Unifying the URR PT approaches and covariance work in a consistent framework

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CSEWG

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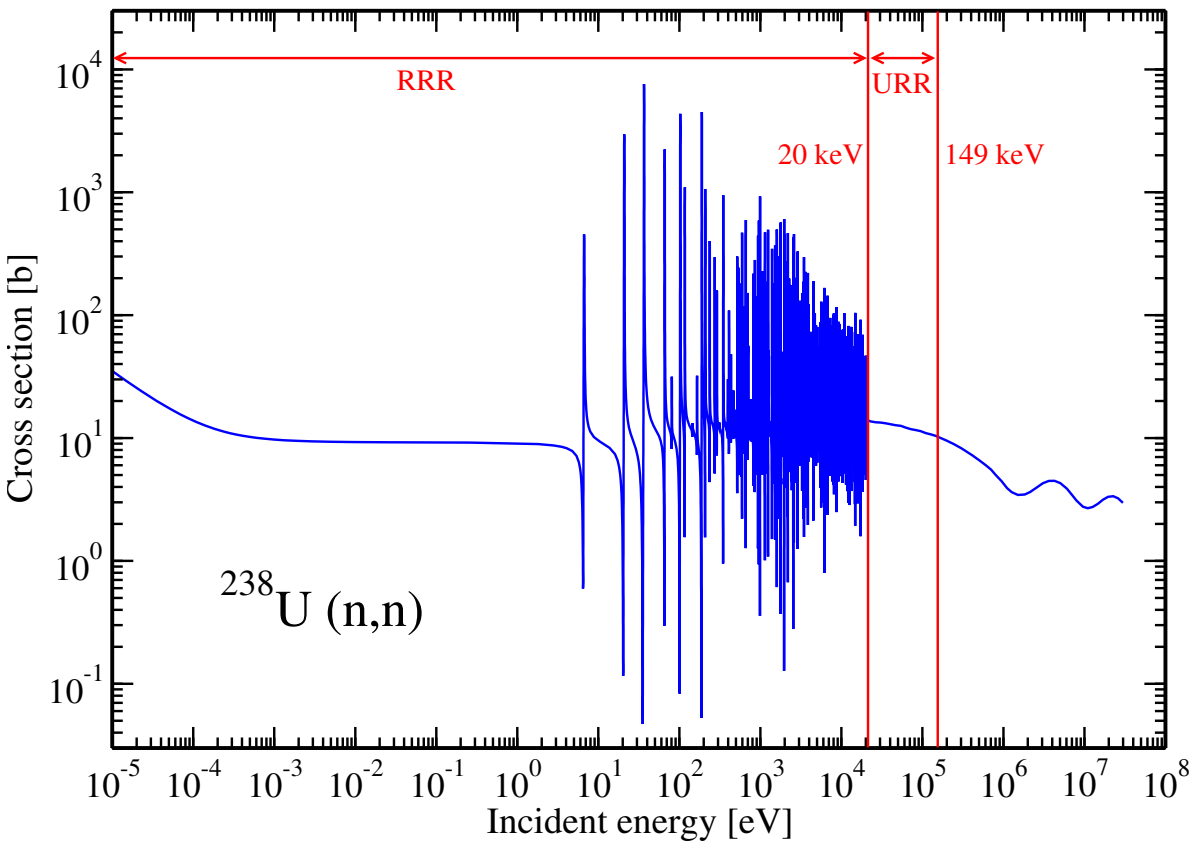
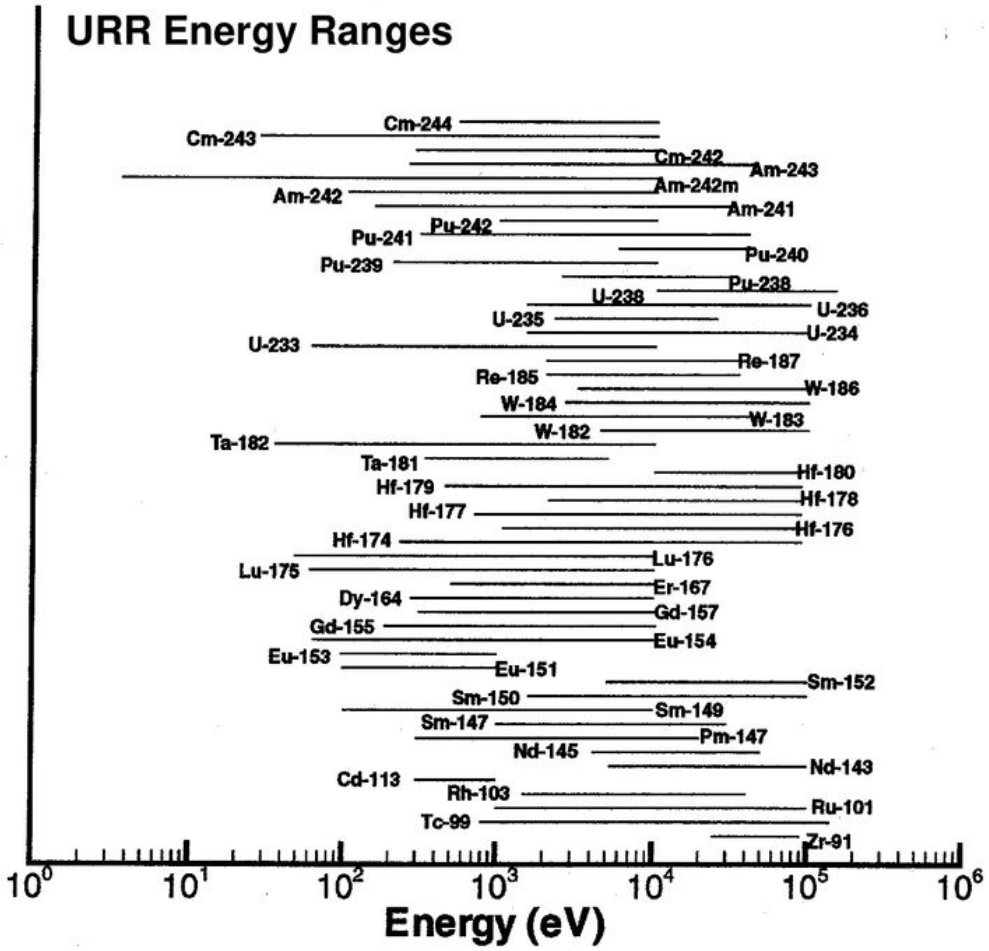
Unresolved resonance region

- Thermalization of neutrons in ^{238}U by elastic scattering requires ~ 2200 collisions
- Energy loss by elastic scattering in the URR amounts to ~ 240 collisions
- ~ 11% of collisions occur in the URR
- This is something we should care about



Unresolved resonance region

- Resonances are too narrow to resolve experimentally
- We cannot determine individual resonance parameters
- We can only determine averages of parameters
- Enough to determine the cross section PDF



Thomas Sutton, KAPL

Cross section probability distributions

The probability distribution is a measure of our ignorance of the cross section

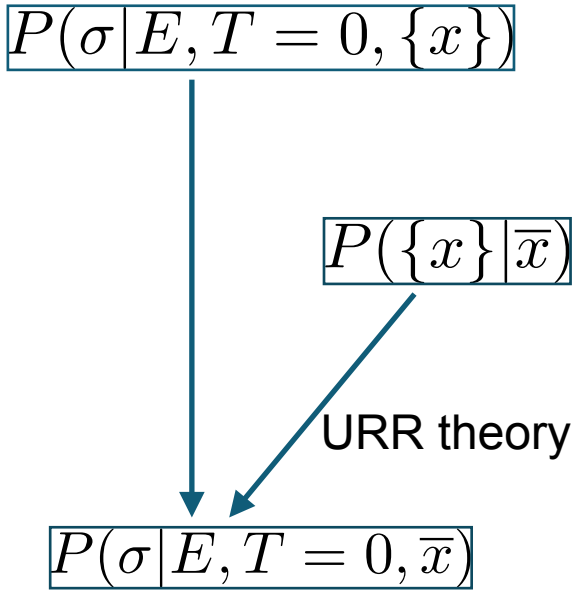
If we know the cross section exactly, the PDF is a delta function

$$P(\widetilde{\sigma}|E) = \delta\big(\widetilde{\sigma} - \sigma(E)\big)$$

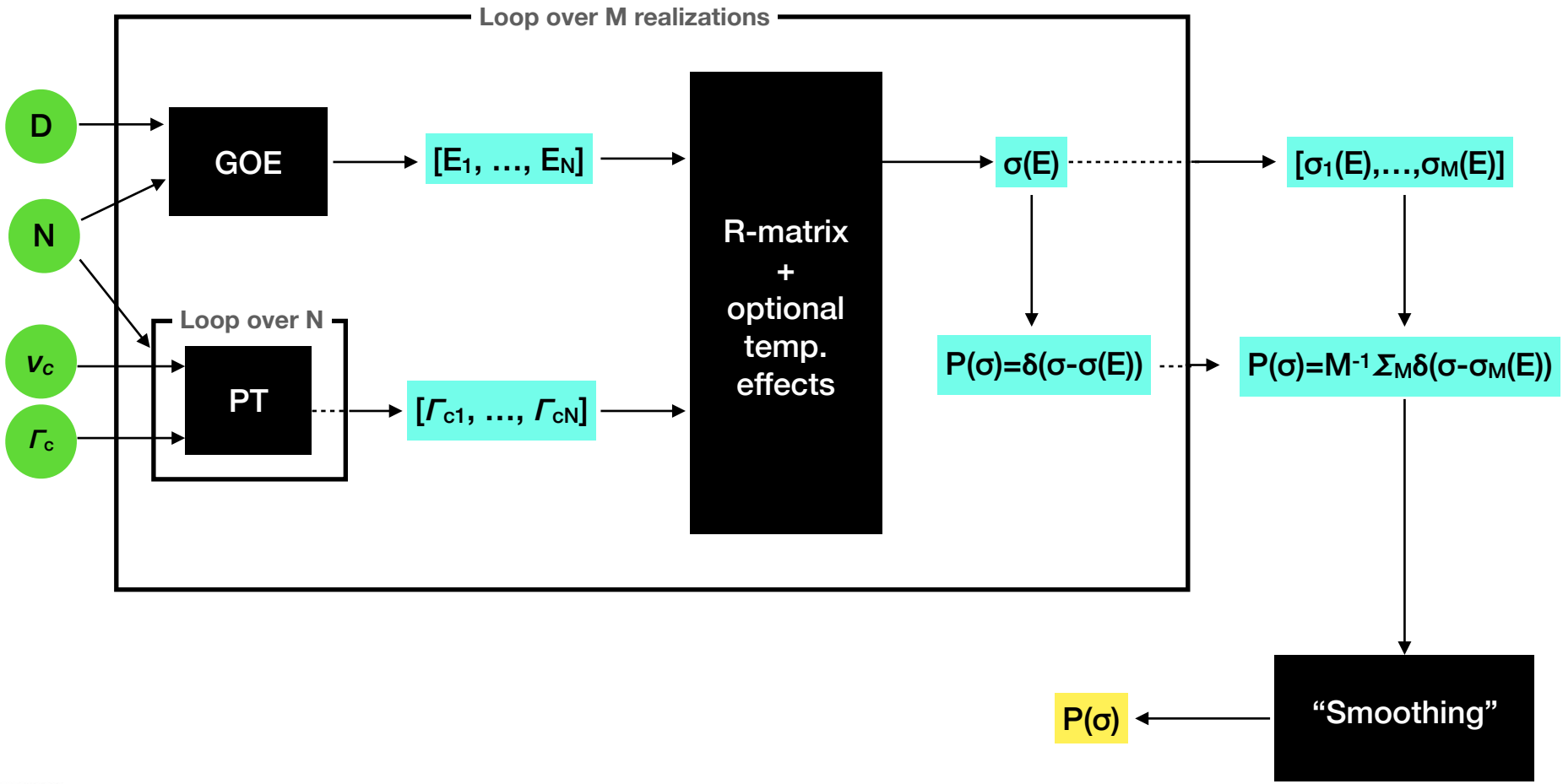
If we want to express our ignorance of the URR parameters

$$P(\widetilde{\sigma}|E, \overline{\boldsymbol{x}}) = \int d\boldsymbol{x}\, P(\boldsymbol{x}|\overline{\boldsymbol{x}})\, \delta\big(\widetilde{\sigma} - \sigma(E, \boldsymbol{x})\big)$$

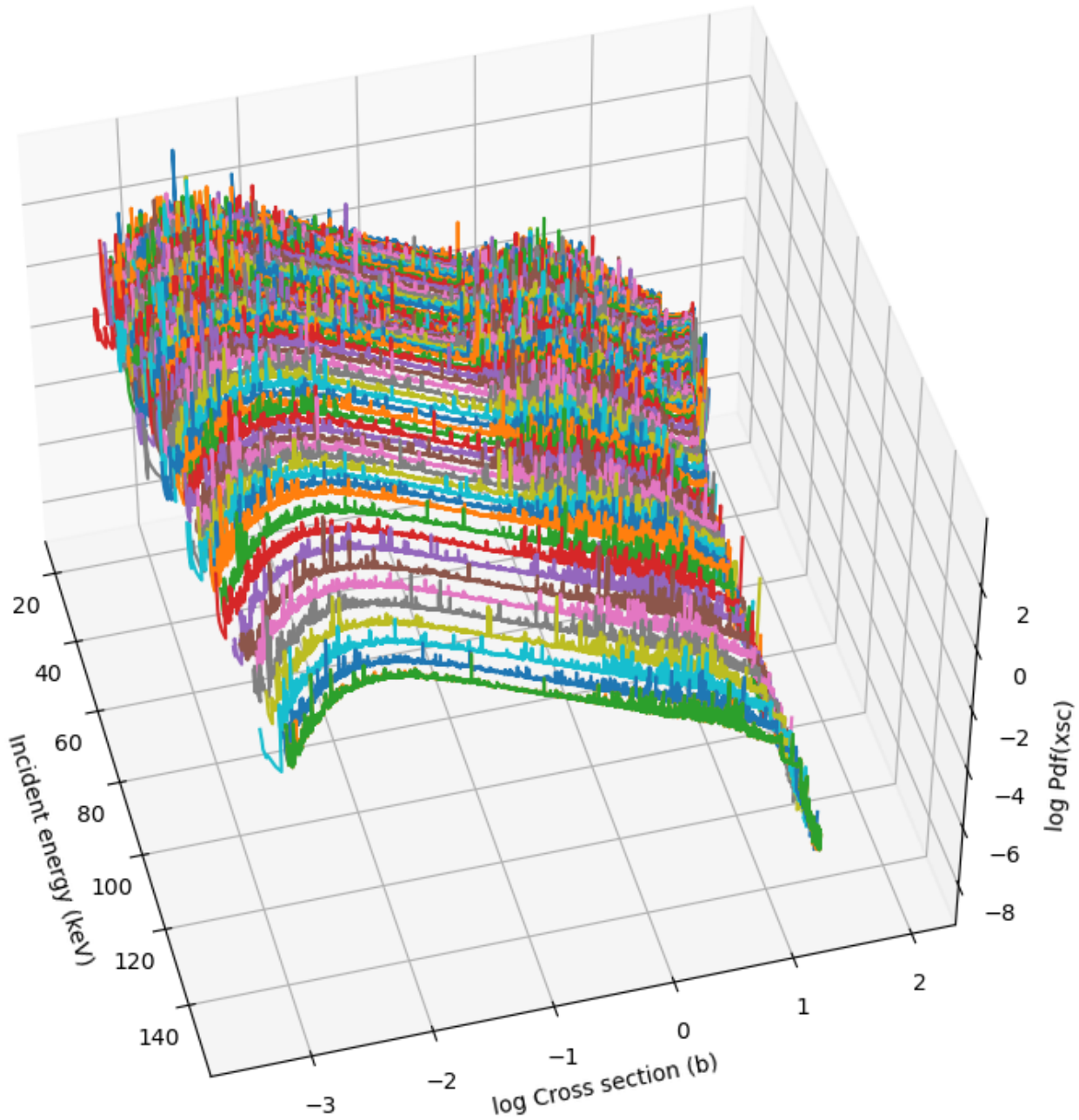
Resonance parameter PDF



Resonance Ladders in FUDGE



U238 capture 0.0K



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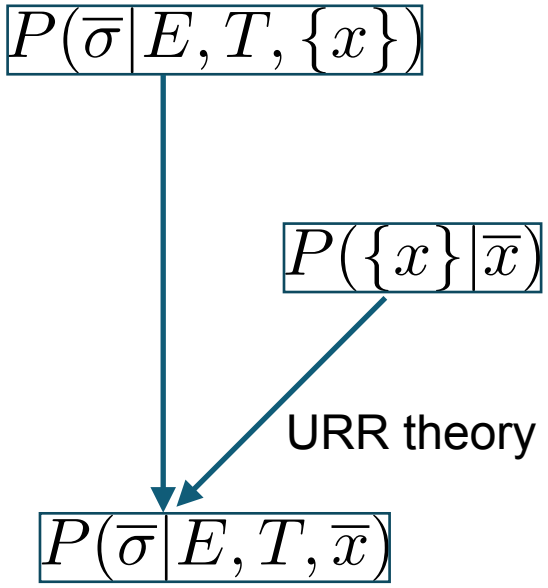
Including target temperature effects

Standard method

$$P_{\mathrm{STND}}(\widetilde{\sigma}|E,T) = \delta\left(\widetilde{\sigma} - \int_{[\mathrm{V_t},\mathrm{V_r}>0]} d\boldsymbol{V}_t\, P(\boldsymbol{V}_t|T)\frac{\mathrm{V_r}}{\mathrm{V}}\sigma(E_\mathrm{r})\right)$$

Including URR parameter variations

$$P_{\mathrm{STND}}(\tilde{\sigma}|E,T,\overline{x}) = \int dx P(x|\overline{x}) P_{\mathrm{STND}}(\tilde{\sigma}|E,T)$$



Standard

1. Sample cross section
2. **Doppler broadening**
3. **Accumulate PDF**

We propose an alternative method

Standard method

$$P_{\mathrm{STND}}(\widetilde{\sigma}|E,T) = \delta\left(\widetilde{\sigma} - \int_{[\mathrm{V_t},\mathrm{V_r}>0]} d\boldsymbol{V}_t\, P(\boldsymbol{V}_t|T)\frac{\mathrm{V_r}}{\mathrm{V}}\sigma(E_\mathrm{r})\right)$$

Alternate method

Zero-temperature PDF

$$P_{\mathrm{ALT}}(\widetilde{\sigma}|E,T) = \int_{[\mathrm{V_t},\mathrm{V_r}>0]} d\boldsymbol{V}_t\, P(\boldsymbol{V}_t|T)\,\delta\left(\widetilde{\sigma} - \frac{\mathrm{V_r}}{\mathrm{V}}\,\sigma(E_r)\right)$$

Standard
1. Sample cross section
2. **Doppler broadening**
3. **Accumulate PDF**

Alternate
1. Sample cross section
2. **Accumulate PDF**
3. **Doppler broadening**

How are these PDF's connected?

An "history" in a reactor simulation represents many "real-world histories" (N >> 10^{10})

Each "real-world history" is assumed to be statistically independent so the central limit theorem applies

$$P_{\mathrm{ALT}}(\widetilde{\sigma}|E,T) = \int_{[\mathrm{V_t},\mathrm{V_r}>0]} d\boldsymbol{V}_t\, P(\boldsymbol{V}_t|T)\, \delta\left(\widetilde{\sigma} - \frac{\mathrm{V_r}}{\mathrm{V}}\,\sigma(E_r)\right)$$

$$\mathrm{stddev} \sim 1/\sqrt{N}$$

$$P_{\mathrm{STND}}(\widetilde{\sigma}|E,T) = \delta\left(\widetilde{\sigma} - \int_{[\mathrm{V_t},\mathrm{V_r}>0]} d\boldsymbol{V}_t\, P(\boldsymbol{V}_t|T)\frac{\mathrm{V_r}}{\mathrm{V}}\sigma(E_\mathrm{r})\right)$$

Our alternate approach is essentially an event-by-event PDF

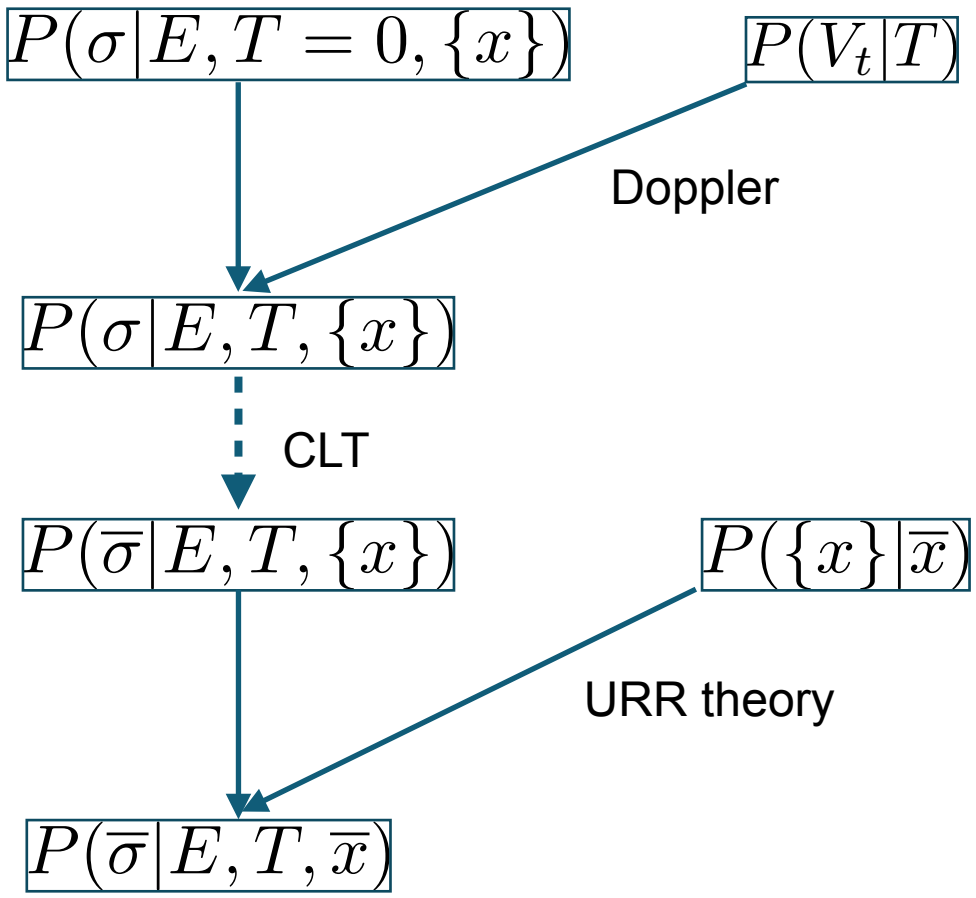
What this means for the standard approach

We’ve rephrased URR PT construction as composition of probabilities:

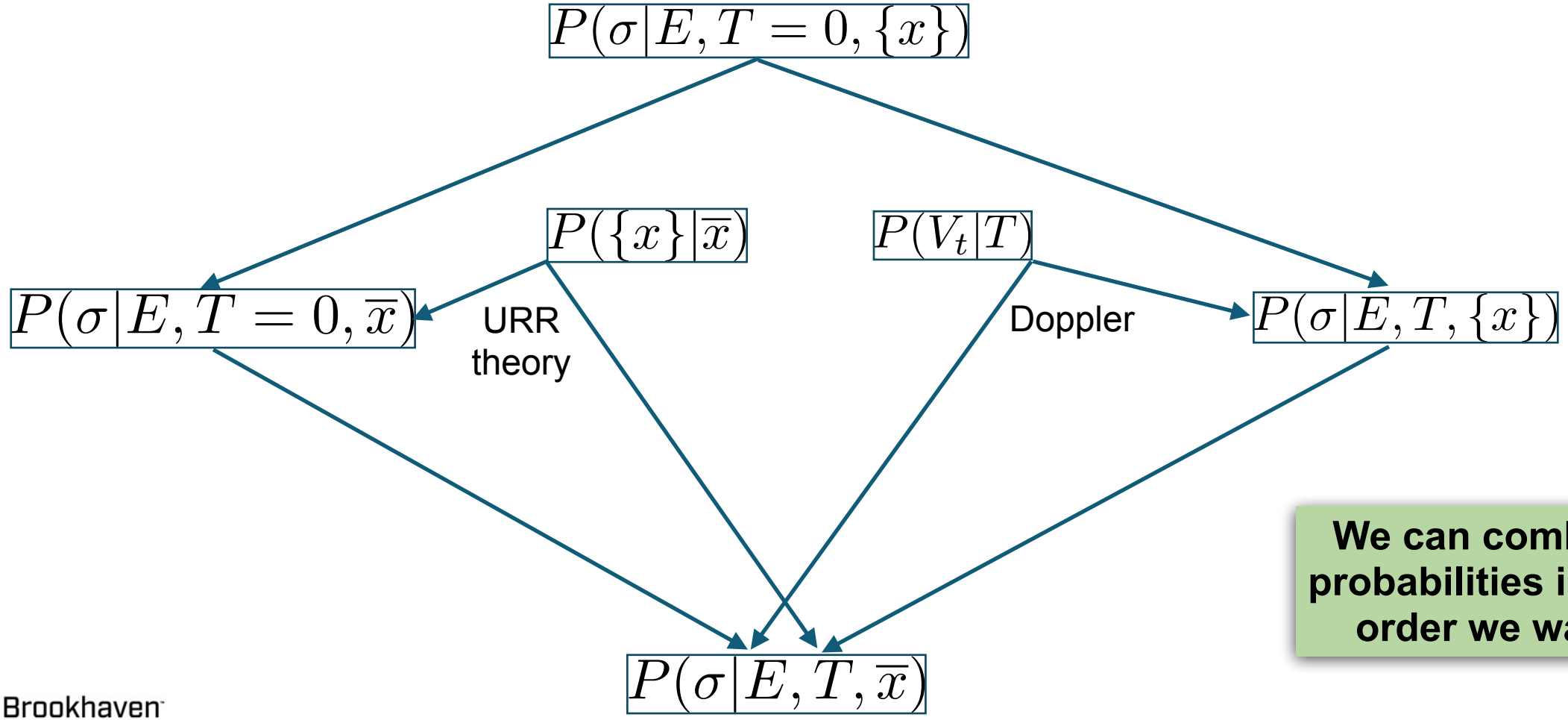
- target temp PDF
- URR parameters

Central Limit Theorem connects alternate(e-by-e) and standard URR PDFs

We can combine other sources of information, namely experiment!

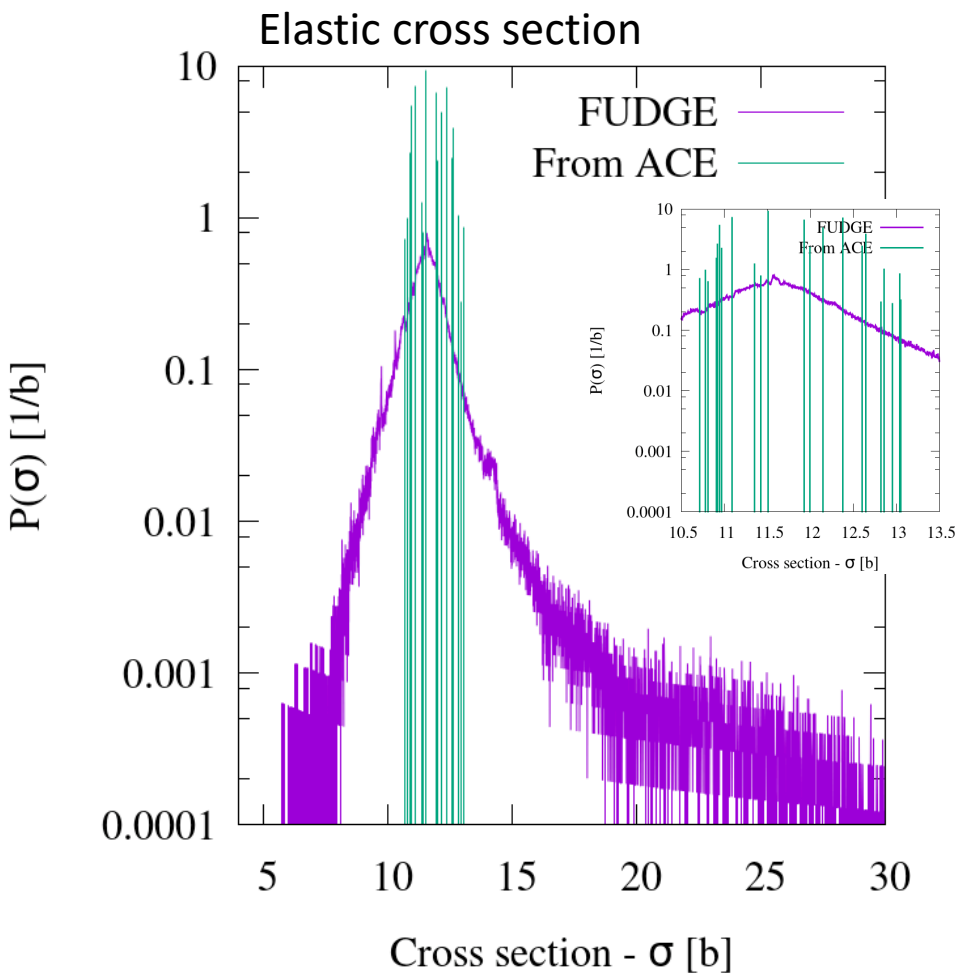


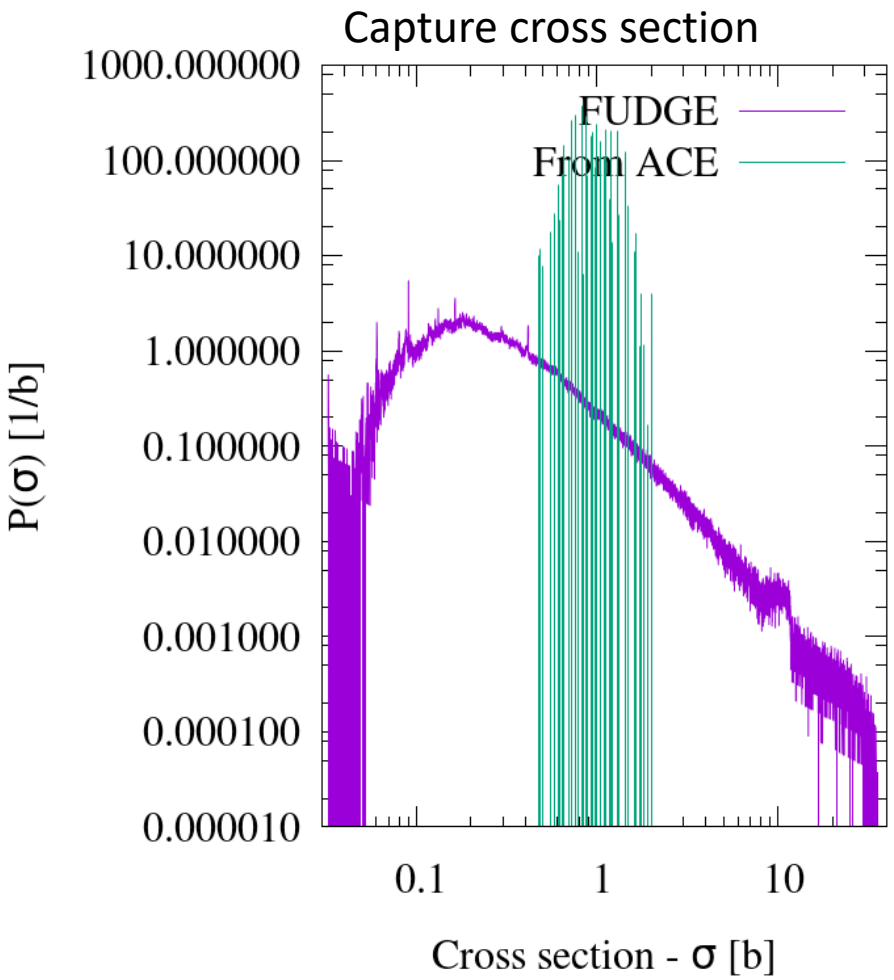
What this means for the alternate (event-by-event) approach



We can combine probabilities in any order we want

FUDGE pdf vs ACE probability tables





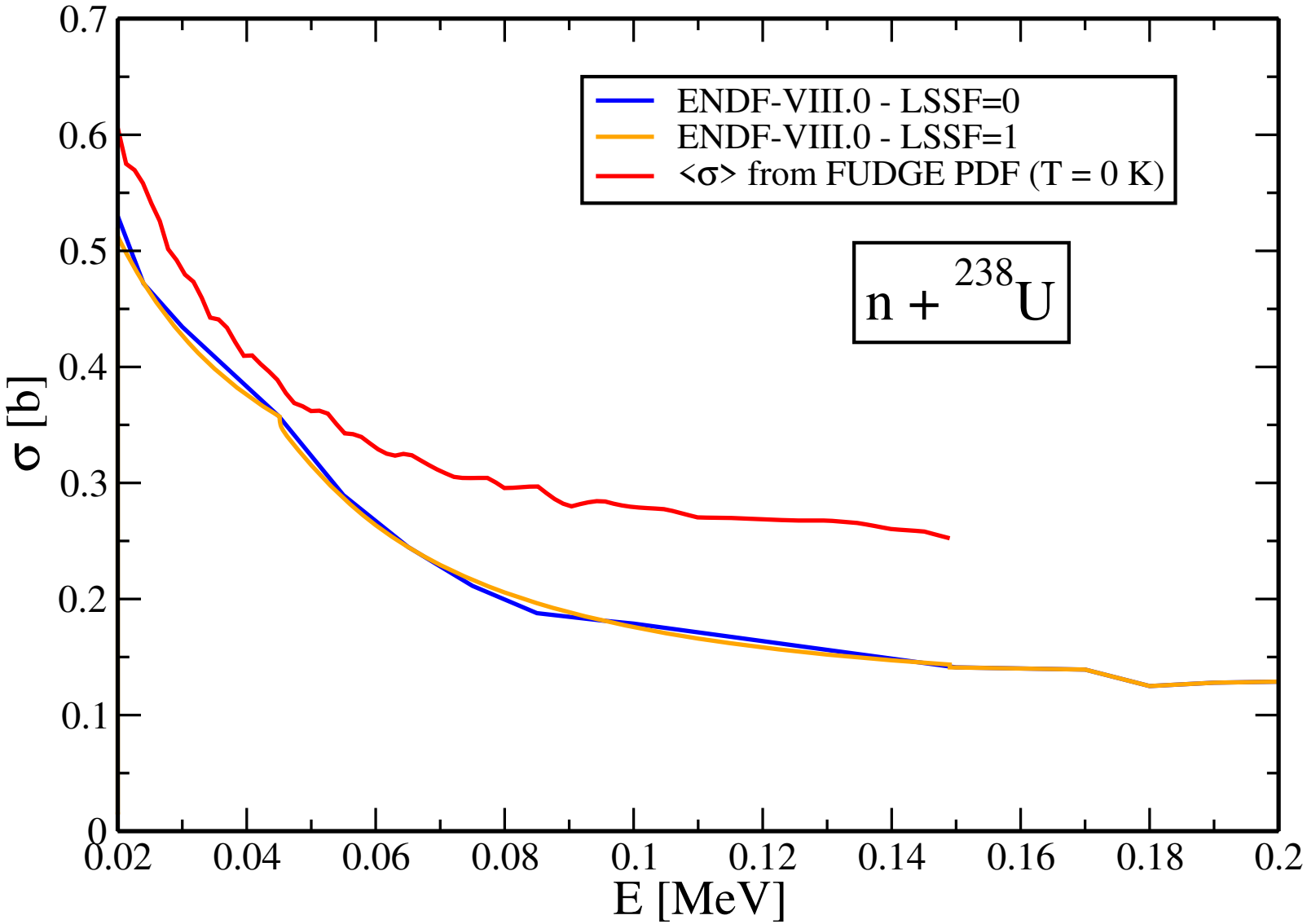
Without CLT, alternate (e-by-e) PDF is very broad and capture peak in wrong place (mean value still same)

Courtesy of Caleb Mattoon

Average cross section

- The e-by-e PDF leads to an average cross section that is in disagreement with the one extracted from ENDF

$$\langle \sigma \rangle = \int d\sigma \, \sigma \, P(\sigma)$$



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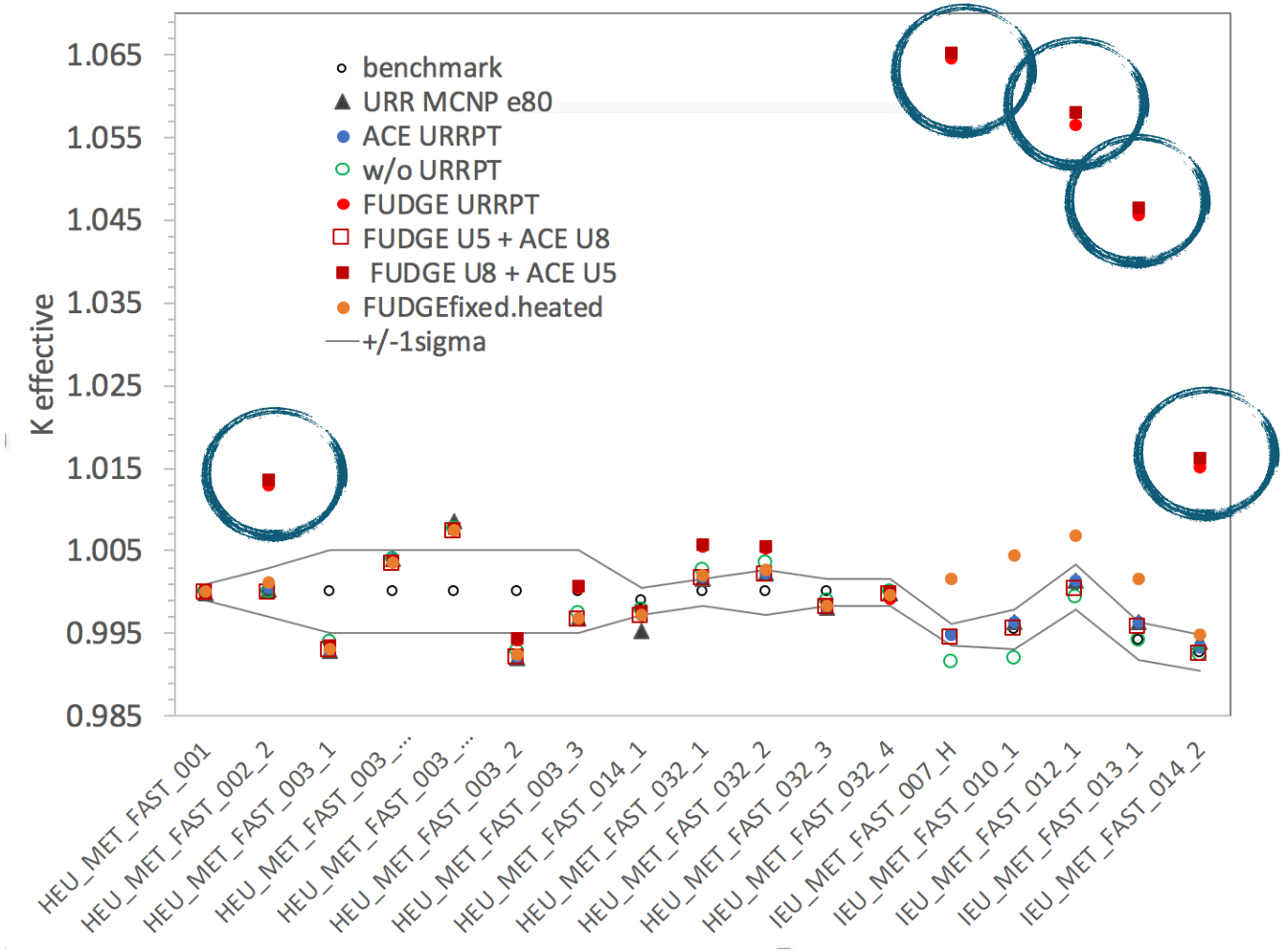
Testing probability tables in V&V suite

Poor initial results for ZPRs and BigTen now much improved

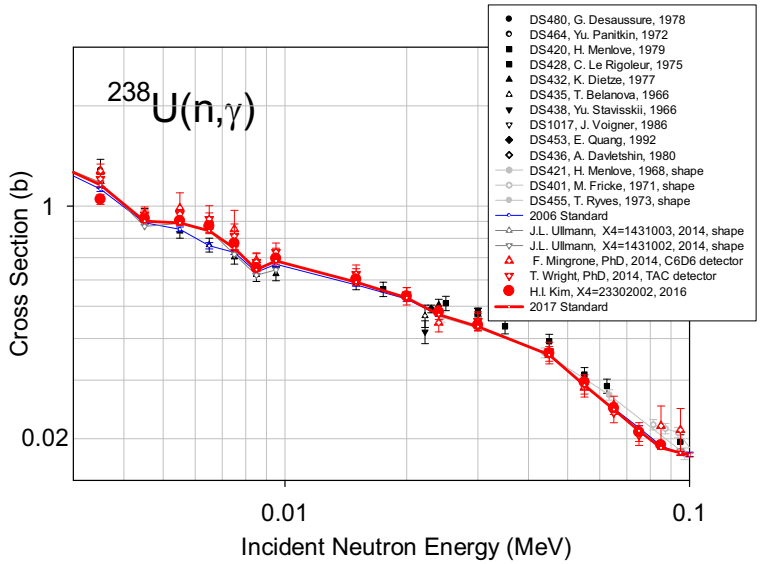


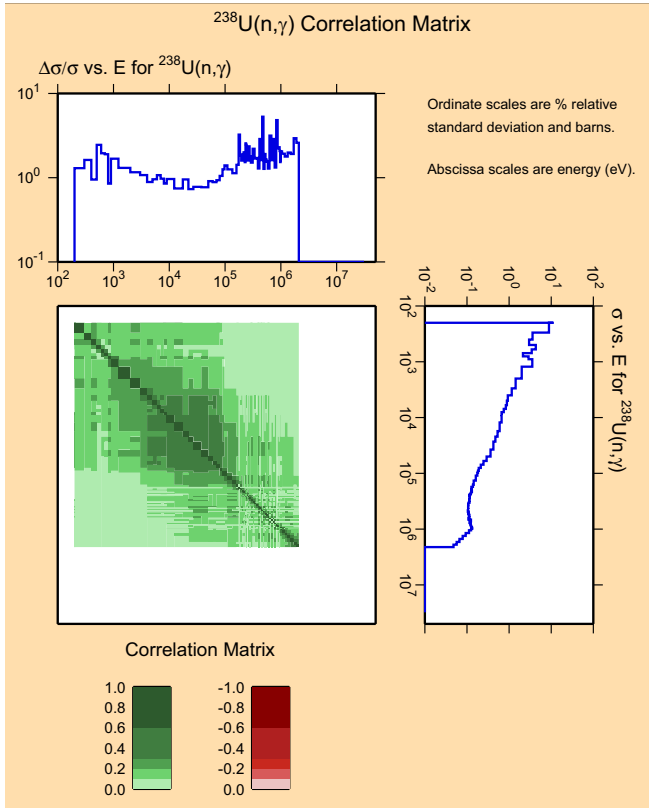
Because alternate (e-by-e) PDF is very broad & peaked in wrong place, it performs poorly in benchmarks

Combining theory and experiment

We can combine theory and experiment at **zero temperature**

$$P_{\mathrm{th-exp}}(\widetilde{\sigma}|E) = P_{\mathrm{th}}(\widetilde{\sigma}|E)\, P_{\mathrm{exp}}(\widetilde{\sigma}|E)$$





Evaluation of the neutron data standards, Nuclear Data Sheets 148 (2018) 143-188

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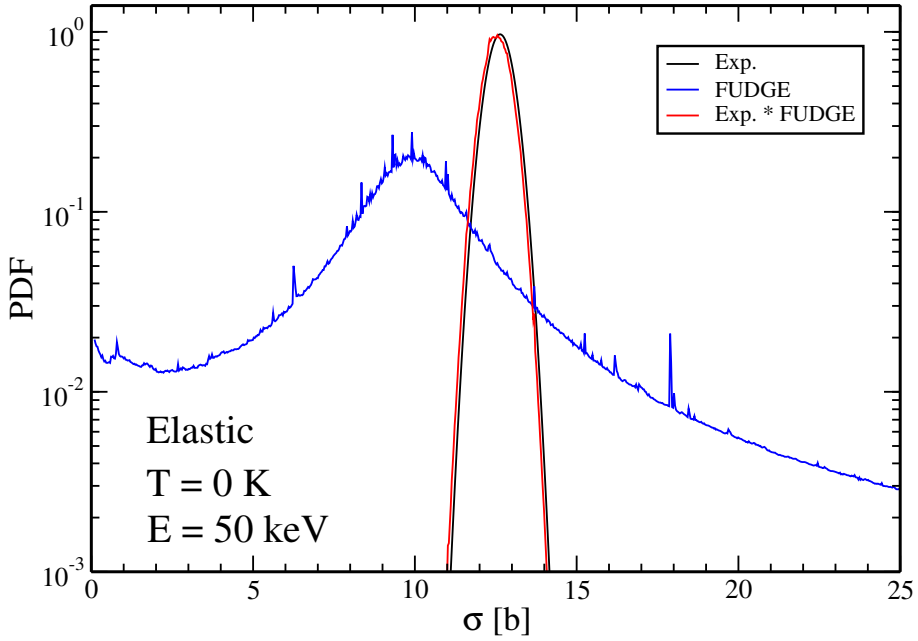
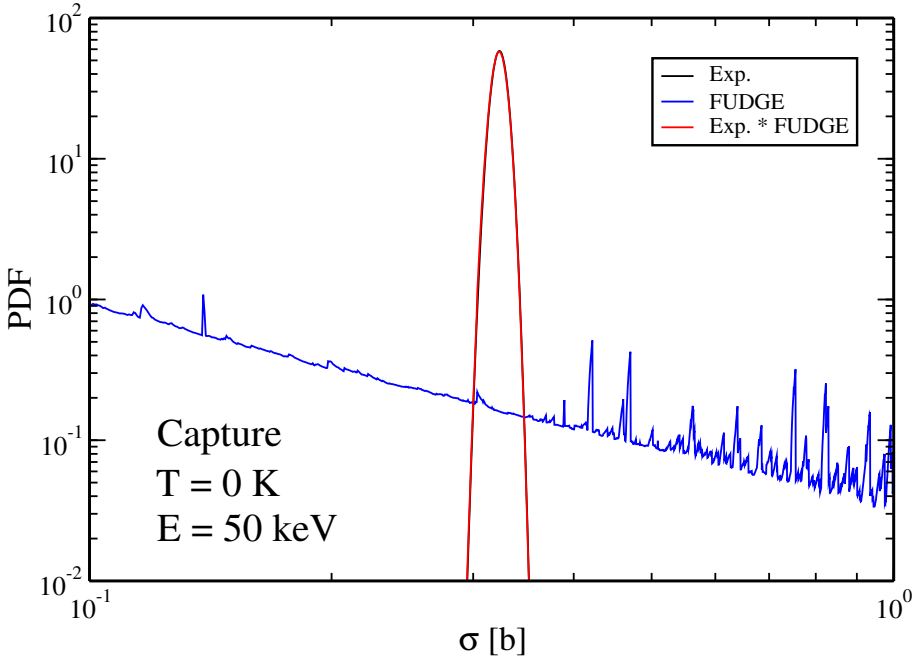
PDF at 0 K for n- ^{238}U

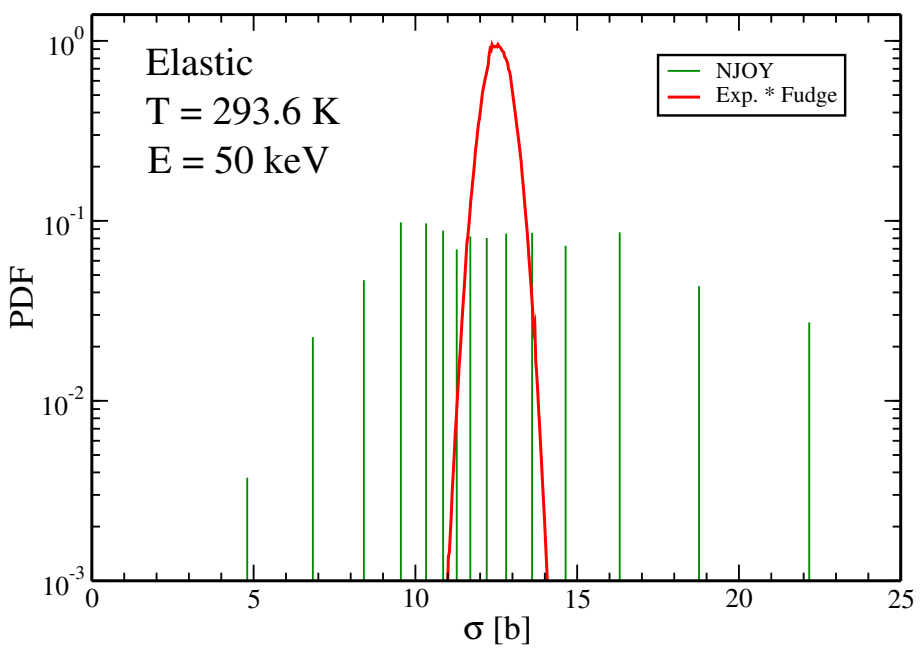
The experimental PDF is a strong constraint for the theoretical one

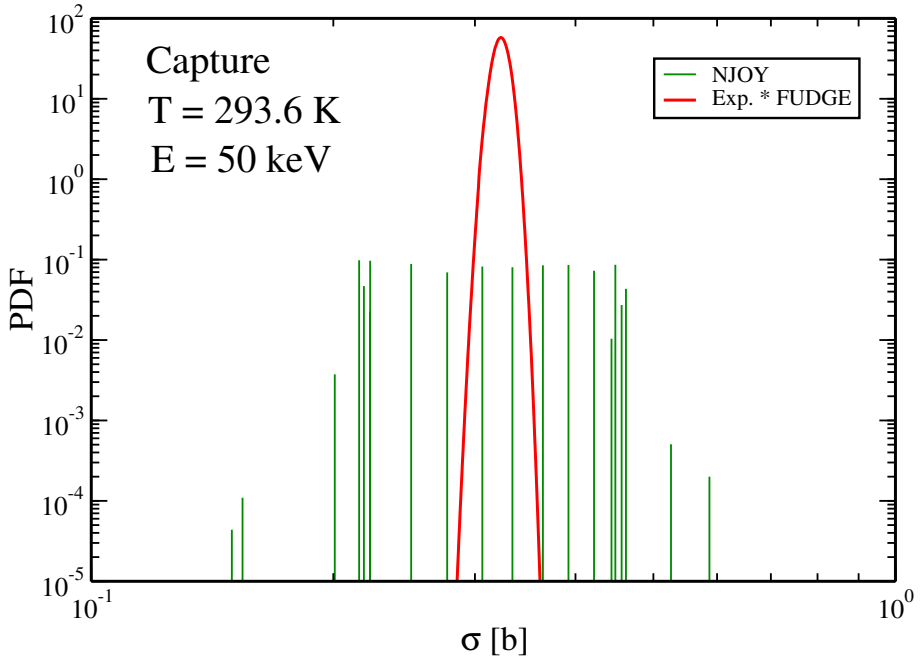
The combined PDF (normalized) is very similar to the experimental one





Heating the PDF for n- ^{238}U





The variance problem seems to be solved!
(we need to run some benchmarks!)

We can combine experiment with either PDF variant!

Summary & outlook

A Bayesian approach is more advisable for the PDF calculation in the URR

- Different probabilities are properly combined together
- Including experiment is straightforward
- Enables event-by-event treatment in URR
- Traditional UQ method and traditional self-shielding method should be interchangeable

Future work will be devoted to

- Speed up numerical calculations of PDFs at higher temperatures
- Fit the zero-temperature PDFs with a “universal” function

What if…

We didn’t need to compute resonance ladders?

How can we fit the PDFs?

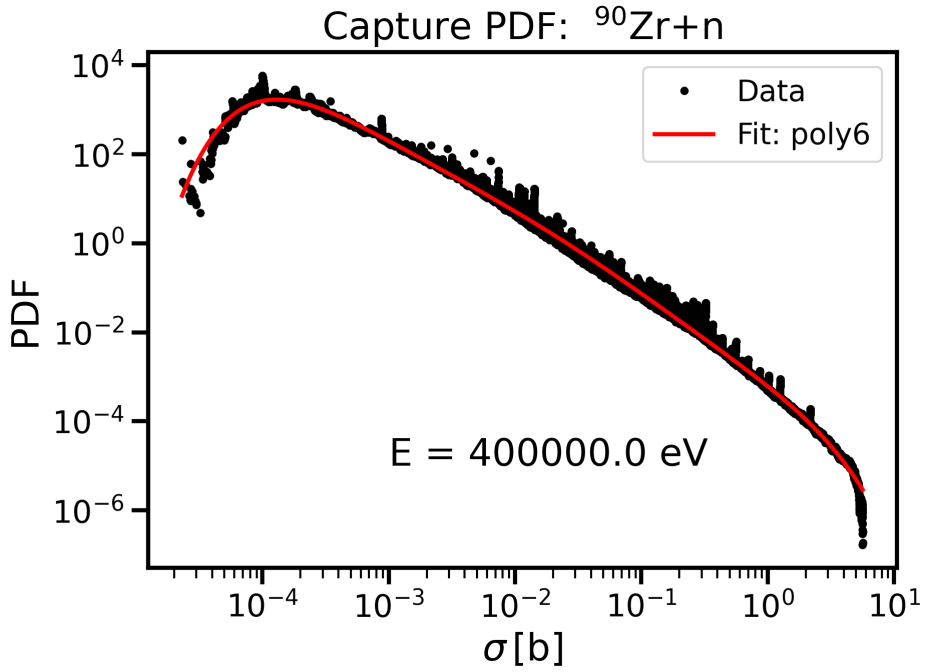
We are focusing on neutron-induced reactions

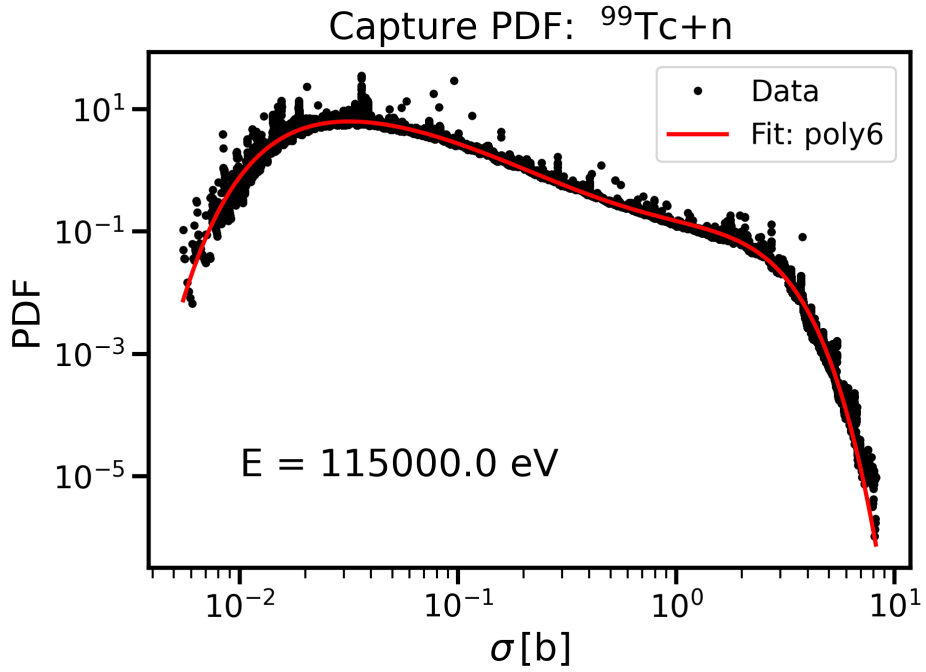
- Many target nuclei
- Different reaction channels (elastic, capture, …)

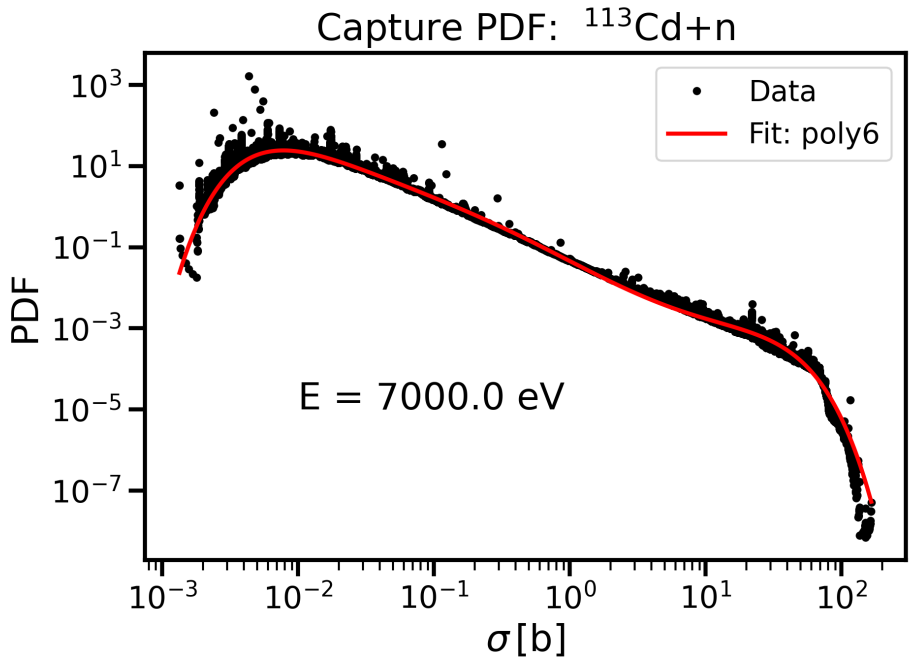
We are looking for a “universal” PDF for each reaction channel

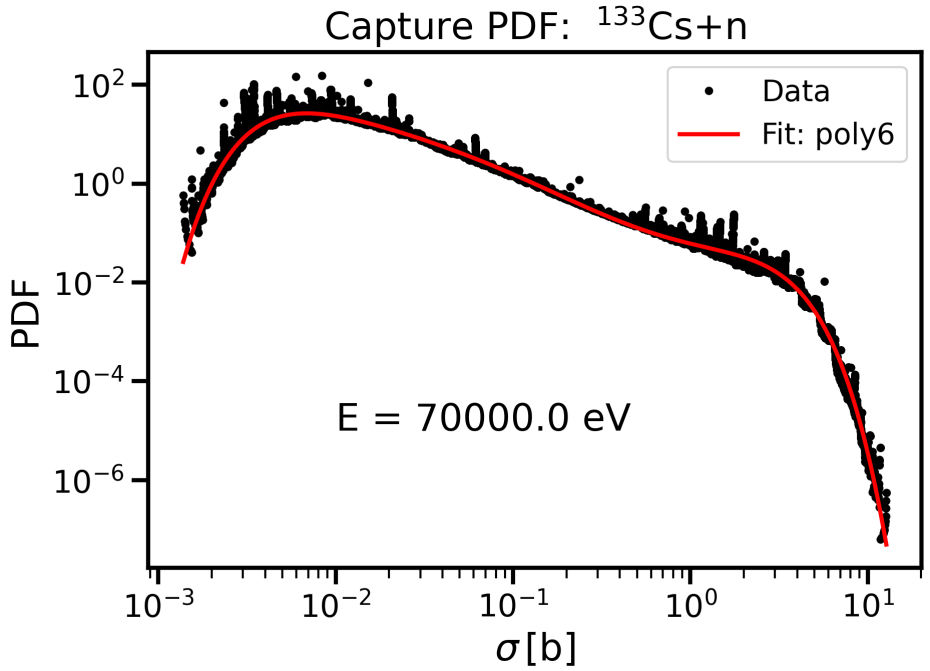
We used standard fitting procedures and also symbolic regression techniques to find a proper function

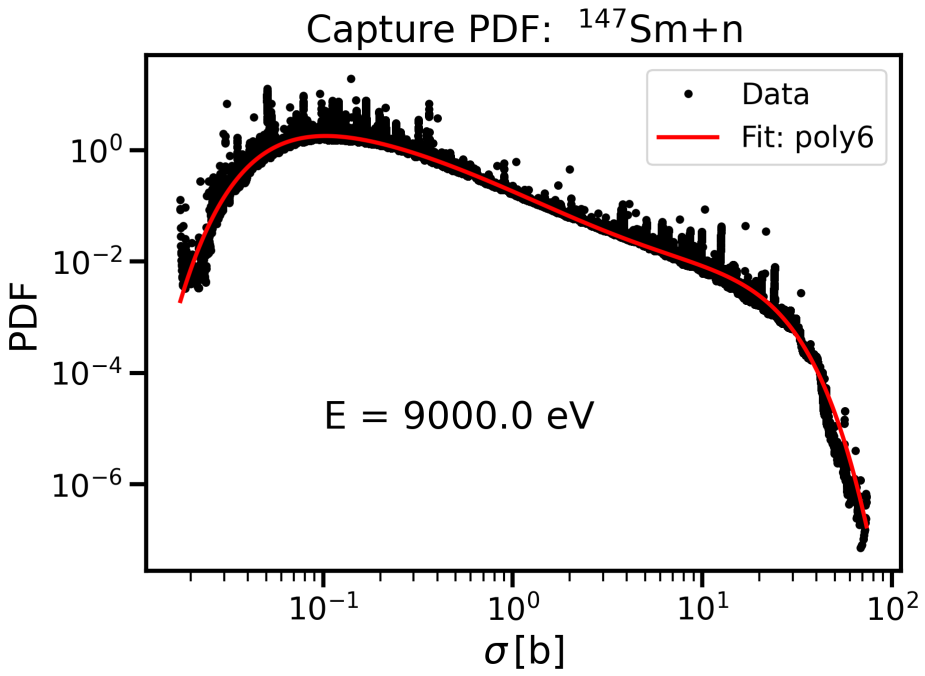
$$P(\sigma, E) = \exp\left\{\sum_{n=0}^{6} p_n(E)\,(\ln\sigma)^n\right\}$$

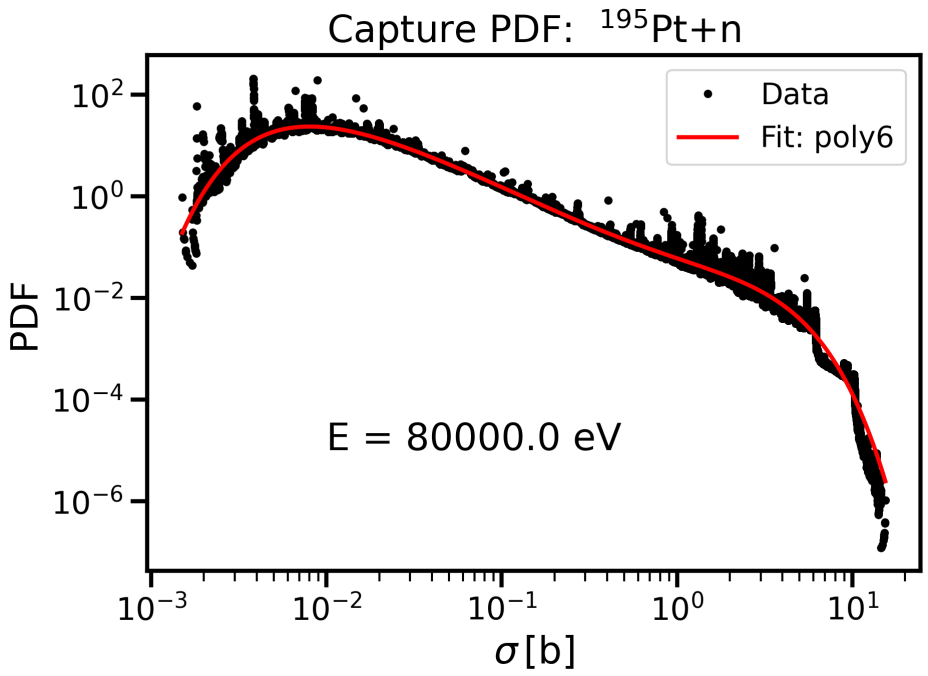

Capture PDF: ^{90}Zr+n
Data
Fit: poly6
E = 400000.0 eV
PDF
σ[b]

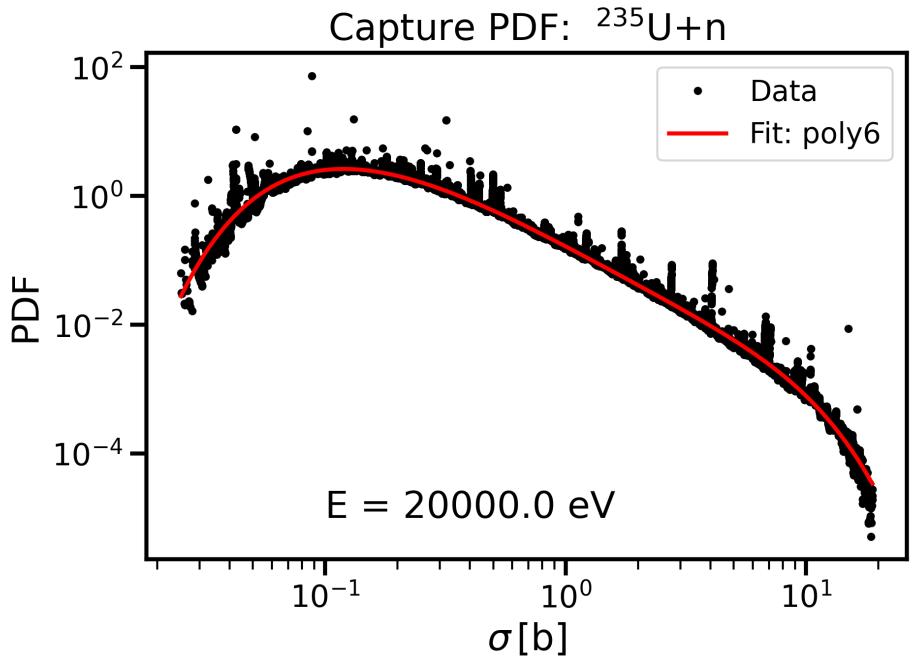

Capture PDF: ^{99}Tc+n
Data
Fit: poly6
E = 115000.0 eV
PDF
σ[b]

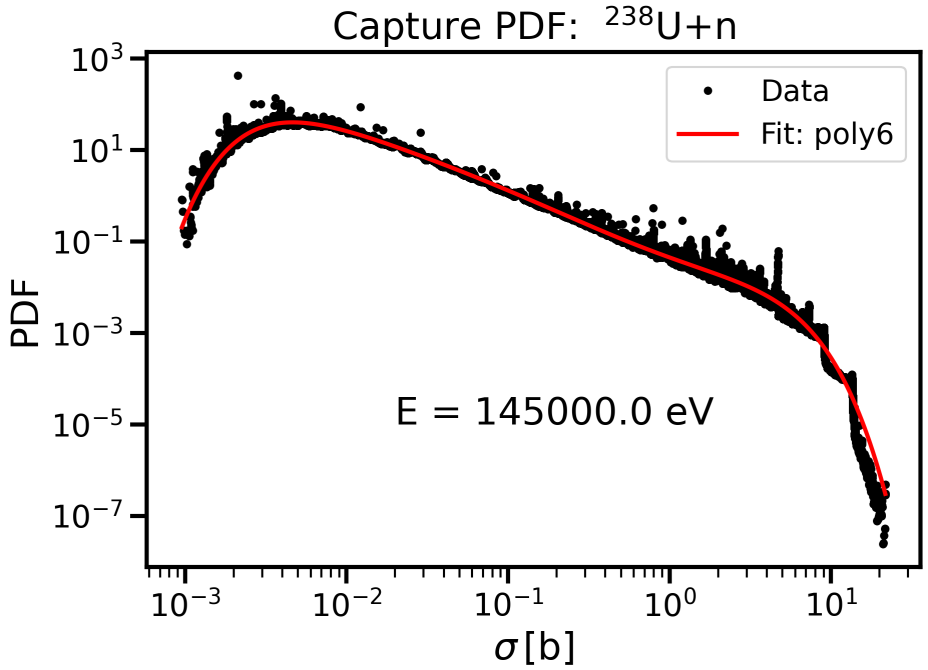

Capture PDF: ^{113}Cd+n
Data
Fit: poly6
E = 7000.0 eV
PDF
σ[b]


Capture PDF: ^{133}Cs+n
Data
Fit: poly6
E = 70000.0 eV
PDF
σ[b]


Capture PDF: ^{147}Sm+n
Data
Fit: poly6
E = 9000.0 eV
PDF
σ[b]


Capture PDF: ^{195}Pt+n
Data
Fit: poly6
E = 80000.0 eV
PDF
σ[b]


Capture PDF: ^{235}U+n
Data
Fit: poly6
E = 20000.0 eV
PDF
σ[b]


Capture PDF: ^{238}U+n
Data
Fit: poly6
E = 145000.0 eV
PDF
σ[b]

Next step

The idea seems to work, but for a full parametrization we need to fit the coefficients $p_n(E)$ as functions of energy

… or store them in a database!!!