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U.S. DEPARTMENT OF ENERGY

Tests of the probability table method for unresolved resonances

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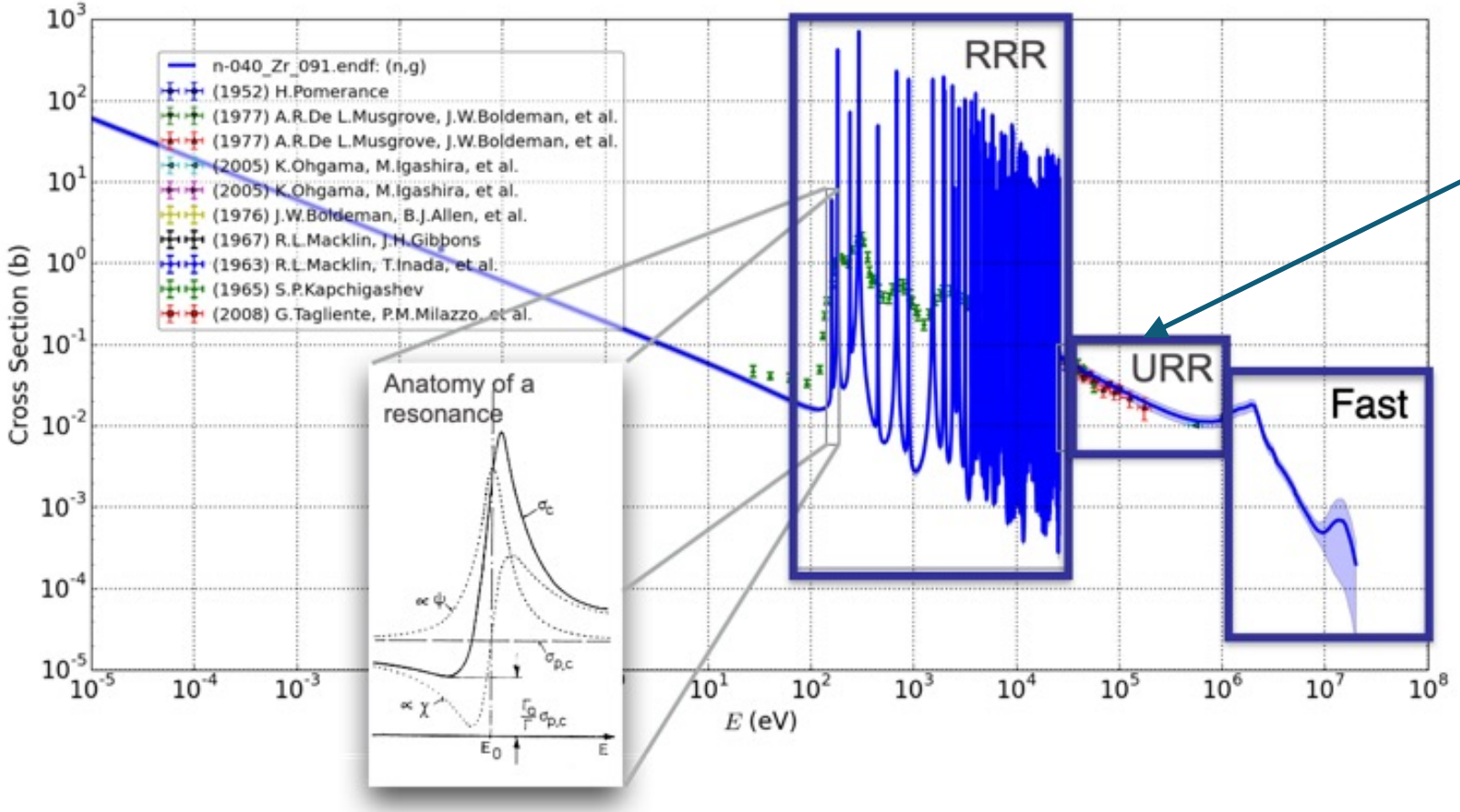
Background

For the past several years as part of an NCSP AM task, a LLNL-BNL collaboration has been working to implement a probability table solution in FUDGE

The FUDGE implementation works, but it is a little bit over-engineered

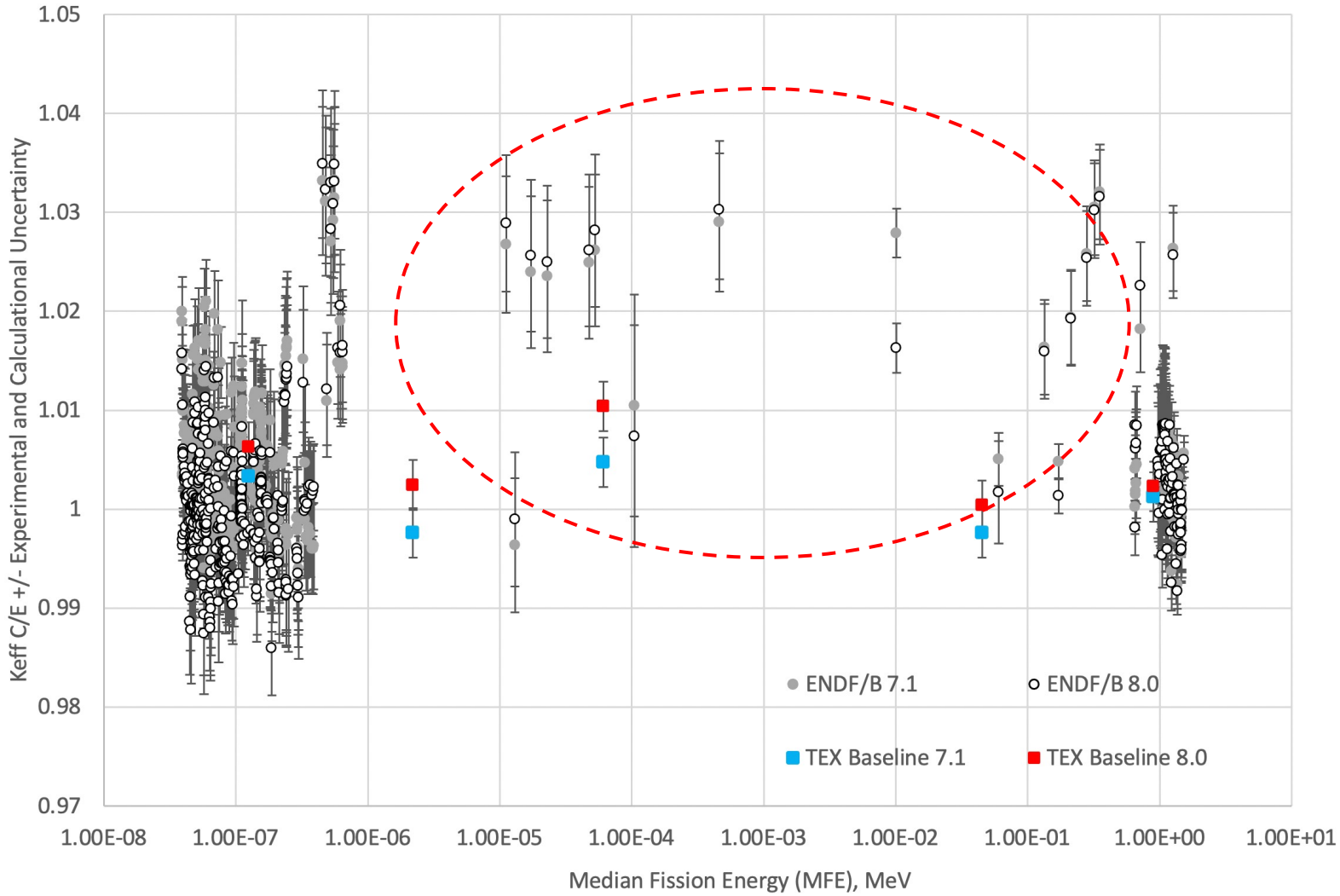
But getting it implemented has led to many questions and a few insights.

The URR is that region just above the RRR where we "don't know anything"!



All we know here are average resonance spacings and widths and maybe an average cross section

Testing suggests systematic bias with assemblies sensitive to the URR



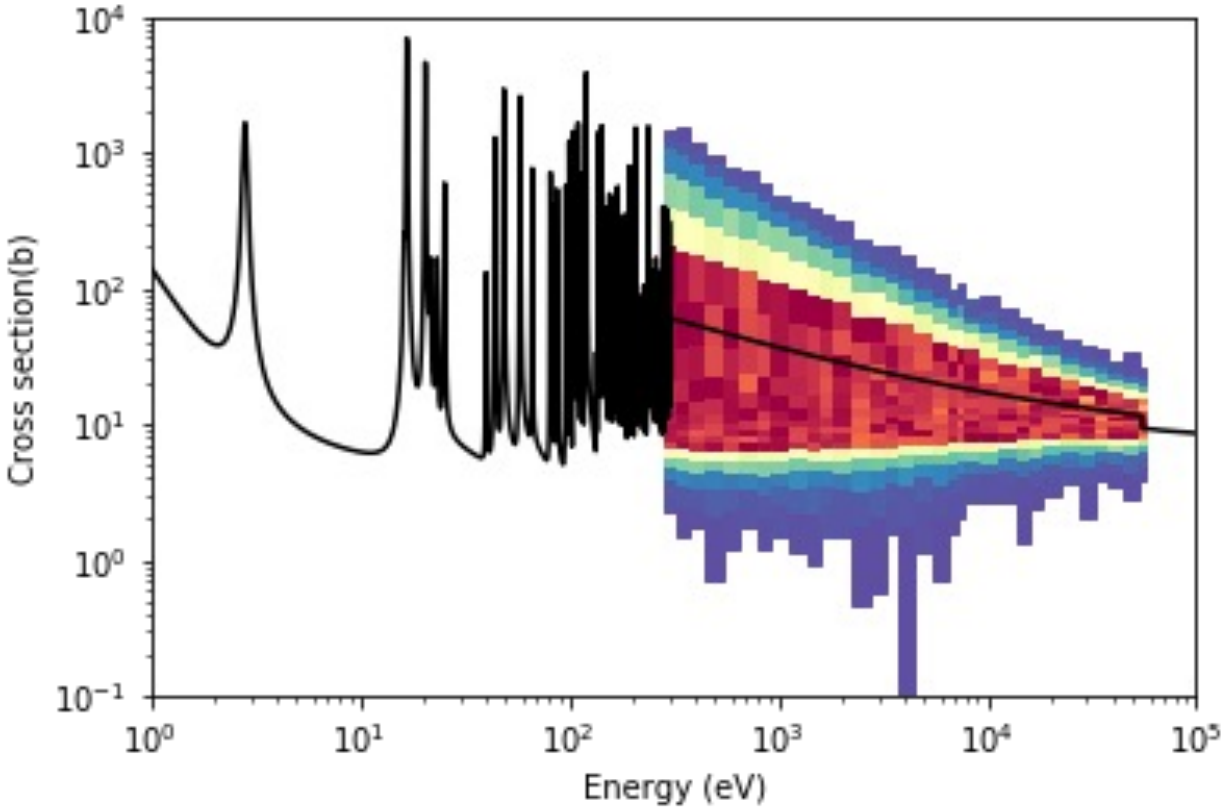
Plot from C. Percher, NCSP TPR 21 Feb 2024

If we “don’t know anything” we must treat probabilistically

In ENDF, we provide the average resonance parameters

These define a cross section probability distribution:

https://docs.openmc.org/en/v0.12.2/examples/nuclear-data.html

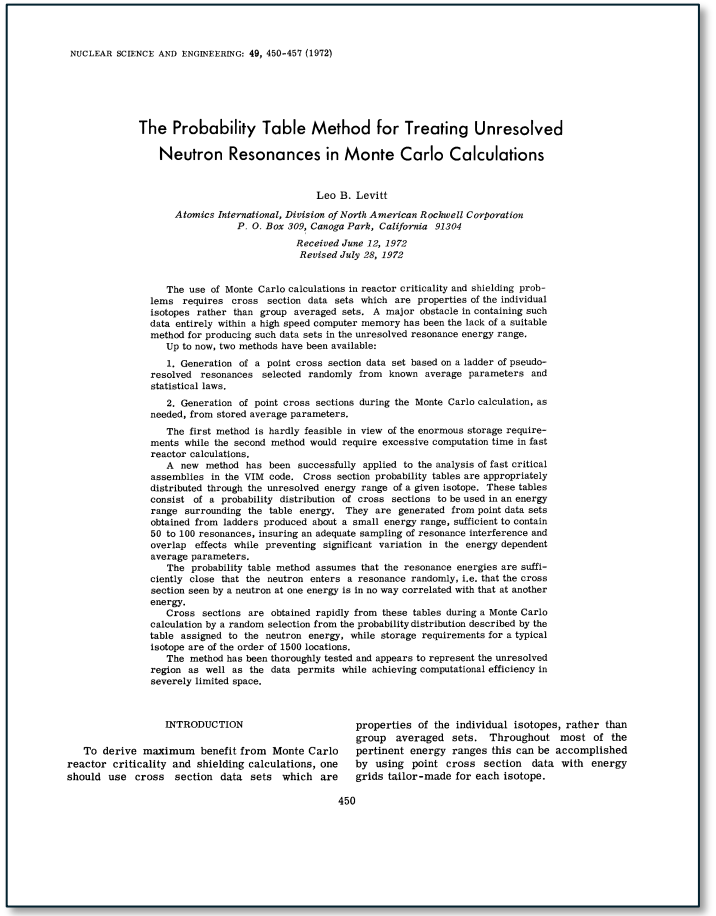


$$P(\sigma_{tot}, \sigma_{cap}, \sigma_{el}) = \delta\left(\sigma_{el} - (\sigma_{tot} - \sigma_{cap})\right) P(\sigma_{tot}, \sigma_{cap})$$

or

$$P(\sigma_{tot}, \sigma_{cap}, \sigma_{el}) = \delta\left(\sigma_{el} - (\sigma_{tot} - \sigma_{cap})\right) P(\sigma_{tot}) P(\sigma_{cap}|\sigma_{tot})$$

Leo Levitt introduced the Probability Table method in 1972



NUCLEAR SCIENCE AND ENGINEERING: 49, 450–457 (1972)

The Probability Table Method for Treating Unresolved Neutron Resonances in Monte Carlo Calculations

Leo B. Levitt

Atomics International, Division of North American Rockwell Corporation
P. O. Box 309, Canoga Park, California 91304

Received June 12, 1972
Revised July 28, 1972

The use of Monte Carlo calculations in reactor criticality and shielding problems requires cross section data sets which are properties of the individual isotopes rather than group averaged sets. A major obstacle in containing such data entirely within a high speed computer memory has been the lack of a suitable method for producing such data sets in the unresolved resonance energy range.

Up to now, two methods have been available:

1. Generation of a point cross section data set based on a ladder of pseudo-resolved resonances selected randomly from known average parameters and statistical laws.

2. Generation of point cross sections during the Monte Carlo calculation, as needed, from stored average parameters.

The first method is hardly feasible in view of the enormous storage requirements while the second method would require excessive computation time in fast reactor calculations.

A new method has been successfully applied to the analysis of fast critical assemblies in the VIM code. Cross section probability tables are appropriately distributed through the unresolved energy range of a given isotope. These tables consist of a probability distribution of cross sections to be used in an energy range surrounding the table energy. They are generated from point data sets obtained from ladders produced about a small energy range, sufficient to contain 50 to 100 resonances, insuring an adequate sampling of resonance interference and overlap effects while preventing significant variation in the energy dependent average parameters.

The probability table method assumes that the resonance energies are sufficiently close that the neutron enters a resonance randomly, i.e. that the cross section seen by a neutron at one energy is in no way correlated with that at another energy.

Cross sections are obtained rapidly from these tables during a Monte Carlo calculation by a random selection from the probability distribution described by the table assigned to the neutron energy, while storage requirements for a typical isotope are of the order of 1500 locations.

The method has been thoroughly tested and appears to represent the unresolved region as well as the data permits while achieving computational efficiency in severely limited space.

INTRODUCTION

To derive maximum benefit from Monte Carlo reactor criticality and shielding calculations, one should use cross section data sets which are properties of the individual isotopes, rather than group averaged sets. Throughout most of the pertinent energy ranges this can be accomplished by using point cross section data with energy grids tailor-made for each isotope.

Levitt, L.B., NSE 49, 450–457 (1972)
https://doi.org/10.13182/NSE72-3

Leo Levitt introduced the Probability Table method in 1972

"At the same time, in appropriate registers with the same band number, the corresponding values of scattering, capture, and fission cross sections are entered. When all points of the data set have been entered we have the following information: the average value of the total cross section in each band of monotonically increasing magnitude, obtained by dividing the sum of the cross section entries in each band by the number of entries in that band. Average cross sections for the other reactions are similarly obtained."

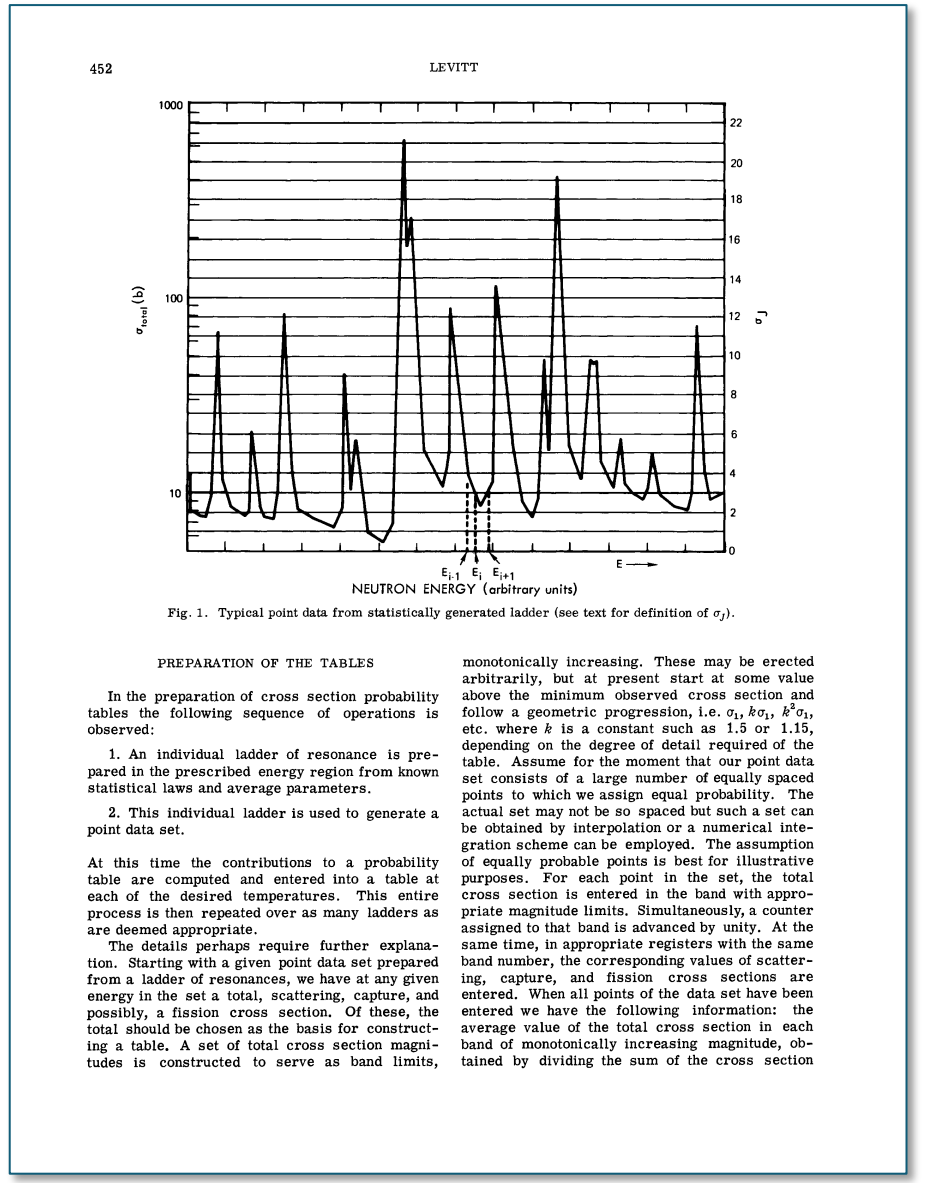


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Fig. 1. Typical point data from statistically generated ladder (see text for definition of σ_J).

PREPARATION OF THE TABLES

In the preparation of cross section probability tables the following sequence of operations is observed:

1. An individual ladder of resonance is prepared in the prescribed energy region from known statistical laws and average parameters.

2. This individual ladder is used to generate a point data set.

At this time the contributions to a probability table are computed and entered into a table at each of the desired temperatures. This entire process is then repeated over as many ladders as are deemed appropriate.

The details perhaps require further explanation. Starting with a given point data set prepared from a ladder of resonances, we have at any given energy in the set a total, scattering, capture, and possibly, a fission cross section. Of these, the total should be chosen as the basis for constructing a table. A set of total cross section magnitudes is constructed to serve as band limits, monotonically increasing. These may be erected arbitrarily, but at present start at some value above the minimum observed cross section and follow a geometric progression, i.e. σ_1, $k\sigma_1$, $k^2\sigma_1$, etc. where k is a constant such as 1.5 or 1.15, depending on the degree of detail required of the table. Assume for the moment that our point data set consists of a large number of equally spaced points to which we assign equal probability. The actual set may not be so spaced but such a set can be obtained by interpolation or a numerical integration scheme can be employed. The assumption of equally probable points is best for illustrative purposes. For each point in the set, the total cross section is entered in the band with appropriate magnitude limits. Simultaneously, a counter assigned to that band is advanced by unity. At the same time, in appropriate registers with the same band number, the corresponding values of scattering, capture, and fission cross sections are entered. When all points of the data set have been entered we have the following information: the average value of the total cross section in each band of monotonically increasing magnitude, obtained by dividing the sum of the cross section

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Leo Levitt introduced the Probability Table method in 1972

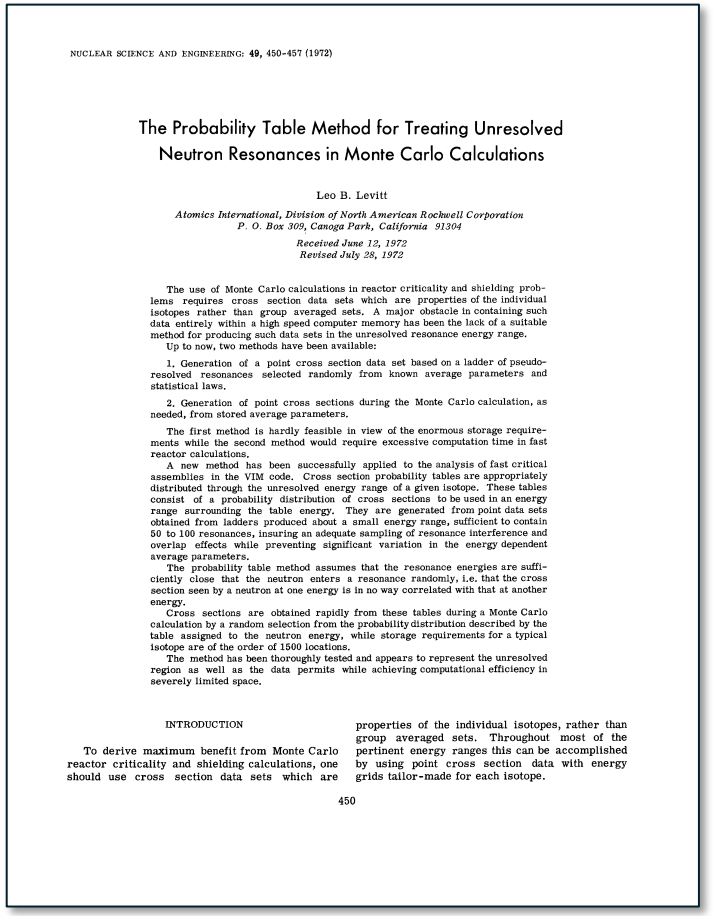
In it, we store

- The total cross section PDF as a ***cumulative distribution function***
- The average cross section(s) for capture, elastic and fission

Essentially, we make this approximation:

$$P(\sigma_{cap}|\sigma_{tot}) \approx \delta\left(\sigma_{cap} - \overline{\sigma}_{cap}(\sigma_{tot})\right)$$

$$\overline{\sigma}_{cap}(\sigma_{tot}) = \int_0^\infty d\sigma_{cap}\sigma_{cap}P(\sigma_{cap}|\sigma_{tot})$$



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How good is this approximation?

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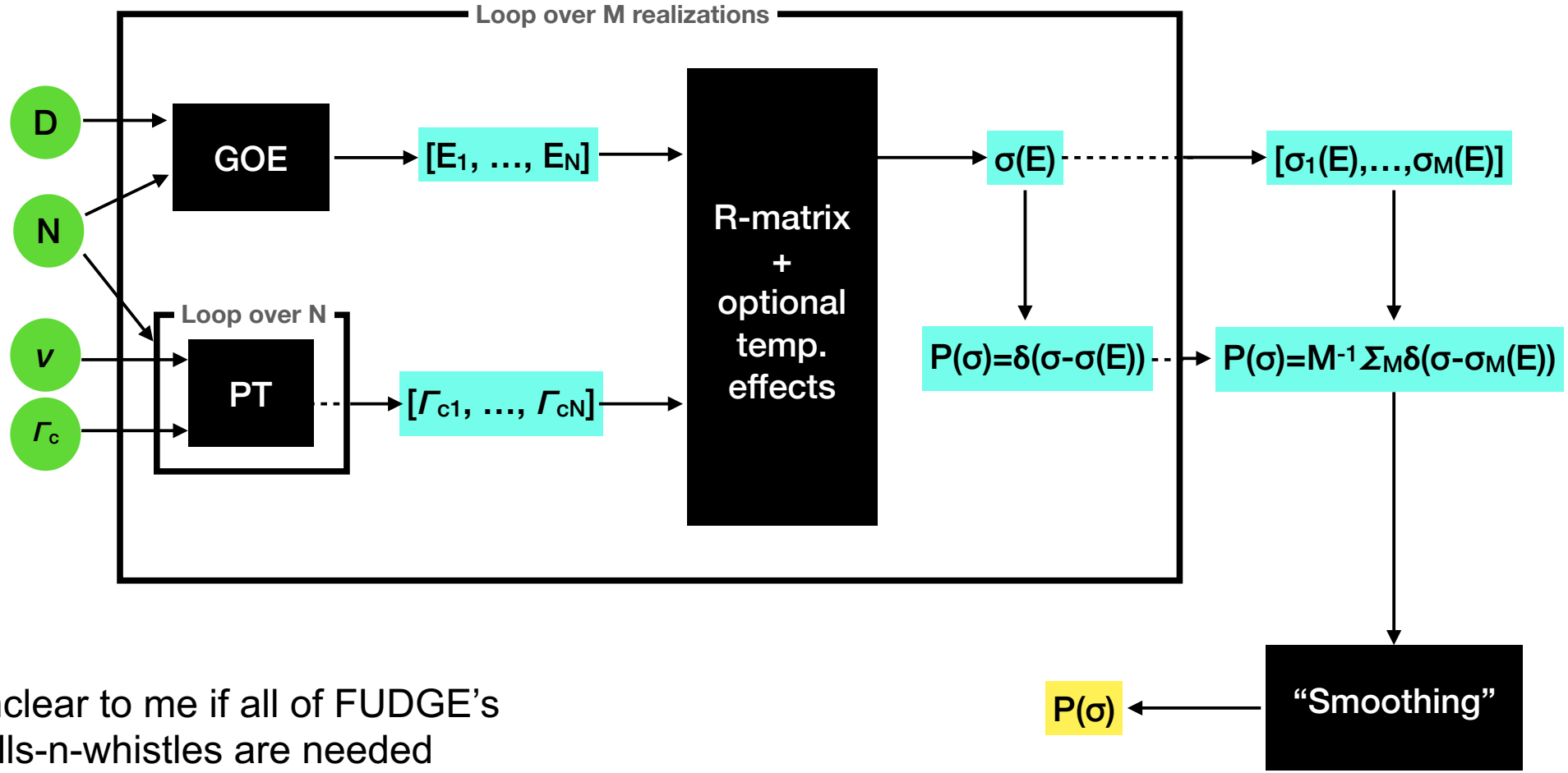
FUDGE ladder generation

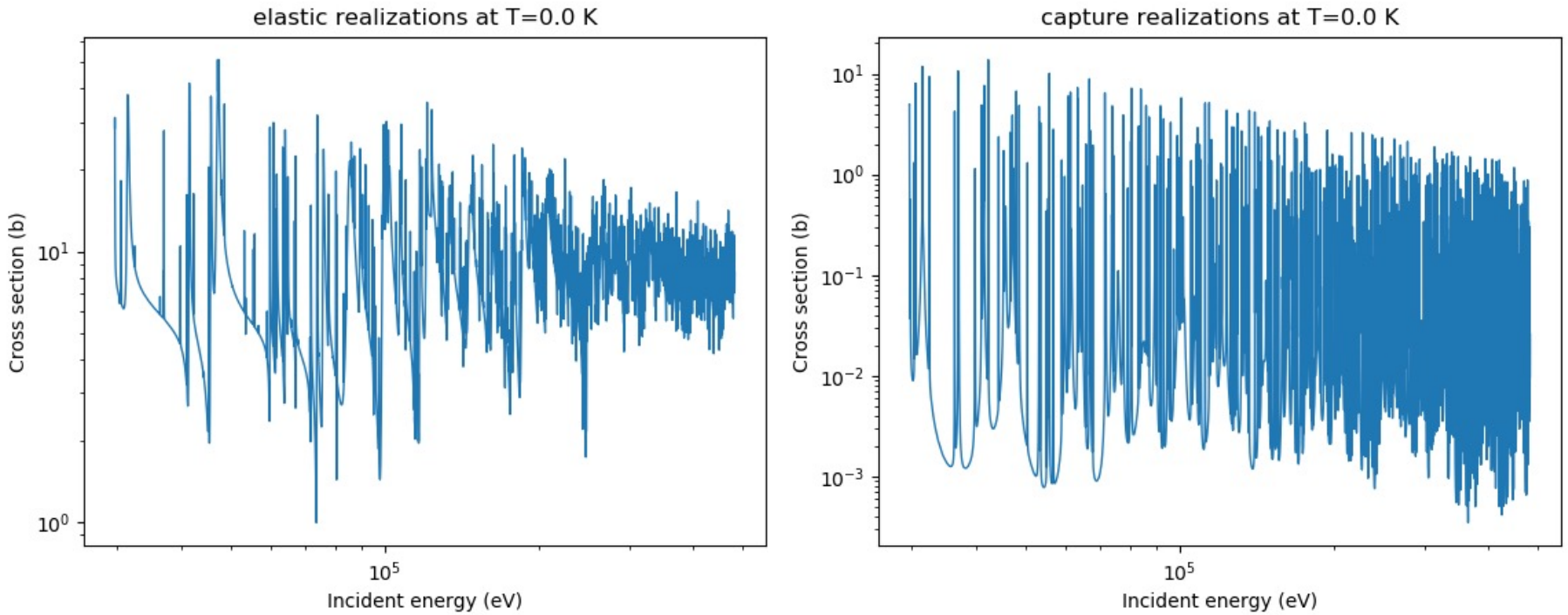
As part of FUDGE's PT generator, we have a generative model for resonances



It is unclear to me if all of FUDGE's bells-n-whistles are needed

"Smoothing" == Doppler broadening

Fe55 realizations: GOE level generator



How to compute pdf(σ) analytically given the functional form of σ(E)

- With cross section at E given by parameters $\{x\}$, the exact pdf(**σ**) is

$$pdf(\sigma) = \delta(\sigma - \sigma(E, x))$$

- Using ergodicity, we do

$$pdf(\sigma) = \int_{\delta E} dE\ \delta(\sigma - \sigma(E, x))$$

- Giving approximate pdf of (E_j's are zeros of delta function)

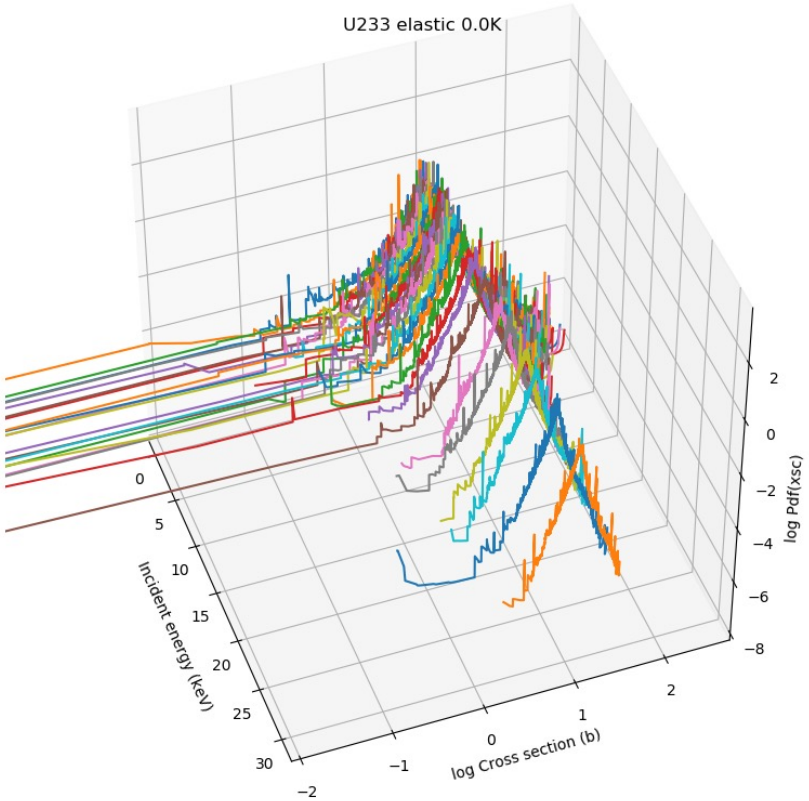
$$pdf(\sigma) = \sum_{j\text{zeros}} \frac{1}{|\partial\sigma(E_i(\sigma), x)/\partial E|}$$

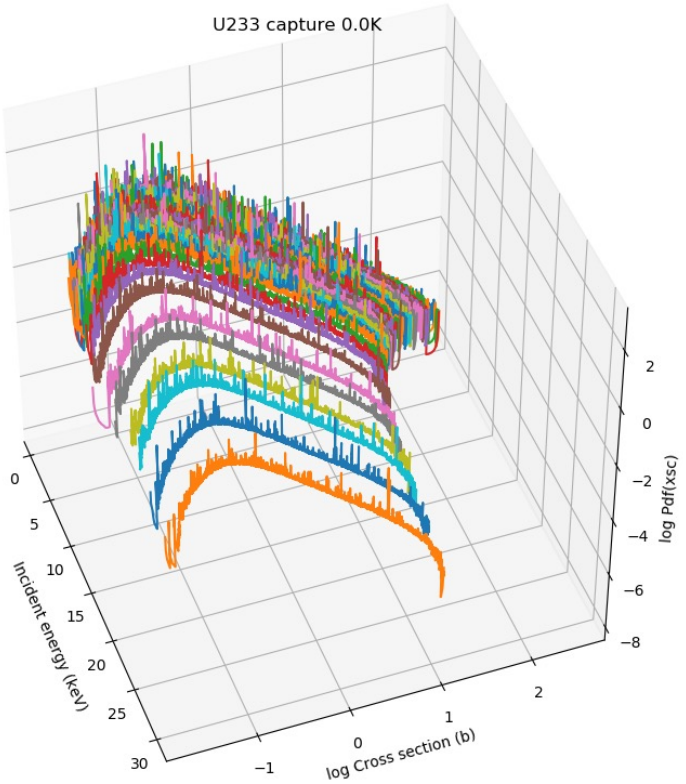
U233 (ENDF-VIII.0) URR cross section probability tables

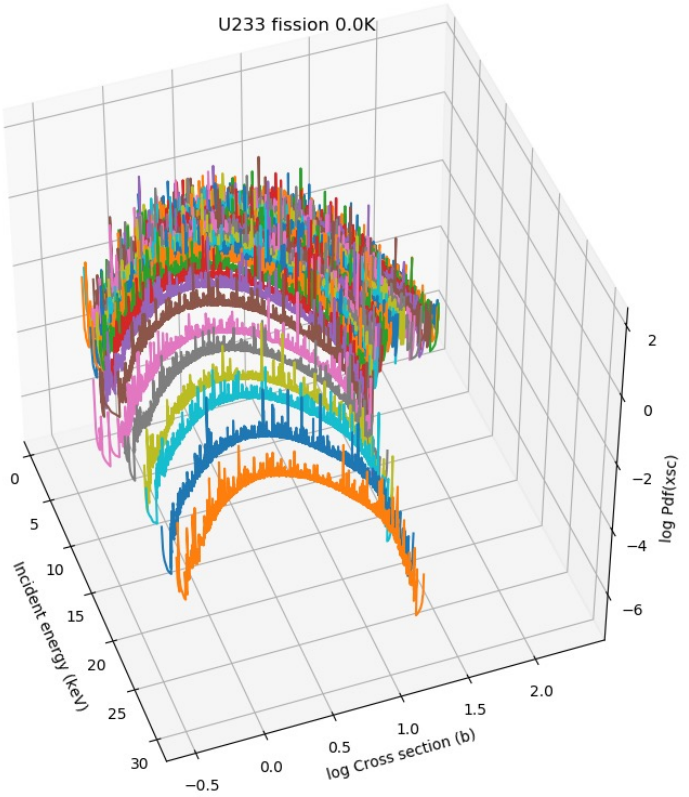
First set of plots generated by FUDGE

- 500 realizations
- sticking with Wigner resonance spacing instead of GOE for now
- heated to 0 K, 300 K and 1200 K
- No smoothing yet, these are ‘raw’ pdfs

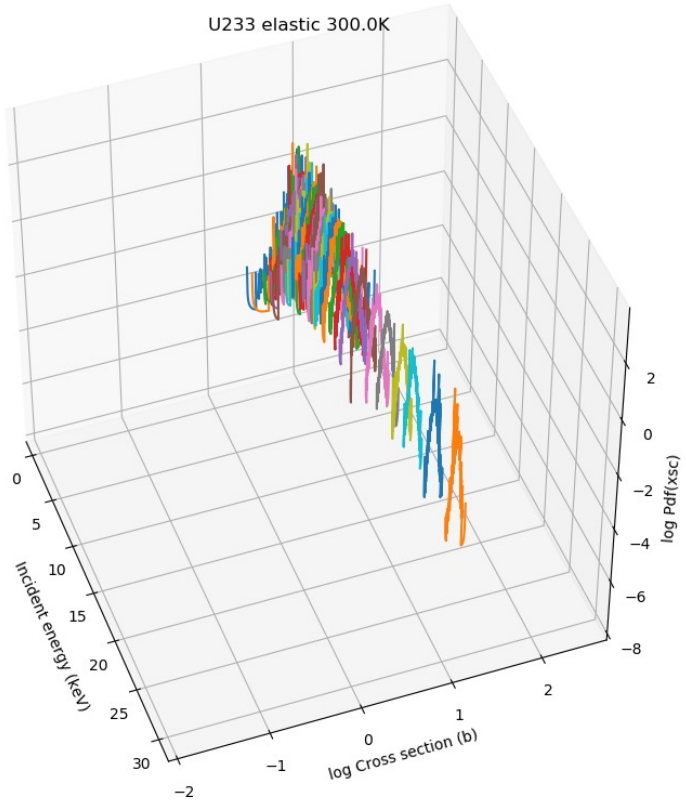
0 K pdfs

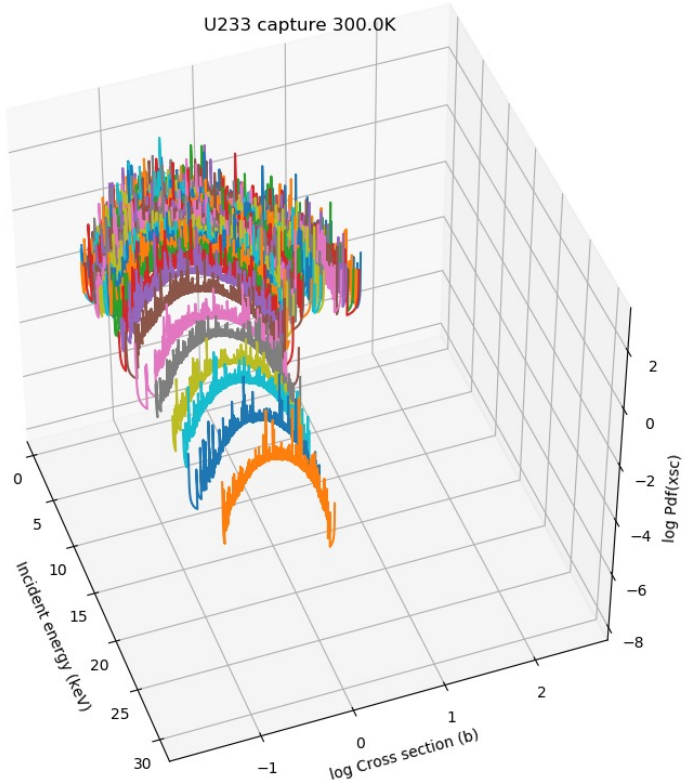

U233 elastic 0.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

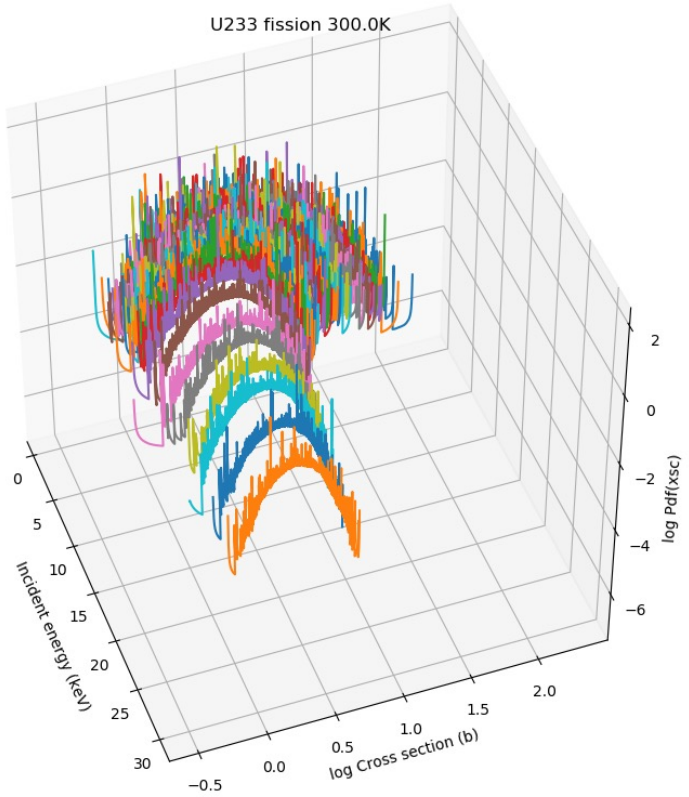

U233 capture 0.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)


U233 fission 0.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

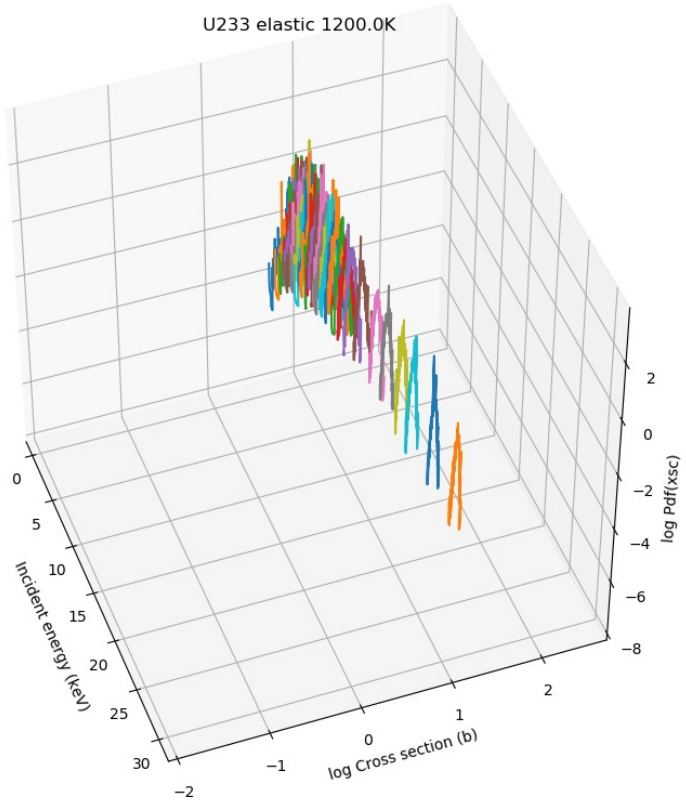
300 K pdfs

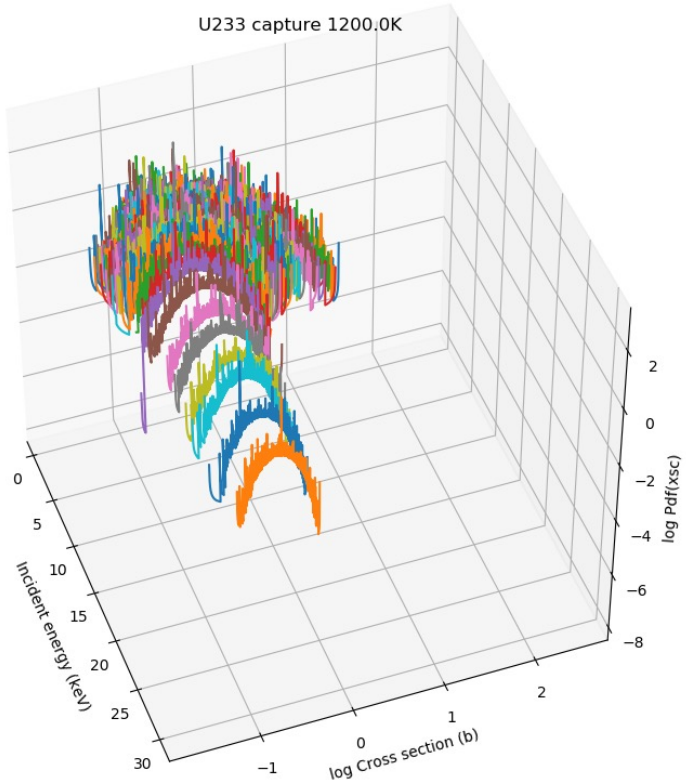

U233 elastic 300.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

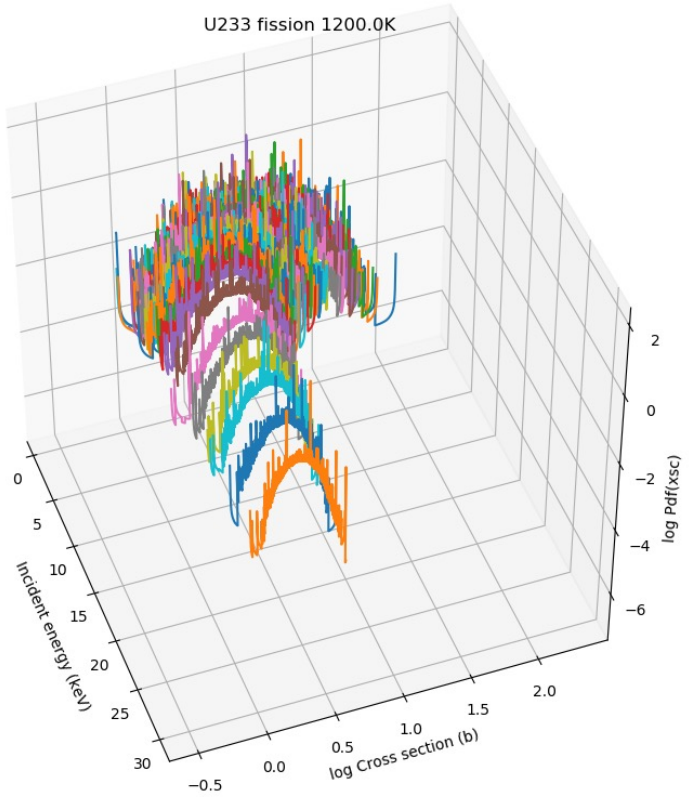

U233 capture 300.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)


U233 fission 300.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

1200 K pdfs


U233 elastic 1200.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

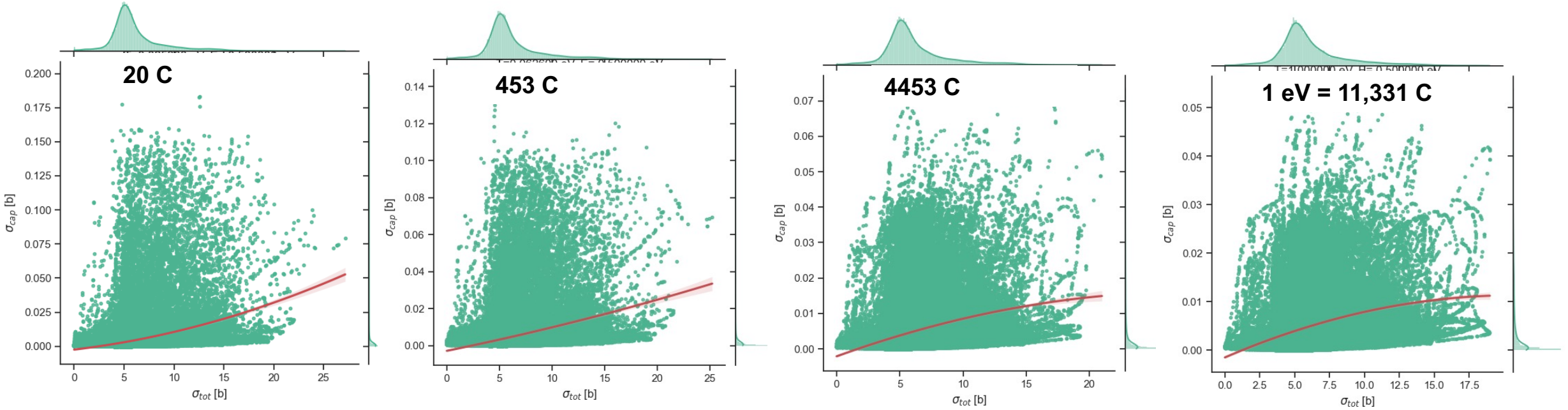

U233 capture 1200.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)


U233 fission 1200.0K
Incident energy (keV)
log Cross section (b)
log Pdf(xsc)

Testing Levitt Approximation

Let's just measure the PDF!

^{90}Zr from ENDF/B-VIII.0
@ E=500 keV
10 realizations (leaning heavily on ergodicity trick)



Temperature increase →

Take aways:

- PDF already very narrow in capture direction
- As temperature increases, it gets even narrower
- Levitt appears to be right-ish?

Need a proper test!

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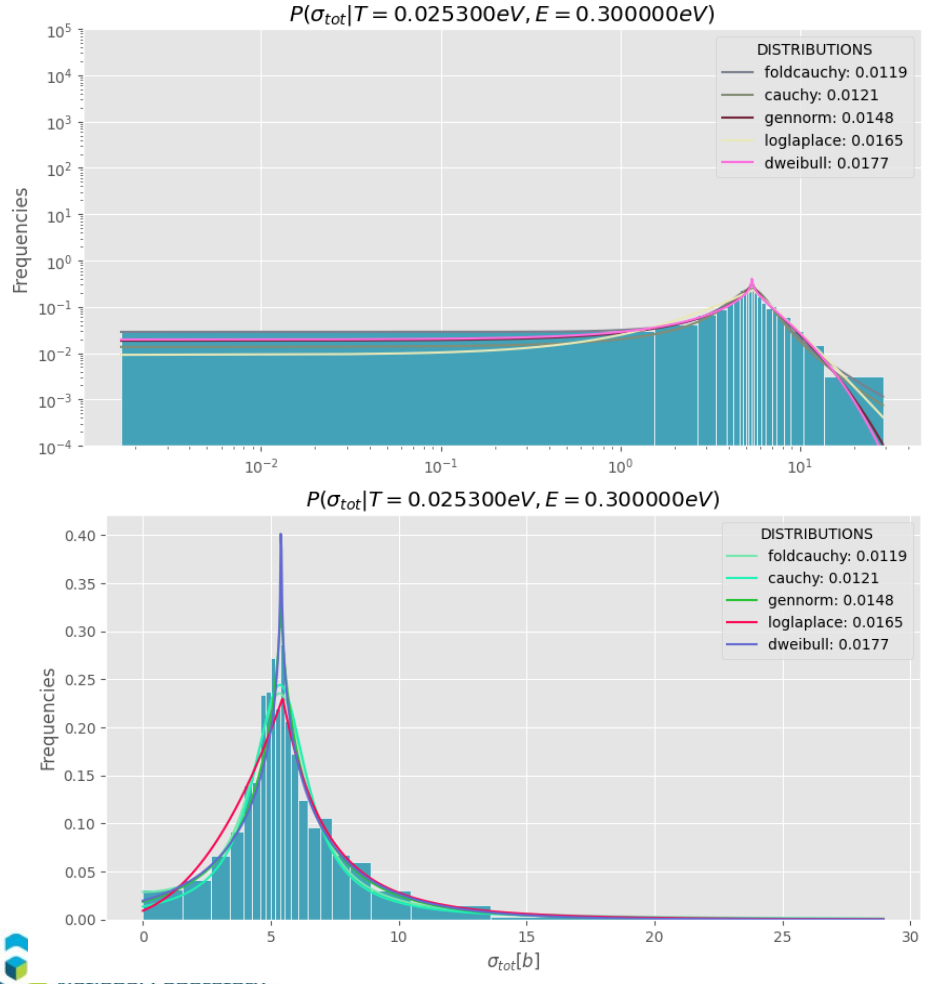
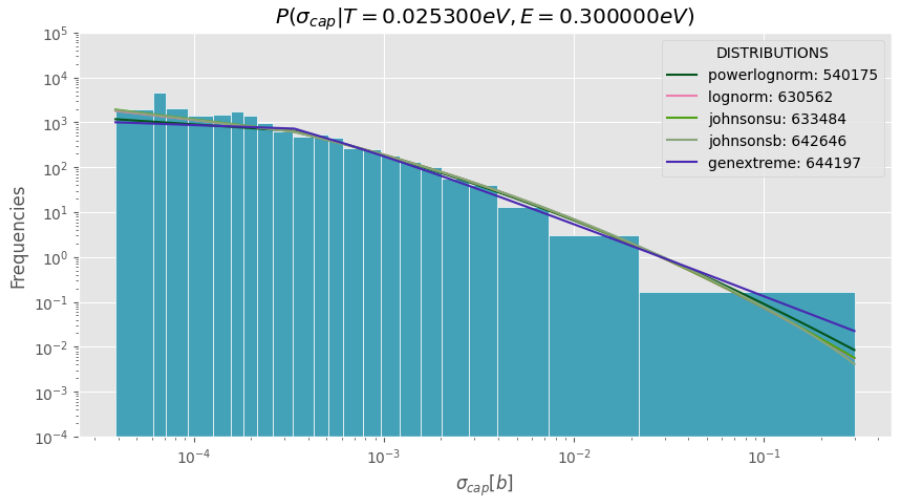
Close ups on the total & capture marginal PDFs





It may be possible to guess a functional form that works for all temperatures, essentially building a surrogate model for the full PDF

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Getting capture PDF in Levitt approximation

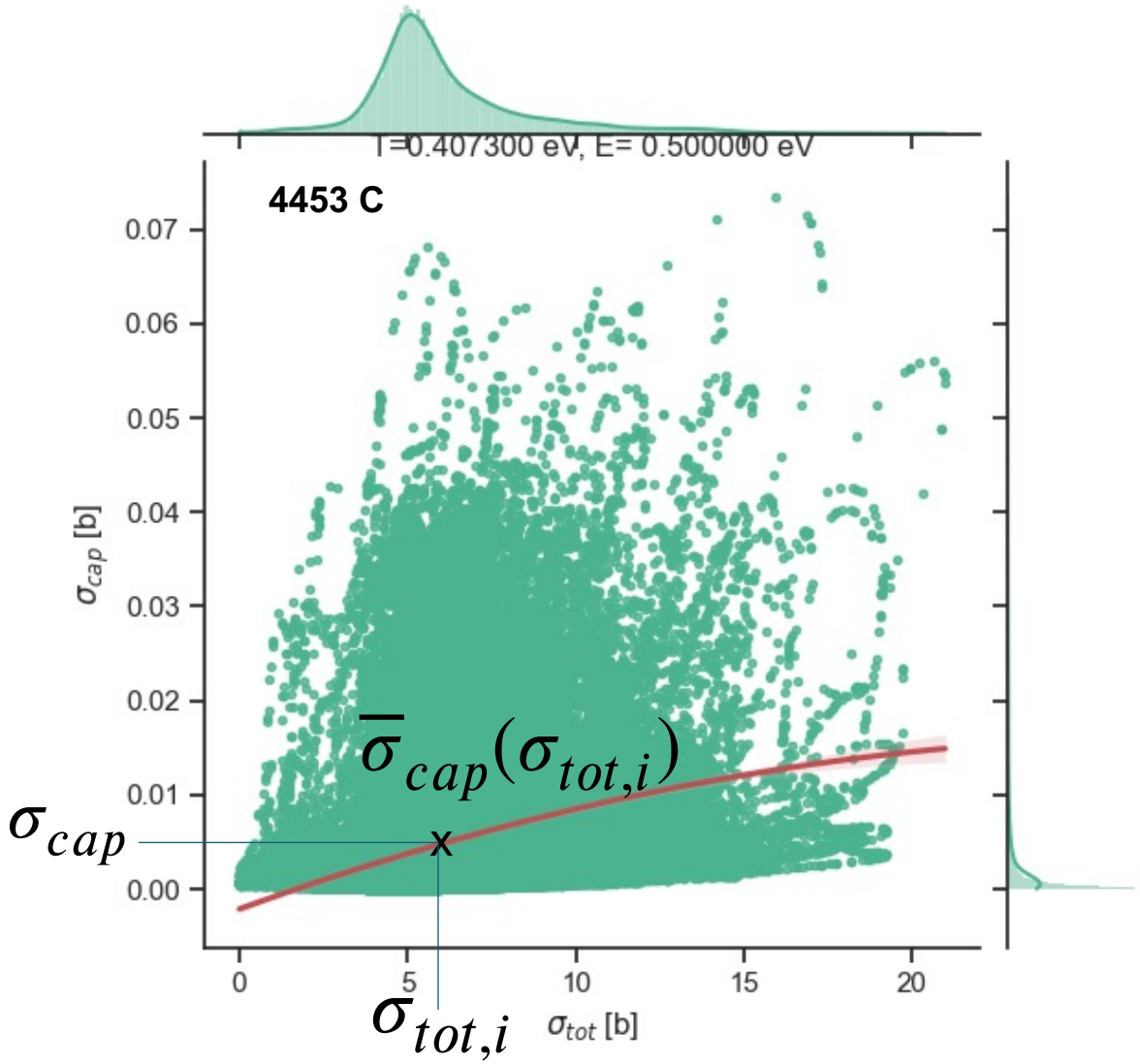
$$P(\sigma_{cap}|\sigma_{tot}) \approx \delta\left(\sigma_{cap} - \overline{\sigma}_{cap}(\sigma_{tot})\right)$$

Integrating Levitt delta function, we have

$$P(\sigma_{cap}) \approx \sum_{\text{zeros}i} \left|\frac{\partial\sigma_{cap}(\sigma_{tot,i})}{\partial\sigma_{tot}}\right|^{-1} P(\sigma_{tot,i})$$

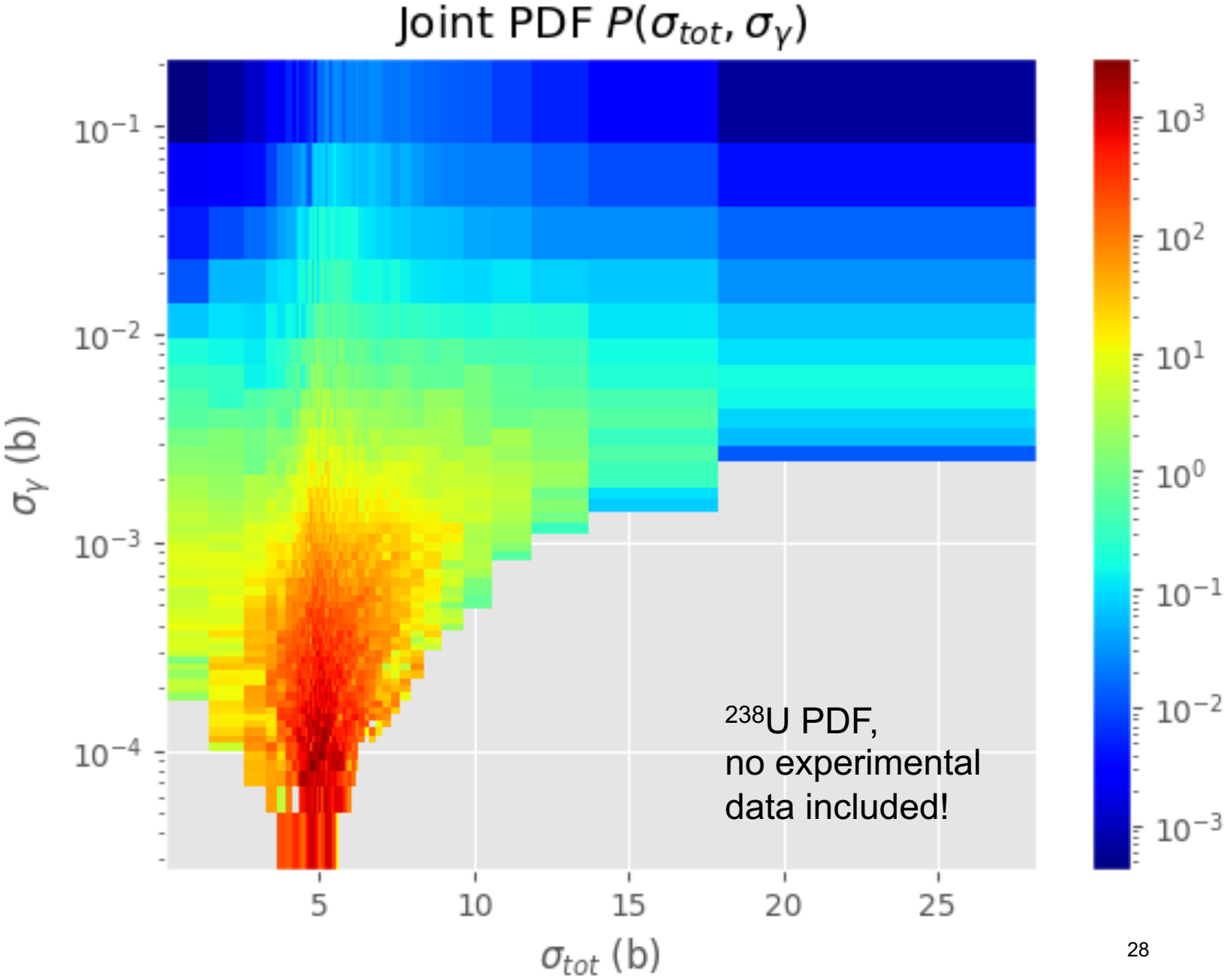
Where zeros are crossings of current capture cross section and regression line

$$\sigma_{tot,i} = \overline{\sigma}_{cap}^{-1}(\sigma_{cap})$$



Here is the full ^{238}U joint PDF

We want to get this into GNDS and McGIDI so can run tests in Mercury



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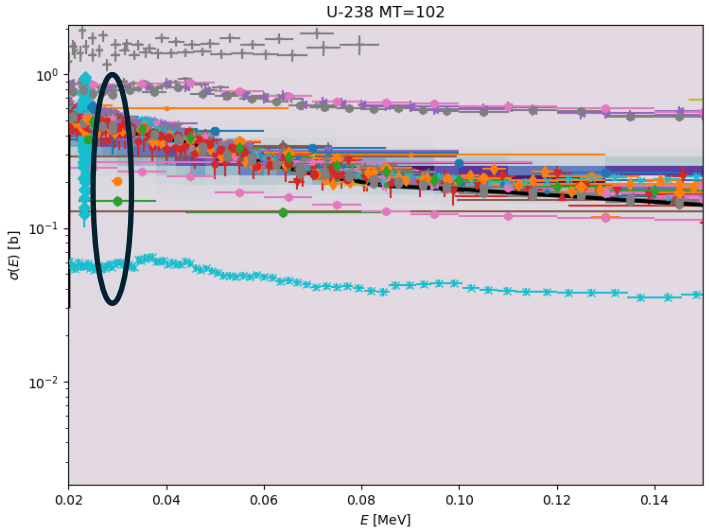
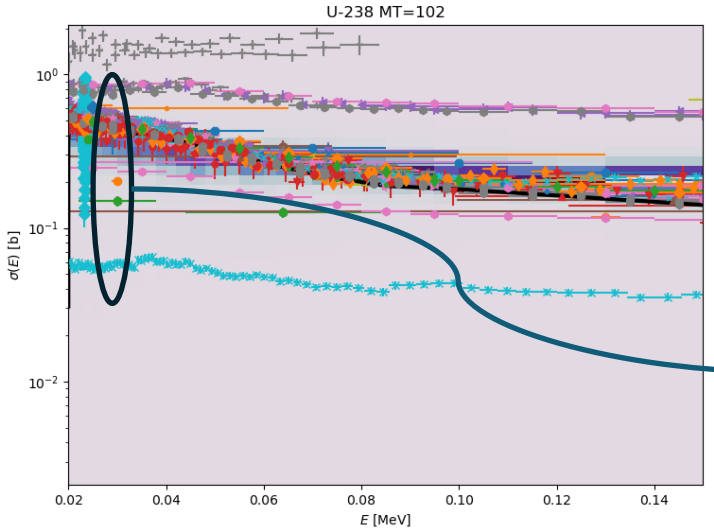
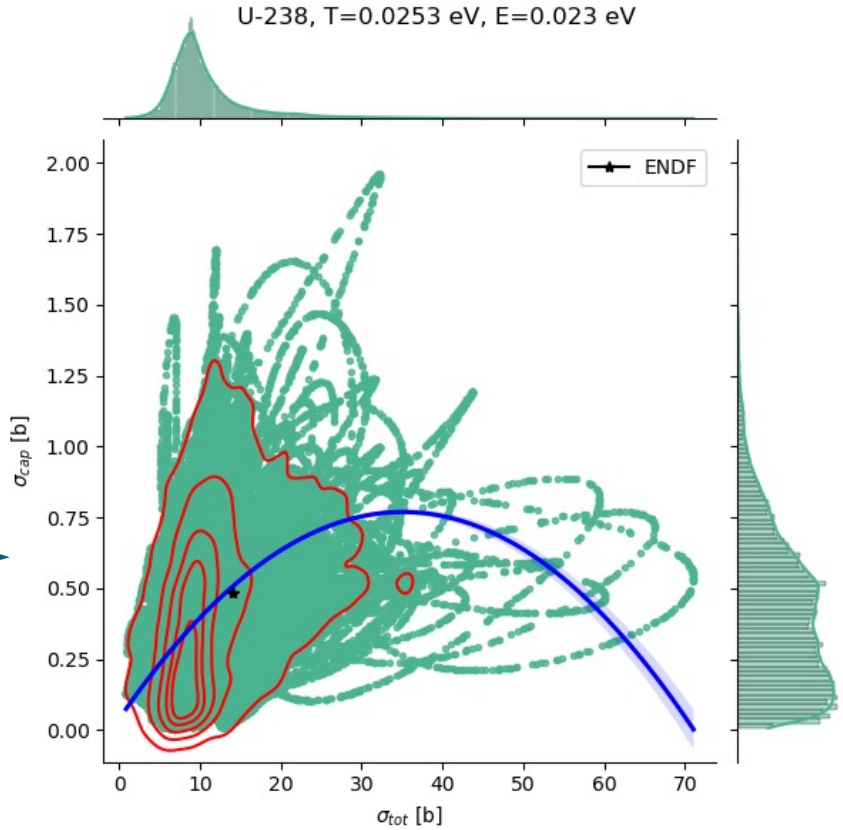
^{238}U



(ugly plot of 238U capture)

^{238}U





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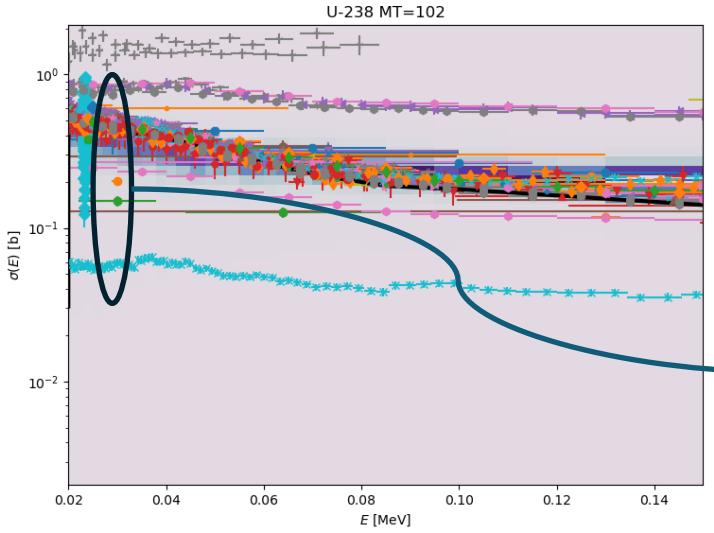
^{238}U



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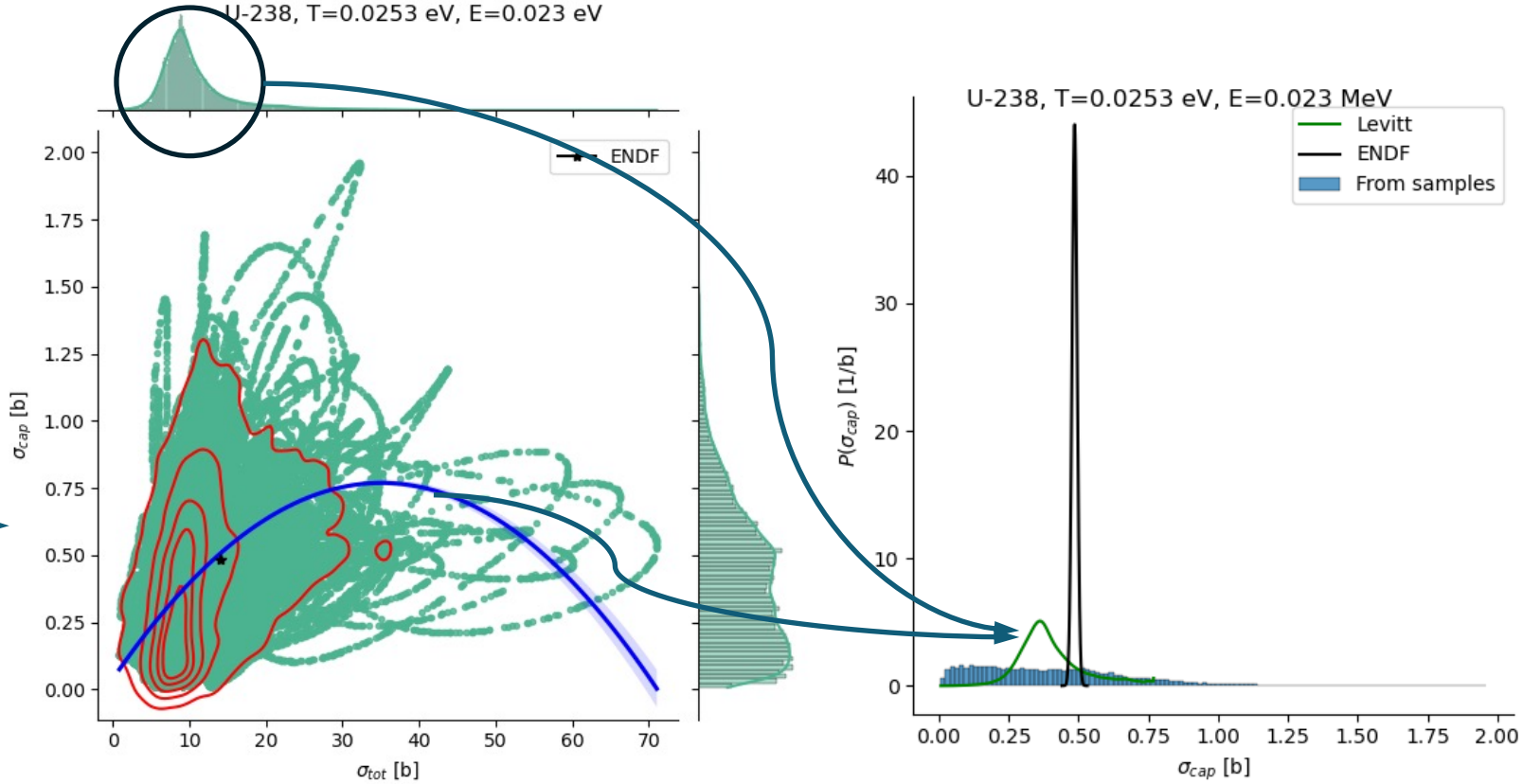

- Mean value in the wrong place, fixable with LSSF=1
- Width & skew very very wrong

Levitt fails?

If Levitt approximation is wrong, does it matter?

Our next step: we need more statistics and to run some crits (esp. BigTen)

Where we are now

Eliminate artifacts of our algorithm at higher temperatures

Fit $P(\sigma_{tot}, \sigma_{cap})$ as a function of T for few interesting isotopes

Examine limits of Leo Levitt approximation for interesting isotopes (^{238}U) in applications (think BigTen)

Develop surrogate model of $P(\sigma_{tot}, \sigma_{cap})$, this would be super useful off-stability (heck, could use it over all energies)