On the Uranium and Plutonium Nuclear Data Evaluations

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OVERVIEW: uraniums

- ^{233}U
  - Motivation: underestimated reactivity for critical assemblies
  - FY20: updates to PFNS, thermal constants, R-matrix[1] improved subset of benchmarks (31 cases)[2]
  - FY21–FY22: RRR extended up to 2.5 keV including fluctuating $\bar{\nu}_p$. Validation including suite of 180 benchmarks[3] showed increased reactivity trend
  - FY23 (current): inclusion of ratio capture-to-fission data recently measured at LANL and updates to URR in the energy range 2.5–40 keV are in progress
- ^{235}U
  - Motivation: investigation of reactivity rates related to depletion calculations
  - FY21–FY22: ^{238}U evaluation[4] affecting the burn-up trend and updated URR evaluation by including recently measured fission data
  - FY23 (current): define strategy to improve the low reactivity at high burnup among the interplay of four nuclides (^{16}O, ^{235,238}U, ^{239}Pu). **Inclusion of sub-thermal measured ratio ^{235}U/^{238}U data (Anton Wallner)**

[1] Upper energy range is 600 eV.
[2] Annals Nuclear Energy **163** (2021) 108595.
[3] Pigni, NCSP TPR 2022.
[4] Updated evaluation released within INDEN collaboration.

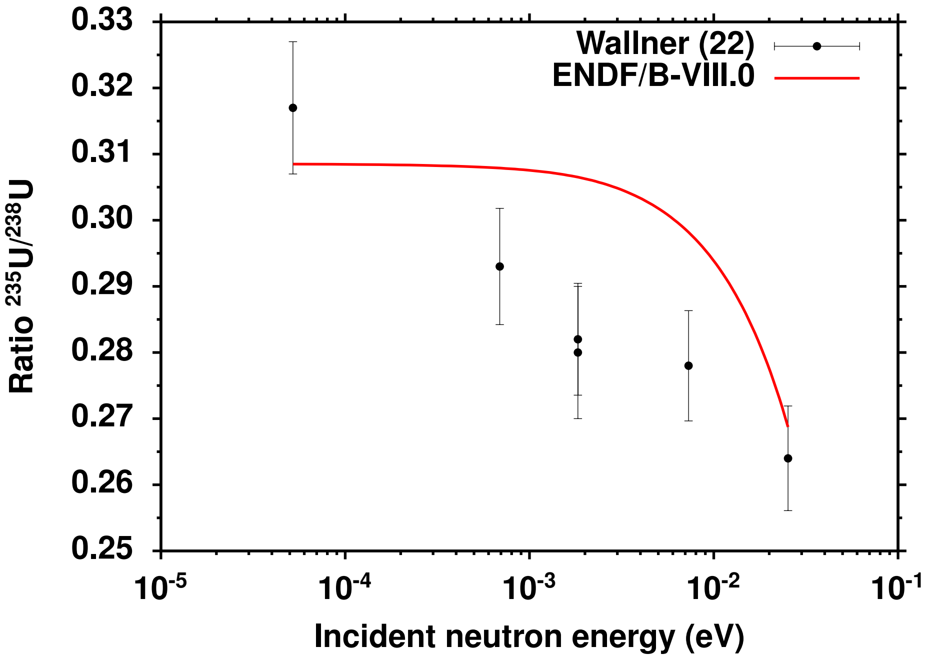
OVERVIEW: plutonium

- Current status in ENDF/B-VIII.0 (<2018):
  - Evaluated resonance parameters and related covariance matrix were adopted from WPEC (SG34)
  - WPEC (SG34) work mainly consists on merging three independent sets of resonance parameters into a single set of parameters by keeping unchanged the performances of the evaluated data on PST benchmarks and MOX fuel calculations
  - No updates in the RRR (up to 2.5 keV) performed within the CIELO collaboration
- Motivation: R-matrix analysis to include TNC values (STD 2017) and PFNS (IAEA+LANL)
- <FY20: updates in TNC and PFNS[5] with partial work to extend RRR up to 5 keV
- FY21: continuing with the extension updates and the coupling RRR and neutron fission multiplicities.
- FY22: RRR extension up to 5 keV completed including fluctuating neutron fission multiplicities.
- FY23 (current): latest ENDF file (up to 5 keV) released and currently under testing, verification, and validation. **Inclusion of Mosby (2014) ratio capture-to-fission data**

[5] INDEN evaluation (`https://www-nds.iaea.org/INDEN/`) including ORNL updates in the RRR as well as IAEA improvements in the fast region was recently adopted for ENDF/B-VIII.1 beta release.

^{235}U: inclusion of sub-thermal data

- Ratio $^{235}U/^{238}U$ data very recently measured at the Accelerator Mass Spectrometry & Isotope Research Helmholtz-Zentrum Dresden (HZDT)[6]



- ENDF/B-VIII.0 evaluations considerably deviates from the measured trend below the thermal neutron energy
- Preliminary work to reproduce the trend by varying bound energy levels and relative widths

[6]Preliminary data from Anton Wallner (TU Dresden) presented at the INDEN meeting 2022.

^{233}U and ^{239}Pu: inclusion of LANL ratio capture-to-fission data

- Simultaneous measurement of coincident fission and anti-coincident capture events performed by Mosby (2014) for ^{239}Pu and by E. Leal (2022) for ^{233}U
  - These data are usually reported as a ratio capture to fission normalized to a specific energy range where resonance levels are well known

$$\alpha(E) = \frac{\sigma_\gamma(E)}{\sigma_\mathrm{f}(E)} = A\, \frac{Y_\gamma(E)}{Y_\mathrm{f}(E)} \tag{1}$$

  - A depends on ENDF capture and fission broadened cross section

$$A = \left(\int \sigma_\mathrm{f}^{\mathrm{ENDF}}\, dE \int Y_\mathrm{f}\, dE\right)\left(\int \sigma_\gamma^{\mathrm{ENDF}}\, dE \int Y_\gamma\, dE\right)^{-1} \tag{2}$$

- However, another option is to work in terms of detector efficiencies ε_x as

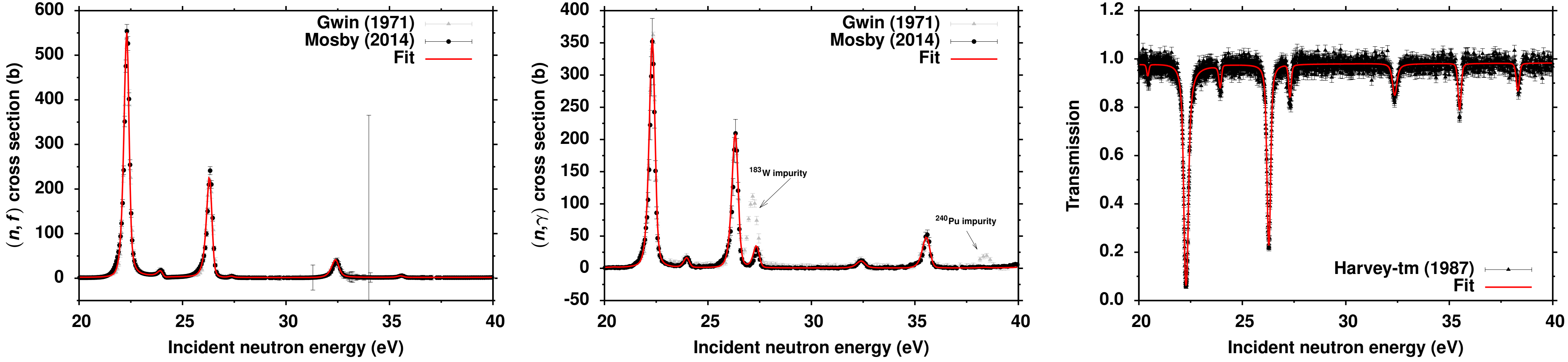
$$\alpha(E) = \frac{C_\gamma(E)}{C_\mathrm{f}(E)} = \frac{\varepsilon_\gamma\, Y_\gamma(E)}{\varepsilon_\mathrm{f}\, Y_\mathrm{f}(E)}\,, \tag{3}$$

  where the detector efficiencies are SAMMY input parameters and the fission and capture yields can be computed including resolution broadening, self-shielding and multiple scattering corrections, …

- With detector efficiencies, SAMMY perfectly compatible to include LANL data for both capture and fission yields

^{239}Pu: preliminary fit of Mosby's data as reported

- Sequential fit of fission[7], capture, and transmission data reveals impurities in Gwin's data and a systematic enhancement in the resonance left wing tail that is typical of a resolution effect[8]



- Particularly for sharp resonances, resolution effects are important to fit peaks and tails of the capture data
- Possible improvements obtained by including optimization of detector efficiencies in the simultaneous fit: compatibility test with other measured data

[7]For Mosby's data, fission data were derived by capture and α data as defined in Eq. (1)
[8]Mosby's data were fitted by including an exponential form for the resolution broadening as implemented in SAMMY.

^{239}Pu: preliminary fit of Mosby's data as reported

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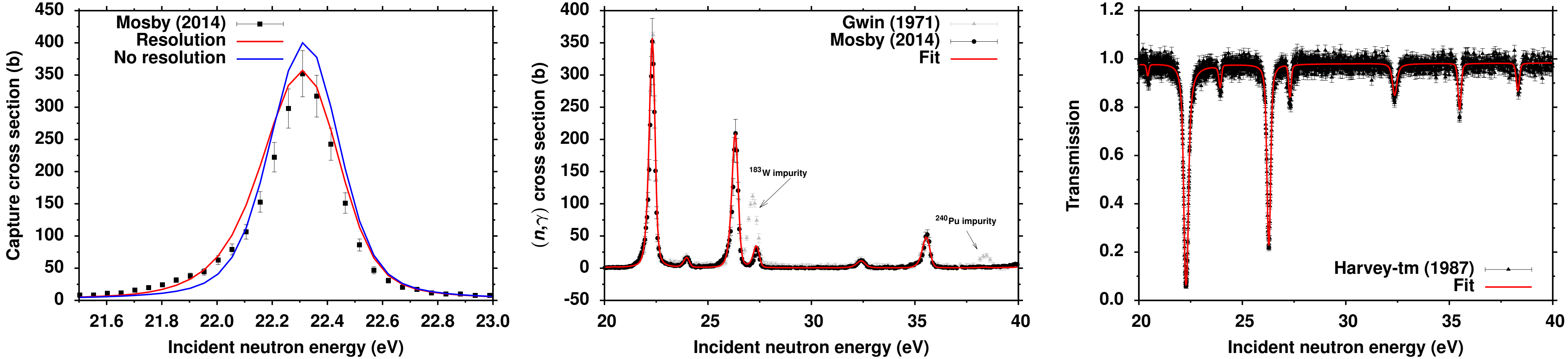


- Particularly for sharp resonances, resolution effects are important to fit peaks and tails of the capture data[10]
- Possible improvements obtained by including optimization of detector efficiencies in the simultaneous fit: compatibility test with other measured data

[9] Mosby's data were fitted by including an exponential form for the resolution broadening as implemented in SAMMY.
[10] In the figure 30% χ^2 reduction between 21-24 eV due to resolution function.

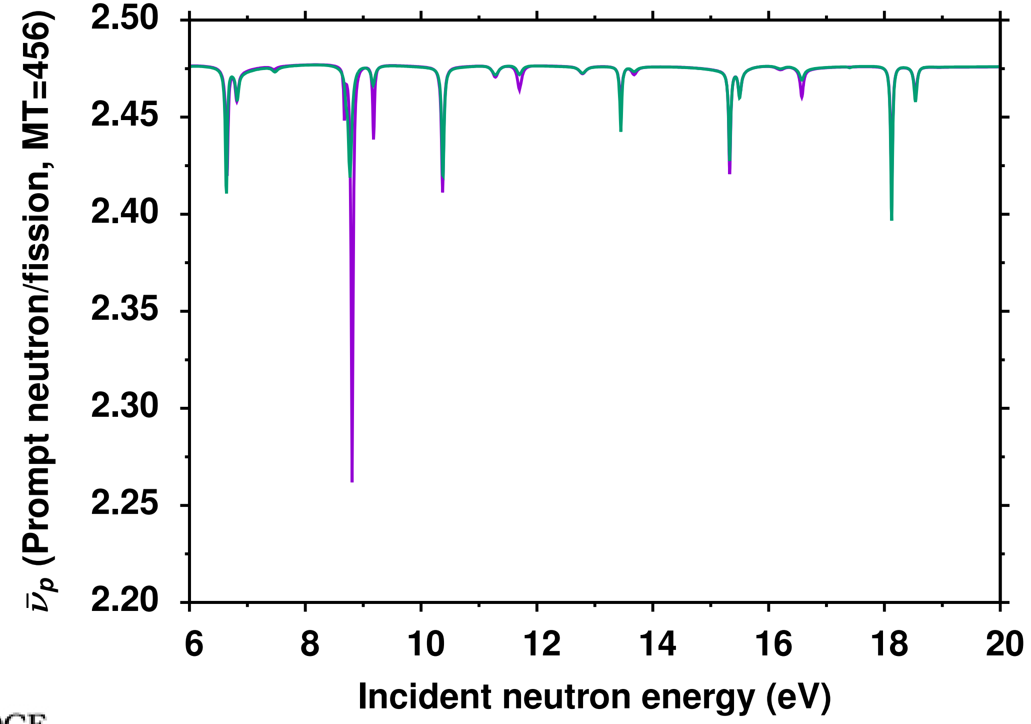
FLUCTUATING NEUTRON MULTIPLICITIES

The fluctuations depend on the corrective term $\Delta\nu^{(n,\gamma f)}$ in Eq. 4

$$\bar{\nu}_p(E) = \nu(E) - \Delta\nu^{(n,\gamma f)}(E)\,, \qquad (4)$$

with

$$\nu(E) = \left[\sum_J \nu_c^J \sum_{k_J} \sigma_f^{k_J}(E)\right] / \sigma_f(E)\,, \qquad \Delta\nu^{(n,\gamma f)}(E) = \left[\sum_J C_J \sum_{k_J} \sigma_f^{k_J}(E)/\Gamma_f^{k_J}\right] / \sigma_f(E)\,, \qquad \sigma_f(E) = \sum_J \sum_{k_J} \sigma_f^{k_J}(E)$$



- The model parameter C_J can be used to tune on average the depth of the fluctuations
- Deep fluctuations occur locally for resonance levels with $\Gamma_f^{k_J} \gg \Gamma_\gamma^{k_J}$
- Dense energy grid

UNCERTAINTY IN EVALUATED LIBRARIES

- Uncertainty (or covariances) reported in evaluated libraries is guided by a systematic knowledge of the experimental uncertainty
  - For instance, a common strategy is to associate relatively small uncertainty (1–2%) to the evaluated total cross sections to match similar experimental accuracy
  - Guidelines for the uncertainty of each reaction channel including related energy dependence are often compiled in the validation and verification of evaluated uncertainty
- Therefore, it is commonly accepted the US ENDF/B-VIII.0 covariance library reflects the accuracy of the measured data
  - This can be seen as a "feature" of nuclear data libraries or an overestimation of the evaluated uncertainty, for instance, when propagated to integral benchmarks
- From the evaluation point of view, the tendency to match the experimental uncertainty can lead to a "boost" of the uncertainty of the theoretical quantities such as resonance parameters reported in ENDF libraries

EXPERIMENTAL EFFECTS[11]

- **Convoluted resolution broadening** $I(t)$: specific experimental facilities (or setups)

$$\tilde{\sigma}(E) = \int_t I(t(E)-t')\,\sigma(E(t');\mathbf{p})dt' \quad \text{with} \quad I(t-t') = \int I_1(t-t_1)dt_1 \left(\prod_{k=1}^{N} \int I_{k+1}(t_k - t_{k+1})dt_{k+1} \right) I_{N+1}(t_{N+1}-t')$$

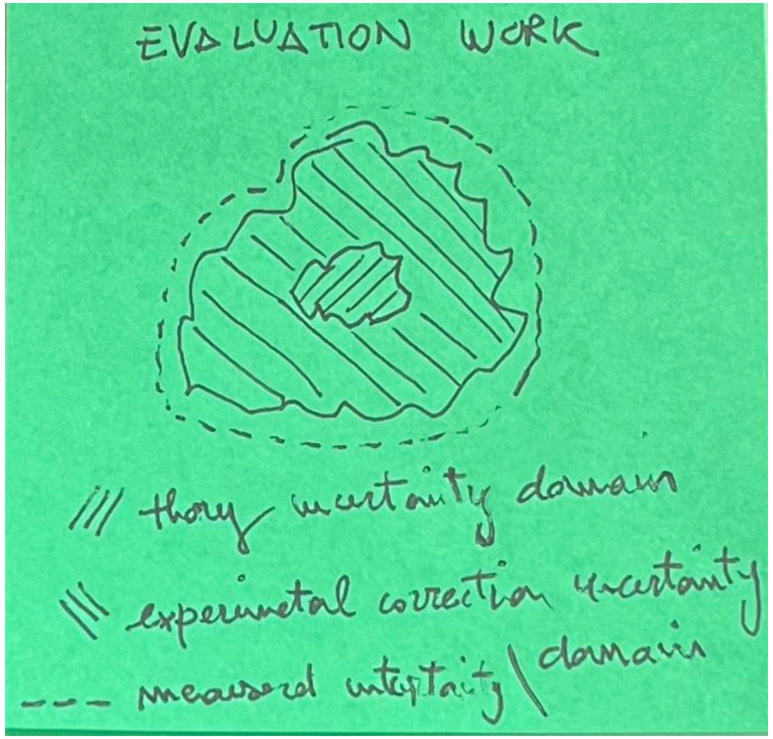
  $I_k(t)$ are functions used to describe *electron burst*, *time-of-flight channel width*, *detector types*, *neutron sources*,...

- **Doppler broadening** : temperature
- **Normalization or background corrections** : $B(t) = B_0 + B_1(t) + \ldots$
- **Self-shielding** : reduction in the measured capture counts due to interactions of incident neutrons with other nuclei
- **Multiple scattering corrections** : finite size sample[12][13]
- **Corrections for nuclide abundances** : relevant because highly enriched sample targets can be costly
- **Peak alignment** : the neutron energy in time-of-flight measurements depend on the flight-path length L and initial time t_0. These can be adjusted to have agreement among data measured sets
- **Detector efficiencies** : (see example on the next slide)

[11] As implemented in the SAMMY code.
[12] A reasonable sized sample is needed to have enough counts.
[13] **Neutron sensitivity** is another experimental effect (not yet treated) for which not only γ-rays but also scattered neutrons reach the detector and create a "false" capture event.

UNCERTAINTY IN EVALUATED LIBRARIES

- Transition from uncertainty domains in the evaluation work to ENDF library



- As long as the ENDF covariance library is guided by the experimental accuracy, the theoretical quantities are inconsistently associated with overestimated uncertainties

SUMMARY: plans for the U and Pu evaluation work

- **^{233}U**
  - Quantity: resolved and unresolved resonance parameter and neutron multiplicities $\bar{\nu}_p$
  - Energy range: 0-2.5 keV for RRR and $\bar{\nu}_p$, 2.5–40 keV for URR, to be decided for $\bar{\nu}_p$>2.5 keV
  - Covariance: preliminary by January 2023 for R(U)RR and $\bar{\nu}_p$
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NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

OAK RIDGE National Laboratory

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Thank you!

ACRONYMS

CIELO	Collaborative International Evaluation Library Organization
EALF	Energy of Average neutron Lethargy causing Fission
ENDF	Evaluated Nuclear Data File
IAEA	International Atomic Energy Agency
INDEN	International Nuclear Data Evaluation Network
LANL	Los Alamos National Laboratory
NCSP	Nuclear Criticality Safety Program
MOX	Mixed Oxide
ORNL	Oak Ridge National Laboratory
PFNS	Prompt Fission Nuclear Spectrum
RRR	Resolved Resonance Region
SG	Sub Group
TNC	Thermal Nuclear Constant
TPR	Technical Program Review
URR	Unresolved Resonance Region
WPEC	Working Party on International Nuclear Evaluation Co-operation