Alternate approach for Calculating URR PDFs

Matteo Vorabbi[1], Dave Brown[1],

Caleb Mattoon[2], Godfree Gert[2], Bret Beck[2]

[1]BNL, [2]LLNL

NDAG, Dec 3 2020

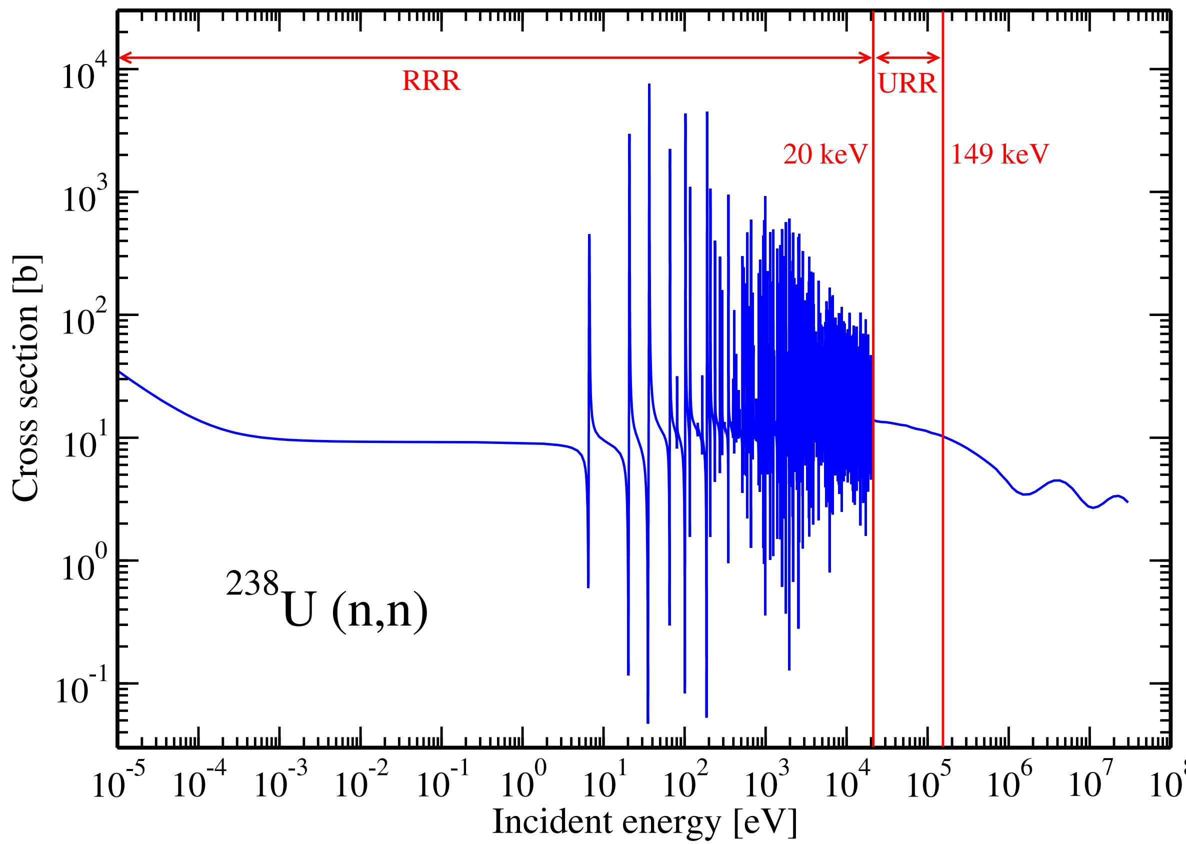
BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

BROOKHAVEN SCIENCE ASSOCIATES

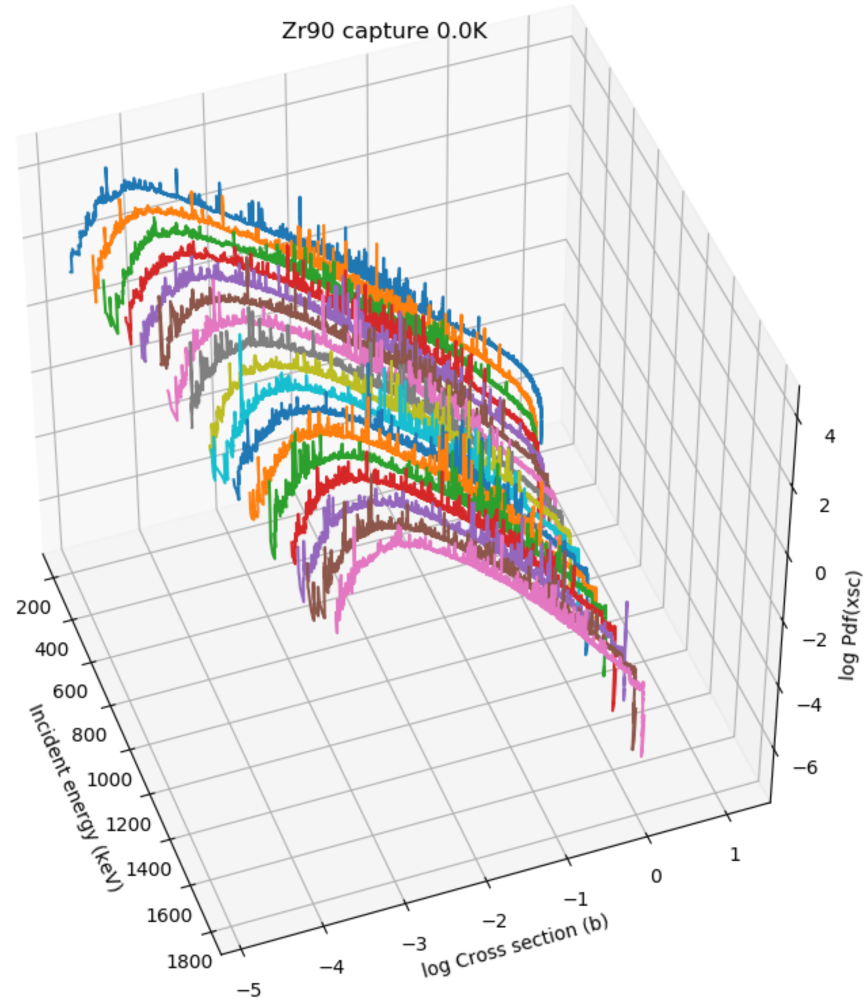
Unresolved resonance region

- 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: $\{\mathbf{x}\}$
- We can only determine averages of parameters: $\overline{\mathbf{x}}$
- Enough to determine the cross section PDF



Generation of the PDF

- Resonance ladders technique
  - Monte Carlo generates resonance
  - Reconstruct cross sections
  - Compute the one-realization PDF by numerically evaluating the delta function integral

$$P(\{\sigma_c\}|\{\overline{\Gamma}_c\},\overline{D},E) = \int \prod_i dE_i \prod_c d\Gamma_{c,i}\, P(\{E_i,\{\Gamma_{c,i}\}\}|\overline{D},\{\overline{\Gamma}_c\},E) \times \delta\big(\sigma_c - \sigma_c(\{E_i,\{\Gamma_{c,i}\}\})\big)$$

  - Accumulate the PDF
  - Repeat steps until converged
- The structure in the plot can be seen as a sampling error

Pre-processing codes

- PDFs are computed with pre-processing codes such as **FUDGE, NJOY**…
- Multi-purpose codes used to convert tabulated data into an interpolable form
- Common feature: calculation of the **Doppler-broadened** cross sections

→ Required to solve the linearized Boltzmann equation in the laboratory system

Doppler broadening

- In neutron transport equation we define an effective temperature dependent cross section

$$\mathrm{V}\sigma(\mathrm{V},T,\mathbf{x}) = \int d\{\mathbf{x}\}\, P(\{\mathbf{x}\}|\mathbf{x}) \int_{[\mathrm{V}_\mathrm{t},\mathrm{V}_r>0]} \left[\mathrm{V}_r\sigma(\mathrm{V}_r,0,\{\mathbf{x}\})\right] P(\overline{V}_\mathrm{t})\, d\overline{V}_\mathrm{t}$$

- Integration over the resonance parameters

$$\mathrm{V}\sigma(\mathrm{V},T,\mathbf{x}) = \int_{[\mathrm{V}_\mathrm{t},\mathrm{V}_r>0]} \left[\mathrm{V}_r\sigma(\mathrm{V}_r,0,\mathbf{x})\right] P(\overline{V}_\mathrm{t})\, d\overline{V}_\mathrm{t}$$

- In the limit $T \to 0$ we have $\sigma(\mathrm{V},T \to 0,\mathbf{x}) \to \sigma(\mathrm{V},0,\mathbf{x})$

Doppler broadening

- In neutron transport equation we define an effective temperature dependent cross section

$$\mathrm{V}\sigma(\mathrm{V}, T, \mathbf{x}) = \int d\{\mathbf{x}\} P(\{\mathbf{x}\}|\mathbf{x}) \int_{[\mathrm{V}_\mathrm{t}, \mathrm{V}_r > 0]} [\mathrm{V}_r \sigma(\mathrm{V}_r, 0, \{\mathbf{x}\})] P(\overline{V}_\mathrm{t})\, d\overline{V}_\mathrm{t}$$

Projectile Speed

Resonance parameter PDF

Cross section at zero temperature

Target-nucleus velocity distribution

- Integration over the resonance parameters

$$\mathrm{V}\sigma(\mathrm{V}, T, \mathbf{x}) = \int_{[\mathrm{V}_\mathrm{t}, \mathrm{V}_r > 0]} [\mathrm{V}_r \sigma(\mathrm{V}_r, 0, \mathbf{x})]\, P(\overline{V}_\mathrm{t})\, d\overline{V}_\mathrm{t}$$

- In the limit $T \to 0$ we have $\sigma(\mathrm{V}, T \to 0, \mathbf{x}) \to \sigma(\mathrm{V}, 0, \mathbf{x})$

Definition of the PDF

- In analogy with the PDF for an ideal case (delta function) we define the following PDF

$$P(\widetilde{\sigma}|\mathrm{V},T,\sigma,\mathbf{x}) \equiv \int d\{\mathbf{x}\}\, P(\{\mathbf{x}\}|\mathbf{x}) \int_{[\mathrm{V}_\mathrm{t},\mathrm{V}_r>0]} d\overline{V}_\mathrm{t}\, P(\overline{V}_\mathrm{t})\; \delta\left(\widetilde{\sigma} - \frac{\mathrm{V}_r}{\mathrm{V}}\,\sigma(\mathrm{V}_r,0,\{\mathbf{x}\})\right)$$

- Properties
  - The expectation value of the variable $\widetilde{\sigma}$ is

$$\mathrm{E}(\widetilde{\sigma}) = \int_0^\infty d\widetilde{\sigma}\; \widetilde{\sigma}\; P(\widetilde{\sigma}|\mathrm{V},T,\sigma,\mathbf{x}) = \sigma(\mathrm{V},T,\mathbf{x})$$

  - The $T \to 0$ has the right behavior

$$\lim_{T\to 0} P(\widetilde{\sigma}|\mathrm{V},T,\sigma,\mathbf{x}) = \int d\{\mathbf{x}\}\, P(\{\mathbf{x}\}|\mathbf{x})\; \delta\big(\widetilde{\sigma} - \sigma(\mathrm{V},0,\{\mathbf{x}\})\big)$$

Combining probabilities (Bayesian approach)

- We can exploit the properties of our PDF to define the following PDF at zero temperature

$$P(\widetilde{\sigma}|\mathrm{V},0,\sigma,\mathbf{x}) \equiv \int d\{\mathbf{x}\}\, P(\{\mathbf{x}\}|\mathbf{x})\; \delta\big(\widetilde{\sigma} - \sigma(\mathrm{V},0,\{\mathbf{x}\})\big)$$

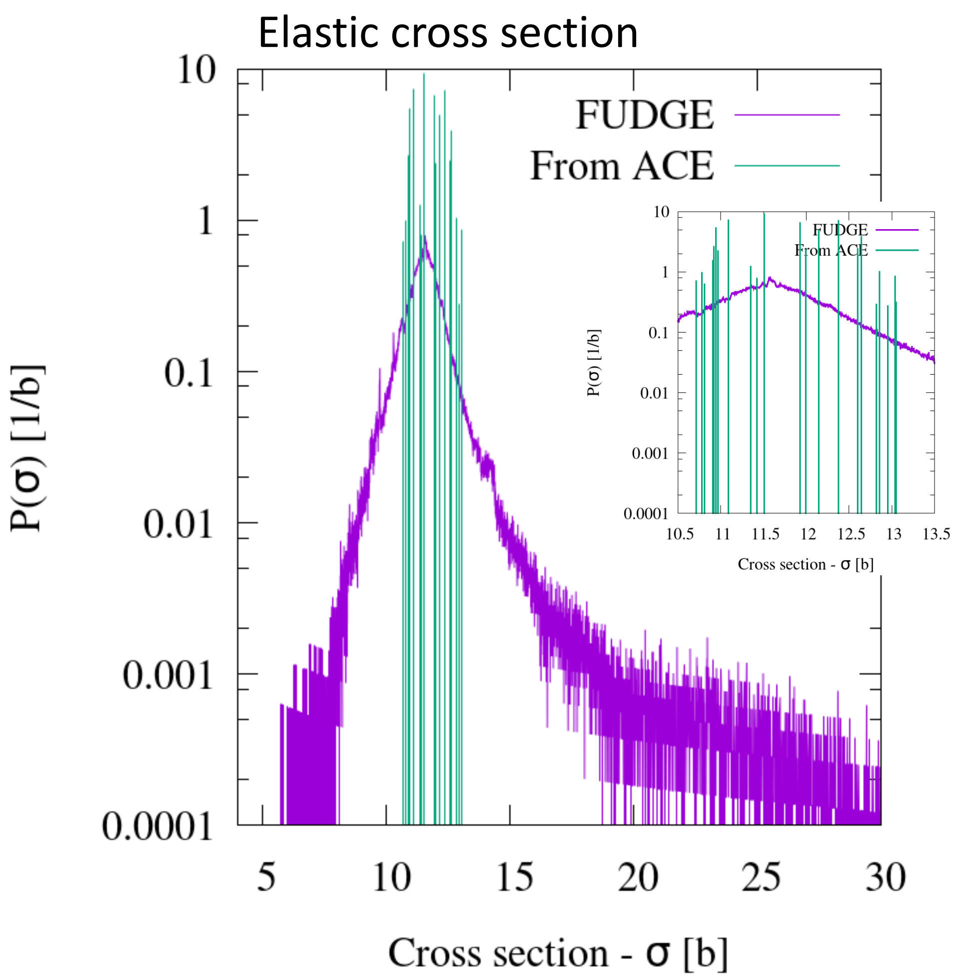
- With this definition we can express our PDF as

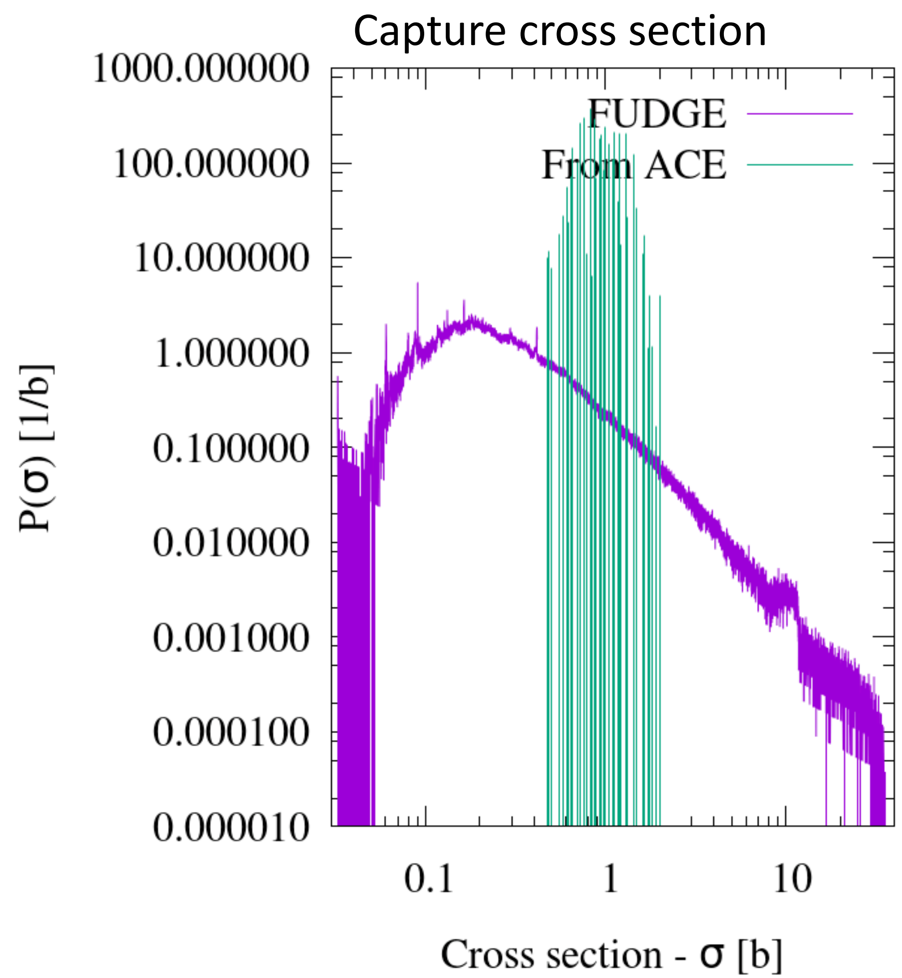
$$P(\widetilde{\sigma}|\mathrm{V},T,\sigma,\mathbf{x}) = \int_{[\mathrm{V}_\mathrm{t},\mathrm{V}_r>0]} d\overline{V}_\mathrm{t}\, P(\overline{V}_\mathrm{t})\, \boxed{P(\widetilde{\sigma}|\mathrm{V}_r,0,\sigma,\mathbf{x})}$$

PDF computed with FUDGE

New computational scheme of the PDF

FUDGE pdf vs ACE probability tables





Understanding the variance problem

- Mean value

$$\mathrm{E}(\widetilde{\sigma}) = \int_0^\infty d\widetilde{\sigma}\;\widetilde{\sigma}\;P(\widetilde{\sigma}|\mathrm{V},T,\sigma,\mathbf{x}) = \sigma(\mathrm{V},T,\mathbf{x})$$

$$\sigma(\mathrm{V},T,\mathbf{x}) = \mathrm{E}_{\mathrm{NJOY}}(\widetilde{\sigma}) = \mathrm{E}_{\mathrm{FUDGE}}(\widetilde{\sigma})$$

- Variance

$$\mathrm{var}\left[\sigma(\mathrm{V},T,\mathbf{x})\right] = \mathrm{E}\left(\widetilde{\sigma}^2\right) - \mathrm{E}^2(\widetilde{\sigma})$$

- **The difference is in the second moment**

→ We show the difference with analytic models

Understanding the variance problem

- Working on analytic models to show the difference between FUDGE and NJOY (1/V and const. cross sections)

  → Analytic proof

- For analytical models (no dependence on $\{x\}$), **the NJOY PDF is always a delta function and the variance is always zero**

- A finite and positive variance is obtained from FUDGE

- Can this explain the variance difference?

Combining theory and experiment

- We can combine there and experiment

$$P_{\mathrm{th-exp}}(\widetilde{\sigma}|E,0,\sigma,\mathbf{x}) = P_{\mathrm{th}}(\widetilde{\sigma}|E,0,\sigma,\mathbf{x})\; P_{\mathrm{exp}}(\widetilde{\sigma}|E)$$

- The experimental PDF can be obtained from standards

$$P_{\mathrm{exp}}(\widetilde{\sigma}|E) = \mathcal{N}\left(\widetilde{\sigma}, \sigma(E), \big(\Delta\sigma(E)\big)^2\right)$$

- where

$$\sigma(E) = \sum_{i=1}^{k} \sigma_i\, B_i(E) \qquad \big(\Delta\sigma(E)\big)^2 = \sum_{i,j=1}^{k} B_i(E)\Sigma_{ij}B_j(E)$$

Summary & outlook

- A theoretical (Bayesian) approach is more advisable for the PDF calculation in the URR (combine probabilities, speed up numerical calculations…)

- The theoretical variance obtained so far is still too large: in benchmarking, the results obtained with NJOY are closer to the right values than those obtained with FUDGE

- Future efforts will be devoted to test our algorithm to shrink the variance