ENDF Project Report to WPEC 2016

M. Herman for CSEWG

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery
U.S. DEPARTMENT OF ENERGY | Office of Science

I will NOT discuss:

- CIELO (SG40)
  - H, ^{16}O, ^{56}Fe, ^{235,238}U, ^{239}Pu
- Fission product yields (SG37)
- New data structure (SG38)
- Thermal scattering law data (SG42)

I will focus on:

- ENDF/B-VIII.0beta1 release
- Non-CIELO evaluations
- Advances in reaction modeling

Plan for reaching ENDF/B-VIII release in 2018

END/B-VII.1, 2011
- Widely used in DOE & around world

CIELO help

Pre-ENDF/B-VIII, 2016
- Base upgrades established (covariances not yet added)
- + numerous variants
- Standards,1H, 16O, 56Fe, 235,8U, 239Pu,
- C,Ne,Ca,Ni,Cu,As,Re,W, …
- Thermal kernels (SG42)

Higher risk:
- Inelastic scattering
- Capture in fast region
- More PFNS upgrades
- …

END/B-VIII.0 2017/18
- Further major upgrades

Draft NDS document 1-year from now, for Jan-2018 publication

END/B-VIII.0 2017/18
- Modest upgrades

Low risk:
- Fission product yields, TKE
- PFGS (fission gammas)
- PFNU (nu)
- …

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ENDF/B-VIII.0beta1 released!

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- **ENDF/B-VIII.0beta1 (25 Apr 2016), rev. 825; Released for testing prior to WPEC meetings, May 2016.**
  - CIELO file updates (^{56}Fe, ^{235}U, ^{239}Pu)
  - Isotopic C: ^{12}C, ^{13}C (LANL)
  - Minor Fe isotopes: ^{54}Fe, ^{57}Fe (BNL)
  - ^{7}Be extended to 20 MeV (LANL)
  - Bug fixes
  - Yb, Os, holes in Dy, Hf (JENDL-4.0)
  - ^{18}O (RUSFOND)
  - ^{236m1}Np (LANL)
  - ^{54}Fe, ^{57}Fe, ^{58}Fe (BNL)
  - n (LANL), yes(!) neutrons as a target.
  - ^{63,65}Cu (ORNL)
  - ^{182,183,184,186}W (ORNL)
  - ^{40}Ar (LANL)
  - Primary g's: ^{6,7}Li, ^{11}B, ^{23}Na, ^{27}Al, ^{28}Si, ^{35,37}Cl
  - Many many bug fixes
- **ENDF/B-VIII.0beta0 (8 Apr 2016), rev. 810; Released for Mini-CSEWG meeting, 11-12 Apr. 2016.**
  - CIELO files (^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U, ^{239}Pu)

Summary of changes to other sub libraries since ENDF/B-VII.1 released

ENDF B-VIII.β1

- **Thermal scattering law evaluations**
  - SiC x2: SiinSiC, CinSiC (NCSU)
  - alpha & beta phase of SiO_2 (NCSU)
  - Lucite (NCSU)
  - H_2O (CAB/CNL)
  - D_2O (CAB/CNL)
- **Electro/photo-atomic, atomic-relaxation**
  - Red Cullen's EPICS2014 library
- **Decay data**
  - Add beta branchings to 24 isotopes (BNL): ^{82,83}Ge, ^{82,86}As, ^{88,89,90,91}Br, ^{90}Kr, ^{93,95,96}Rb, ^{95}Sr, ^{95,98,98m1,99}Y, ^{134}Sb, ^{138}I, ^{140,141}Cs, ^{143}Ba, ^{143,144,145}La
- **Minor bugfixes:**
  - gammas, deuterons
- **Unchanged:**
  - SFY, NFY, protons, tritons, helium3s

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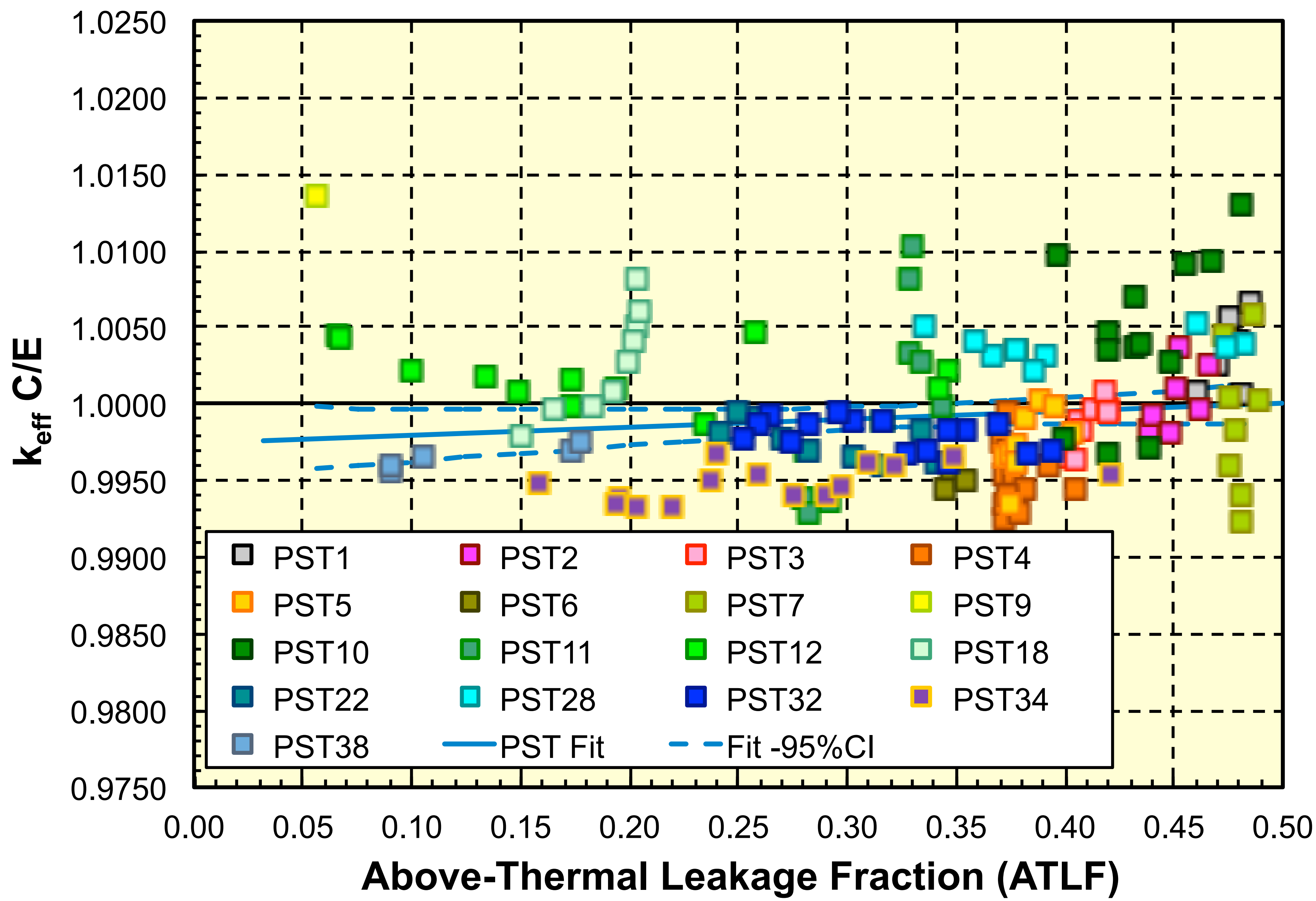
ENDF/B-VIII.beta1 validation

Pu-SOL-THERM 158 critical configurations

Skip Kahler



ENDF/B-VIII.0β1

Pu-SOL-THERM test suite … 158 critical configurations.

Trend with ATLF is statistically insignificant.

Average k_{eff} C/E with endf/b-vii.1 was 1.0045(4). Sub-Group 34 work reduced the k_{eff} C/E bias by about 2/3rd.

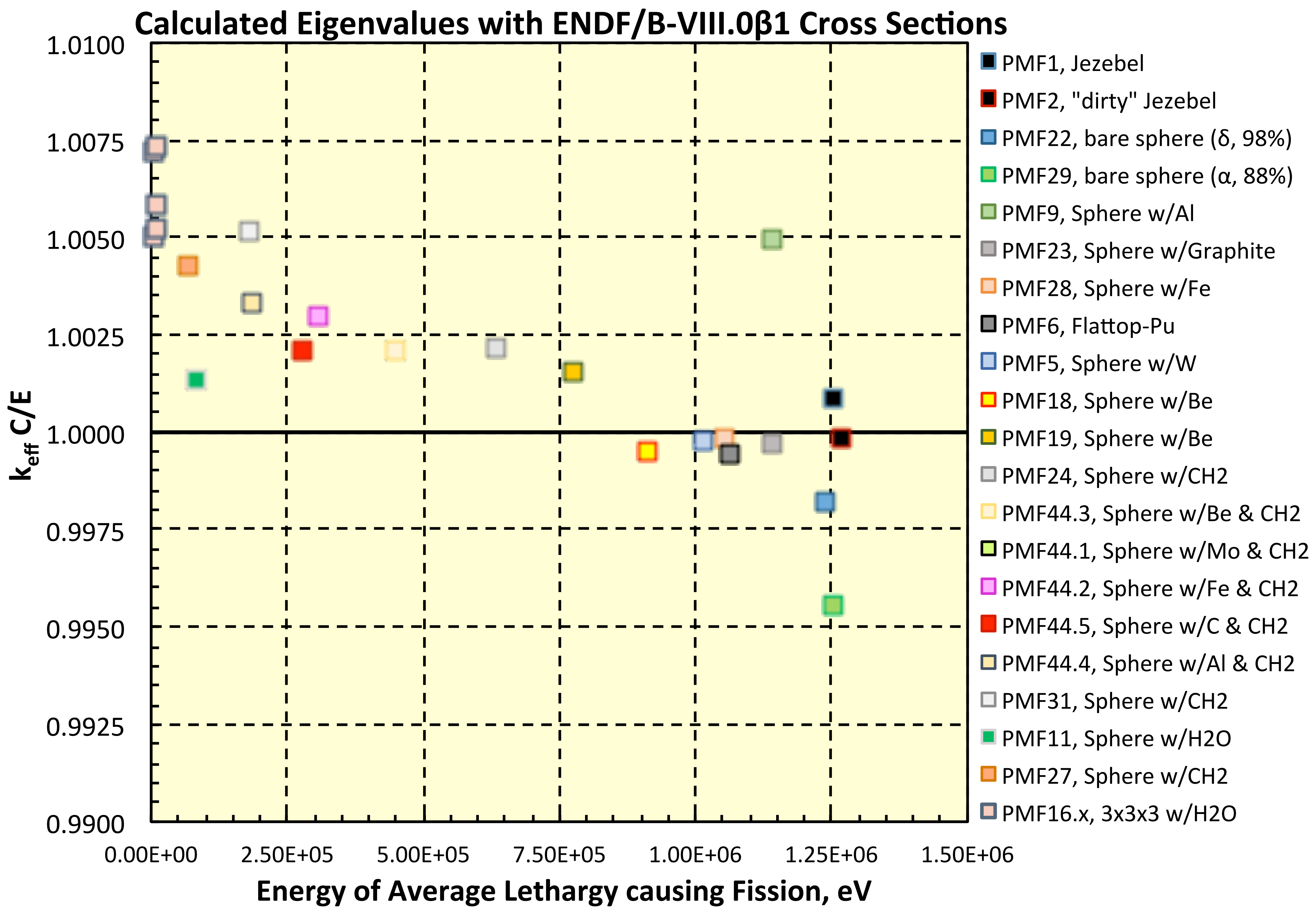
These new results represent a further improvement on the average k_{calc}.

Average k_{eff} C/E is 0.9992(4).

ENDF/B-VIII.beta1 validation

Partial PMF benchmark suite

Skip Kahler



Partial PMF benchmark suite results …

Increasing trend in k_{eff} C/E seen in endf/b-vii.1 remains, but some individual improvements …

k_{eff} C/E for PMF28, a steel reflected assembly, improves from 0.9990 (e71) to 0.9999 (e80β1); PMF6 (Flattop-Pu) improves from 1.0011 (e71) to 0.9995 (e80β1).

Summary of data testing of new pre-mini-CSEWG (Apr. 2016) files

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- Fast region
  - Unreflected: Jezebel, Godiva - equally good
  - Pu & HEU Flattops, and iron reflectors - equally good/slightly improved
  - Bigten - equally good
- Thermal region
  - Pu solutions - much better
  - U5 solutions - reasonably good (similar to VII.1)
  - LEU - equally good

Phase space of evaluation trial files, for testing, is very large. Much ENDF testing work done by Kahler (LANL) and Trkov, Capote (IAEA), and SG39 (Ian Hill):

- **Single Substitutions of new files into VII.1**
- **Substitutions of ensembles into VII.1 (U5,8,Pu9,O16, …)**

Conclusions

Much progress, with improved physics

We have a base set of files that perform adequately in integral simulations

- future improvements in integral performance still a goal

Much work will be also needed to add credible covariances

This creates optimism that we can release ENDF/B-VIII in the 2017/2018 time frame

- NDS big paper for CIELO & VIII planned for Jan 2018.

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QA of ENDF/B is essential part of our process

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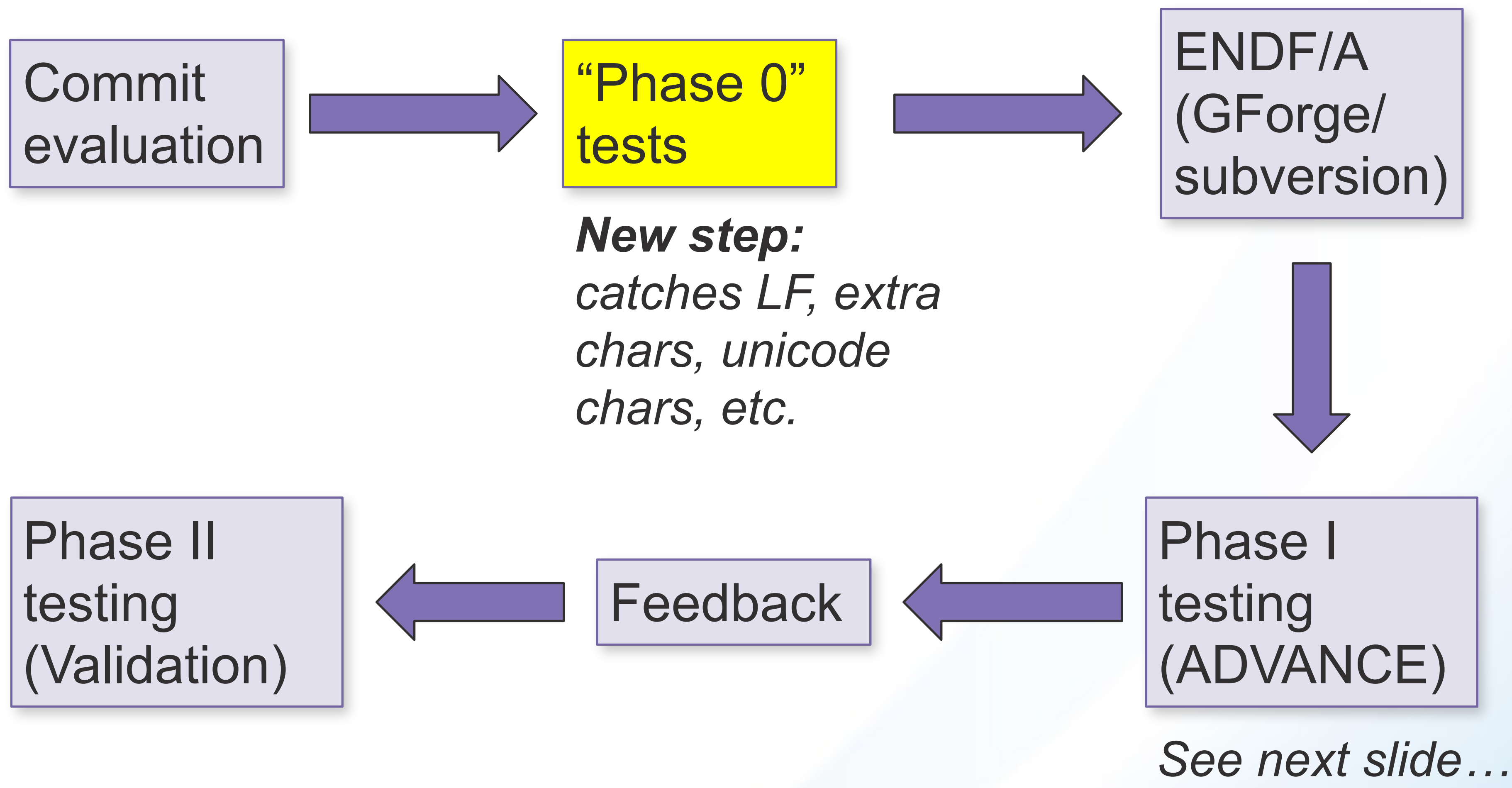

Phase 0 testing: evaluations are now rejected automatically if…

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- Commit contains illegal characters (non-printing ASCII like TAB characters and BACKSPACE)
- Non-UNIX LF feeds used
- svn keywords in first line missing

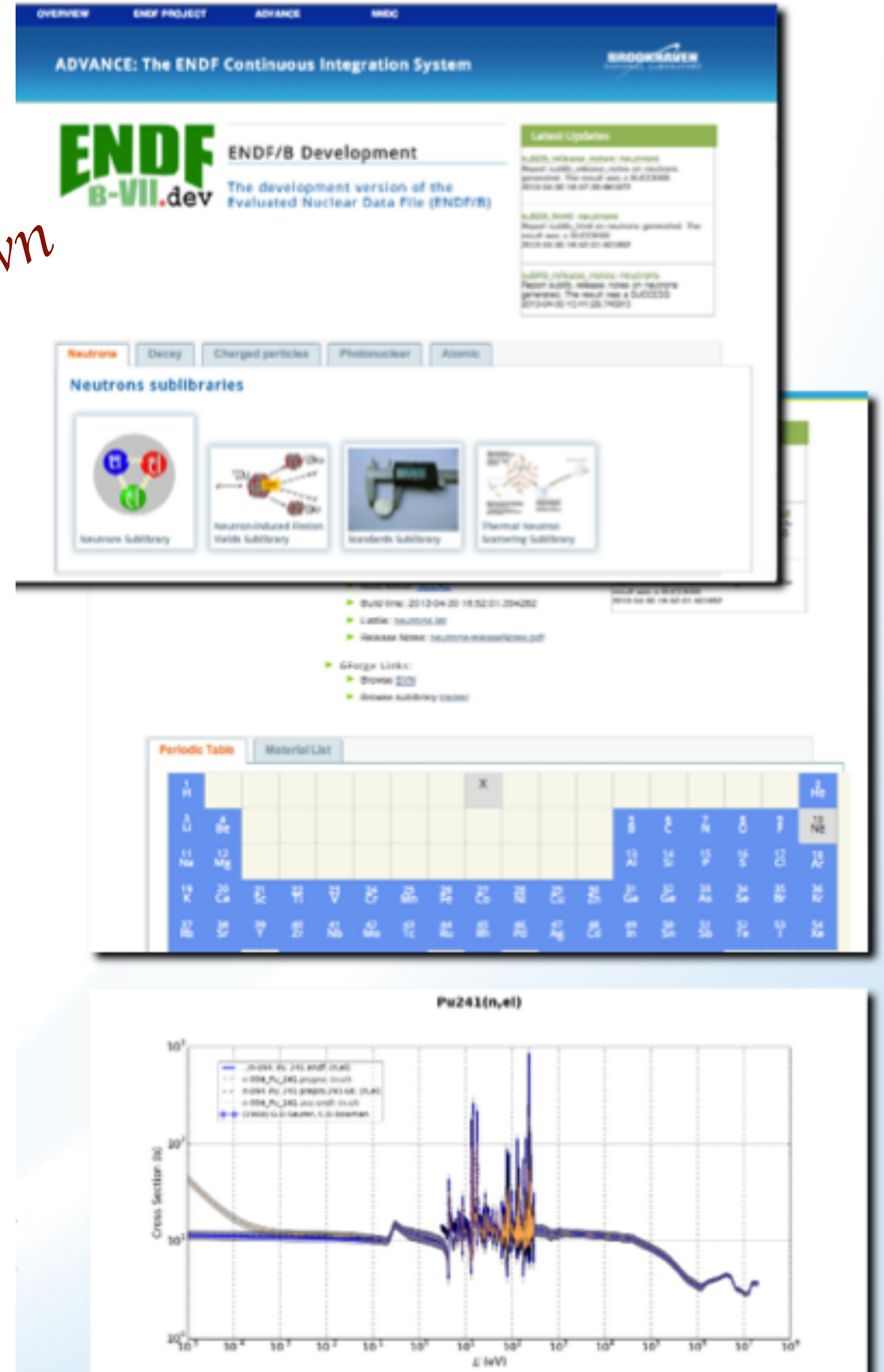
Other administrative changes

- We have stripped line numbers from every file in the library
  - commits are *much* faster
  - GForge diffing to works properly
- svn keywords forced in 1^{st} line in all files
  - helps to identify the file
  - helps to avoid overwriting corrections

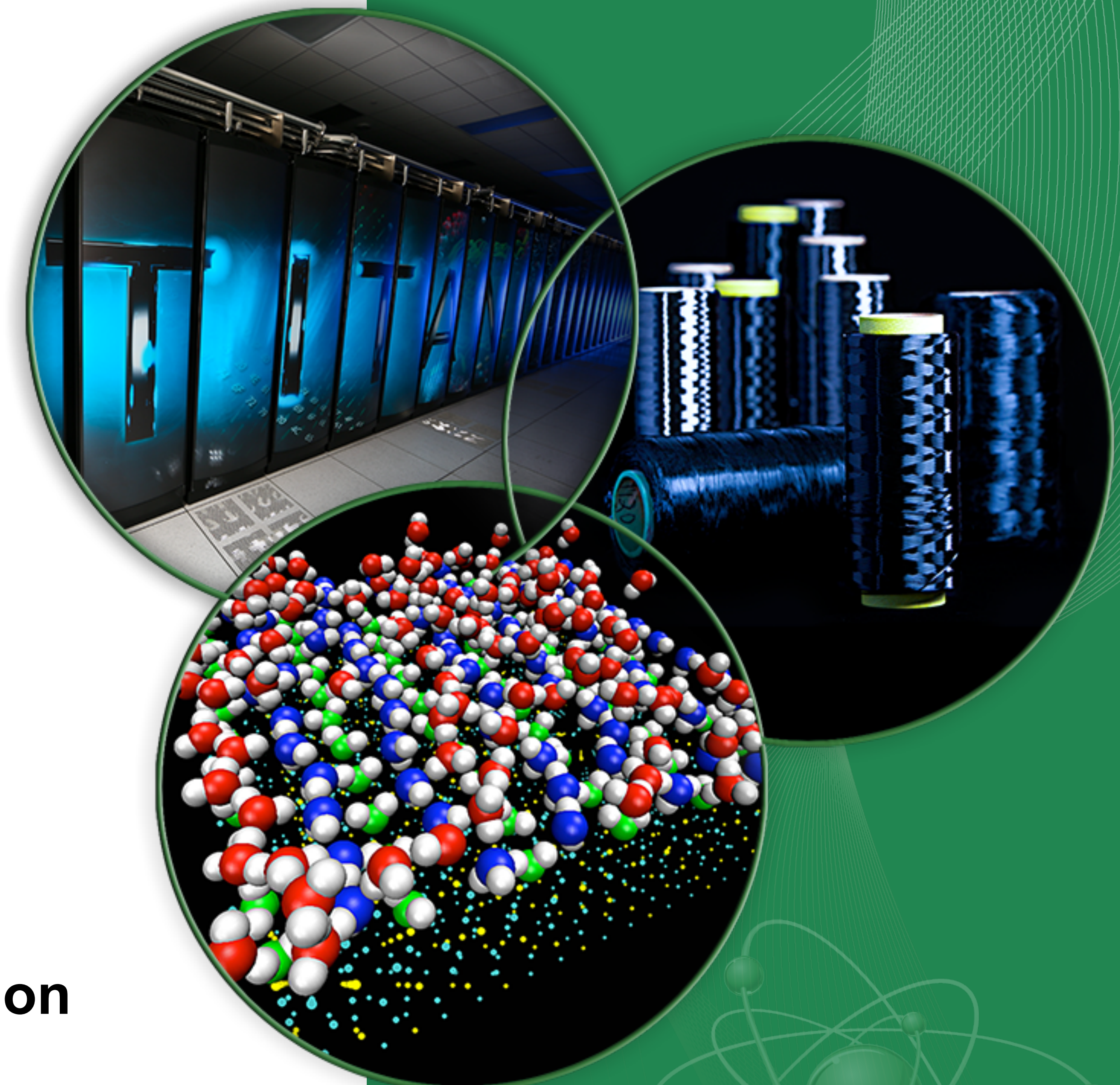
ADVANCE quality assurance system for ENDF

D. Brown

- **On every commit of every evaluation in ENDF**
  - Check out evaluation
  - Run through a battery of tests
  - Process with customer processing codes
  - Generate comparison plots
  - Generate HTML report of evaluation
- **Automation is better!**
  - Find data problems before the customers!
  - Far faster/better than old PHASE I review
- **Available at http://www.nndc.bnl.gov/endf/b7.dev/qa/index.html**



ORNL EVALUATION REPORT



M.T. Pigni, K.H. Guber, V. Sobes, D. Wiarda, G. Arbanas, M.E. Dunn
Oak Ridge National Laboratory
Oak Ridge, TN

L.C. Leal
IRSN
Fontenay-aux-Roses, 92260, France

CSEWG Meeting – Cross Section Session
Brookhaven National Laboratory
November 2015

RRR evaluation status

M. Pigni

Resolved Resonance Region (RRR) Cross Section Evaluations							
No.	**Nucleus (I^{π})**	$E_{min} - E_{max}^{ORNL} (E_{max}^{existing})$	**Method**	**No. Levels(*)**	**J_0**	**J_1**	**Evaluator**
1 ✓	^{182}W (0^+)	10^{-5} eV–10 (5.0) keV	RM	306	171	135	L. C. Leal
2 ✓	^{183}W ($1/2^-$)	10^{-5} eV–5 (2.2) keV	RM	387	346	21	M. T. Pigni
3 ✓	^{184}W (0^+)	10^{-5} eV–10 (4.0) keV	RM	178	94	84	L. C. Leal
4 ✓	^{186}W (0^+)	10^{-5} eV–10 (8.3) keV	RM	169	95	74	L. C. Leal
5 ✓	^{63}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	1093	545	548	V. Sobes
6 ✓	^{65}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	952	337	615	V. Sobes

RM – Reich-Moore Approximation (*) bound and external levels not included

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Tungsten Isotope Evaluations

M. Pigni

- Transmission and capture cross section measurements performed at Geel for 182,183,184,186W for energy up to 10 keV and for 183W up to 5 keV
- Early high-resolution total cross section measurements by Harvey at ORELA for natural tungsten
- Reich-Moore approximation
- Cross section covariance matrices (compact format)
- Submitted ENDF files (LRF=7) to NNDC/BNL in August 2014 (revisions 633 to 636 in GForge ENDF)

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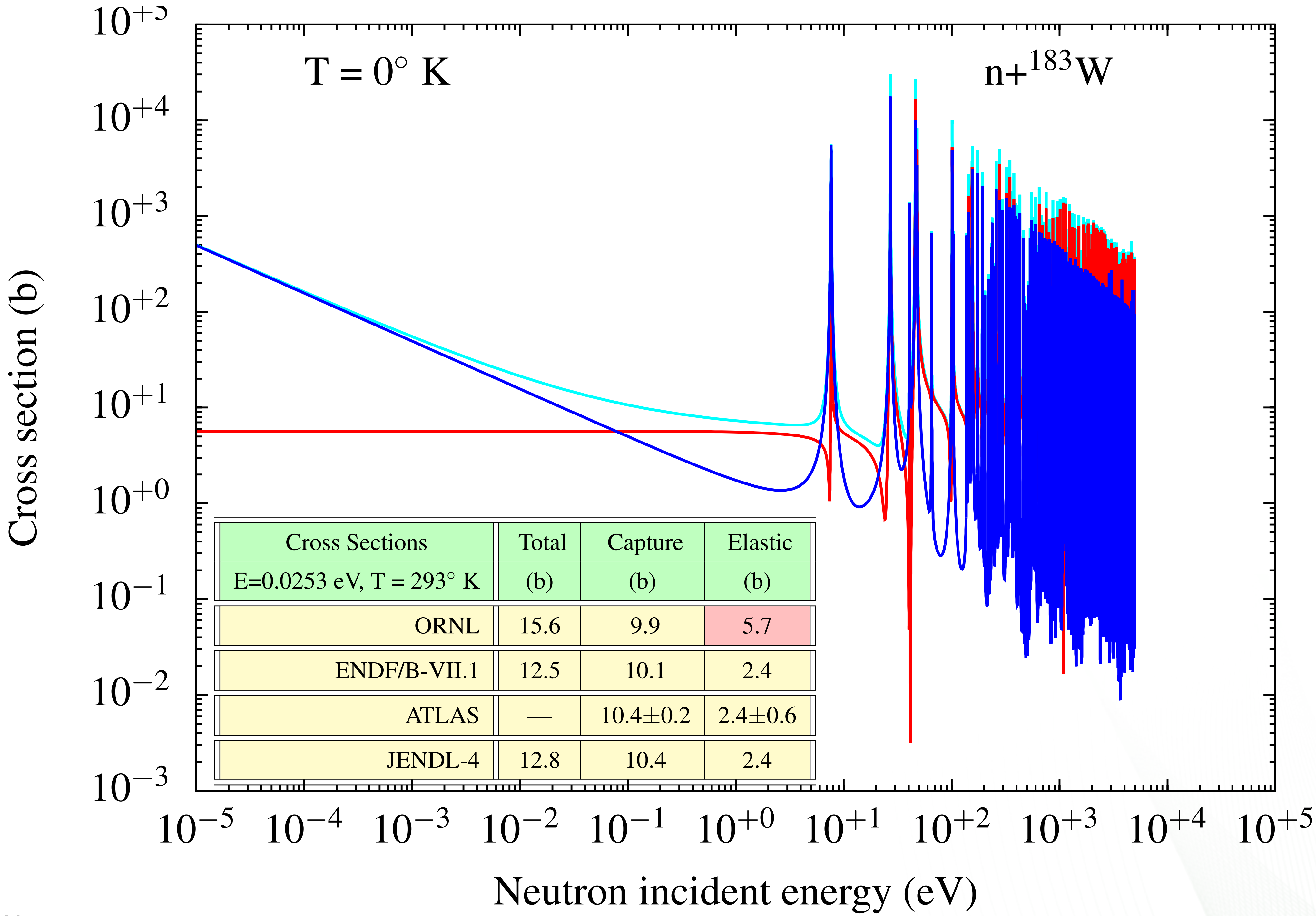
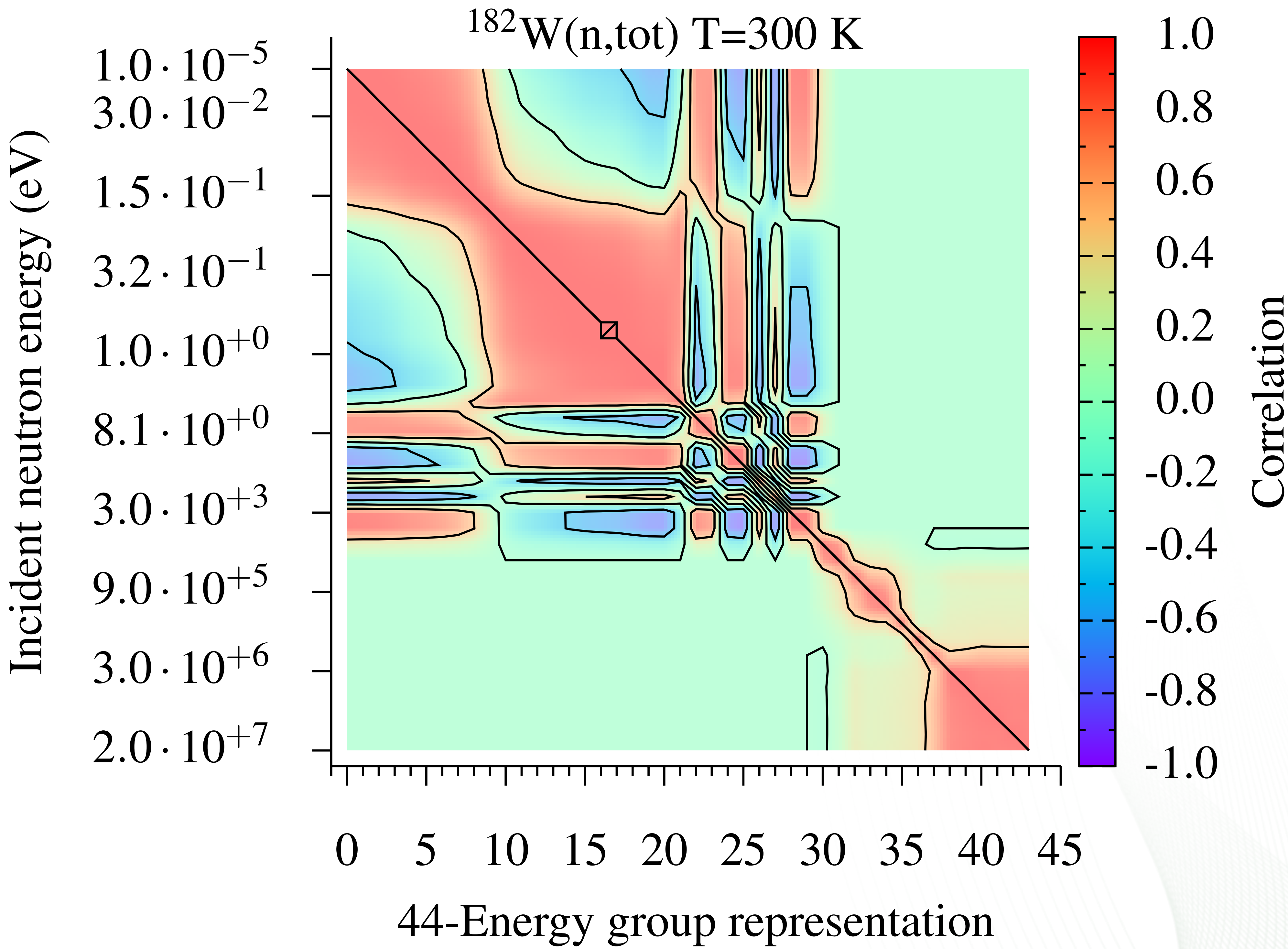
Cross sections: n+^{183}W



Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	15.6	9.9	5.7
ENDF/B-VII.1	12.5	10.1	2.4
ATLAS	—	10.4±0.2	2.4±0.6
JENDL-4	12.8	10.4	2.4

(*) **M.T. Pigni et al., PHYSOR 2012 – Advances in Reactor Physics – Knoxville, TN April 15-20 2012 (published)**
M.T. Pigni et al., International Conference on Nuclear Data for Science and Technology (ND2013), New York, NY March 4-8 2013 (published)
M.T. Pigni et al., International Conference on Nuclear Criticality Safety (ICNC2015), Charlotte, NC September 13-17, 2015 (accepted)

Covariance for $^{182}W(n,tot)$



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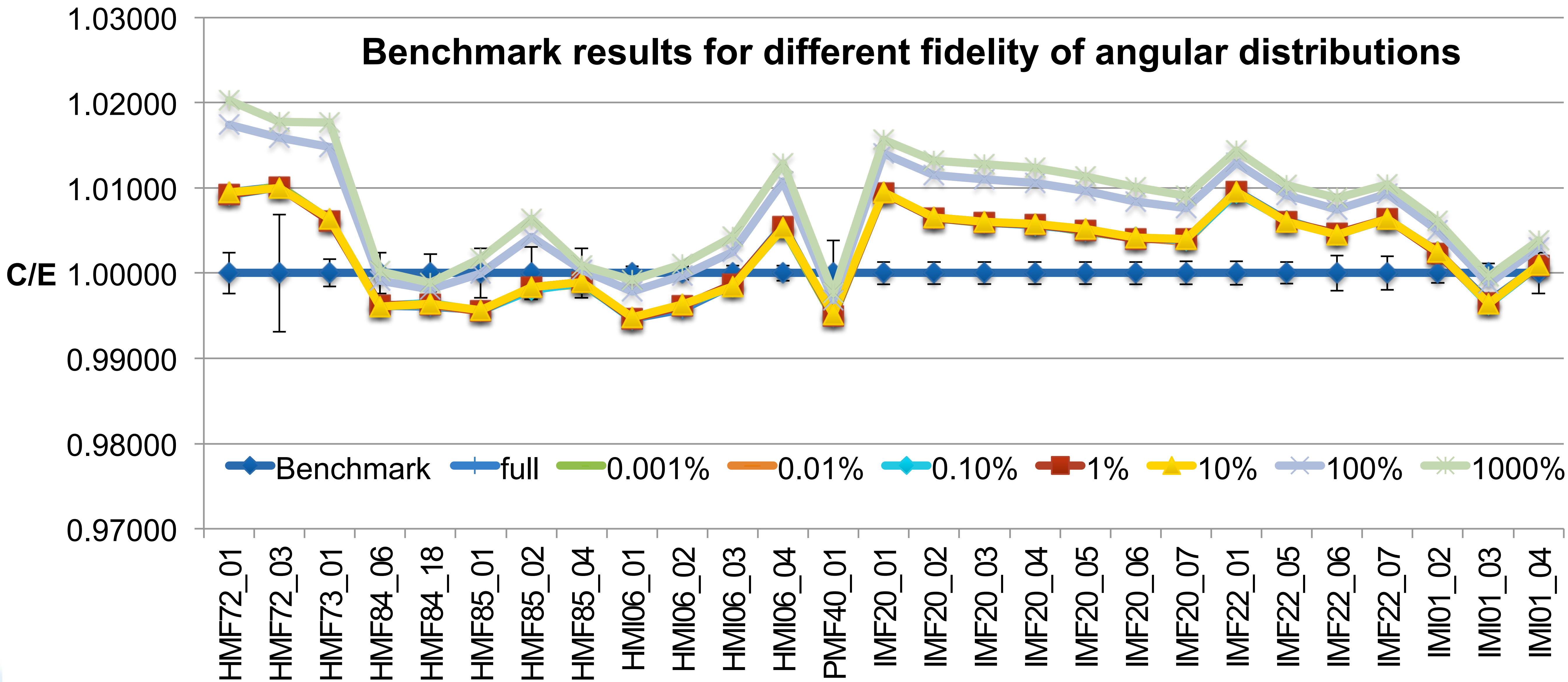
Copper resonance evaluations

- Major improvements
  - RRR extended up to 300 keV
    - Data in the thermal range (Sobes, MIT)
    - Transmission data (Pandey, ORELA)
    - Capture data (Guber, GELINA)
  - Corrected capture cross sections (in rev. 620 and 622 above 220 keV cross sections were underestimated)
  - Detailed elastic angular distributions
    - Point-wise description of angular distribution reconstructed from resonance parameters
    - Test on benchmarks

Copper resonance evaluations

Benchmark Test on Point-wise Angular Distribution



Error	0.001%	0.01%	0.1%	1%	10%	100%	1000%
Points	107 000	102 500	94 000	83 000	76 500	17 500	10 000

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^{40}Ca resonance evaluation

- Transmission and capture measurements at Geel for ^{nat}Ca up to 1 MeV (Guber)
  – Measurements of Calcium using metallic samples
  – The samples are in Al canning due to reactivity with air
  – Transmission experiments w/ different sample thickness (path 50 m)
  – Neutron capture using path 60 m
- Early high-resolution total cross section measurements by
  – Cierjacks (1968, KIC): natCa(n,tot)
  – Perey (1972, ORELA): natCa(n,tot)
  – Singh (1975): $^{nat}Ca(n,tot)$
  – Johnson (1978, ORELA): 40Ca(n,tot)
- Used formalism of Reich-Moore approximation
- Included (n,α) and (n,p) channels

Updates to the ENDF/B Decay Data Sub-library

A.A. Sonzogni, E.A. McCutchan, T.D. Johnson

National Nuclear Data Center

Updates to the decay data sub-library

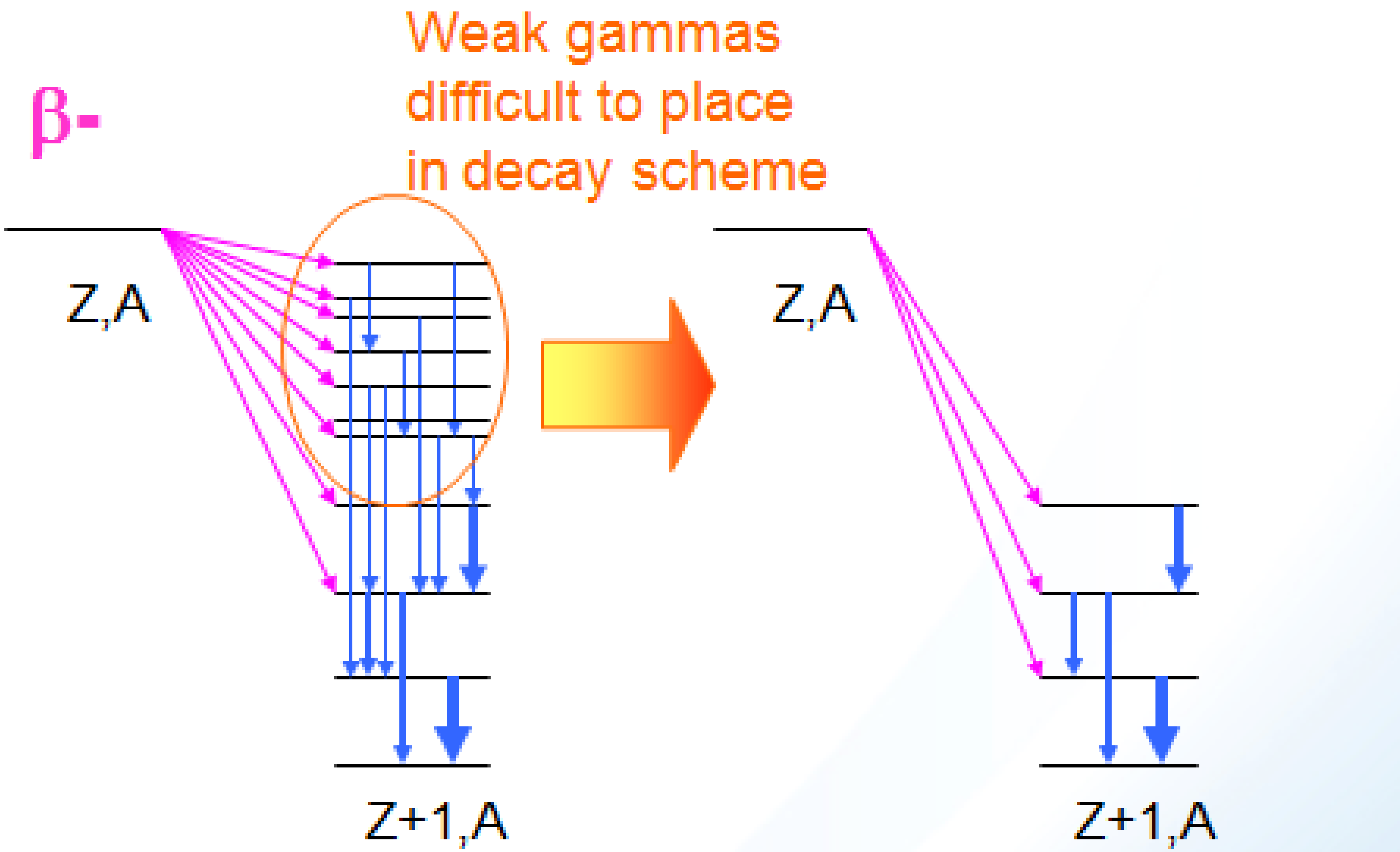
Beta intensities from TAGS experiments were used for the following nuclides:
91Rb, 92Rb, 93Rb, 94Rb, 95Sr, 140Cs,141Cs, 95Y, 143La, 144La, 145La, 143Ba.

Beta intensities from beta spectra measurements were used for:
82As, 88Br, 89Br, 90Br, 95Rb, 96Rb, 98Y, 99Y, 134Sb, 138I.

Additionally, the files for the following nuclides were modified.
82Ge, 83Ge, 91Br, 90Kr, 98mY, 86As.

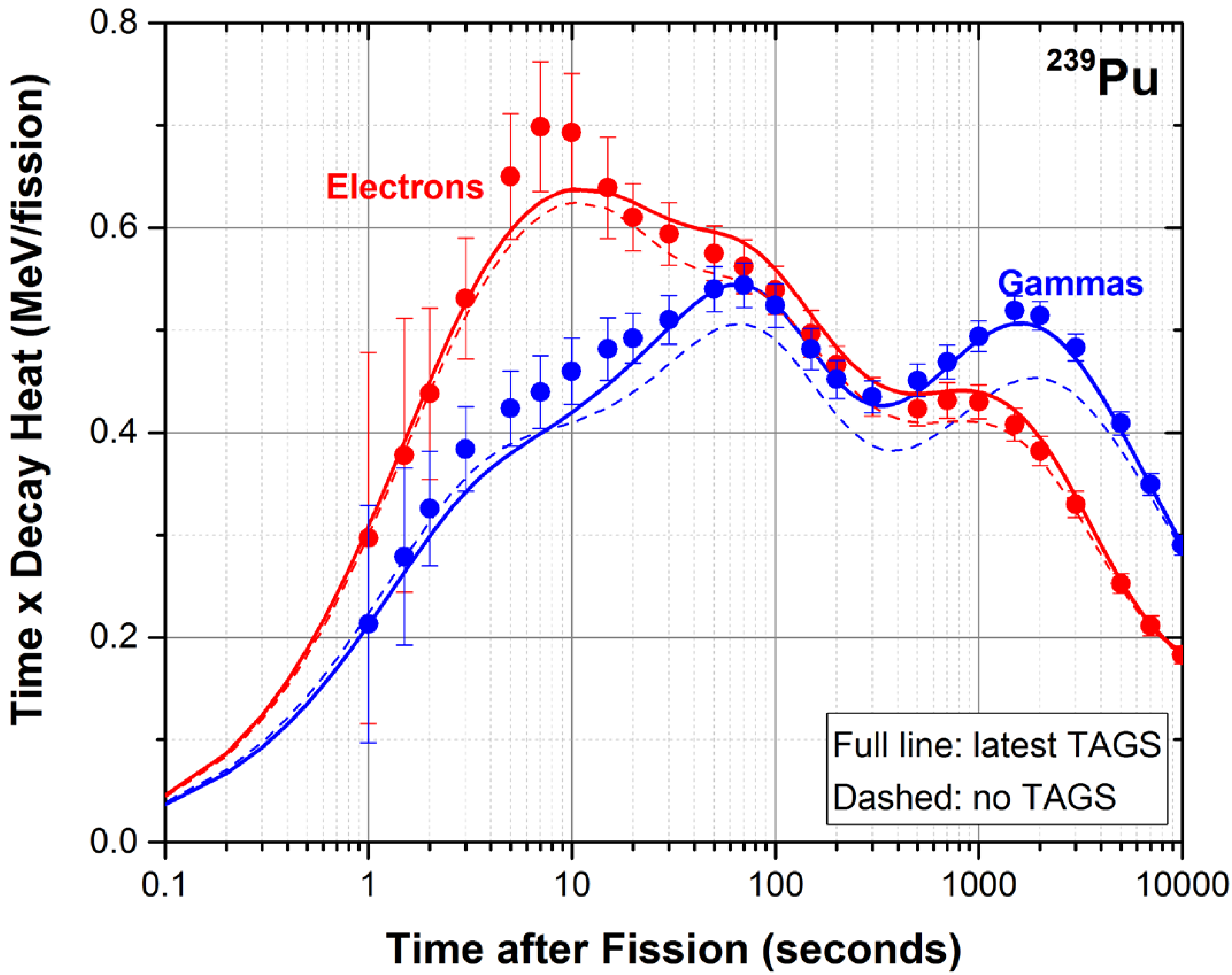
Total Absorption Gamma Spectroscopy

It has been known that Total Absorption Gamma Spectroscopy (TAGS) data in the average gamma and beta energies helps solve the Pandemonium effect.



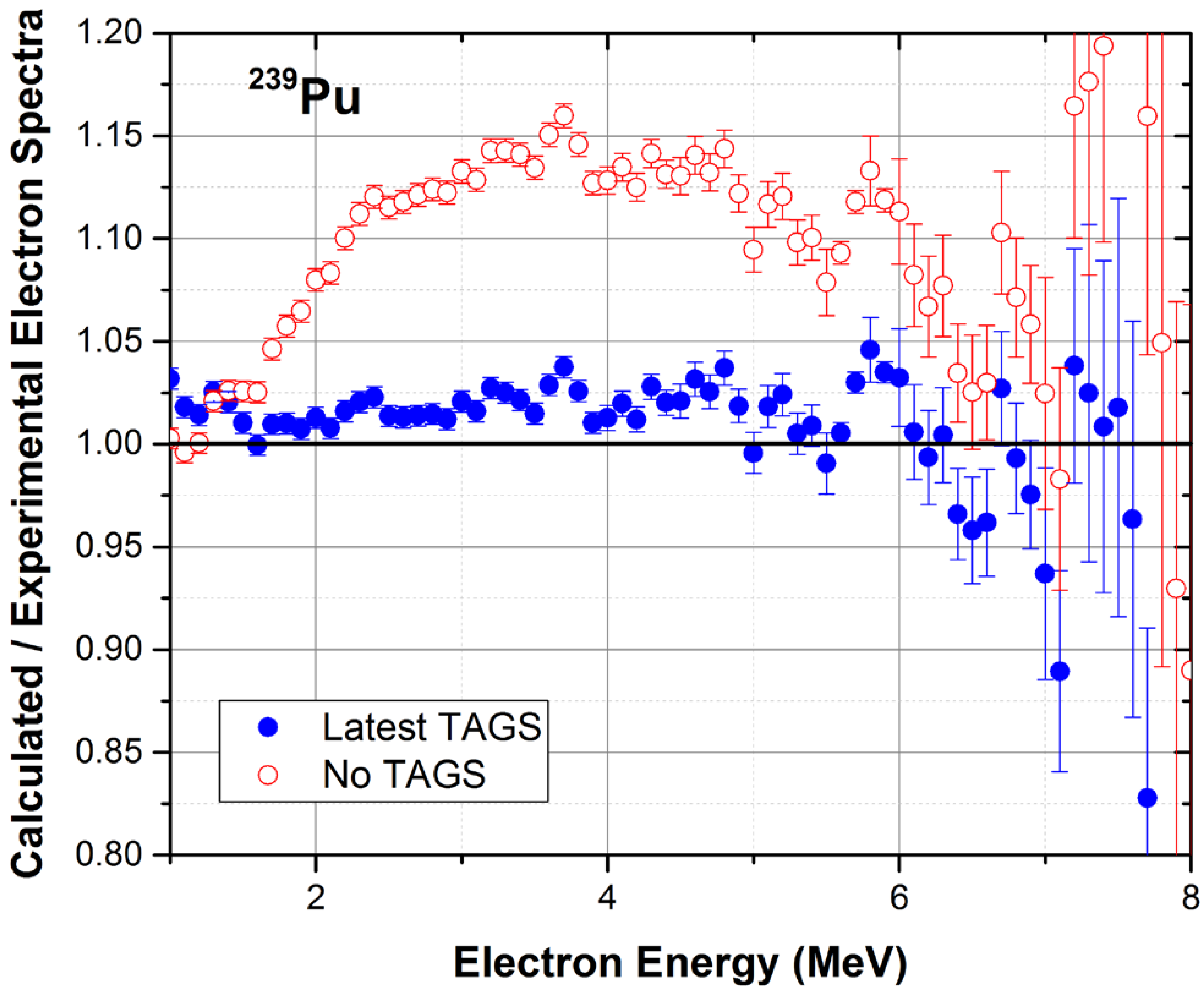
A. Algora et al., Phys. Rev. Lett. 105, 202501 (2010).

^{239}Pu Decay Heat



Much improved agreement for times larger than 10 seconds

Comparison with Exp. Data (ILL)



Conclusions and future work

- Most of our recent work has centered around the short-lived fission products that are relevant in reactor antineutrinos.

- We plan to use McGill Univ. data for beta spectrum (Iafigliola thesis)

- There are new ENSDF evaluations for 241Pu and 227Th that will be incorporated.

Fission Yields Effect on the Calculation of Antineutrino Spectra

A.A. Sonzogni, E.A. McCutchan, T.D. Johnson

National Nuclear Data Center

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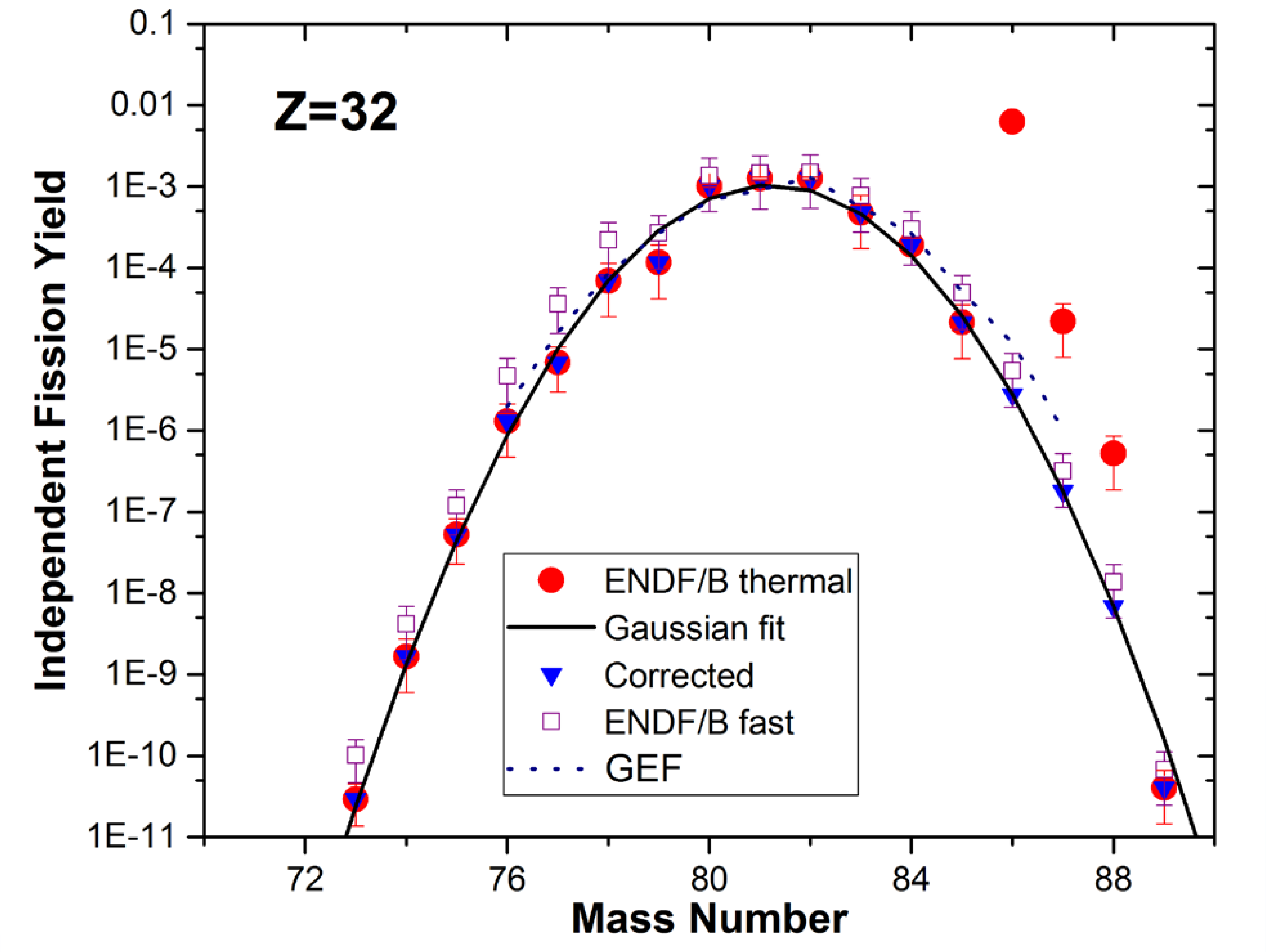
ENDF/B-VII.1 yields were released in 1992,

- A few yields seem anomalous.
- Isomeric ratios could be updated
- Yields are not fully compatible with modern decay data.

We explored correcting the independent fission yields, and then obtain cumulative yields with the decay sub-library, to finally perform some calculations.

For more details see A.A. Sonzogni et al, PRL 116, 132502 (2016).

We concluded that the $^{86,87,88}Ge$ yields are anomalous, and corrected them using a weighted Gaussian fit.



Conclusions

There is currently plenty of interest on the reactor antineutrino spectrum. What we have learned from our research is:

- There have been new measurements of fission yields since 1992, and more are expected to come soon.
- There have been many measurements on the fission products decay properties since 1992.
- Funding is needed to ensure that these data are included the fission yields sub-library.

Advances in Nuclear Reaction Theory for Deformed Nuclei (Actinides)

T. Kawano

Theoretical Division
Los Alamos National Laboratory

Nuclear Data Week 2015,
Brookhaven National Laboratory, 11/2 – 6, 2015

Los Alamos

Statistical Model for Strongly Deformed Systems

- Hauser-Feshbach with coupled-channels model essential
  - collective states (rotational band levels) strongly excited
    - neutron inelastic scattering process modified by S-matrix unitarity limit
    - Engelbrecht-Weidenmüller transformation is required
  - M1 giant resonance (scissors mode) at a few MeV
    - neutron radiative capture cross section in the fast energy range enhanced
  - fission is a key process for nuclear data of actinide
    - fission penetration calculation, as well as the barrier parameters, still not accurate enough to predict fission cross sections
- Overview of recent upgrades in nuclear reaction theory for deformed systems, particularly for actinides
  - combining nuclear structure information crucial

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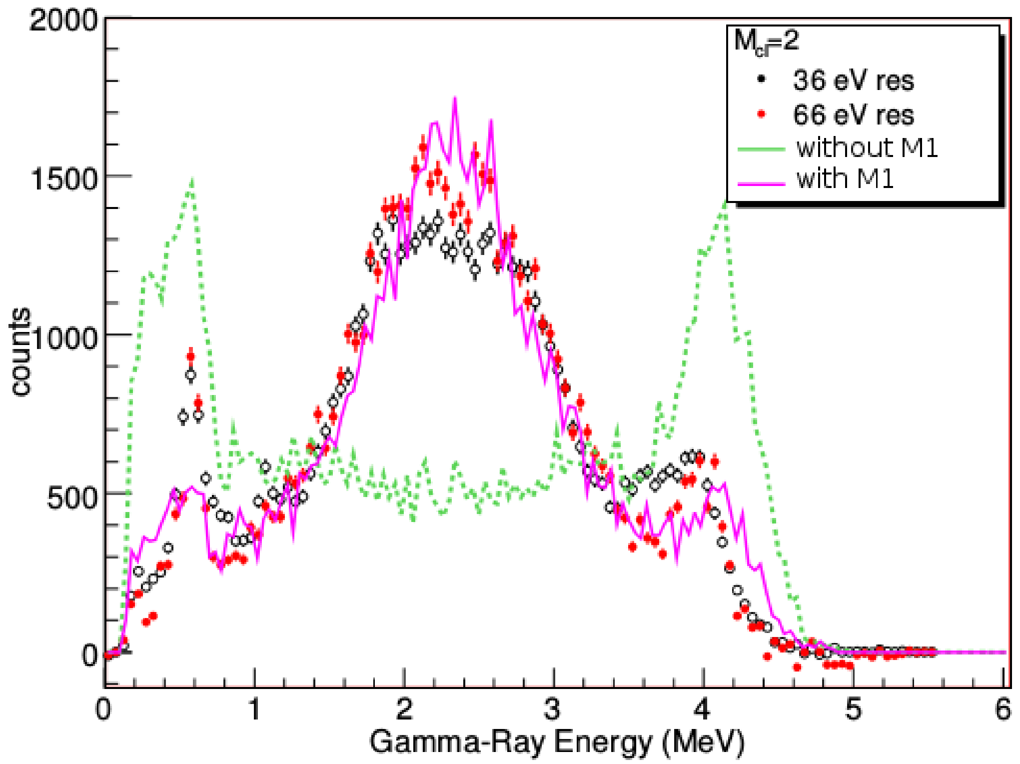
γ-Ray Cascade and Capture Cross Section

T. Kawano



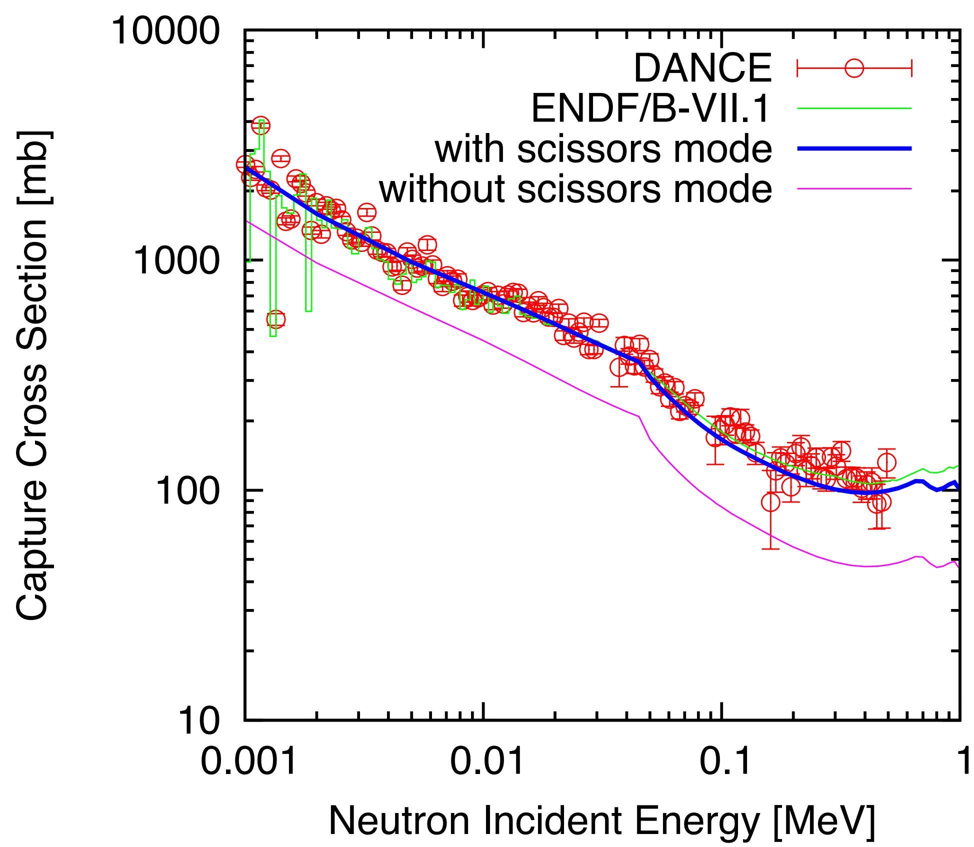
J. Ullmann, et al. PRC **89**, 034603 (2014)

DANCE γ-ray spectrum for multiplicity two

- an additional strength in the low energy region needed
- we assume this is an M1 scissors mode

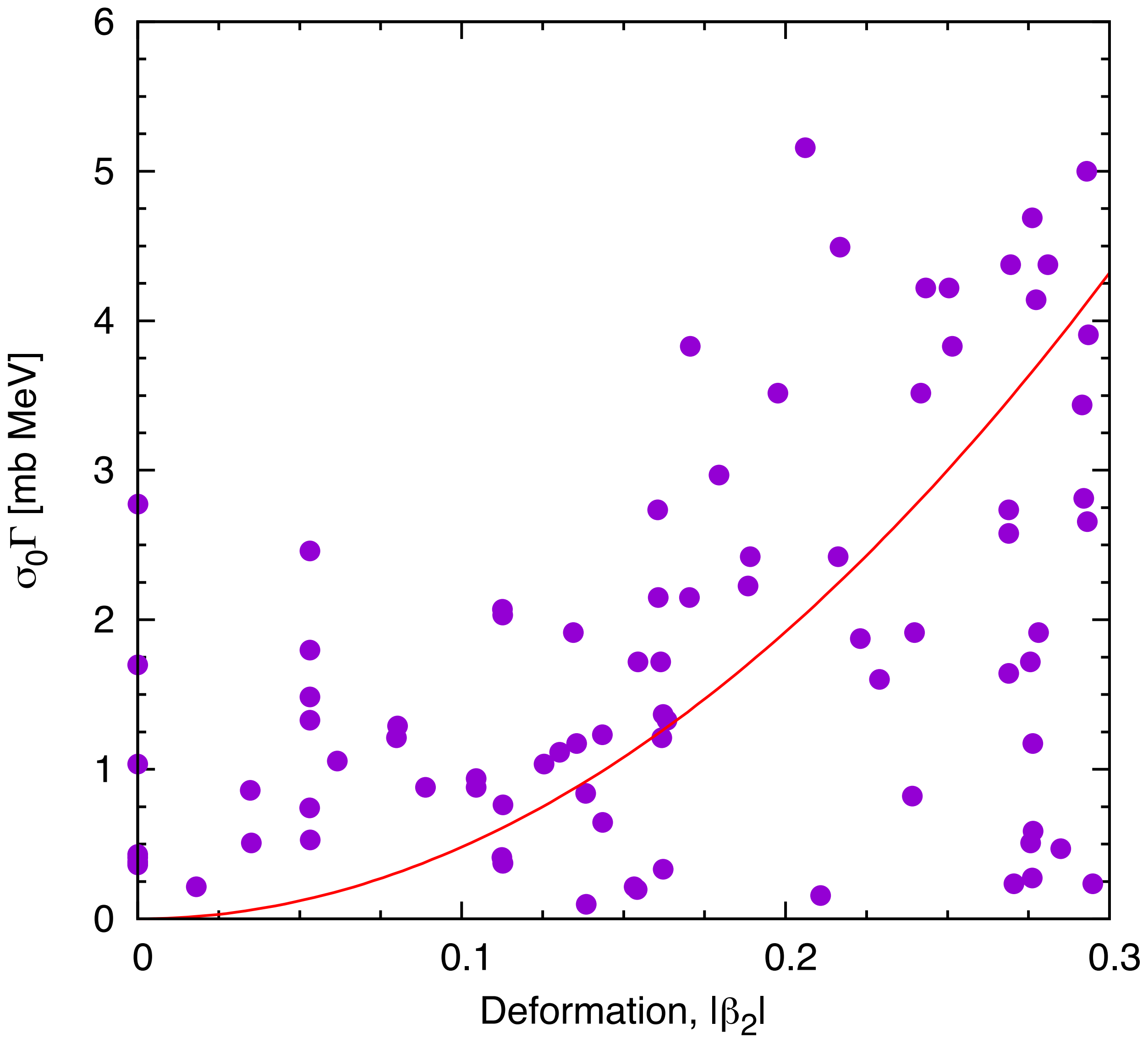
Including a small M1 component at low energies, the ^{238}U(n,γ) data are well-reproduced without artificial re-normalization of photon strength function

Does correlation exist between M1 and nuclear deformation?



M1 Strength vs. Nuclear Deformation

M1 strength required to reproduce evaluated capture cross section at 100 keV, in addition to the generalized Lorentzian E1



Resonance Energy

- assume oscillation amplitude proportional to the resonance energy
- analysis of ^{238}U DANCE data gave $E \simeq 2$ MeV

$$E_{\mathrm{M1}} = 80|\beta_2|A^{-1/3} \quad \mathrm{MeV}$$

$66\delta A^{-1/3}$ in [D.R. Bes, Phys. Lett. **137B**, 141 (1984)]

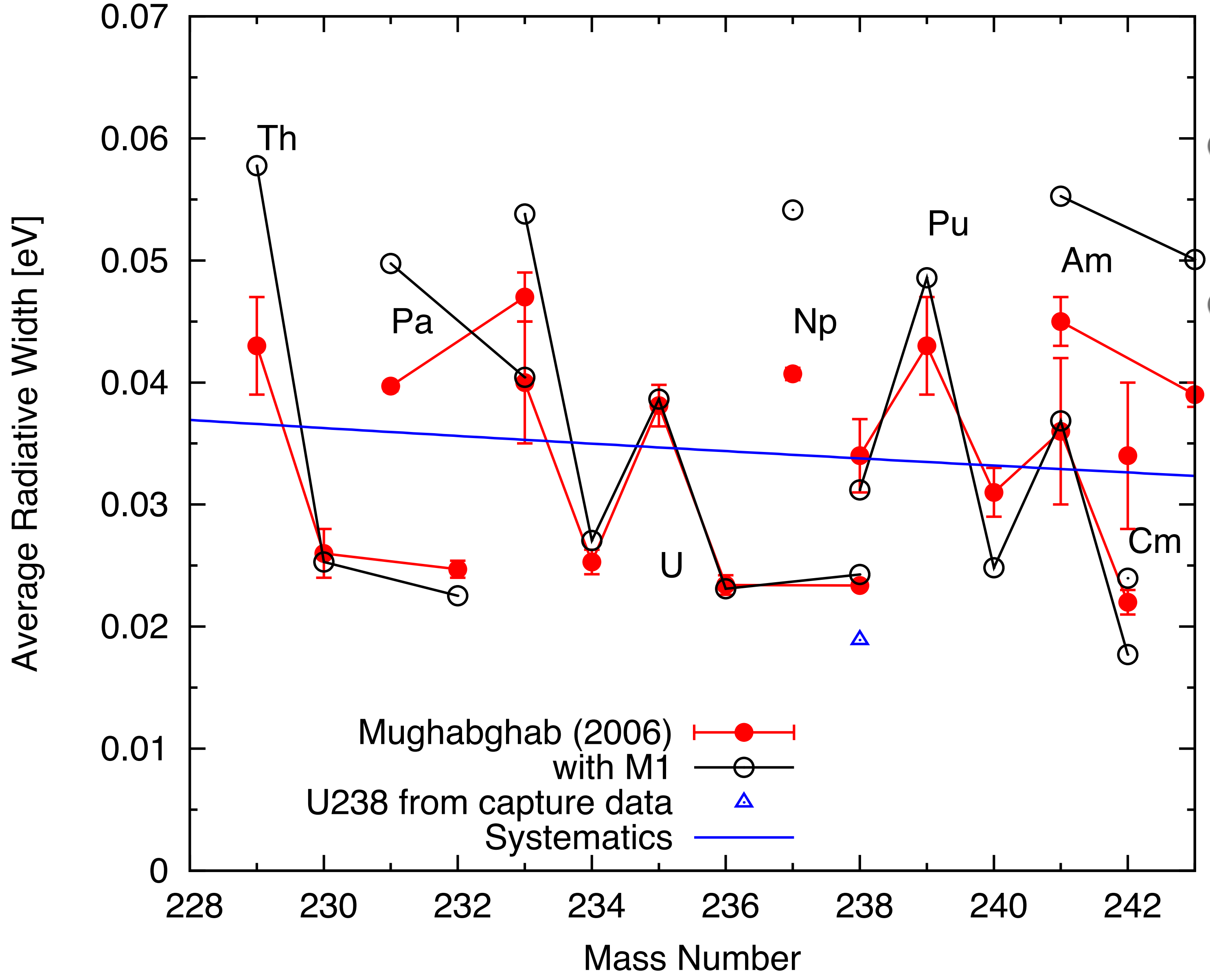
Peak Cross Section and Width

$$\sigma_{\mathrm{M1}}\Gamma_{\mathrm{M1}} = 50\beta_2^2 \quad \mathrm{mb\ MeV}$$

T. Kawano

Average Gamma Width, Actinide Region

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{XLJ'} \int_0^{S_n+E_n} T_{XL}(E_\gamma)\rho(S_n + E_n - E_\gamma, J')dE_\gamma \quad (1)$$



- actinide data not included in the search
- ^{238}U value
  - 23.36±0.31 meV (ATLAS)
  - 23.6 meV (RIPL)
  - 24.3 meV (this work)
  - 18.9 meV from $\sigma_{\rm capt}$

Inclusion of Direct Channel in Hauser-Feshbach

Cross section calculations for strongly deformed systems

- Approximated Method
  - calculate transmissions from Coupled-Channels S-matrix

$$T_a = 1 - \sum_c |\langle S_{ac} \rangle \langle S^*_{ac} \rangle|^2 \tag{2}$$

  - $\sum_a T_a$ gives correct compound formation cross section
  - HF performed in the direct-eliminated cross-section space
- Engelbrecht-Weidenmüller (EW) transformation
  - diagonalize S-matrix to eliminate the direct channels
  - HF performed in the diagonal channel space
  - transform back to the cross section space

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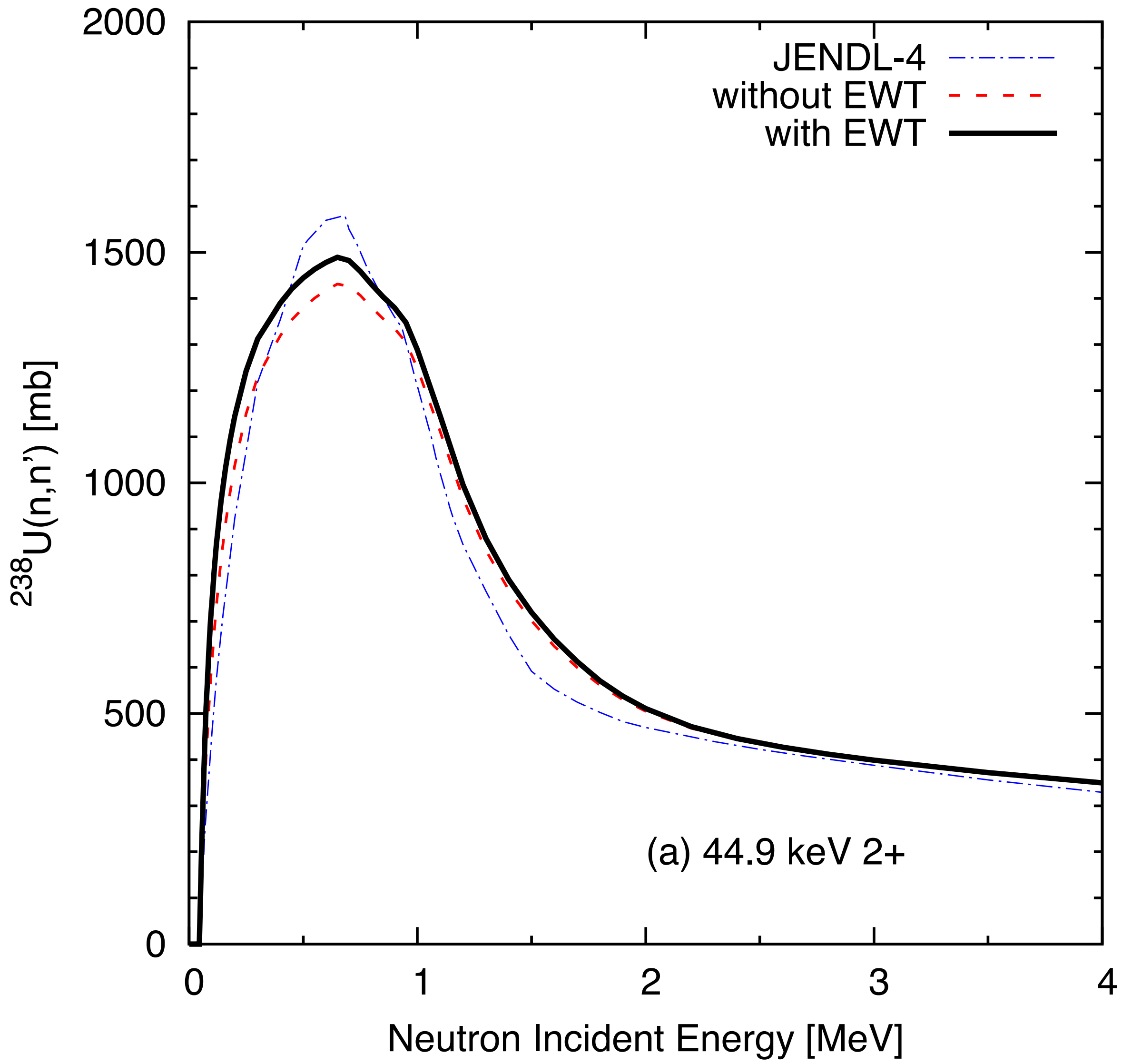
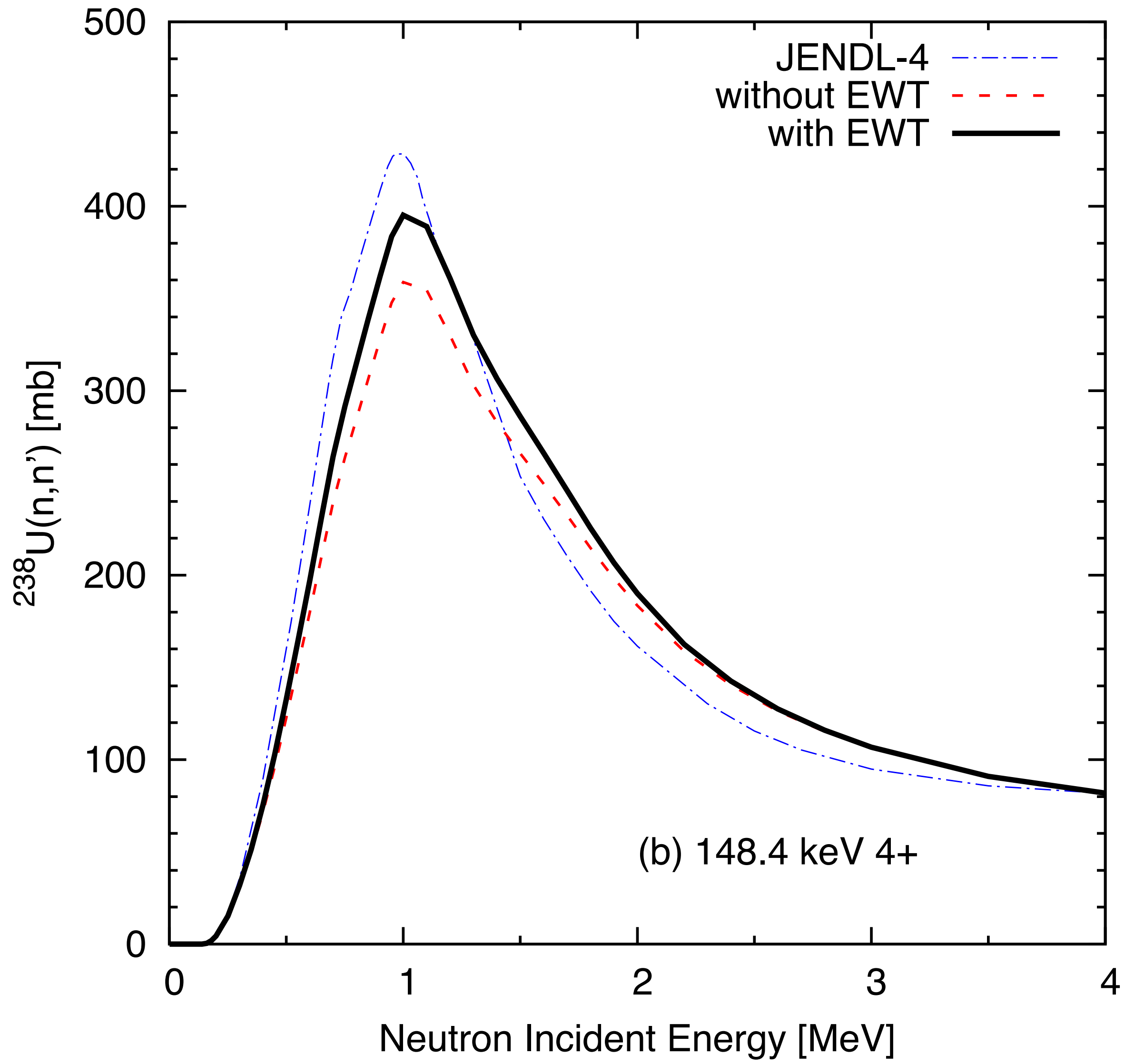
U-238 Inelastic Scattering Cross Section

T. Kawano

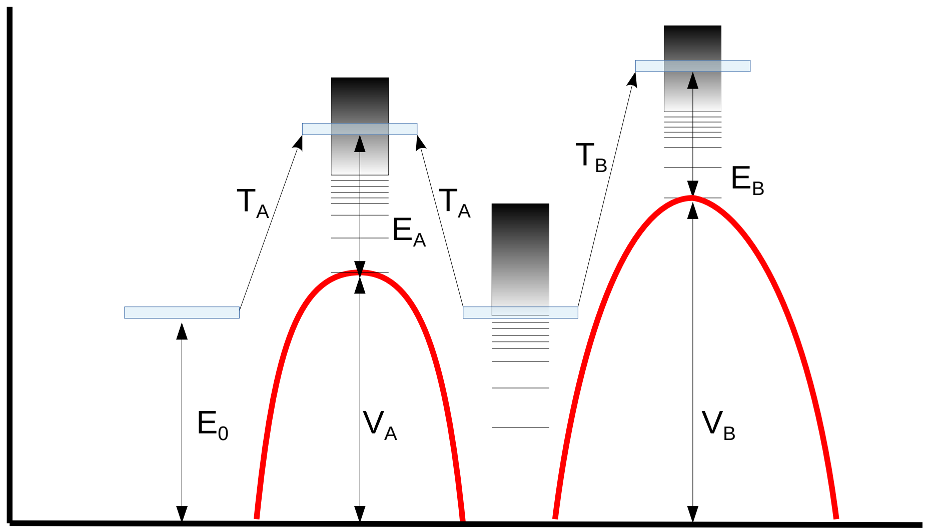
Full EW transformation implementation into the CoH_3 code (MH: EMPIRE under way)

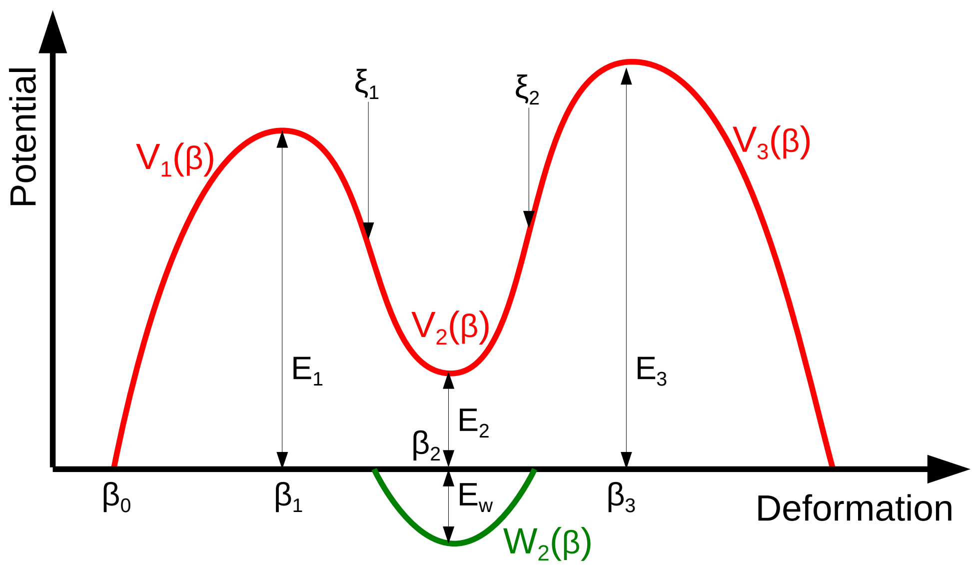




Probably we have been underestimating the inelastic scattering cross sections of actinides by 10 – 15%.

Fission Transmission for Arbitrary Potential Shape





Solving One-dimensional Schrödinger equation

J.D. Cramer, J.R. Nix, Phys. Rev. C **2**, 1048 (1970)

$$\frac{d^2}{d\beta^2}\phi(\beta) + \frac{2\mu}{\hbar^2}\left\{E - (V(\beta) + iW(\beta))\right\}\phi(\beta) = 0 \qquad (6)$$

with the boundary conditions of

$$\phi(\beta) \simeq \begin{cases} u^{(-)}(k\beta) - S\,u^{(+)}(k\beta) & \beta > \beta_{\max} \\ Au^{(-)}(k\beta) & \beta < \beta_0 \end{cases} \qquad (7)$$

where

$$u^{(\pm)}(k\beta) = \cos(k\beta) \pm i\sin(k\beta) \qquad (8)$$

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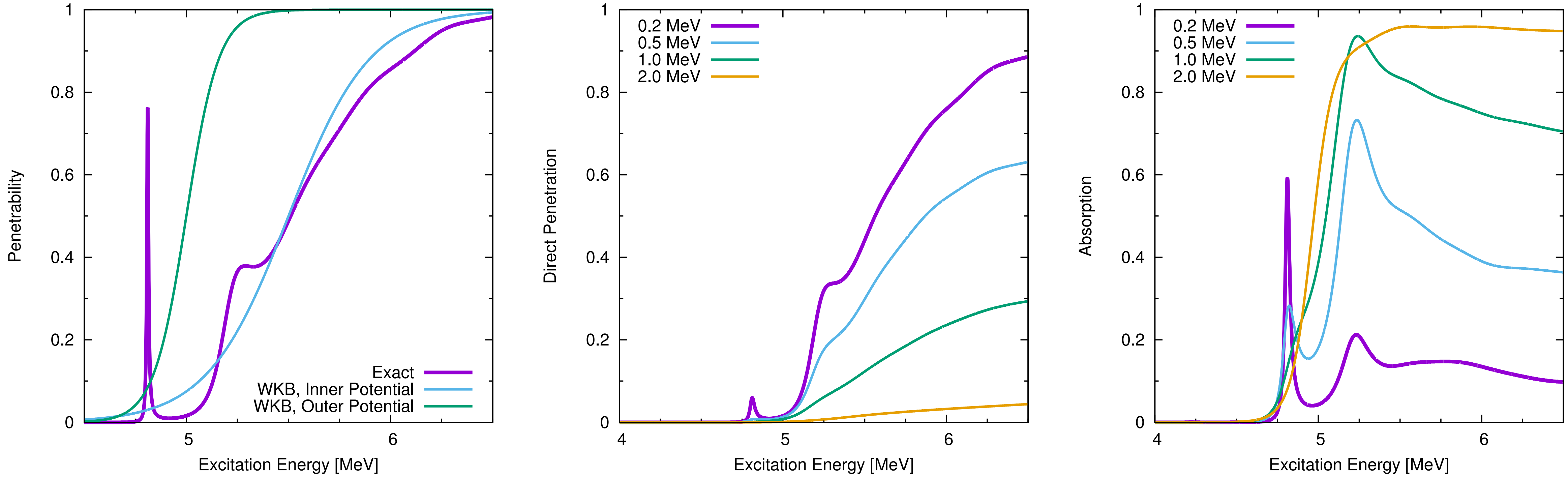
Fission Transmission Coefficients

T. Kawano



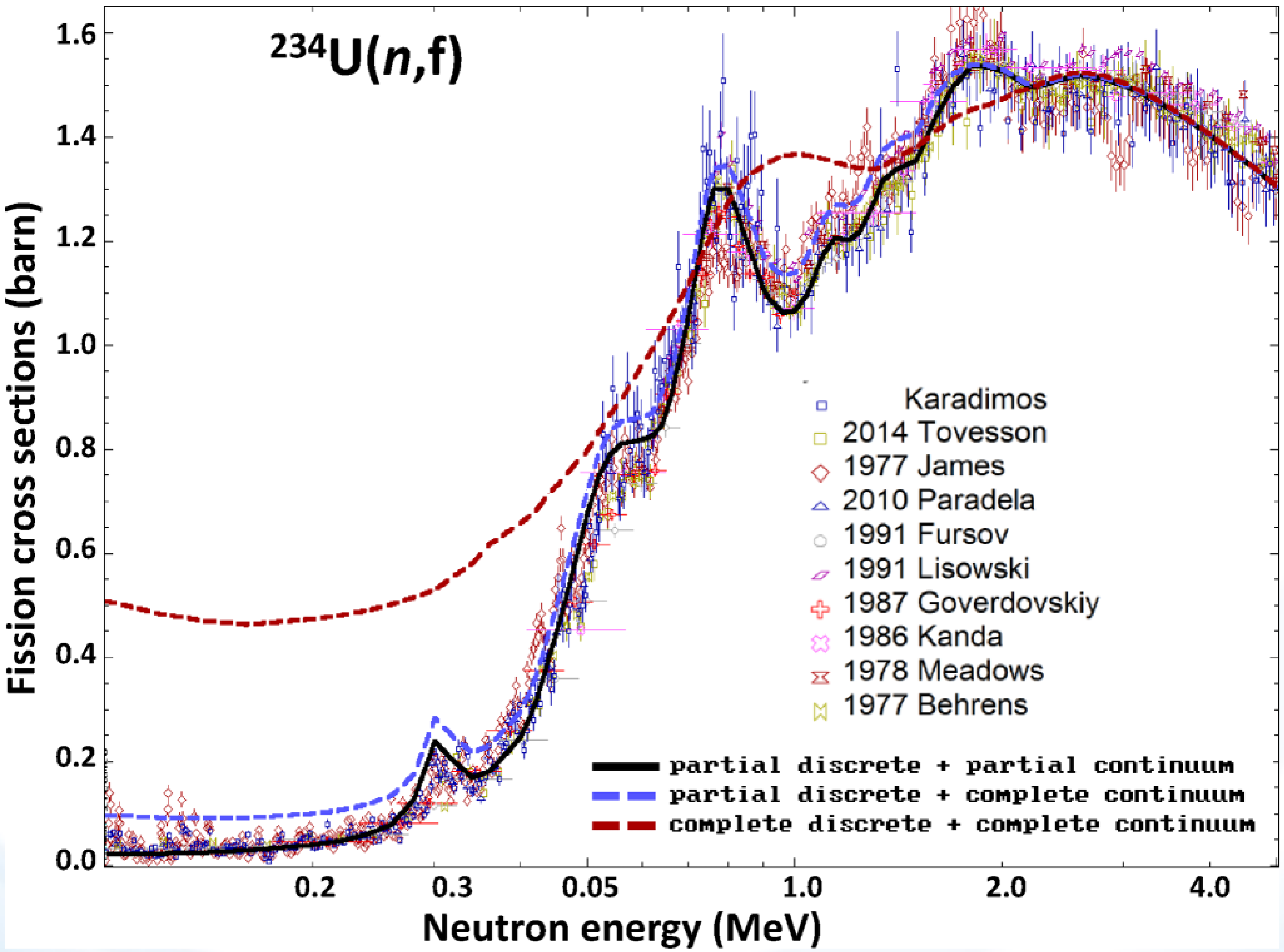
- Empire has a similar capability, but WKB approximation
- T_f solver already implemented in CoH_3
- We still need to model indirect fission for the complex potential case
  - absorbed flux goes into the fission channel,
  - or come back to the initial compound nucleus (capture or inelastic)

MH: Implemented in EMPIRE

PHYSICAL REVIEW C **93**, 034605 (2016)

Extended optical model for fission

M. Sin,[1,*] R. Capote,[2,†] M. W. Herman,[3] and A. Trkov[2]



Partial damping of class-II/III states, and of direct transmission through discrete and continuum fission channels, is critical for a description of 234,235,238 U(n,f).
239 Pu(n,f) can be calculated in the complete damping approximation.

Calculated cross sections for 235,238U(n,f) and 239Pu(n,f) agree within 3% with the Neutron Standards derived from experimental data.

Conclusion

- Hauser-Feshbach calculations for actinide significantly improved in the last decade
- However, model parameters still need to be refined for better prediction
  - photon strength functions — generalized E1, enhanced E1, M1 scissors
  - level density with realistic spin and parity distributions
  - realistic fission path
    - coupled-channels calculation for rotational-vibrational nuclei, and potential parameters
- Mean-field theories may help better understanding
- Exchange expertise among similar code projects important
  - Empire at BNL and IAEA, TALYS at CEA/DAM, CCONE at JAEA, CoH_3 at LANL, and LLNL code

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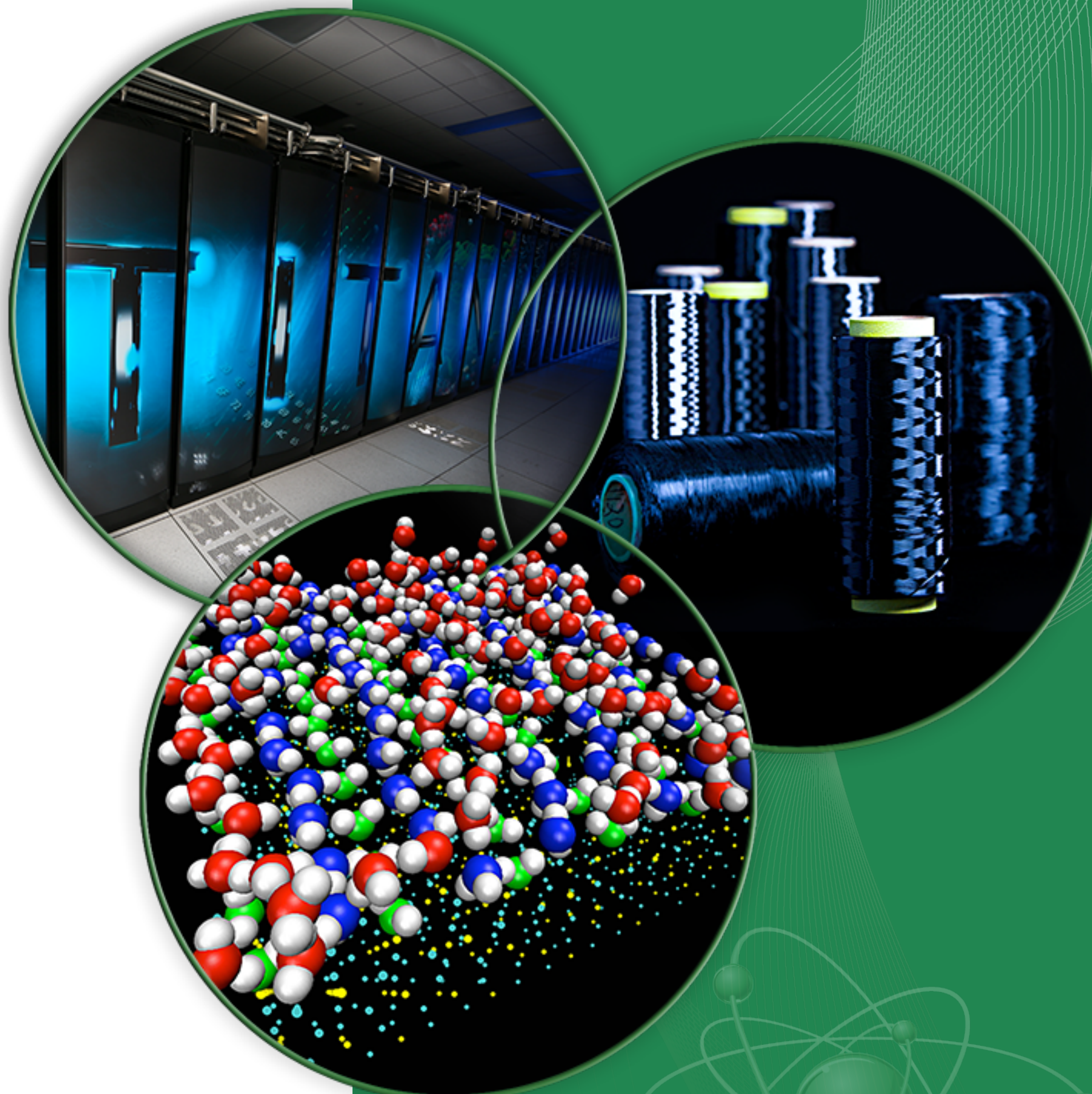
SAMMY Modernization



Goran Arbanas, ORNL

Doro Wiarda,ORNL

Vlad Sobes, ORNL

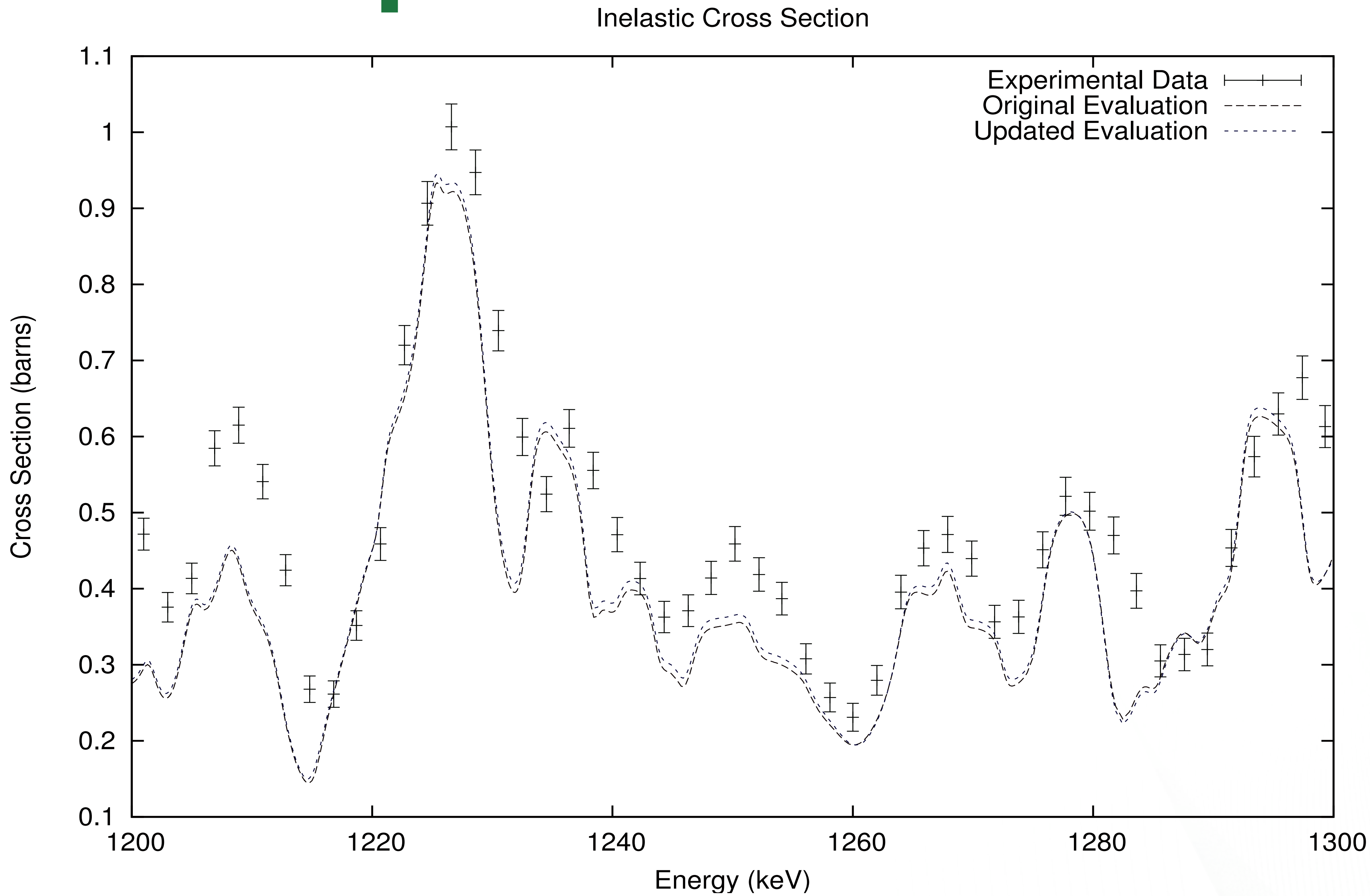
Mike E. Dunn, ORNL

Cross Section Evaluation Working Group,
U.S. National Nuclear Data Week 2015
BNL, November 2-6, 2015

SAMINT: Nuclear Data Adjustment Based on Integral Experiments

- SAMINT is an auxiliary program designed to allow SAMMY to adjust nuclear data parameters based on integral data.
- Allow coupling of differential and integral data evaluation in a continuous-energy framework
- Update the parameters of a resolved resonance region evaluation directly based on integral benchmark experiments
- http://www.osti.gov/scitech/biblio/1185560/

Cross Section Changes: Finer Scale than Differential Experimental Data



Inelastic cross section of ^{56}Fe before (χ^2 = 23.6023) and after (χ^2 = 22.9036) the adjustment based on integral experimental data plotted on top of differential experimental data of Perey, presented with one standard deviation error bars.

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