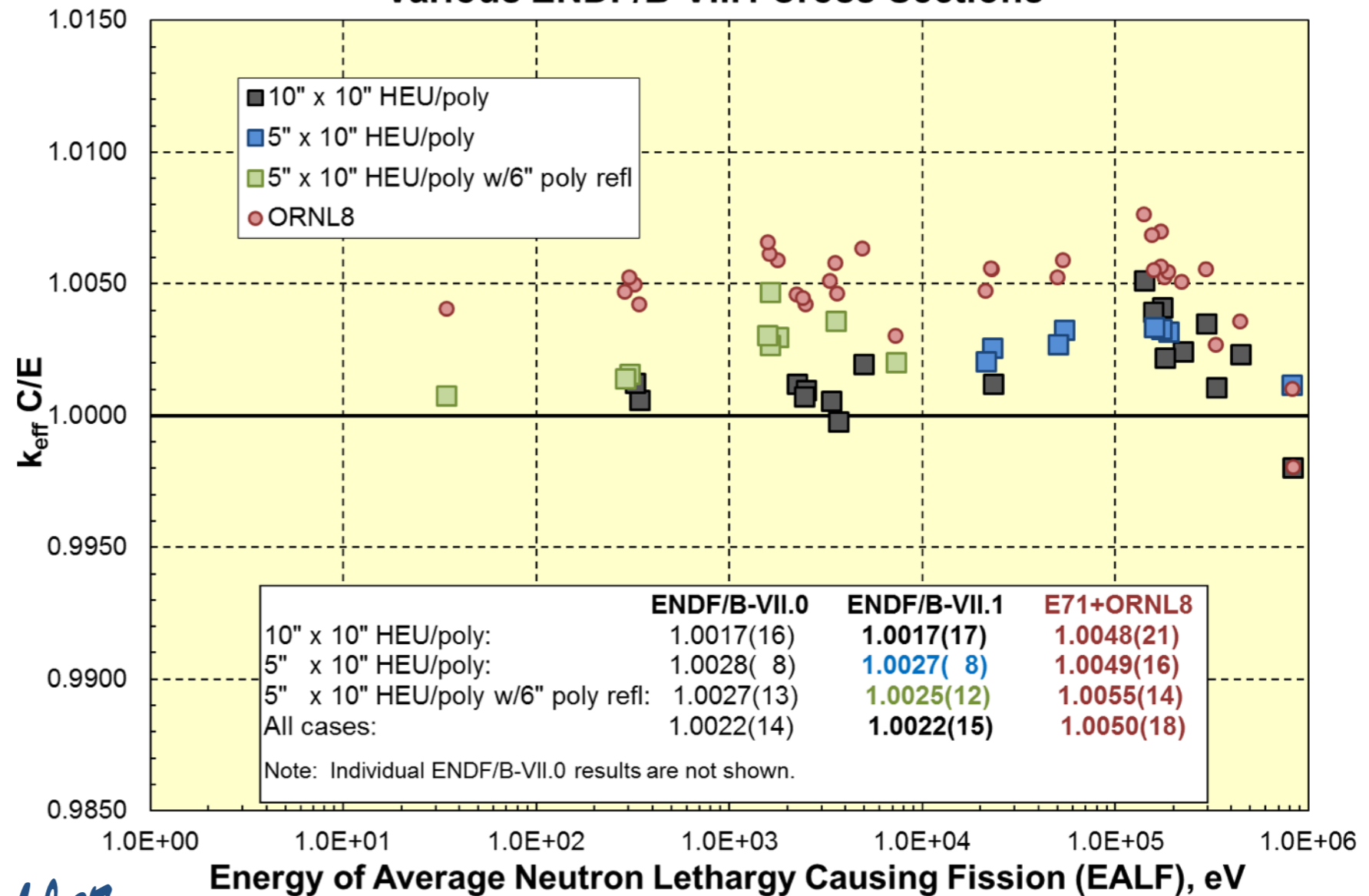




HMF7 (HEU + CH₂) Benchmarks

- HEU + poly system tests xs data over several orders of magnitude.
- E70 & E71 results are near unity at either energy extreme but are biased high in the intermediate energy range.
- This bias is worsened with the latest ORNL8 ²³⁵U evaluated file.

HEU-MET-FAST-007 Calculated Eigenvalues with Various ENDF/B-VII.1 Cross Sections



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LANL

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Validation



Data Testing Revised ^{235}U and ^{239}Pu Files with ICSBEP Benchmarks

A. C. (Skip) Kahler
Los Alamos National Laboratory

L. C. Leal
Oak Ridge National Laboratory

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^{239}Pu – WPEC SG34

- Revised resolved resonance
- Revised $v_p(E)$ data, up to 650 eV
- Revised PFNS
- Differences between JEFF and ENDF remain, ☹.

Although the Sub-Group is near an end, this work remains a “work in progress” that will continue under CIELO.

WPEC Subgroup 34 - Mozilla Firefox

File Edit View History Bookmarks Tools Help

WPEC Subgroup 34

https://www.oecd-nea.org/science/wpec/sg34/

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NEA Nuclear Energy Agency

NEA search engine Go

OECD

Nuclear science > Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

Coordinated evaluation of ^{239}Pu in the resonance region

WPEC Subgroup 34 (SG34)

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- SG34 proposal by R.D. McKnight and C. De Saint Jean, WPEC meeting, June 2009
- SG34 mailing list for questions, comments or to consult archives

Meetings

- NEA, Issy-les-Moulineaux, France, 2 June 2010
- NEA, Issy-les-Moulineaux, France, 21 May 2012

Test evaluation

- New resolved resonance parameters in ENDF format

Publications and documents

- L.C. Leal et al., ^{239}Pu Resonance Evaluation for Thermal Benchmark System Calculations, ND2013 contribution (Draft Feb. 2013).
- A.C. Kahler et al., Critical Eigenvalue Calculations of Selected ICSBEP Benchmarks with Various ^{239}Pu Evaluated Data Files, WONDER 2012, Aix en Provence, France, September 25-28, 2012.

Related links

- WPEC Home Page

Co-ordinator: Cyrille De Saint Jean
NEA contact: Emmeric Dupont (wpec@oecd-nea.org)

Last update: 30 April 2013

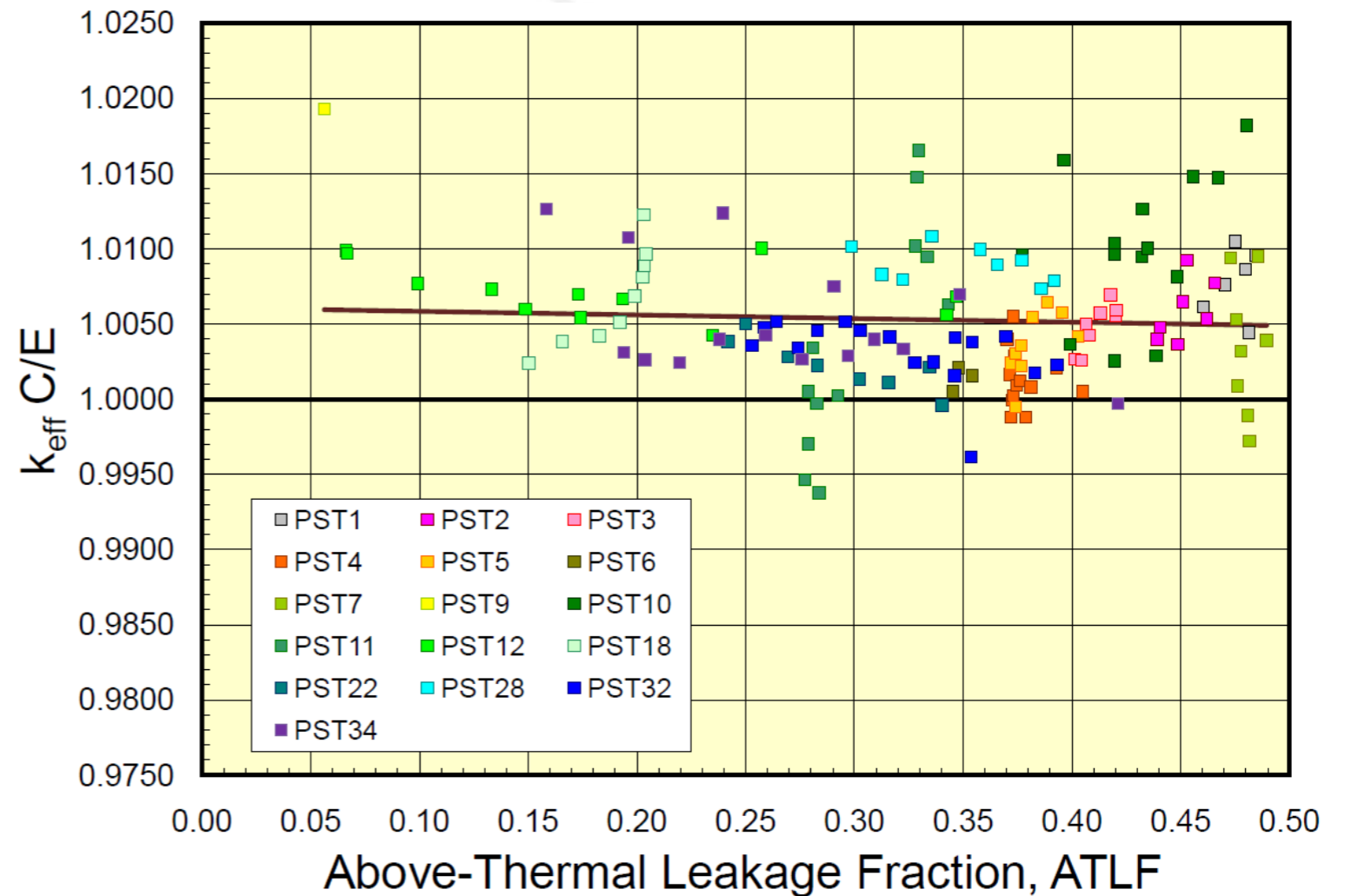
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Pu-SOL-THERM Benchmarks - I

- A ~500 pcm bias in calculated PST reactivity is a long-standing issue.
- WPEC Sub-Group 34 was tasked with defining a new (better?) set of resolved resonance parameters for ^{239}Pu in an attempt to resolve this issue.
- Can define a sub-set of these 150 benchmarks to test revised data files.



Consider benchmark attributes such as (i) ATLF; (ii) ^{239}Pu atom-% in Pu; (iii) Above-Thermal Fission Fraction (ATFF); (iv) H/Pu number density (or gPu per liter) to define this sub-set.

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Analysis of VNIITF Mo Benchmarks

M. L. Zerkle
Bettis Atomic Power Laboratory

Cross Section Evaluation Working Group Meeting
November 20-22, 2013
Brookhaven National Laboratory



VNIITF Mo Benchmarks

- ^9Be – new evaluation by G. Hale
- ^{92}Mo – new evaluation by Mughabghab + JENDL-3.3
- ^{95}Mo – new evaluation by Kim, Herman, Mughabghab
- New ICSBEP Mo Benchmarks
 - HMF092 – fast, Mo reflected
 - HMF093 – fast, Mo reflected/diluted
 - HMF094 – fast, Mo diluted, Be/BeO mod, DU/Be/BeO Reflected
 - HMM020 – mixed, Mo diluted, CH₂ mod/reflected
- Analyzed with MC21
 - ENDF/B-VII.0 cross section
 - ENDF/B-VII.1 cross section
 - 108 active neutron histories ($\sim 0.0001 \Delta k$ 95% CI)

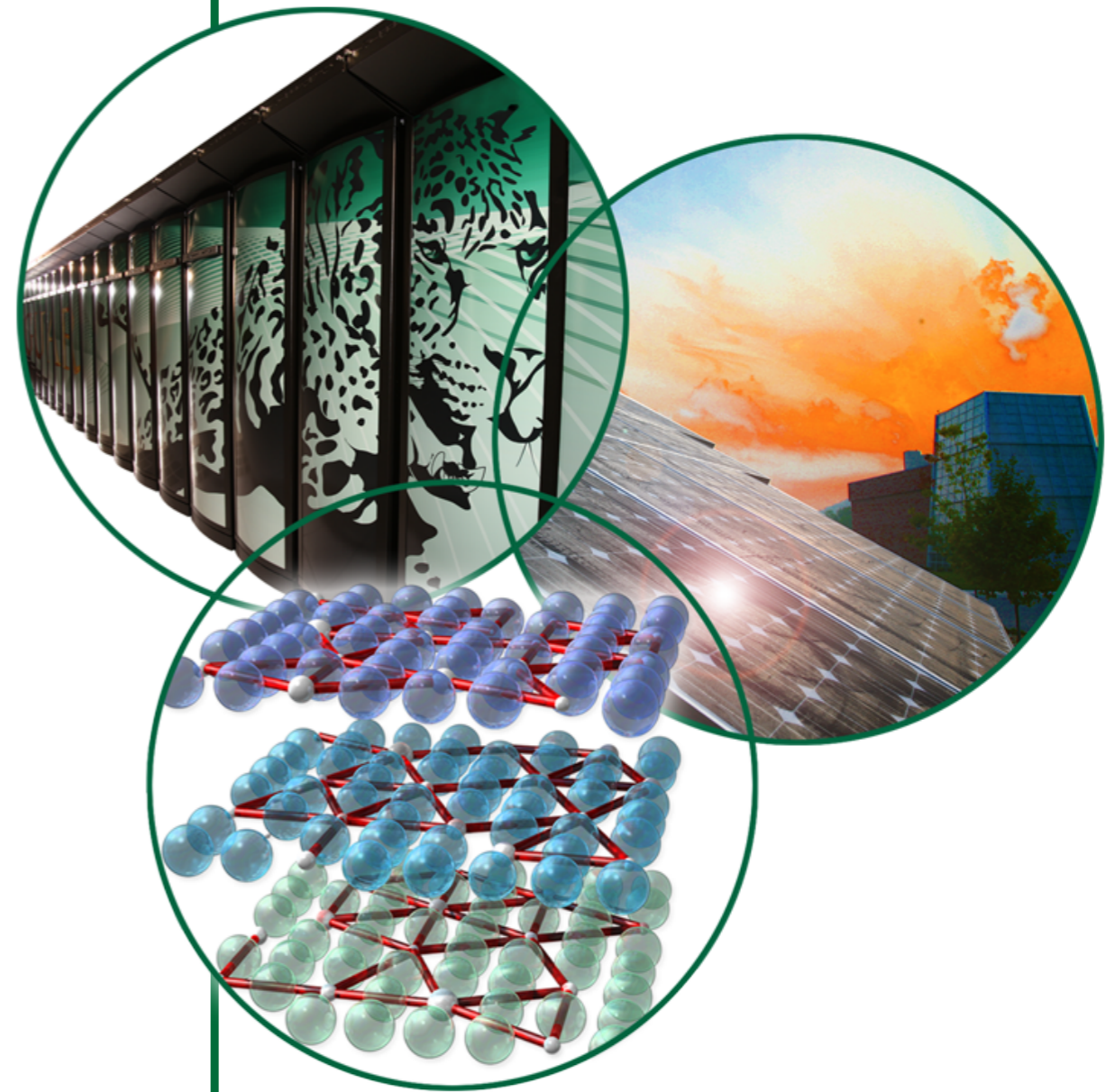


Conclusions

- ENDF/B-VII.0 and ENDF/B-VII.1 results consistent except for Be moderated/reflected cases (HMF094)
 - Implies improvement in ENDF/B-VII.1 Be evaluation
- Positive k_{calc} bias with Mo reflector thickness
 - Bias grows from +0.4% to +0.6% Δk for HMF092
 - Mo elastic ang. distributions insufficiently forward peaked and/or
 - Mo fast capture too low
- Bias increases to +0.7% Δk when Mo dilution added (HMF093)
 - Mo fast capture too low
- k_{calc} biased high in moderated cases
 - +0.6% Δk bias for Be/BeO moderated cases (HMF094)
 - +0.64% to 0.74% Δk bias for CH₂ moderated cases (HMM020)
 - capture too low (RR, fast)
 - Spectral dependence on bias in RR (bias reduced for softer spectrum CH₂ moderated cases)

Investigation of ENDF/ B-VII.1 Covariance Data for SCALE-6.2

Mark Williams, B.J. Marshall, Doro
Wiarda, Brad Rearden
Oak Ridge National Laboratory



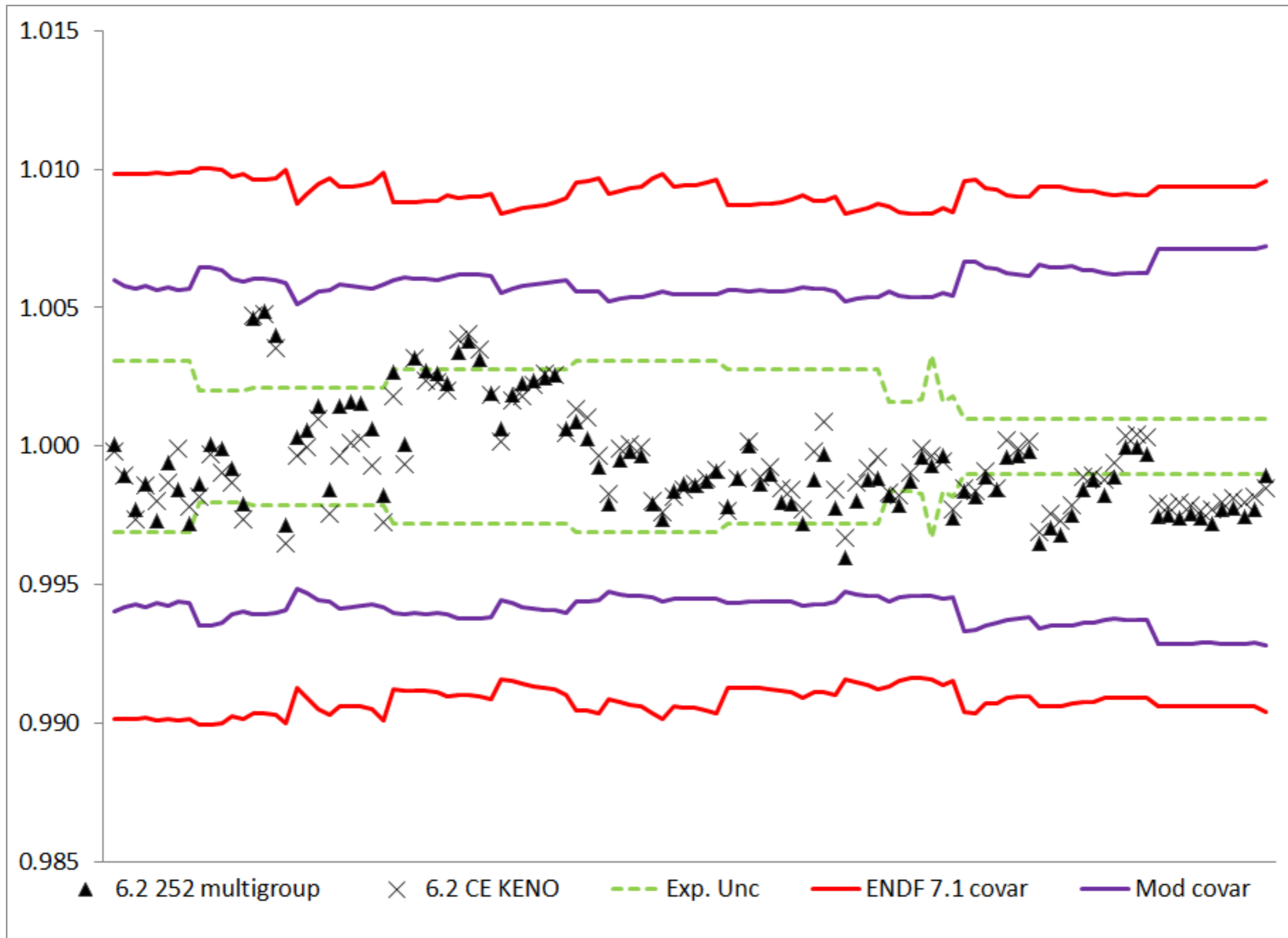
SCALE-6.2 Will Include Cross Section Libraries and Covariance Data Processed from ENDF/B-VII.

1

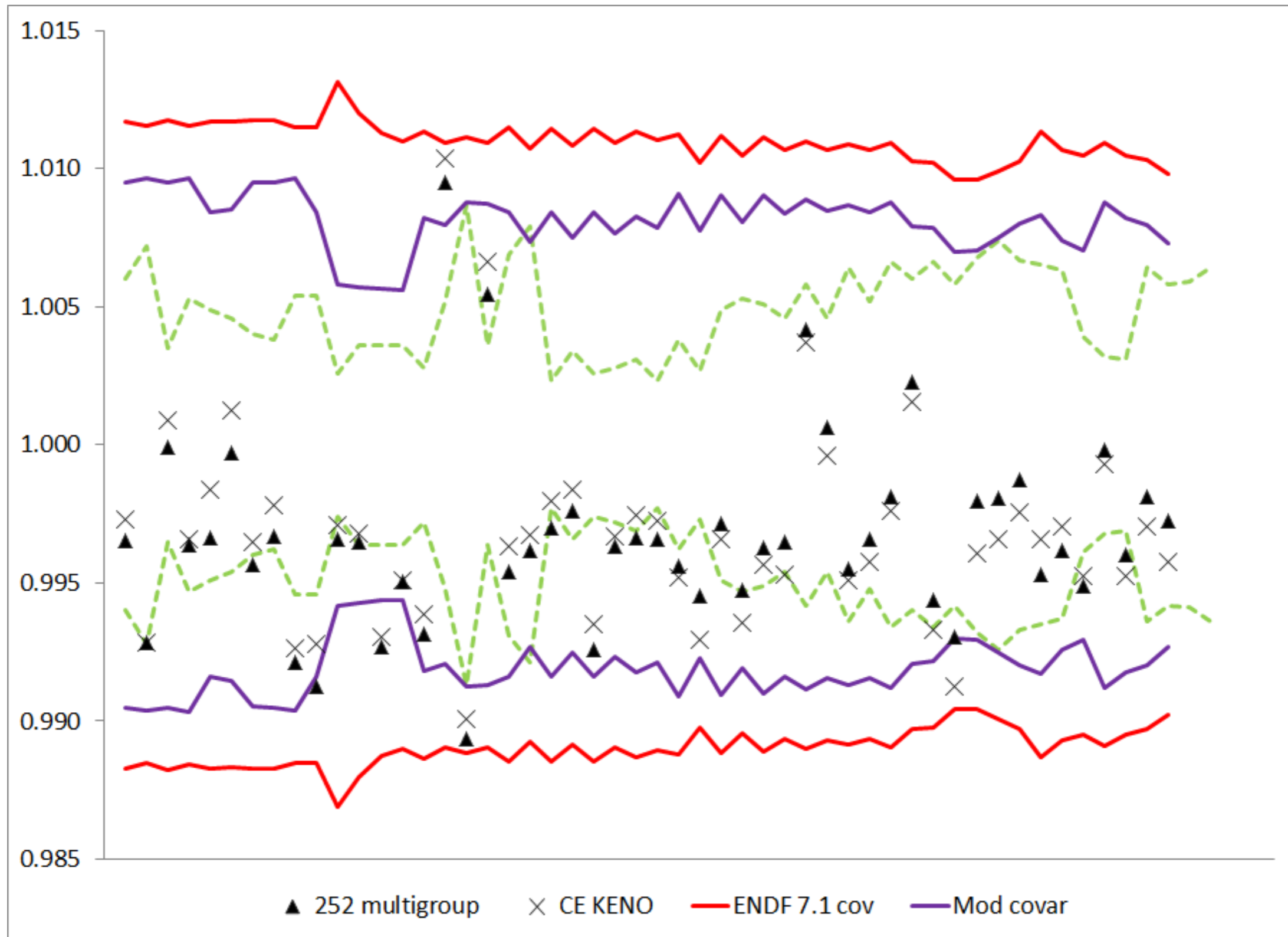
Validation studies performed for 320 benchmark experiments

- Continuous energy (CE), 252g multigroup, and covariance data were processed using AMPX
- Critical eigenvalues computed with Keno Monte Carlo code using both 252g and CE
- Covariance library generated by replacing covariances in SCALE-6.1 with ENDF-VII.1 data, if available. Variations were made in some ENDF-VII.1 values
- S/U calculations with 252g TSUNAMI-3D (Keno)

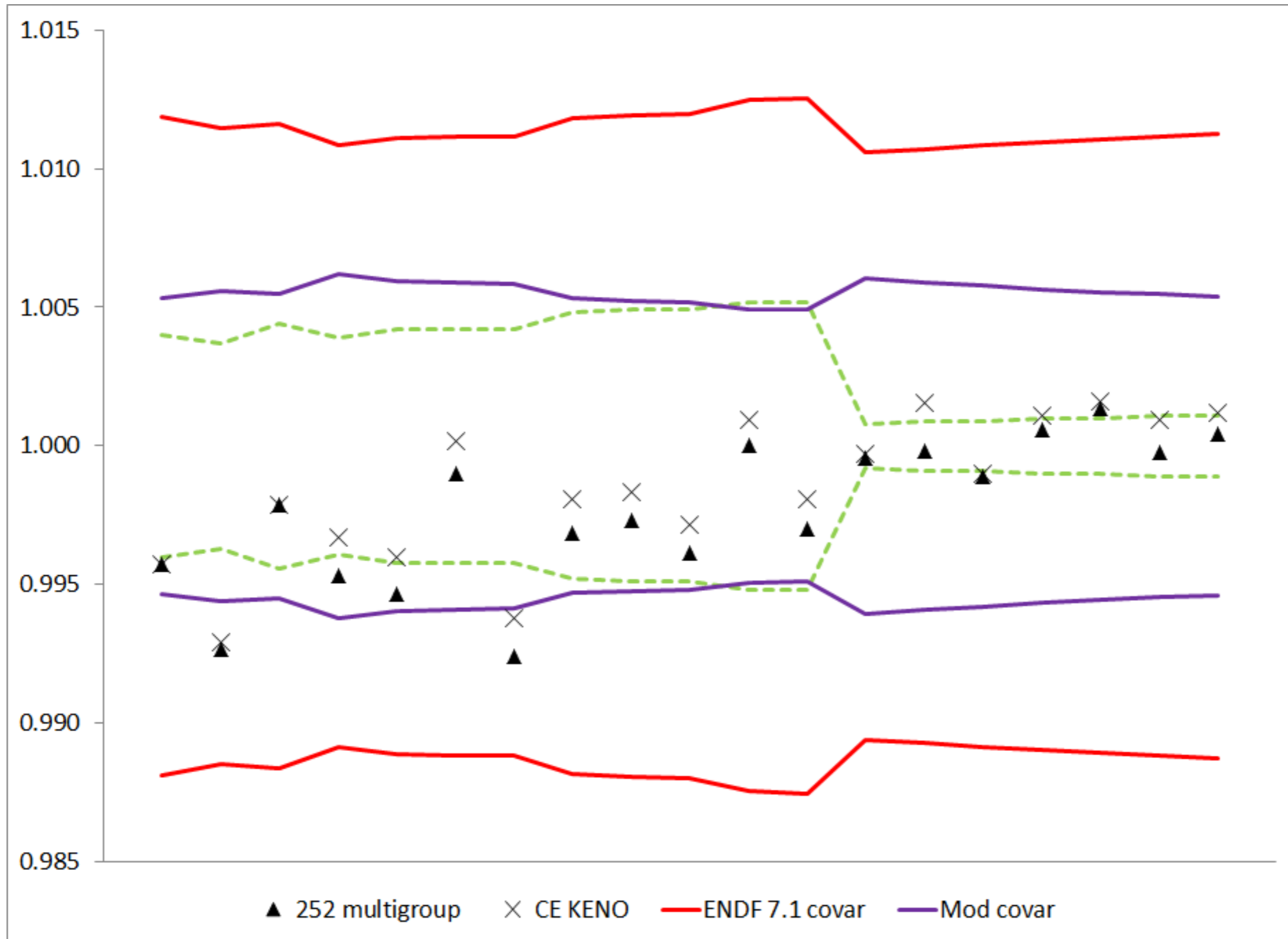
Uncertainties for LEU-COMP-THERM Benchmarks



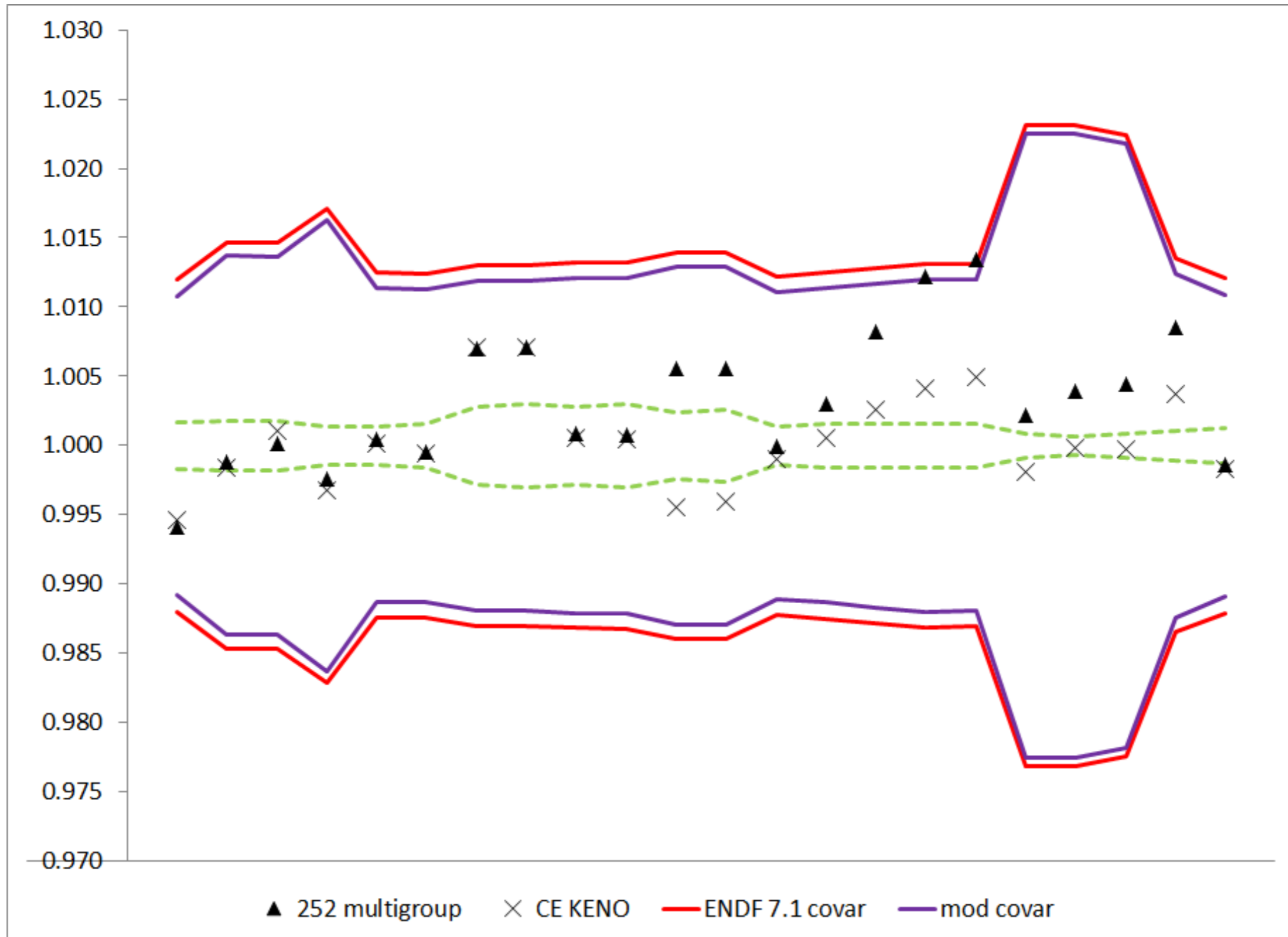
Uncertainties for HEU-SOL-THERM Benchmarks



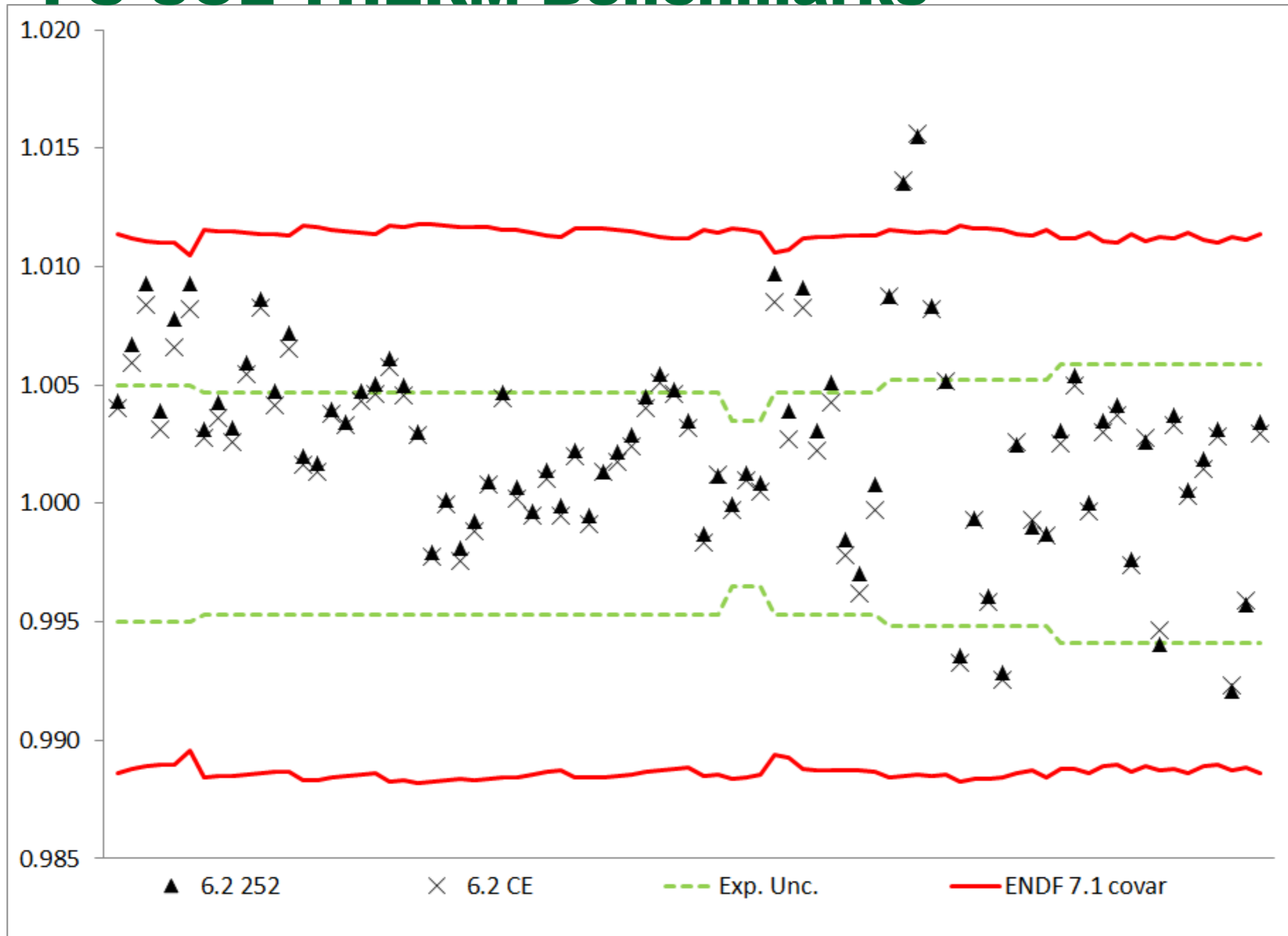
Uncertainties for LEU-SOL-THERM Benchmarks



Uncertainties for HEU-MET-FAST Benchmarks



Uncertainties for PU-SOL-THERM Benchmarks



Observed Standard Deviations are Less Than Predicted from Nuclear Data Covariances

Cases	St. Dev (pcm) from C/E Values	St. Dev (pcm) from S/U
<i>HST</i>	<i>590</i>	<i>800</i>
<i>LST</i>	<i>259</i>	<i>556</i>
<i>LCT</i>	<i>185</i>	<i>583</i>

Modernizing infrastructure

LA-UR-13-28858

CGMF and CoH3 Nuclear Reaction Codes

Toshihiko Kawano, Ionel Stetcu, Patrick Talou

T-2, Nuclear Physics Group
Los Alamos National Laboratory



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Slide 1

Operated by Los Alamos National Security, LLC for NNSA

USNDP Meeting, BNL, Nov. 19, 2013

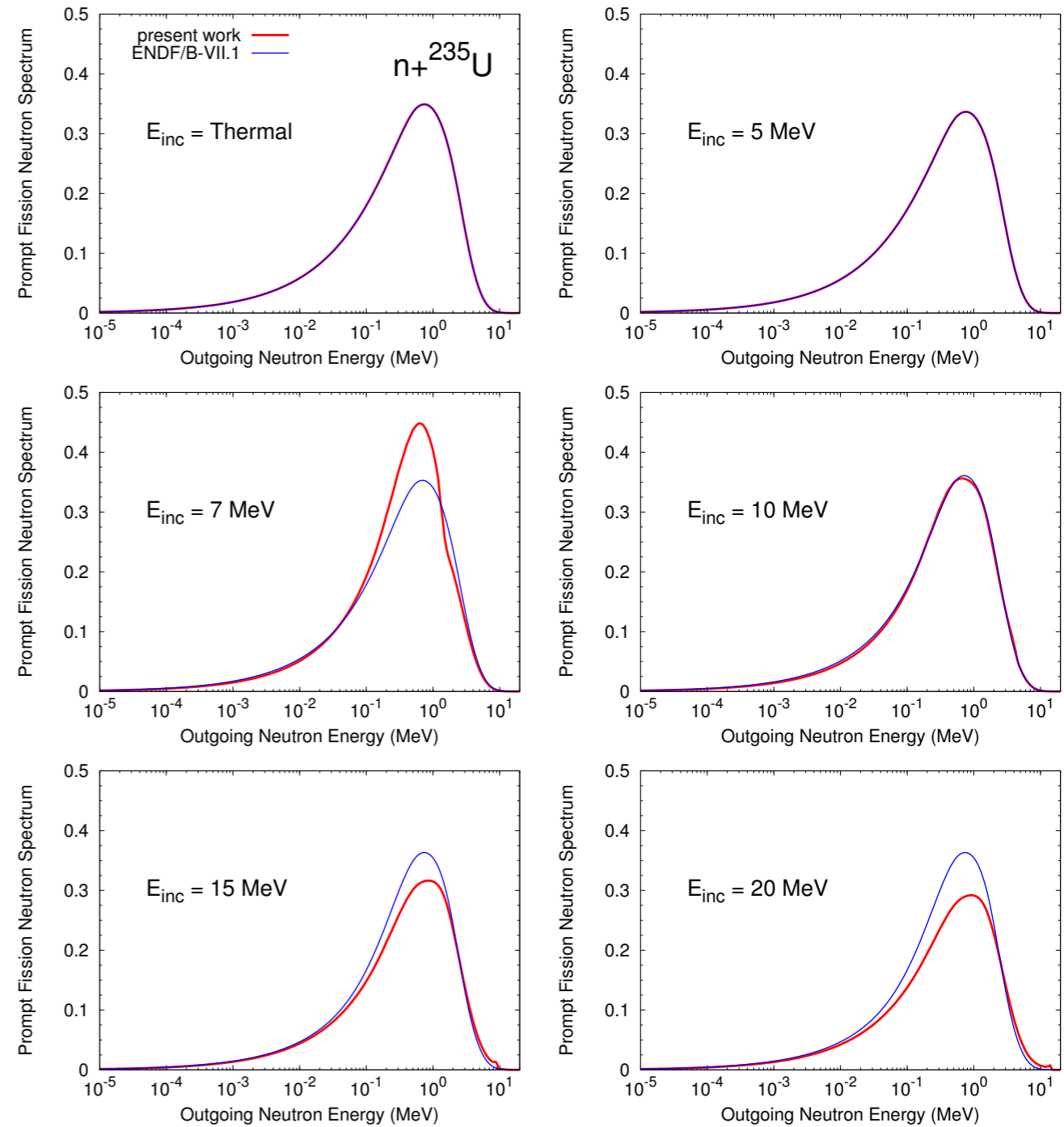
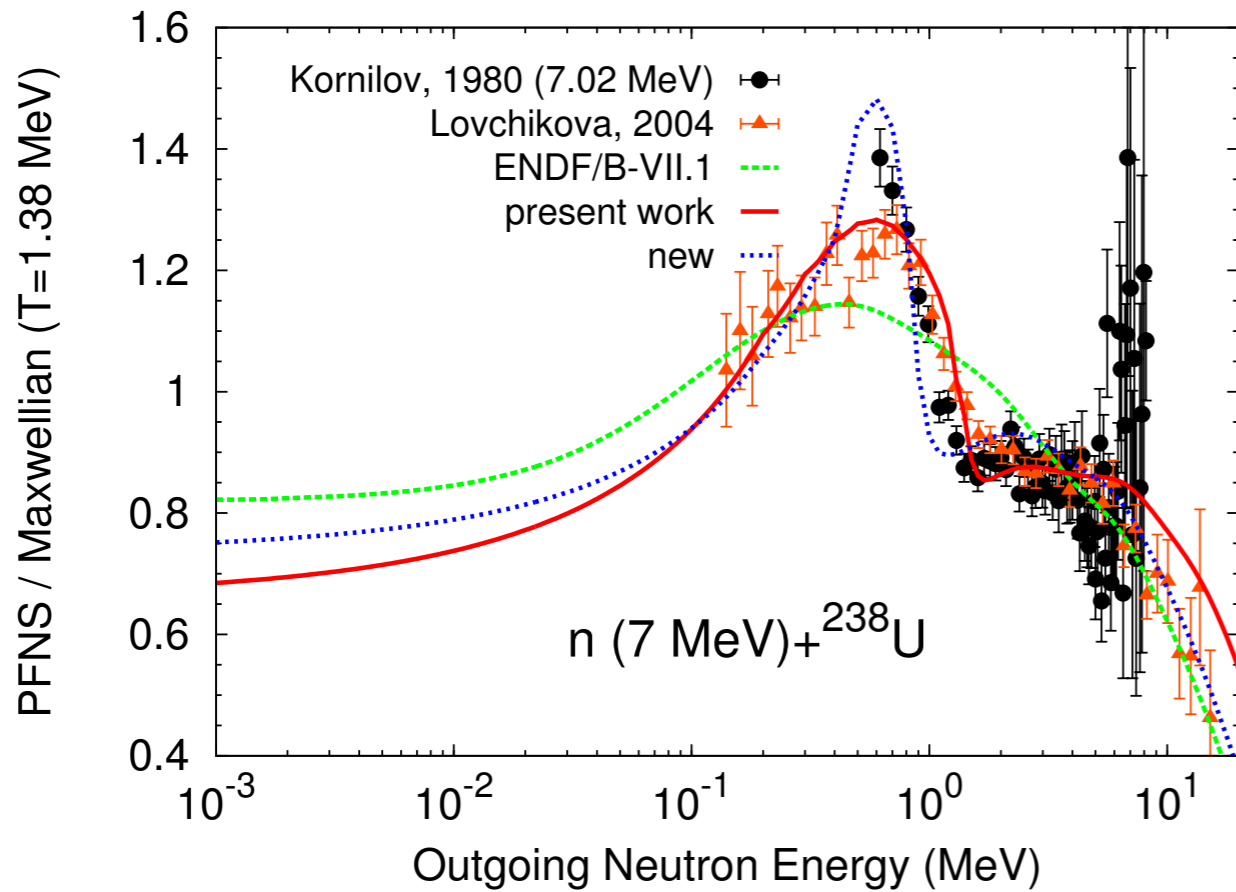


CoH3

- **What is it?**
 - Optical model and coupled-channels calculations (spherical and deformed)
 - Exciton pre-equilibrium model
 - Direct and semi-direct capture model
 - Hauser-Feshbach statistical model
 - Calculates nuclear reaction cross sections for medium and heavy targets
 - keV and MeV energy regions
- **Written in C++**
- **Input files or... “super-lazy mode”:** `coh -z 26 -a 56 -e 10.0`
- **Newest addition:**
 - **prompt fission neutron spectrum** calculated with the Los Alamos model equations.
 - Pre-fission neutrons included

CoH3 calculations of PFNS

$n+^{235}\text{U}$



CGM

Cascading Gamma Multiplicities

- T.Kawano, P.Talou, M.B.Chadwick and T.Watanabe, "Monte Carlo Simulation for Particle and γ -Ray Emissions in Statistical Hauser-Feshbach Model," J. Nucl. Sci. Tech. 47, 462 (2010).
- **Monte Carlo Hauser-Feshbach code**

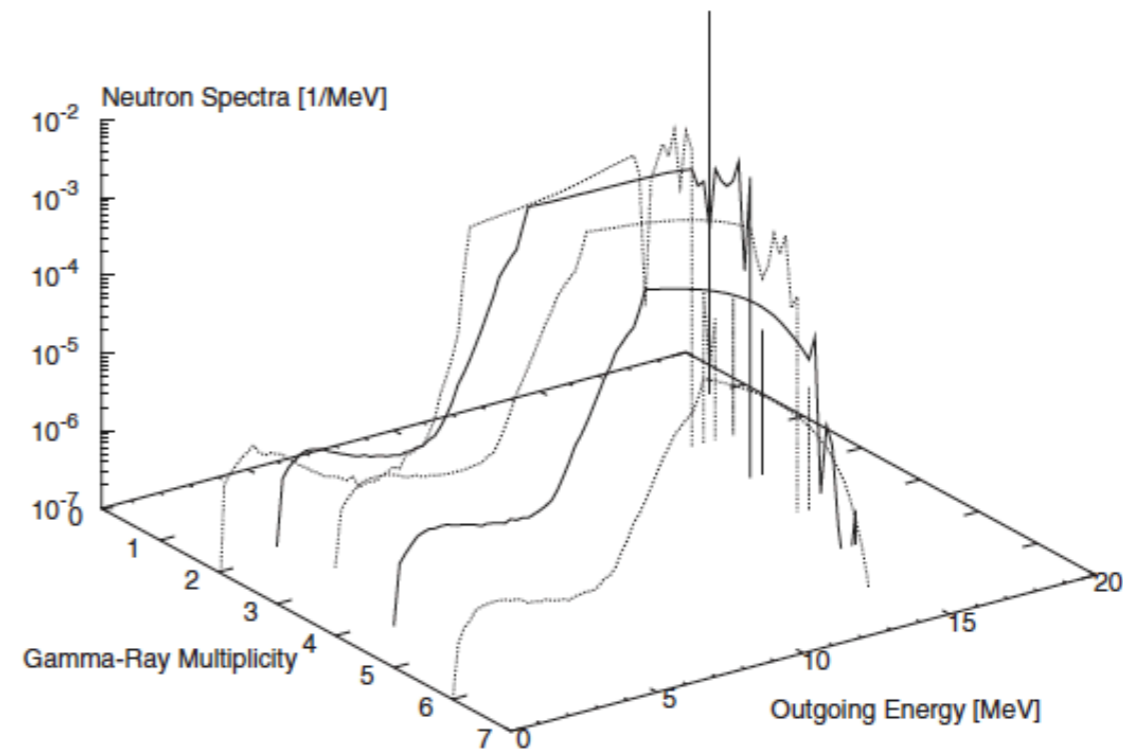
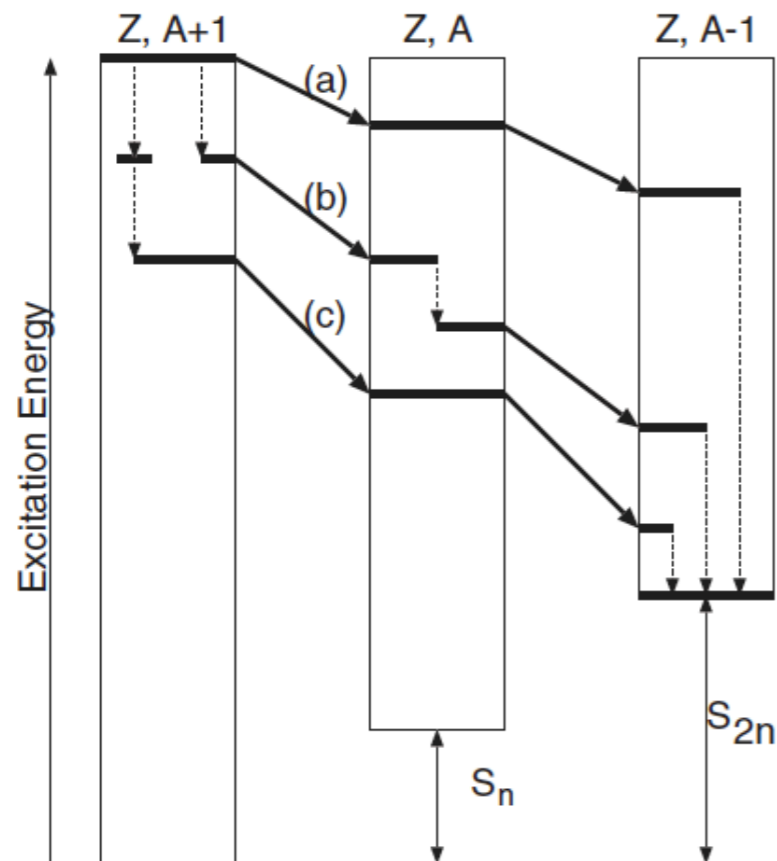


Fig. 6 Inelastic scattering neutron energy spectra from ^{56}Fe by 20-MeV incident neutron. The outgoing neutrons are virtually gated by a γ -ray transition from 847 keV 2^+ state to the 0^+ ground state, as well as a fixed number of γ -ray multiplicities. The spectra are shown alternately by solid and dotted lines.

Summary

- New in CoH3: prompt fission neutron spectrum with the Los Alamos model, including pre- fission neutron emissions.
- CGMF code: Monte Carlo Hauser-Feshbach approach to the prompt fission neutrons and gamma-rays, applied to:
 - Cf-252 spontaneous fission neutrons,
 - fission gamma-rays, and
 - other observables.
- Integration with MCNP6 is planned for near future.

Multilevel Breit-Wigner (MLBW) elastic angular distributions

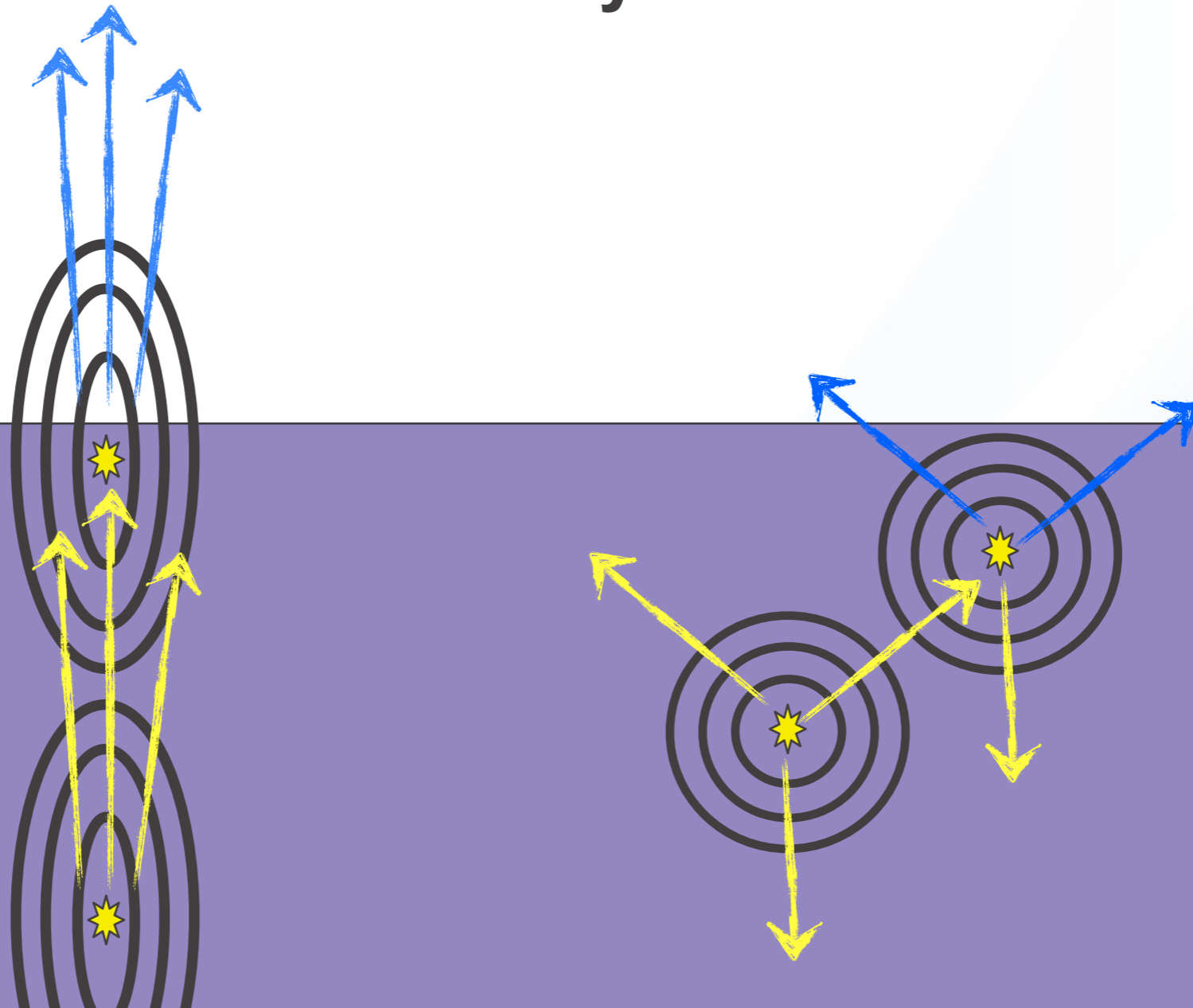
D.A. Brown, NNDC



Leakage from a critical assembly depends greatly on angular dists.

D. Brown
BNL

- A forward peaked distribution lets more particles escape from collision events on boundaries than an isotropic one
- Most evident in small critical systems



What angular distributions are available in the resonance region?

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Format	Number occurrences	Number with angular distributions enabled
scattering radius only	66	0
SLBW	8	0
MLBW	270	0
Reich Moore (LRF=3)	54	46
R Matrix Limited (LRF=7)	1	0
URR only	26	0

What angular distributions are available in the resonance region?

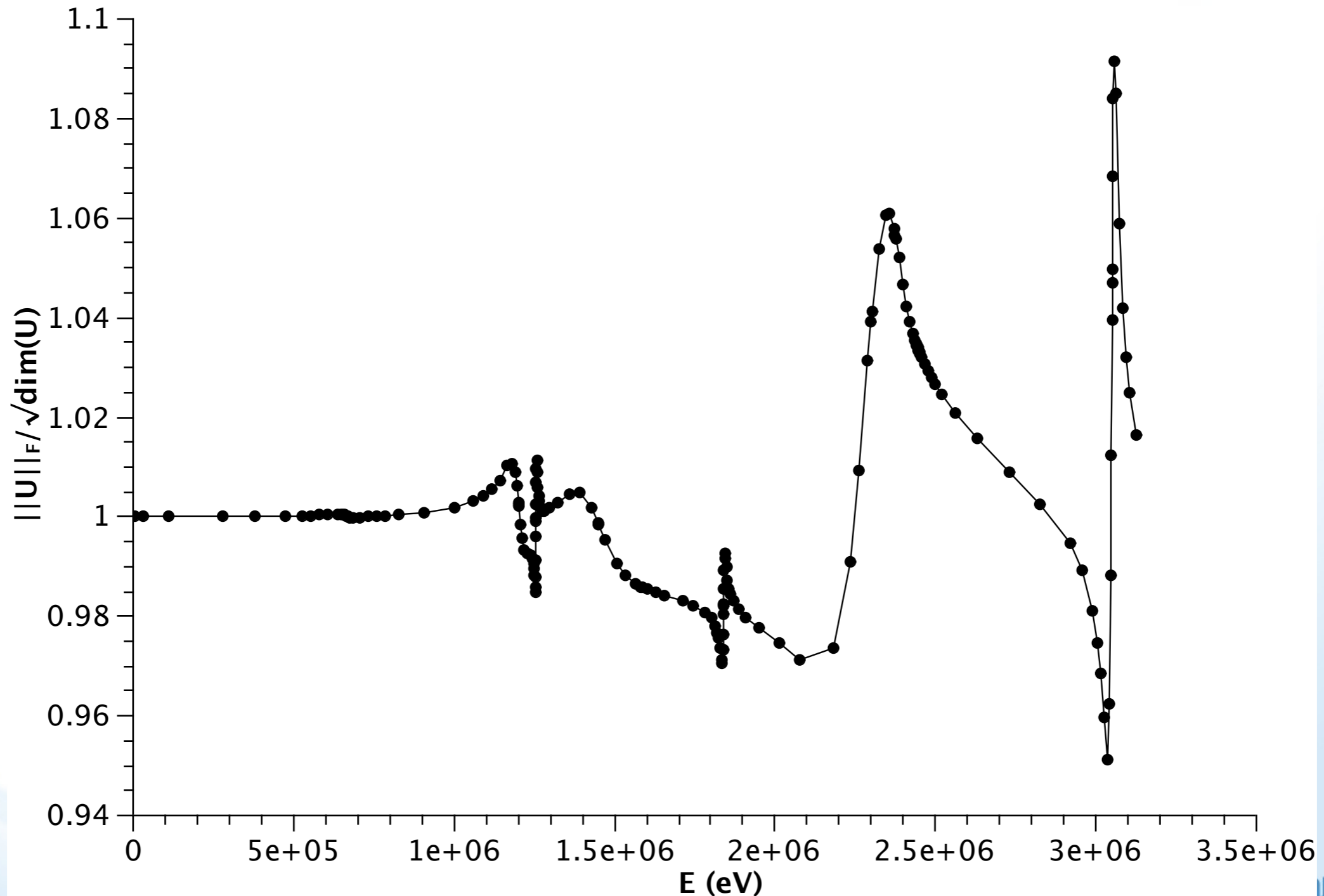
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BNL

Format	Number occurrences	Number with angular distributions enabled
scattering radius only	66	0
SLBW	8	0
MLBW	270	0
Reich Moore (LRF=3)	0	0
R Matrix Limited (LRF=7)	1	0
URR only	26	0

can we salvage these guys?

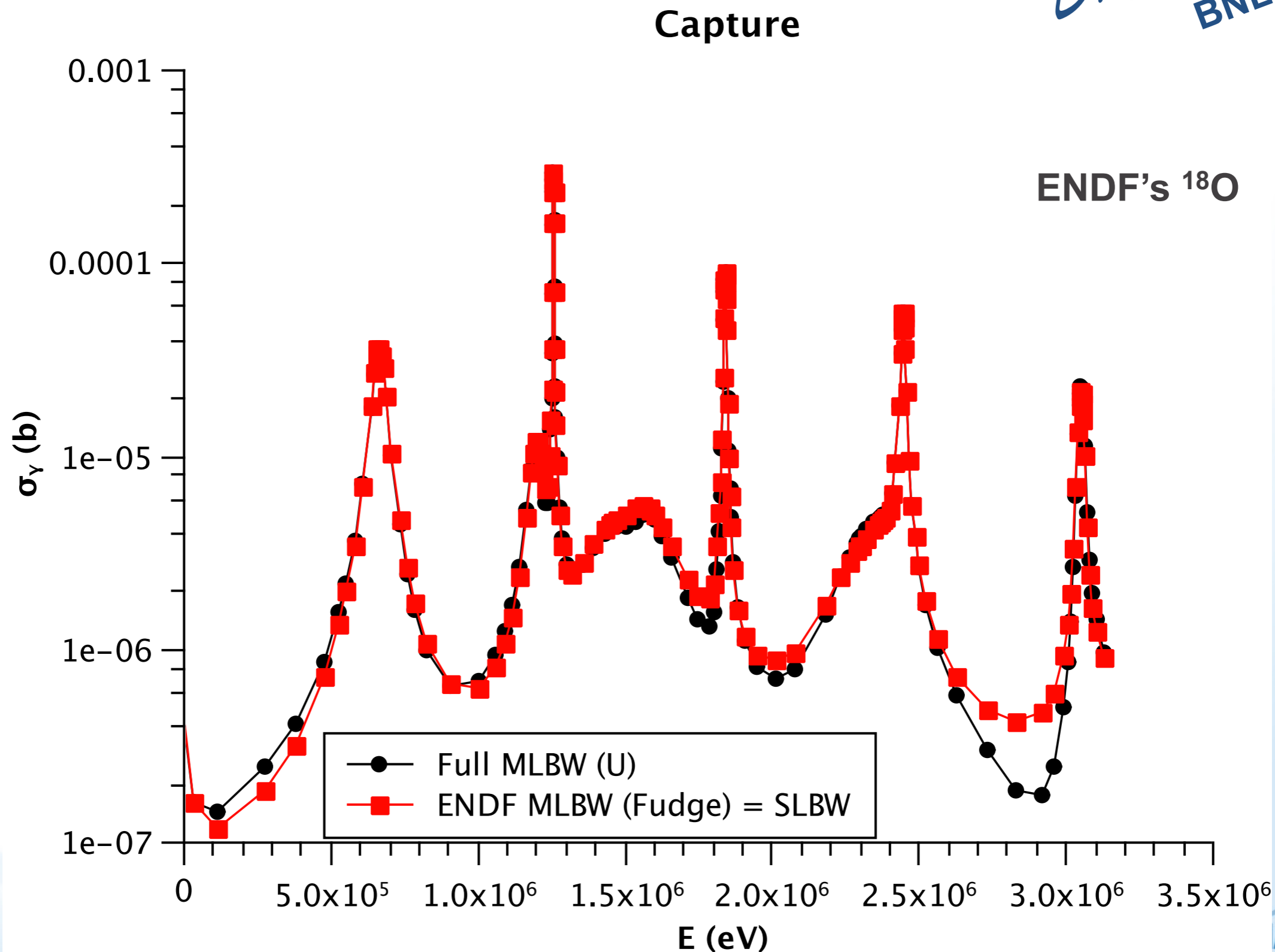
MLBW is not unitary - Is this a problem?

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ENDF's MLBW capture is clearly different

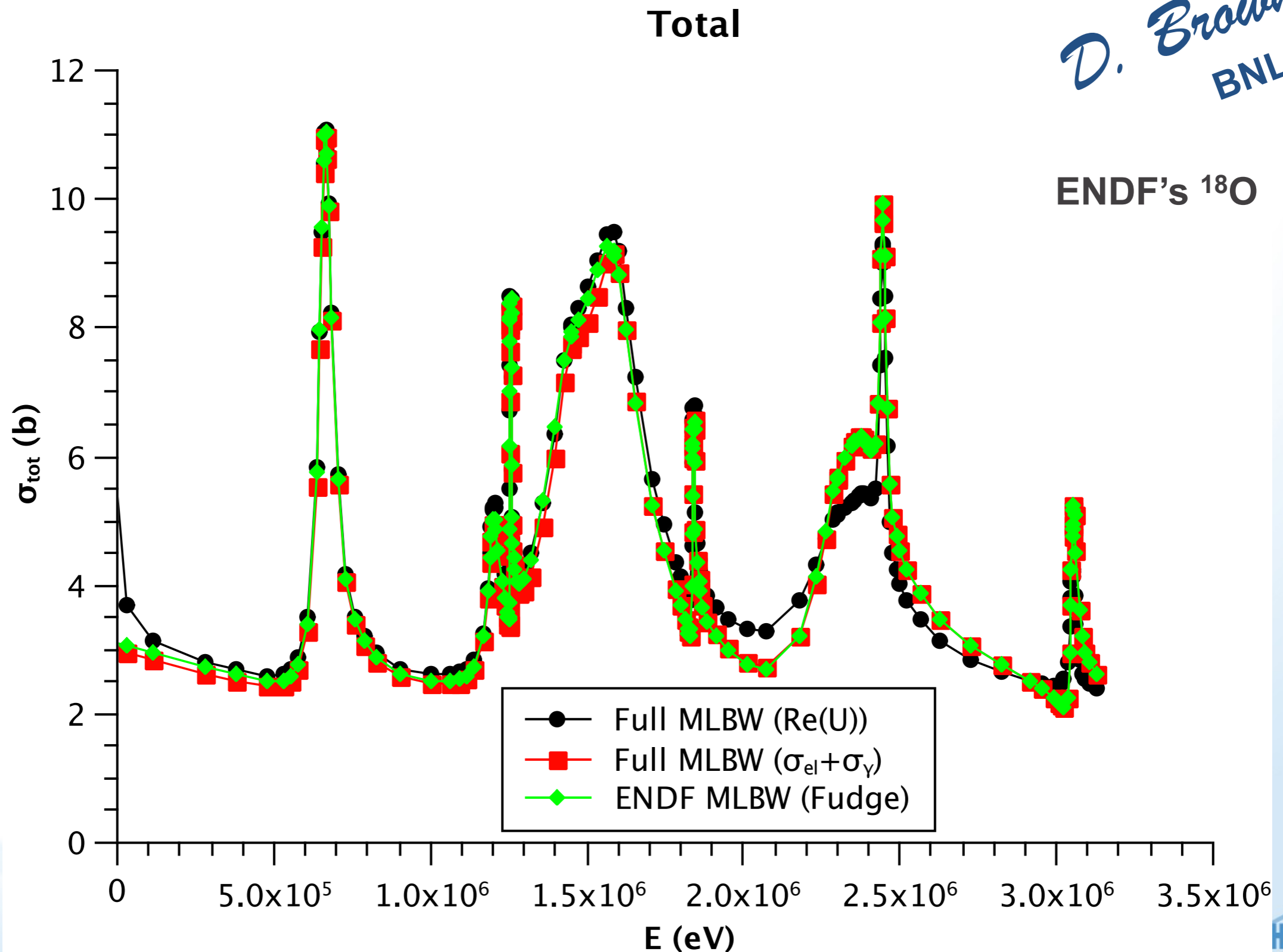
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This naturally impacts the total too

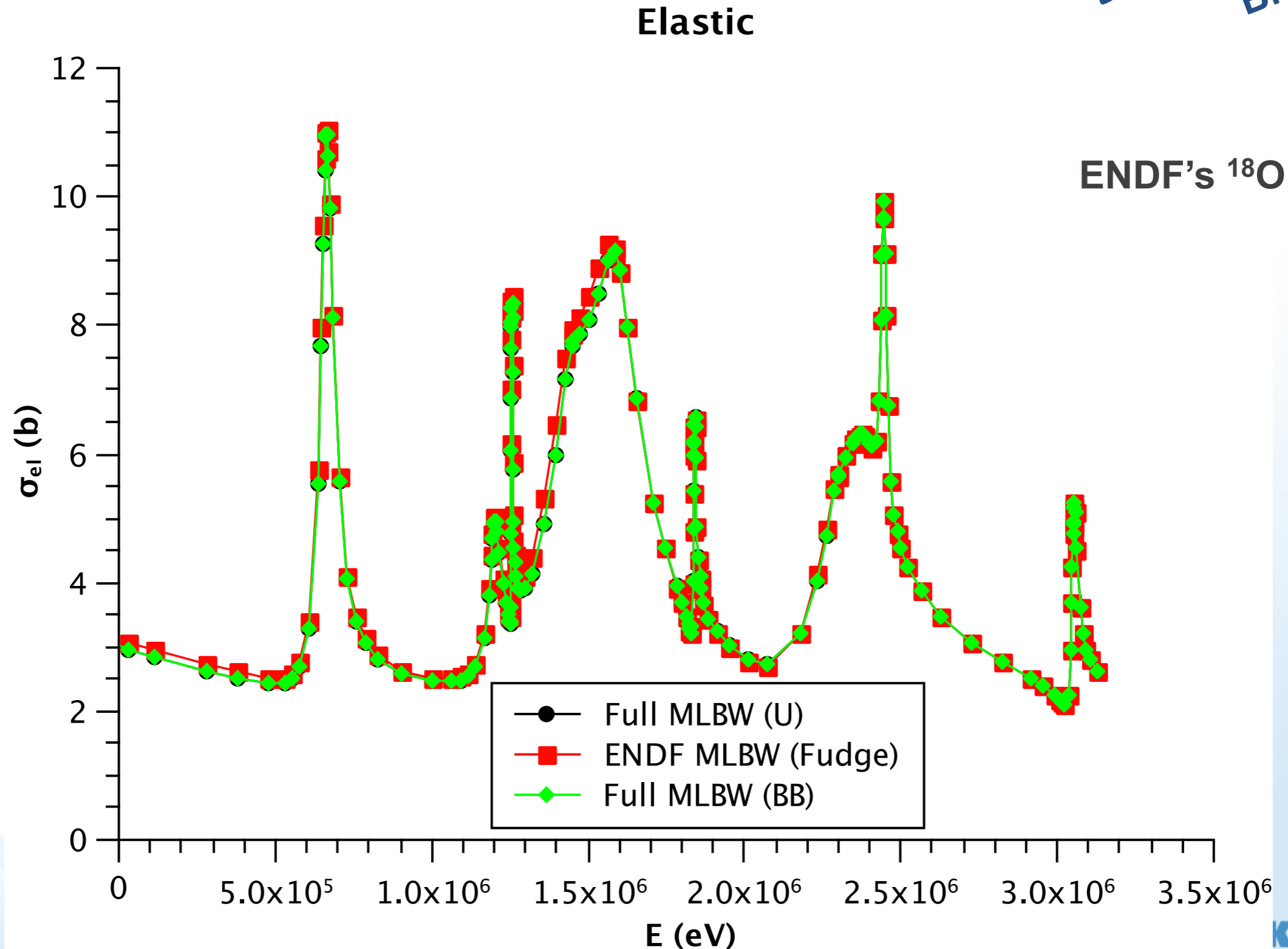
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ENDF's ^{18}O



ENDF MLBW elastic is the same as the R matrix MLBW elastic

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We can get MLBW angular distributions!!!

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According to Blatt-Biedenharn formalism, we only need a collision matrix in order to compute an angular distribution:

$$\frac{d\sigma_{\alpha,\alpha'}(E)}{d\Omega} = \frac{1}{k^2(2i+1)(2I+1)} \sum_{s,s'} \sum_{L=0}^{\infty} B_L(\alpha s, \alpha' s'; E) P_L(\mu)$$

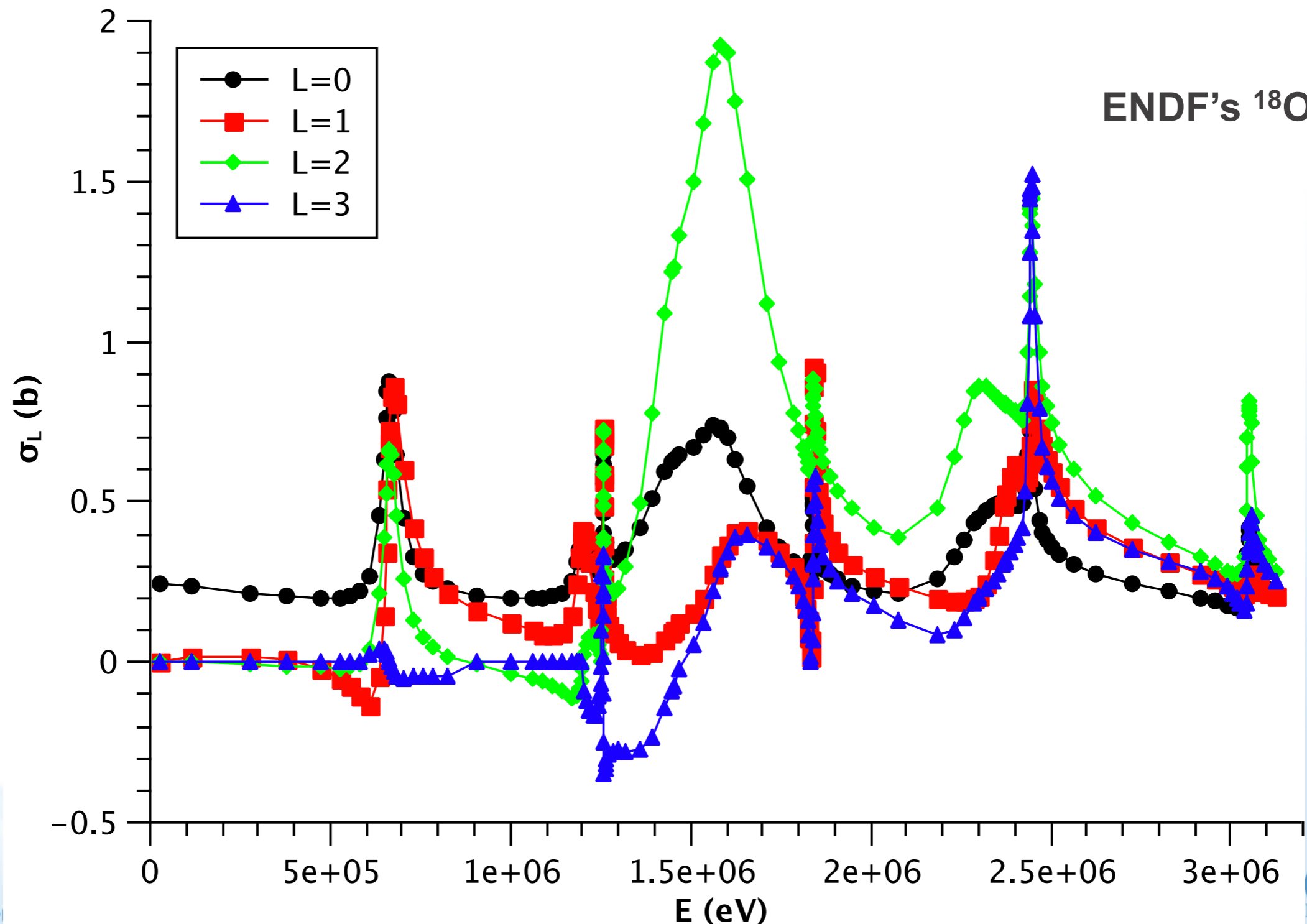
where

$$B_L(\alpha s, \alpha' s'; E) = \frac{(-)^{s-s'}}{4} \sum_{c_1=\{\alpha l_1 s_1 J_1\}} \sum_{c'_1=\{\alpha' l'_1 s'_1 J'_1\}} \sum_{c_2=\{\alpha l_2 s_2 J_2\}} \sum_{c'_2=\{\alpha' l'_2 s'_2 J'_2\}} \bar{Z}(\ell_1 J_1 \ell_2 J_2 s L) \bar{Z}(\ell'_1 J_1 \ell'_2 J_2 s' L) \\ \times \delta_{s s_1} \delta_{s' s'_1} \delta_{J_1 J'_1} \delta_{s s_2} \delta_{s' s'_2} \delta_{J_2 J'_2} (\delta_{c_1 c'_1} - U_{c_1 c'_1}(E))^* (\delta_{c_2 c'_2} - U_{c_2 c'_2}(E))$$

The angular distribution directly from ENDF MLBW parameters

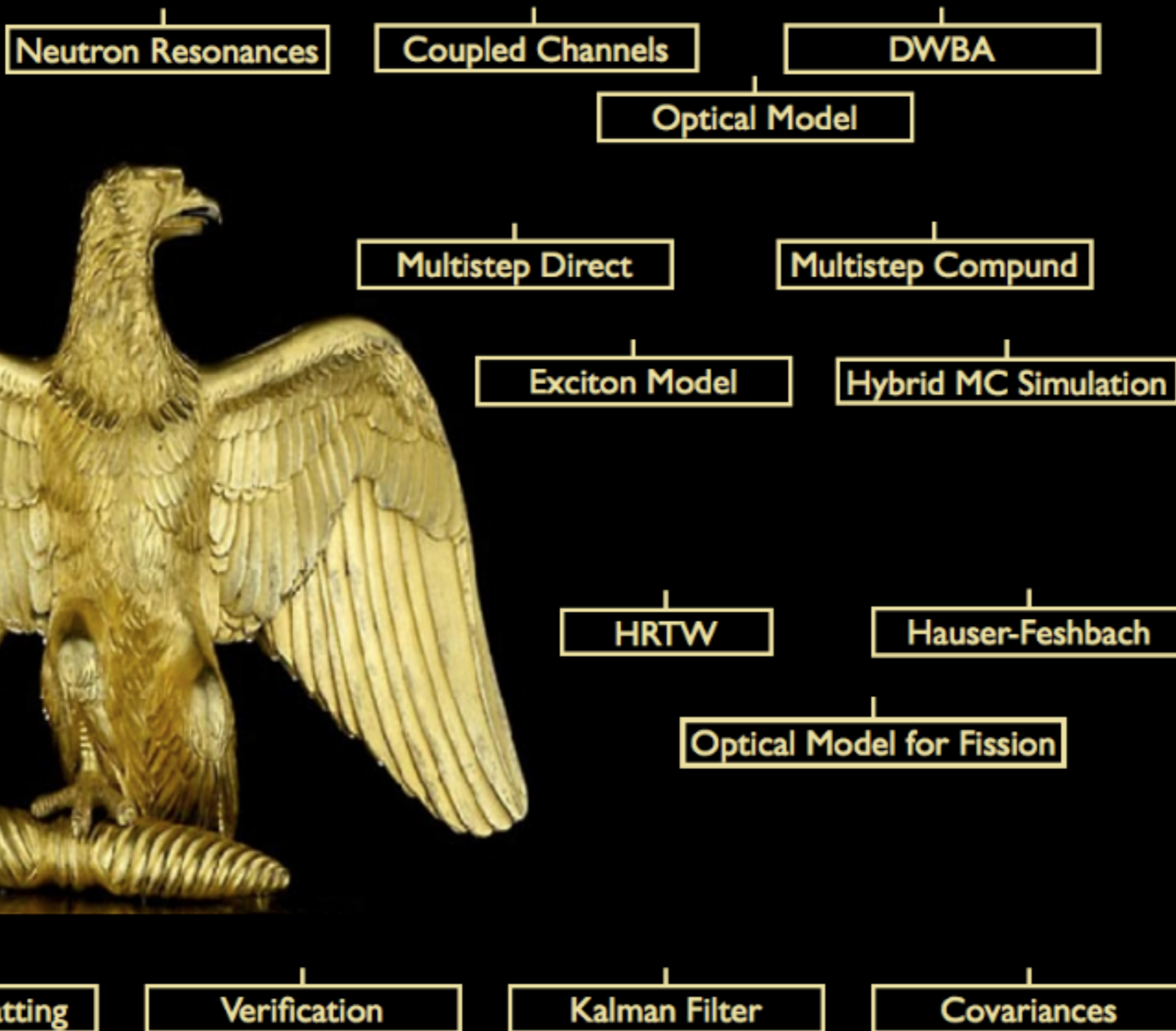
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$$d\sigma_{el}/d\Omega = (4\pi)^{-1} \sum_L \sigma_L P_L(\mu)$$



EMPIRE-3.2 (Malta)

Nuclear Reaction Model Code



EMPIRE-3.2 (Malta)



Capture of Malta by French army heading for Egypt in 1798

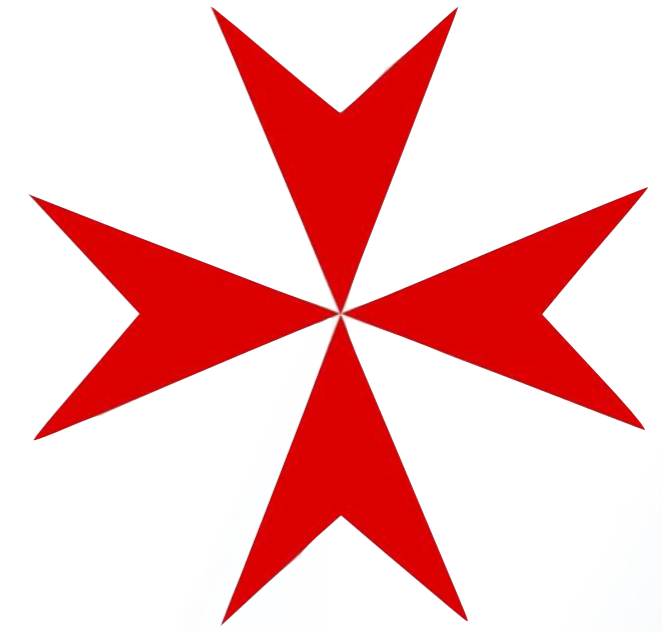
■ A bit more of physics

- T_{ij} rather than T_I used for the CN formation & decay
- Native angular distributions for CN elastic and inelastics
- Simulation of the Engelbrecht-Weidenmuller transformation.
- Kalbach parameterizations for breakup and transfer reactions of complex projectiles

■ A bit better numerics

- Fixing fluctuations due to the gap between the last level and the continuum
- Improving x-sec & energy balance

EMPIRE-3.2 (Malta)



- **A bit newer FORTRAN**
 - HRTW-comp.f90, kalend.f90, kalman.f90, genkal.f90, newinp.f90
 - Improved gfortran compatibility
- **A bit more functionality**
 - Improved support for assimilation procedure
 - Improved qsubEmpire.py for running on a cluster
 - GUI that applies Kalman results back to Empire input file.
- **A bit better formatting**
 - Making line numbers in ENDF files optional

FREYA Update



Ramona Vogt (LLNL) & Jørgen Randrup (LBNL)
w/input from C. Hagmann & J. Verbeke (LLNL), M. James (LANL)

LLNL-PRES-646392

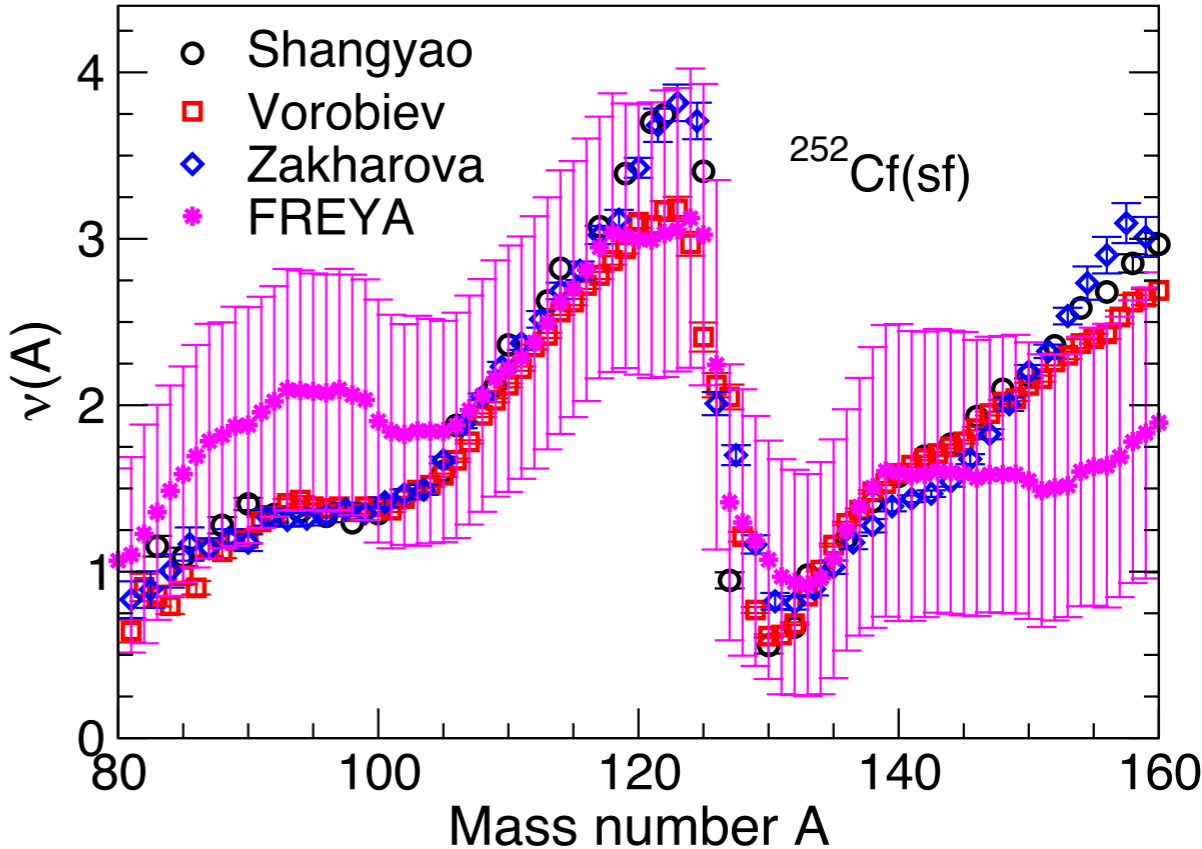
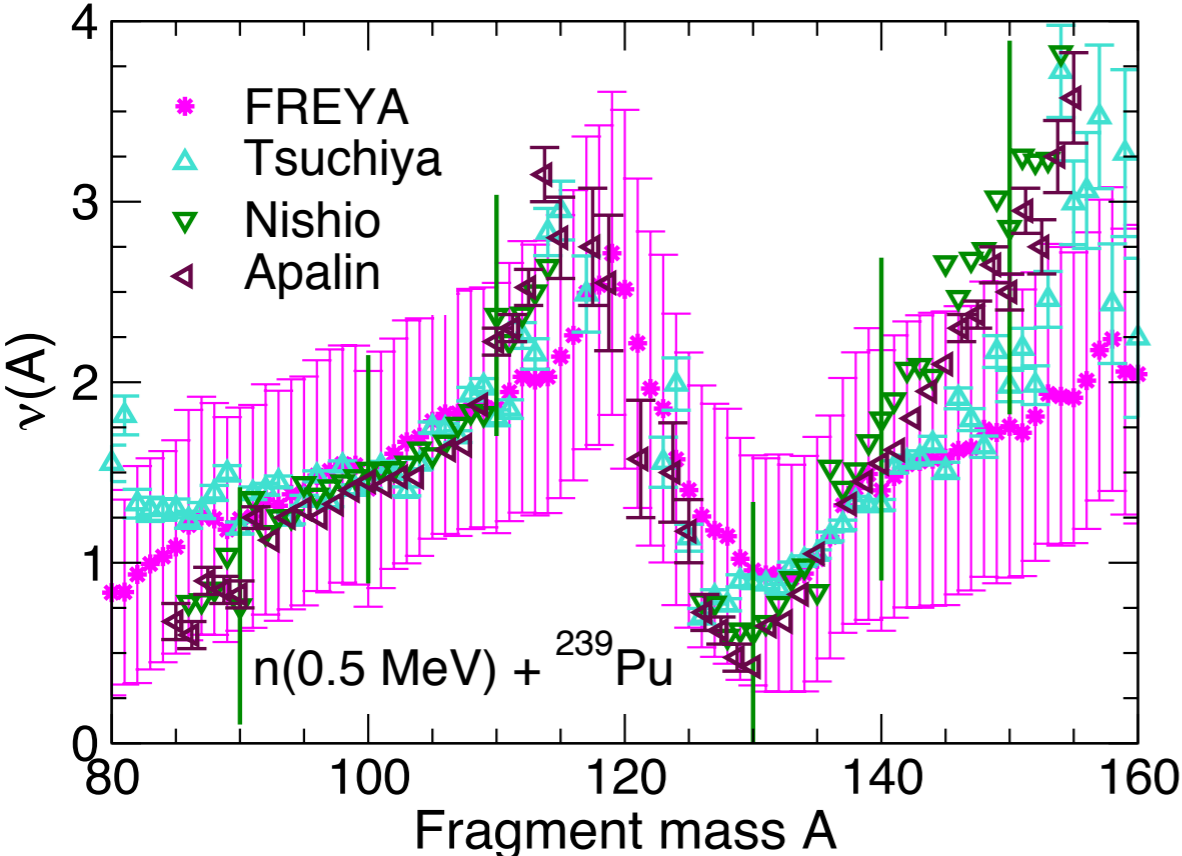
This work performed under the auspices of the U.S. Department of Energy by
Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344



Neutron observables: sawtooth $\nu(A)$

Mean neutron multiplicity as a function of fragment mass; agrees with sawtooth shape of data

$\nu(A)$ calculation shows dispersion in Z for a given mass (**FREYA** 'error bars')



Summary

- Event-by-event treatment shows significant correlations between neutrons that are dependent on the fissioning nucleus
- **FREYA** agrees rather well with most neutron observables for several spontaneously fissioning isotopes and for neutron-induced fission
- Comparison with n-n correlation data very promising
- Photon data do not present a very clear picture – clearly more experiments with modern detectors needed to verify older data
- Refined modeling of photon emission in **FREYA** is planned
- Plans to incorporate **FREYA** into **MCNP6**, **FREYA1.0** with neutrons released as open source in July 2013

Optical Model Potential in Rare-earth Region

G. P. A. Nobre*, A. Palumbo, M. Herman,
D. Brown and S. Hoblit
NNDC, Brookhaven National Laboratory

F. S. Dietrich
Lawrence Livermore National Laboratory

*Nuclear Data Week at BNL, USNDP and CSEWG meetings
November 18-22, 2013*

*gnobre@bnl.gov

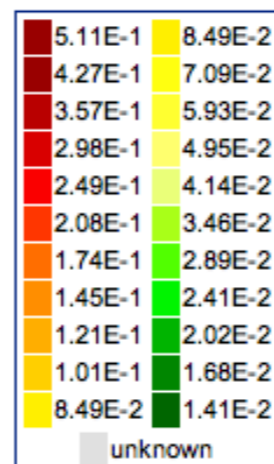


Motivation

- Why seek an optical potential for this region?
 - Lack of existing regional OP's for deformed nuclei
 - Recent work* shows scattering from highly deformed nuclei is near adiabatic limit → deforming a spherical global potential may be suitable with only minor modifications

We deform the Koning-Delaroche spherical global potential and couple g.s. rotational band

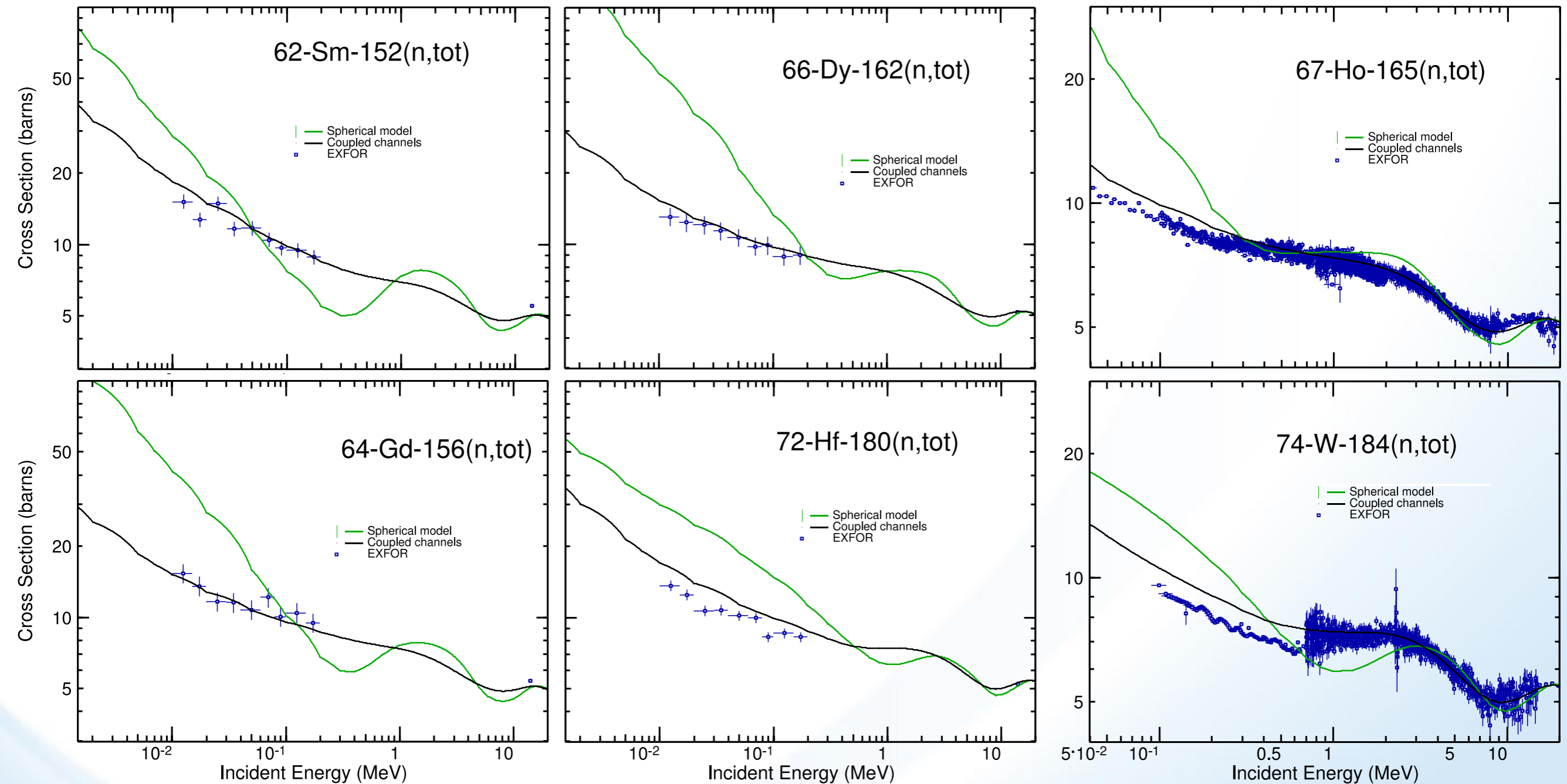
β_2



rotors

- * Phys. Rev. C 85 (2012) 044611
- § J. Nucl. Sci. Tech. 44 (2007) 838

Comparison between spherical and CC: Total cross sections

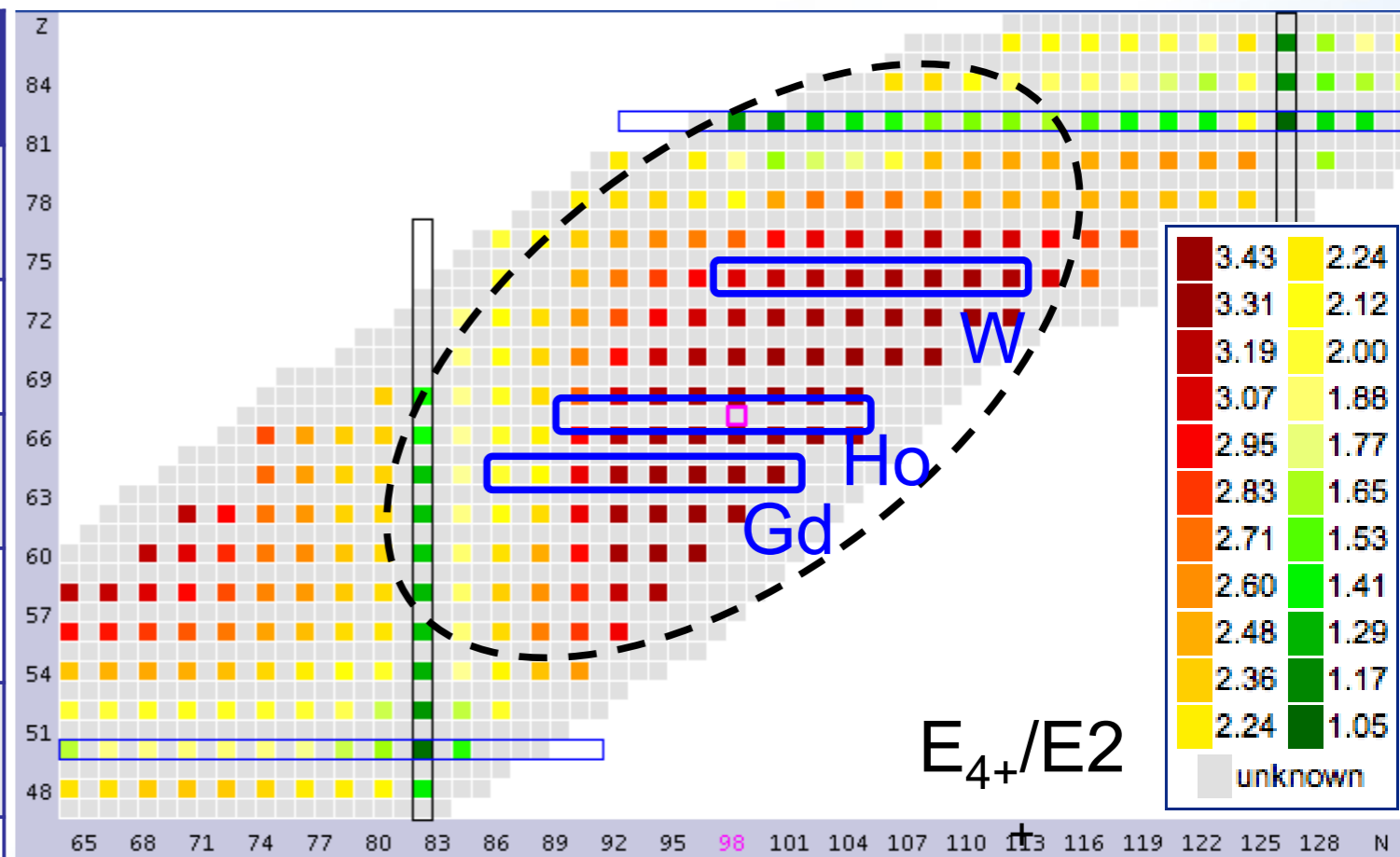


Spherical approach fails at low energy and its shape is often in disagreement with experimental data, while deforming KD potential provides a good description of the observed total cross sections

Angular distributions: Gd, Ho, W

- More detailed analysis on the experimental data sets
- Some elastic ang. dist. data actually contained inelastics
- Ensured convergence regarding number of rotational channels

nucleus	β_2^*	β_4^{\S}	Δ_R	$\beta_2^{(sys)\P}$
^{158}Gd	0.348	0.056	0.990	0.362
^{160}Gd	0.353	0.056	0.990	0.372
^{165}Ho	0.293	-0.020	0.993	0.385
^{182}W	0.251	-0.080	0.995	0.268
^{184}W	0.236	-0.080	0.996	0.255
^{186}W	0.226	-0.080	0.996	0.226



* At. Data. Nucl. & Data Tables, 78, (2001) 1

§ Ann. Nucl. Energy, 31 (2004) 1813;

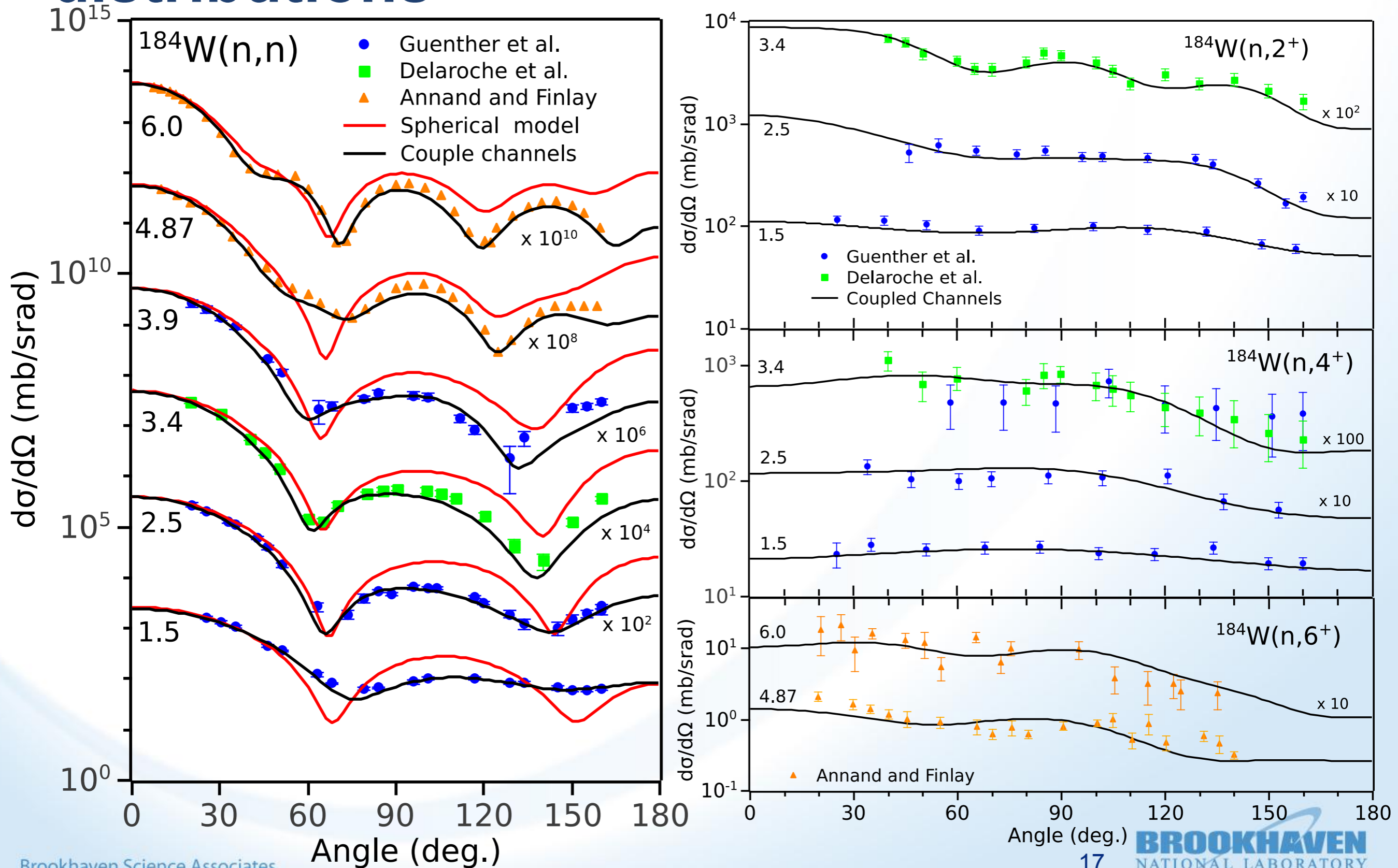
Phys. Lett. 26B (1968) 127;

Ann. Nucl. Energy, 28 (2001) 1745

¶ Phys. Rev. C 70 (2004) 014604;

Phys. Rev. C 76 (2007) 024605

^{184}W – Elastic and inelastic angular distributions



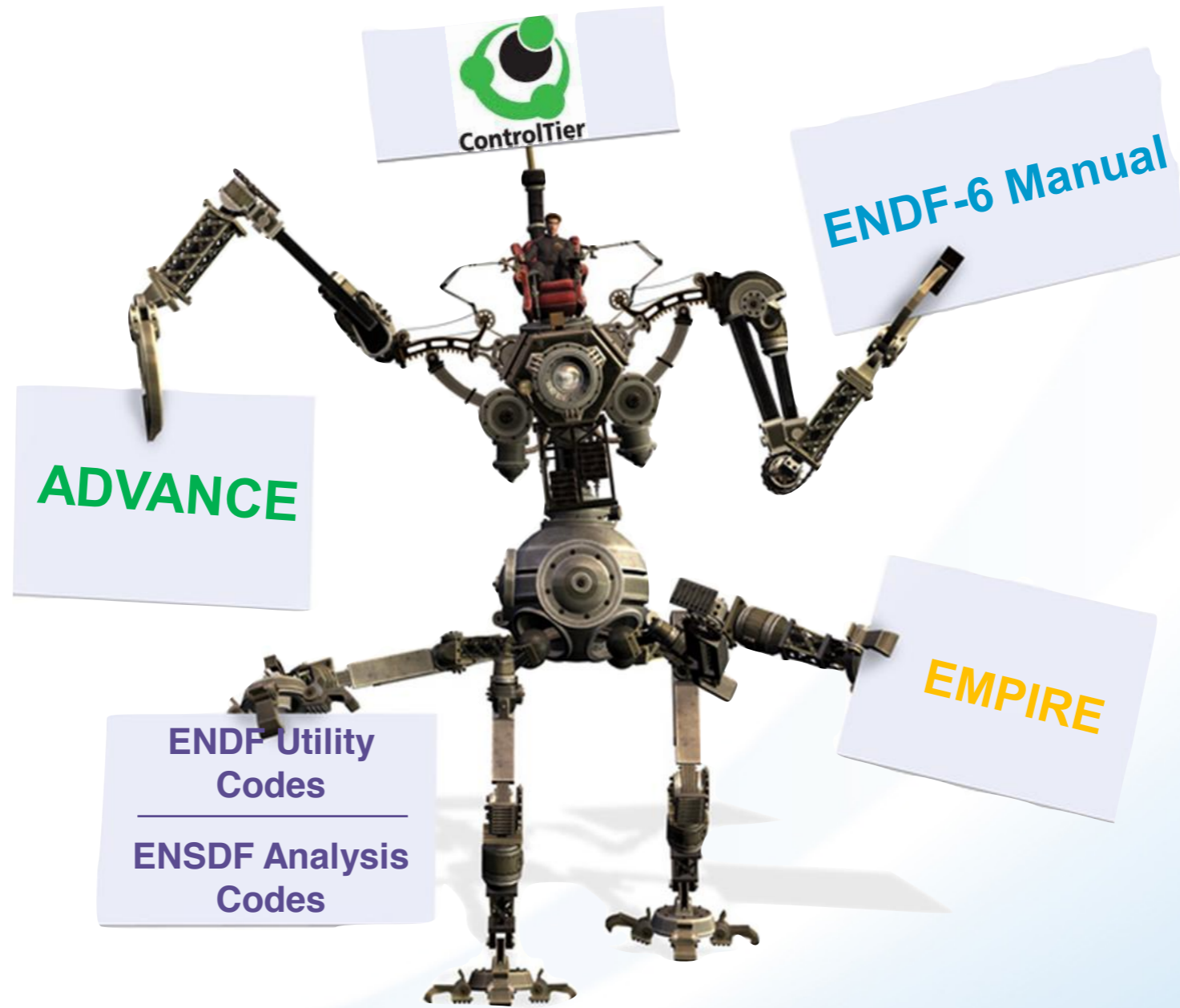
Conclusion

- We deformed spherical KD potential in CC calculations to describe statically-deformed nuclei
 - No free parameters (experimental deformations)
 - Radius correction gives (small but) noticeable effect
- This approach provides remarkable results for
 - Total, elastic, inelastic cross sections
 - Elastic and inelastic angular distributions
- Improvement of capture cross sections, in particular their shape

This simple method is a good, consistent and general step towards an OP capable of fully describing the rare-earth region, filling the current lack in this important region.

Continuous verification & validation (ADVANCE system)

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BNL



ADVANCE system for ENDF quality assurance

- Ensuring that all ENDF files get checked
- Every commit, all changed files subjected to a battery of tests including
 - NNDC checking codes (PSYCHE, CHECKR, FIZCON, STANEF, STAN and INTER)
 - NJOY
 - Fudge
 - PREPRO
- Results collected in an easy to use HTML report:
<http://www.nndc.bnl.gov/endl/b7.dev/qa/index.html>

ADVANCE: The ENDF Continuous Integration System



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BNL



ENDF/B Development

The development version of the Evaluated Nuclear Data File (ENDF/B)

Latest Updates

sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 15:41:29.746913

Neutrons

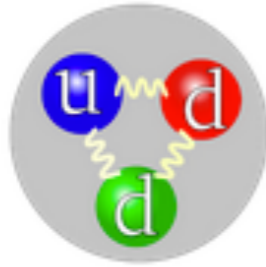
Decay

Charged particles

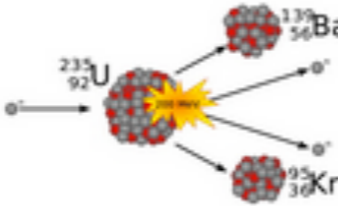
Photonuclear

Atomic

Neutrons sublibraries




Neutrons Sublibrary



Neutron-Induced Fission Yields Sublibrary



Standards Sublibrary



Thermal Neutron Scattering Sublibrary

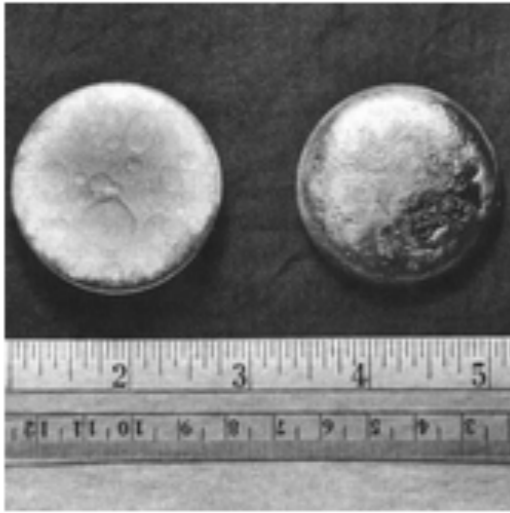


Image of plutonium from <http://images-of-elements.com/>

239 Pu

Neutrons Sublibrary

- ▶ General Information:
 - ▶ ENDF MAT designator: 9437
 - ▶ Evaluated by Young, Chadwick, MacFarlane, Derrien (LANL), SEP06
 - ▶ Natural abundance: 0.0 +/- 0.0 %
 - ▶ Check out Wikipedia's entry for [plutonium](#)
- ▶ Revision Number: 611M
- ▶ Last Modified Revision: 532:611M
- ▶ Build Status:
 - ▶ Build status: **ERROR** ([Submit tracker item](#))
 - ▶ Build time: 2013-04-30 06:17:38.108808
- ▶ GForge Links:
 - ▶ Browse [SVN](#)
 - ▶ View current [revision](#)
 - ▶ Download current [revision](#)

Latest Updates

evaluation_summary: n-094_Pu_239.endf
Code evaluation_summary completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:17:39.392055

njoy2012: n-094_Pu_239.endf
Code njoy2012 completed run on n-094_Pu_239.endf. The result was a ERROR
2013-04-30 06:17:36.872836

inter: n-094_Pu_239.endf
Code inter completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:10:24.995505

*D. Brown
BNL*

← GForge links

← RSS activity feed

Code Results

ENDF Overview

ACE Overview

Integral Quantities

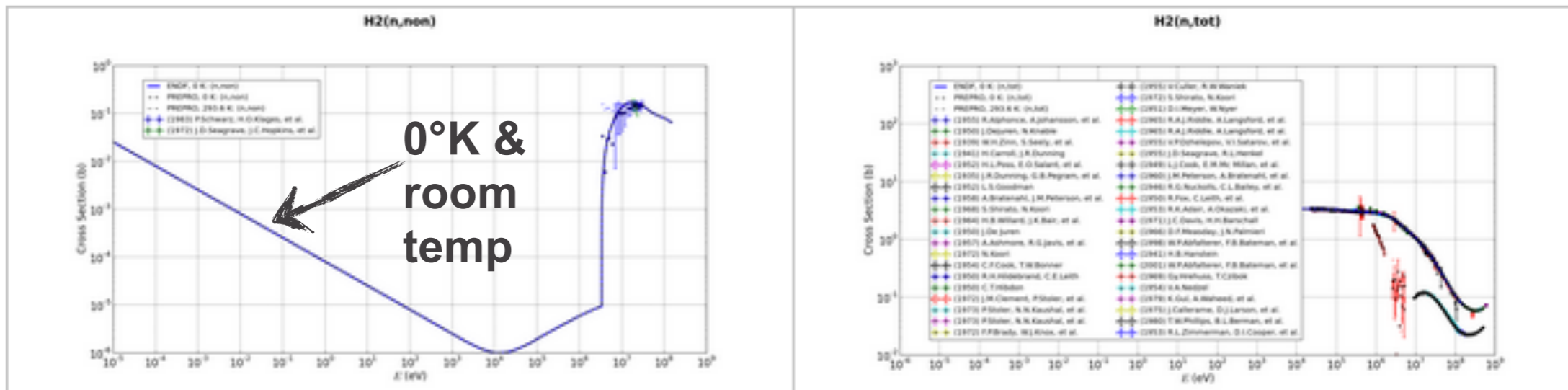
Cross Section Plots

Summary of all tests on this evaluation.

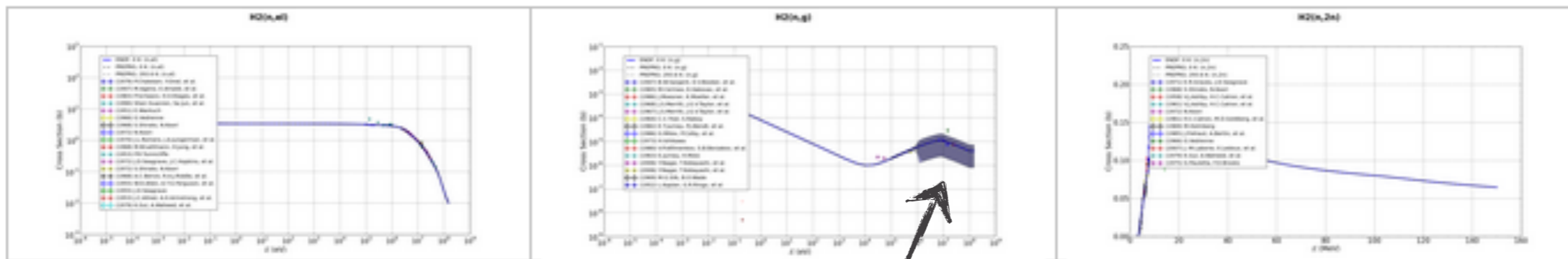
Use checking code button to show/hide errors.

Status	Code	# Tests	# Failures	# Errors	Run time (sec)	Files
✓	STAN	0	0	0	31.533	STN File
✓	STANEF	0	0	0	29.316	

Comparison between cross section data in this ENDF file and data retrieved from EXFOR Aggregate channels:



Regular channels:



ADVANCE Version 0.7 (svn rev: 669)

Error band!