Deployment of Gaussian Surrogate Model for Ad-Hoc Adjustments to Elastic Scattering Angular Distributions

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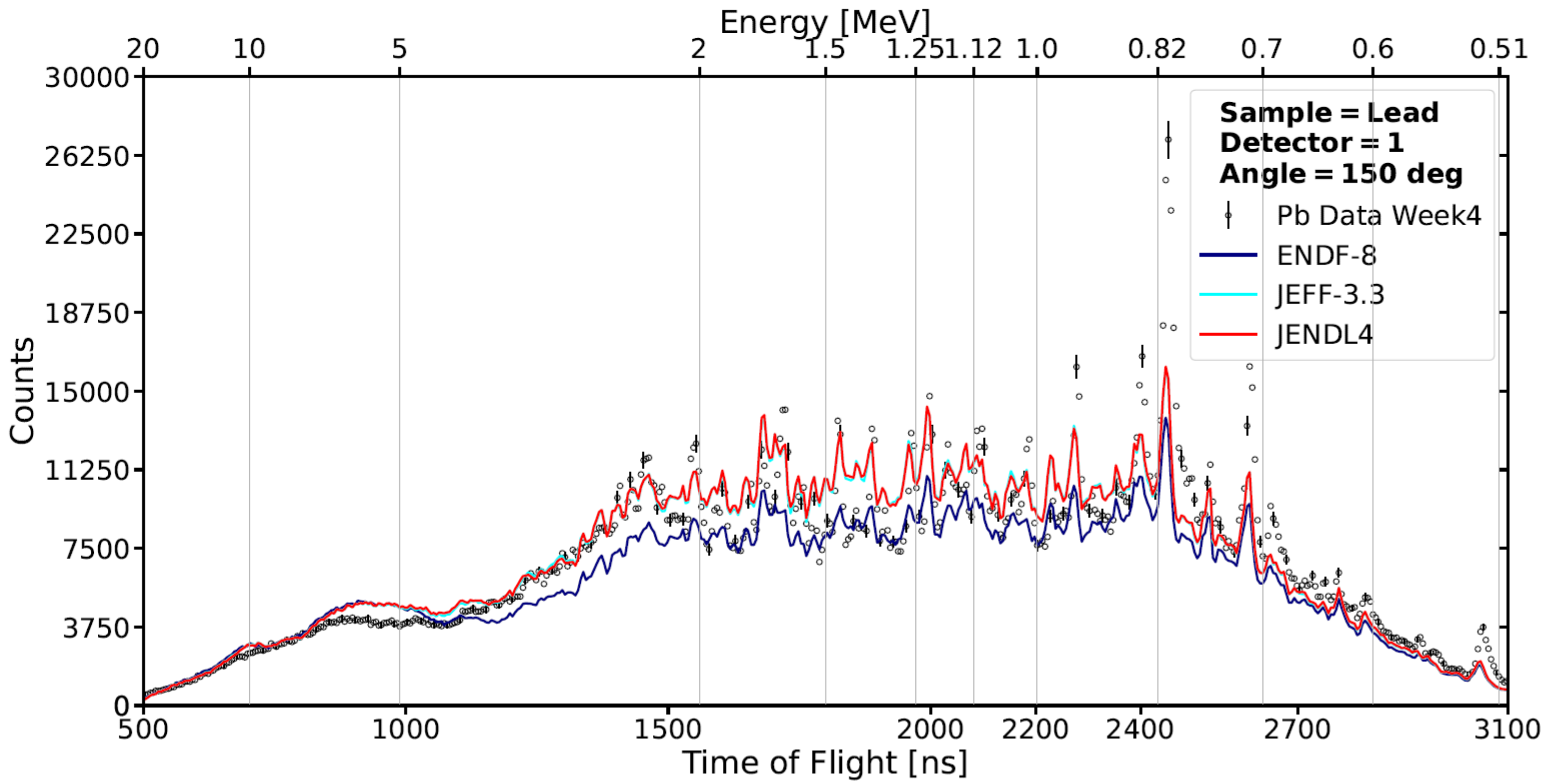
WINS 2023 | Rensselaer Polytechnic Institute

- Motivation
- Gaussian Surrogate Models
- Validation of Method with Pb-208
- Application on Be-9
- Summary

- In nuclear data evaluations there are often difficulties in replicating experimental phenomena with the theories, models, or formats available to evaluators
- Even in the best circumstances evaluators might have to adjust ENDF outside of their models

Lead Quasi-Differential Scattering Data



- In the previous talk, I used the Blatt-Biedenharn (BB) formalism to get ESAD which are derived from resonance parameters.
- These could constitute the “True” solution to the ESAD since its based on scattering physics over resonances
- What happens when the BB treatment isn’t available but there’s structure that should be replicated in scattering?

- Option 1: Fit data directly
  - Quasi-differential scattering is not a true double differential measurement of a partial channel → Not Possible
- Option 2: Brute force
  - Sample all possible combinations of secondary neutron distributions, problem goes expensive as polynomial order increases
- Option 3: Surrogate Process Modeling
  - Define objective function based on scattering simulation/data and Legendre polynomials coefficients, optimize this objective.

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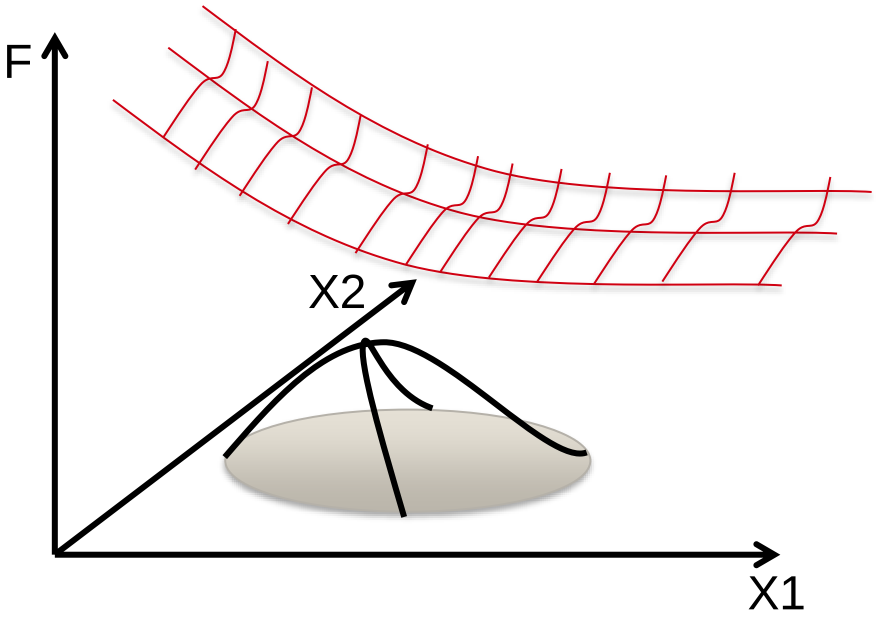
- Numeric method to approximate the important responses of a function that is normally expensive to evaluate

$$F(x,y,z) \xrightarrow{Surrogate\ Process} f(w)$$

$$F(x,y,z) \approx f(w)$$

- Surrogates can be constructed with any semi-positive definite function, here Gaussian distributions will be used
- These multivariate Gaussians can replicate any smooth function and enables several orders of differentiation for optimization



- MCNP transport calculations are expensive, come with statistical noise, and have hundreds of variable inputs
- Looking to develop a function dependent only on the scattering distribution coefficients

$$F(\sigma, \Omega, E) \approx f(a_0, a_1, a_2, \ldots a_n)$$

Objective Function

- The objective is to minimize a chi-square-like FoM between simulation and experiment, using coefficients to Legendre Polynomials $a_l = [a_0, a_1, a_2, a_n]$

$$\text{Obj.} = \min(a_l) \sum_{i=0}^{\#\,detectors} \sum_{j=E_{res,min}}^{E_{res,max}} \frac{(C_{sim,i,j}(a_l) - C_{exp,i,j})^2}{\sigma_{exp}^2}$$

Such that

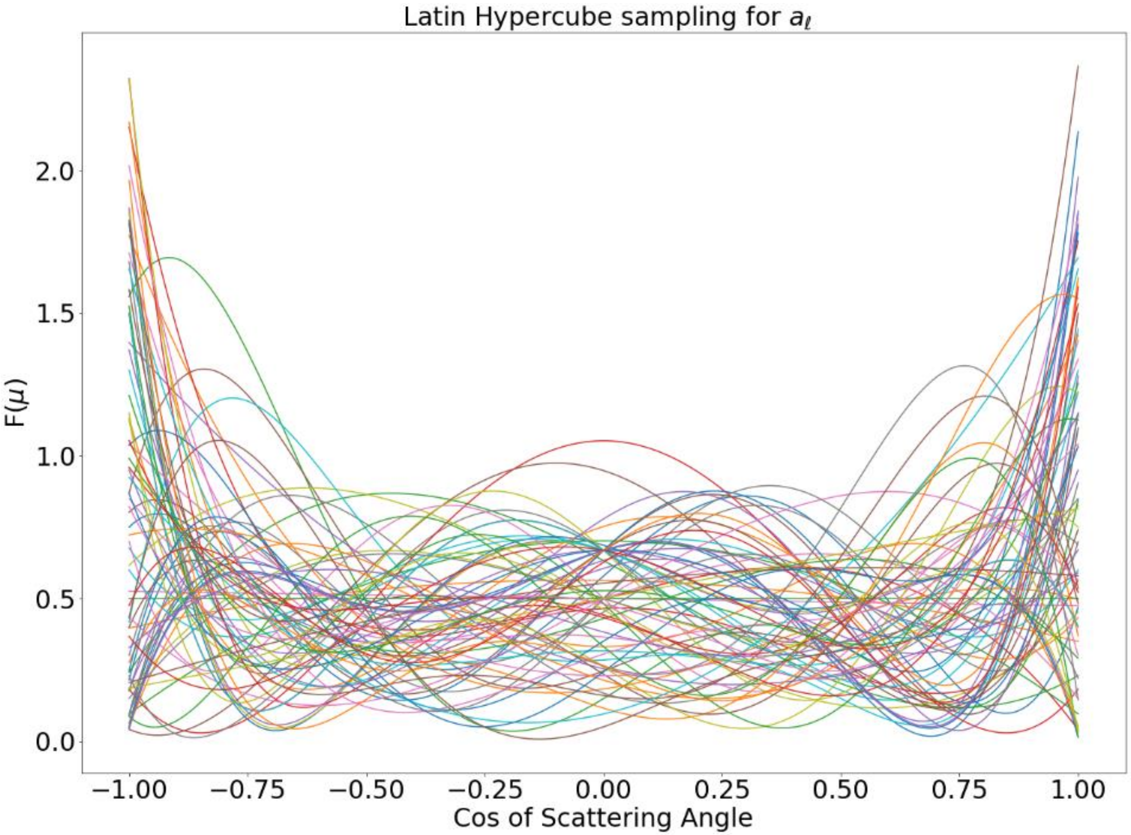
$$\int_{-1}^{1} \sum_{l=0}^{N} \frac{2l+1}{2} a_l P_l(\mu) d\mu = 1 \qquad \sum_{l=0}^{N} \frac{2l+1}{2} a_l P_l(\mu) d\mu \geq 0 \qquad \mu = [-1,1]$$

- Assumptions
  - Fit between simulation and experiment is solely dependent on elastic scattering angular distribution
  - Can use one elastic scattering angular distribution (ESAD) in the energy range of interest

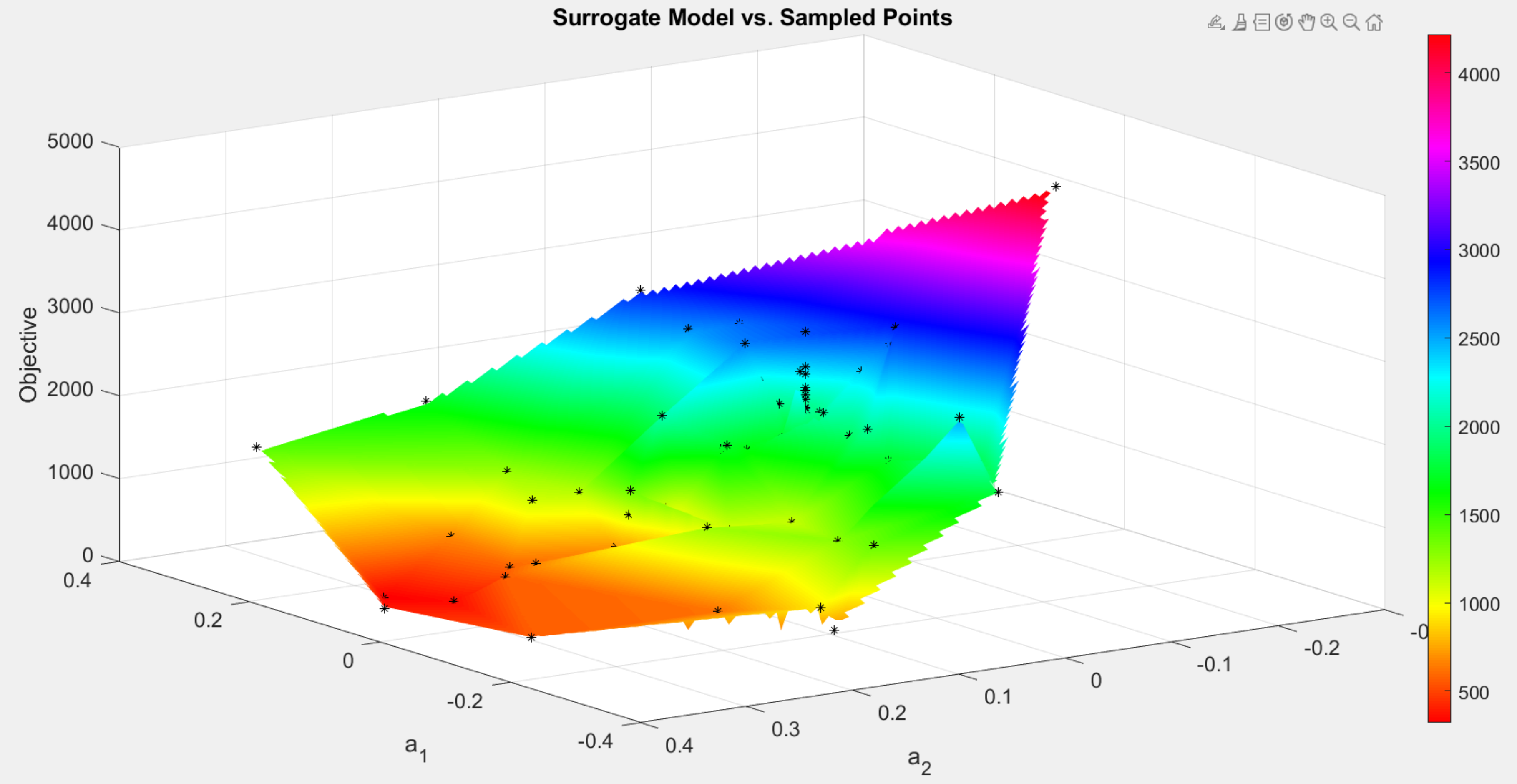
- With the objective function defined, need a minimum data set of the calculated function to form the model
- This involves choosing the order of Legendre polynomials and the step-size for evaluating each coefficient

Sampling scattering coefficients

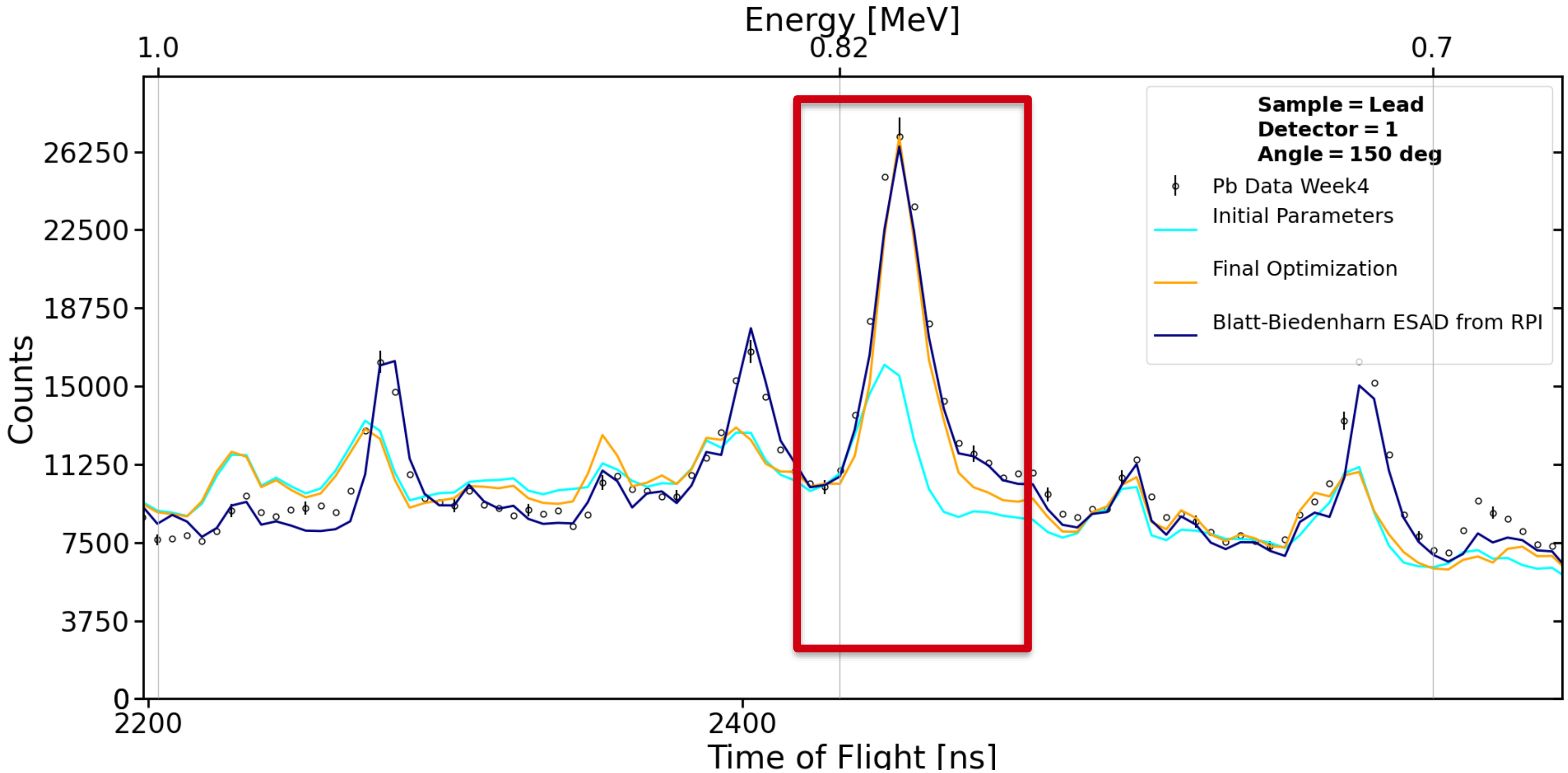
- Use sixth term Legendre polynomial (a0 – a5)
- Sampling done using Latin hypercube sampling
- This defines minimal set of scattering distributions from fully backscattering to forward scattering



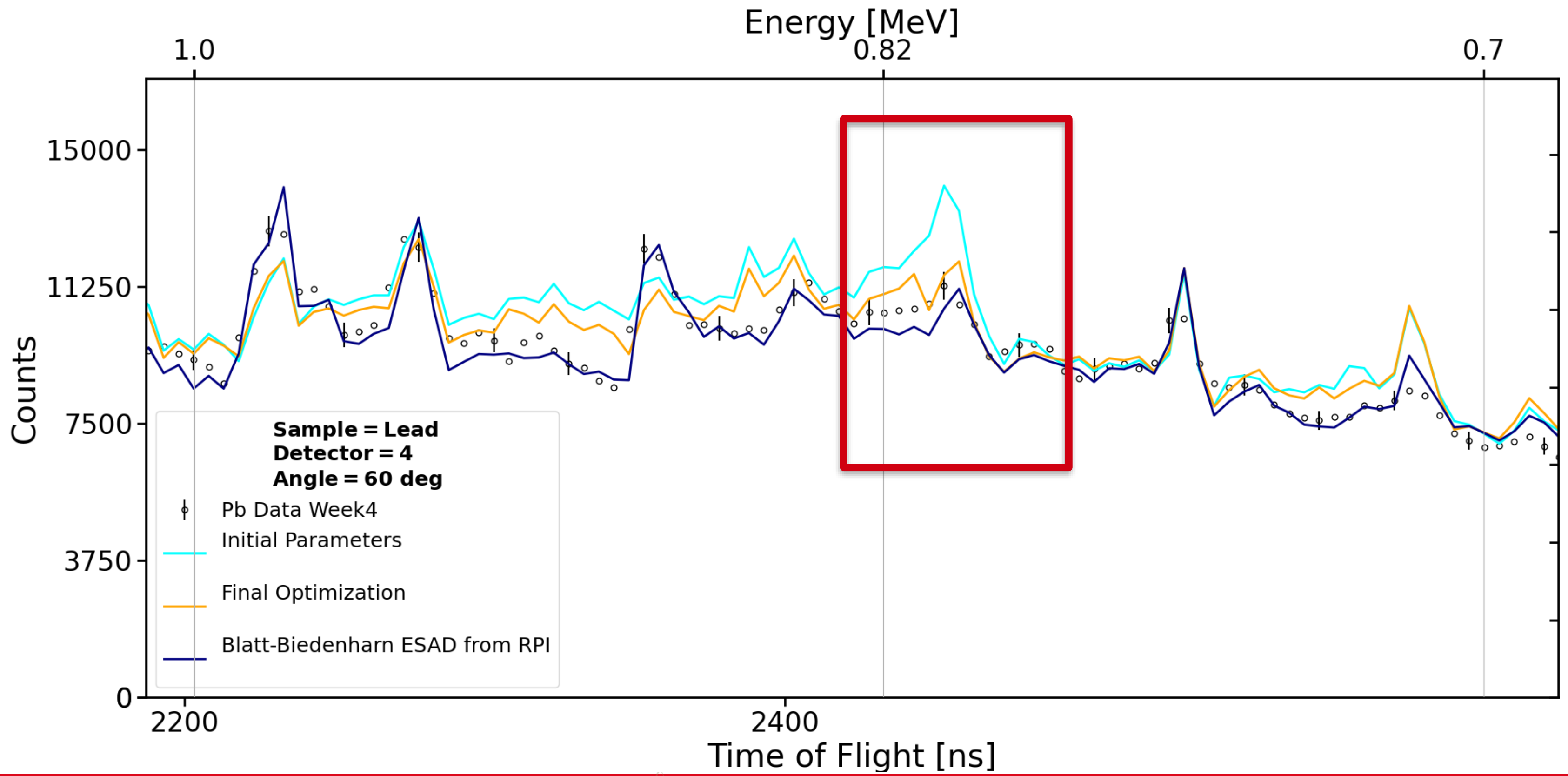
- To validate this methodology, employ the surrogate model to fix ESAD for Pb-208 resonance at 814 keV
- The outcome of optimization should provide similar level of agreement to the Blatt-Biedenharn derived ESAD
- Surrogate model and optimization done with MATLAB


Surrogate Model vs. Sampled Points
Objective
5000
4000
3000
2000
1000
0
0.4
0.2
0
-0.2
-0.4
a_1
0.4
0.3
0.2
0.1
0
-0.1
-0.2
a_2
4000
3500
3000
2500
2000
1500
1000
500

Pb-208 Scattering Optimization



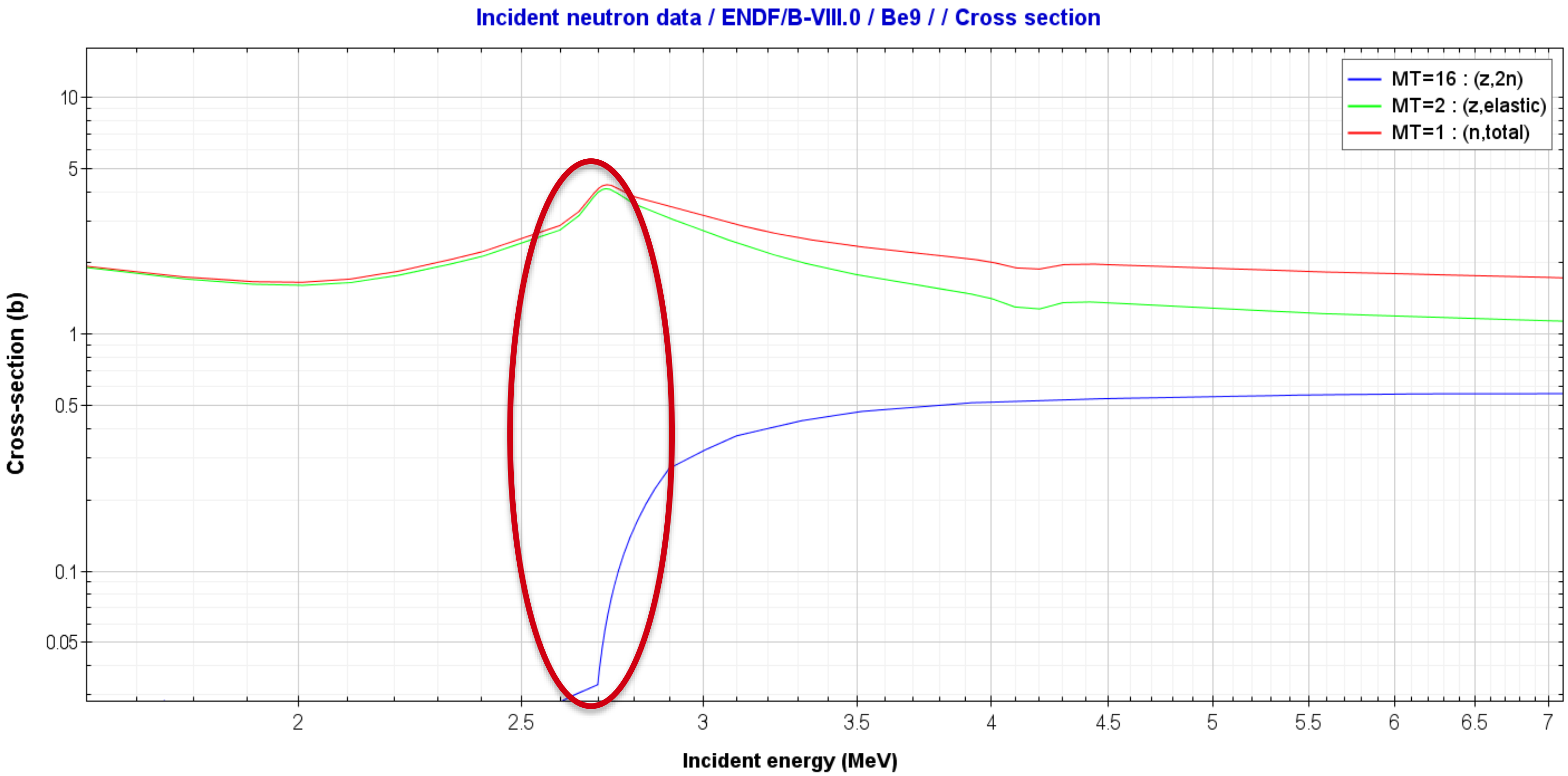
Pb-208 Scattering Optimization



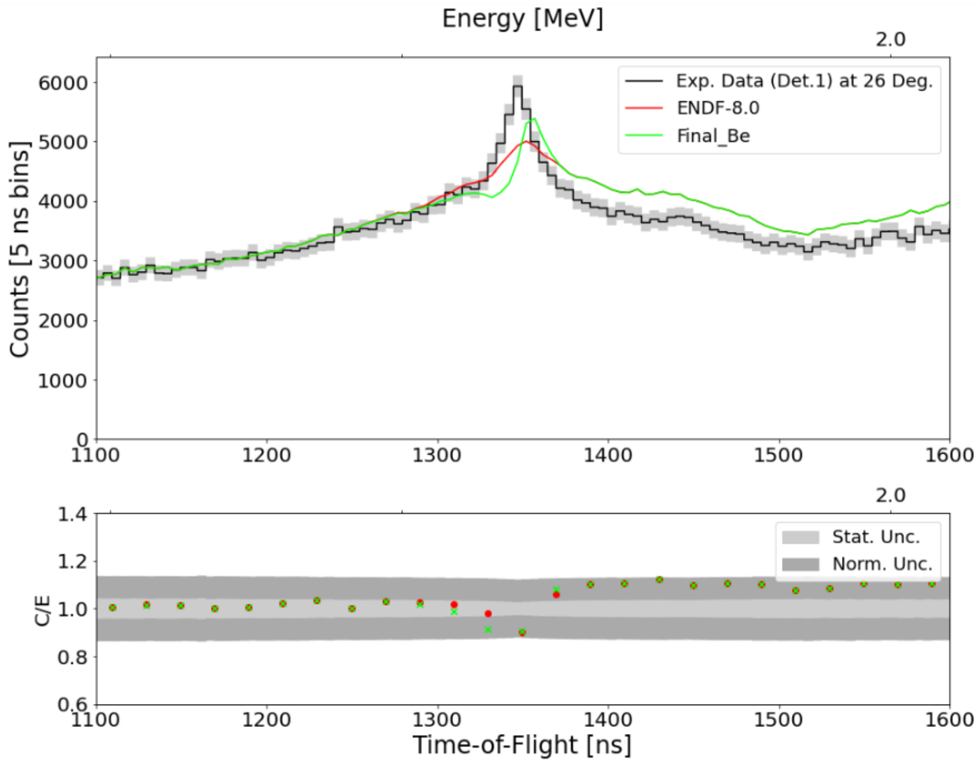
- MATLAB constructed the surrogate model hypersurface and found a global minima of scattering coefficients
- ESAD for 814 keV resonance was adjusted to align better with experimental data
- With method validated, can other isotopes be explored?

- Be-9 is a pesky isotope to evaluate due to the R-matrix needing to handle both uncharged and charged particle channels
- At the beginning of the (n,2n) threshold there appears to be disagreement between the simulation and data for ENDF/B-VIII.0

Be-9 Cross Sections



Be-9 Quasi-Differential Scattering



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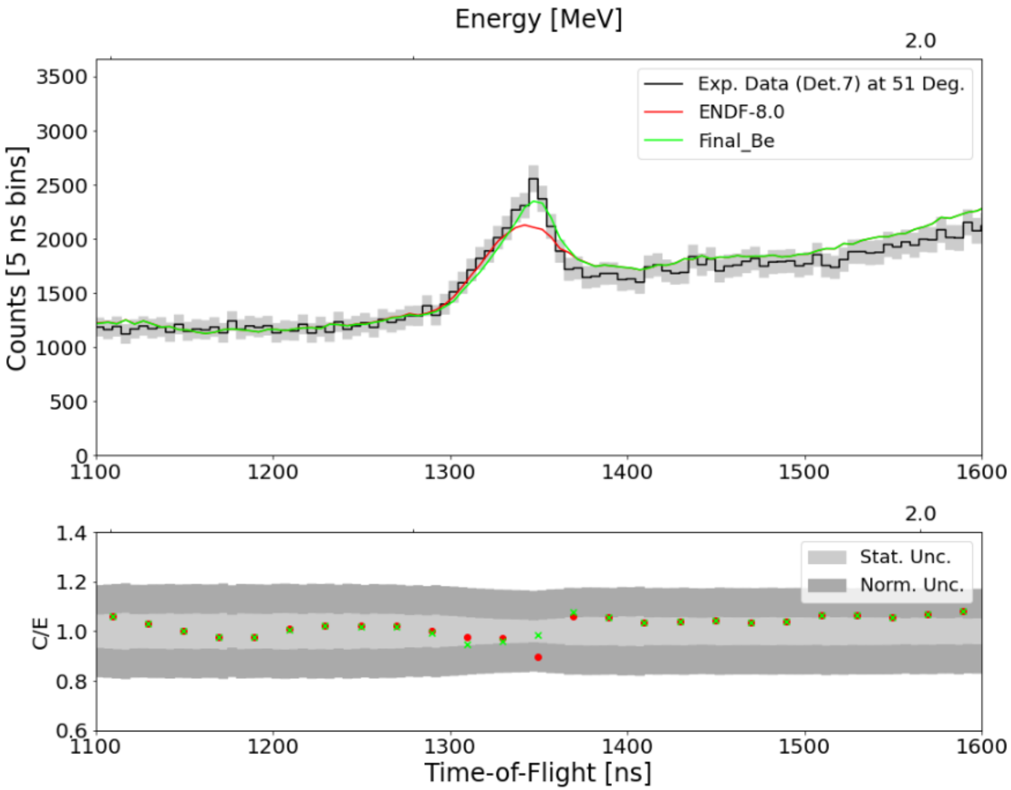
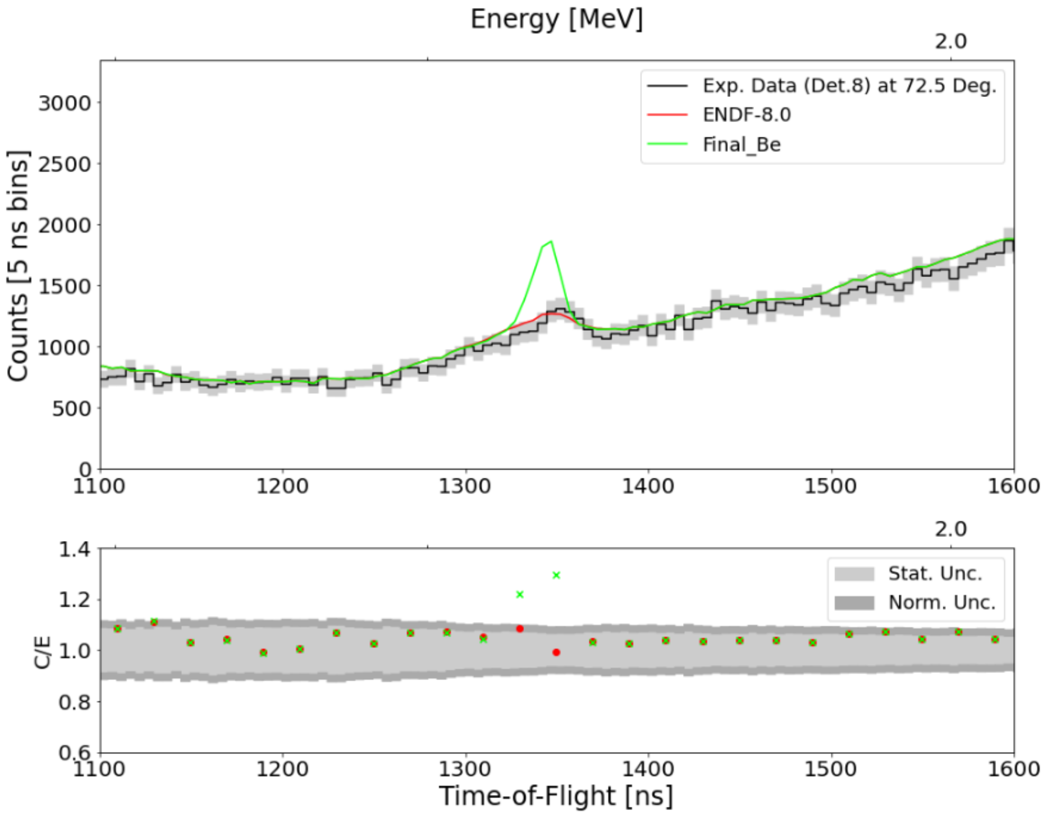
Be-9 Quasi-Differential Scattering

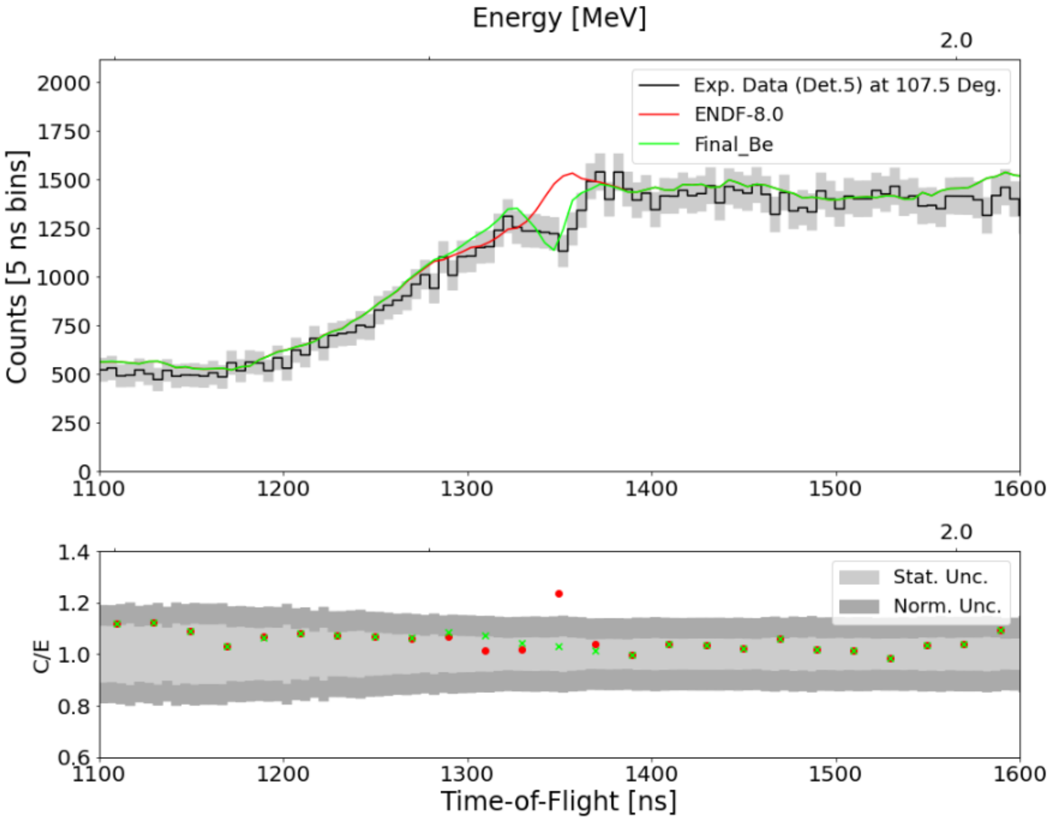


Be-9 Quasi-Differential Scattering

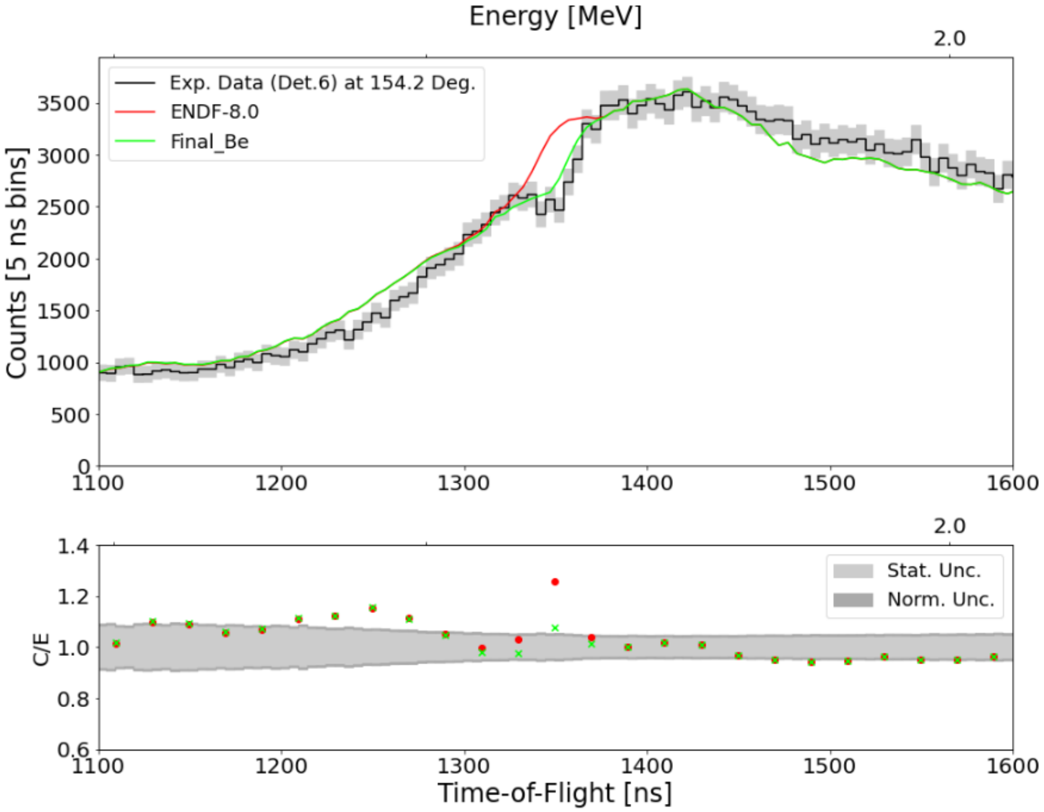
Not all angles are improved! Scattering to 70-90º is poorer than original evaluation



Be-9 Quasi-Differential Scattering



Be-9 Quasi-Differential Scattering



- Performing the adjustment for 2.7 MeV resonance does show overall improvement
- However, at perpendicular scattering there is a worsening of response, possibly need different order Legendre or elastic scattering assumption is incorrect

Conclusion

- Surrogate Process Modeling proves a useful tool in adjusting ESAD when its appropriate
  - Poor prediction of scattering data due to single isotope
  - Issue with single isotope is the ESAD
  - Possible issues with fitting arise from normalization between simulation and experiment, poor detector responses
- Since the number of simulations is constant for polynomial order, disconnected energy regions can be simulated and fit for no additional cost
- Future work is expanding to multiple energies and isotopes

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