Unresolved resonance region cross section measurements and validation

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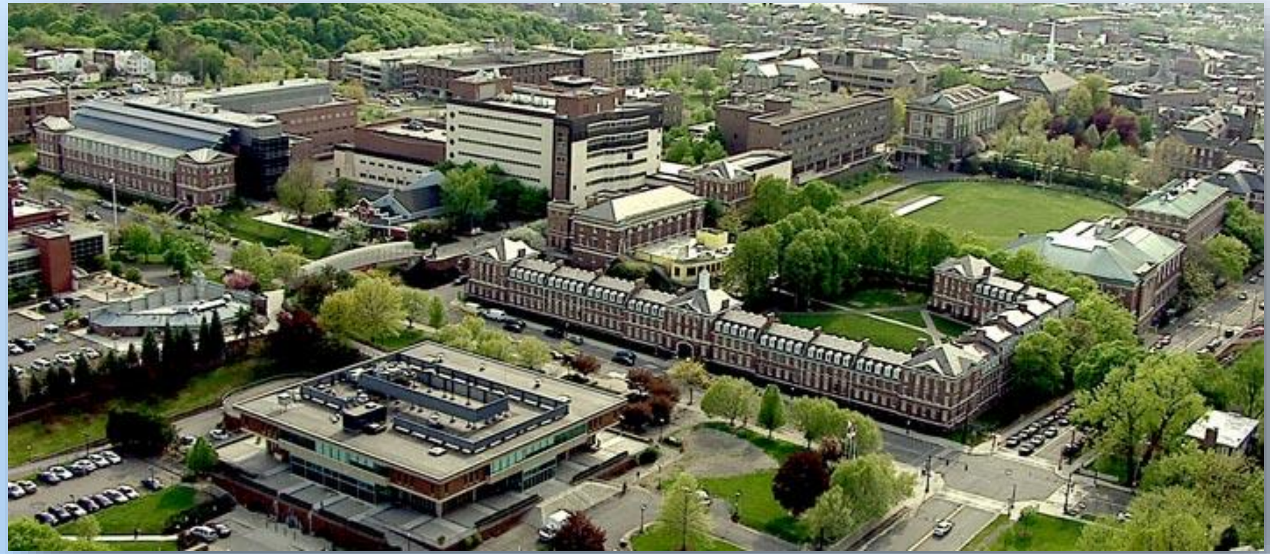

SG51, WPEC, May 15, 2024, NEA, 46, quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

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Outline

- The ENDF format and its implication for experimental data
- The effect of self-shielding on measured cross sections
  – Some call this effect transmission enhancement (to be explained)
- From experiment to evaluation
- Processing “high energy resolution” transmission for URR evaluation
- Examples
  – Ta-181 transmission, capture, and validation
  – U-238 transmission and self-indication

Unresolved resonance region experiments

- The URR energy range starts where resonances can no longer be experimentally resolved
- In the URR:
  - Observed resonances overlap
  - Some resonances are small and not observable (higher *l*-values)
- Quantities of interest for evaluation (more on this later)
  - Average cross section (we measure neutron transmission and capture/fission yield)
  - Angular distributions
- Issues
  - Measured average transmission or yield have some amount of self-shielding
  - Intermediate structure results in broad fluctuations (valid for some nuclides)
  - Difficult to handle more than one isotope in a measured sample
  - Information from partly resolved cross sections is lost (need smooth data)
    - Improvement might be possible but is it needed?
  - URR has a relatively small effect in most applications, thus approximations are often used.

URR options in ENDF

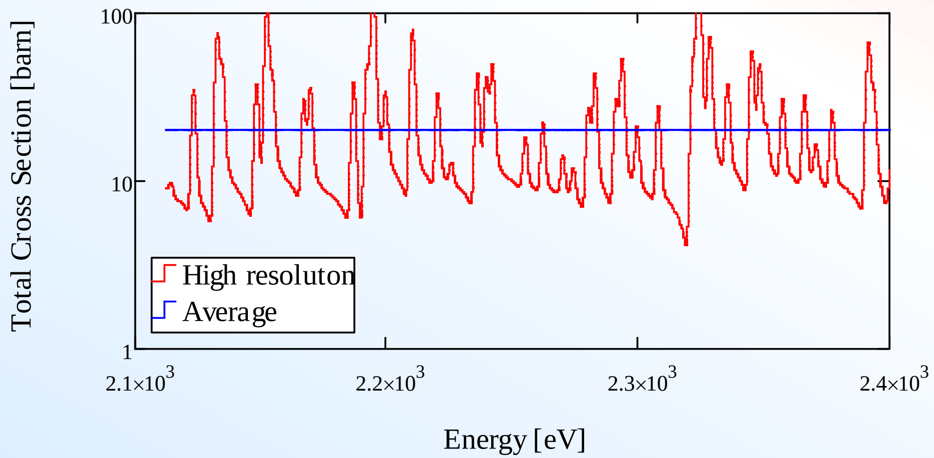
- **LSSF**=0
  - File 2 – URR parameters
    - Used to generate probability tables (or self-shielding factors)
  - File 3 – background cross section (usually zero)
  - Cross section = (File 2 generated cross section) + (File 3 background)
- **LSSF**=1
  - File 2 – URR parameters
    - Used to calculated self-shielding factor SF= <σ from F2 shielded>/<σ from F2 not shielded>
  - File 3 – Gross structure infinite dilution cross section (with covariance in file 33)
  - Cross section = SF (File 2) x cross section(File 3) (fixes the energy grid)
- Probability tables and self-shielding factors are generated in application codes like NJOY
- URR average cross section is generally represented as **smooth function** of average URR parameters in a certain energy range around energy E_s.

$$\langle \sigma_x(E) \rangle = f(E_s, \bar{D}^{J,l}, \bar{\Gamma}_n^{J,l}, \bar{\Gamma}_\gamma^{J,l}, \bar{\Gamma}_f^{J,l}, others)$$

URR transmission enhancement example

- Example calculating neutron transmission through a 6 mm Ta sample
- If the cross-section was known in high energy resolution, the “true” transmission (what we measure):

$$\langle T \rangle = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} e^{-n \cdot \sigma_t(E)} dE = 0.59$$



- If we use only the average cross-section :

$$\bar{T} = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} e^{-n \cdot \langle \sigma_t \rangle} dE = e^{-n \cdot \langle \sigma_t \rangle} = 0.51$$

- Fluctuations enhance (increase) transmission and thus reduce the effective cross section (relative to the average) hence the term cross section self-shielding
- When measuring the total cross section with a “thick” sample, a correction for the self shielding is needed.
  - Can use two sample thicknesses →

    Froehner, et al, “Cross-section fluctuations and self-shielding effects in the unresolved resonance region “, International Evaluation Co-operation volume 15 (NEA-WPEC--15), Nuclear Energy Agency of the OECD, NEA, (1995).
  - Can use a model-based approach → SESH

    Froehner, Fritz, and Brown, Jesse, *SESH*, Computer Software. https://github.com/brownjm1968/sesh. 01 Oct. 2021. Web. doi:10.11578/dc.20211001.4.

More on URR transmission enhancement

Neutron transmission through a sample: $T(E) = e^{-n\sigma_t(E)}$

The "true" average transmission from energy E_1 to E_2

$$\langle T\rangle = \frac{1}{E_2-E_1}\int_{E_1}^{E_2} e^{-n\sigma_t(E)}dE = \frac{1}{E_2-E_1}\int_{E_1}^{E_2} e^{-n[\sigma_t(E)+\langle\sigma_t\rangle-\langle\sigma_t\rangle]}\,dE$$

Enhancement due to $\sigma_t(E)$ fluctuations

$$\langle T\rangle = e^{-n\langle\sigma_t\rangle}\frac{1}{E_2-E_1}\int_{E_1}^{E_2} e^{-n[\sigma_t(E)-\langle\sigma_t\rangle]}dE$$

Note: positive and negative contributions

$$T_{sf}(E) = \frac{1}{E_2-E_1}\int_{E_1}^{E_2} e^{-n[\sigma_t(E)-\langle\sigma_t\rangle]}dE$$

$$\bar{T} = e^{-n\langle\sigma_t\rangle}$$

Self-shielded

True average

$\langle T\rangle = \bar{T} * T_{sf}(E)$ where $T_{sf}(E) > 1, \rightarrow$ $\langle T\rangle > \bar{T}$ $\rightarrow$ $\sigma_{measured} = \frac{-1}{n}\ln(\langle T\rangle) < \langle\sigma_t\rangle$

Evaluation procedure must correctly preserve the observed fluctuations of $\sigma_t(E)$

What is measured?

- To generate a measurement suitable for evaluation, it is sufficient to measure cross sections in wide energy bins such that there are statistically enough resonances in each bin.
  - Practically we measure with much better energy resolution than needed because the data can be averaged later.
- A high energy resolution measurement will be averaged for evaluations.
- We measure neutron transmission and yield not cross sections

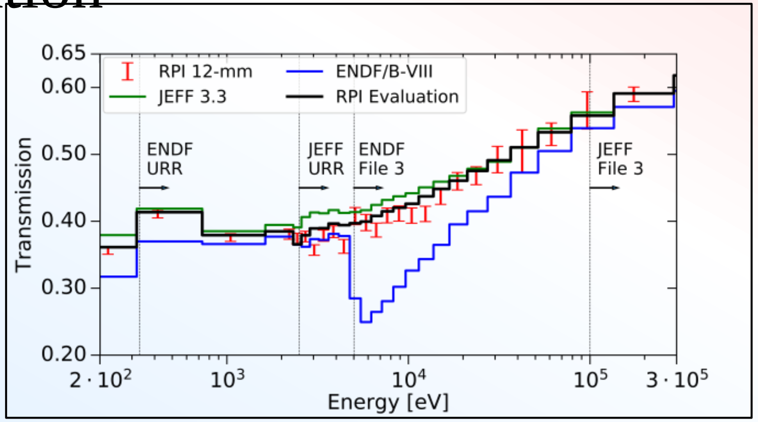
$$\langle T \rangle = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} e^{-\mathrm{n} \cdot \sigma_t(E)} \, dE \qquad \langle Y_x \rangle = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} \left(1 - e^{-\mathrm{n} \cdot \sigma_t(E)}\right) \frac{\sigma_x(E)}{\sigma_t(E)} + Y_{ms} dE$$

The big picture

Measurements

T

Validation

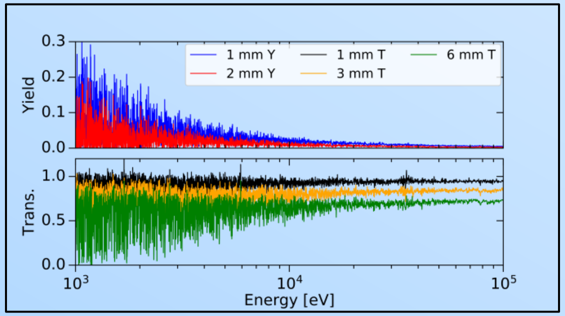


Use Thick-Sample Transmission Measurement: Validating the URR self-shielding

MCNP 6.x

NJOY 2016

Evaluation



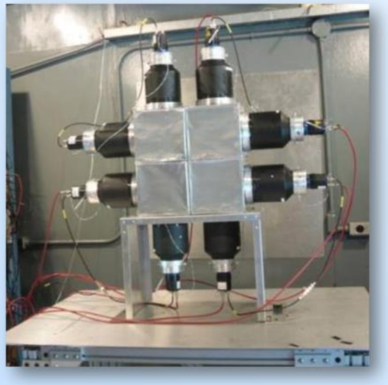
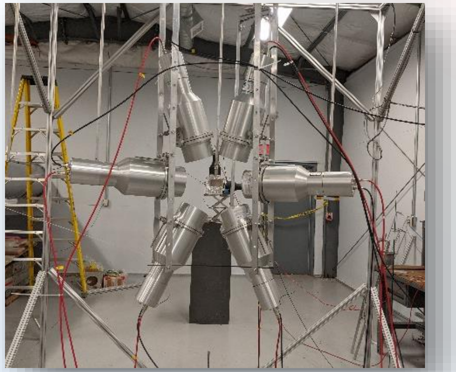
Grouped T and or Y

URR Parameters

SESH / SAMMY / FITACS

Updated URR parameters

Detectors for cross section measurements

MELINDA (100m)	^{6}Li glass (35m)	C_6D_6 Detector (45m)
		

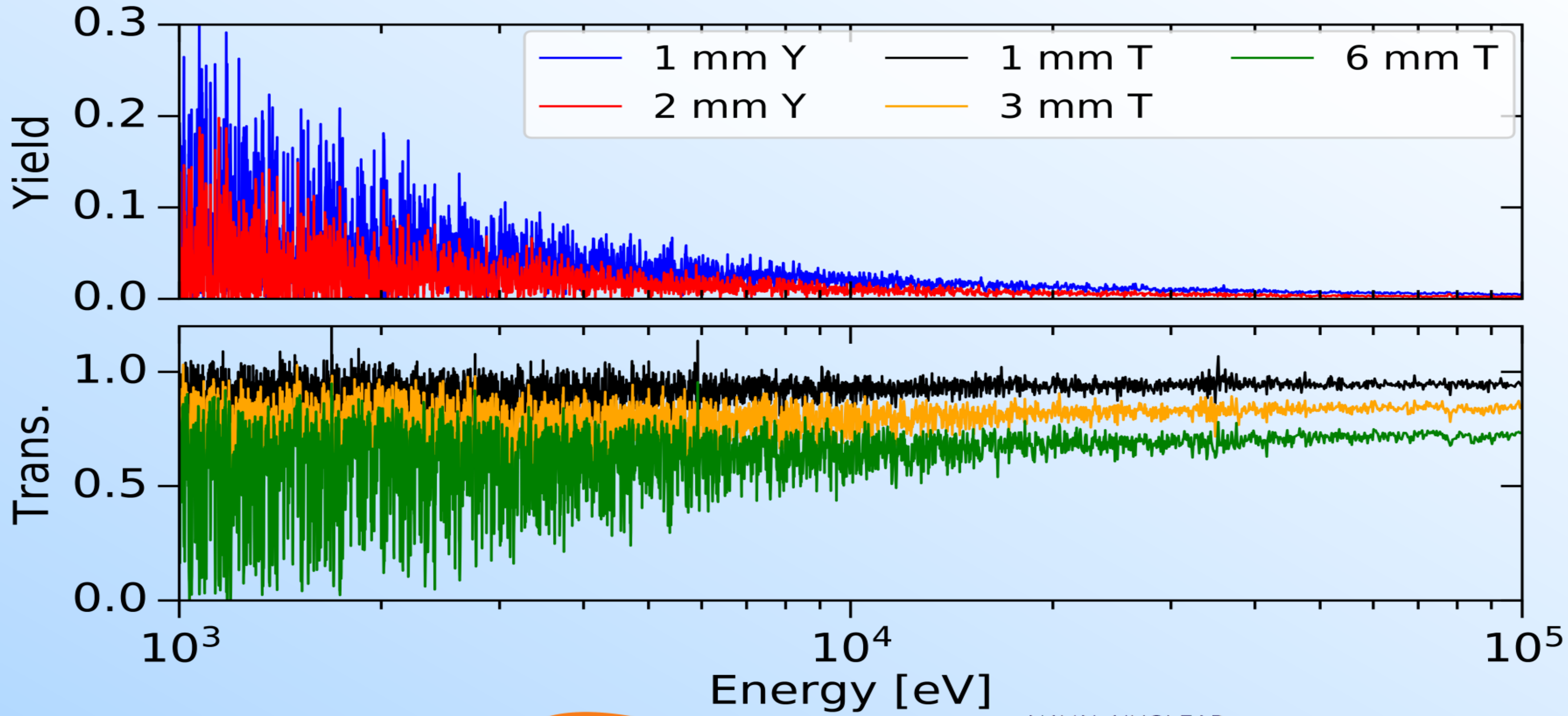
Transmission
- High energy resolution
- Fast timing
- Large active detector area
- Data-processing well understood

Transmission
- Relatively good energy resolution
- Fast timing
- Shorter flight-path enables greater count rate
- Better count rate allows freedom of neutron targets

Capture
- Highest energy resolution for capture at RPI
- Low neutron sensitivity
- Designed with digital acquisition system

Example ^{181}Ta

- ^{181}Ta Evaluation Datasets:
  - Capture Yield: 1 and 2 mm
  - Transmission: 1, 3, and 6 mm
  - URR in ENDF/B-8.1 is for E>2200 eV and structure is clearly visible in the measurements.



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How to process experimental data in the URR Transmission example

Current

Measure T in high or low resolution

↓

Group T (in TOF)

↓

Correct T for self shielding using SESH

↓

Convert T to σ_t

- To use the current (green) route
  - Need average transmission
  - If EXFOR entry has uncorrected high resolution cross section
    - Convert to transmission, group, self shielding correct, and converted back to cross section
    - Or use another method to self-shielding correct grouped cross section

A path with less self shielding correction

Measure T in high resolution

↓

Convert T to σ_t

↓

Group σ_t

↓

Correct σ_t for self shielding

- Self Shielding correction of the blue path:
  - With more then one sample use the Froehner method:

$$\overline{\langle\sigma\rangle} = \frac{n_2\overline{\sigma_1} - n_1\overline{\sigma_2}}{n_2 - n_1}$$

  - For single sample **need to know the experimental energy resolution**

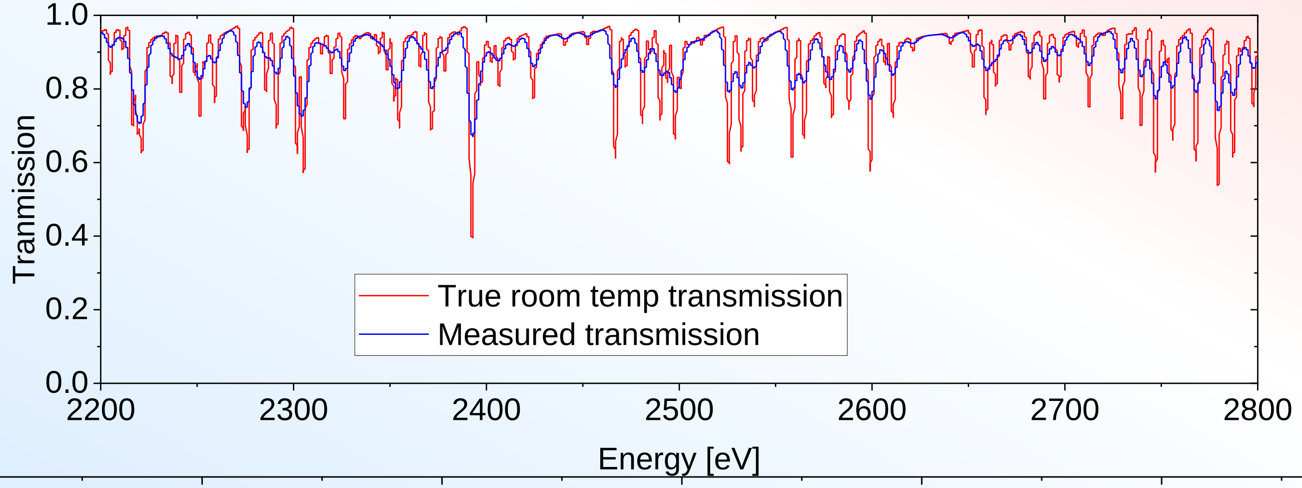
Fit averaged cross section

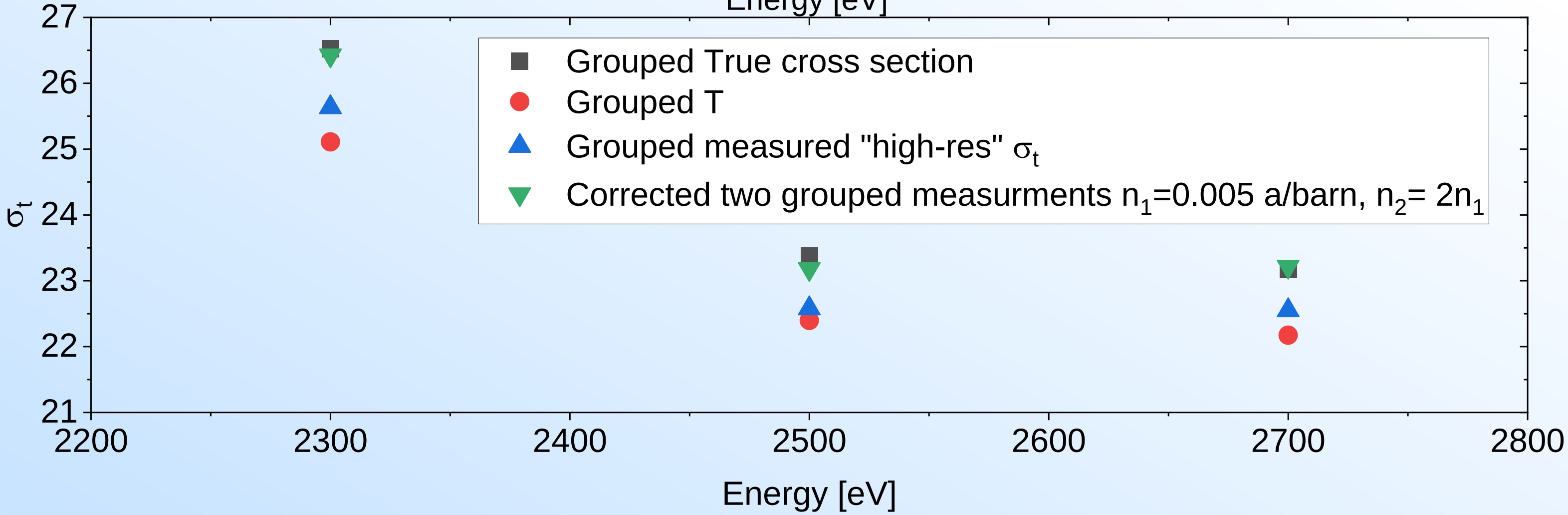
Fit σ_t with SAMMY

Recent updates to SAMMY will make thing simpler (discussed later)

Example when high resolution transmission was measured

- Assume we know the true cross section
- Include some experimental resolution
- Process in 3 ways
  1. Average the true cross section to get the true average
  2. Average transmission and convert to cross section
  3. Convert transmission to cross section and average
- No. 3 above results in close answer to the true cross section
  - However, the correction requires knowledge of the experimental energy resolution, or can be accomplished with the Froehner method if two sample thicknesses were measured
  - Correction of the average transmission requires URR parameters and a code like SESH or MCNP and can work when only on sample is available





Evaluators need to be aware of which quantity they use and how to correct SF

SAMMY Evaluation

RRR

Input:
- Resonance Parameters
- Data Reduction Parameters
- Experimental Conditions
- Experimental Data: Transmission and Capture Yield

SAMMY:
R-matrix Bayesian Fitting Program

New Resonance Parameters

URR

Input:
- Average Resonance Parameters
- Experimental Conditions
- Experimental Data: Total and Capture cross section

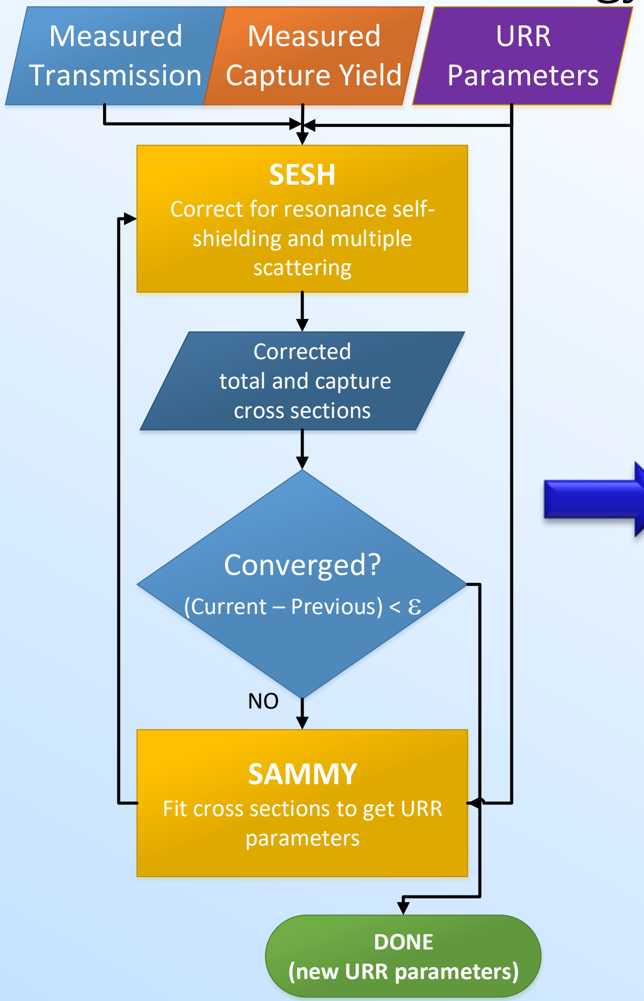
SAMMY/FITACS & SESH:
- **Hauser Feshbach Bayesian Fitting Program**
- **MC Self-Shielding Code**

New Average Resonance Parameters

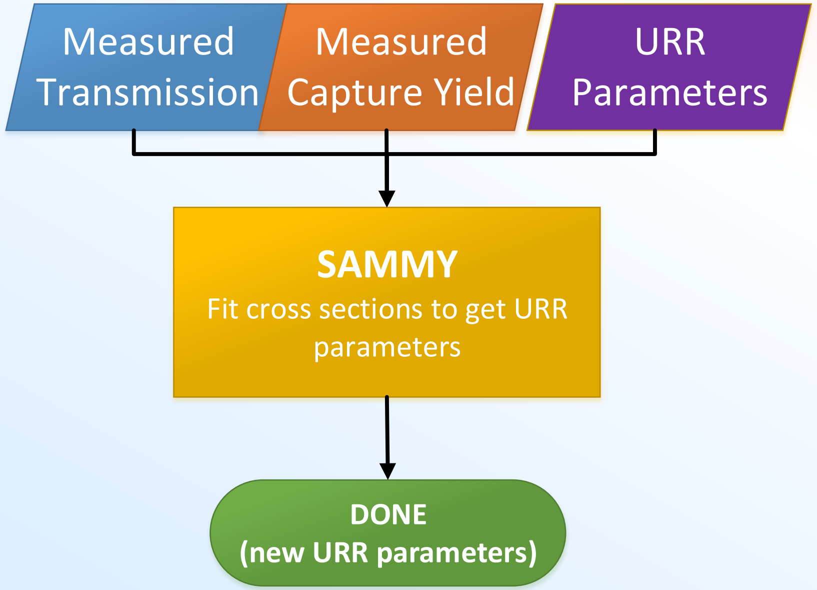
SAMMY SESH Integration

- PhD student thesis
- Collaboration with ORNL/NNL
- Help modernize SAMMY URR analysis
- Integration of a SESH like code into SAMMY
- Eliminate external iterations
- Directly fit transmission (T) and capture yields (Y) like SAMMY can do in the RRR
- SAMMY capabilities like the RRR in the URR
  - Include samples with multiple isotopes and multiple samples
  - Mix transmission and capture yield in one fit
- Completed
  - Transmission
  - Capture
  - Multiple samples
- In-progress
  - Multiple isotopes in a sample

Current URR methodology



New SAMMY

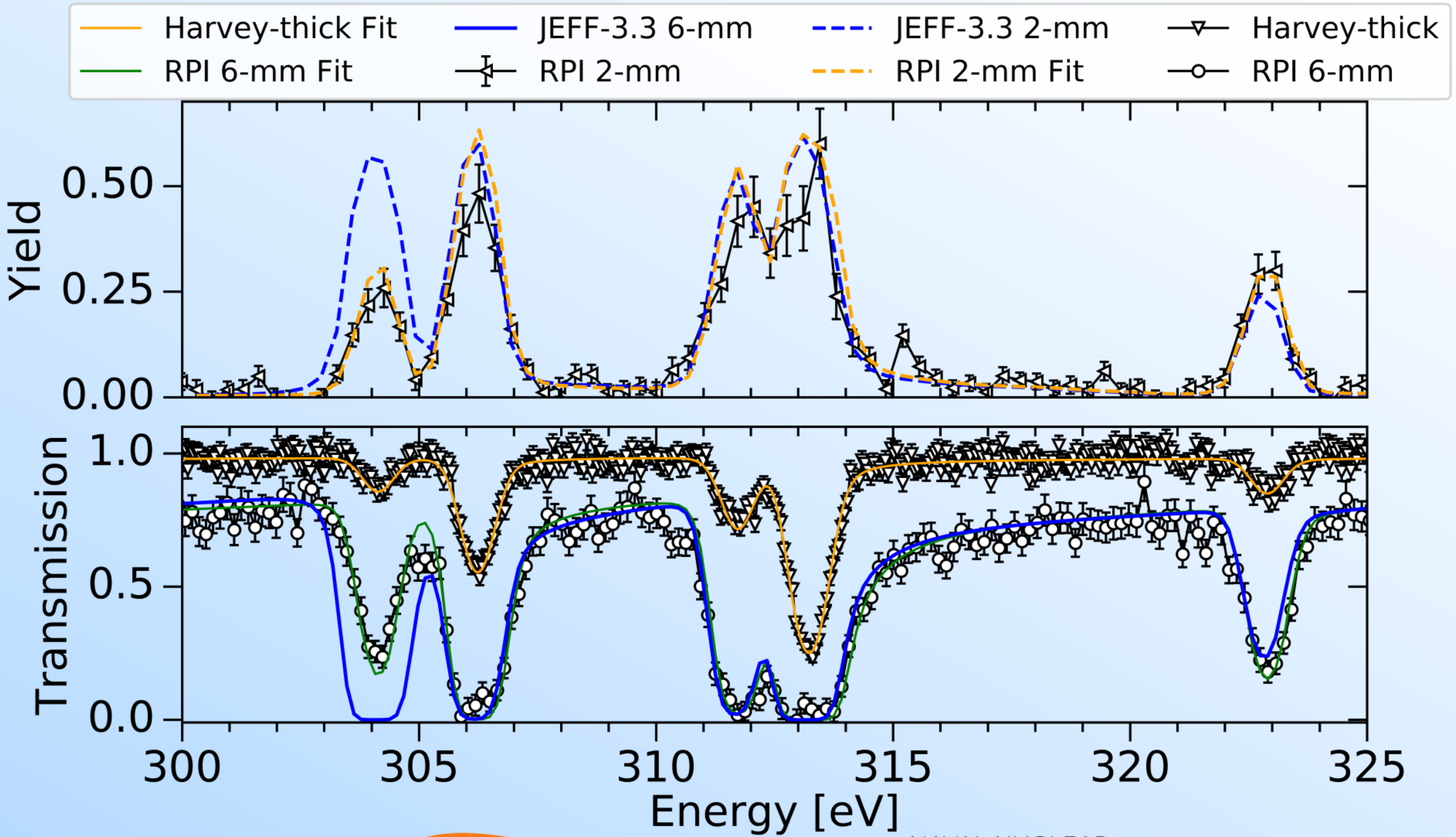


Examples from previous work

^{181}Ta Data to Evaluate: RRR (one example)

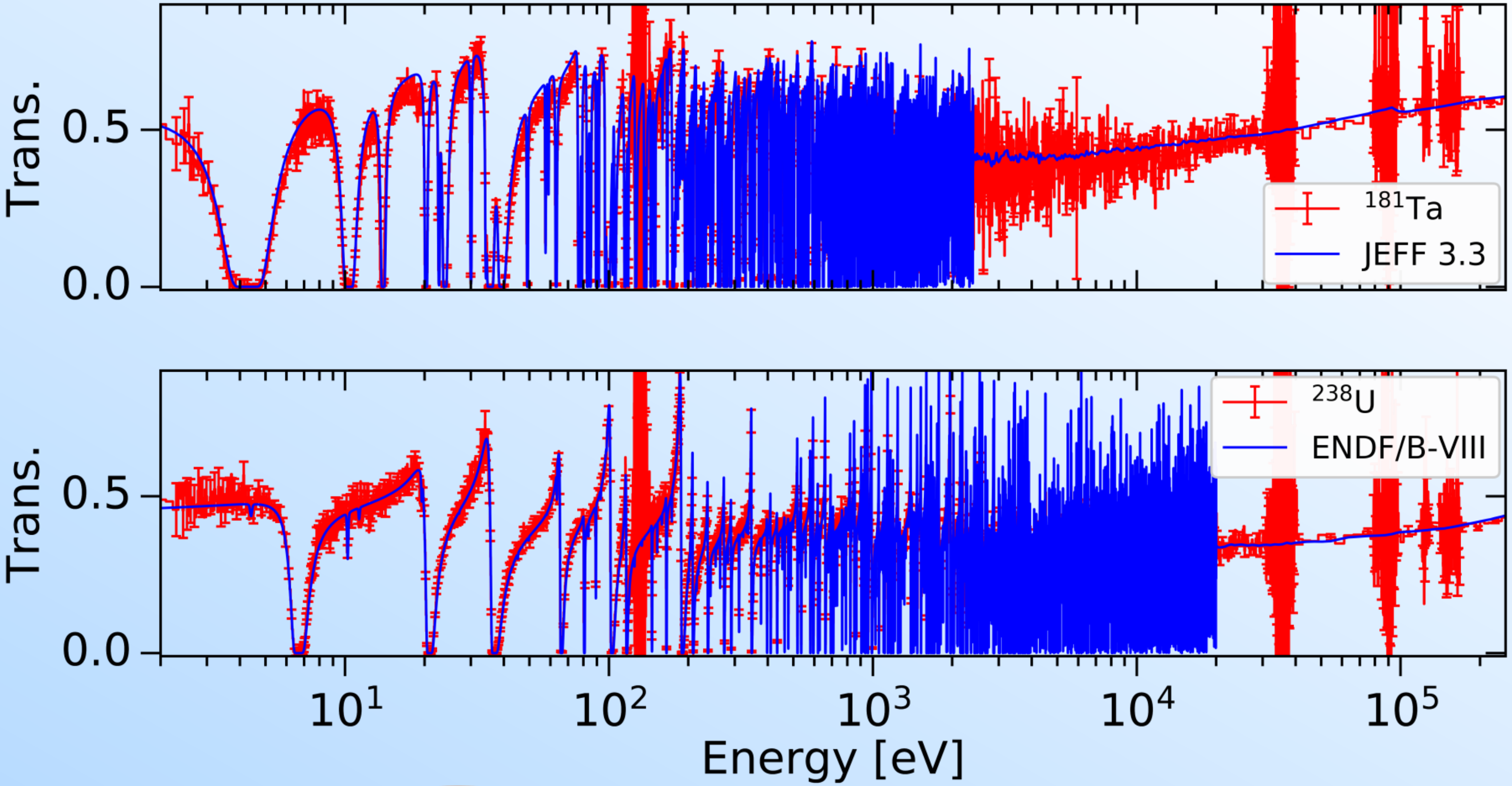
End of ENDF/B-VIII.0 RRR:

- 304 eV resonance updated
- Transmission and capture yield are well resolved



Validation of ^{181}Ta transmission data using ^{238}U

- ^{181}Ta Validation Dataset:
  - ^{181}Ta: 12 mm used as URR validation sample due to heavy self-shielding
  - ^{238}U verification dataset



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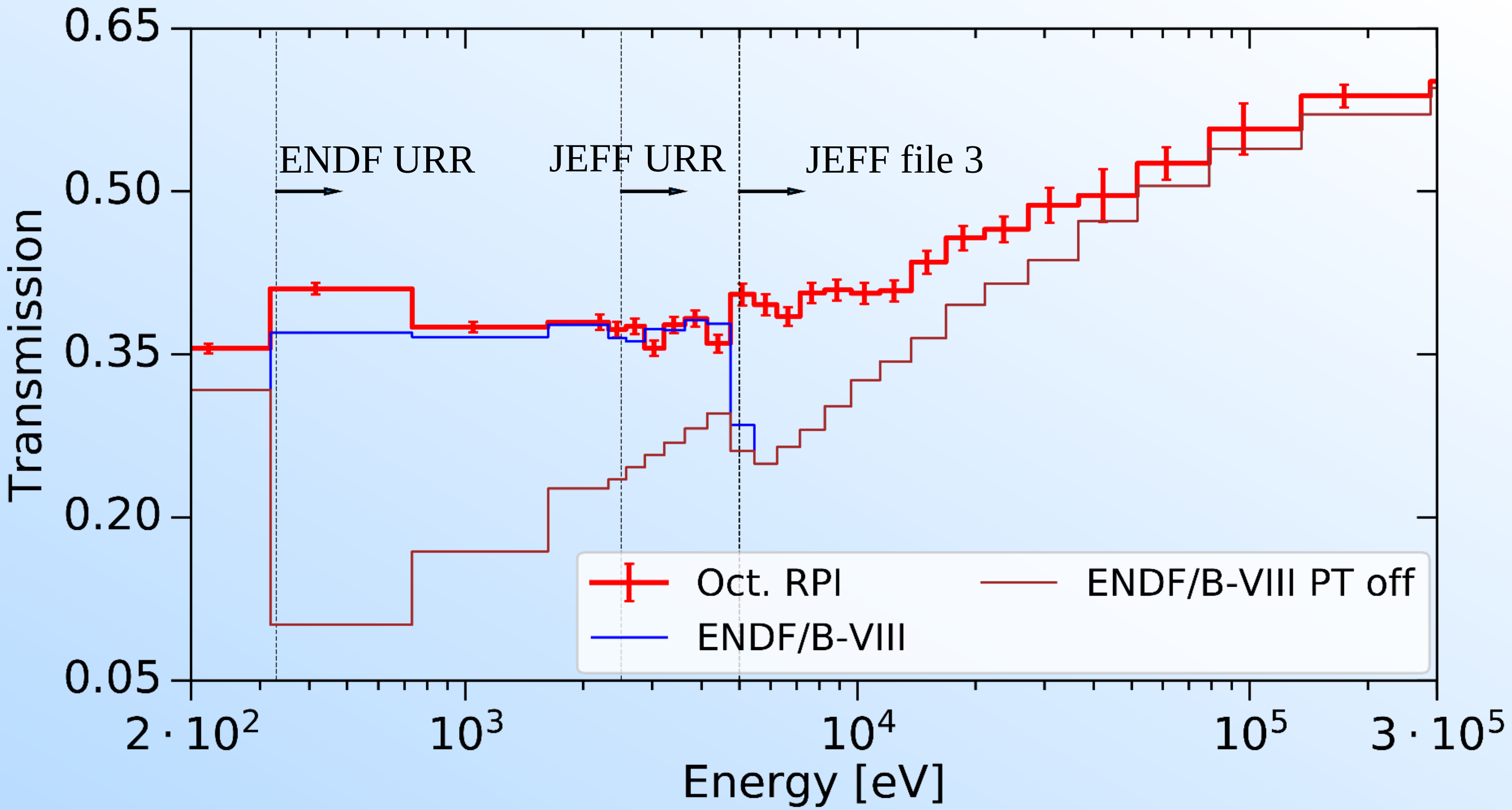
Resonance Self-Shielding effect in Ta

- The effect of self shielding is shown by turning off the URR treatment in MCNP
- Near 400 eV self-shielding increase the transmission by a factor of about 4



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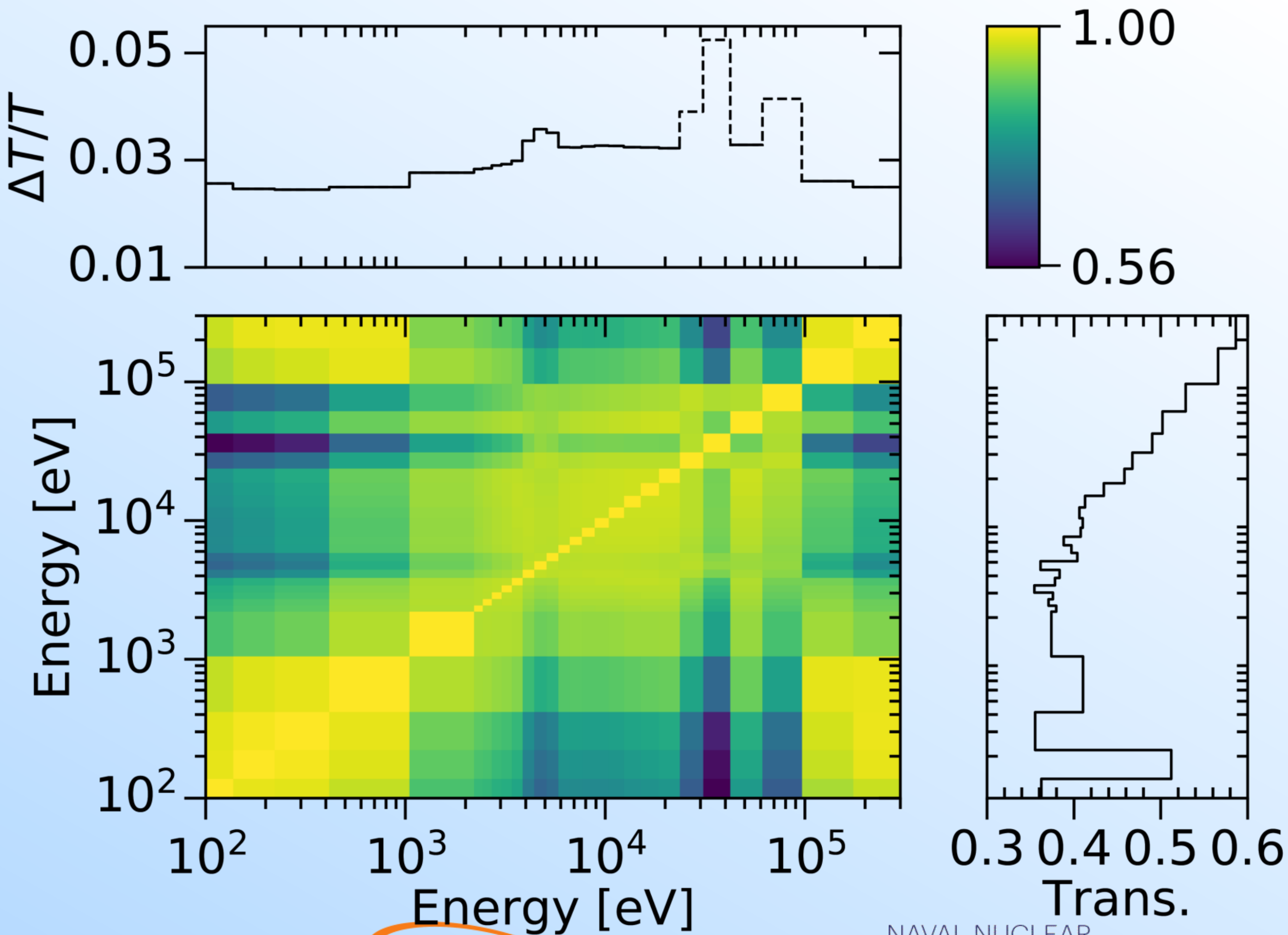
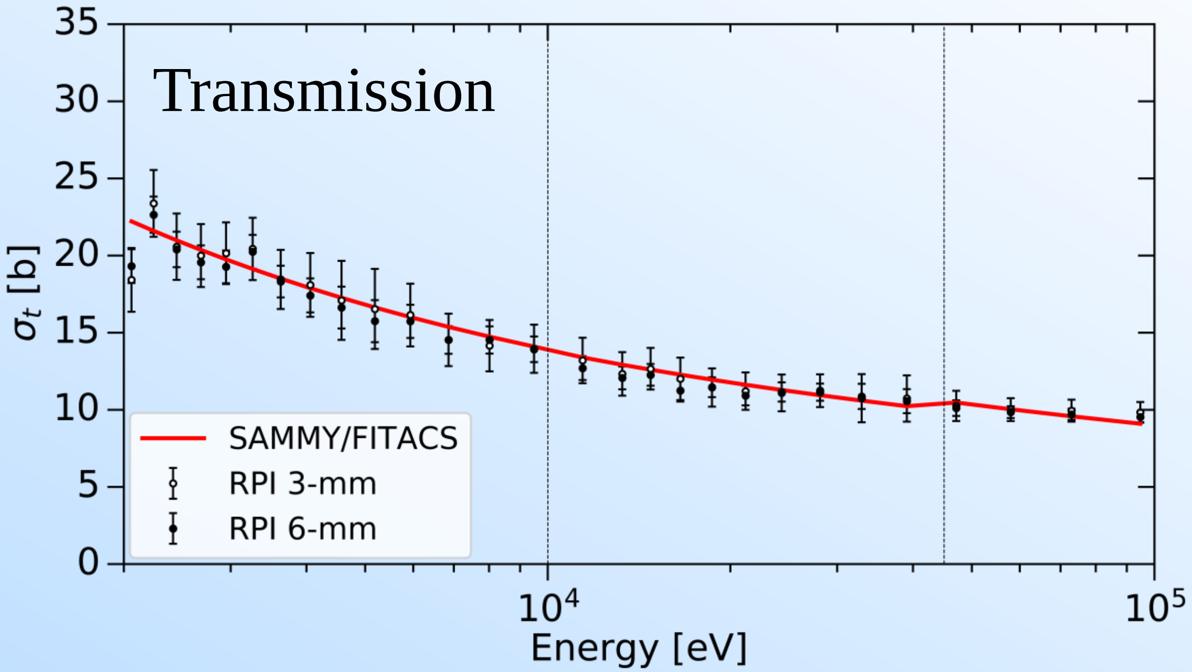
We also generate an experimental covariance (Ta-181)

$$C_y = F_x C_x F_x^T = F_{x,stat} C_{x,stat} F_{x,stat}^T + F_{x,sys} C_{x,sys} F_{x,sys}^T$$

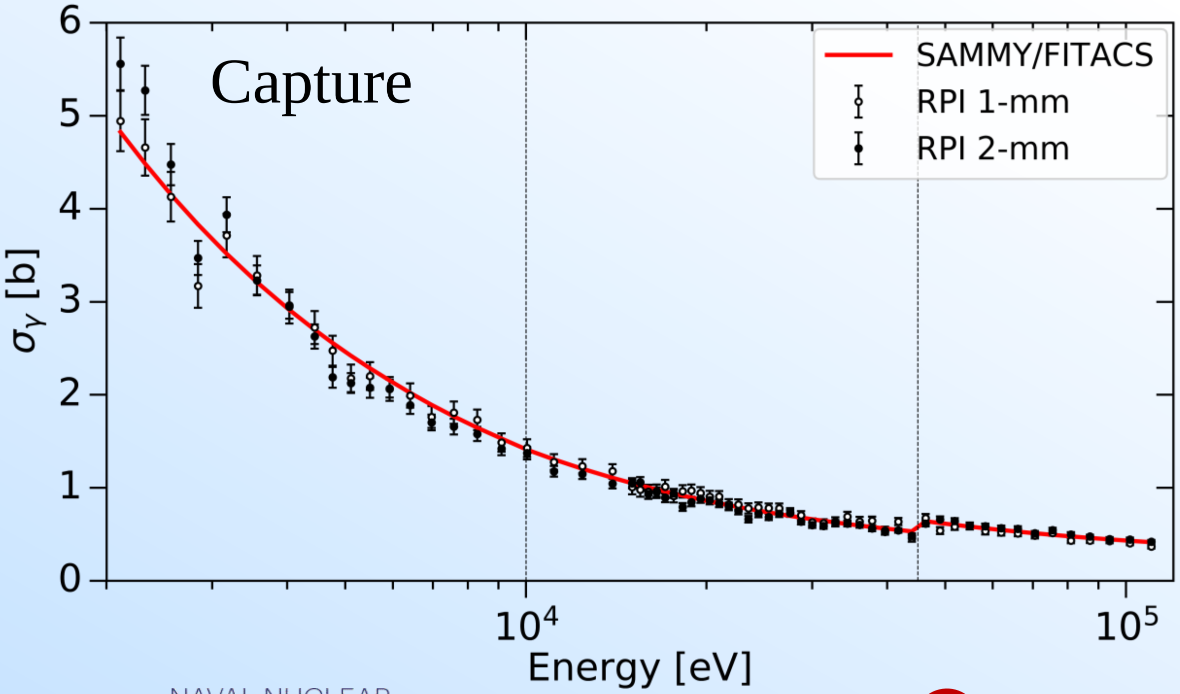


Multi-Region URR (Ta-181)



Fit options considered

1. One region URR
2. Multi Region URR
3. Extended RRR



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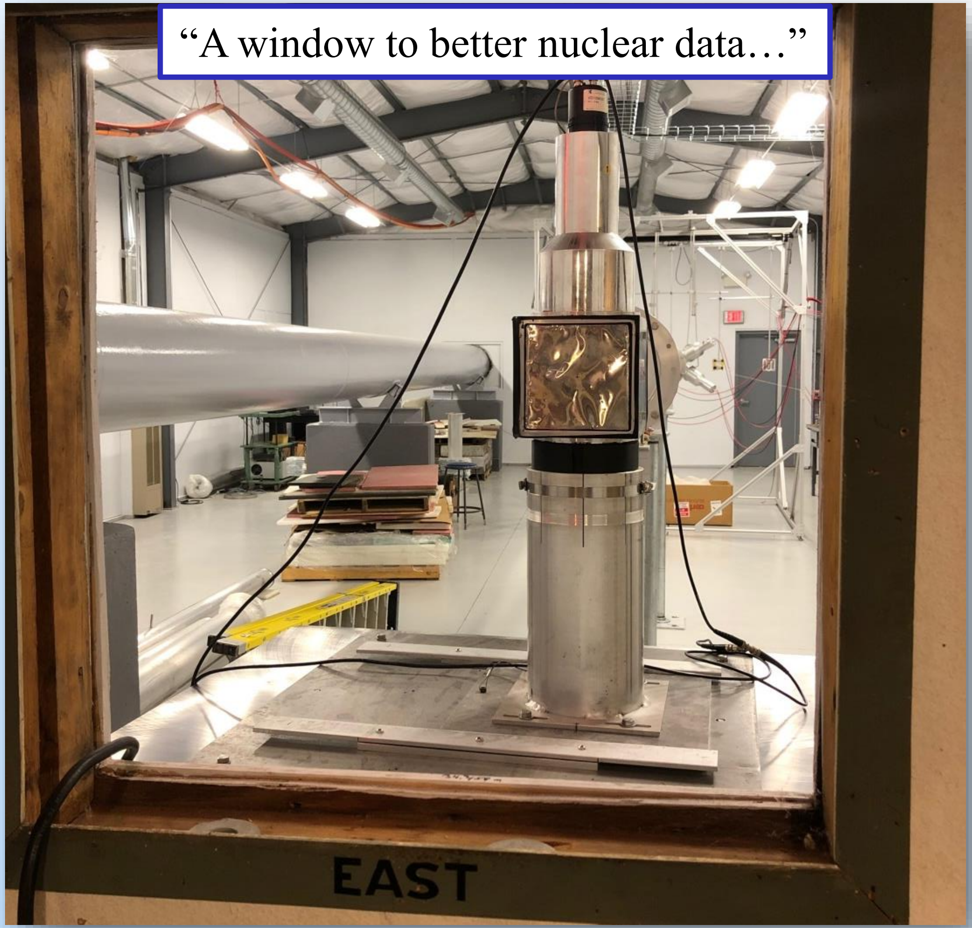
Thick sample transmission for validation

^{6}Li doped scintillating glass detector

- 2 PMT's viewing a light tight aluminum case



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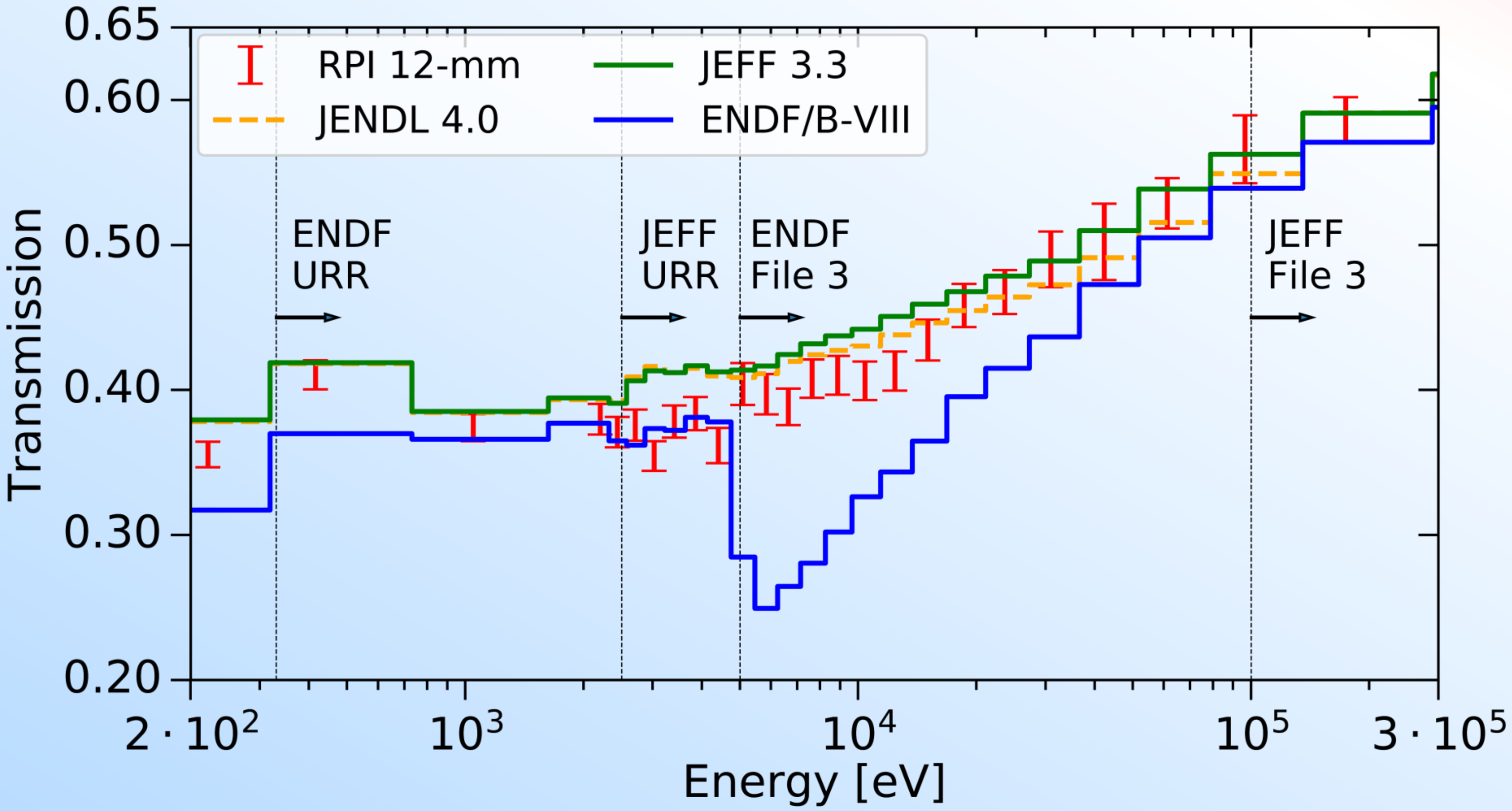
Validation Transmission and evaluations

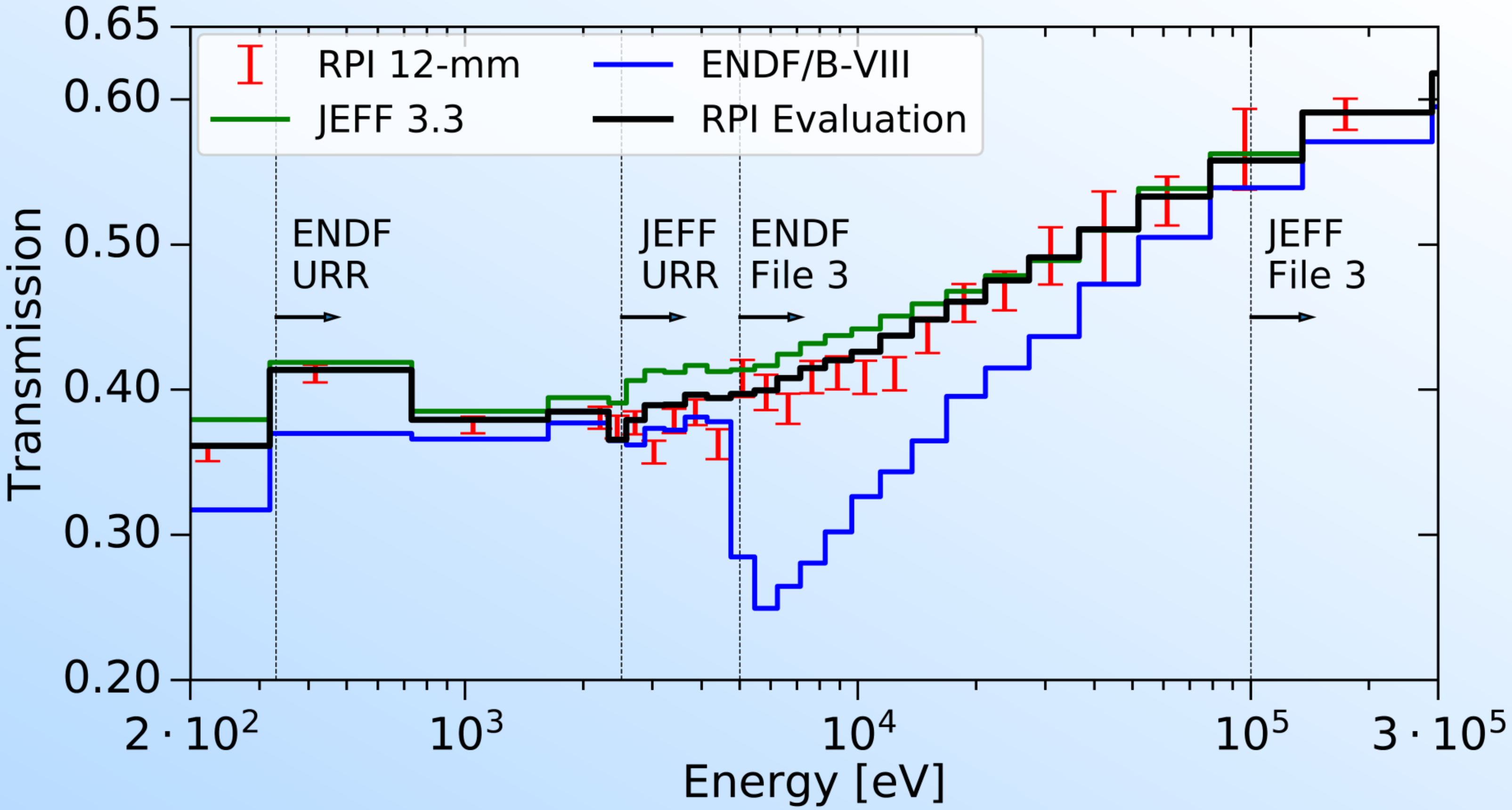
- Transmission for 12 mm sample grouped to have about 50 resonances per bin
- Observe the limitations of the URR treatment using JEFF-3.3, JENDL-4.0, and ENDF/B-VIII.0



Jesse M. Brown, R. C. Block, A. Youmans, H. Choun, A. Ney, E. Blain, D. P. Barry, M. J. Rapp and Y. Danon, “Validation of Unresolved Neutron Resonance Parameters Using a Thick-Sample Transmission Measurement”, Nuclear Science and Engineering, vol. 194, no. 3, pp. 221-231, 2019, DOI:10.1080/00295639.2019.1688087

RPI Evaluation: Updated JEFF-3.3

- Updated RRR and URR parameters
- Very sensitive to a_c, D and other $\langle Pars \rangle$
- Using the RPI evaluation we can improve agreement with measured data



Validation of URR evaluations using transmission and self indication for ^{238}U and Ta

- Revisit the data in the PhD thesis of Byoun
  - Tae Y. Byoun, Experimental investigation of the resonance self-shielding and Doppler effect in uranium and tantalum, PhD thesis, Rensselaer Polytechnic Institute, Troy, N. Y. May 1973
- Data on EXFOR was recently updated and some errors were removed.
- Includes transmission and self-indication measurements for depleted U and Ta
- Temperature dependent measurements at 77, 295, and ~l000K

What is self indication

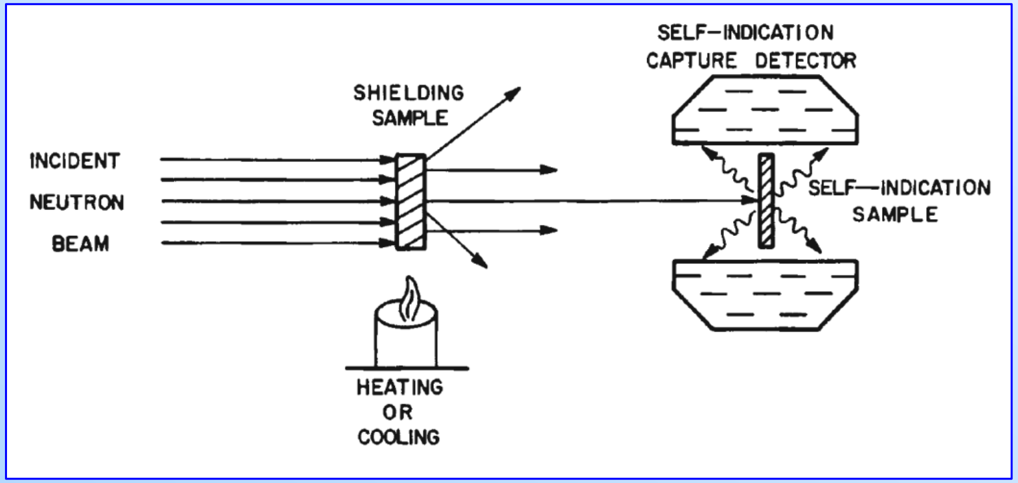
- Self-indication is a transmission experiment where a capture detector with the sample material is used to detect neutrons
- Provides information on the self shielding effect in the sample material

Transmission

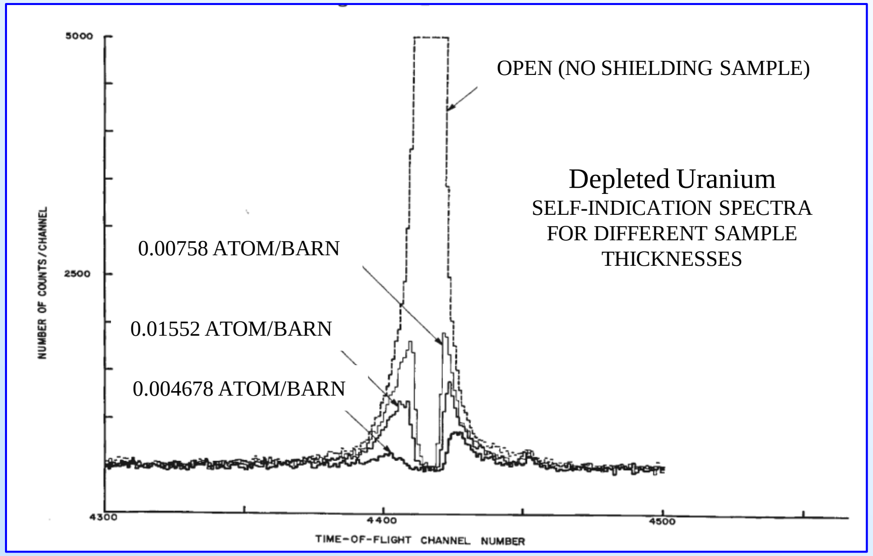
$$T = \int_{E_1}^{E_2} e^{-n\sigma_t(E)} dE$$

Self-shielded capture yield

$$Y_{si} = \int_{E_1}^{E_2} \left(1 - e^{-n\sigma_t(E)}\right) \frac{\sigma_\gamma(E)}{\sigma_t(E)} e^{-n\sigma_t(E)} dE$$



Figures from Byoun's PhD thesis



Self indication ratio (SIR)

Theory (1st order)

$$SIR = \frac{\int_{E_1}^{E_2} \left(1 - e^{-n\sigma_t(E)}\right) \frac{\sigma_\gamma(E)}{\sigma_t(E)} e^{-n\sigma_t(E)} dE}{\int_{E_1}^{E_2} \left(1 - e^{-n\sigma_t(E)}\right) \frac{\sigma_\gamma(E)}{\sigma_t(E)} dE}$$

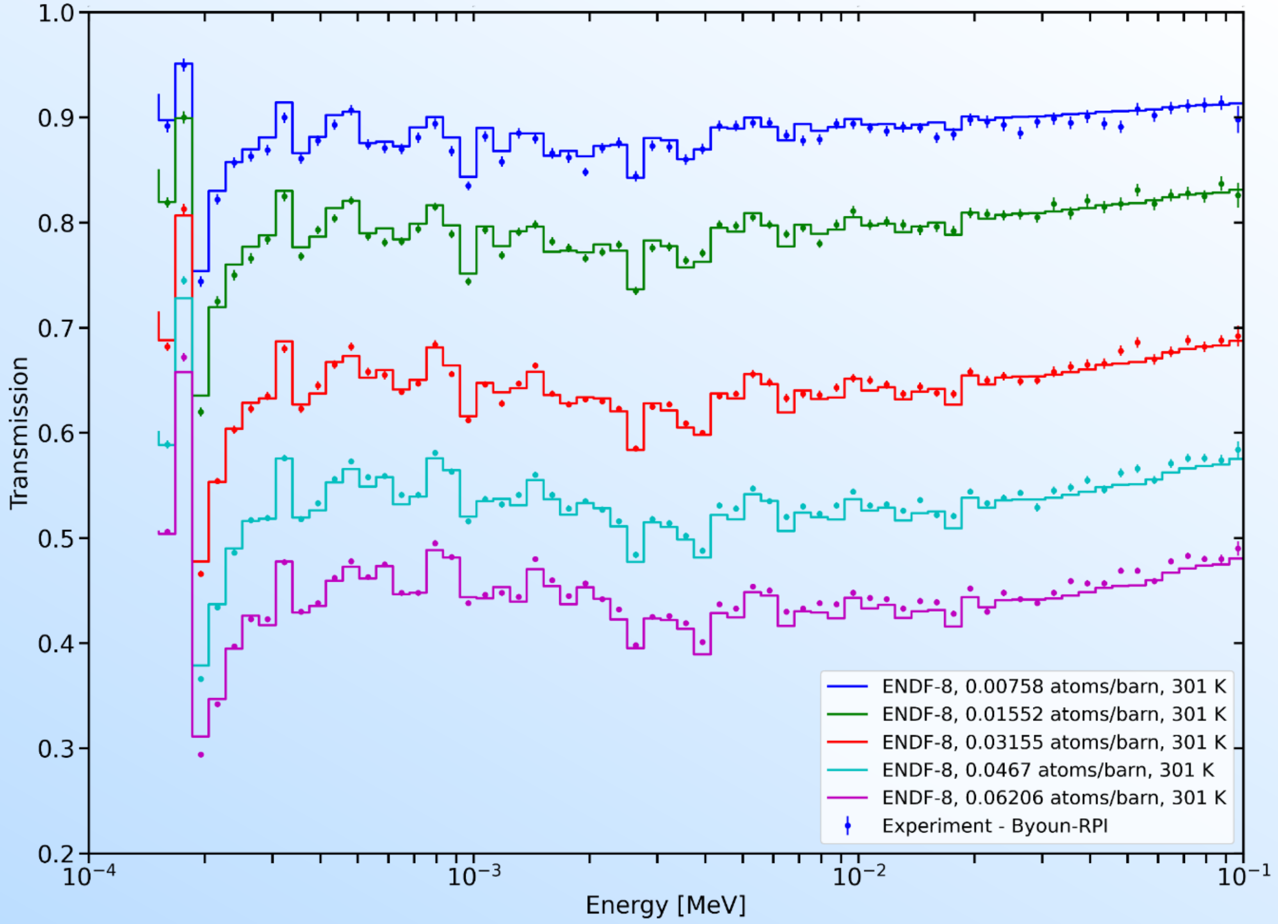
Experiment

$$SIR = \frac{\sum_{i=E_1}^{E_2} \left(C_i^s - B_i^s\right)}{\sum_{i=E_1}^{E_2} \left(C_i^0 - B_i^0\right)}$$

- C_i^s and B_i^s are measurements with the transmission sample, C_i^0 and B_i^0 without it
  - Use of a thin capture sample can simplify the math
- Increased sensitivity to resonance wings and capture interactions
- Unlike capture measurements, normalization is not needed
- The temperature of the transmission sample can be changed

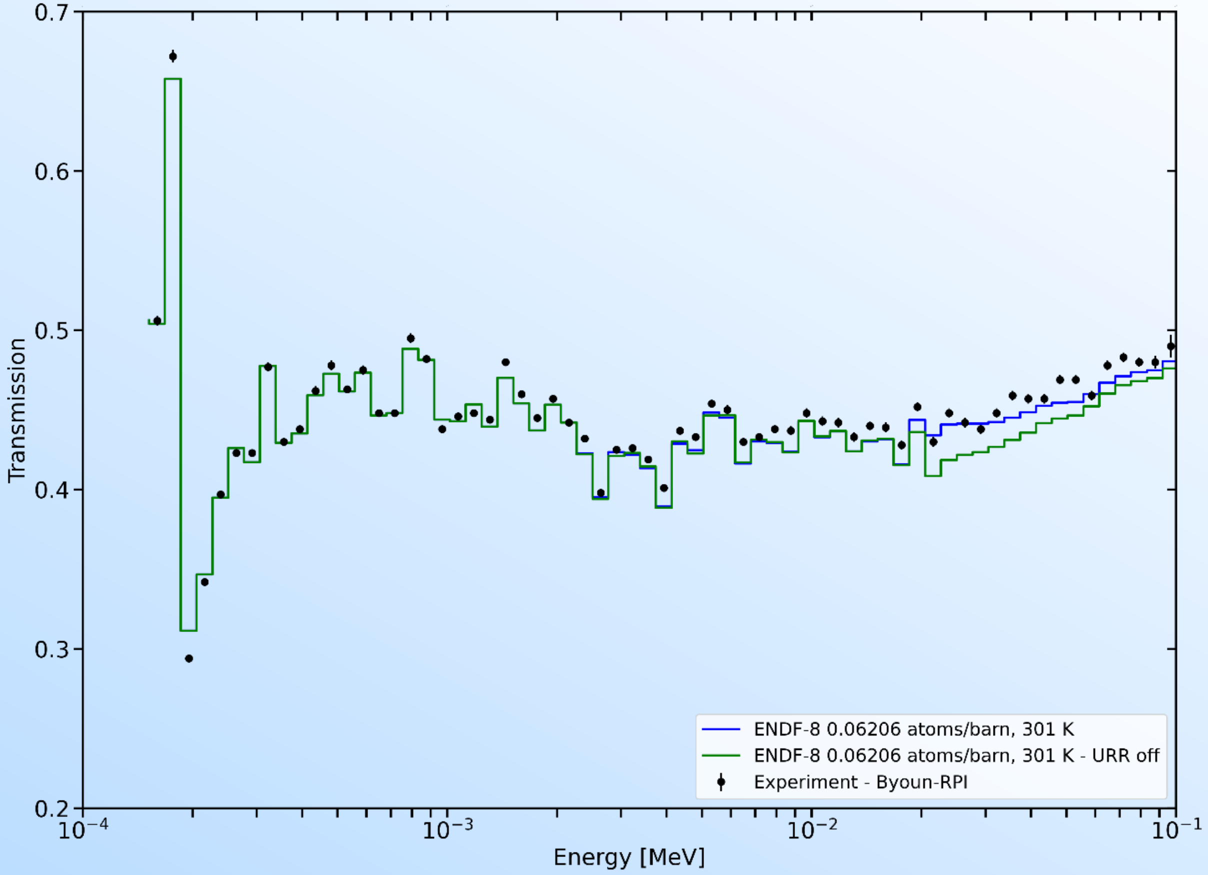
^{238}U transmission at room temp

- Overall good agreement between experiments and calculations including URR (E>20 keV)



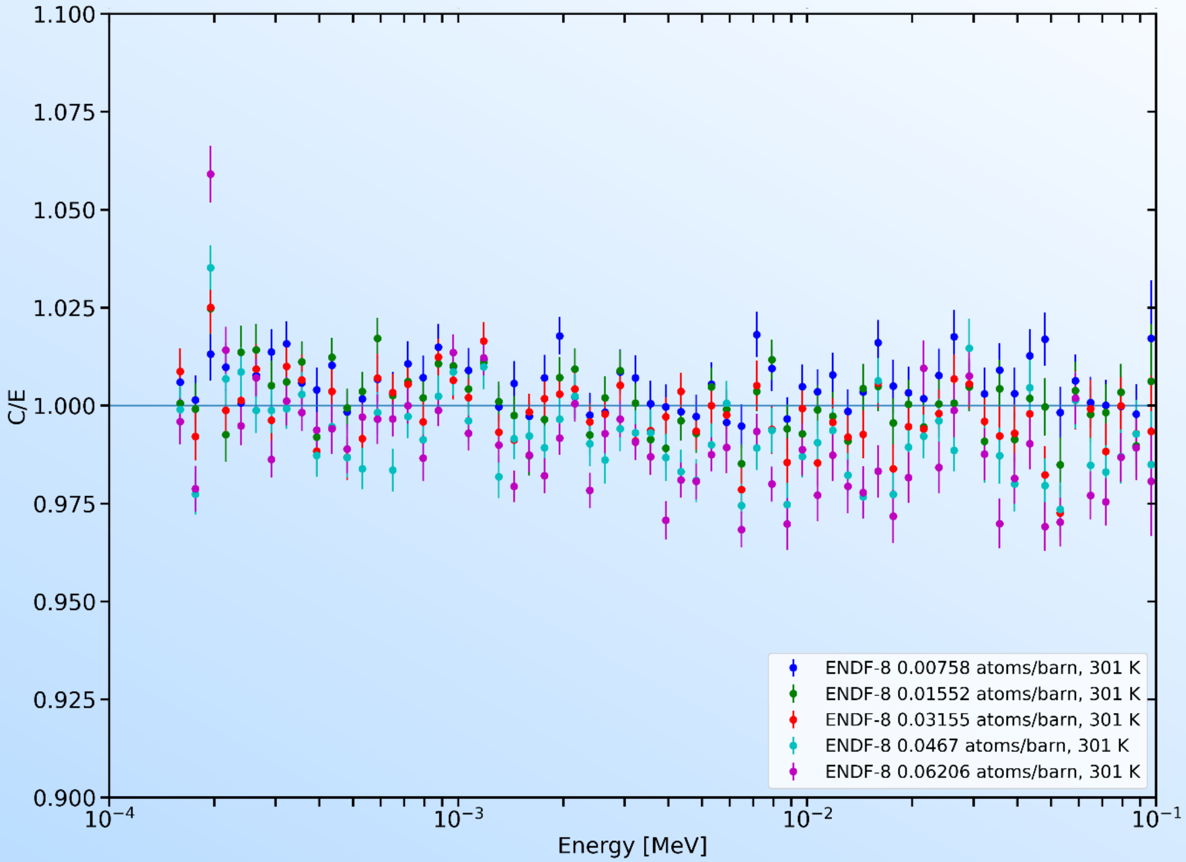
^{238}U effect of probability tables

- Probability tables are necessary to better match the experimental transmission URR
- Sample thickness and energy bin size affect the amount of resonance self shielding



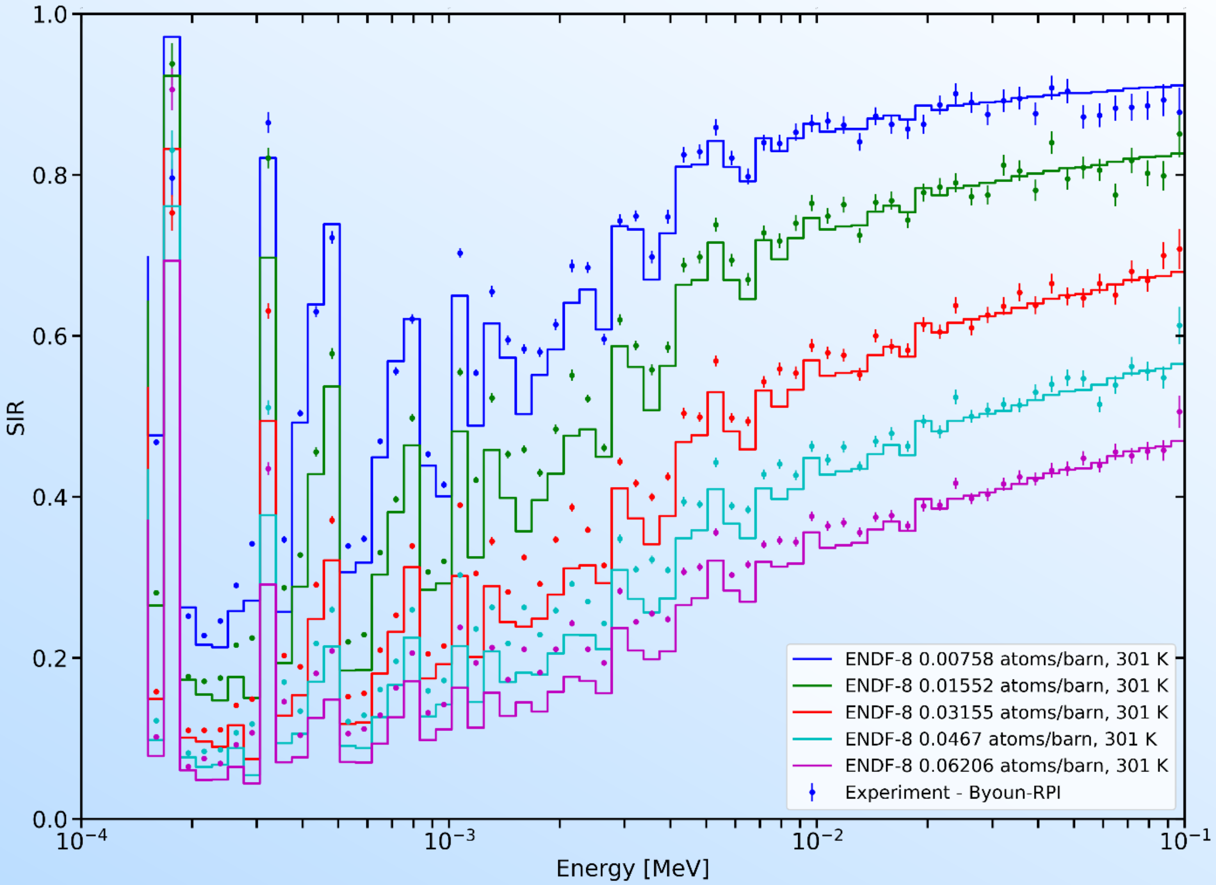
C/E for transmission

- Difference between evaluation and experiments is less then 2.5%
- The evaluation seems to get a bit lower with increasing thickness



^{238}U Self indication ratio

- The evaluation and experiment seems to agree well in the URR
- Differences are visible in the RRR, possible issues with the capture cross section??



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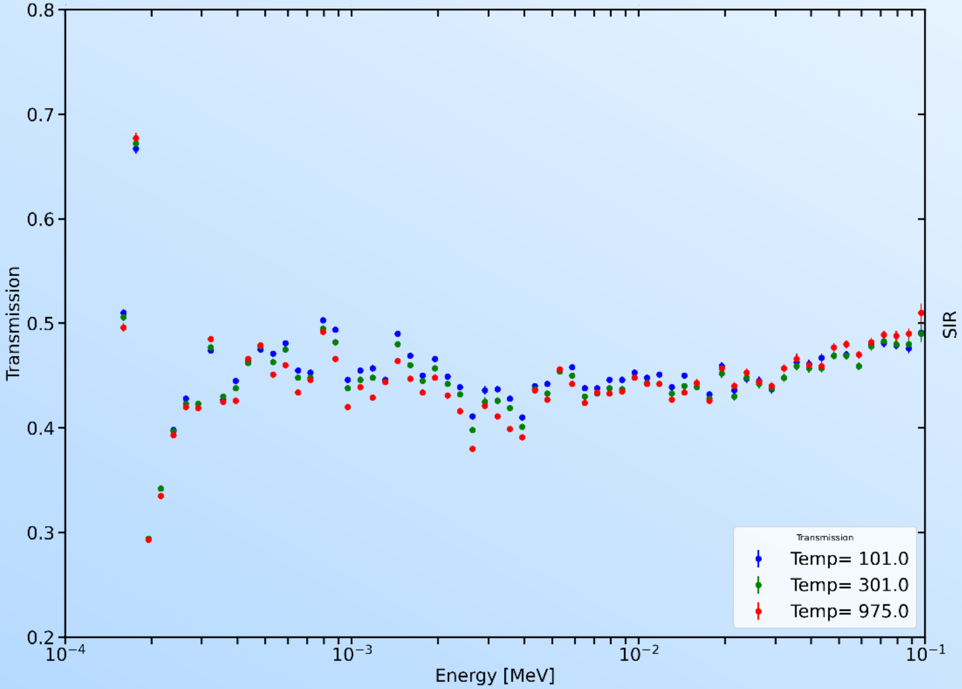
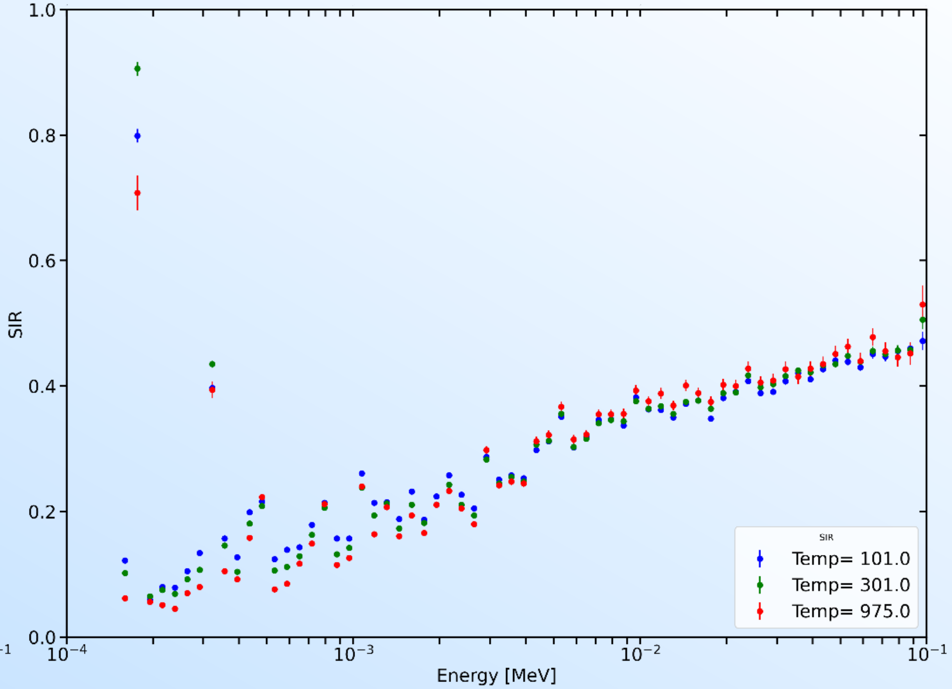
U-238 at different temperatures

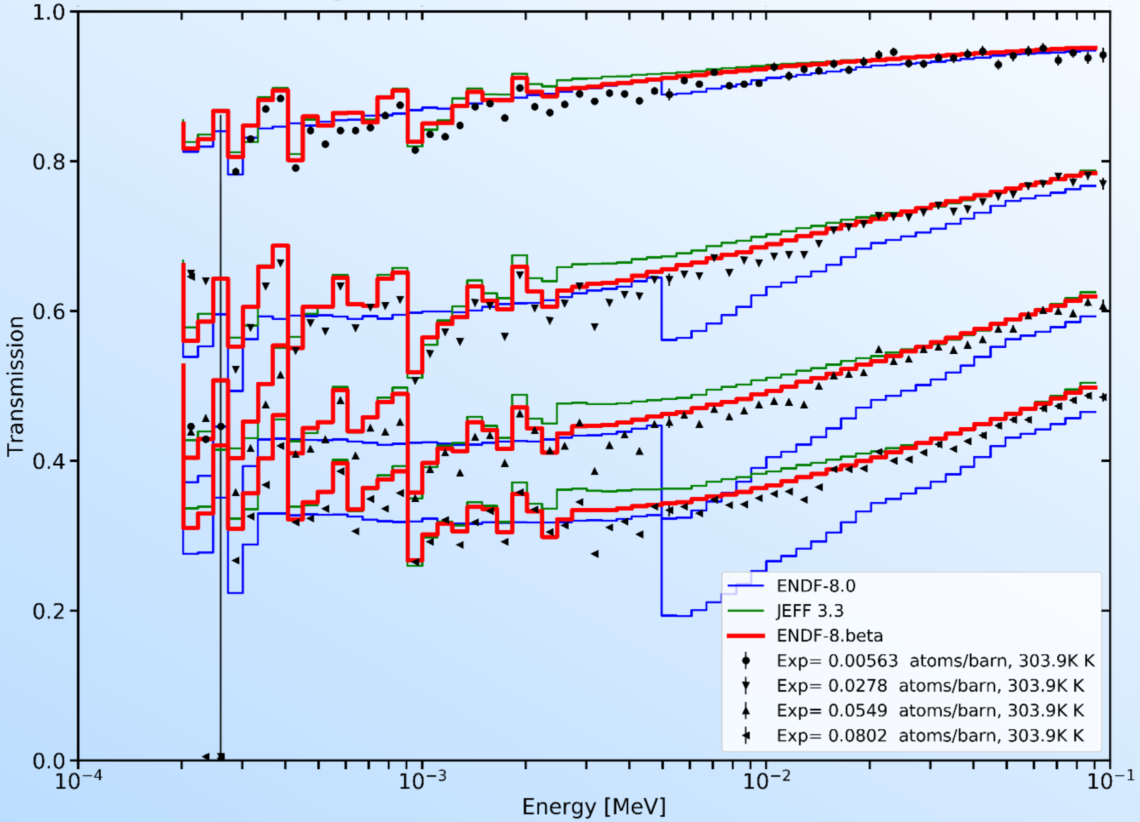
- Two effects: changes to both areal density (expansion) and self-shielding
  - Density: Temperature↑ → N↓ → Transmission↑
  - Self-shielding: Temperature↑ → σ→σ_{av}→ Transmission↓
- Larger changes observed in SIR, shows a clear trend with temperature with cross at about 5 keV
- Need to compare to evaluations…





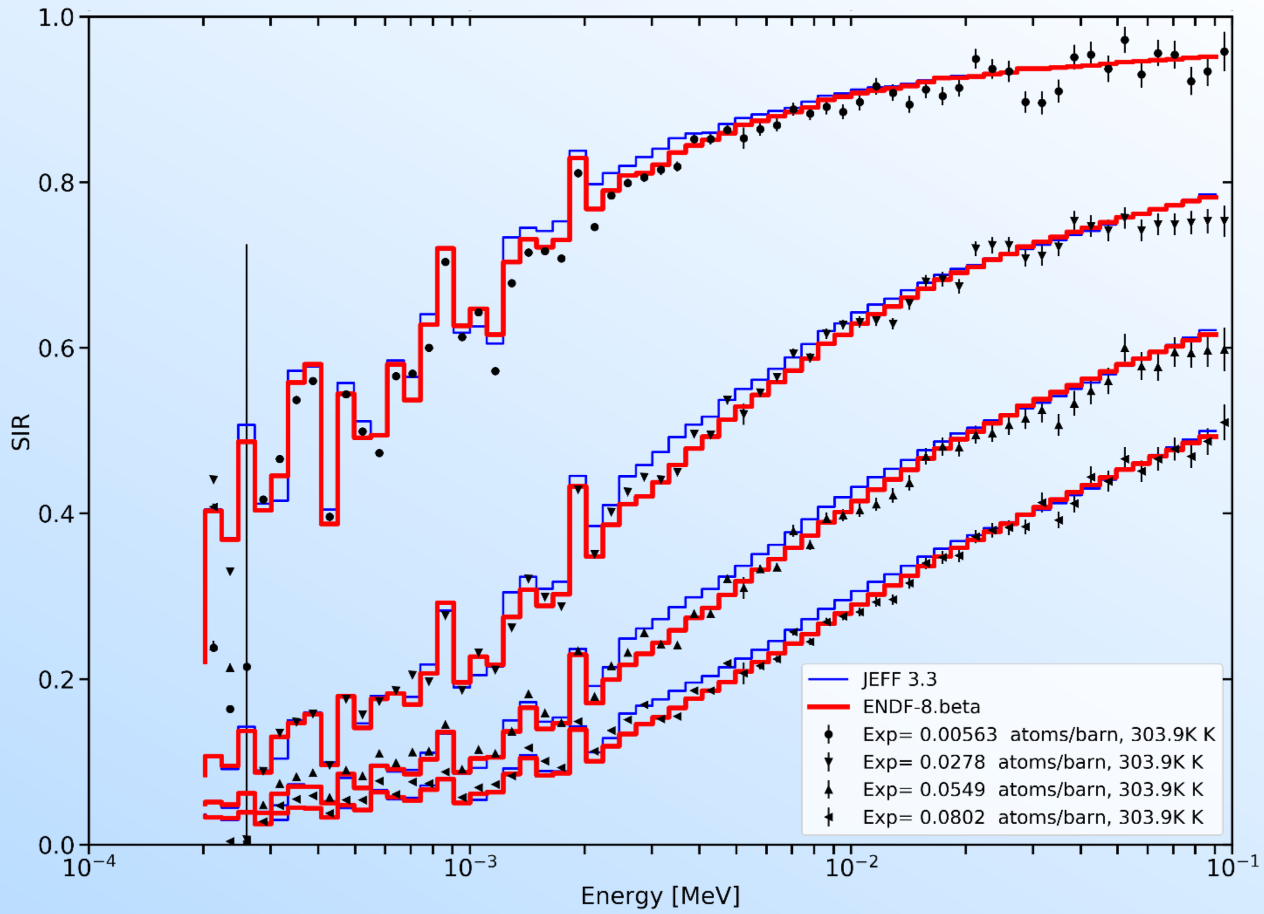
Ta Transmission

- Known problem with ENDF-8
  - See: Jesse M. Brown, R. C. Block, A. Youmans, H. Choun, A. Ney, E. Blain, D. P. Barry, M. J. Rapp and Y. Danon, “Validation of Unresolved Neutron Resonance Parameters Using a Thick-Sample Transmission Measurement”, Nuclear Science and Engineering, vol. 194, no. 3, pp. 221-231, 2019, DOI:10.1080/00295639.2019.1688087
- JEFF-3.3 and ENDF-8.beta show good agreement in URR
- ENDF-beta seems to agrees better, but there is room for improvement



Ta- Self indication ratio

- The new ENDF evaluation shows better agreement in the URR



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Conclusions

- URR experiment provide average transmission or yield data that can be used for evaluations
- Self shielding correction of the experiment might be needed (depends mostly on sample thickness)
- High energy resolution experiments in the URR can produce a less self shielded average cross section but methodology for correction in requires more knowledge of the experiment
- Examples for ^{181}Ta, ^{238}U including transmission, capture and self indication were provided.
- A method for URR cross section validation using a thick sample was demonstrated Brown et al.