Windowed Multipole

An introduction to a novel nuclear data formalism

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Introduction and Motivation

- Cross sections are wrong (Inherently)
- "Inaccuracies in the evaluated nuclear cross-section data are responsible for the majority of errors in modeling and simulation results"
- Data will always have inaccuracies
- Evaluators are tasked with trying to improve our lives(aka work) by getting those numbers closer to the "correct" value

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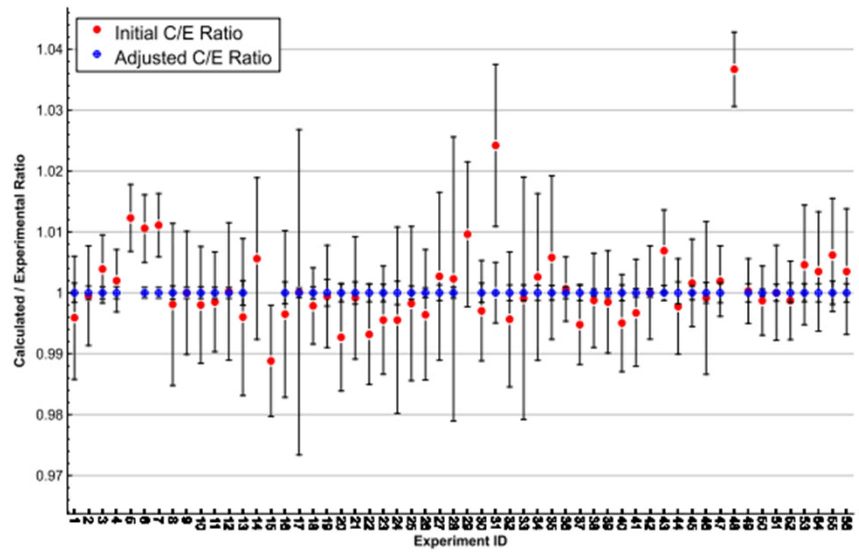
How can we help?

Introduction and Motivation

- Evaluating a nuclear data library has often been a qualitative process
  - Look at a test suite of “MOX-MET-INT” test cases and we might find out that (JEFF) overestimates k consistently
  - Maybe PU-MET-THERM integral benchmarks are consistently off
  - Finagle the data (scientifically)



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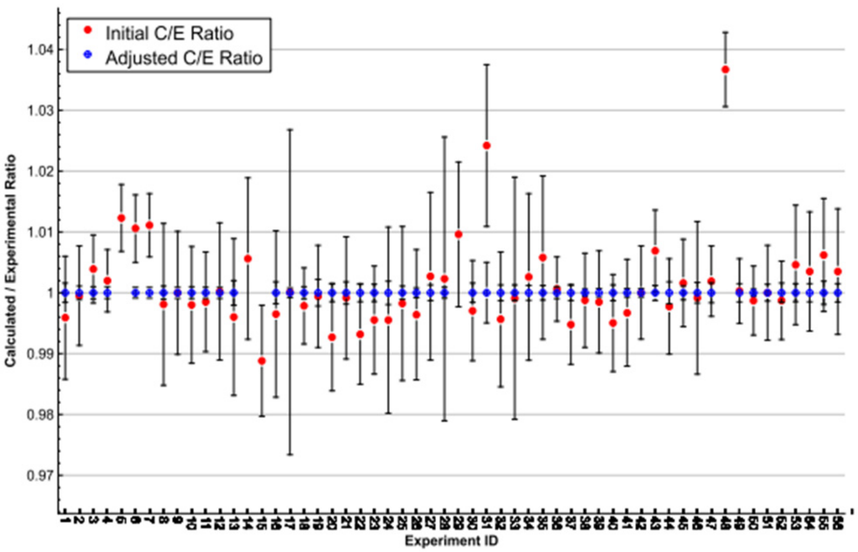
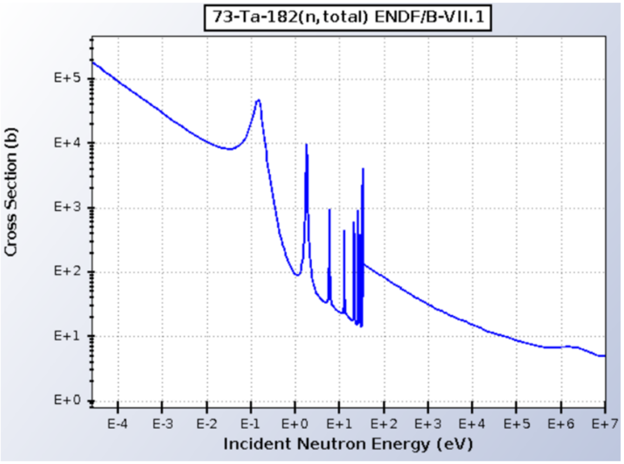
- I want to add a tool that can help quantitatively finagle the data



Introduction and Motivation

- Introduction to nuclear data
  - Continuous Energy (CE) cross sections are built up from Resonance parameters*
    - “Mathematical” resonances at negative energies introduced to get the 1/v behavior

eV	J	GT	GN	GG	GF
-2.000000+1	2.500000+0	6.970000-1	6.300000-1	6.700000-2	0.000000+0
1.470000-1	3.500000+0	6.731500-2	3.151000-4	6.700000-2	0.000000+0
1.820000+0	2.500000+0	6.835400-2	1.353700-3	6.700000-2	0.000000+0
5.980000+0	3.500000+0	6.740600-2	4.062000-4	6.700000-2	0.000000+0
1.293000+1	2.500000+0	6.767100-2	6.710000-4	6.700000-2	0.000000+0
2.150000+1	3.500000+0	6.842000-2	1.420100-3	6.700000-2	0.000000+0
2.666000+1	2.500000+0	7.091500-2	3.915300-3	6.700000-2	0.000000+0
2.940000+1	3.500000+0	6.832800-2	1.328200-3	6.700000-2	0.000000+0
3.297000+1	2.500000+0	8.039800-2	1.339800-2	6.700000-2	0.000000+0
3.465000+1	2.500000+0	9.400000-2	2.700000-2	6.700000-2	0.000000+0



Σ_t for Ta-184

nndc.bnl.gov/sigma

Introduction and motivation

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- We know resonances impact cross sections
- We know evaluators adjust cross sections to fit reality
- Can we use our knowledge of resonance parameters to increase the "resolution" of these evaluations?

Mission Relevance

- The goal of this work is to increase the fidelity of fission cross sections to further our ability to detect and intercept fissile material
  - Cross sections are inconsistent with experimental benchmark measurements
  - This work will allow for a more quantitative approach to evaluating nuclear data

- *NNSA Mission*
  - *Website:* https://www.energy.gov/nnsa/missions/nonproliferation

  Preventing nuclear weapons proliferation and reducing the threat of nuclear and radiological terrorism around the world are key U.S national security strategic objectives that require constant vigilance.

  NNSA's Office of Defense Nuclear Nonproliferation works globally to prevent state and non-state actors from developing nuclear weapons or acquiring weapons-usable nuclear or radiological materials, equipment, technology, and expertise.

Technical Approach

- The start of the adventure!
  - We need to know how these parameters impact cross sections
  - That sounds a lot like sensitivity information
  - Perhaps we could use sensitivity information to dial in a more accurate value for these resonance parameters

Technical Approach

- What do I mean by sensitivity information?
  - $S_{R,\Gamma} = \frac{\partial R / R}{\partial \Gamma / \Gamma}$
  - The sensitivity coefficient ($S_{R,\Gamma}$) describes "the fractional change in the response(R) of a system induced by changes to a system parameter(Γ)"
    - Response can be k, fission rate, nuclide generation rate
  - We want to use this information to "dial in" the values for a given evaluation

$$S_{k,\Gamma_n} = \frac{\partial R / R}{\partial \Sigma_x / \Sigma_x} \frac{\partial \Sigma_x / \Sigma_x}{\partial \Gamma_n / \Gamma_n}$$

Technical approach

- Our method of finding this sensitivity information,
  - Windowed Multipole – A novel nuclear data formalism
  - Based on Richard Hwang's work from the 80's
  - Capable of "on-the-fly" analytic doppler broadening
    - As a byproduct we can produce our ${\partial \Sigma_x}/{\partial \Gamma}$ term

- Not implemented into MCNP
  - Well now I have a new project
  - Implementing a method of finding those sensitivities

Technical Approach

- Nuclear data crash course
  - Majority of nuclear data evaluations are done through the lens of R-matrix theory
    - 2 bodies in/2 bodies out
    - Assumes a "compound" nucleus
    - Internal region dominated by strong force/ external dominated by coulomb

  - From there we Parameterize
    - Dominant parametrization is Wigner - Eisenbud
    - $E_\lambda, E_{Tc}, a_c, B_c, \gamma_{\lambda,c}$
    - Real, measurable, but arbitrary

Technical Approach

- Nuclear data crash course
  - Parametrization defines how we interact with our model
    - What “dials” we can play with
    - Given a formalism(set of simplifications) we use these parameters to build up cross sections
  - Windowed multipole uses a different set of parameters
    - We need a way translate one set into another

r_j, p_j → $E_\lambda, E_{Tc}, a_c, B_c, \gamma_{\lambda,c}$

Technical Approach

- Turns out translating between different nuclear data parameters can be tricky
  - A method of going between parametrizations was included in the Hwang paper
    - Calculated the wrong number of poles
    - Ignored Energy threshold – good assumption at the time
  - Eventually Pablo Ducru wrote a series of papers detailing how to do it correctly

Technical Approach

- How to swap between resonance parameter?
  - First realization was that transmission probabilities can be represented as sums of poles and residues
    - Poles of what?

  - R-Matrix uses resonance parameters to build up matrices
    - $U_{cc'}$ Transmission matrix shows the likelihood of going from one channel to another
    - This U matrix is often expressed in terms of the Level Matrix A
    - The level matrix is key to going between both different formalisms and parametrizations

Technical Approach

- Finding the poles and residues, comes down to solving a radioactive states problem, namely

$$\boldsymbol{A}^{-1}(E)\Big|_{E=\mathcal{E}_j}\overrightarrow{\boldsymbol{r}_j} = \boldsymbol{0}$$

  - Here A is our level matrix, $\mathcal{E}_j$ are our poles and $\overrightarrow{\mathrm{r}_j}$ are our residue width vectors
    - So our poles are the values that make A^{-1} singular and then our residue width vectors are the null space of $A(\mathcal{E}_j)$

Technical Approach

- The problem then comes from A

$$A^{-1}(\mathcal{E}_j) = \vec{\boldsymbol{e}} - \mathcal{E}_j \cdot \mathbb{I} - \boldsymbol{\gamma}\big(\boldsymbol{L}(\mathcal{E}_j) - \boldsymbol{B}\big)\boldsymbol{\gamma}^{\boldsymbol{T}}$$

  - Where $\boldsymbol{\gamma}$ is a full matrix of resonance parameters and **L** is also a function of energy and momentum number

  - Result is a full matrix with a complex dependence on energy

GT	GN	GG	GF
6.970000-1	6.300000-1	6.700000-2	0.000000+0
6.731500-2	3.151000-4	6.700000-2	0.000000+0
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Technical Approach

- Can we simplify this Problem?
  - Majority of cross sections in thermal energies use either
    - Multi-level Breit Wigner(MLBW)
    - Reich-Moore(RM)
    - It turns out only difference is how we define this A matrix

Ex.

$$A(\mathcal{E}_j)^{-1}_{MLBW} = A(\mathcal{E}_j)^{-1} \cdot \mathbb{I}$$

Technical Approach

- For MLBW that just becomes solving a series of quadratic equations
  - Since it's diagonal, any diagonal entry being zero gives us our singular matrix
  - Results in

$$E_{\lambda} - p_j^2 - \Sigma_{c=1}^{N_c} \gamma_{\lambda,c}^2 (L_C(p_j) - B_c)) = 0$$

- For RM it ends up being similar

National Nuclear Security Administration

Technical Approach

- Once poles and residues are calculated we can generate cross 0K sections
  - Then we can produce the $\frac{\partial \Sigma_x}{\partial \Gamma_x}$ term and generate sensitivities
  - Sensitivities can then be used in data evaluations

National Nuclear Security Administration

Expected Impact

- If successful, this work will not only produce the discussed sensitivities but also may draw more attention to windowed multipole
  - This is beneficial as it has applications for GPU as it is more FLOP intensive than memory intensive

MTV Impact

- The MTV has helped by introducing me to new connections that I might be able to call upon
- Personnel transitions: This coming summer I hope to work with Los Alamos to continue this work
- Technology transitions
  - This work has been in collaboration with Los Alamos,
  - Interest has been expressed in the on-the-fly doppler broadening capability for GPU based Monte Carlo

Conclusion

- Despite the work nominally being towards sensitivity based nuclear data evaluations, the work done to convert between the parameters has found uses in other areas of the field such as GPU computing and cross sections as a whole
- A more accurate and consistent methodology for evaluating nuclear data will improve our ability to detect fissile material

Next Steps

- Steps forward
  - Generate poles and residues regardless of nuclear data formalism
    - Solve radioactive states problem for dense matrices
  - Use these to produces sensitivities

$$S_{k,\Gamma_n} = \frac{\partial R / R}{\partial \Sigma_x / \Sigma_x} \frac{\partial \Sigma_x / \Sigma_x}{\partial \Gamma_\mathrm{n} / \Gamma_\mathrm{n}}$$

Acknowledgements

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