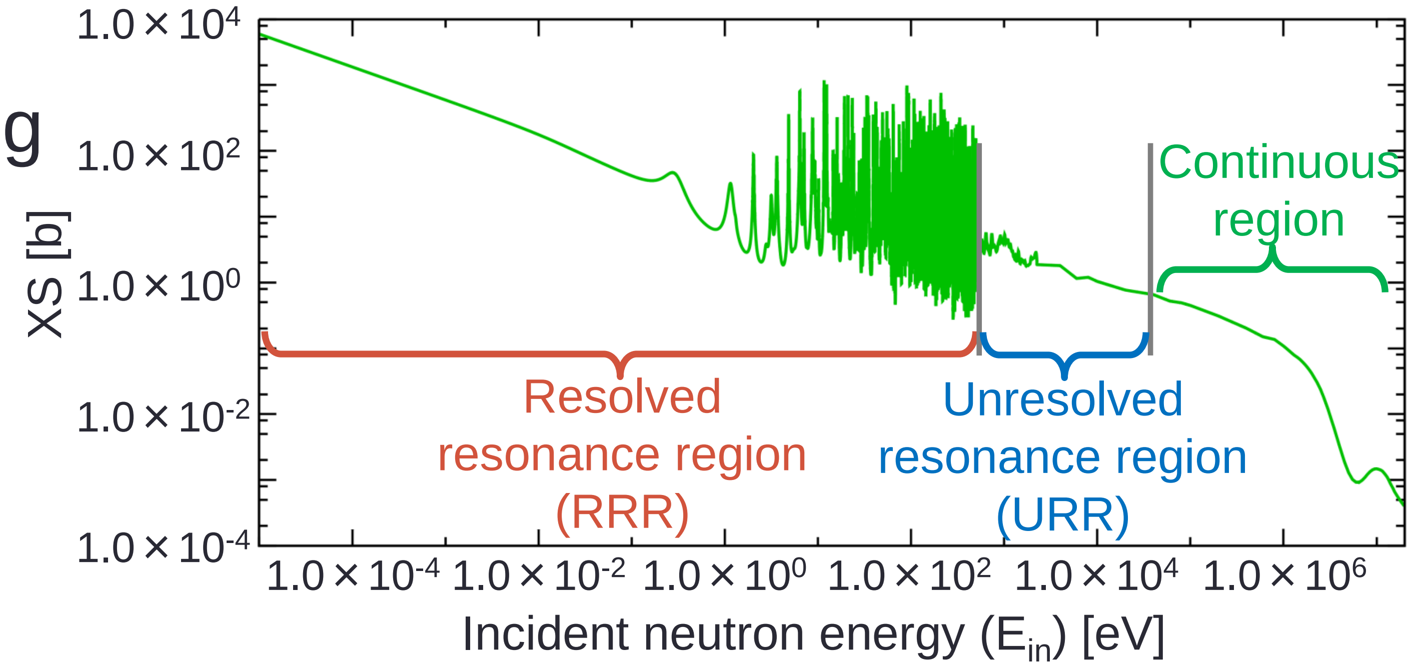
Statistical Uncertainty Quantification of Probability Tables for Unresolved Resonance Cross Sections

Japan Atomic Energy Agency Kenichi TADA
Nagoya University Tomohiro ENDO

Self-shielding effect in URR

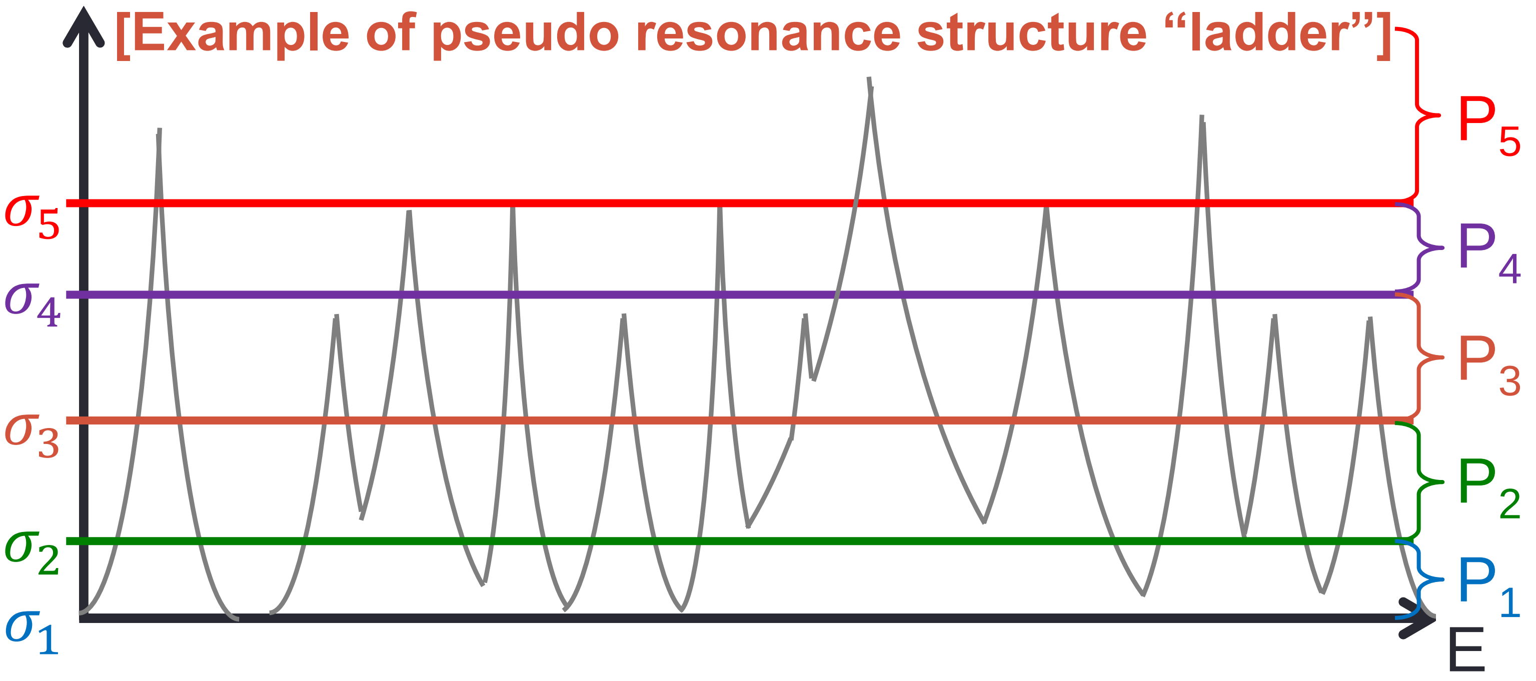
- Averaged resonance parameters are given in the unresolved resonance region (URR).
  - Nuclear data processing code cannot reconstruct resonance structure in URR.
  - Consideration of the self-shielding effect in URR is important for accurate neutronics calculations.
- Probability table method is used to treat the self-shielding effect in URR.

[Radiative capture XS of U-235 from JENDL-4.0 (0 K)]



Calculation of probability table

- Probability table is the probability distribution of cross section (σ_i, P_i) in given energy grid points.
- Probability table requires the generation of a lot of pseudo resonance structures called "ladder".
  - Calculation of probability table requires a long calculation time.
  - Reduction of the number of ladders is important to reduce the calculation time.



Importance of statistical uncertainty quantification

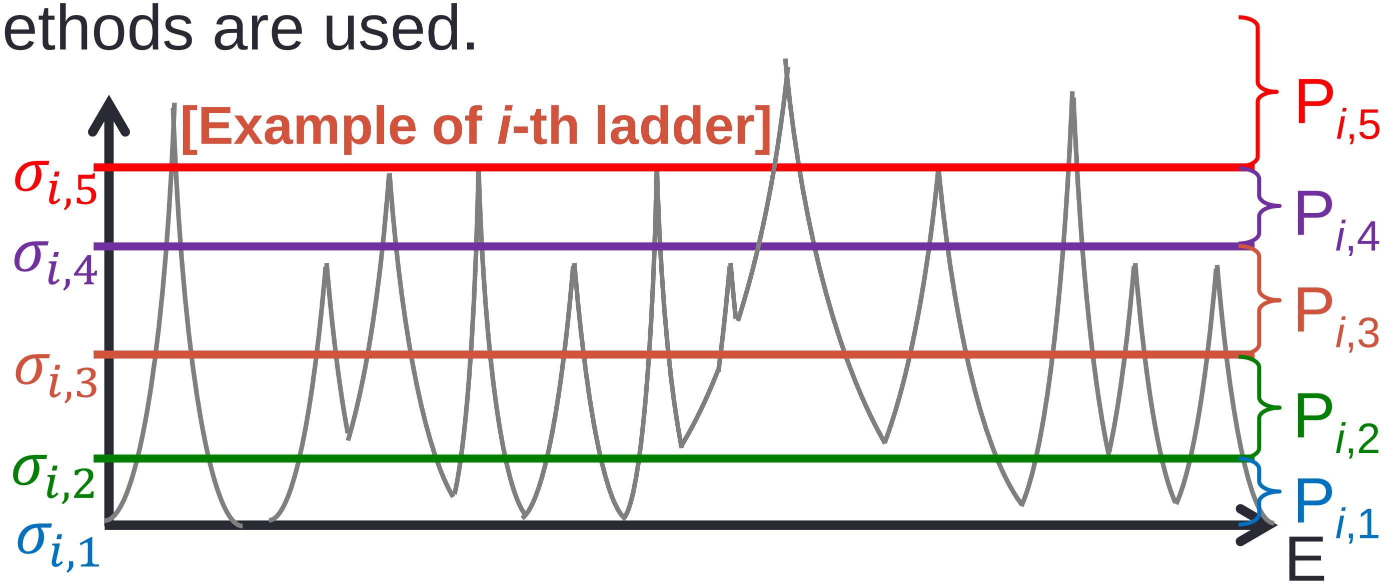
- Conventional nuclear data processing codes use number of ladders as an input parameter to generate probability table.
  - Users have to set large number of ladders since there is no information about the optimal number of ladders.
  - We investigated the optimal number of ladders.
    - Optimal number of ladders is different to each nuclide.
    - K. Tada, Proc. Physor2022 (https://doi.org/10.1051/epjconf/202124709002).
- Probability table is generated by Monte Carlo method.
  - Statistical uncertainty of probability table will be good information for estimation of convergence.
  - Optimization of number of ladders using statistical uncertainty will be available.

Statistical uncertainty quantification of probability table

- Target of statistical uncertainty of probability table.
  - Product of probability P and average cross section $\bar{\sigma}$.
  - Both probability and cross section are important for neutronics calculation.
- Calculation method of statistical uncertainty
  - Central limit theorem (CLT)
  - Bootstrap method
  - Jackknife method
    - Bootstrap and jackknife methods are available for non-normal distribution.
    - Calculation time of these methods are longer than that of CLT since these methods require the resampling process.
  - Statistical uncertainties using these methods are compared to reference results.

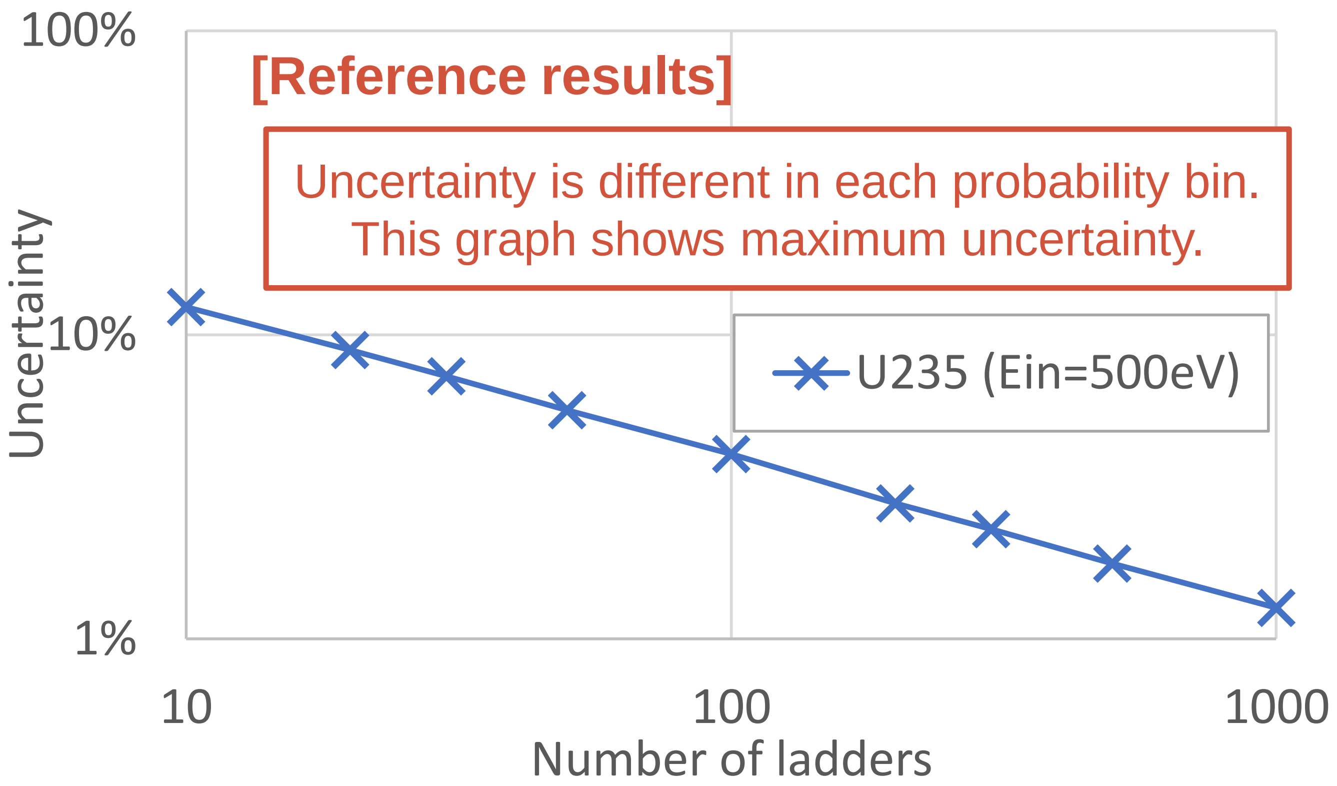
Calculation flow of statistical uncertainty quantification

- Calculation of probability $P_{i,j}$ and average cross section $\overline{\sigma_{tot}}_{i,j}$, $\overline{\sigma_{sc}}_{i,j}$, $\overline{\sigma_{rad}}_{i,j}$, and $\overline{\sigma_{fis}}_{i,j}$.
  - i: *i*-th ladder index, j: *j*-th probability bin
- Calculation of statistical uncertainty $u_{tot,j}$, $u_{sc,j}$, $u_{rad,j}$, and $u_{fis,j}$.
  - $P_{0,j}\overline{\sigma_{tot}}_{0,j}$, $P_{1,j}\overline{\sigma_{tot}}_{1,j}$, …, $P_{i-1,j}\overline{\sigma_{tot}}_{i-1,j}$, $P_{i,j}\overline{\sigma_{tot}}_{i,j}$ are used to calculate $u_{tot,j}$.
  - CLT, bootstrap, and jackknife methods are used.
- Generation of *i+1*-th ladder.



Comparison of statistical uncertainty: Conditions

- U-235 from JENDL-4.0 was used for comparison.
  - Consideration of probability table of U-235 has a large impact on neutronics calculation.
- Statistical uncertainties obtained by CLT, bootstrap, and jackknife methods were compared to reference results.
  - 1,000 probability table sets were generated with 1,000 different random seeds.
    - Statistical error of 1,000 probability table sets is used as reference results.



Comparison of statistical uncertainty: Results

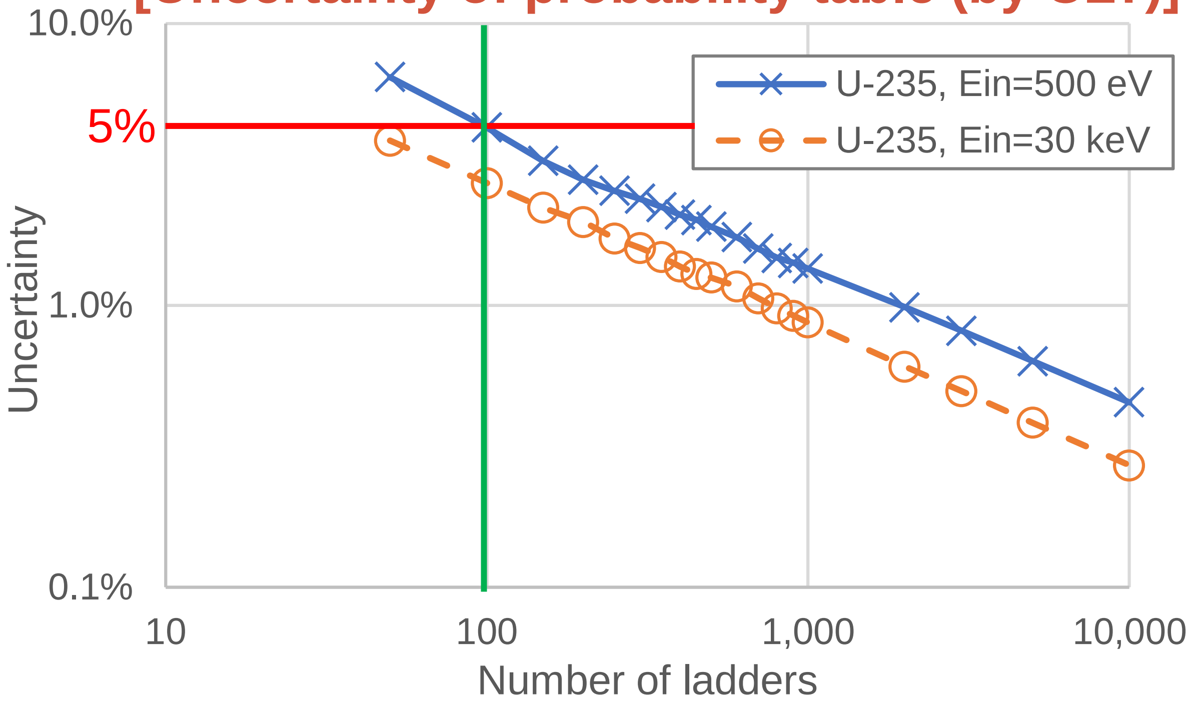
- Statistical uncertainties of each method show good agreement to reference results.
  - Calculation time of CLT is faster than that of other methods.
  - FRENDY uses CLT for statistical uncertainty quantification of probability table.

Ein	No. of Ladders	Statistical uncertainty			
		Ref.	CLT /Ref.	Bootstrap /Ref.	Jackknife /Ref.
Ein = 500 eV	50	5.65%	1.01	1.00	1.02
	100	4.05%	1.00	0.99	1.01
	300	2.30%	1.02	1.02	1.02
	500	1.77%	1.03	1.03	1.03
	1000	1.27%	1.02	1.01	1.02
Ein = 30 keV	50	5.45%	0.97	0.95	0.98
	100	3.73%	1.00	0.99	1.01
	300	2.05%	1.05	1.05	1.05
	500	1.68%	0.99	0.99	1.00
	1000	1.20%	0.99	0.99	0.99

Speeding up of probability table generation

- Statistical uncertainty is different with incident energy.
  - Optimum number of ladders is different with incident energy.
    - Lower incident energy has larger uncertainty.
    - Calculation time of the probability table becomes longer when incident energy becomes higher.
  - Number of ladders in each incident energy can be optimized if tolerance of statistical uncertainty is used as an input parameter.
- Default number of ladders in FRENDY is 100
  - Statistical uncertainty should be less than or equal to 5%.
    - Default tolerance in FRENDY is 5%.
  - Calculation time becomes less than half when the input parameter is changed from the number of ladders to the tolerance of statistical uncertainty.

[Uncertainty of probability table (by CLT)]



Conclusions

- Statistical uncertainty quantification of probability table was developed.
  - For optimization of number of ladders and speeding up of probability table generation.
- Product of probability P and average cross section $\bar{\sigma}$ was used as the target of statistical uncertainty of probability table.
  - Central limit theorem (CLT), bootstrap, and jackknife methods were adopted for statistical uncertainty quantification.
    - Statistical uncertainties of each method show good agreement to reference results.
    - CLT is the best method from the viewpoint of calculation time.
- Statistical uncertainty quantification of probability table is available in FRENDY Ver. 2.
  - FRENDY Ver. 2 can be downloaded from the JAEA website:
    - https://rpg.jaea.go.jp/main/en/program_frendy/index.html
  - Default tolerance of statistical uncertainty in FRENDY is 5%.
  - Calculation time becomes less than half when the input parameter is changed from the number of ladders to the tolerance of statistical error.

Background

- JAEA developed a nuclear data processing code FRENDY.
  - **FR**om **E**valuated **N**uclear **D**ata librar**Y** to any application
- FRENDY Version 2 was released from the JAEA website in Jan. 2022.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
  - 2-clause BSD open-source software.
  - FRENDY ver. 2 can generate cross section library for continuous-energy Monte Carlo and multi-group codes.
- Speeding up of nuclear data processing is an important issue.
  - Statistical uncertainty quantification of the probability table will contribute to reducing the processing time.