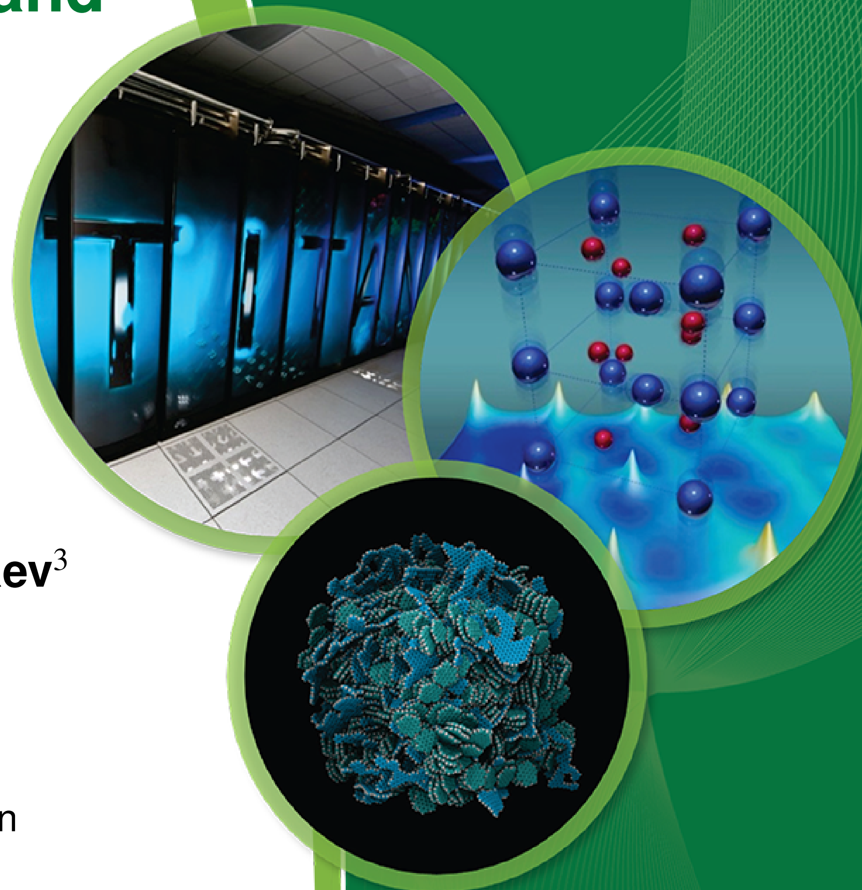
n+^{235}U Resonance Parameters and Neutrons Multiplicities in the Energy Region below 100 eV and Future Plans



M.T. Pigni[1], R. Capote[2], A. Trkov[2], V.G. Pronyaev[3]

[1] Oak Ridge National Laboratory, USA

[2] IAEA Nuclear Data Section, Austria

[3] State Corporation Rosatom, Moscow, Russian Federation

CSEWG2016 - Evaluation session
Upton, NY, November 2016

Outline

- Introduction : motivation and background
- Nuclear data evaluation overview for ^{235}U
- Brief description of the evaluation procedure with SAMMY
- Results
  - Work on n+^{235}U cross sections
  - Neutron multiplicities $\bar{\nu}(E)$ (Pronyaev/Capote)
  - Benchmark simulations (Trkov/Capote)
- Future plans
- Summary and conclusions
- Acknowledgments

Introduction

Motivation

- For nuclear critcality applications and many others, the existing evaluated data perform well in transport simulations partly owing to *compensating errors* in the nuclear data libraries
- CIELO collaboration provides a framework for nuclear data evaluation aimed to establish the highest fidelity general purpose nuclear database
- ^{235}U among ^{1}H,^{16}O,^{56}Fe,^{238}U, ^{239}Pu is one of the highest priority isotopes

Background

- Current status of ^{235}U evaluation in ENDF/B-VII.1 library (2011)
  - Resonance parameters are the same as ENDF/B-VI.8 release (ORNL/TM-13516)[1]
  - Description of the ^{235}U resonance evaluation can be found in NEA/WPEC-18
- ^{235}U ORNL resonance evaluation(=CIELOb18=**o23**) is part of the ENDF/B-VIII.0β2 and β3 releases (2016)

[1] See also L. C. Leal, H. Derrien, N. M. Larson, R. Q. Wright, *Nucl. Sci. Eng.*, **131** 230 (1999).

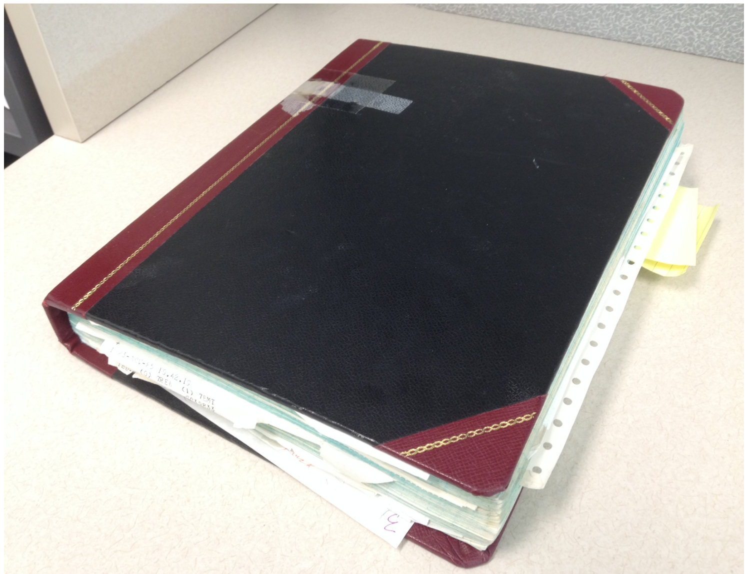
Nuclear Data ORNL Evaluation Overview

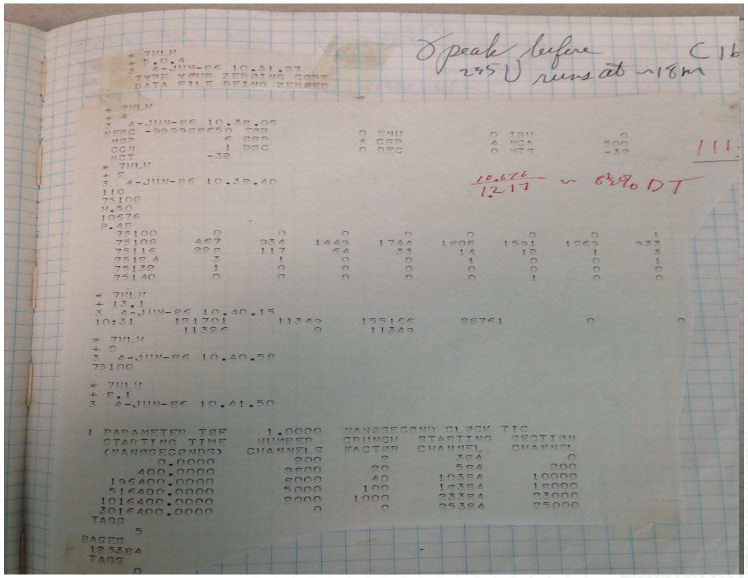
No.	Nucleus (I^{π})	E_{max}	Method	J_{3^-}	J_{4^-}
1	^{235}U $(7/2^-)$	2.25 keV	Reich-Moore	1433	1731

- The current ORNL resonance evaluation **o23** (ORNLv23) is an intermediate step of the evaluation process within CIELO
- The current **o23** resonance evaluation started from a set of resonance parameters (**o17**)
  - **o17** was documented in the ORNL presentation at the mini-CSEWG meeting (LANL, April 2016) and released in May 2016 as part of the ENDF/VIII.0β1 release.
- Particular emphasis in producing **o23** was devoted to
  - *Sub-thermal and thermal* : Thermal Constants (Pronyaev, micro. data)
  - *Fission integrals (7.8-11 eV)*
  - Neutron incident energies up to 20 eV for *measurements of* $\alpha = \sigma_\gamma/\sigma_f$ *(or* η*)*

Nuclear Data ORNL Evaluation Overview

- The current ORNL resonance evaluation **o23** is generated by the SAMMY code using the *Reich-Moore approximation*
  - All SAMMY inputs included in the current evaluation procedure are written using the most recent key-word for particle-pair definitions.
  - Isotopic impurities included
  - Parameters for the resolution functions (crunch data, γ-peak) of transmission experimental data (J. A. Harvey) retrieved from ORELA logbook (special thanks to K. Guber).
- Residuals and chi-squared of all experimental data





OAK RIDGE National Laboratory

SAMMY Algorithm

The various reaction cross sections $\sigma_{cc'}$ for an incoming channel c and outgoing channel c' can be written in terms of the matrix

$$X_{cc'} = \sqrt{P_c} L_c^{-1} \sum_{c''} [(L^{-1} - R)^{-1}]_{cc''} R_{c''c'} \sqrt{P_{c'}} \delta_{JJ'} \,, \qquad (1)$$

where, in the eliminated-channel approximation, the matrix R (or R-matrix) for the channel spin group defined by the total spin J^{π} is

$$R_{cc'} = \left[\sum_{\lambda=1}^{n} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E - \imath \bar{\Gamma}_{\lambda\gamma}/2} + R_c^{\text{ext}} \delta_{cc'} \right] \delta_{JJ'} \qquad (2)$$

SAMMY derives from the best fit of experimental data the reduced-width amplitude $\gamma_{\lambda c}$ related to the channel width using

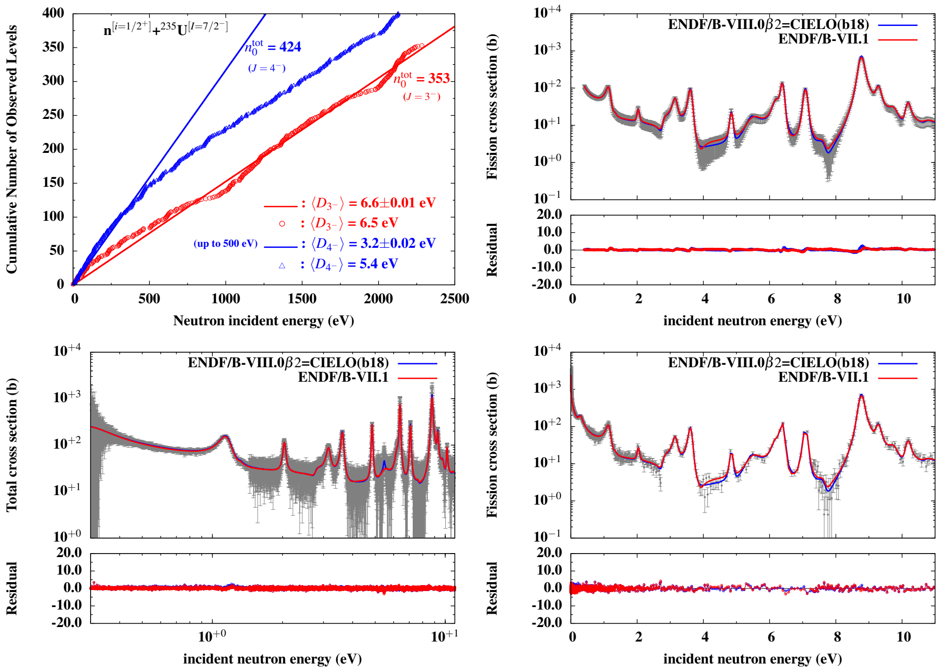
$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 P_c(E) \,, \qquad (3)$$

where the penetrability factors depend on the Coulomb functions F_ℓ, G_ℓ as $P_c(E) = ka/[F_\ell^2(ka,\eta) + G_\ell^2(ka,\eta)]$.

Differential and Integral Data

Differential data

- Application of the R-matrix SAMMY method (Reich-Moore) to determine a consistent set of neutron resonance parameters (RP) based on the fit of available experimental data (transmission, capture, angular distribution, ...)
- Statistical properties of RP such as average spacing $\langle D_\ell \rangle$ and strength function S_ℓ



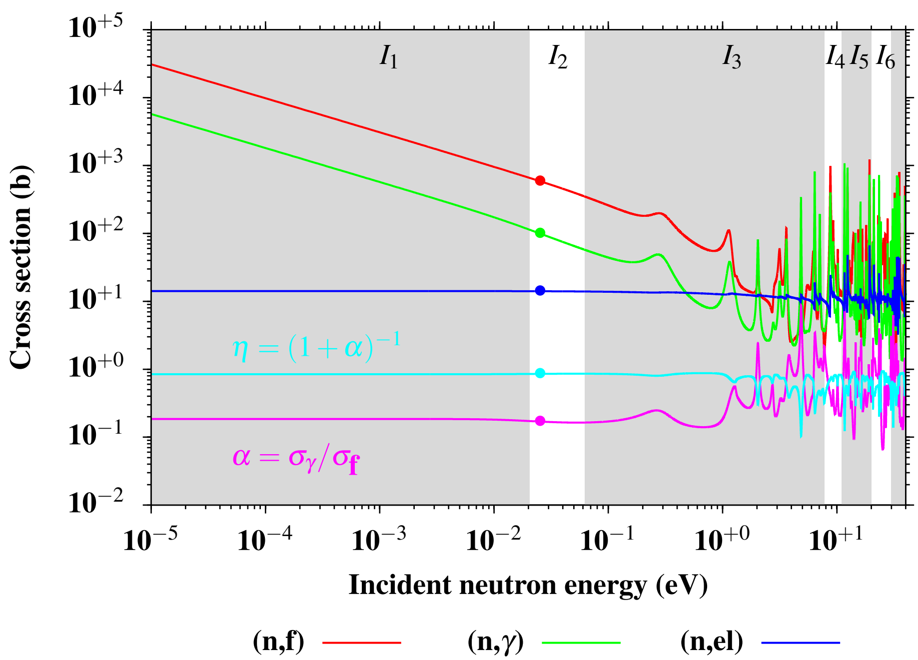
Integral data

- Resonance parameter and covariance are converted into the ENDF/B format - file 2 (parameter) and 32 (covariance matrix)
- Process ENDF/B file with processing codes as NJOY or AMPX in order to generate cross section in point-wise and/or group representation
- Test evaluations against integral benchmarks (e.g. reaction rate) sensitive to a specific energy range (RRR)

$$R = \int_{\mathrm{RRR}} \sigma(E)\phi(E)dE \qquad (4)$$

Thermal Cross Sections and Integrals

- **o23** values for fission and capture thermal cross sections are based on ^{235}U(n,f) thermal constants obtained on the basis of microscopic data (i.e., only considering Wallner thermal capture measurements)
- Fission integral (I_4=247.0 b·eV in the Figure below) between 7.8 and 11 eV based on recommendation of Neutron Standards (246.4 b·eV)

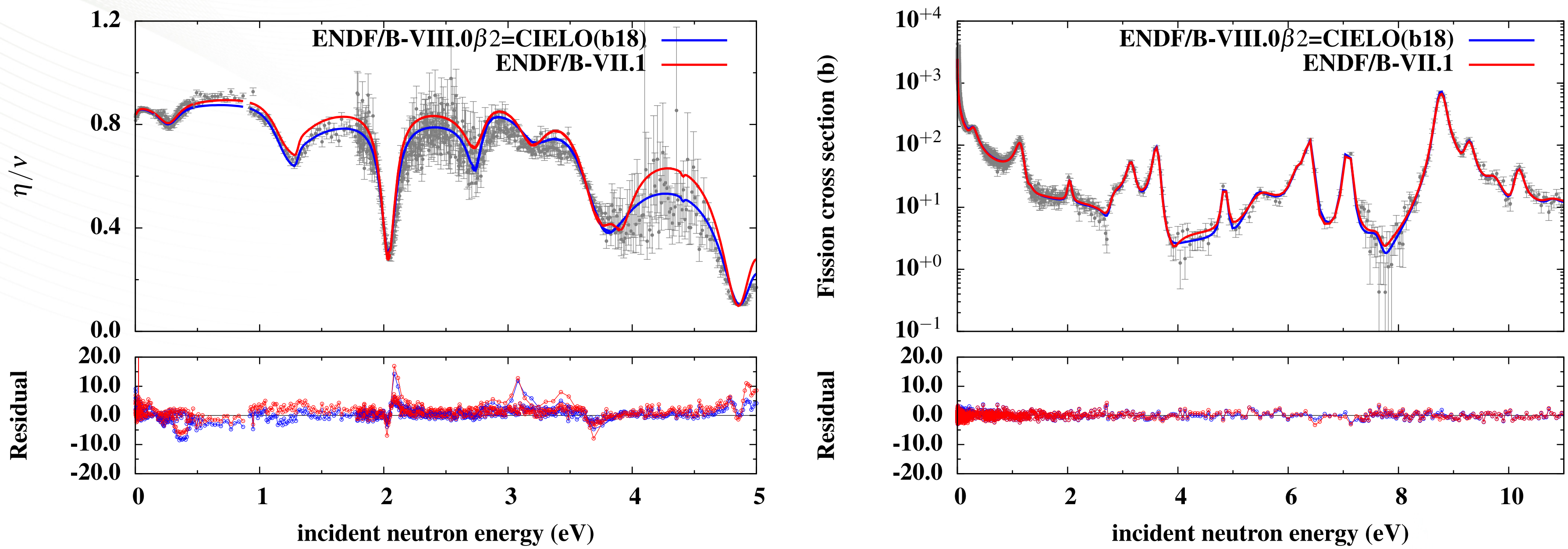


o23[a]	Standards	CONRAD	Quantity
586.6	587.15±1.36	586.4±1.5	σ_f
99.4	99.26±1.36	99.1±2.1	σ_γ
14.08	14.09±0.21	14.05±0.22	σ_{el}
0.855	0.855	0.855	η[b]
0.1694	0.1690	0.1689	α[b]

[a] T=0 K

[b] Calculated from σ_f and $\sigma\gamma$

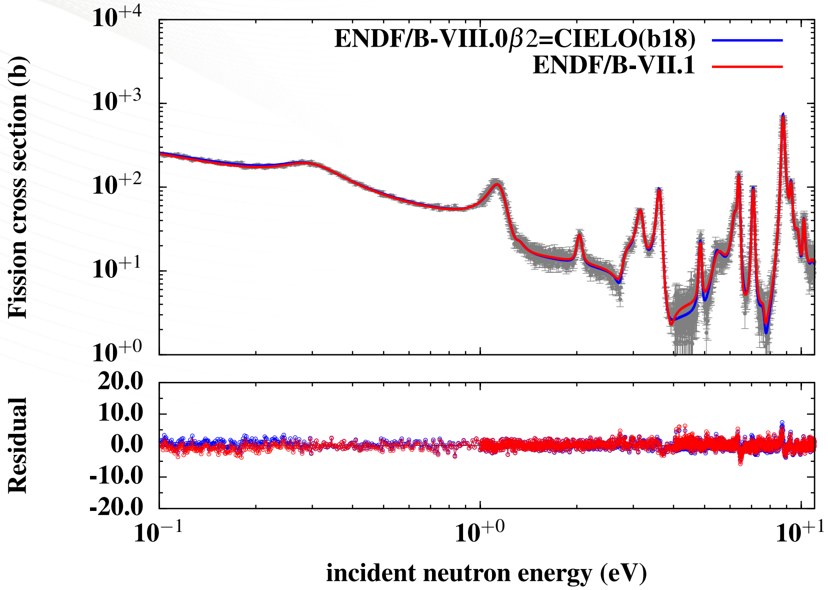
Results

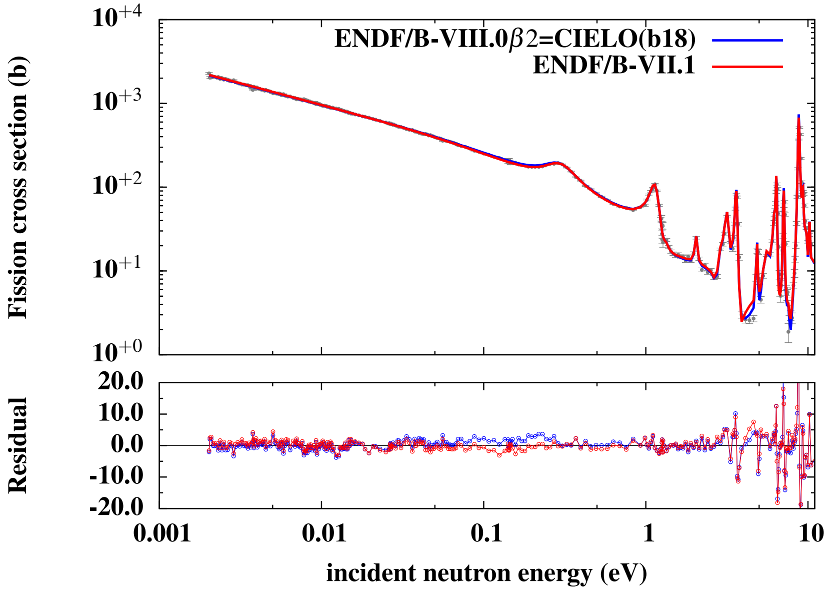


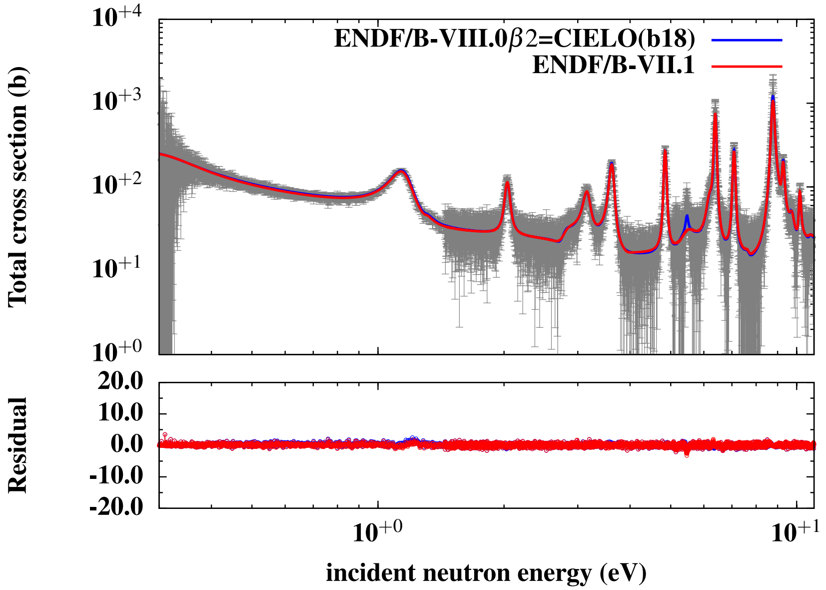
- n+^{235}U η measurements of Brooks, Wartena, and Weigmann (left) and Gwin's fission measured cross sections (right) compared to ENDF/B-VII.1 and ENDF/B-VIII.0β2 values.
- the CIELO η (decreased) values are, on average, in better agreement with the experimental data
  - achieved by increasing the capture cross sections, mostly in the valley of the resonances while keeping their peak values unchanged. The resonance at E_n=2 eV is clearly an example.
- The sensitivity of the resonance parameters to fission cross sections seems to be more relevant than to capture cross sections at neutron energies $\gtrsim 4$ eV (see fission cross sections shown in blue continuous line).

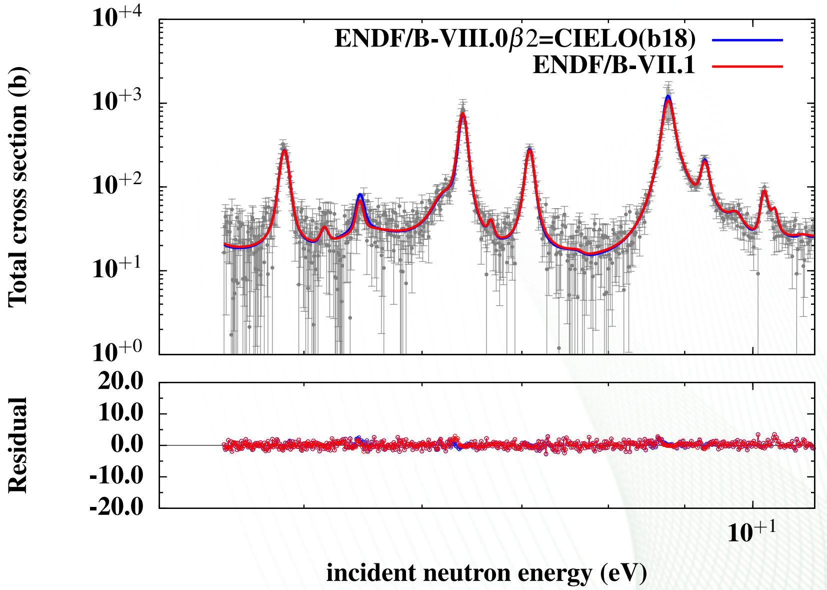
OAK RIDGE National Laboratory

Other Results









Neutron multiplicities $\bar{\nu}(E)$[2]

- In the observed $\bar{\nu}(E)$ there are clear fluctuations roughly correlated with the energy of compound nucleus resonances, but also partially explained by the influence of the (n,γf) process, where a γ is emitted prior to the fission event

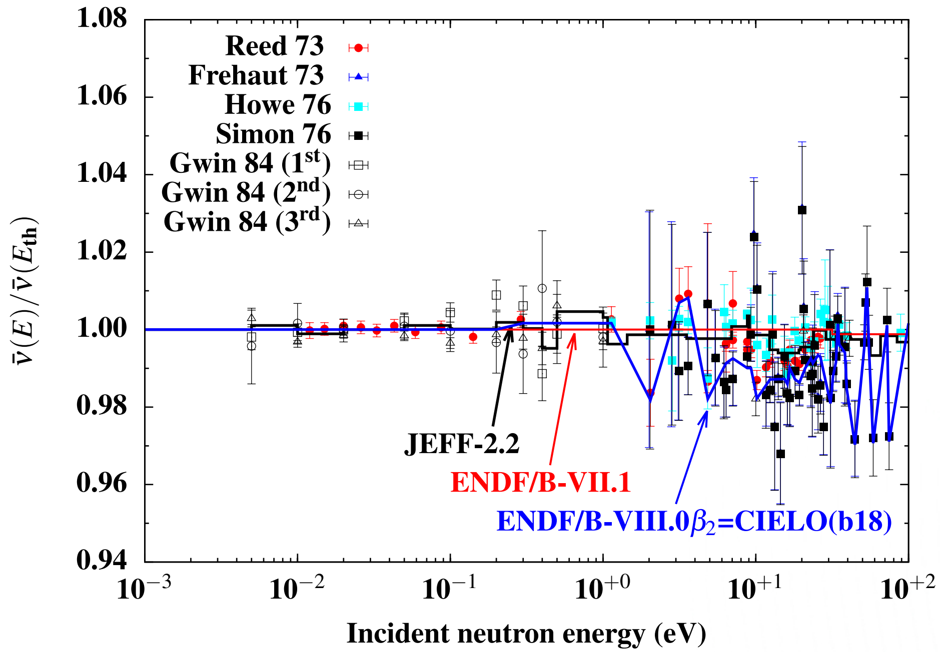


Figure 1: $\bar{\nu}(E)$ relative to $\bar{\nu}(E_{\mathrm{th}})$ calculated at thermal energy (0.0253 eV) for n+^{235}U reactions. Several experimental data sets are compared to three evaluated data.

[2]Pronyaev/Capote

ATLF benchmark simulations[3]

- Results of the suite of integral benchmarks for thermal solutions of highly enriched uranium (HEU-SOL-THERM)
- Results displayed as a function of the above-thermal-leakage fraction (ATLF)

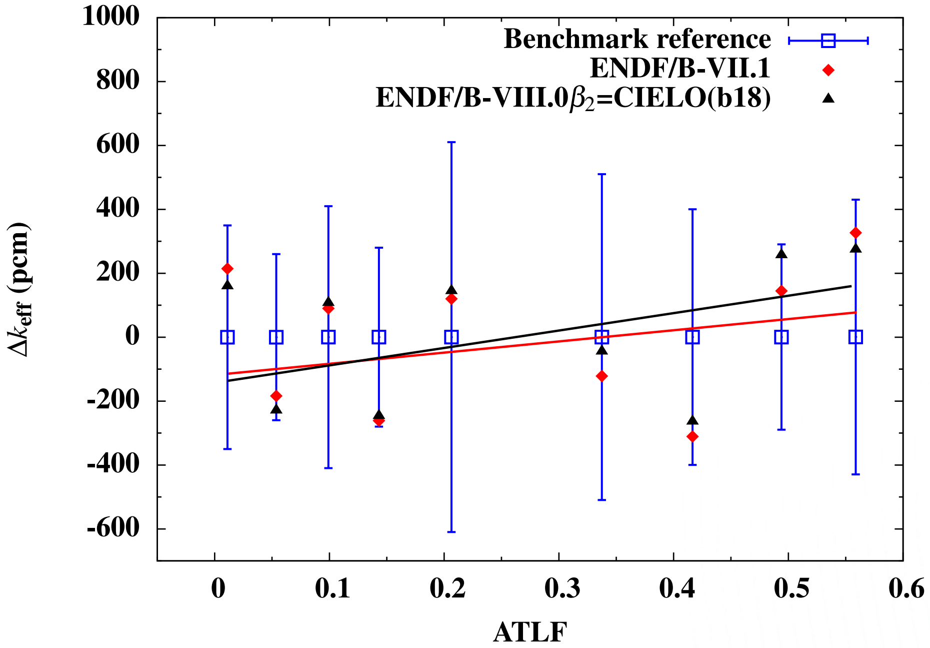
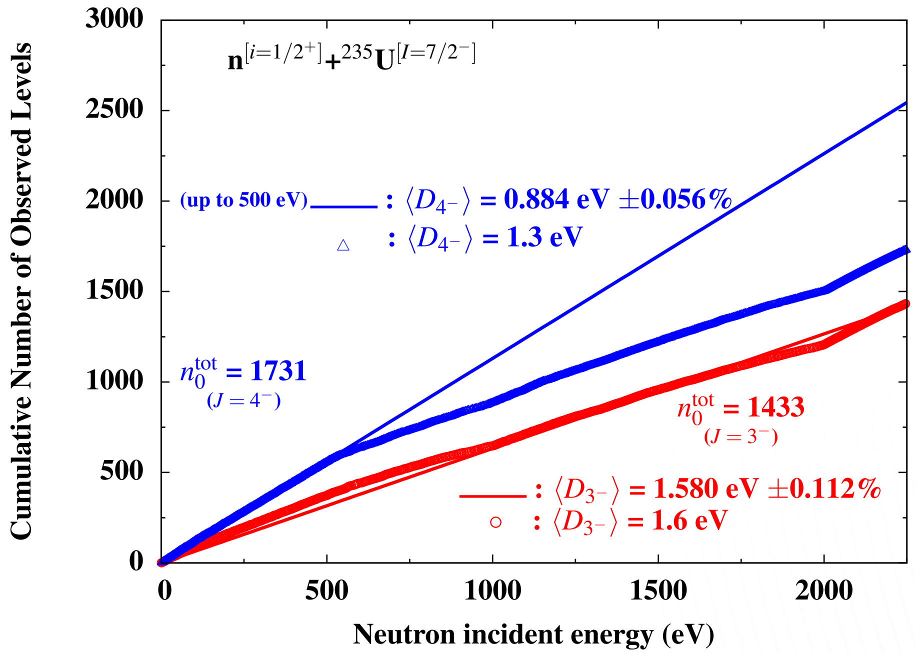


Figure 2: Differences (in pcm) between predicted and measured k_{eff} of ATLF benchmarks using ENDF/B-VII.0 (in red) and the ENDF/B-VIII.0β_2 evaluation (in black).

[3] Trkov/Capote

Future plans

- To improve the evaluation work by including newly measured data for fission and capture cross sections, namely from the RPI and nTOF collaborations
- To include an improved set of resonance parameters for incident neutron energies above 500 eV. The present evaluation is based on the ENDF/B-VII.1, in which the set of resonances are pseudo-resonances with different statistical properties than the true resonances in the energy range up 100 eV



- To include improved distribution of the fission widths. Analyses of the ^{235}U fission widths showed that the number of degrees of freedom does not obey the chi-squared distribution

OAK RIDGE National Laboratory

Summary and Conclusions

- We applied the R-matrix SAMMY method using the Reich-Moore approximation to determine a consistent set of neutron resonance parameters for ^{235}U
- The **o23**=CIELOb18 is currently part of the ENDF/B-VIII.0β3 (October 2016)
- Constraints applied on the **o23** resonance parameter evaluation are
  - Brooks'η experimental data
  - Standard thermal cross sections and the fission integral between 7.8–11 eV
  - New thermal Prompt Fission Neutron Spectra (PFNS)
- The present set of resonance parameters yields cross sections still in reasonable agreement with the suite of experimental data
- The validation analysis on the thermal benchmarks showed good agreement with the experimental response and that the **o23** resonance parameters are compatible with the current values of $\bar{\nu}$ (from thermal constants) and thermal PFNS (average energy 2.00$\pm$0.01)
- Paper submitted to ND2016 conference proceedings

Conclusion : new resonance analysis allowed to combine new evaluation of Thermal Neutron Constants, the recommended value of the fission resonance integral from 7.8-11 eV, new PFNS evaluation, and to describe Brooks data while keeping an excellent agreement with existing fission, capture and transmission measurements.

Acknowledgments

This work was supported by the US Department of Energy (DOE), Nuclear Criticality Safety Program (NCSP) funded and managed by the National Nuclear Security Administration for DOE.

Thank you!