Enabling URR Self Shielding Functionality in SAMMY

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FY2022 Milestones

- Identified bug in doppler broadening subroutine that caused SESH to miscalculate correction factors

- Replaced doppler broadening subroutine with new implementation

- Completed validation of transmission self shielding correction

- Completed validation of capture self-shielding correction

Motivation
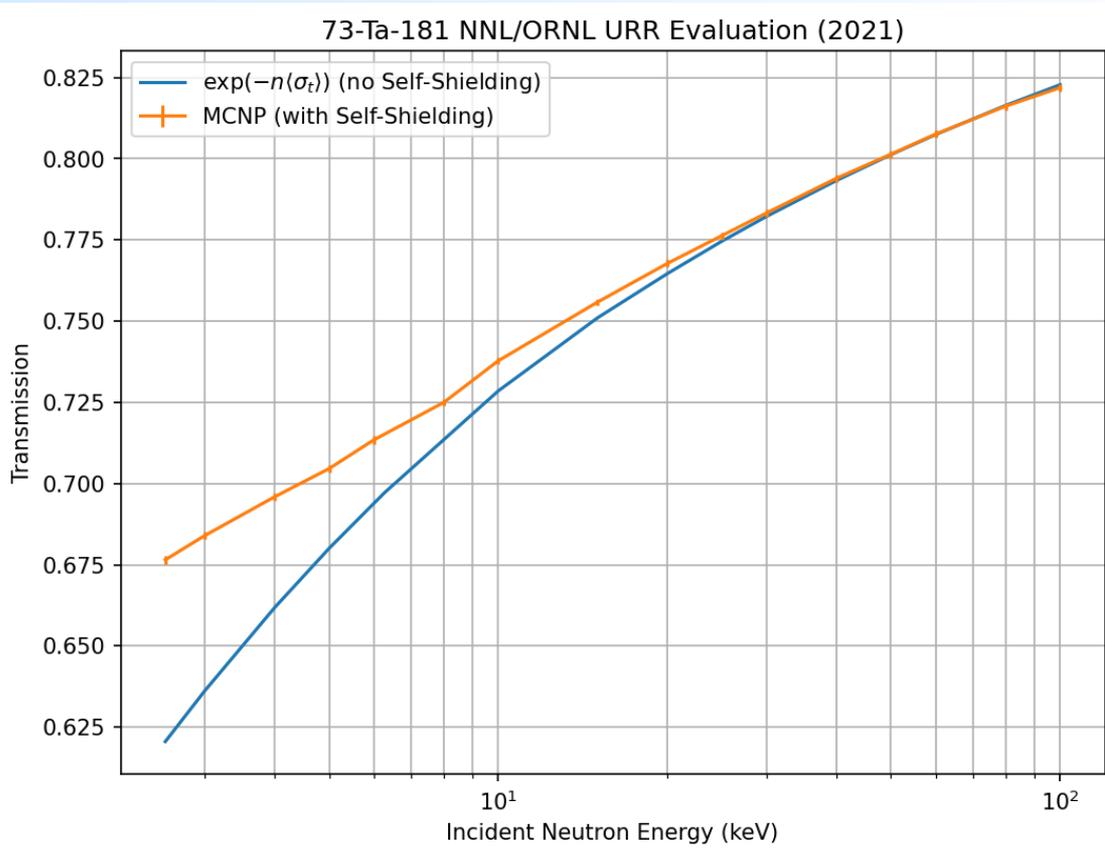
- Self Shielding is phenomena which occurs in the unresolved resonance region

- Because only average parameters can be obtained in the URR, a correction factor must be calculated in order to fix transmission and capture data and properly fit resonance parameters

- A 4mm Ta181 transmission simulation is used to demonstrate self shielding

Motivation

$$\langle T \rangle_{experiment} = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} e^{-n\sigma(E)} dE$$

$$= \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} e^{-n(\sigma(E) + \langle \sigma \rangle - \langle \sigma \rangle)} dE$$

$$= \frac{e^{-n\langle \sigma \rangle}}{E_2 - E_1} \int_{E_1}^{E_2} e^{-n(\sigma(E) - \langle \sigma \rangle)} dE$$

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

The correction factor defines the average difference between the average cross section and "true" cross section

such that
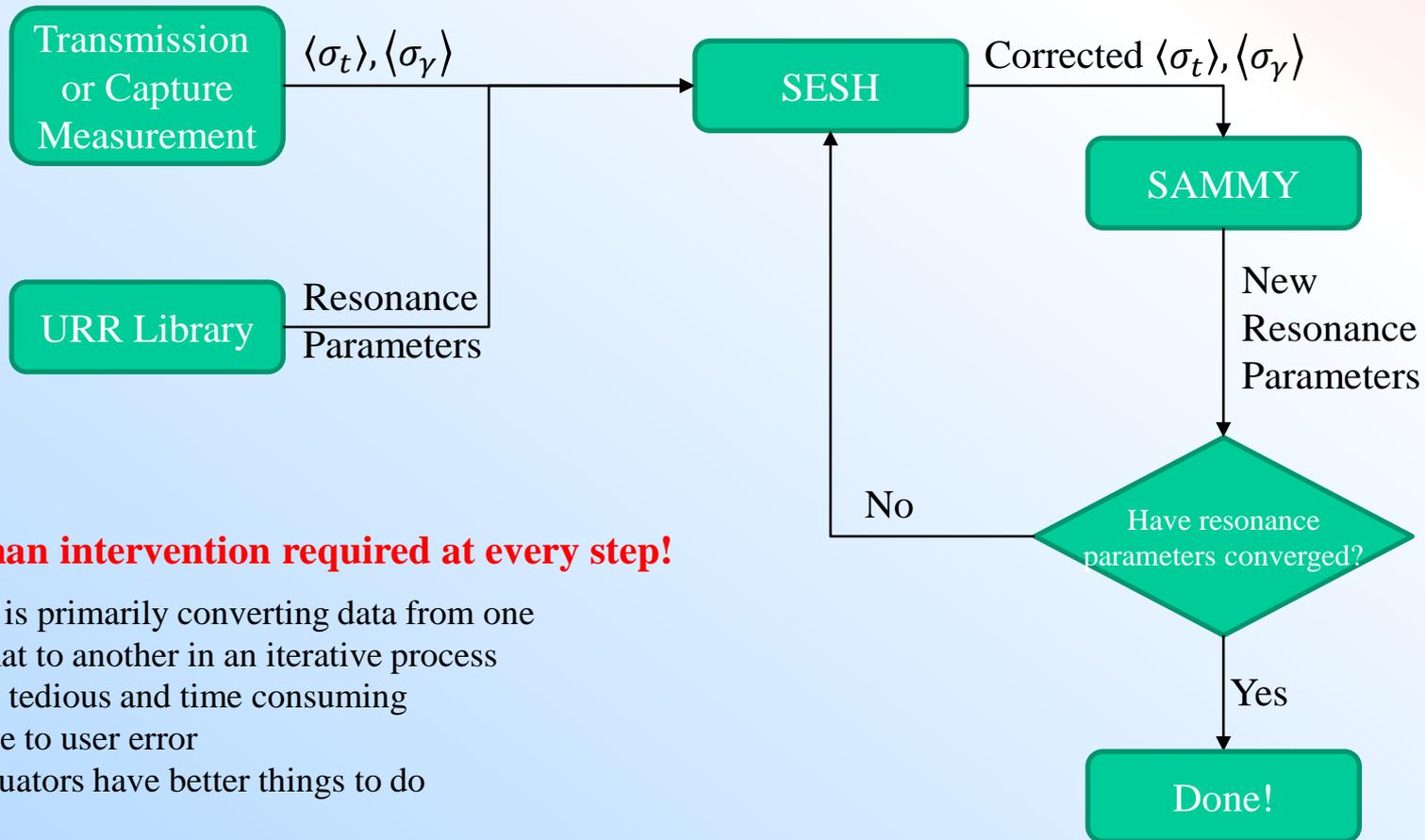
$$\langle T \rangle_{experiment} = e^{-n\langle \sigma \rangle} C_T$$

And then rearranging C_T, we get

$$C_T = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} \frac{e^{-n\sigma(E)}}{e^{-n\langle \sigma \rangle}} dE = \frac{\langle e^{-n\sigma(E)} \rangle}{e^{-n\langle \sigma \rangle}}$$
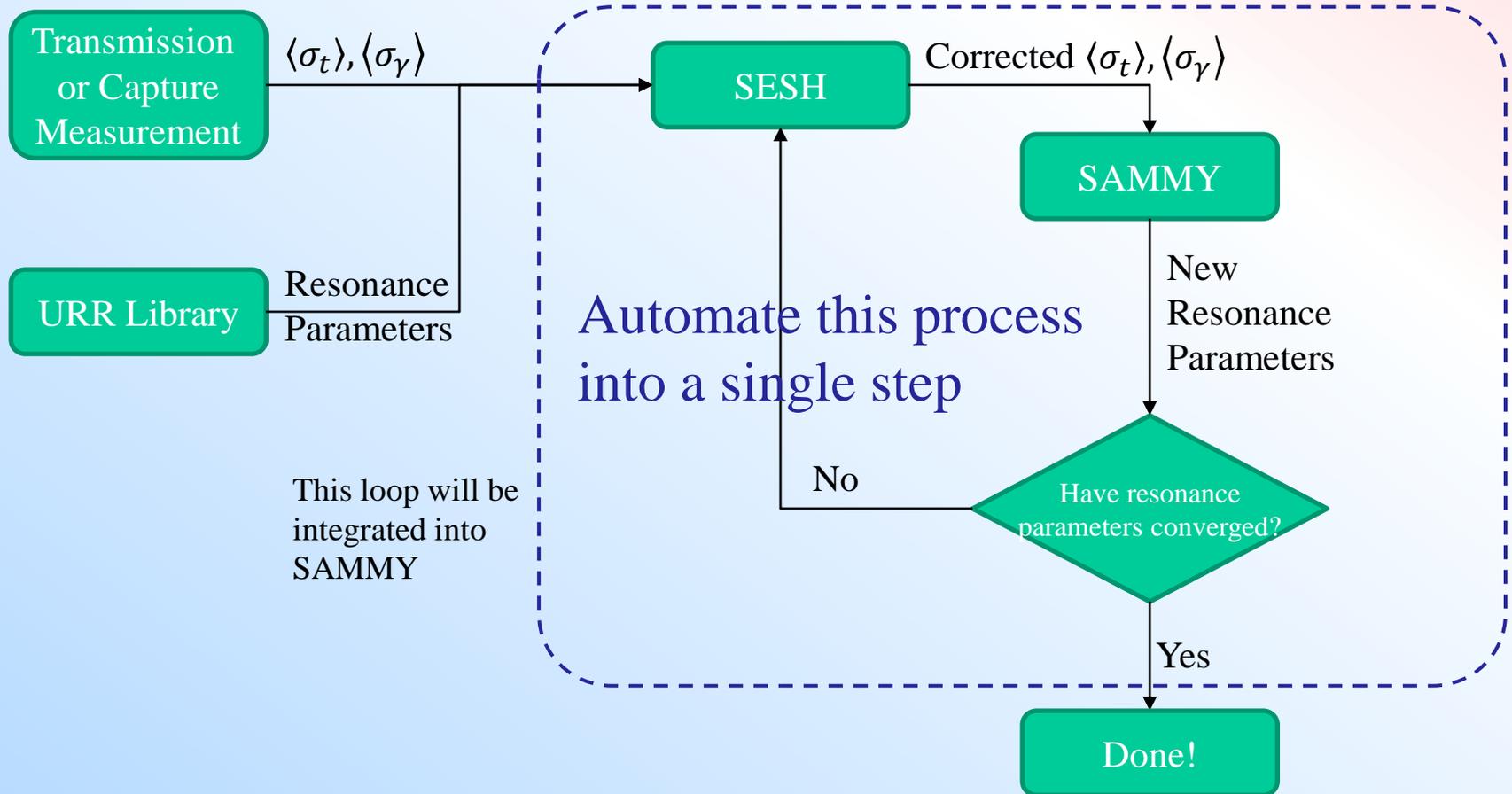
Current Self Shielding Correction Workflow

Transmission or Capture Measurement → $\langle\sigma_t\rangle, \langle\sigma_\gamma\rangle$

URR Library → Resonance Parameters

SESH → Corrected $\langle\sigma_t\rangle, \langle\sigma_\gamma\rangle$

SAMMY → New Resonance Parameters

Have resonance parameters converged?

No → (back to SESH)

Yes → **Done!**

Human intervention required at every step!

This is primarily converting data from one format to another in an iterative process
Very tedious and time consuming
Prone to user error
Evaluators have better things to do

Current Self Shielding Correction Workflow

```
┌──────────────┐   ⟨σₜ⟩,⟨σᵧ⟩
│ Transmission │ ────────────→          ┌─────────┐  Corrected ⟨σₜ⟩,⟨σᵧ⟩
│  or Capture  │                        │  SESH   │ ───────────────────→ ┌─────────┐
│ Measurement  │                        └─────────┘                      │  SAMMY  │
└──────────────┘                                                         └─────────┘

┌──────────────┐  Resonance        Automate this process                    New
│ URR Library  │  Parameters       into a single step                    Resonance
└──────────────┘                                                         Parameters

                   This loop will be         No          ◇ Have resonance
                   integrated into        ──────────────   parameters converged? ◇
                   SAMMY

                                                                         Yes

                                                                    ┌─────────┐
                                                                    │  Done!  │
                                                                    └─────────┘
```

The equations shown in the diagram:

$\langle\sigma_t\rangle, \langle\sigma_\gamma\rangle$

Corrected $\langle\sigma_t\rangle, \langle\sigma_\gamma\rangle$

Transmission or Capture Measurement

URR Library — Resonance Parameters

SESH

SAMMY — New Resonance Parameters

Automate this process into a single step

This loop will be integrated into SAMMY

Have resonance parameters converged?

No

Yes

Done!

Methodology: Transmission Correction Factor

SESH functions by generating random resonances cross section based on average resonance parameters and their known distributions

$$\sigma_{tot}^i \equiv i^{th} \text{ instance of the total cross section}$$

$$\langle \sigma_{tot} \rangle = \frac{1}{N} \sum_{i=1}^{N} \sigma_{tot}^i$$

$$\langle T \rangle = \frac{1}{N} \sum_{i=1}^{N} \exp(-n\sigma_{tot}^i)$$

$$C_T = \frac{\langle T \rangle}{\exp(-n\langle \sigma_{tot} \rangle)}$$

$$\langle \sigma_{tot} \rangle_{new} = \langle \sigma_{tot} \rangle_{experiment} + \frac{1}{n} \ln C_T$$

where

$$\langle \sigma_{tot} \rangle_{experiment} = -\frac{1}{n} \ln(\langle T \rangle_{experiment})$$

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Verification of Transmission

- Compared with MCNP run of a transmission experiment using NNL/ORNL 73-Ta-181 (2021) Evaluation

- Multiple thicknesses (4mm, 8mm, and 12mm) were examined to determine operating parameters of SESH without changing theoretical models

- MCNP self shielding was determined by running with and without probability tables enabled, and taking the ratio of the two

- SESH and MCNP produced essentially identical results for all thicknesses

73-Ta-181 NNL/ORNL URR Evaluation (2021)
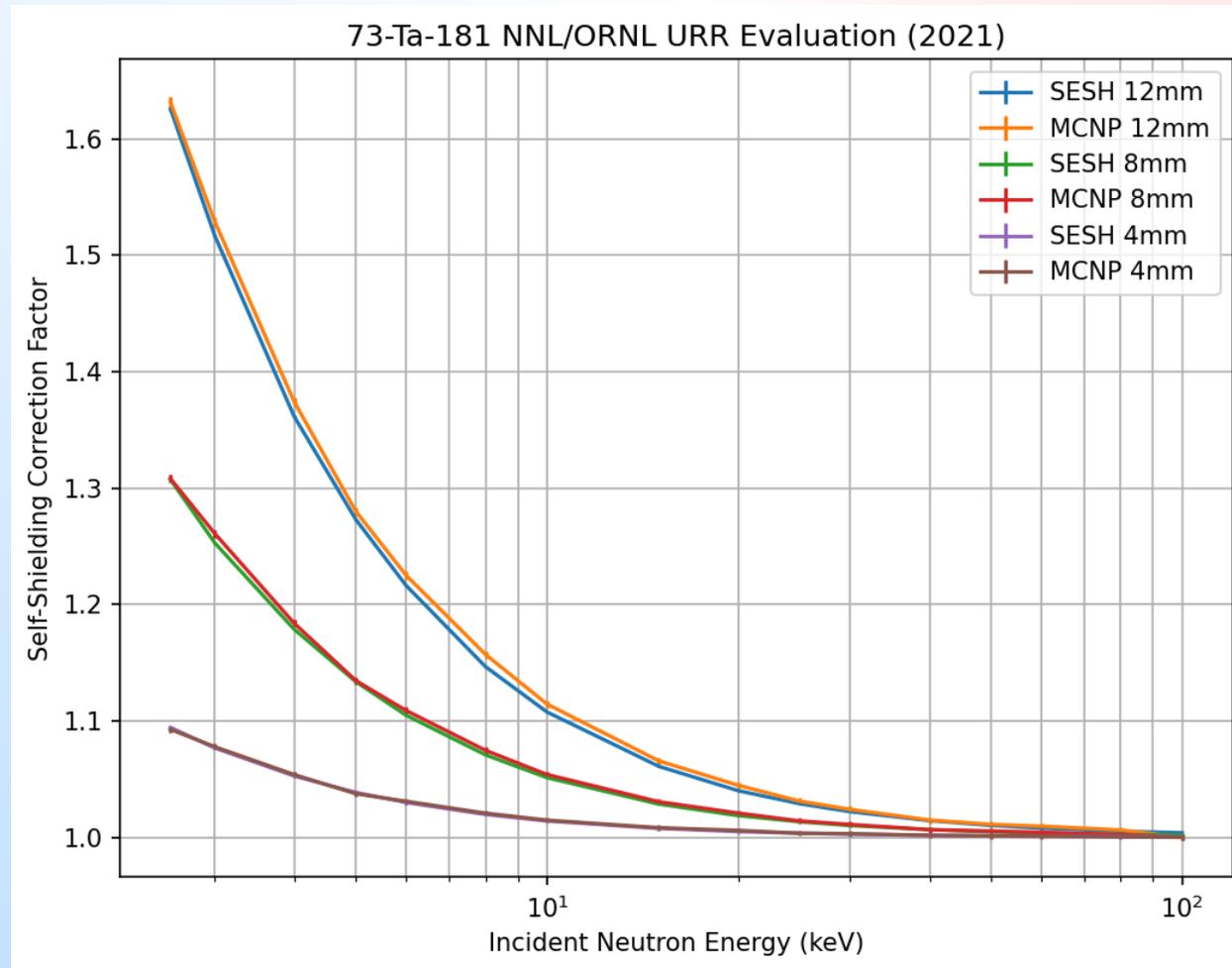
Methodology: Capture Correction Factor

$$P_0^i = \left(1 - e^{-n\sigma_{tot}^i}\right) \frac{\sigma_\gamma^i}{\sigma_{tot}^i}$$

$\equiv$ the probability that a neutron is absorbed without scattering

$P_1^i \equiv$ the probability that a neutron is absorbed after scattering once

$P_k^i \equiv$ the probability that a neutron is absorbed after scattering k times

$$\langle p \rangle = \sum_{i=1}^{N} \sum_{k=0}^{10} P_k^i \equiv \text{the average probability of a neutron being absorbed}$$

$$C_C = \frac{\langle p \rangle}{n \langle \sigma_\gamma \rangle}$$

$$\langle \sigma_{\gamma, new} \rangle = \frac{\langle Y_{experimental} \rangle}{n C_C}$$

Inaccurate Capture Correction Factor Observed

- Performed capture comparison with identical simulation parameters to transmission calculation

- Strong agreement between SESH and MCNP at lower energies

- However, SESH and MCNP produced very different results at increasing thicknesses and high energies

- ~10% error at 100keV energies and 12mm thick capture sample
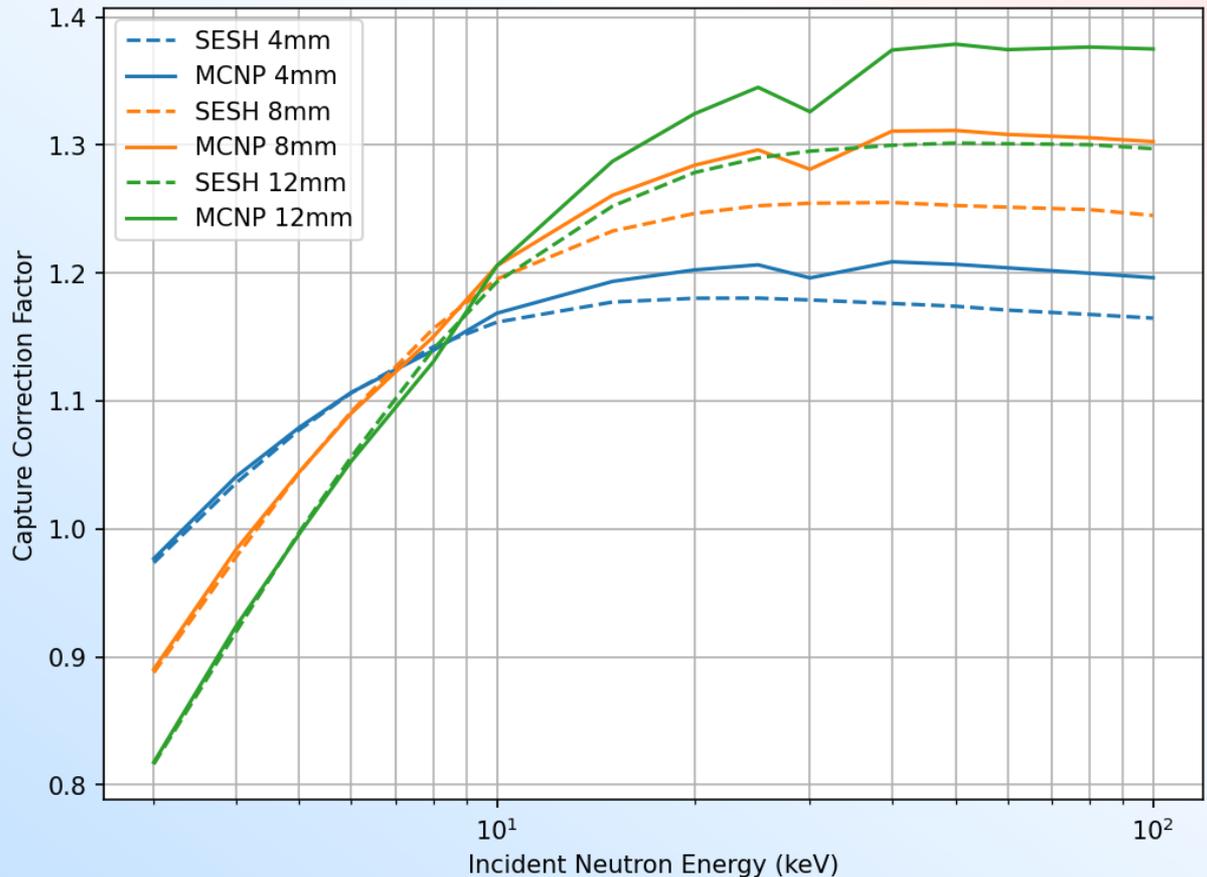
Doppler Broadening Issue

- The reason for the lack of agreement at high energies was ultimately found to be due to SESH's doppler broadening algorithm

- SESH uses the Psi-Chi method to perform doppler broadening which uses the Faddeeva Function

- $\psi + i\chi = w(x + i\beta)$

- x, β are functions of temperature and resonance width

- SESH calculates the actual ψ value somewhat accurately most of the time

- However, SESH also regularly fails, and instead returns the 0K cross section
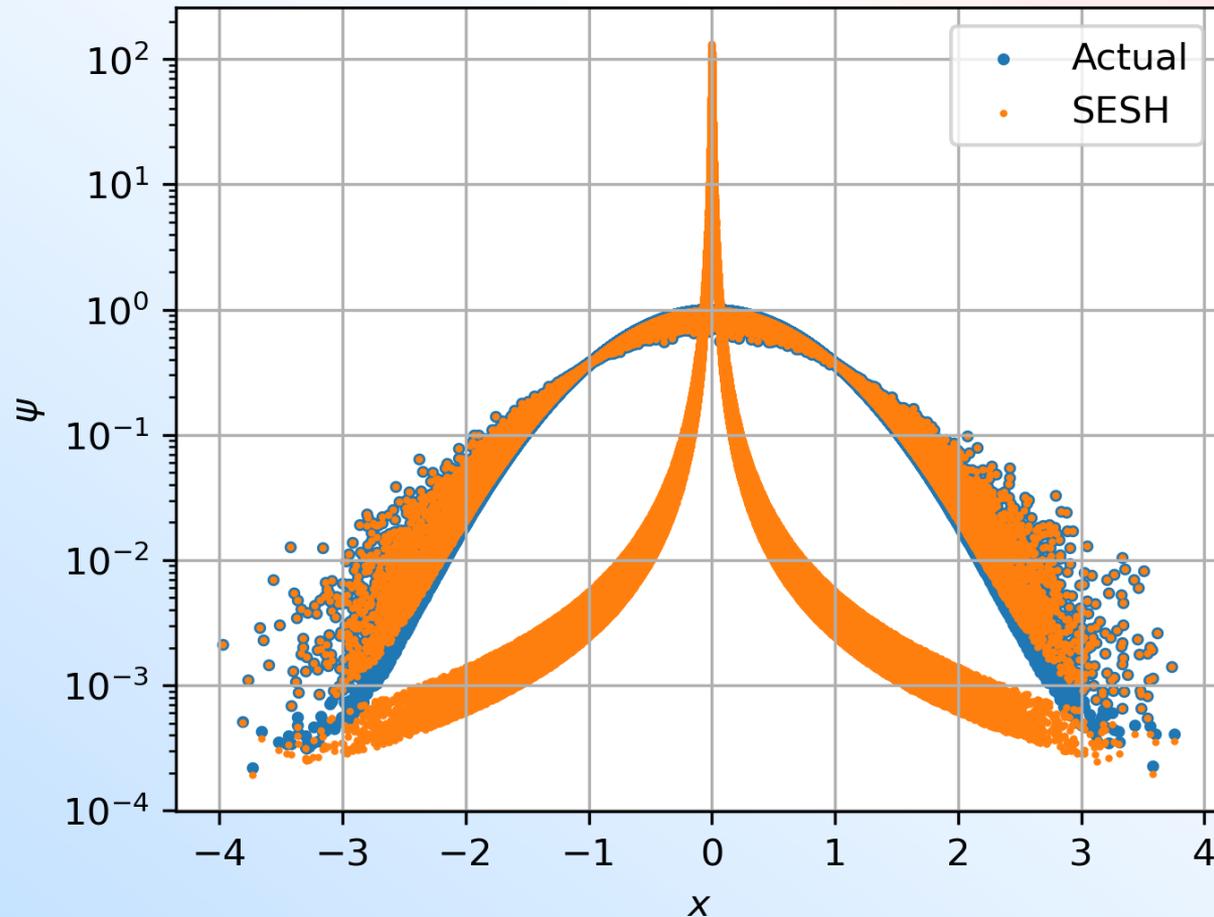
Doppler Broadening Issue

- SESH's original Faddeeva function failed if beta were less than 0.01
- Beta decreases with increasing energy, so higher energy resonances will encounter bug more frequently and increase correction factor error
- Implemented a new Faddeeva function algorithm into SESH
- This new algorithm resolved the low beta bug present in original algorithm
- New algorithm is much more accurate at all values
- Speed was not tested, but no noticeable performance change
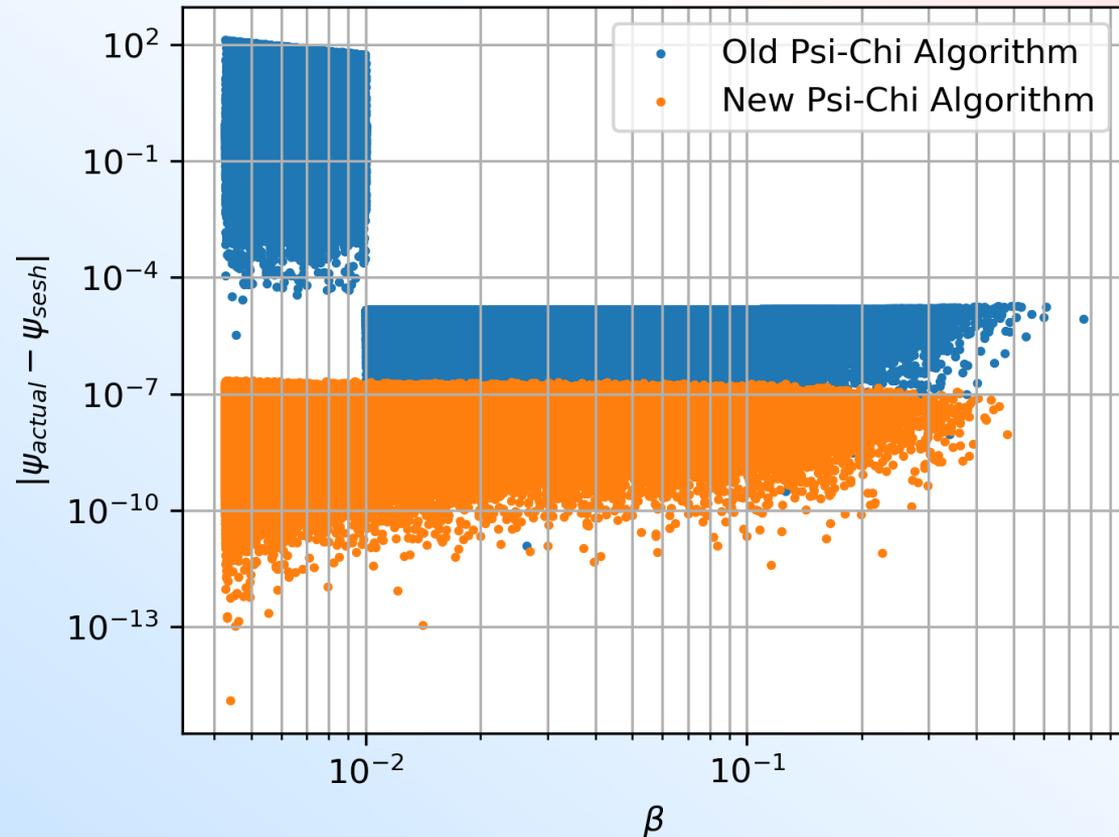
Verification of Capture

- Implementing the new Psi-Chi algorithm resolved the differences between MCNP and SESH

- Now the capture correction factor is accurate at all energies, not just low energies

- SESH is also now accurate at all thicknesses for capture, as is the case with transmission
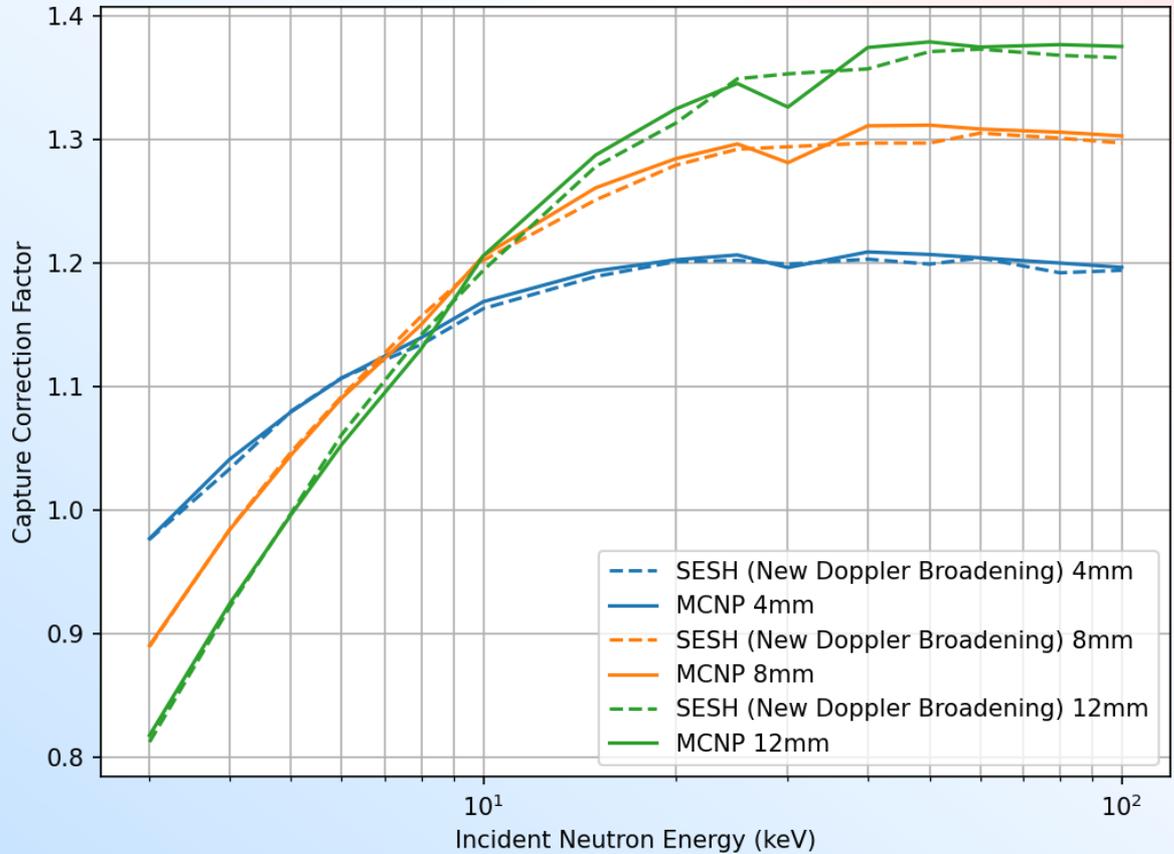
Future Work

- SESH has been sufficiently validated with MCNP – now ready for integration into SAMMY

- Currently working on wrapping SESH as-is into SAMMY

- Once SESH is fully integrated and a testing suite has been setup, ease-of-use improvements to the SESH codebase to ensure future development is relatively straightforward and easy

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