Automatic Determination of Resonance Parameters from Self-Shielded Measurements

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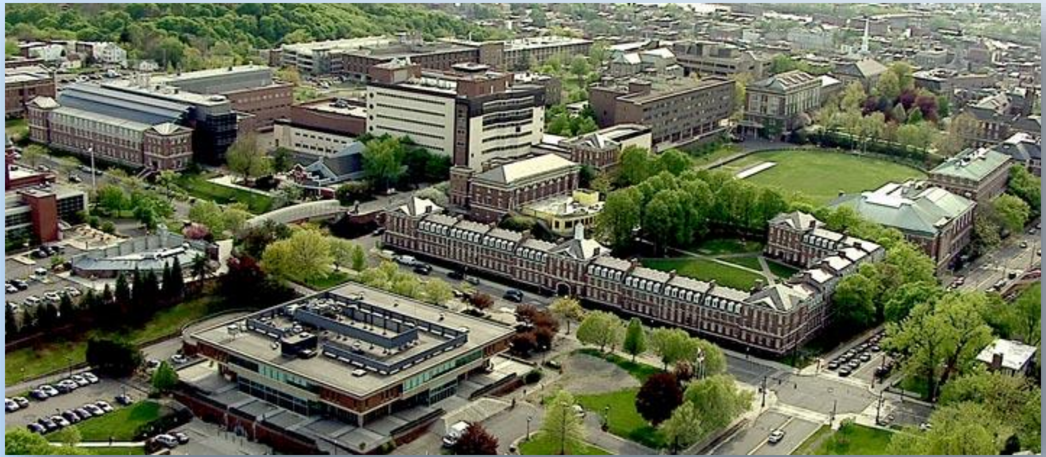

NCSP Technical Program Review
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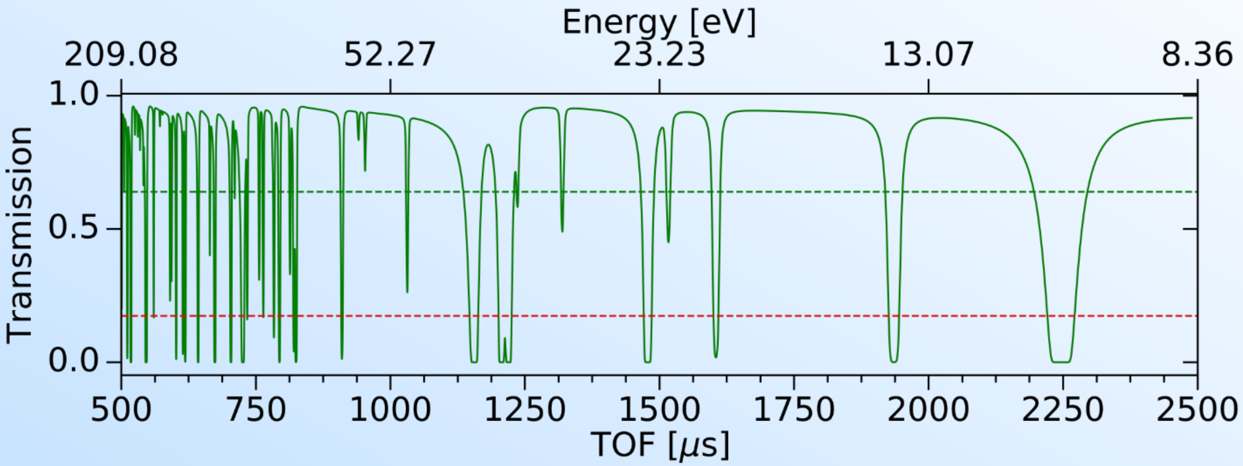
Motivation



$\boxed{\langle T \rangle \approx 0.6}$

$\boxed{e^{-n\langle \sigma \rangle} \approx 0.2}$

$C_T \approx 3.0$

$\langle T \rangle = e^{-n\langle \sigma \rangle} C_T$

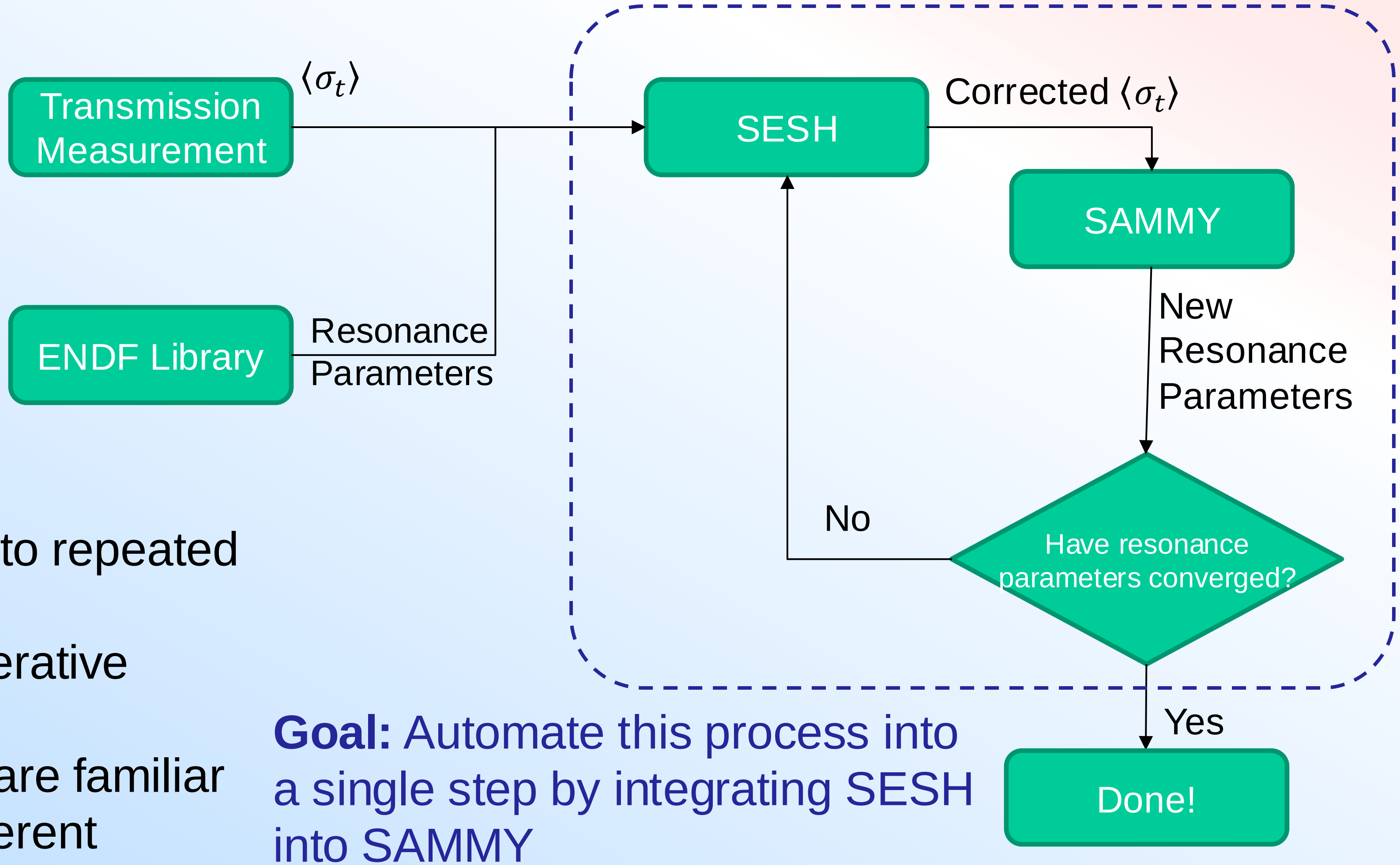
Goal: Define $\langle T \rangle$ as a function of $\langle \sigma \rangle$

$$\langle T \rangle \neq e^{-n\langle \sigma \rangle}$$

SESH

- Calculates C_T, the self-shielding correction factor
- Simulates resonances with Monte Carlo sampling from:
  1. Average resonance parameters
  2. Their known statistical distributions
- Uses Monte Carlo sampling to compute $\langle \sigma \rangle$ and $\langle T \rangle$
- Uses these values to determine C_T

Previous Self-Shielding Workflow



Challenges:

- **Tedious and time-consuming** due to repeated manual steps
- **Prone to user error,** especially in iterative cycles
- **Limited expertise:** Few evaluators are familiar with fitting in URR – significantly different workflow than RRR evaluations

Goal: Automate this process into a single step by integrating SESH into SAMMY

SESH/SAMMY Integration Roadmap

Fitting Monotopic URR Transmission

Milestone	Done	Doing	To Do
Characterize Resonance Pair Effect	●		
Characterize Sample Thickness Effect	●		
Characterize Sample Temperature Effects	●		
Write converter from SAMMY .par parameters to SESH parameters	●		
Enable SESH input parameters in SAMMY input	●		
Validate SAMMY/SESH transmission fitting	●		
Characterize limitations on fitting derivatives	●		
Write verification tests for transmission fitting	●		

Fitting Monotopic URR Capture Yield

Milestone	Done	Doing	To Do
Improve collision handling approximations for multiple scattering	●		
Resolve Psi-Chi doppler broadening issue	●		
Write verification tests for capture yield fitting	●		

Enabling Multi-Isotope Data Processing

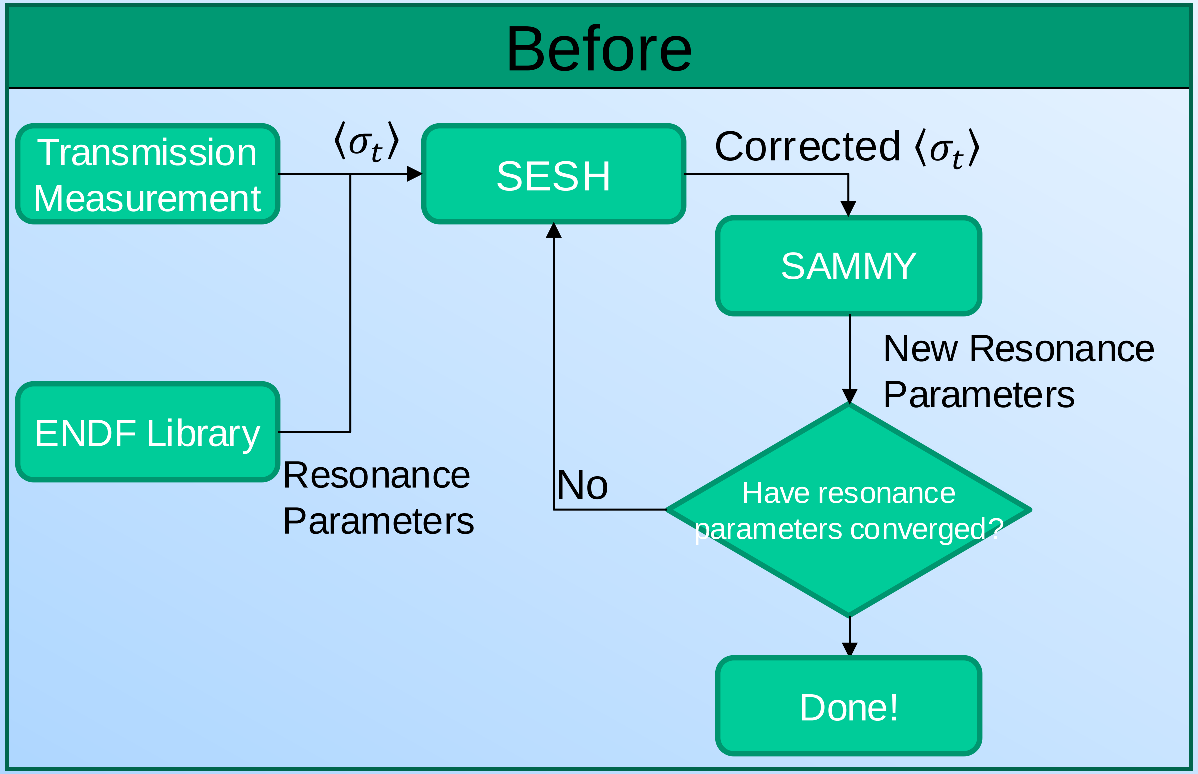
Milestone	Done	Doing	To Do
Characterize impact of multi-isotope self-shielding	●		
Write new .par parser for SAMMY in URR to handle multiple isotope parameters	●		
Remove global parameters from FITACS modules	●		
Write FORTRAN interface module for using SAMMY/FITACS subroutines	●		
Merge cross section energy dependent parameters with NJOY and MCNP models	●		
Implement NJOY resonance pair contribution model	●		
Calculate *u*-parameter matrix from .par file parameters		●	
Add fitting loop to multi-isotope formatted data		●	
Add Read/Write covariance matrix subroutines			○
Add output text file generator subroutines			○

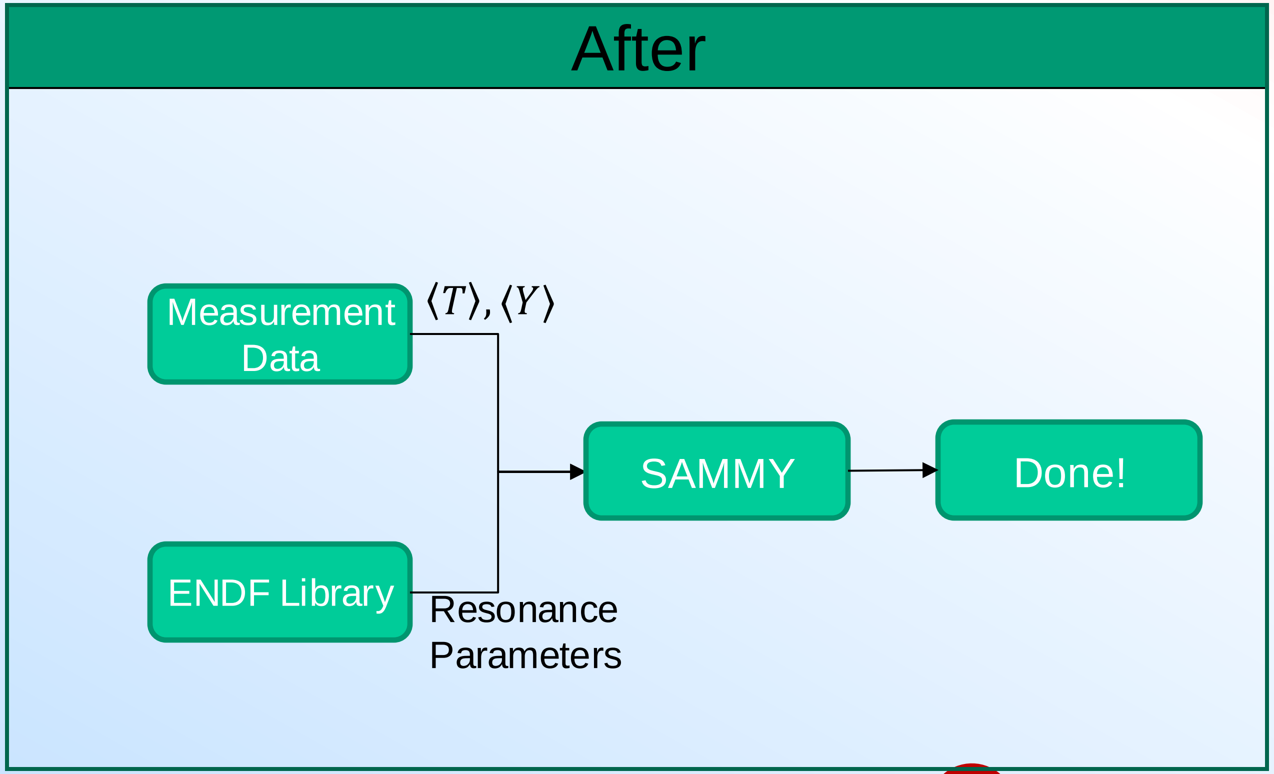
Miscellaneous

Milestone	Done	Doing	To Do
Write LCG PRNG subroutines	●		
Change to implicit capture weighting scheme	●		
Add unit tests to SESH subroutines		●	
Write Documentation for SESH inputs		●	

2024 Accomplishments

- Transmission and capture correction factors both validated and integrated into the main SAMMY branch
- Developed uncertainty quantification method for self-shielding correction factor
- Implemented new Multi-Isotope scheme for URR





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Multi-Isotope Motivation

Current Limitation:

- SAMMY can only perform self-shielding corrections for monotopic samples

Need for Thicker Samples:

- Thicker samples measurements are necessary for more accurate URR measurements

Challenges with Thick Samples:

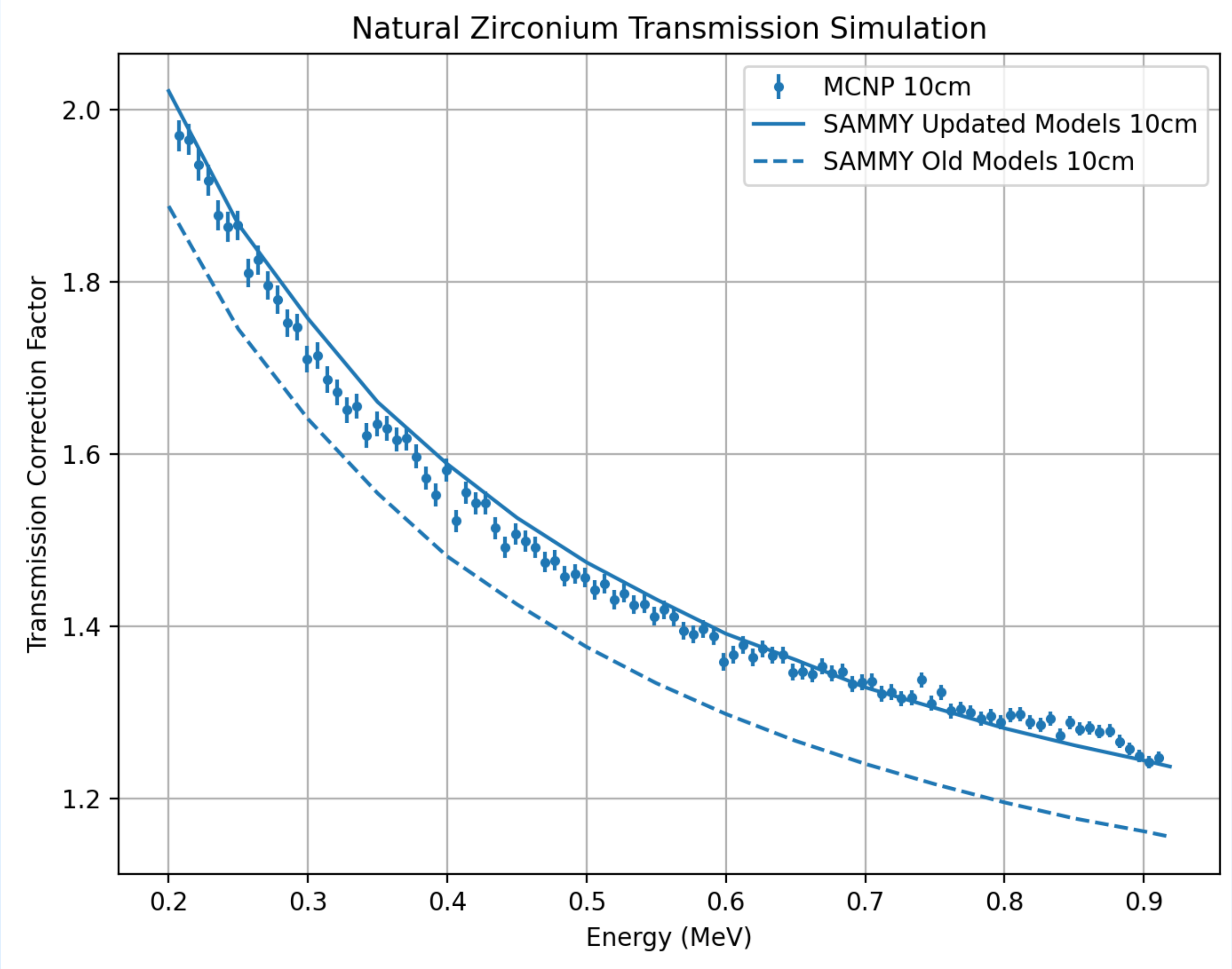
- Significant self-shielding – affects measurements, must be corrected for
- Very high cost for producing enriched, monotopic thick samples

Natural Multi-Isotopic Samples:

- Much more cost-effective alternative

Implementing multi-isotope self-shielding corrections into SAMMY is non-trivial and complicated. Necessitated significant validation of SESH's algorithms.

Transmission Correction: Resolving Modeling Issues



Needed to validate the accuracy of Multi-Isotope processing for transmission correction

Transmission Correction Validation Process

- Natural Zr used as basis for validation
- Compared samples ranging from 1-10cm

Initial Challenges:

- *Significant* disagreement between SESH and MCNP
- Attributable to differences in energy-dependent parameter models between SESH and NJOY
- Issues were not present when validating Mono-isotopic model with Ta-181
- Ta-181 has much narrower URR compared to Zr, model discrepancies less impactful

Outcome:

- Model discrepancies were resolved – SAMMY and MCNP now show *much* stronger agreement on transmission correction
- Sufficient agreement to proceed to capture correction validation

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Capture Correction: Fixing Multiple Scattering

- Capture correction factor corrects the thin sample approximation for yield

$$\langle Y \rangle \approx n\langle \sigma_\gamma \rangle$$
$$\langle Y \rangle = n\langle \sigma_\gamma \rangle C_C$$

- Accounts for two effects: **resonance self-shielding** and **multiple scattering**
- Two aspects of SESH's multiple scattering model led to discrepancies between SAMMY and MCNP in capture yield simulations

Weight Cutoff Scheme

- SESH used an analog particle simulation scheme to simulate scattering events
- Inefficient and underestimated multiple scattering correction

Current Status:

- Replaced analog with implicit capture weighting
- Improved efficiency
- More precisely matches MCNP simulations

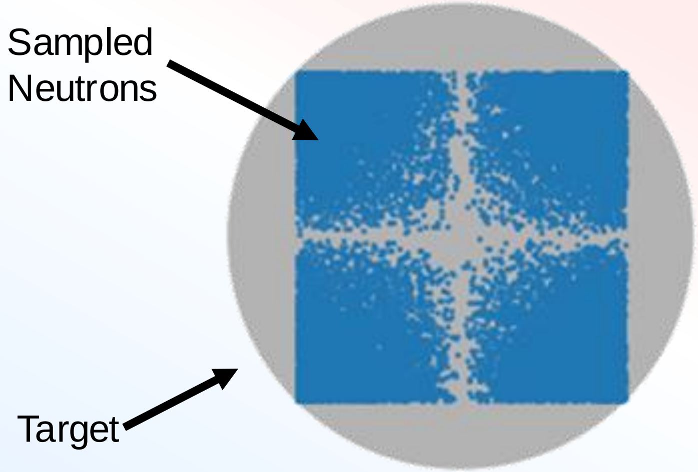
Incident Neutron Sampling

- Requires (x, y) coordinates for incident neutrons
- *Should* uniformly distribute neutrons across target
- Original algorithm had sampling bug: underestimated multiple scattering contribution

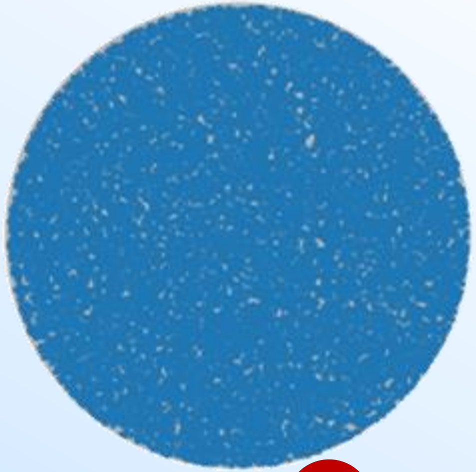
Current Status:

- Now uses uniform distribution
- much more accurate scattering representation

Original Sampling Algorithm



Improved Sampling Algorithm



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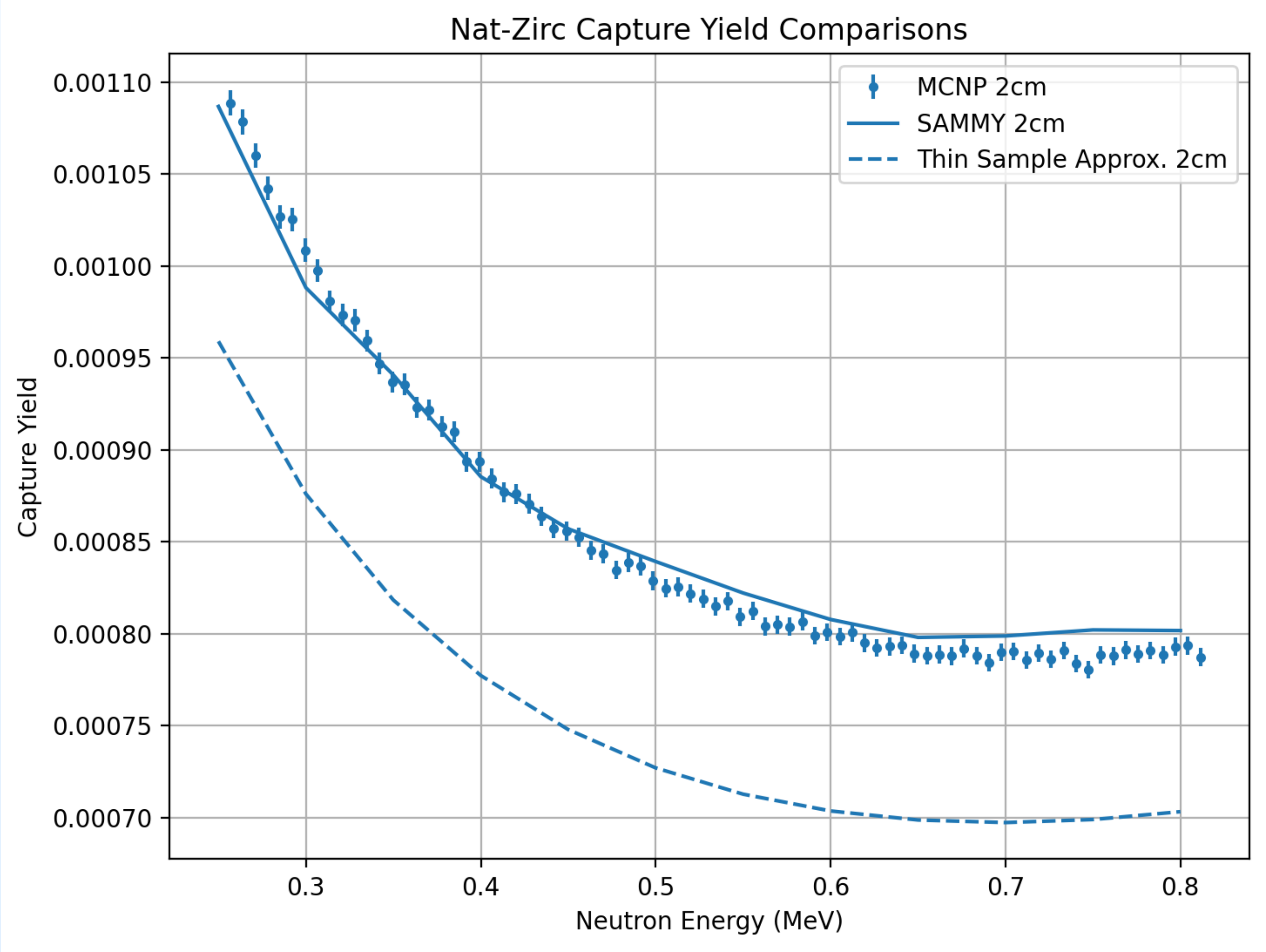
Validating Capture Correction



Capture Correction Validation Process

- Natural zirconium cylindrical discs simulated to compare capture correction

Challenges:

- $\langle\sigma_\gamma\rangle \ll \langle\sigma_{tot}\rangle$ for all Zr isotopes in URR
- Highly sensitive to multiple scattering effect
- Resolving the location sampling issue was essential to matching MCNP and SESH
- Differences are attributable to weight cutoff factor in scattering algorithm - can be tuned even closer to fit by adjusting weighting and cutoff

Outcomes:

- Strong agreement between SAMMY and MCNP now for both **capture** and **transmission** corrections

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Evaluating Self-Shielded Measurements

Two assumptions are used for correcting self-shielded measurements:

1. There are a statistical number of resonances in an energy bin
2. Energy bin is narrow enough to ignore energy dependent effects

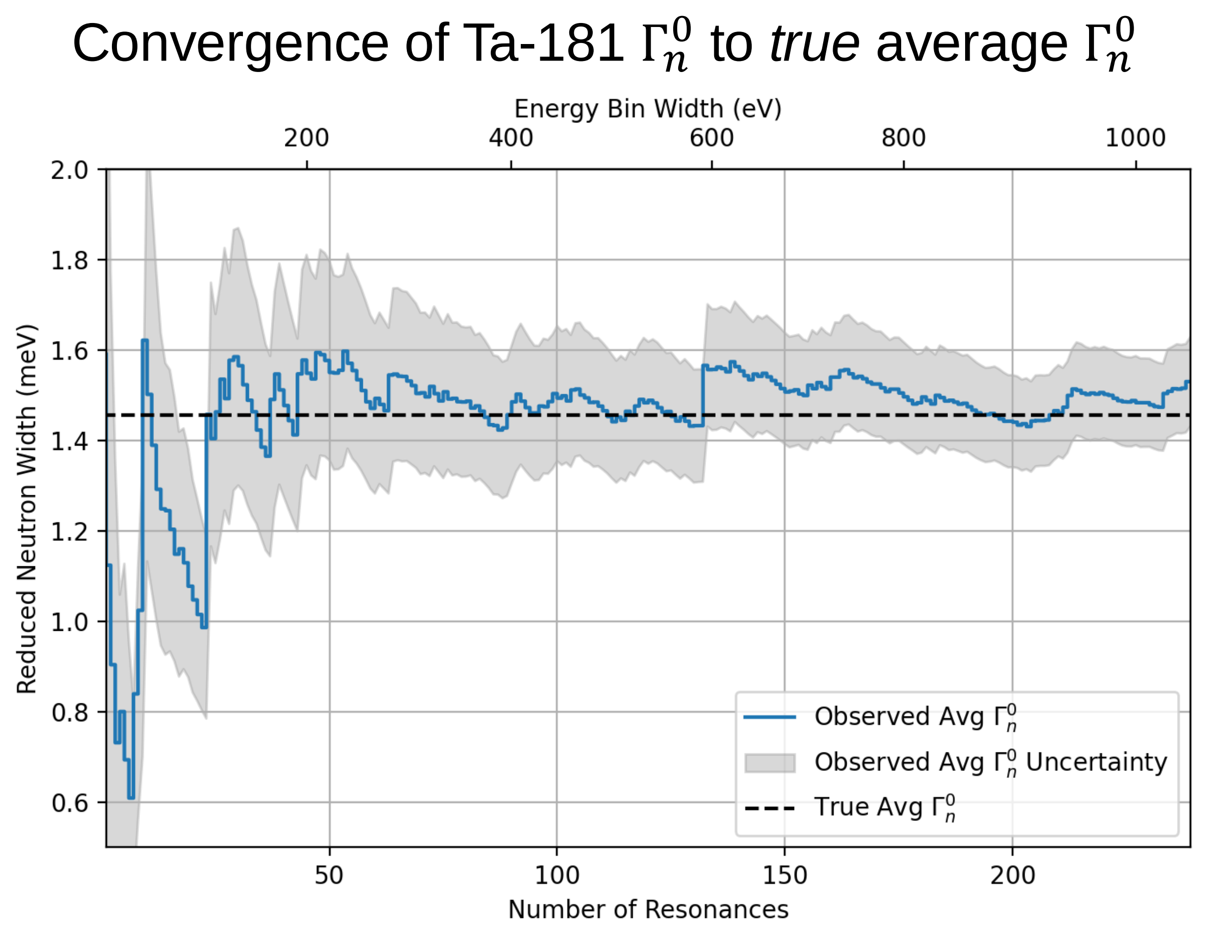
Ta-181 meets both assumptions

– $\langle\Gamma_n^0\rangle$ starts to converge at ~250 resonances
– Equivalent to 1 keV energy bin width

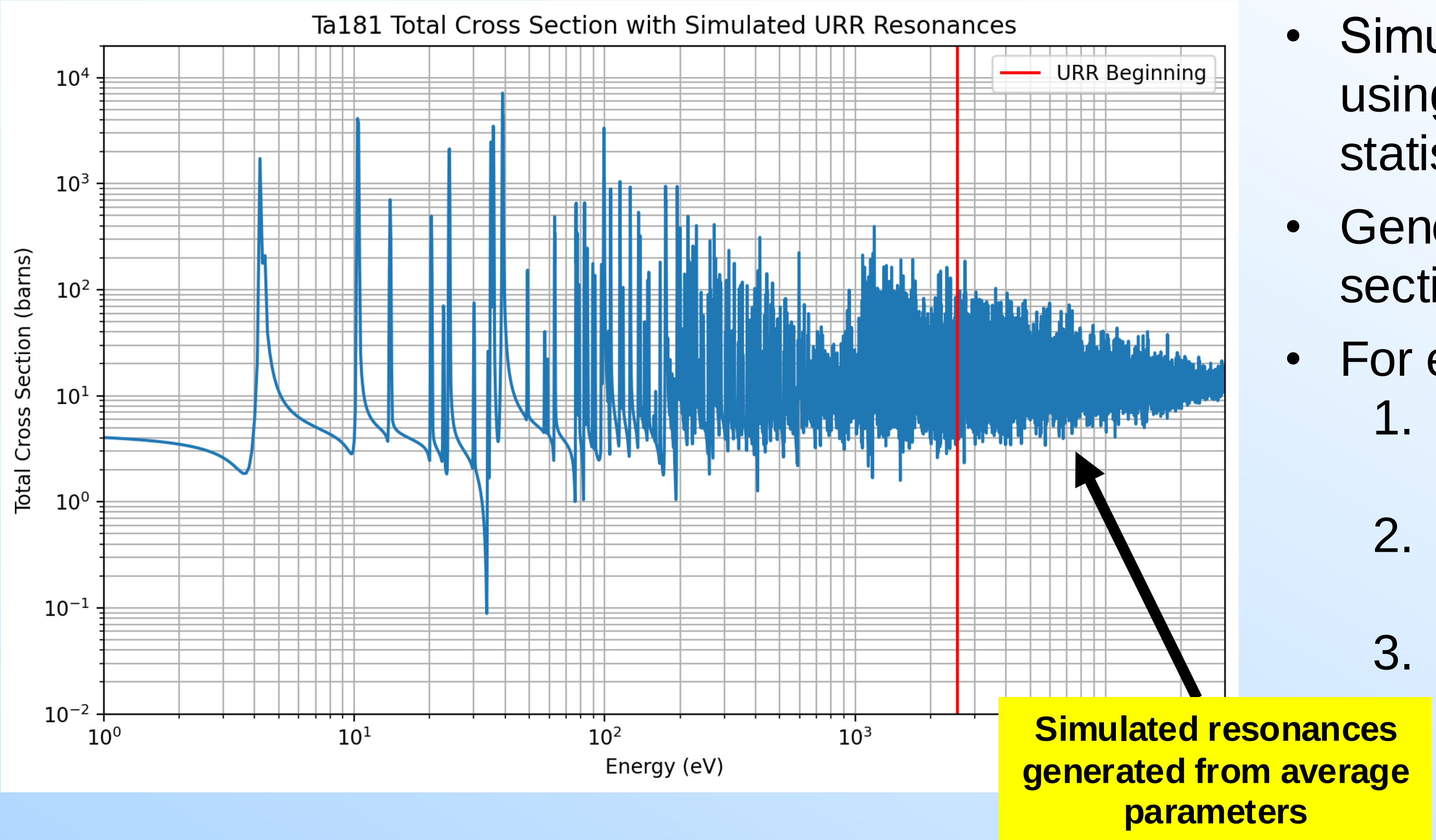
Zr-90 cannot meet both assumptions

– 6.0 keV average level spacing
– 200 resonances would require a 1.2 MeV energy bin (!!)

Issue: Finite number of resonances per energy bin can inaccurately represent average parameters – introduces uncertainty on correction factor



Uncertainty Quantification of Finite Resonance Effects



- Simulated 'resolved' URR cross sections using resonance parameters derived from statistical distributions
- Generated realizations of pointwise cross sections from these resonance parameters
- For each realization:
  1. Calculated pointwise transmission using thickness n
  2. Calculated energy-averaged $\langle \sigma_t \rangle$ and $\langle T \rangle$ from 3-4 keV
  3. Determined C_T via

$$C_T = \langle T \rangle \cdot \left(e^{-n\langle \sigma \rangle} \right)^{-1}$$

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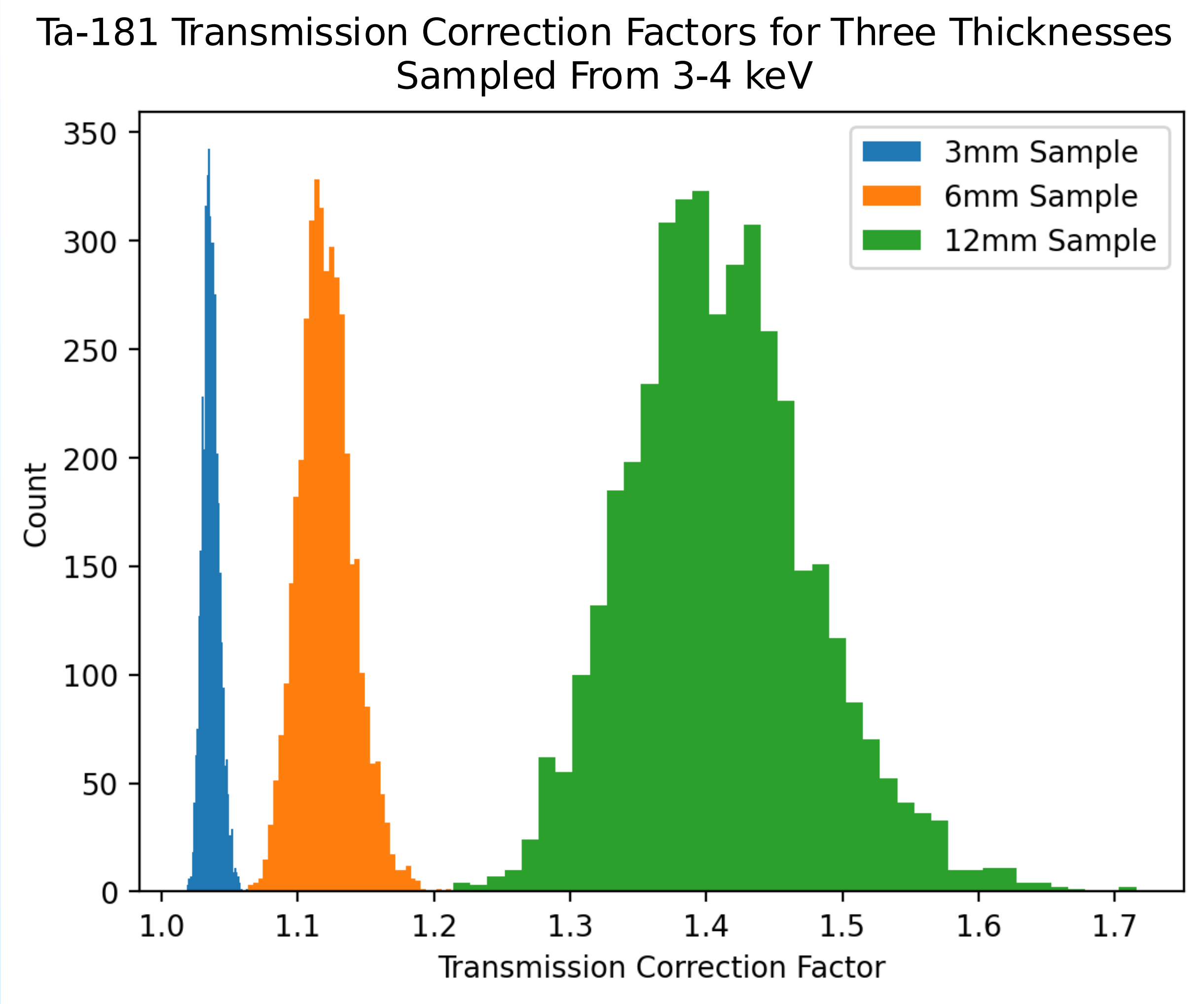
Sampling Resolved Realizations of the URR

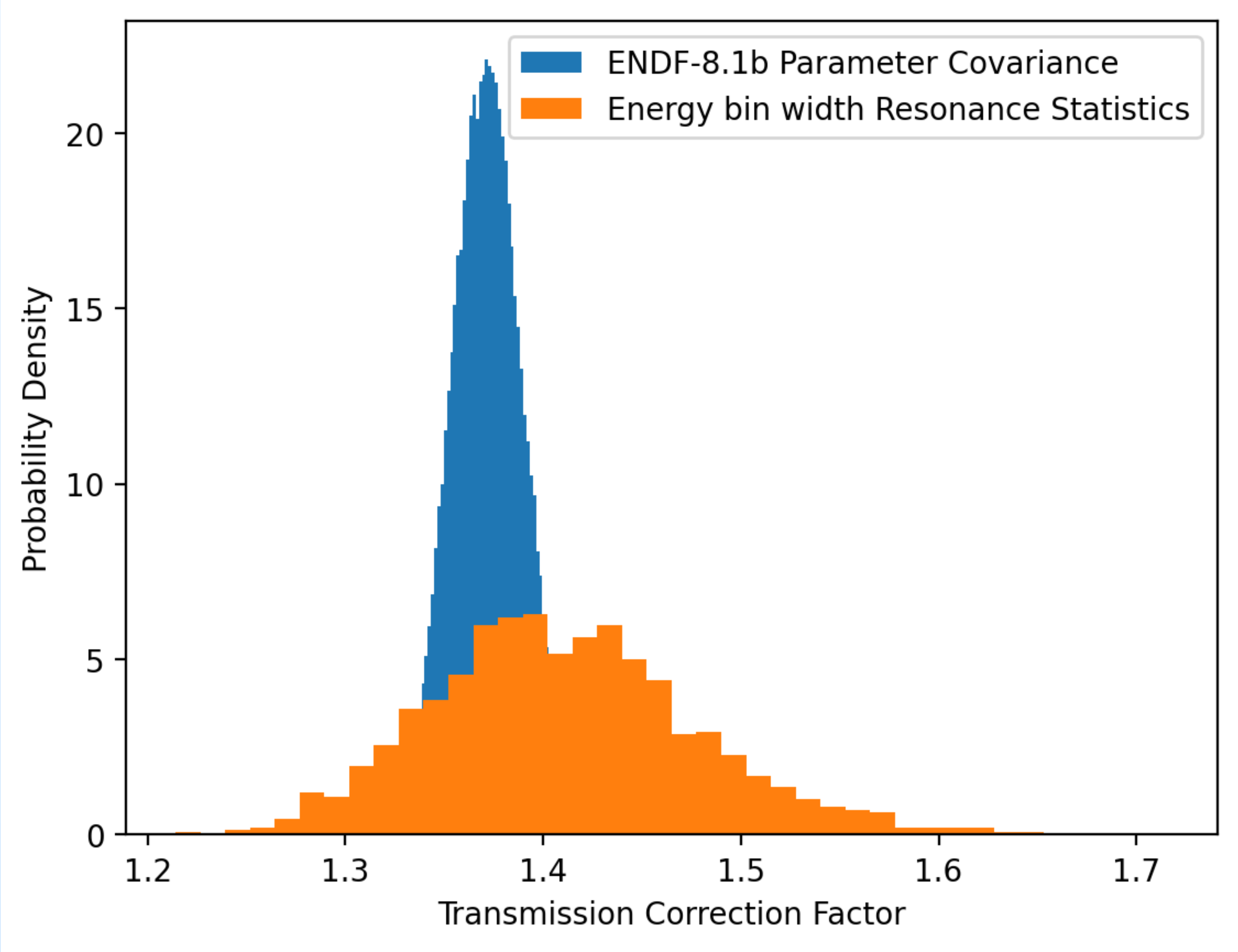
- Simulated transmission for three thicknesses: 3mm, 6mm, and 12mm
- 4100 realizations per thickness used to calculate C_T
- C_T values show significant uncertainty due to finite resonance effects

Thickness	C_T	$\frac{\sigma_{C_T}}{C_T}$
3mm	1.036	0.600%
6mm	1.121	1.764%
12mm	1.411	4.800%

- This is ***only*** due to finite resonance effects – there is no uncertainty on the average parameters



Comparing Self-Shielded Uncertainty to Evaluation



- Covariance on URR Resonance parameters was calculated from Ta-181 ENDF-8.1 evaluation, used to sample 100k realizations of URR resonance parameters
- SESH was run with these parameters to compute variance on C_T (12mm sample)
- ENDF-8.1 evaluation significantly underestimates C_T uncertainty for this case
- Fortunately, Ta-181 level spacing is small – can use wider bins to reduce effect significantly without violating energy independence assumption
- This is not true for Zr-90 – finite resonance uncertainty must be accounted for when performing self-shielding correction

Source of Uncertainty	$\frac{\sigma_{C_T}}{C_T}$
ENDF-8.1 URR Covariance	1.44%
Finite Resonances	4.80%

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Conclusion and Future Work

Current Progress:

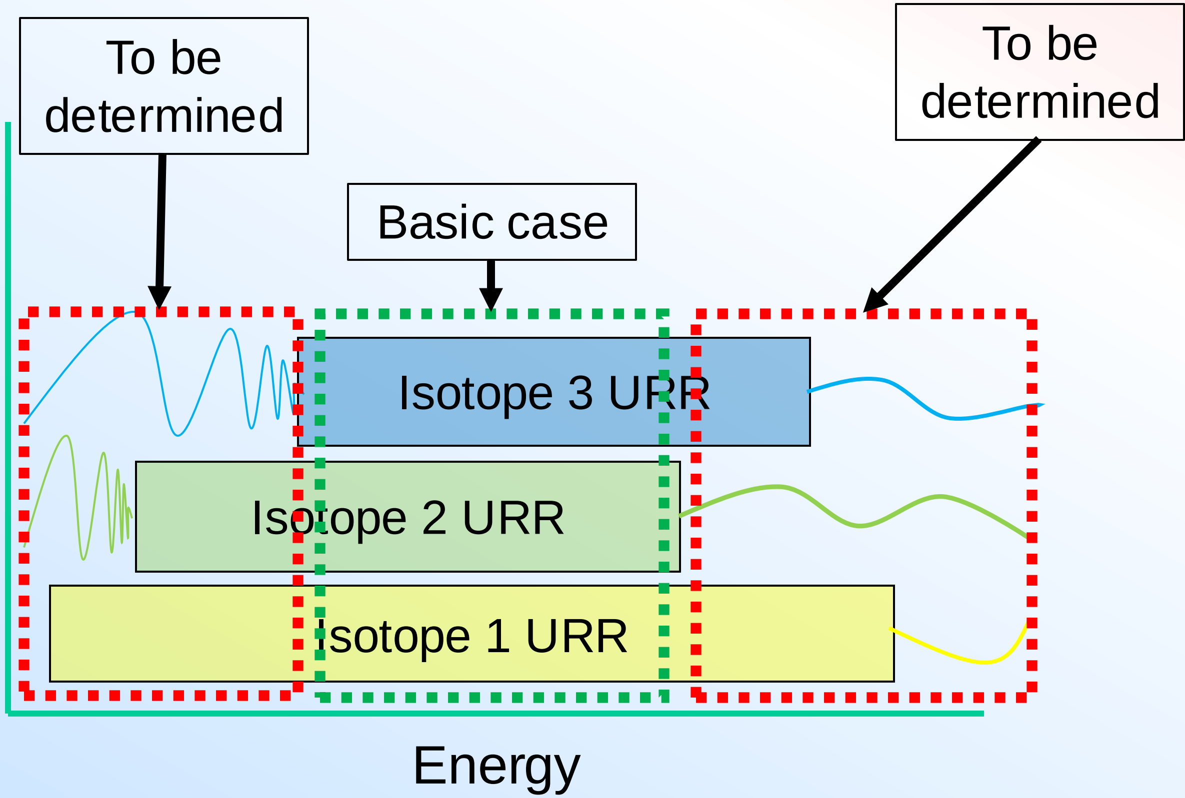
- Transmission and capture correction factors are being accurately accounted for with new multi-isotope processing scheme
- Moving onto fitting procedure

Finite Resonance Effects in URR:

- Significant uncertainties can and should be attributed to finite resonances
- Minimizing this can be used to optimize energy bin widths in evaluation
- Work underway to apply methodology to Zr and propagate uncertainties to URR parameters

Future Goals:

- Develop methodology for processing non-overlapping URR in multi-isotope samples
- Add fission yield fitting



Acknowledgements

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