Automatic Determination of Resonance Parameters from Self-Shielded Measurements

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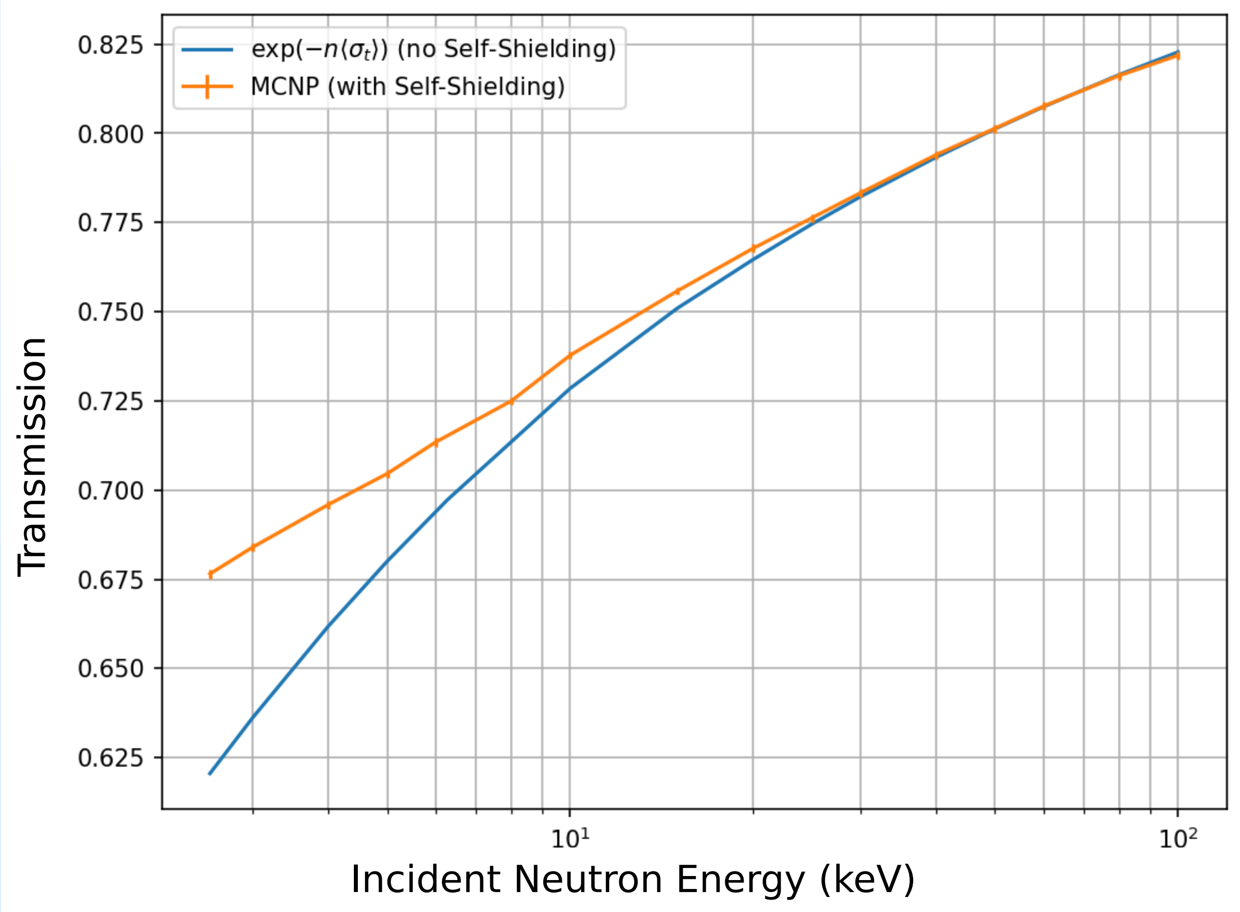
Achievements

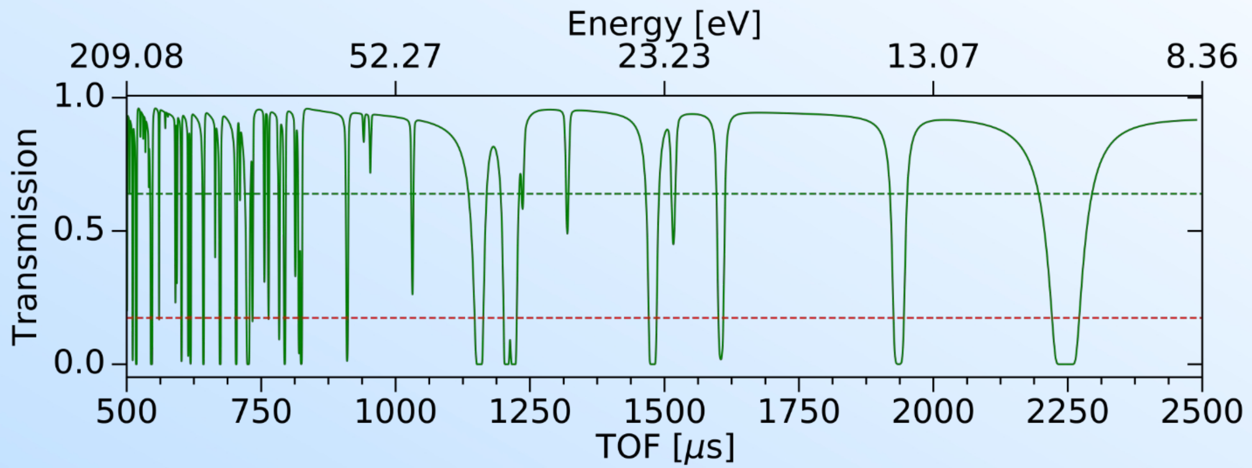
- Developed functionality to fit URR parameters from self-shielded transmission measurements
- Improved physics for calculating self-shielded capture yield correction factor
- Developed functionality to fit URR parameters from self-shielded capture yield measurements
- Validated fitting performance for both capture and transmission measurements

Motivation



- Self Shielding is phenomena which occurs in the unresolved resonance region
- Function of the resonance structure of the cross section we are unable to resolve
- Because only average parameters can be obtained in the URR, a correction factor must be calculated to fix transmission data and properly fit resonance parameters
- A 4mm Ta-181 transmission simulation is used to demonstrate self shielding

Motivation



$\langle T \rangle \approx 0.6$

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

$C_T \approx 3.0$

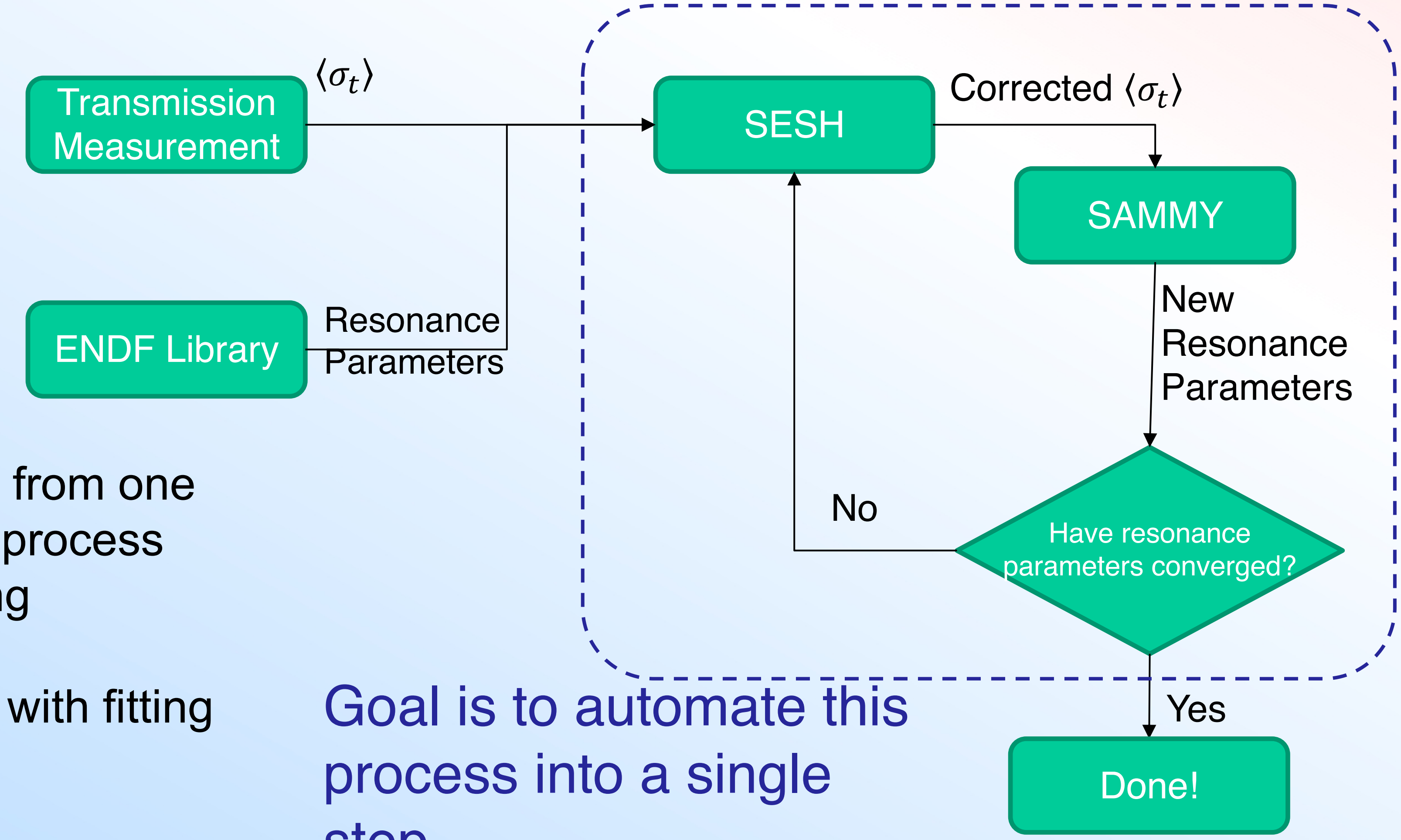
$$\langle T \rangle = e^{-n\langle \sigma \rangle} C_T$$

- Goal is to define $\langle T \rangle$ as a function of $\langle \sigma \rangle$

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

- Code exists called SESH which calculates C_T, the self-shielding correction factor
- SESH simulates resonances using average parameters and their known distributions
- Calculates $\langle \sigma \rangle$ and $\langle T \rangle$ from Monte Carlo sampling
- Uses these quantities to calculate C_T

Previous Self-Shielding Workflow



- This is primarily converting data from one format to another in an iterative process
- Very tedious and time consuming
- Prone to user error
- Very few evaluators are familiar with fitting URR

Goal is to automate this process into a single step

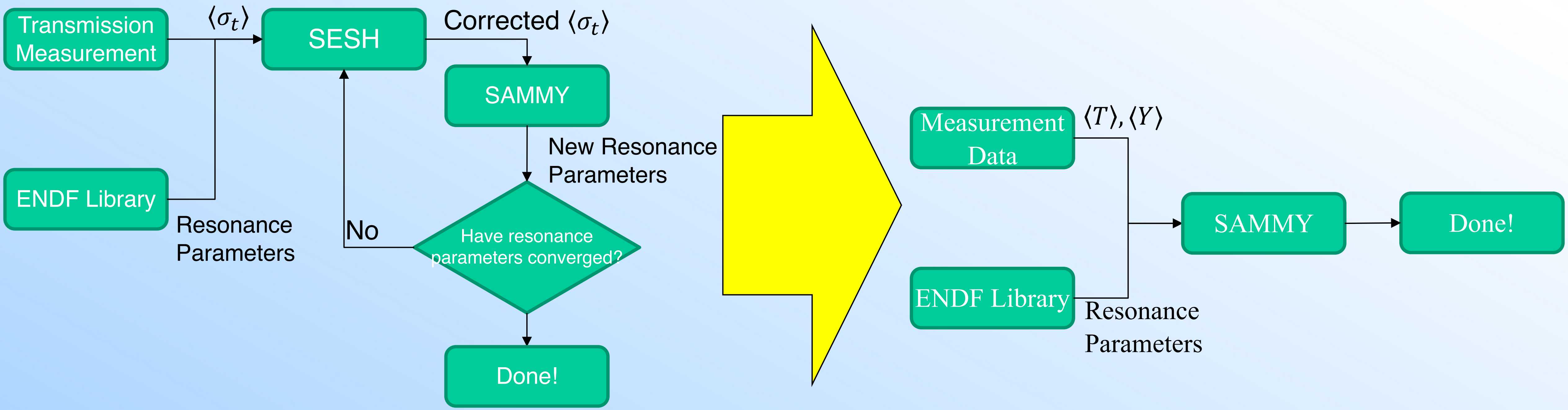
Previous Work

- Validated SESH performance for transmission correction
- Validated SESH performance for capture correction
- Rewrote doppler broadening subroutine to fix correction factor underprediction

CURRENT PROGRESS

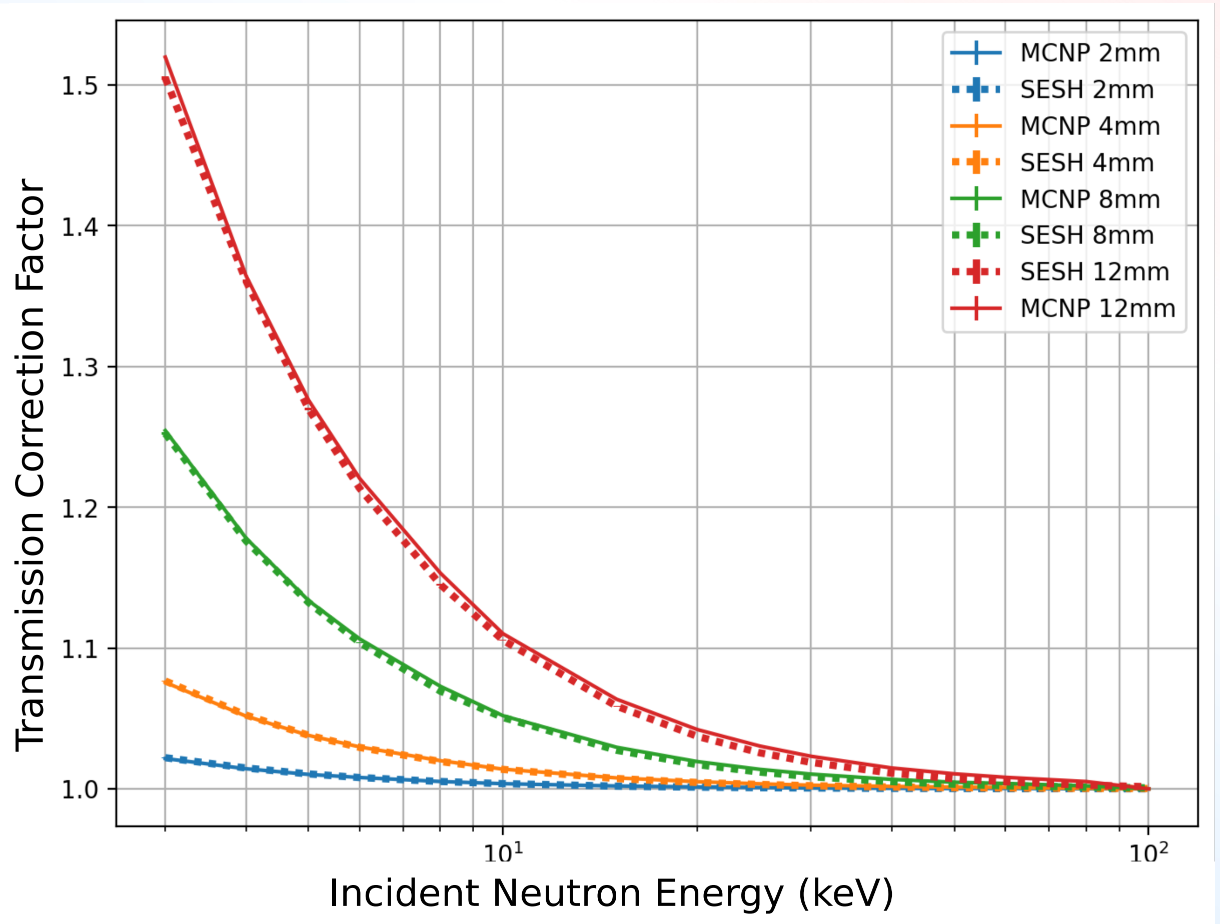
Calculating Self-Shielded Measurements with SAMMY

- SAMMY is now able to calculate theoretical self-shielded transmission and yield from resonance parameters
- Functionally identical to fitting in resolved resonance region
- A functioning example for transmission can be found in a new SAMMY test tr191



Verifying Transmission Fitting

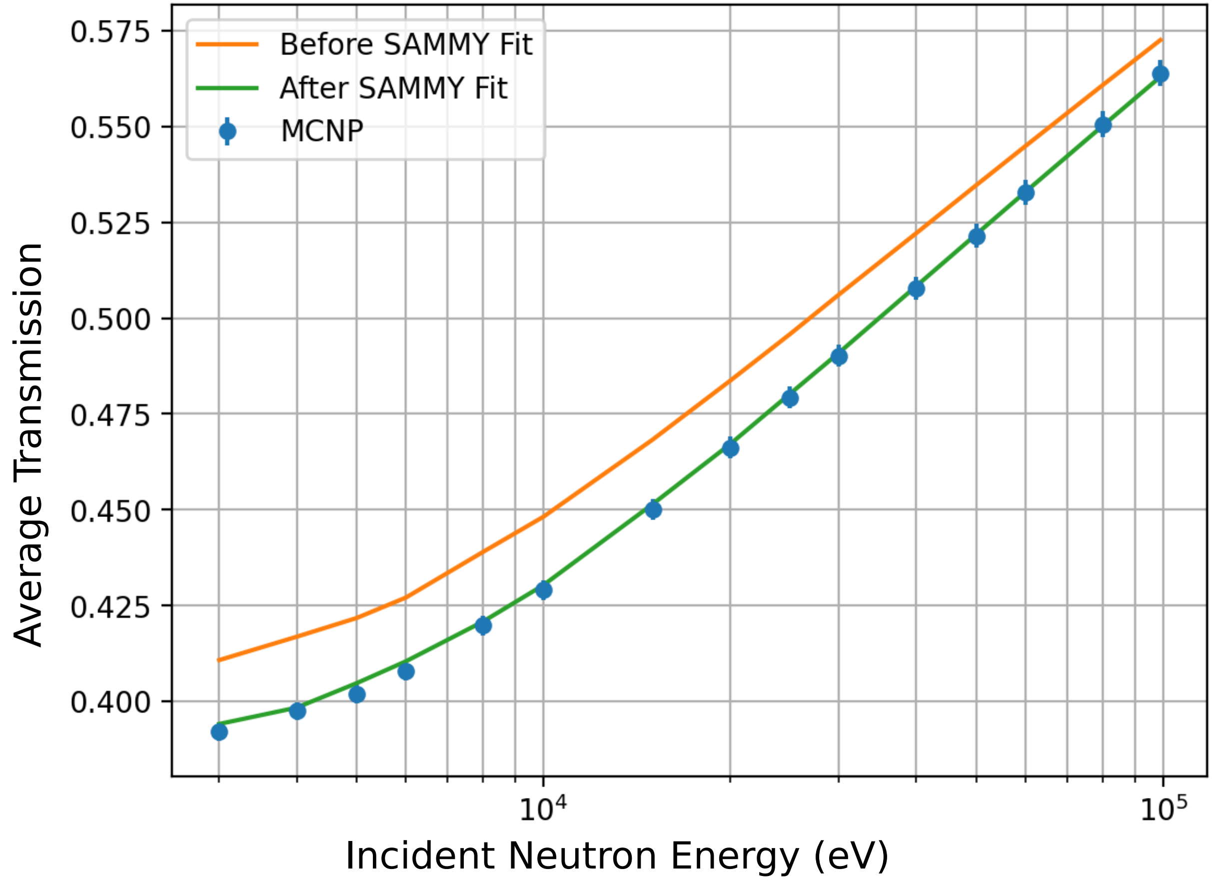
- To test this, compared to simulated transmission measurements in MCNP with Ta-181 using ENDF-8.1b2 evaluation
- Assuming NJOY+MCNP is completely correct
- Used four different thicknesses: 2mm, 4mm, 8mm, and 12mm



Verifying Transmission Fitting

	2mm	4mm	8mm	12mm	ENDF-8.1b2
$S_0(\times 10^4)$	1.753	1.752	1.739	1.723	1.740 ± 0.03
$S_1(\times 10^4)$	0.823	0.808	0.799	0.801	0.800 ± 0.07
$S_2(\times 10^4)$	1.527	1.632	1.741	1.787	1.690 ± 0.18

- Goal was to perturb the parameters such that the initial value was incorrect, and then obtain the correct parameters.
- Final fits fell within the range of error of the ENDF-8.1b2 evaluation for all thicknesses
- Fitting self-shielded URR transmission measurements in SAMMY is working correctly



Capture Correction: Multiple Scattering

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

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

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

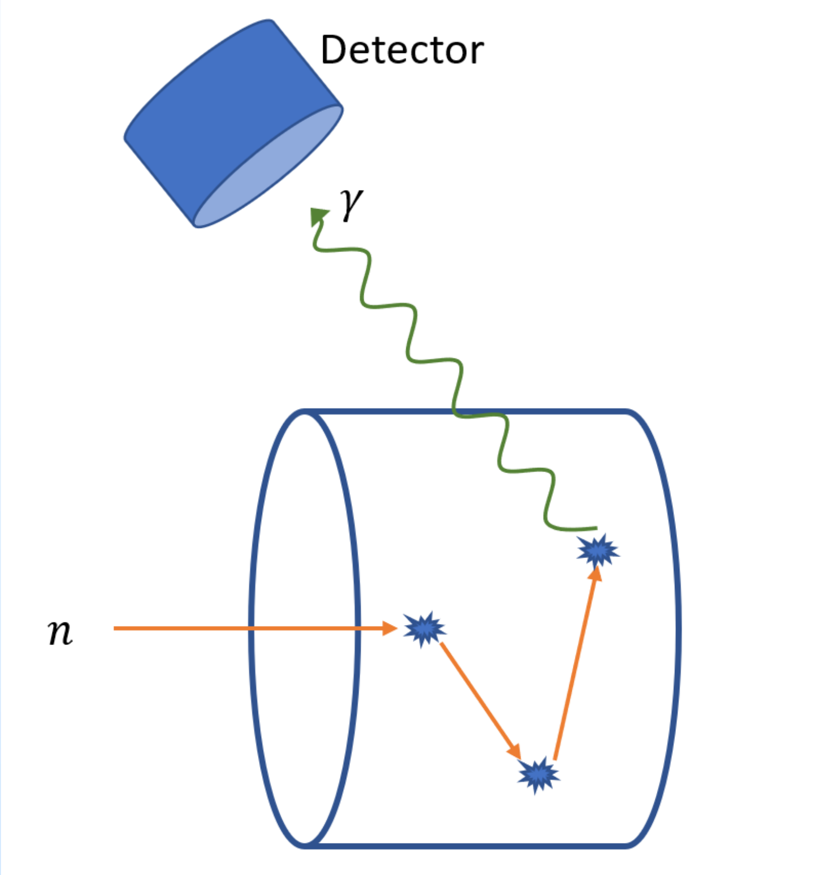
$P_k^i \equiv$ the probability that a neutron is absorbed after scattering k times

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

$Y \approx n\sigma_\gamma \equiv$ thin sample approximation

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

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



Improving Multiple Scattering Physics

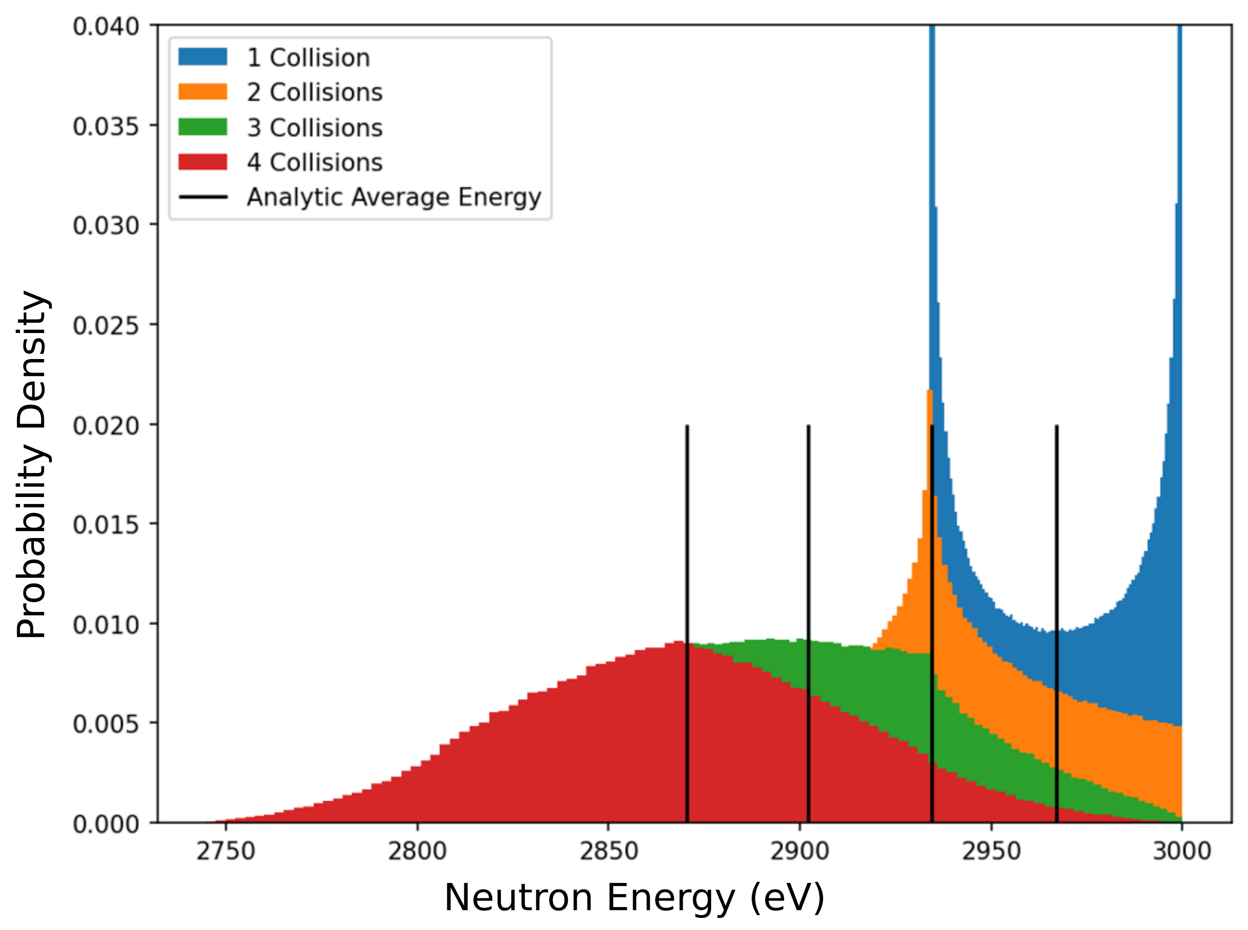
- SESH previously assigned every scattered neutron with the average scattering energy, independent of scattering angle
- Substituted with an angle-dependent energy sampling procedure:
  1. The scattering angle of each post collision neutron would be sampled assuming an isotropic scattering distribution
  2. post collision energy would be calculated as a function of the scattering angle

$$E' = E\,\frac{A^2 + 2A\mu_c + 1}{(A+1)^2}$$

Where

$\mu_c = \cos\phi_c$; $\phi_c \equiv$ scattering angle in CMS

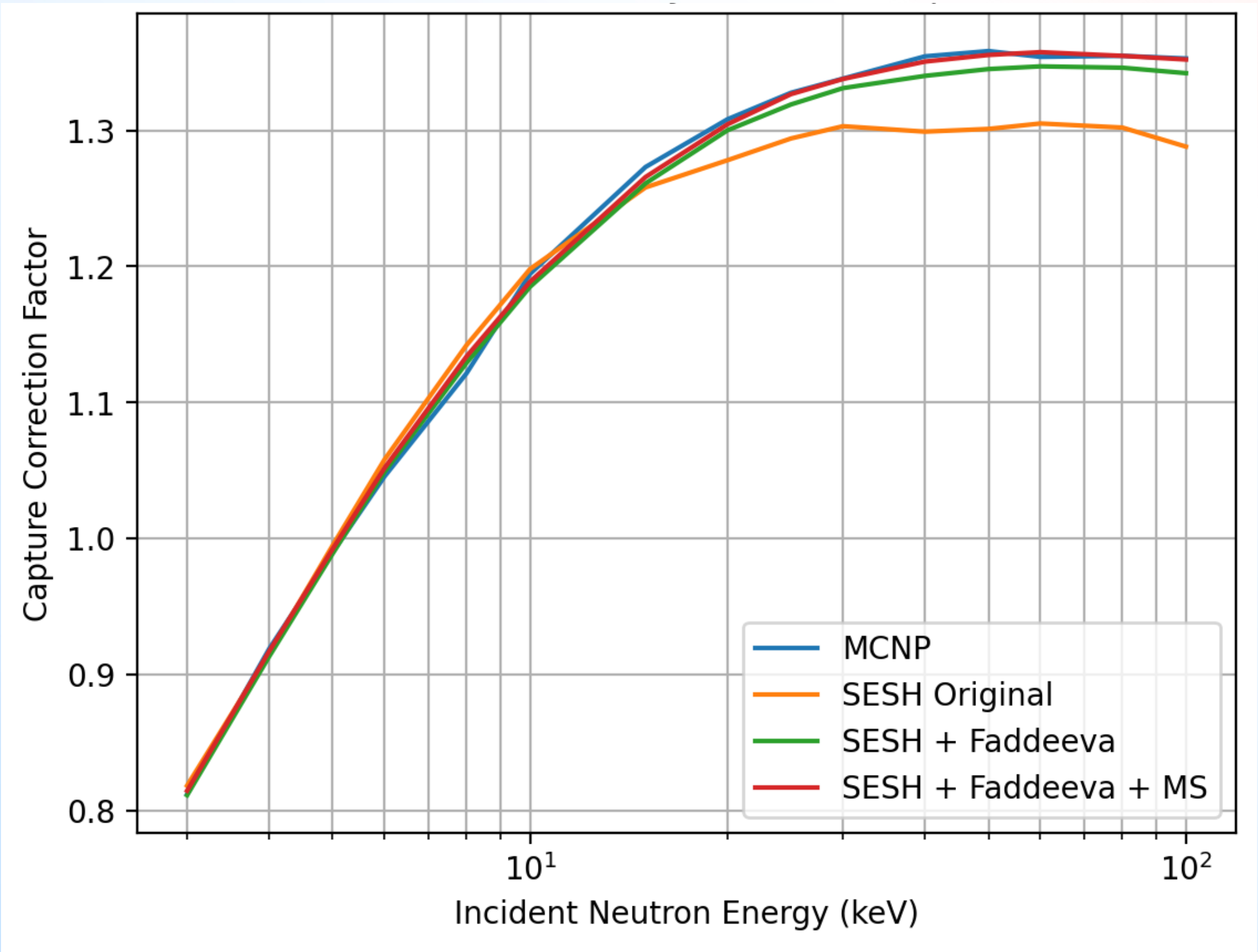
Increased maximum number of scattering events per neutron from 10 to 100



Improving Capture Correction

- Previously fixing the doppler broadening issue resolved majority of disagreement between SESH and MCNP

- Improving multiple scattering calculation improved agreement even further for all energies



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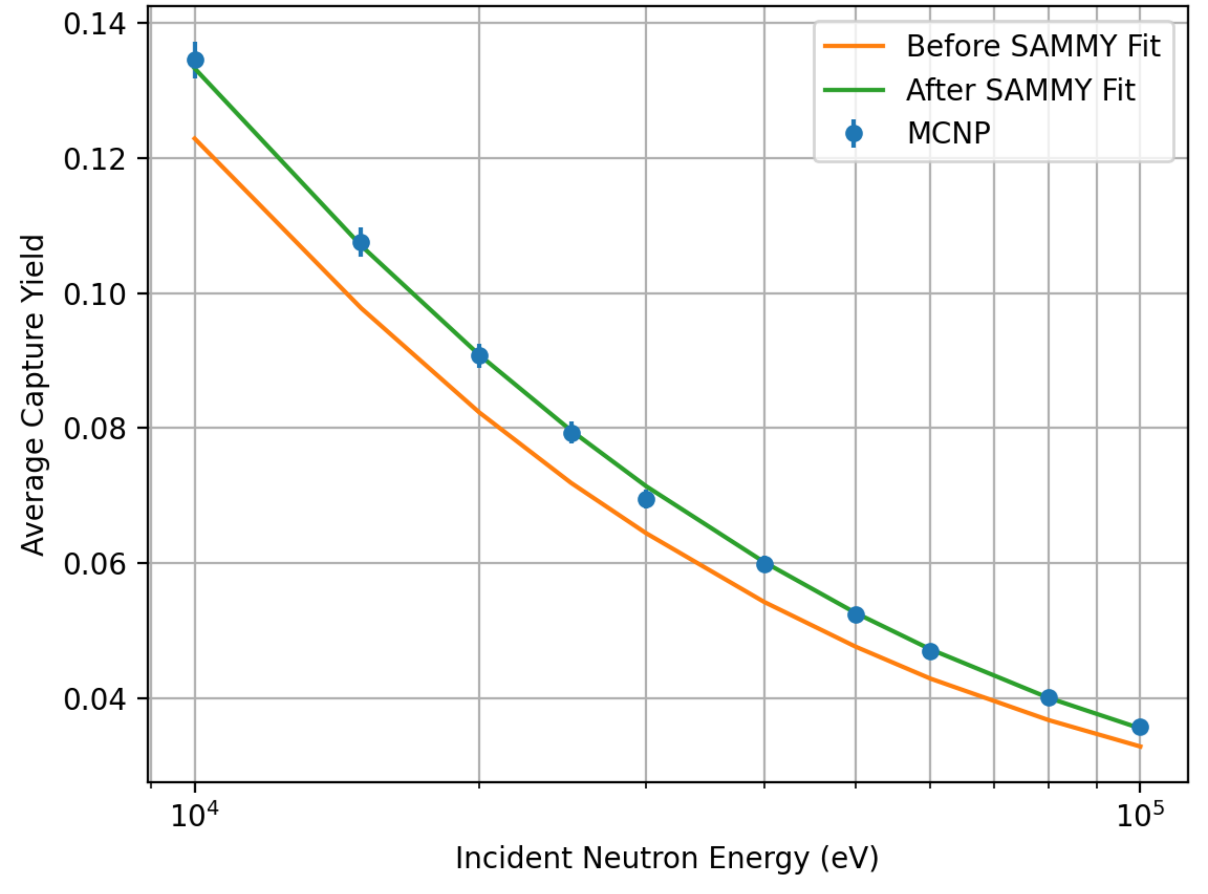
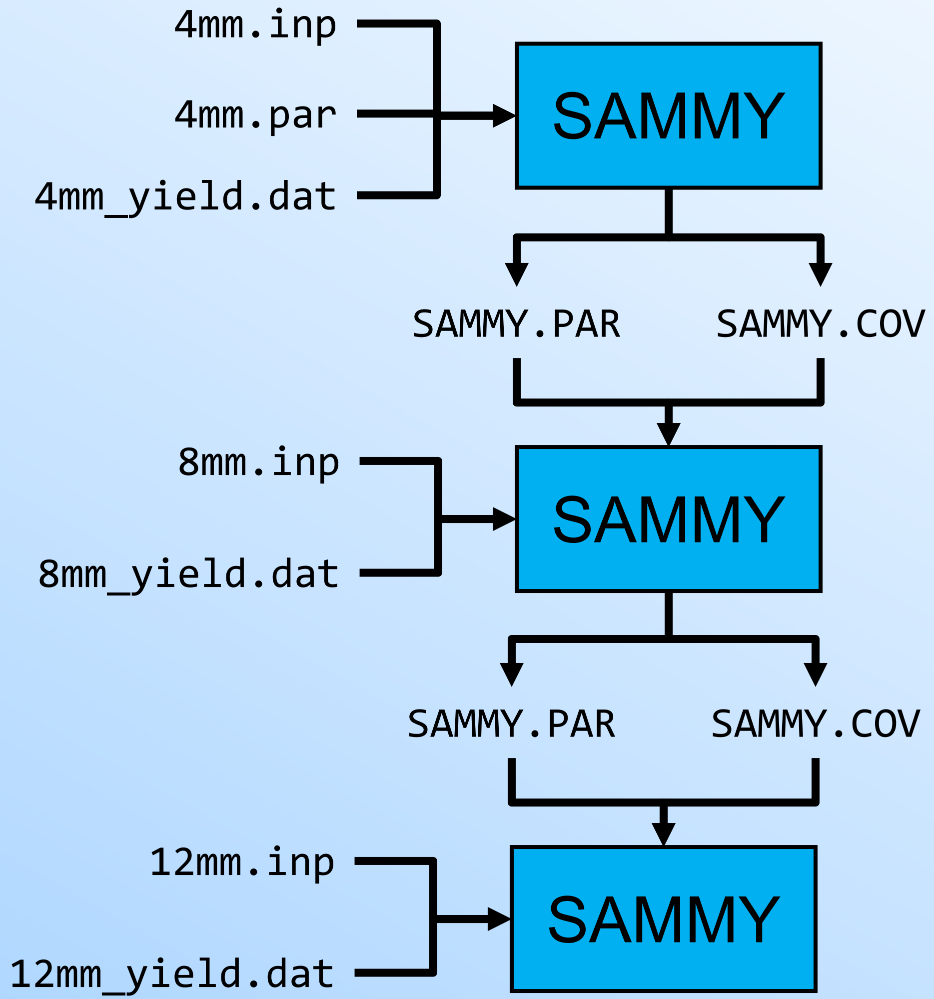
Verifying Capture Fitting

	4mm	8mm	12mm	ENDF-8.1b2
$S_0(\times 10^4)$	1.739	1.751	1.745	1.740 ± 0.03
$S_1(\times 10^4)$	0.927	0.897	0.892	0.800 ± 0.07
$S_2(\times 10^4)$	1.573	1.632	1.596	1.690 ± 0.18

- Proceeded with fitting capture in same method as transmission
- P-wave strength fits outside of error bounds from ENDF-8.1b2 Ta-181 evaluation



Verifying Capture Fitting: Processing Multiple Samples



- Wanted to ensure that inclusion of SESH into SAMMY did not break functionality to process multiple samples
- Should also increase fitting performance

	SAMMY	ENDF-8.1b2
$S_0(\times 10^4)$	1.737	1.740 ± 0.03
$S_1(\times 10^4)$	0.857	0.800 ± 0.07
$S_2(\times 10^4)$	1.614	1.690 ± 0.18

- Fits increased accuracy significantly – much stronger agreement with ENDF-8.1b2 parameters
- Capture performance and multiple sample processing performance successfully verified

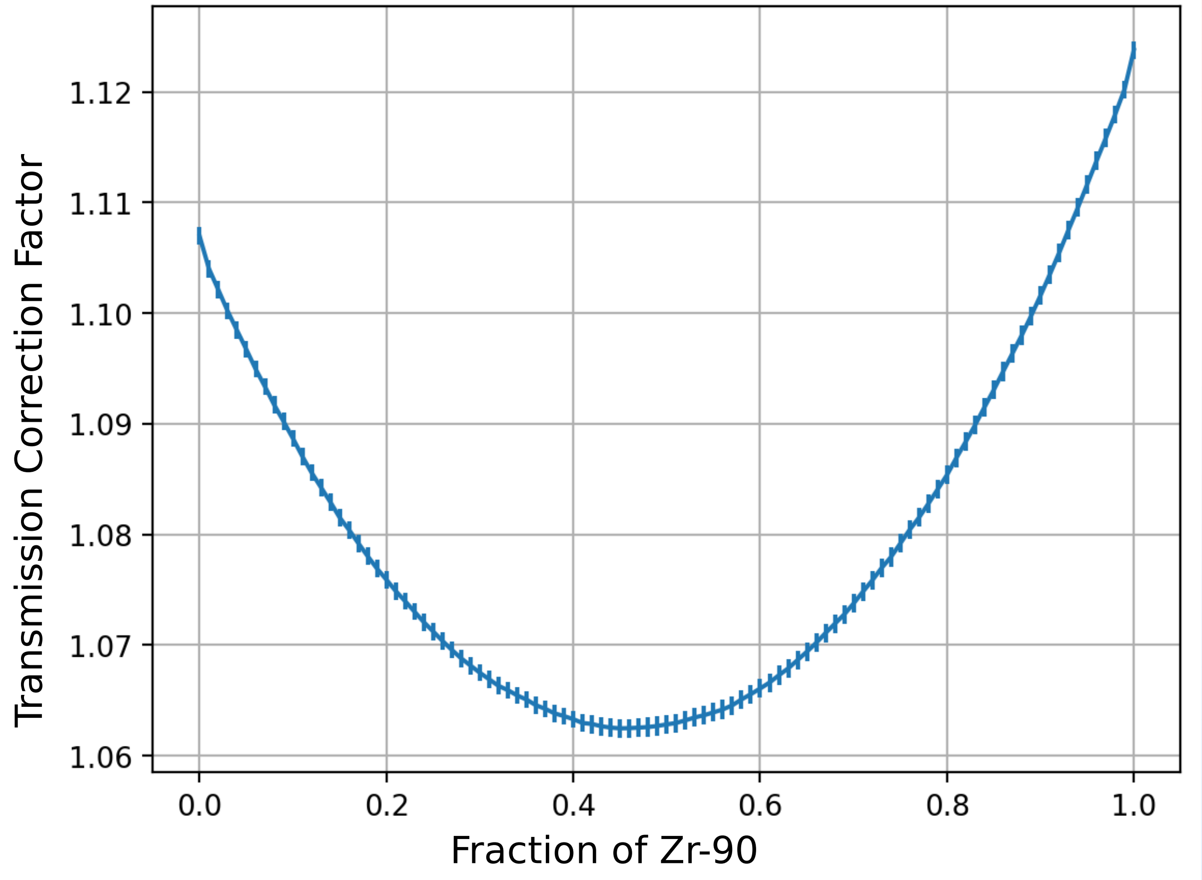
ONGOING WORK

Multiple Isotope Sample Corrections

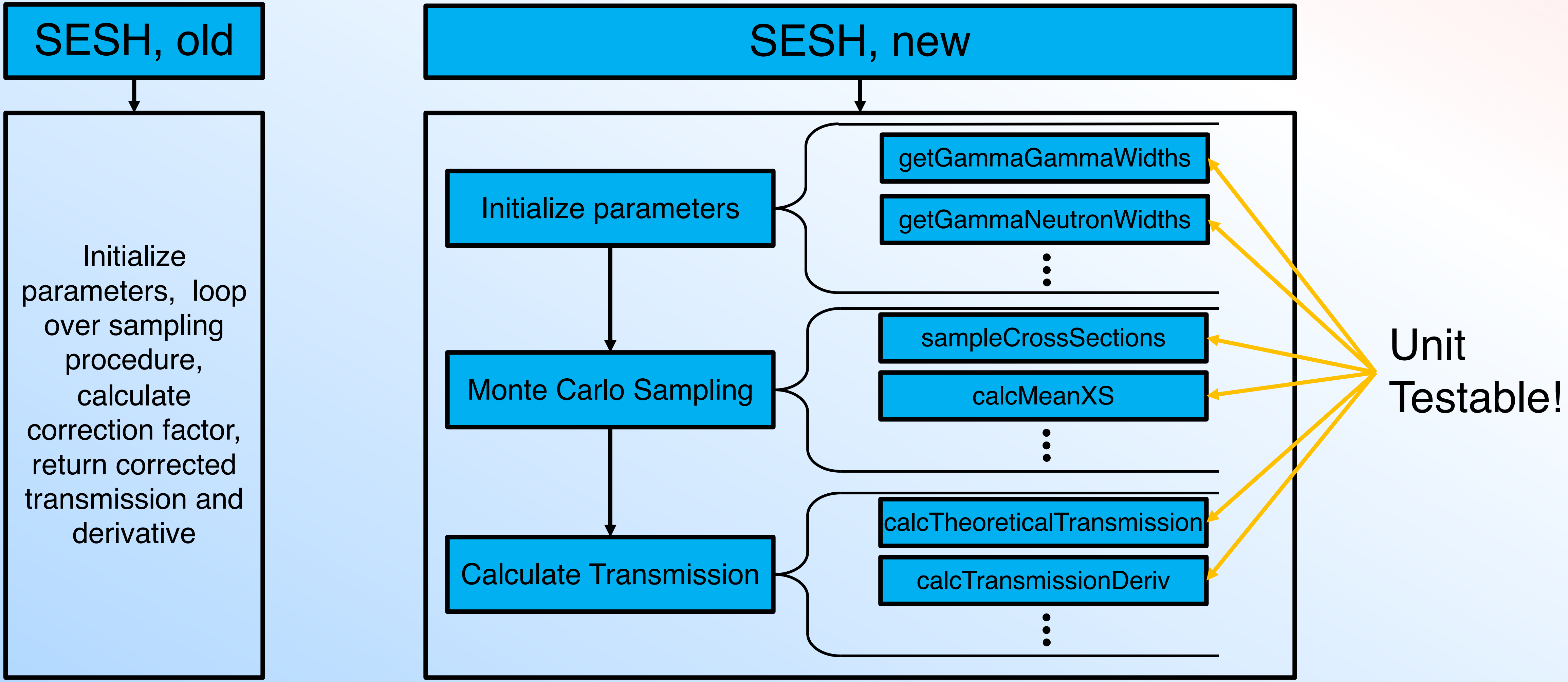
- Looking at modeling capture correction for samples with multiple isotopes
- As basis, looked at transmission correction through a sample of Zr-90 and Zr-92 at varying enrichments
- Mixed isotope samples in simulation exhibit dampening of correction factor
- No simple functional relationship between the constituent isotope's individual correction factors, i.e.,

$$C_{T,mix} \neq \gamma_1 C_{T,1} + \gamma_2 C_{T,2}$$

- Calculating correction factor of mixtures will require more intensive altering/refactoring of SESH code



Functionalizing SESH



Before/After Refactoring Subroutines

```
17        GNS=0.
          GNINS=0.
          DO L = L1,L2,2
!
            CALL PORTER(GNE(NC,J,L),GNL(L))
            GNS=GNS+GNL(L)
            GNINS=GNINS+GNINE(NC,J,L)
          end do
          GT=GNS+GNINS+GGE(NC,L1)
          ETA=GT*DOP(NC)
          XI=2.*ETA*H/GT
          CT=C0*ETA/GT
          CG=CT*GNS*GGE(NC,L1)/GT
!
          CALL WOFZ(XI, ETA, UU, VV)
!
          SCC=CG*UU
          SN=SN+SCC
!           EFFECTIVE CAPTURE CROSS SECTION
          SC=SC+SCC
!         TOTAL CROSS SECTION
          do L=L1,L2,2
            ST=ST+CT*GNL(L)*(UU*COSE(NC,L)+VV*SINE(NC,L))
          end do
          IF(MP.EQ.1)GO TO 18
!                   CHECK IF SECOND MEMBER OF PAIR IS ALREADY INCLUDED
          IF(H.LT.0.)GO TO 16
!
          CALL WIGNER(DE(NC,J,L1),DD)
!
          HNEG=HNEG-DD
          H=HNEG
          GO TO 17
!                   CHECK IF SECOND MEMBER OF PAIR IS ALREADY INCLUDED
18        IF(H.LT.0.)GO TO 16
          HPOS=H
          HNEG=H-DD
          H=HNEG
          GO TO 17
!                   INCLUDE ANOTHER PAIR OF RESONANCES IF REQUIRED
16        IF(MP.EQ.NP)GO TO 93
          MP=MP+1
!
          CALL WIGNER(DE(NC,J,L1),DD)
!
          HPOS=HPOS+DD
          H=HPOS
          GO TO 17
```

```
do n = 1,params%NumPairs
    if(n.eq.1) then
        CALL SPACE(endep_params%DE(J,L1),DD)
        HPos=DD*random()
        HNeg= HPos - DD
    else
        call wigner(endep_params%DE(J,L1),DD)
        HPos = HPos + DD
        call wigner(endep_params%DE(J,L1),DD)
        HNeg = HNeg - DD
    end if

    Hvals(1) = HPos
    Hvals(2) = HNeg

    do h_i=1,2
        H = Hvals(h_i)
        GNS = 0.
        GNINS = 0.

        do L=L1, L2, 2
            call porter(endep_params%GN(J,L), GNL(L))
            GNS=GNS+GNL(L)
            GNINS= GNINS + endep_params%GNIN(J,L)
        end do

        GT=GNS + GNINS + endep_params%GGE(L1)
        ETA=GT*endep_params%dop
        XI=2.*ETA*H/GT
        CT=C0*ETA/GT
        CG = CT*GNS*endep_params%GGE(L1)/GT

        CALL WOFZ(XI,ETA,UU,VV)
        SC = SC+CG*UU

        do L=L1,L2,2
            ST=ST+CT*GNL(L)*(UU*endep_params%COS2(L)+VV*endep_params%SIN2(L))
        end do
    end do
end do
```

Future Work

- Uncertainty Quantification
  - It is unclear how to propagate uncertainty using self-shielded parameters in the URR
  - Previously no self-shielding uncertainty was propagated at all
  - More study must be done to figure out how to translate this to an evaluation

Conclusion

- Fitting procedures working correctly for self-shielded transmission and capture measurements inside of SAMMY
- Working on functionalizing and adding test coverage to all components in SESH
- Multi-Isotope sample fitting soon to be enabled

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