16TH NUCLEAR DATA
FOR SCIENCE AND TECHNOLOGY CONFERENCE
JUNE 22ND – 27TH | MADRID (SPAIN) | 2025

Estimation of Maxwellian averaged cross-sections with machine learning methods

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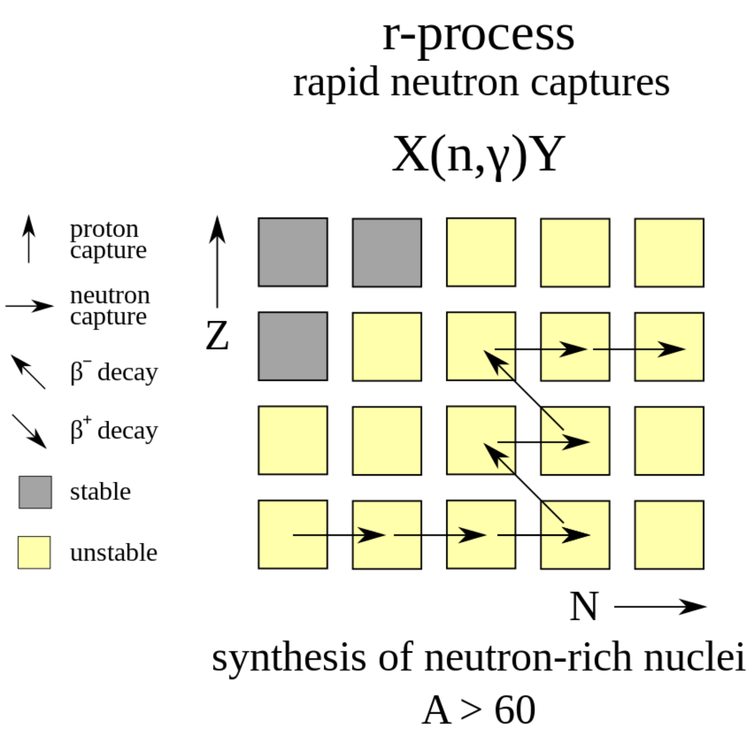
[d] Stony Brook University, USA

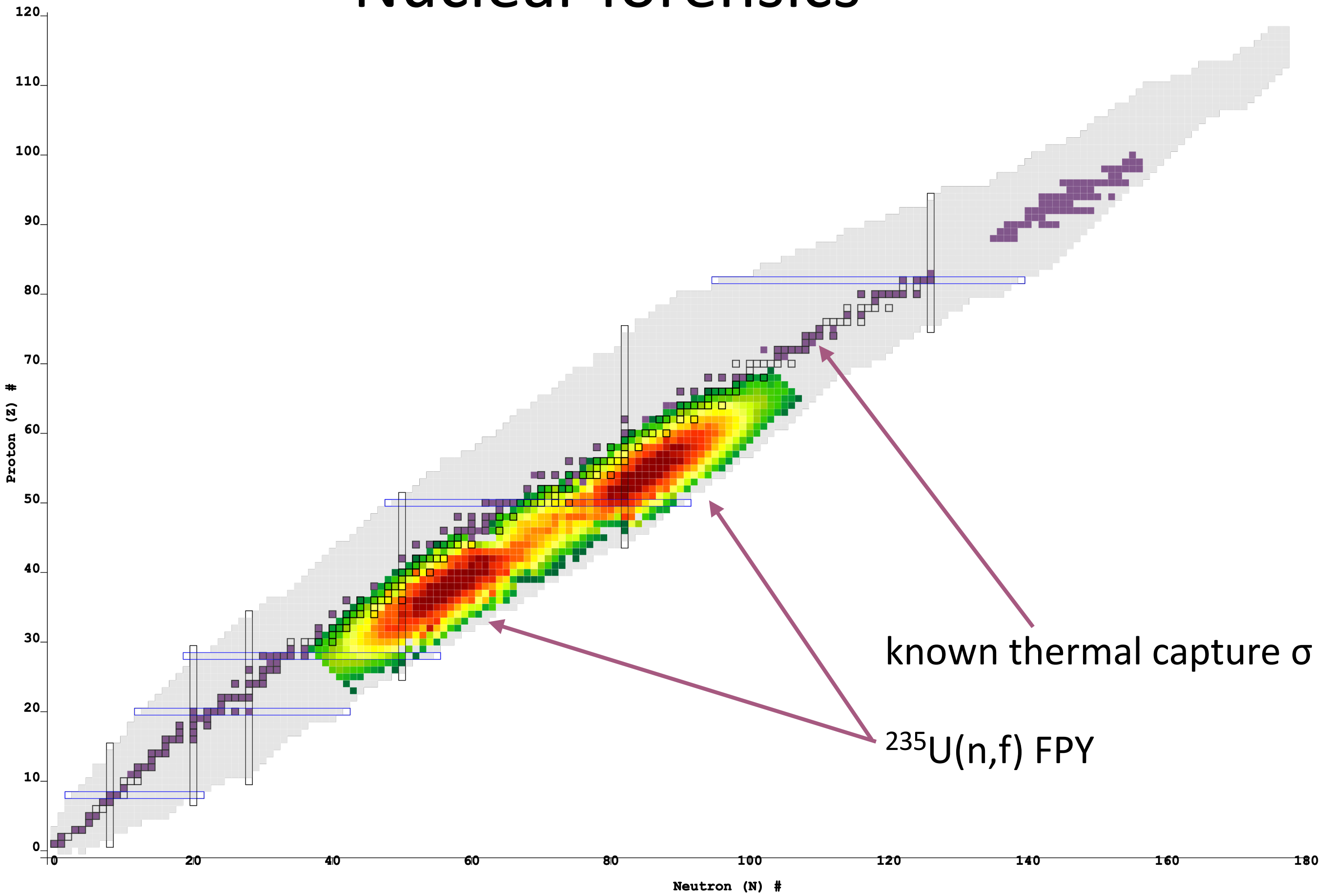
ND 2025

There are times where we need a capture cross-section but what we've got is garbage

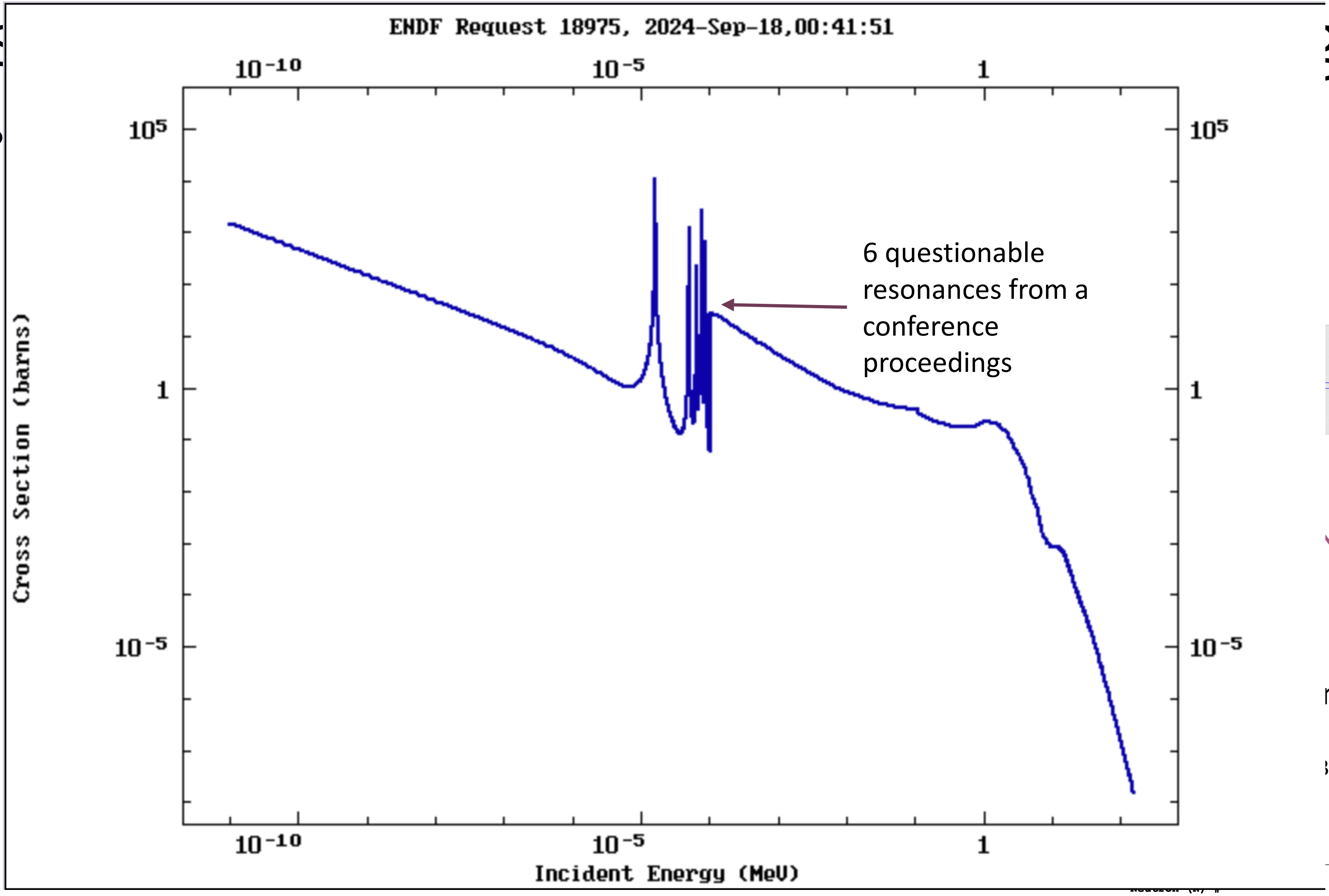
- Nucleosynthesis

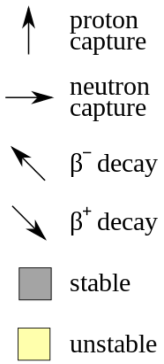


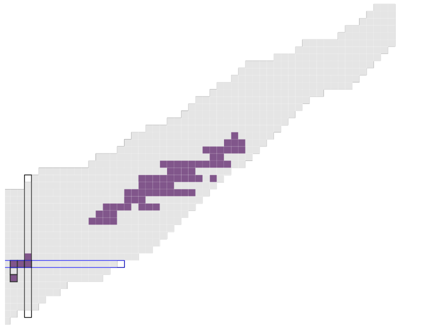
Nuclear forensics



There are times where we need a capture cros… …ge



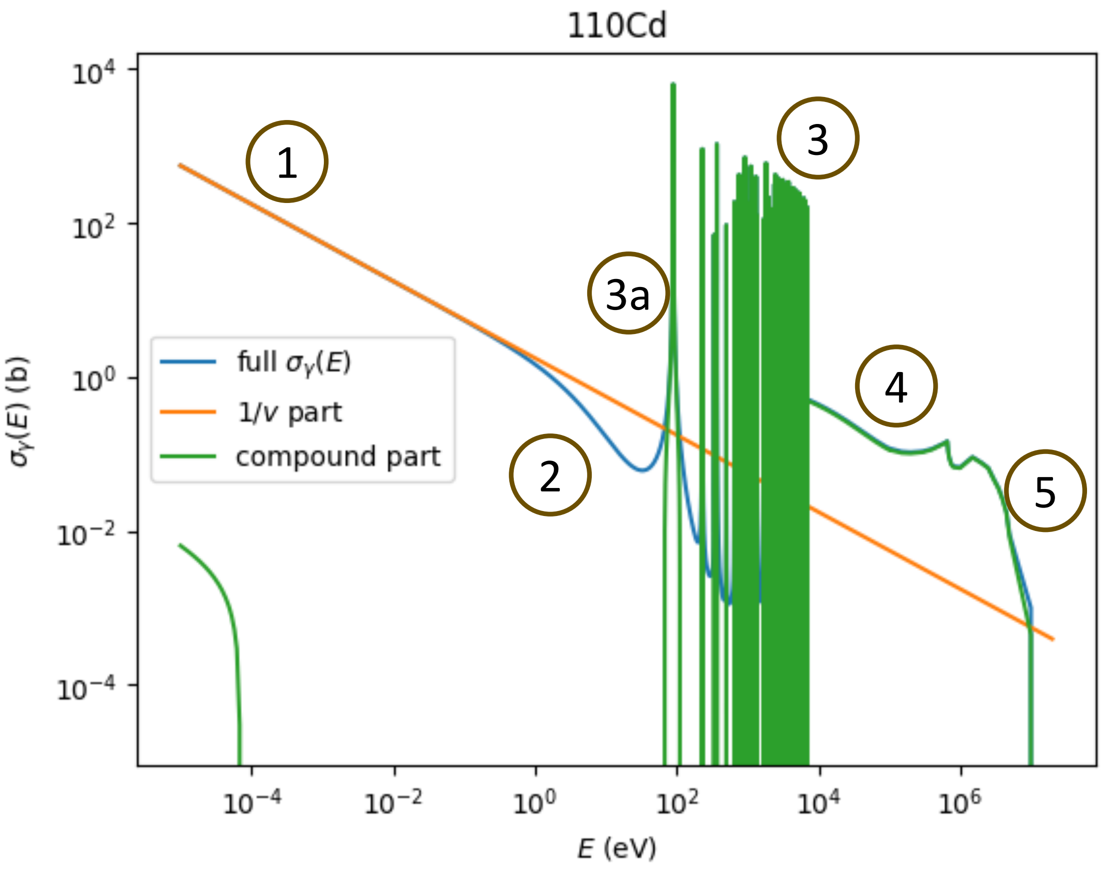




…nown thermal capture σ

…⁵U(n,f) FPY

Anatomy of a capture cross-section



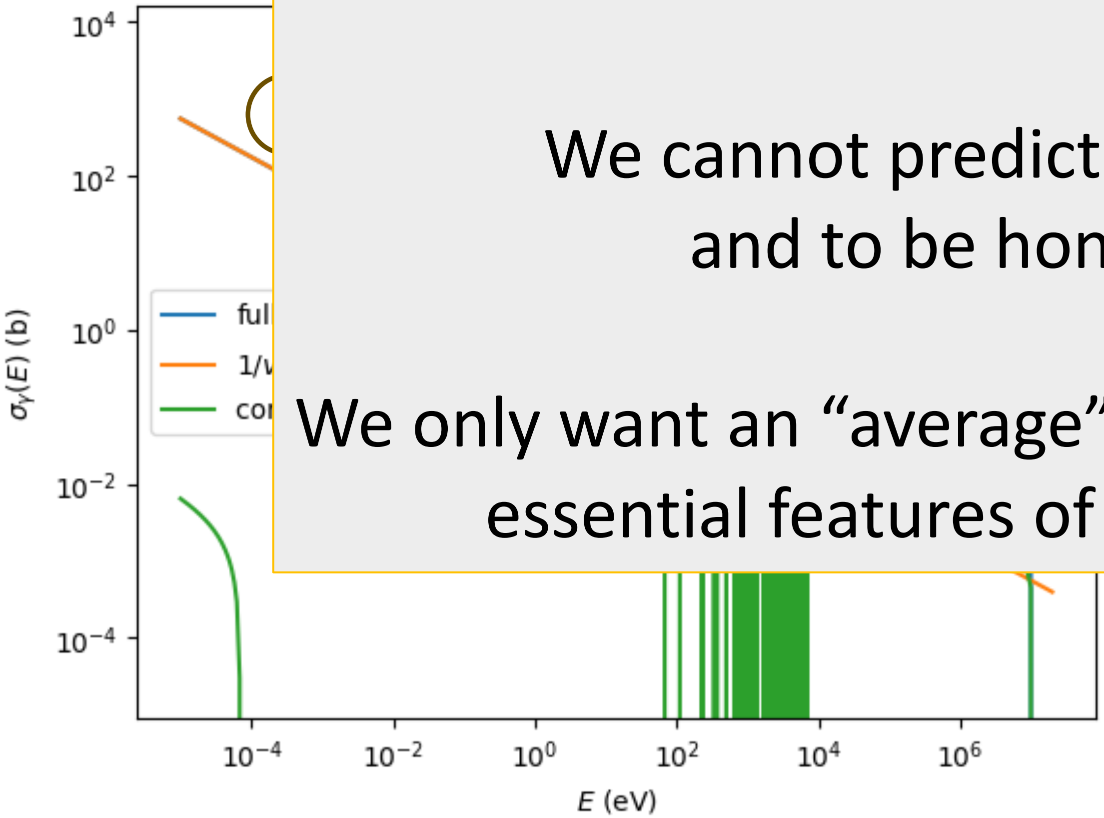
1. “the 1/v part” – S-wave direct capture; the shape is analytic, the magnitude must be measured
2. ”the dip” – direct capture turning off
3. “the RRR” - A compound nuclear part consisting of resolved resonances
   a. Often one or more resonances separated from main pack
4. “the URR” - A compound nuclear part consisting of unresolved resonances
5. “the fast part” A smooth high-energy part that peaks around 14 MeV

Anatomy of a capture cross-section

There are too many resonances.

We cannot predict their position or width,
and to be honest, we don't care.

We only want an "average" cross-section that captures the essential features of the capture cross-section



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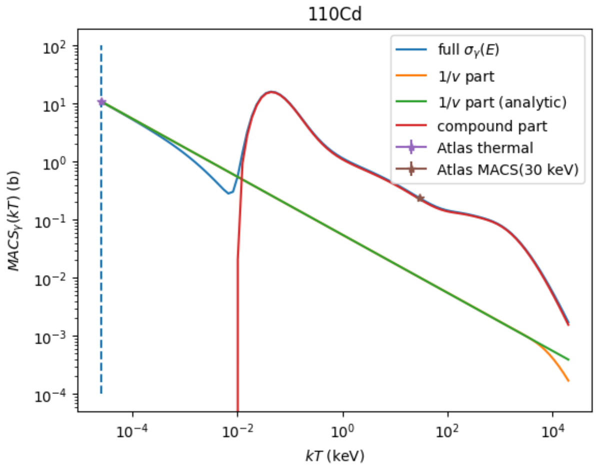
consisting of unresolved resonances

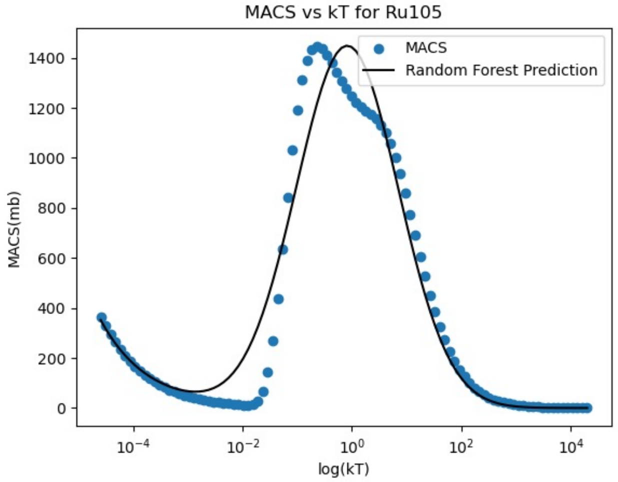
5. "the fast part" A smooth high-energy part that peaks around 14 MeV

Our approach

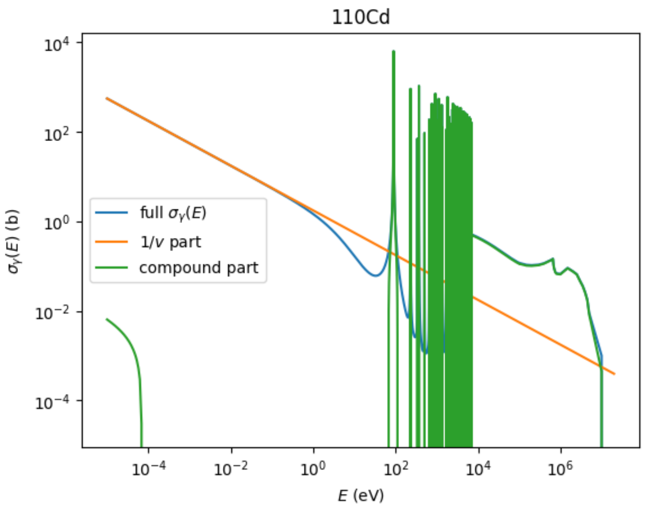
Build reduced order model of MACS



Learn parametric (Z,A) dependence of reduced order model



Transform model back to cross-section space



Test against original cross-sections or MACS

"magic" function $\sigma_\gamma(Z,A,E)$

Training set statistics

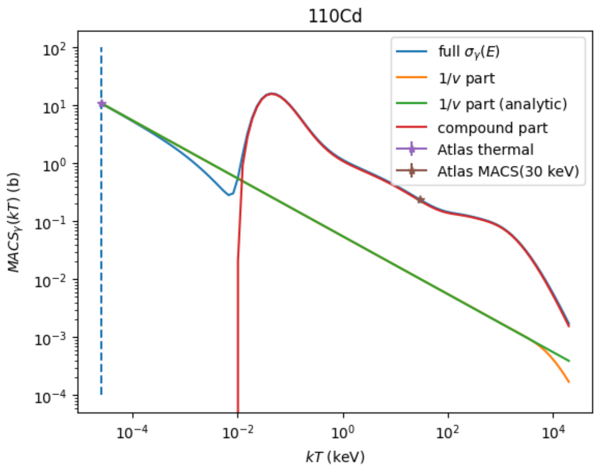
- Capture data from ENDF/B-VIII.1's neutron sublibrary (i.e. n+ZA)
  - Our best understanding of theory + experiment
  - 558 isotopes total (^{1}H-^{255}Fm), along valley of stability and up valley walls
  - Has warts and gotchas
- Unusable sets:
  - 4 with no capture reaction (n, t, a, ^{7}Be)
  - 52 taken from TENDL and therefore fictitious
- Tricky sets:
  - 11 with Westcott g<1. These have direct capture and/or low-lying resonances, fouling up the behavior at low energies – cut-off model should fix
  - 19 with very high energy resonances (> 2 MeV)

475 usable isotopes, another 30 recoverable with effort
Eliminating low quality sets leaves us with ~430 sets

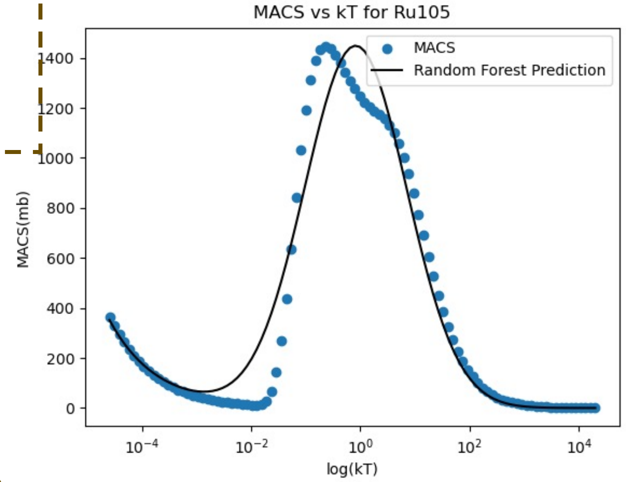
With such a small training set, we must invest most of our time in data curation and perfecting our reduced order model

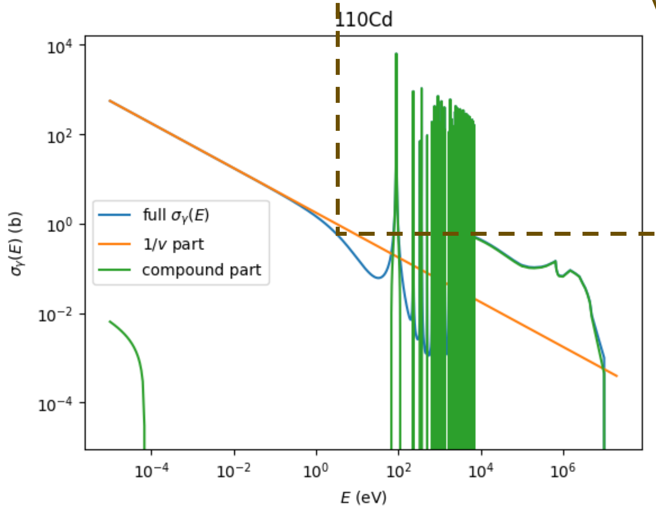
Our approach

Build reduced order model of MACS



Learn parametric (Z,A) dependence of reduced order model





Transform model back to cross-section space

Test against original cross-sections or MACS

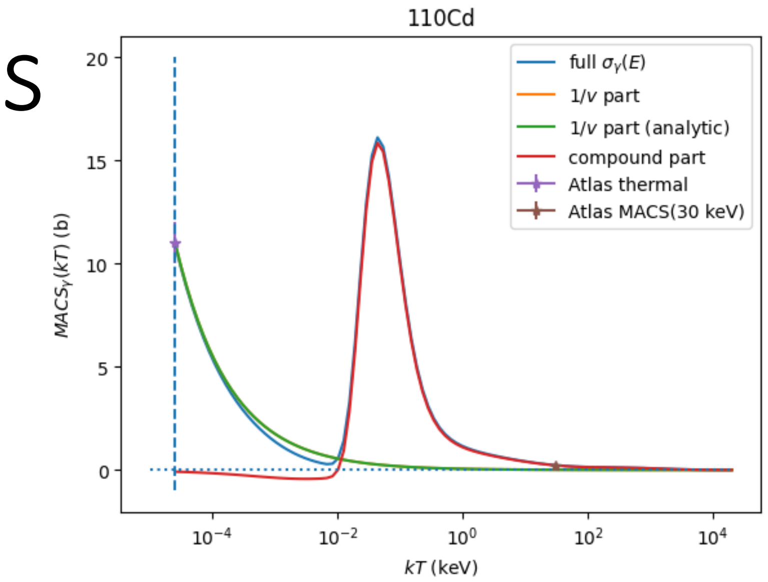
"magic" function $\sigma_\gamma(Z,A,E)$

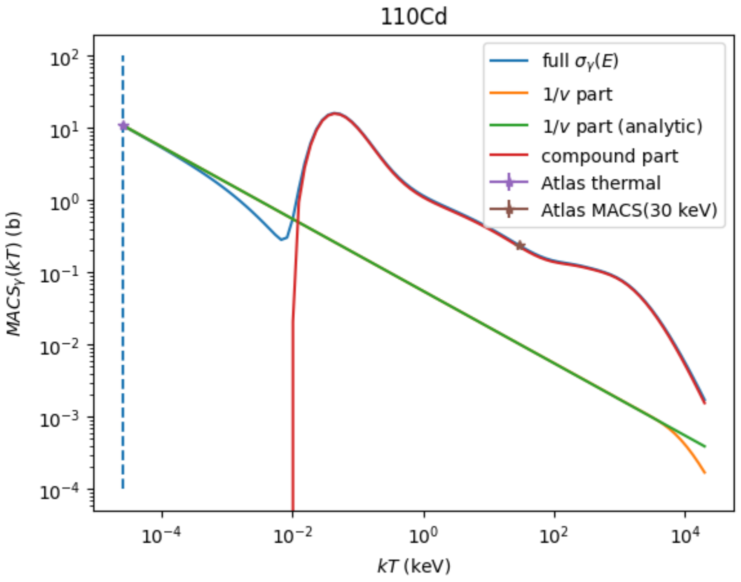
Maxwellian Averaged Cross-Sections

- Maxwellian averaging is one way to smooth
- The MACS is given by

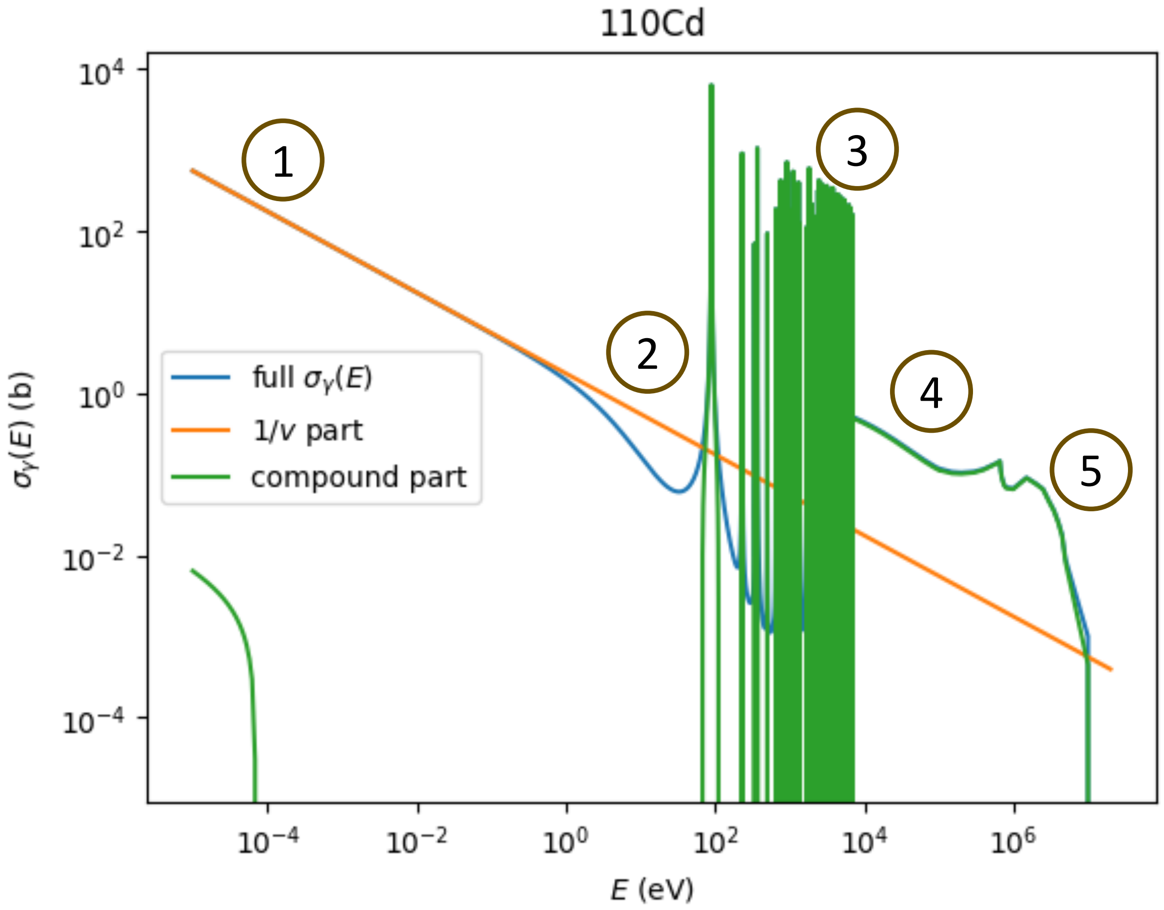
$$\mathrm{MACS}(k_BT) = \frac{2}{\sqrt{\pi}}\frac{a^2}{(k_BT)^2}\int_0^\infty E\sigma(E)\mathrm{e}^{-\frac{aE}{k_BT}}dE$$
$$= \frac{\langle\sigma v\rangle}{v_T}.$$

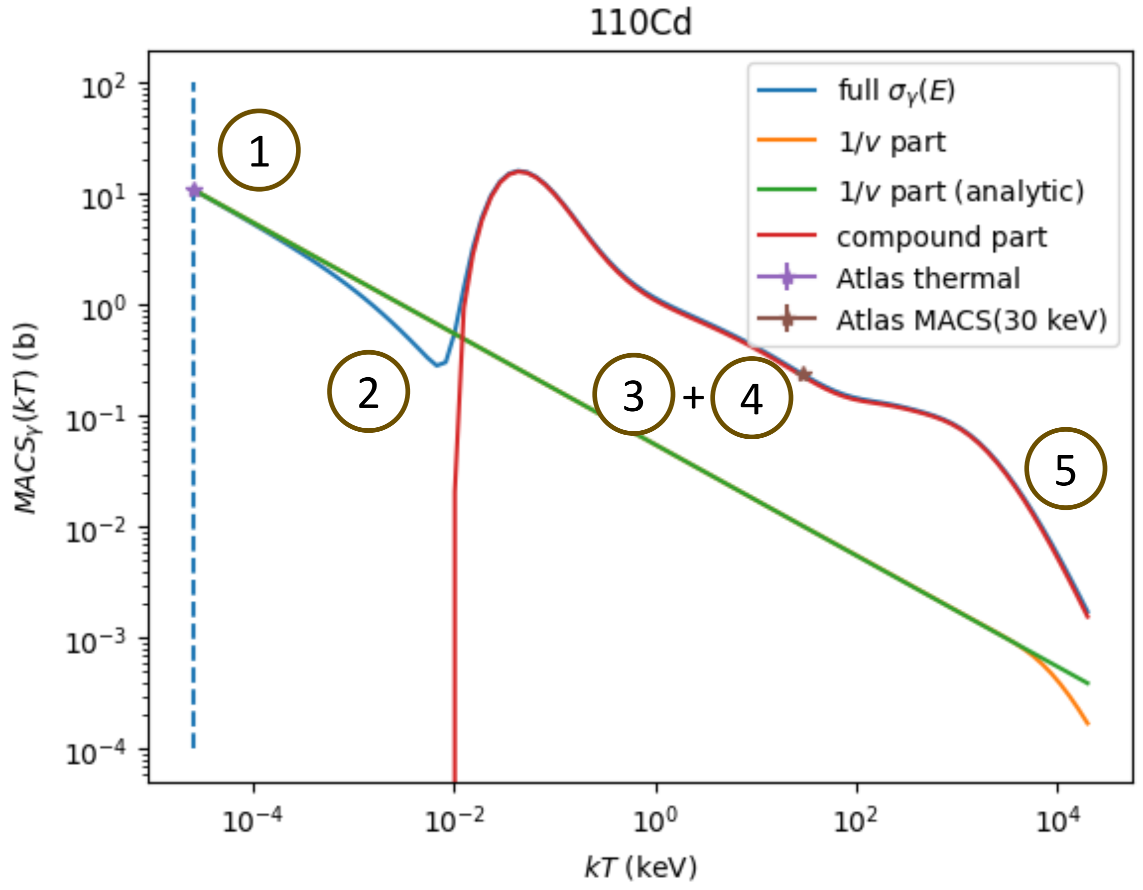
- Note: the MACS are all smooth bumps sitting on top of a “1/v-like” baseline.
- Side benefit: can use in nucastro calcs. as-is



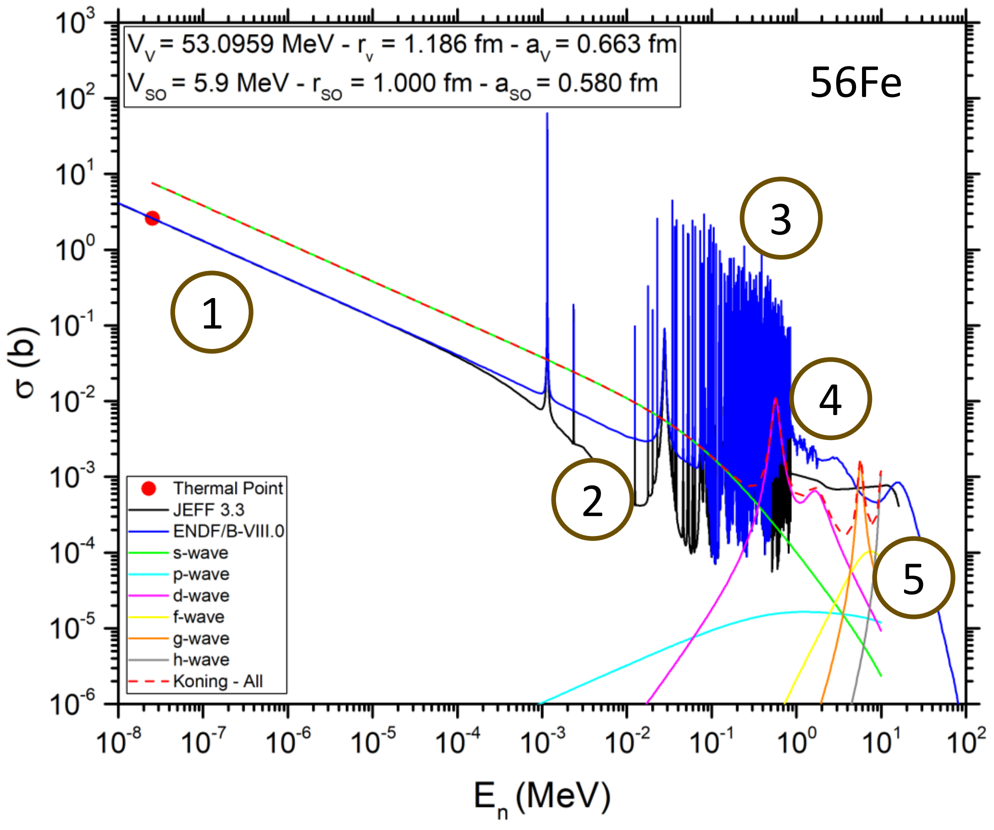


Features in the MACS can be traced to features in the original cross-section

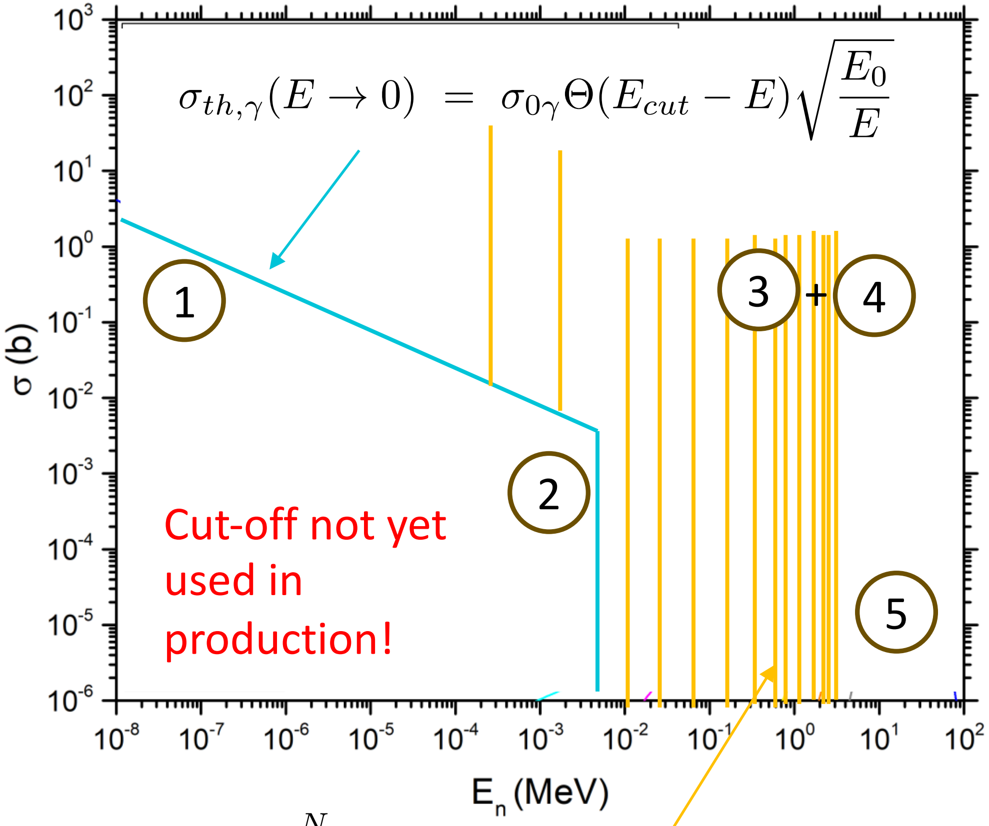




We can build this mapping into a crude model



M. Diakaki, G. Gkatis, A. Mengoni, G. Noguere, P. Tamagno, "First Results on the DRC calculations for the 56Fe isotope" Consultants Meeting on Structural Materials for the INDEN collaboration (2021)



$$\sigma_{cn,x}(E) = \sum_{n=1}^{N} A_{xn}\delta(E - nD) \qquad A_\gamma \;=\; 2\pi^2\lambda^2\frac{g\Gamma_n\Gamma_\gamma}{\Gamma}$$

The MACS for the crude model can be done analytically

- Without a direct reaction cut-off:

$$MACS_{th,\gamma}(kT) = \sigma_{0\gamma}\sqrt{\frac{aE_0}{kT}} = \sigma_{0\gamma}\sqrt{\omega E_0}$$

- With a cut-off energy:

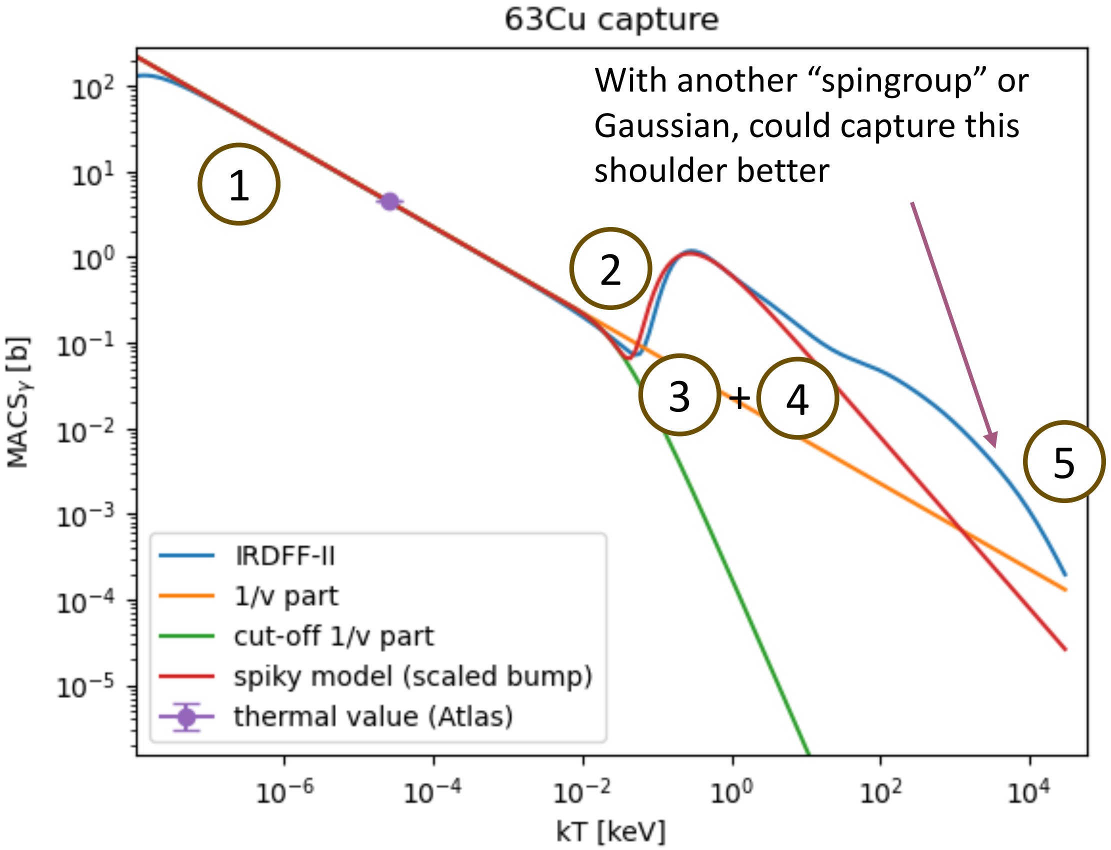
$$MACS_{th,\gamma}(kT) = \sigma_{0\gamma}\left[\sqrt{\omega E_0}\,\mathrm{erf}\left(\sqrt{\omega E_{cut}}\right) - \frac{2}{\sqrt{\pi}}\omega\sqrt{E_0 E_{cut}}\exp(-\omega E)\right]$$

not yet used in production!

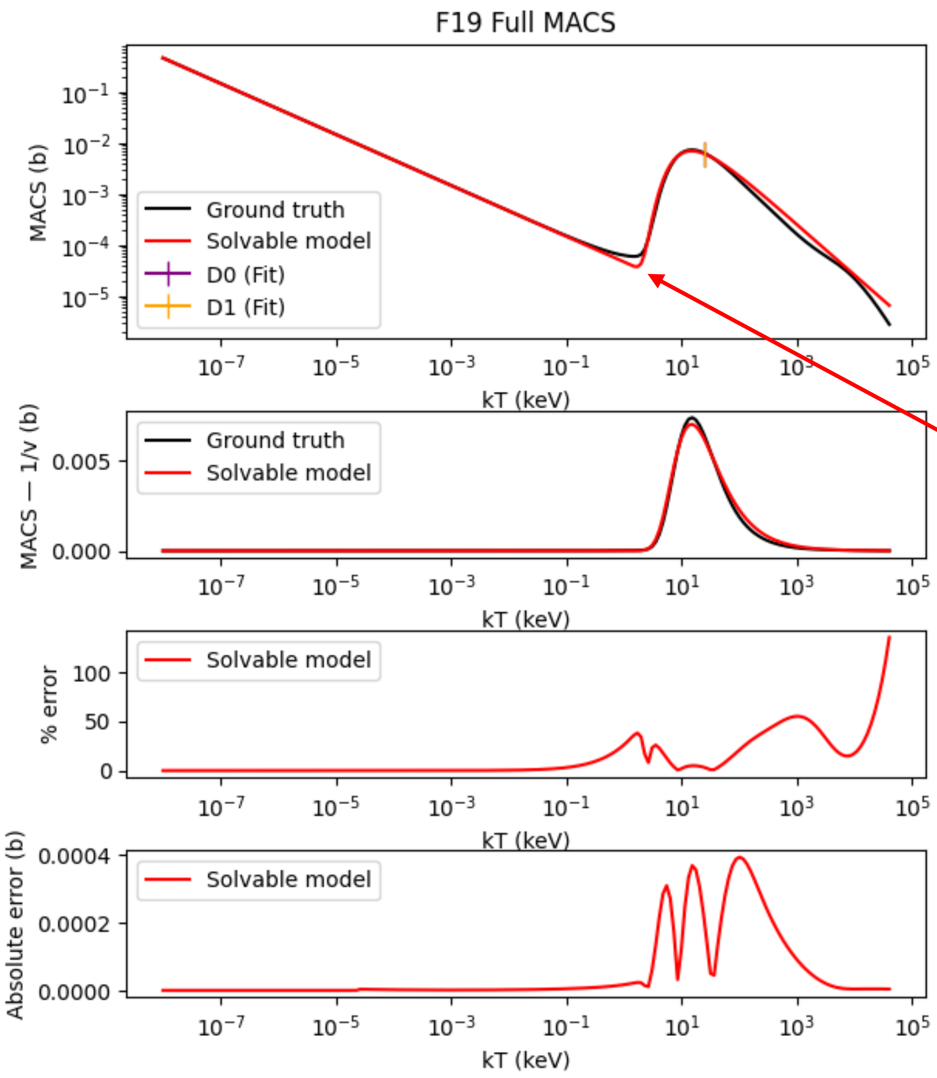
- Compound part:

$$MACS_{cn,\gamma}(kT) = B\left(\frac{a}{kT}\right)^2\left(\exp\left(\frac{aD}{kT}\right) - 1\right)^{-1}$$

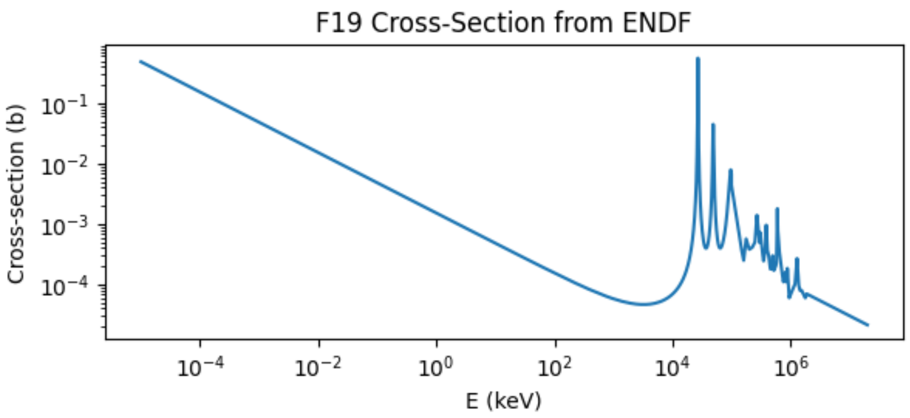
$$\omega = a/kT \qquad B = 2\pi^{3/2}\frac{(\hbar c)^2}{m_n}\frac{g\Gamma_n\Gamma_\gamma}{\Gamma}$$



F19

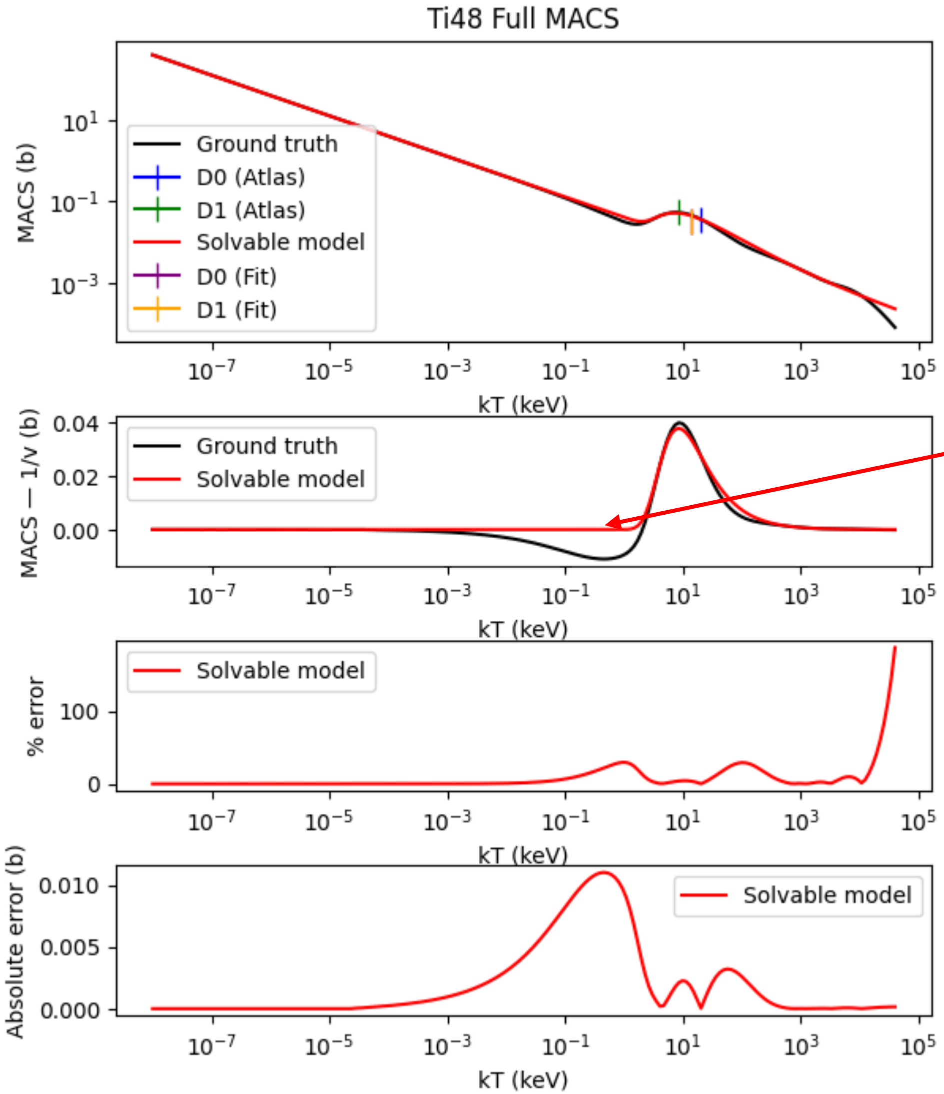


Needs cutoff!

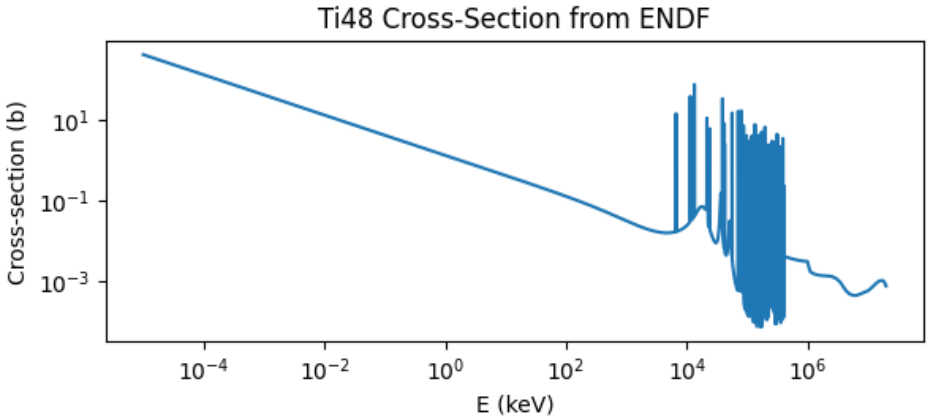


	Parameters
Z	9
A	19
Westcott g	nan
Number of peaks	0
Number of dips	0
TENDL flag	0
NRes	14
NNegRes	0
D0 [keV]	nan
D1 [keV]	60.0
Fit D0 [keV]	24.8141635
Fit D1 [keV]	24.7040562
Bump height 0 [keV]	0.0014514
Bump height 1 [keV]	0.0
R^2, log modified	0.9982171959647976

Ti48

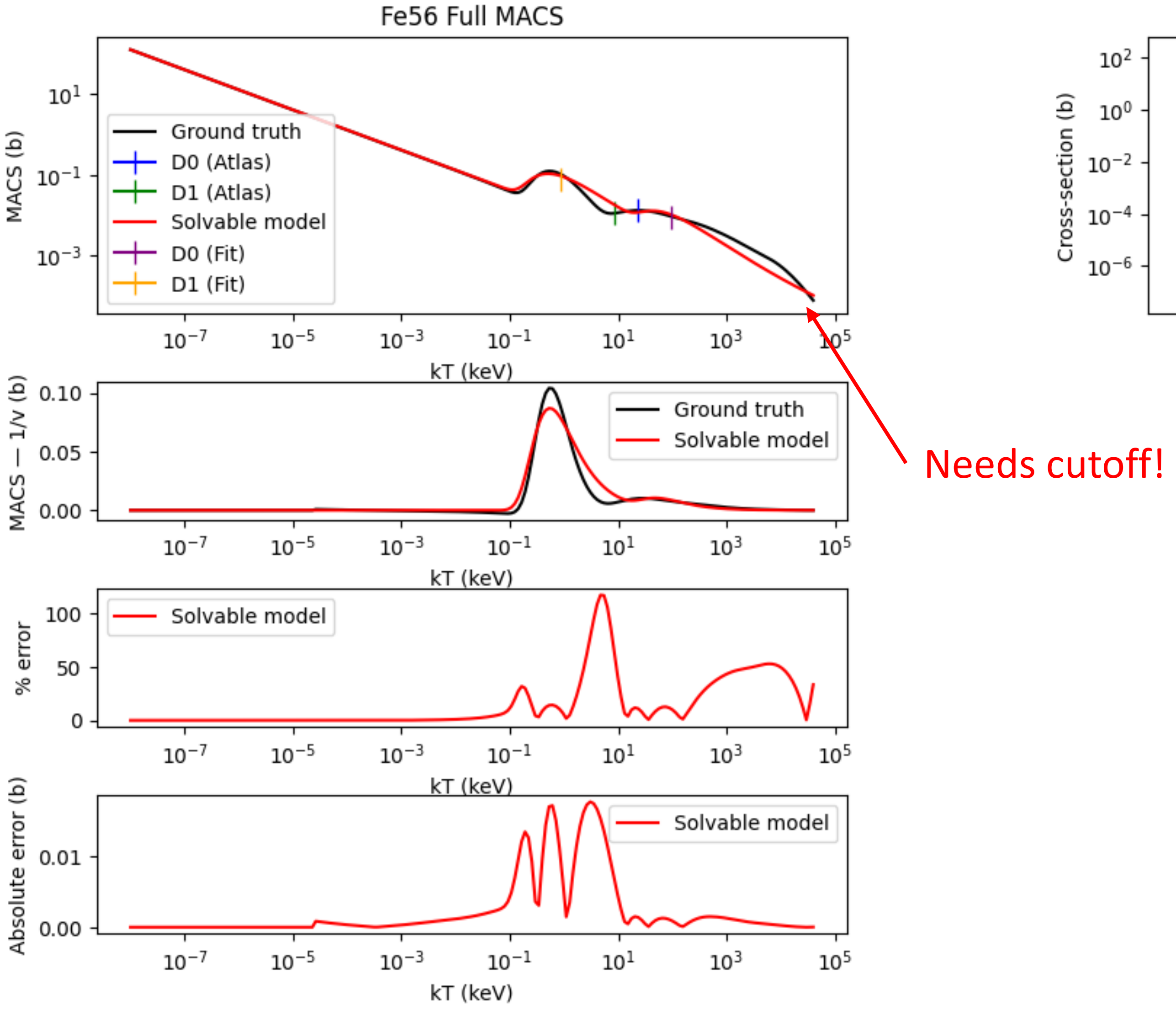


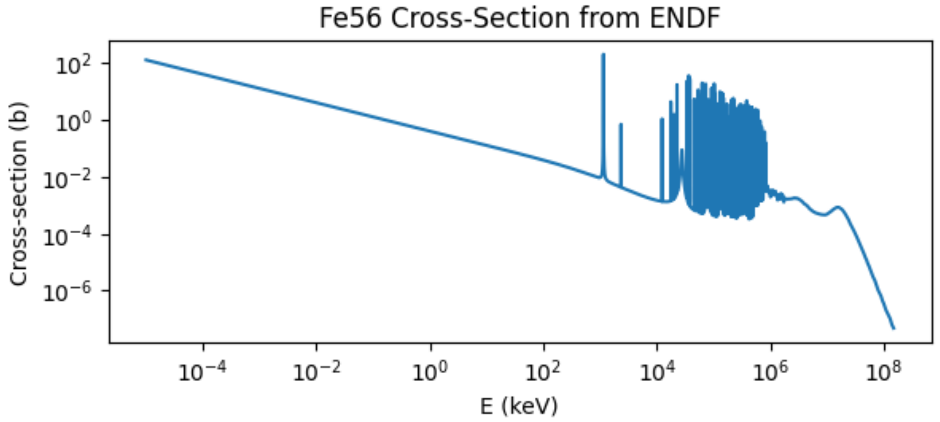
Needs cutoff!



	Parameters
Z	22
A	48
Westcott g	nan
Number of peaks	1
Number of dips	0
TENDL flag	0
NRes	120
NNegRes	1
D0 [keV]	20.8
D1 [keV]	8.7
Fit D0 [keV]	13.928875
Fit D1 [keV]	13.8307746
Bump height 0 [keV]	2e-07
Bump height 1 [keV]	0.002419
R^2, log modified	0.9997214269580116

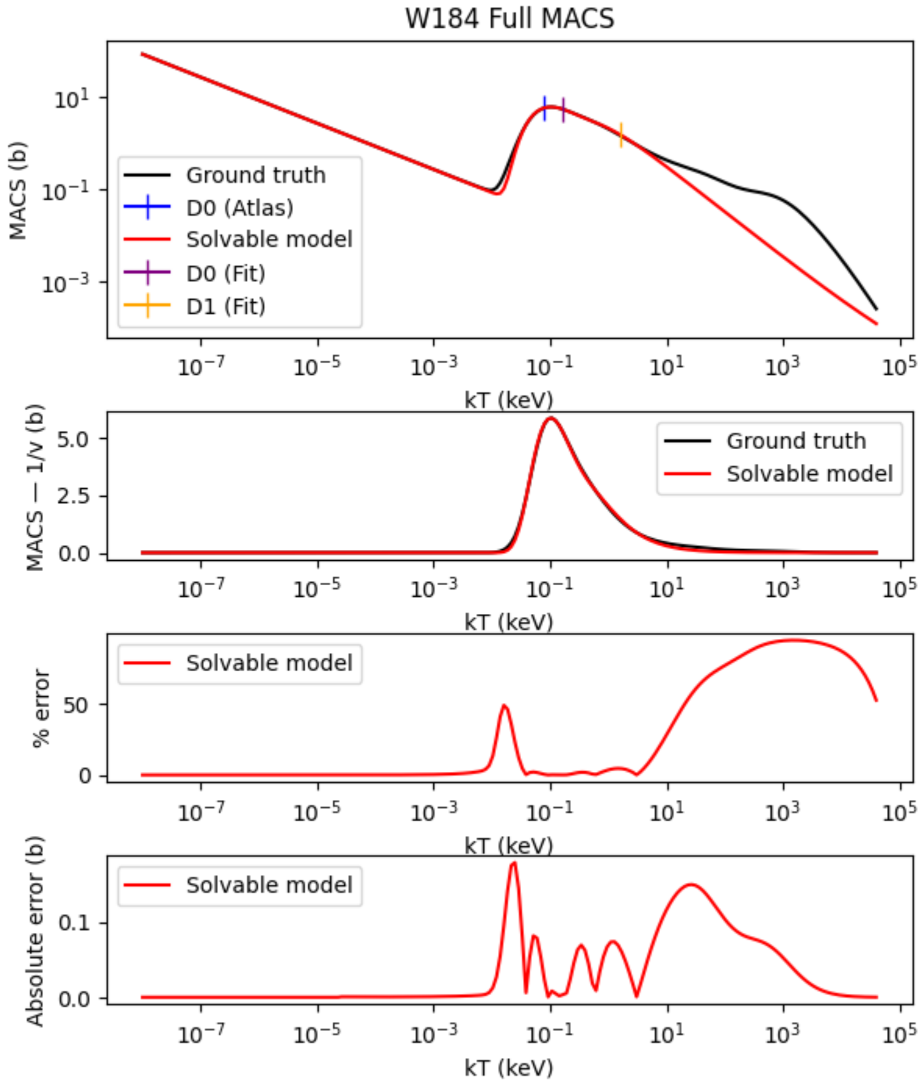
Fe56

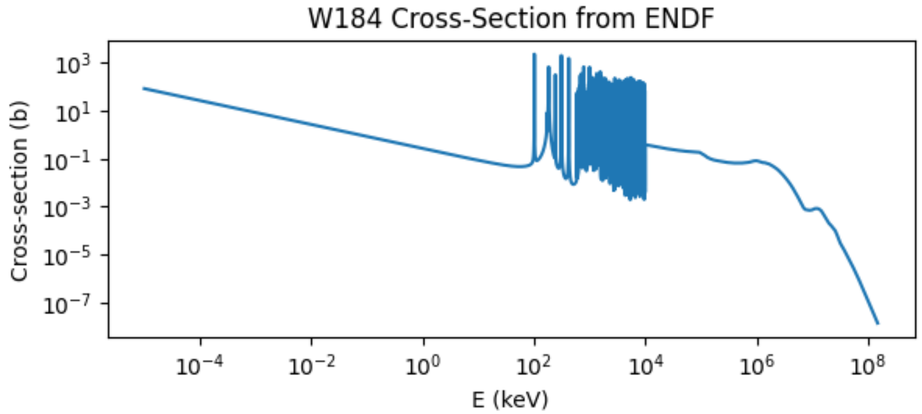




	Parameters
Z	26
A	56
Westcott g	1.004
Number of peaks	1
Number of dips	1
TENDL flag	0
NRes	312
NNegRes	3
D0 [keV]	22.0
D1 [keV]	8.21
Fit D0 [keV]	96.037885
Fit D1 [keV]	0.8947984
Bump height 0 [keV]	0.0257382
Bump height 1 [keV]	2.33e-05
R^2, log modified	0.9970409245444716

W184

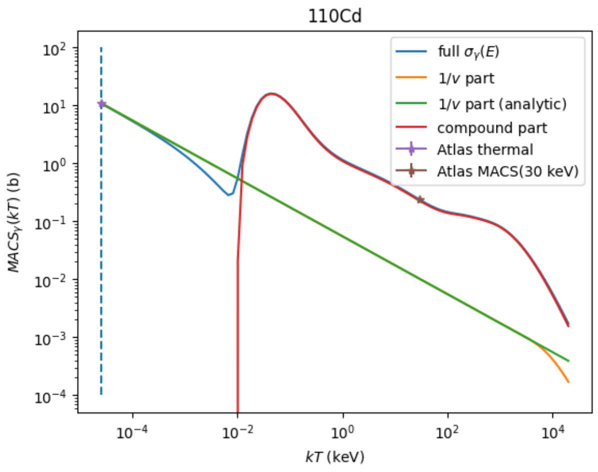




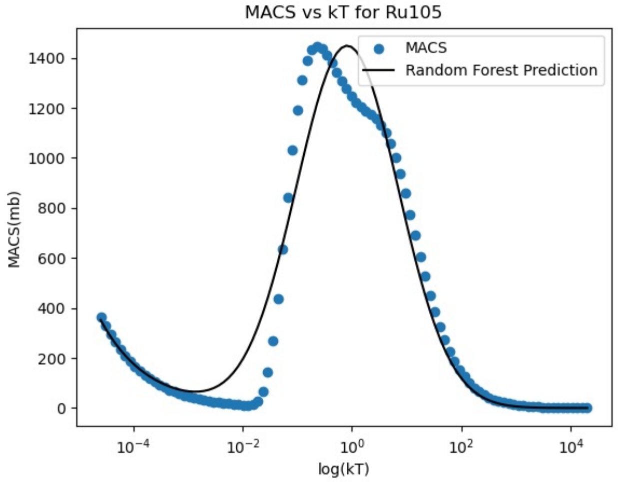
	Parameters
Z	74
A	184
Westcott g	1.004
Number of peaks	1
Number of dips	0
TENDL flag	0
NRes	218
NNegRes	1
D0 [keV]	0.081
D1 [keV]	nan
Fit D0 [keV]	0.1646915
Fit D1 [keV]	1.5696948
Bump height 0 [keV]	5.31e-05
Bump height 1 [keV]	0.0005502
R^2, log modified	0.896065371751298

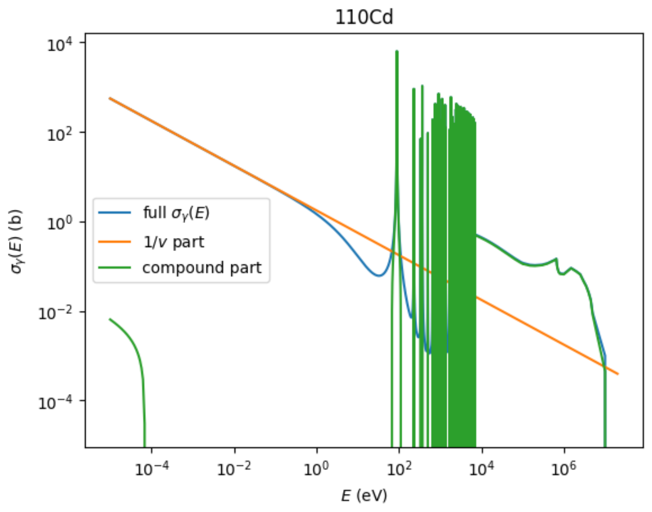
Our approach

Build reduced order model of MACS



Learn parametric (Z,A) dependence of reduced order model





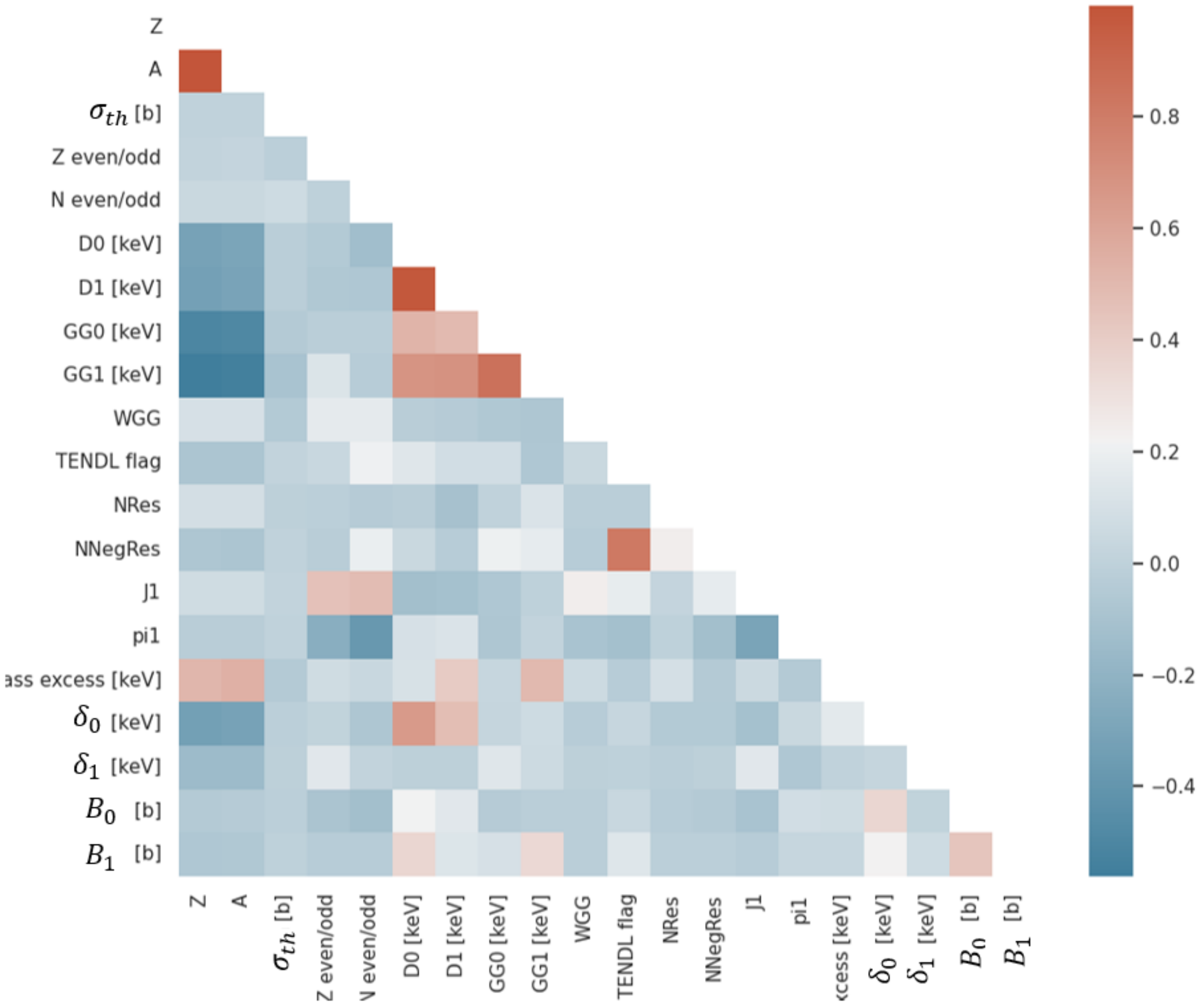
Test against original cross-sections or MACS

"magic" function $\sigma_\gamma(Z,A,E)$

Transform model back to cross-section space

Fitted parameters are strongly correlated with physics parameters

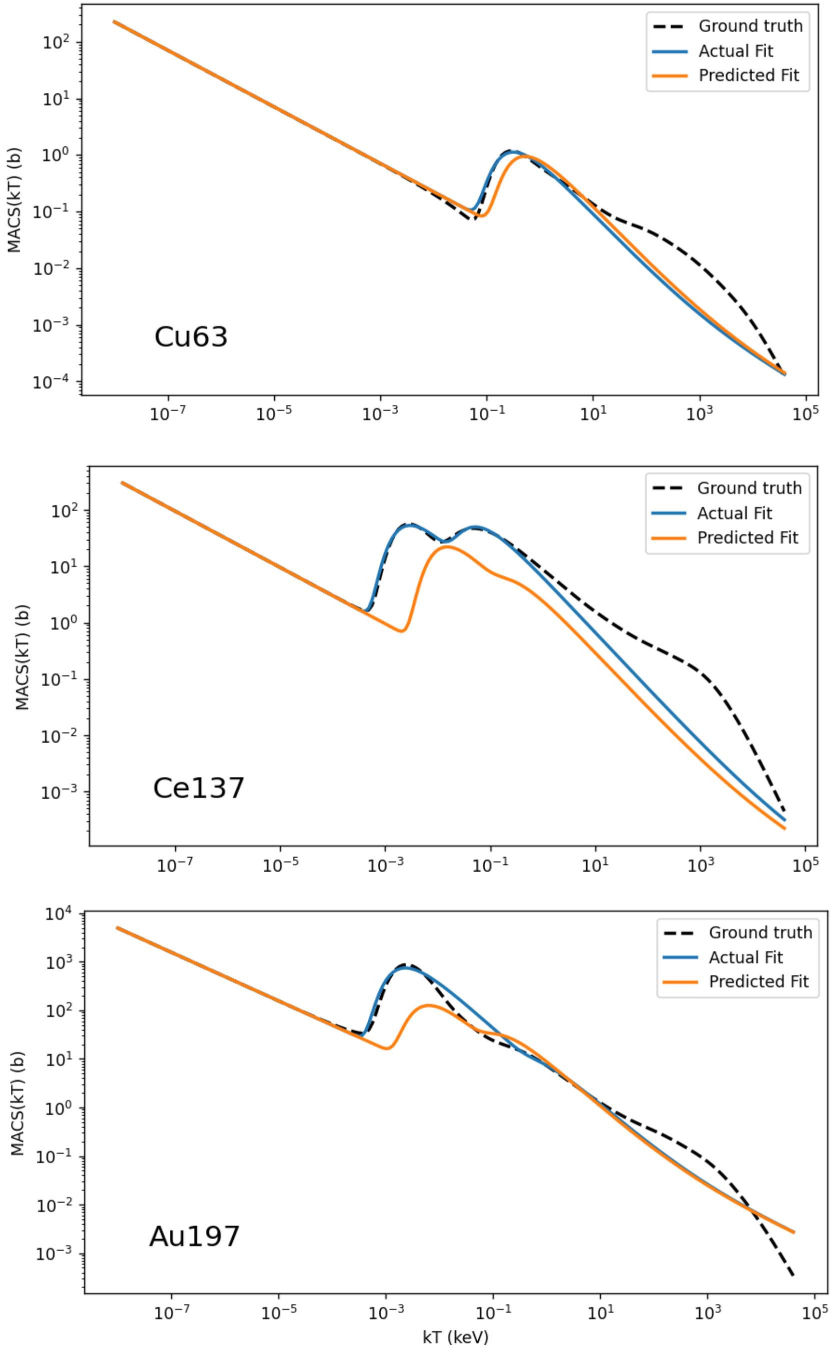
- Leads to our default feature choice: Z, A, Z even/odd, N even/odd, Jπ, mass excess



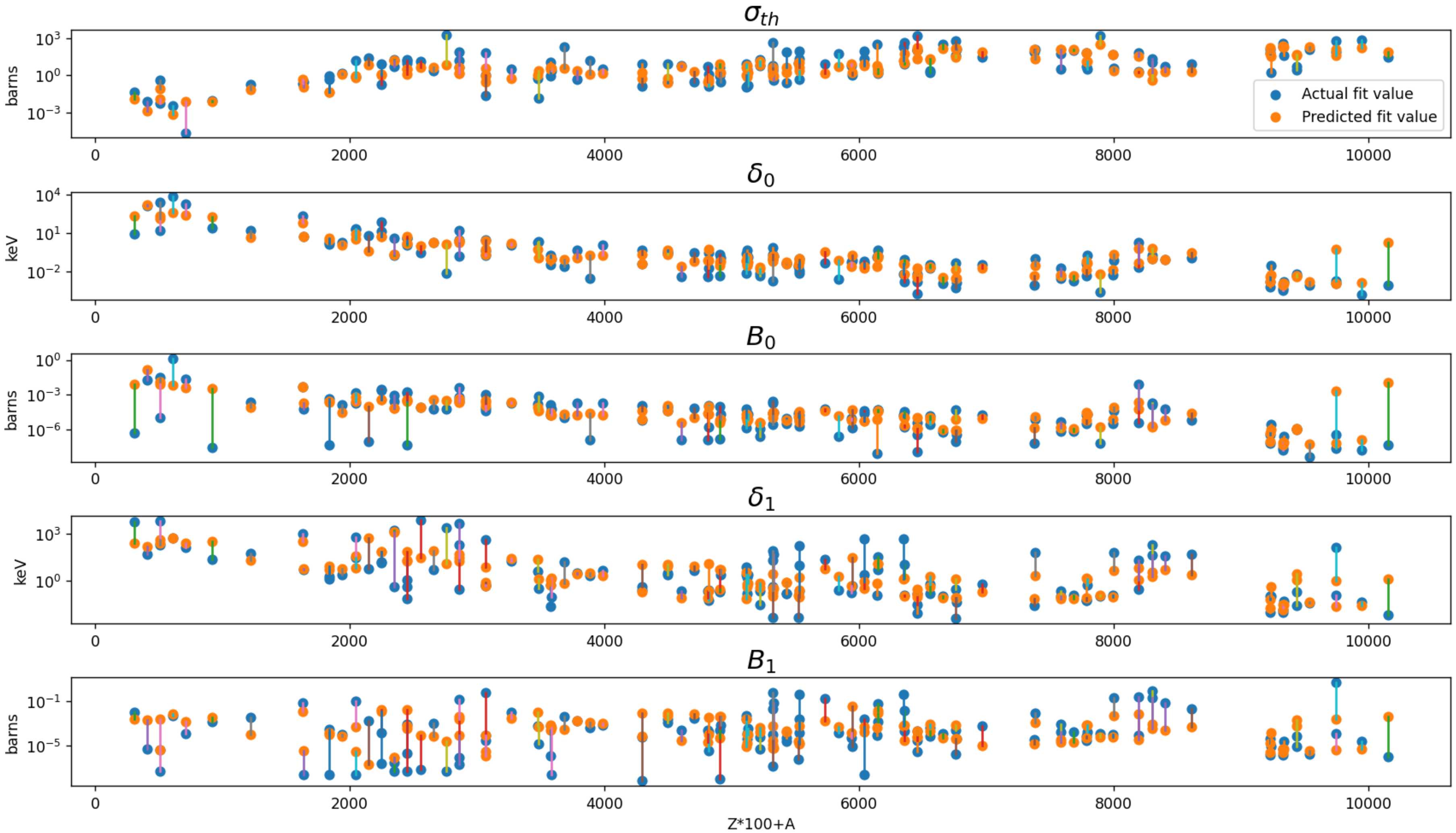
Typical performance

- Predictions are generally accurate within an order-of-magnitude for σ_{th} and 1st bump
- Some isotopes' MACS are predicted reasonably well (e.g. Cu63), many others not
- Changing input feature space did not significantly impact performance, but…
- Hope improving training set with cut-off model makes impact

Regressor: Gradient-Boosted DecisionTree Ensemble Regressor
Features: Z, A, Z even/odd, N even/odd, Jπ, mass excess



Quality of prediction

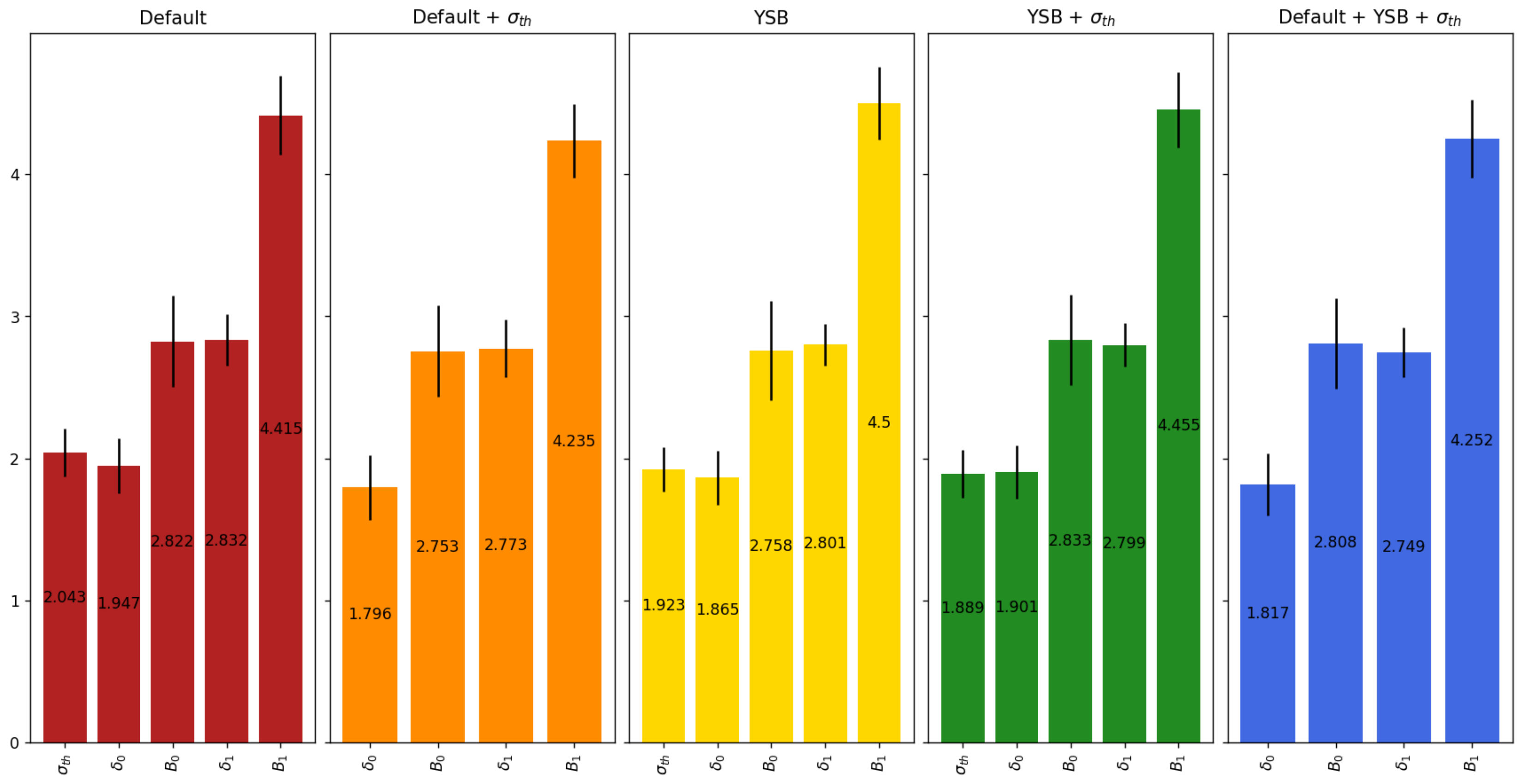


Thermal cross-section
(no cut-off yet!)

1st bump

2nd bump

Comparing feature choices



Intriguingly, Yuskel, Soydaner, Bahtiyar (YSB)* input features: Z, N, A, $A^{2/3}$, (N−Z)/A, ν_Z, ν_N, Z_{shell}, N_{shell} show modest improvement over other options.

(N−Z)/A is a measure of isospin asymmetry, ν_Z and ν_N are the proton/neutron valence numbers, and Z_{shell} and N_{shell} are the shell model orbitals of the last proton/neutron.

$$\mathrm{RMSLE} := \left(\frac{1}{N}\sum^{N}(\log(y_i+\epsilon)-\log(\hat{y}_i+\epsilon)^2\right)^{1/2}$$

* Phys. Rev. C 109, 064322 (2024); https://doi.org/10.1103/PhysRevC.109.064322

Need to do more work on curating our training data:

- use cut-off in direct capture model,
- watch for 1st cluster of resonances,
- use humans in fitting!

Project status

- ✓ Reworking training set
- ✓ Proper test/train split using medium-high quality data
- ✓ Train regressors and tune hyperparameters
- ✓ Propagate ENDF covariance data
- ○ Switch to cut-off model & rerun ML with varied feature sets
- ○ Write paper
- ○ Try MACS in astrophysical network code
- ○ Try in forensics inventory codes

We need help!

Acknowledgements

This research was funded by the National Nuclear Security Administration, Defense Nuclear Nonproliferation Research and Development. The views expressed in the article do not necessarily represent the views of the U.S. Department of Energy or the U.S. Government. The work at Brookhaven National Laboratory was sponsored by the Office of Nuclear Physics, Office of Science of the U.S. Department of Energy under Contract No. DE-SC0012704 with Brookhaven Science Associates, LLC.

Brookhaven National Laboratory

SRNL SAVANNAH RIVER NATIONAL LABORATORY

Stony Brook University

INDIANA UNIVERSITY

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Backup slides

Established scoring rubric

	Very Poor (0)	Poor (1)	Acceptable (2)	Excellent (3)
Experimental data quality **(EXP)**	No experimental data	Sparse/conflicting data	Data in reasonable agreement with itself and with evaluations. Enough data for R-matrix fit.	High -quality and -volume data allowing for R-matrix analysis. Data is self-consistent and in agreement with evaluations, outliers do not impact results.
Resonance evaluation **(RES)**	No evaluated resonances	Few or purely-theory resonances. Includes those derived from TEFAL (in TENDL).	Experimentally measured resonances. Data may indicate missing resonances or high-energy direct capture. Includes data taken from Atlas of Neutron Resonance [4]. Transmission data used to determine resonances, capture widths "schematic".	All resonances backed by measurement. Documentation of direct capture treatment and impact of missing or distant resonances.
Integral metrics **(INT)**	No experimental data	Sparse/conflicting data	Data in reasonable agreement with itself and with evaluations	Data in excellent agreement with data and systematics
Covariance **(COV)**	No covariances included	Values optimistically small; Covariances for background cross section only. Includes COMMARA or LoFi covariances	Values reasonable, but misclassified as reaction MT32, NJOY/FUDGE cannot parse	Detailed MT32 covariances, converted to MT33 NJOY/FUDGE can parse, plot
Fission Product **(FPY)**	Iso. is fission product yield > 1%	Iso. is fission product 1%>yield> 0.001%	Iso. is fission product 0.001% > yield	Isotope is not a fission product
Documentation **(DOC)**	No details	Some resonance region discussion	More resonance region discussion, a list of experimental sources. SG-23 evaluations generally fall here.	Detailed discussion of evaluation and experimental issues, if any.

BNL-224135-2023-INRE

Review of capture cross sections relevant for intentional nuclear forensics

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(Dated: March 7, 2023)

The NA-22 Intentional Forensics Venture is developing a system for tagging nuclear fuel using various methods of information encoding. One of the main methods under development is the insertion of isotopically enriched tracers into the fuel. In order to aid in the understanding of the neutronic performance of these taggants, we assess the quality of the nuclear data underpinning simulations, which are driven by the neutron-capture cross sections. We present these cross sections of naturally occurring isotopes of the elements provided in the neutron sublibrary of the planned ENDF/B-VIII.1 Feb. 2023 library release. We make this assessment using a rubric designed for this effort, which quantifies orthogonal features related to the overall quality. The quality metric highlights 6 aspects: experimental data, resonance evaluations, integral metrics, covariances, fission products, and documentation. We focus on energy ranges relevant for reactor applications. We also discuss additional sources for new, high-quality cross-section data that may be utilized on the time scale of the venture, including existing global data, new experiments, and computational methods. Finally, overall outlook is presented with conclusions.

CONTENTS

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I. INTRODUCTION

NA-22's Intentional Forensics (IF) Venture project is an effort to develop a *taggant* technology for nuclear fuel. An ideal taggant is a well-characterized additive to the fuel that will encode some unique identifier, corresponding to a set of optimal information related to features such as manufacturer, location, age, fuel stage, and others to be decided. The primary goal of this first IF venture is to develop a proof of concept suite of candidate-taggants whose initial suitability has been vetted from the various important perspectives and specialties of the venture members.

This taggant technology should provide several benefits to global stakeholders from public and private interests. It will establish provenance and tracking, identify extra-regulatory material, highlight security lapses, aid law enforcement, and deter future trafficking [1]. Candidate taggants have two primary qualifications. Firstly, they must have an entirely predictable response to a high neutron fluence environment, relative to persistence and/or transmutation. Second, and perhaps most important, they must not detrimentally impact nuclear fuel performance.

Results of cross-section quality review