Overview of FRENDY Ver. 2

Japan Atomic Energy Agency (JAEA)
Kenichi TADA

https://rpg.jaea.go.jp/main/en/program_frendy/index.html

tada.kenichi@jaea.go.jp

Outline

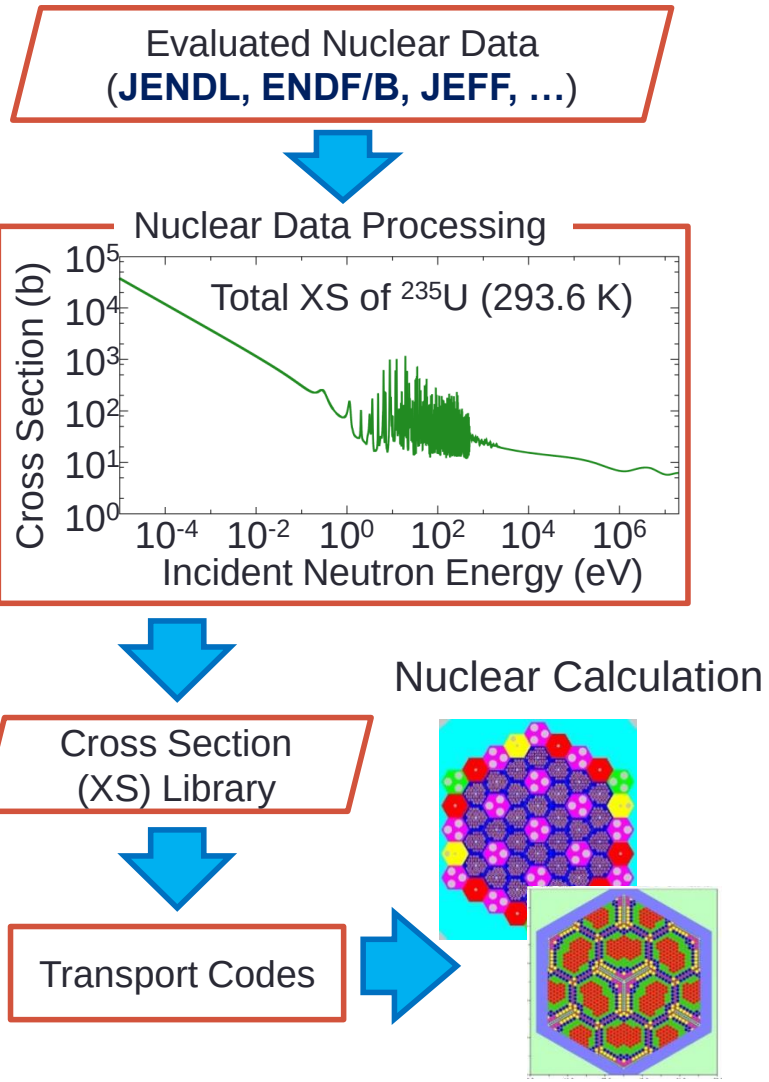
- Overview of nuclear data processing
- Development of FRENDY
- Features of new functions in FRENDY Ver. 2
- Input format of FRENDY
- Future work

Overview of nuclear data processing

What is nuclear data processing?

- Nuclear data processing generates cross section (XS) libraries for particle transport codes.
  - Not just a converter
  - It performs many processes.
    - Linearization, Resonance reconstruction, Doppler broadening, …
- NJOY (LANL) and PREPRO (IAEA) are well-known in the world.

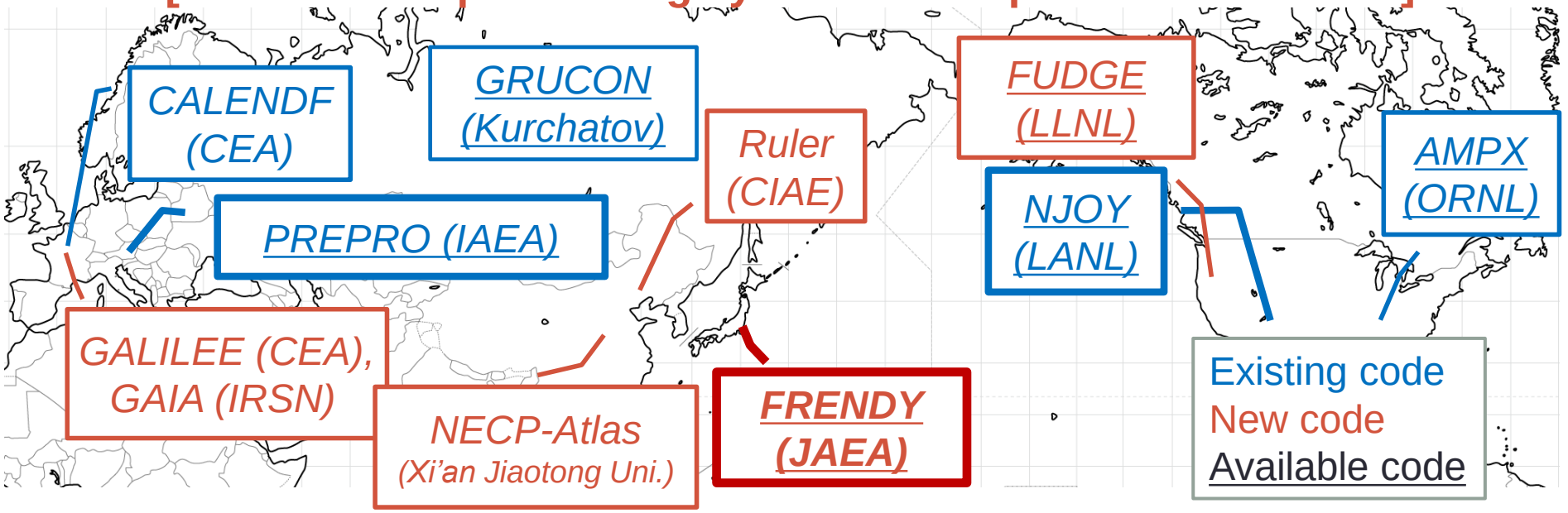
[Example of processing]



Status of nuclear data processing system development

- Development of nuclear data processing system has been started in many institutes.
  - To process their own nuclear data library
  - To handle new nuclear data format GNDS
    - GNDS: Generalized Nuclear Data Structure

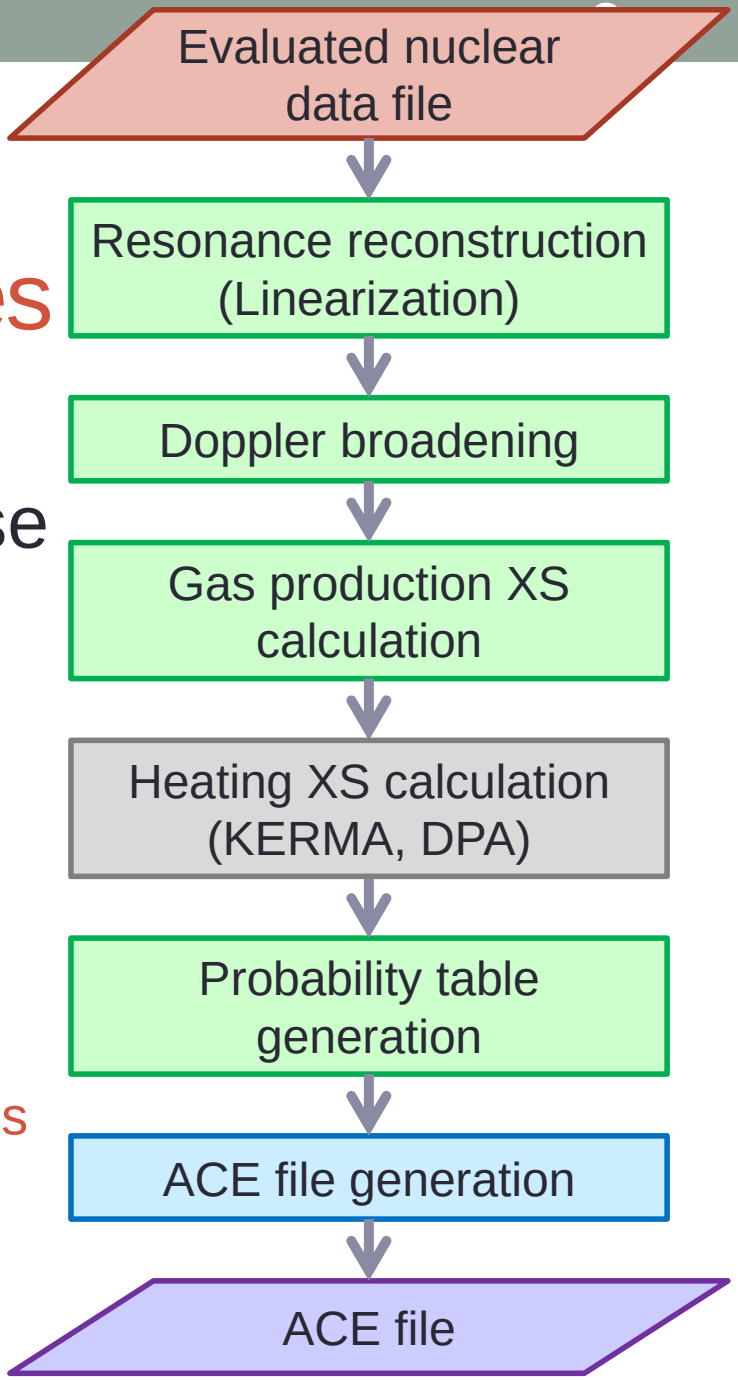
[Nuclear data processing system development in the world]



Ref. D. Brown, "The New Evaluated Nuclear Data File Processing Capabilities," *INDC(NDS)-0695*.

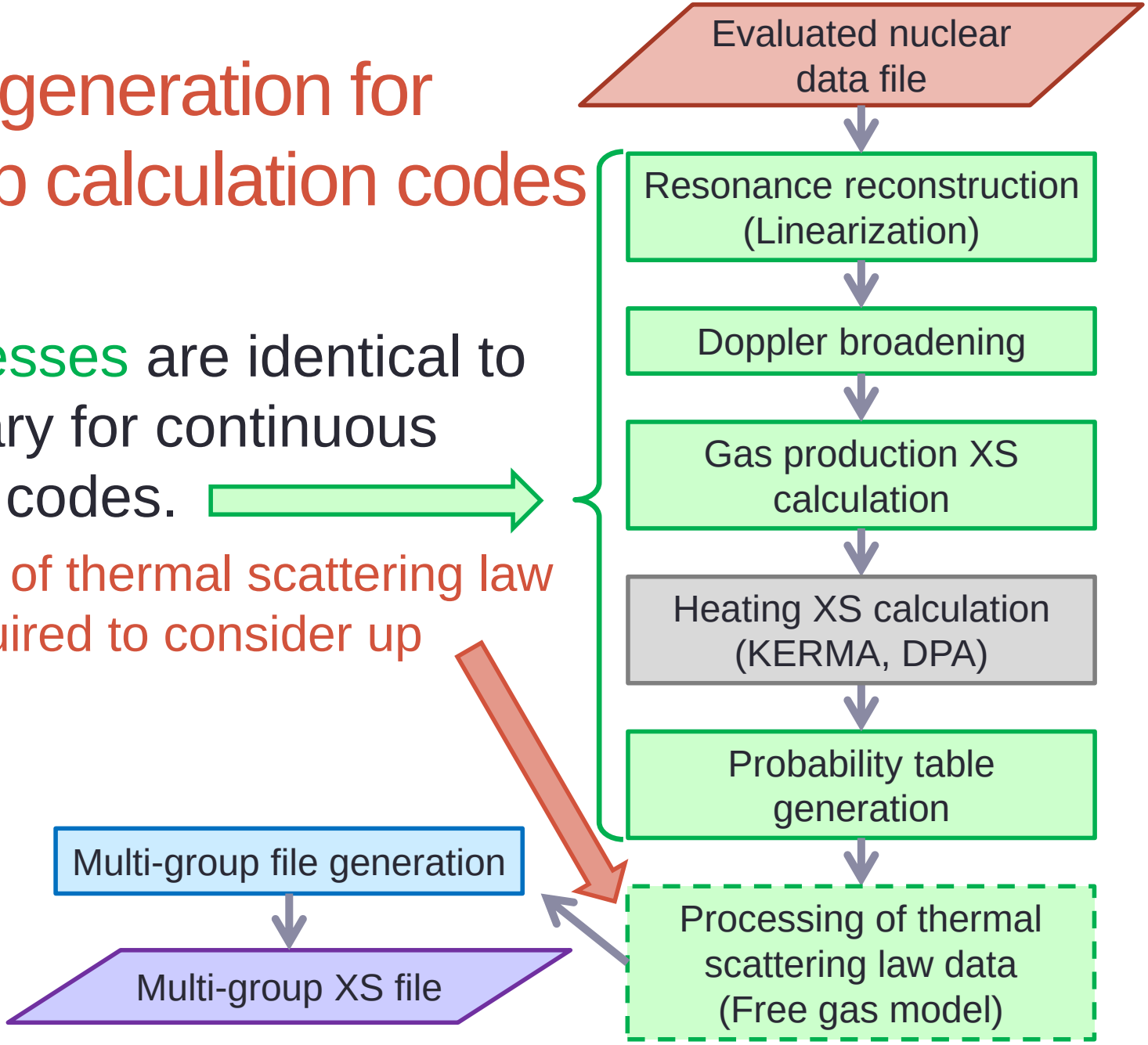
XS library generation for continuous energy MC codes

- Many Monte Carlo (MC) codes use ACE file.
  - MCNP, PHITS, Serpent2, OpenMC, SuperMC, …
  - Current version of FRENDY does not implement Heating XS calculation function.
    - KERMA : kinetic energy release in materials
    - DPA : displacement per atom



XS library generation for multi-group calculation codes

- Many processes are identical to the XS library for continuous energy MC codes.
  - Processing of thermal scattering law data is required to consider up scattering.



Development of FRENDY

Development of nuclear data processing system FRENDY

- JAEA started developing a new nuclear data processing system FRENDY in 2013.
  - **FR**om **E**valuated **N**uclear **D**ata librar**Y** to any application
  - To process nuclear data library by JAEA's nuclear application code users **with simple input file**.
- FRENDY Version 2 was released in 2022.
  - https://rpg.jaea.go.jp/main/en/program_frendy/

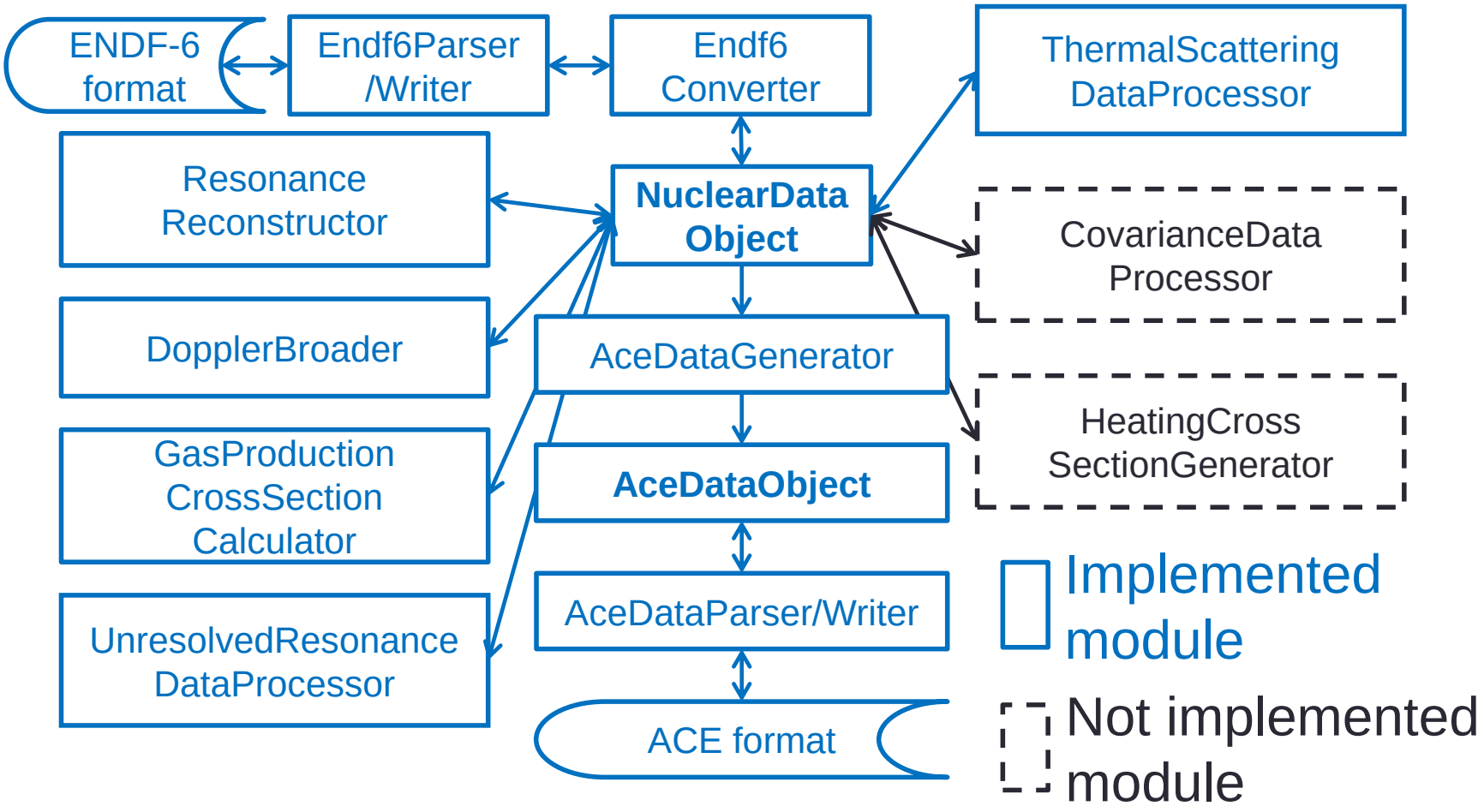
Features of FRENDY

- Utilization of modern programming techniques
  - C++, BoostTest library, Git
  - Improvement of quality and reliability
- Consideration of maintainability, modularity, and flexibility
  - Encapsulate all classes
  - Minimize the function of module
  - Maintain the independence of each module
- Processing methods of FRENDY are similar to NJOY.

Ref. K. Tada, et. al., “Development of nuclear data processing code FRENDY version 2,” *J. Nucl. Sci. Technol.* (2023). (https://doi.org/10.1080/00223131.2023.2278600)

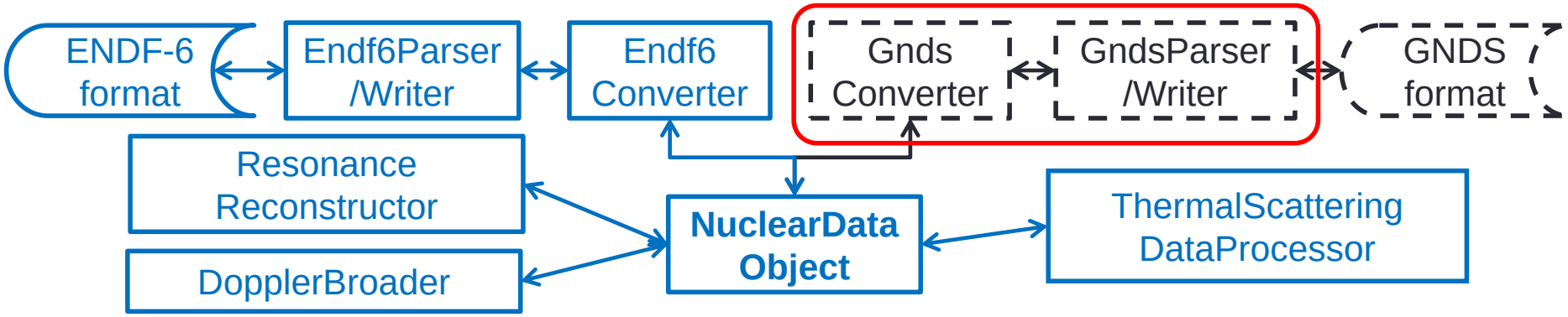
Structure of FRENDY

- Modularity is carefully considered.
  - Modules of FRENDY can be used other calculation codes by adding only a few lines.



Advantage for using the FRENDY's original nuclear data object

- FRENDY has original format of the nuclear data for efficient management.
  - NuclearDataObject class
- Minimizing the impact by the change of nuclear data format
  - Developer and users are not necessary to consider the nuclear data format.
  - Consideration of a new data format GNDS
    - GNDS format can be addressed if another set of parser, writer and converter classes are implemented.



Input format of FRENDY

- FRENDY treats two types of the input formats.
  - FRENDY original input format
  - NJOY compatible
    - RECONR, BROADR, GASPR, PURR, UNRESR, THERMR, GROUPR, MATXSR, MODER
- Simple and easy input data
  - The simplest input: Nuclear data file name and processing mode are **only** required for the processing.
    - FRENDY has recommended parameters in the source code.
    - User can also change (override) parameters.

Input format of FRENDY and NJOY

- Input parameters of FRENDY consist of “input data name” and “input data”.
  - Comment line is similar to C/C++.
    - //~ or /* ~ */
- Input format of FRENDY is easy to understand.
  - This input format is suitable for beginners.

[Sample input of FRENDY]

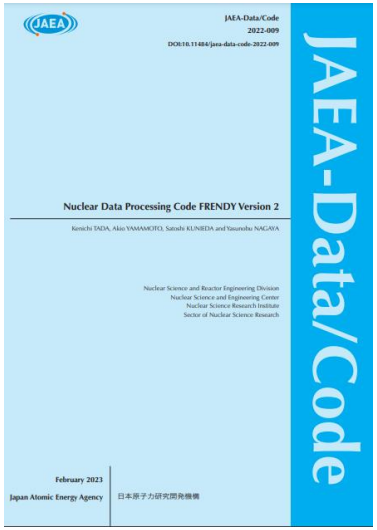
```
ace_fast_mode  // Processing mode
  nucl_file_name   U235.dat
  ace_file_name    U235.ace
  temp             296.0
```

[Sample input of NJOY]

```
reconr                              / command
 20  21                             / input(tape20), output(tape21)
'pendf tape for JENDL-4 U235'       / identifier for PENDF
 9228                               / mat
 1.00e-03  0.00                     / err, temp
 0                                  /
broadr                              / command
 20  21  22                        / endf, pendf(in), pendf(out)
 9228  1                           / mat, temp no
 1.00e-03  -5.0E+2                  / err, thnmax
 296.0                              / temp
 0                                  /
gaspr                               / command
 20  22  23                        / endf, pendf(in), pendf(out)
purr                                / command
 20  23  25                        / endf, pendf(in), pendf(out)
 9228  1  10  20  500               / mat, temp no, sig no, bin no, lad no
 296.0                              / temp
 1E10  1.0E6  1E4  1E3  300  100  35  10  1.0  0.1    / sig zero
 0                                  /
acer                                / command
 20  25   0  30  31                 / nendf, npend, ngend, nace, ndir
 1   1   1  0.30                    / iopt(fast), iprint(max), itype, suffix
 'ACE file for JENDL-4 U235'        / descriptive character
 9228  296.0                       / mat, temp
 1  1                               / newfor(yes), iopp(yes)
 1  1  1                           / thin(1), thin(2), thin(3)
stop                                /
```

Release of FRENDY

- FRENDY was released from our website.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
  - Open-source software
    - 2-Clause BSD license
  - Presentations of FRENDY training course and exercise are also found in this website.
- Manual of FRENDY
  - JAEA-Data/Code 2022-009
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2022-009.pdf
    - There are many sample input files in this manual.



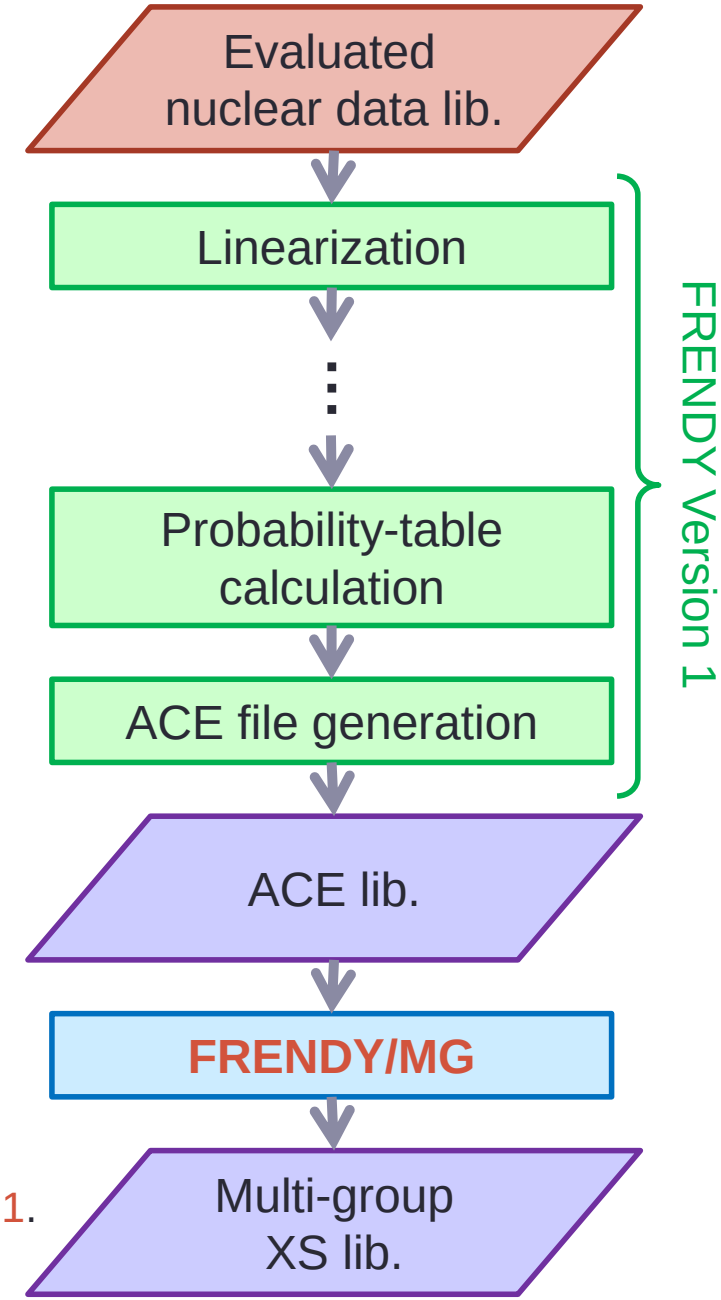
Development of FRENDY Ver. 2

- FRENDY Ver. 1 only generates ACE file.
- Many capabilities are prepared after FRENDY Ver. 1.
  - Neutron induced multi-group cross section generation
  - Perturbation of ACE file for uncertainty quantification
    - This function was implemented in FRENDY Ver.1.01.001.
  - Modification of evaluated nuclear data file
  - Uncertainty quantification for probability tables
  - Improvement of input checker to reduce input errors
- FRENDY version 2 was released including these functions in Jan. 2022.

Features of new functions in FRENDY Version 2

Multi-group XS generation

- FRENDY/MG*) is used for a multi-group XS files.
  - FRENDY/MG generates multi-group XS files from ACE files.
    - FRENDY/MG can also generate a multi-group XS library from the existing ACE library.
- NJOY input is also available for multi-group XS file generation.
  - Input of GROUPR and MATXSR modules are available.



*) A. Yamamoto, K. Tada, G. Chiba, T. Endo, "Multi-group neutron cross section generation capability for FRENDY nuclear data processing code," J. Nucl. Sci. Technol., 2021. https://doi.org/10.1080/00223131.2021.1921631

Major capabilities of multi-group generation

- Output format of multi-group cross sections
  - GENDF and MATXS
- Angular/energy distributions
  - LAW=3, 4, 7, 9, 11, 44, 61, and 66 in ACE file
  - All nuclides in JENDL-4.0, -5, ENDF/B-V, B-VII.1, B-VIII.0, JEFF-3.3, and TENDL-2019, -2021 are available.
- Calculation function of multi-group photoatomic cross section, KERMA factors, and group-to-group photon scattering matrix is not implemented.
  - GAMINR of NJOY

New functions of multi-group generation

- Back-ground cross-section set can be automatically set with minimum number of background cross-sections*).
- A compound of different isotope can be specified to explicitly consider the resonance interference effect.
  - For example, U-235, U-238, and O-16 in UO_2.
- Any energy grid points can be used for ultra-fine group slowing down calculation.

*) A. Yamamoto, T. Endo, K. Tada, “Adaptive setting of background cross sections for generation of effective multi-group cross sections in FRENDY nuclear data processing code,” J. Nucl. Sci. Technol., 2021. https://doi.org/10.1080/00223131.2021.1944930

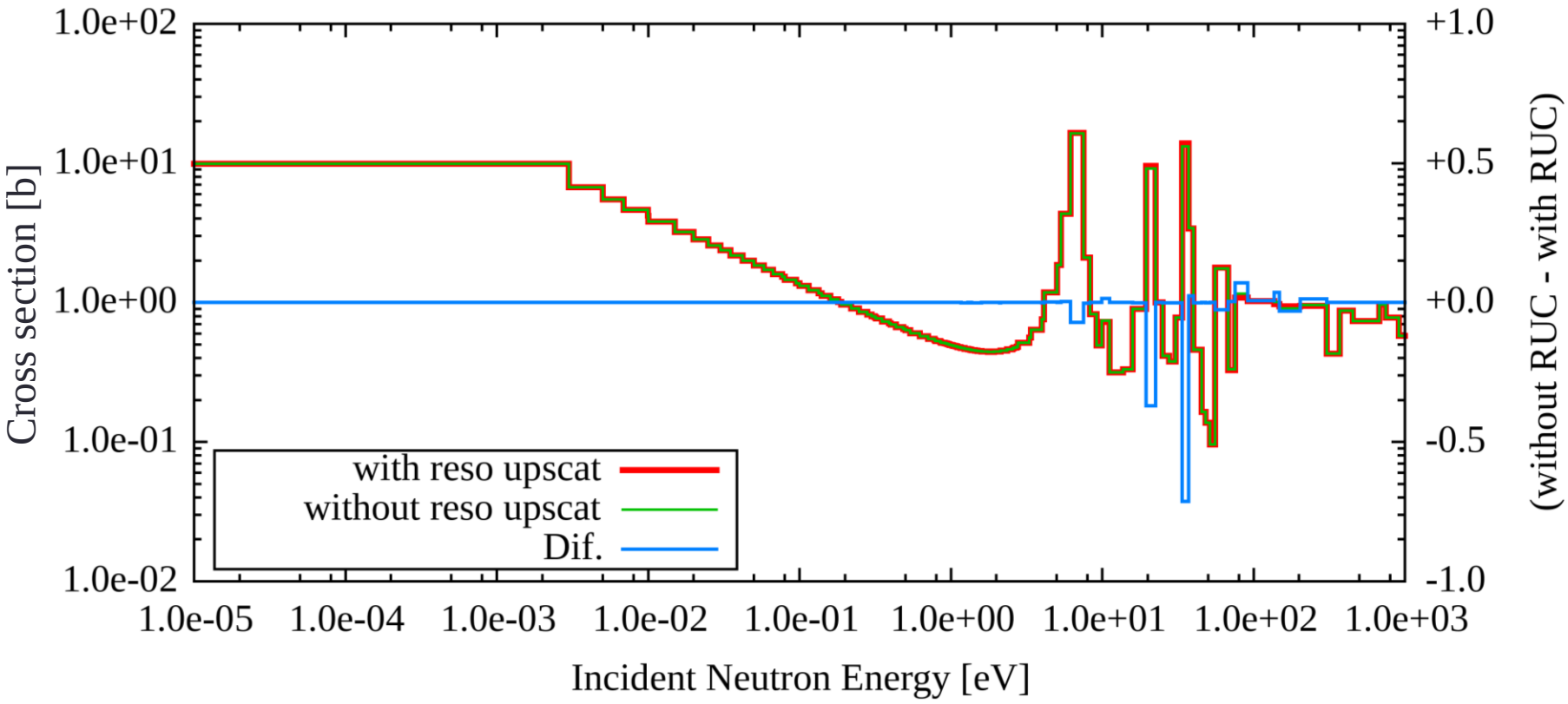
Resonance up-scattering correction (RUC)

- Calculation of elastic scattering cross section and scattering kernel using 0 K scattering cross section data generated by FRENDY.
  - Mixed nuclide is also available to explicitly consider the resonance interference effect.
    - For example, U-235 with RUC, U-238 with RUC, and O-16 without RUC in UO_2.
  - Sample input files to use RUC are found in the FRENDY manual.
- Neutronics calculation codes can consider RUC without any modification.

Comparison of XS with and without RUC

- Larger differences are found at the large resonances below 100 eV.

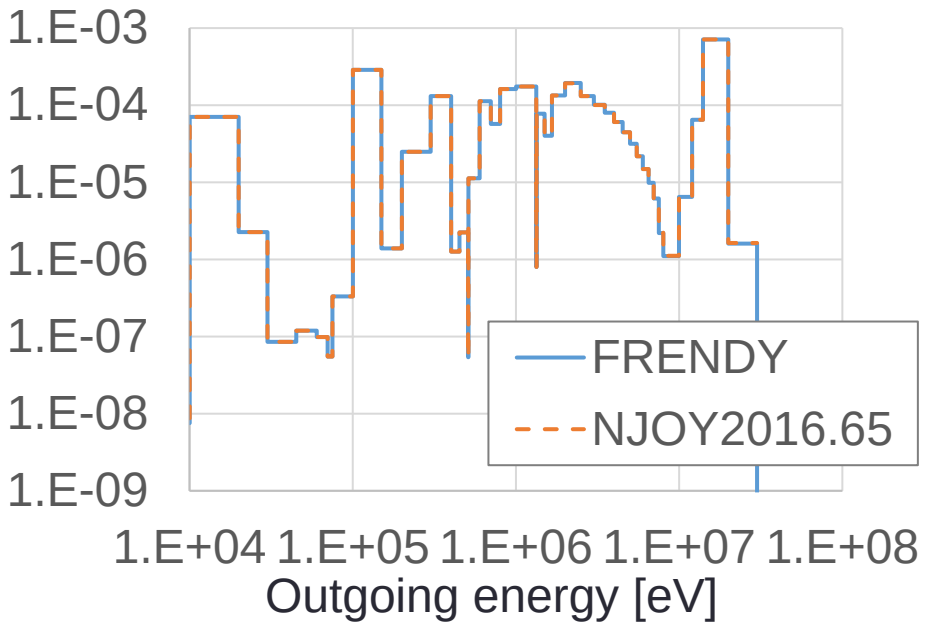
<Comparison of cross section with and without RUC (U-238, MT=102)>



Multigroup generation of secondary gamma spectrum

- FRENDY results show good agreement with NJOY results.
  - All nuclides in JENDL-4.0, JENDL-5, ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.3, and TENDL-2018 are available.

Secondary gamma spectrum of Fe-56 from J5
(MT=102, Ein=13.840-14.191MeV, vitamin-j 42g)



2D interpolation scheme of FRENDY

- ENDF-6 format recommends using unit base interpolation for 2D interpolation.
- FRENDY uses MCE for 2D interpolation.
  - Method of Corresponding Energy
  - MCE is identical to unit base interpolation when the number of divisions *N* is 1.

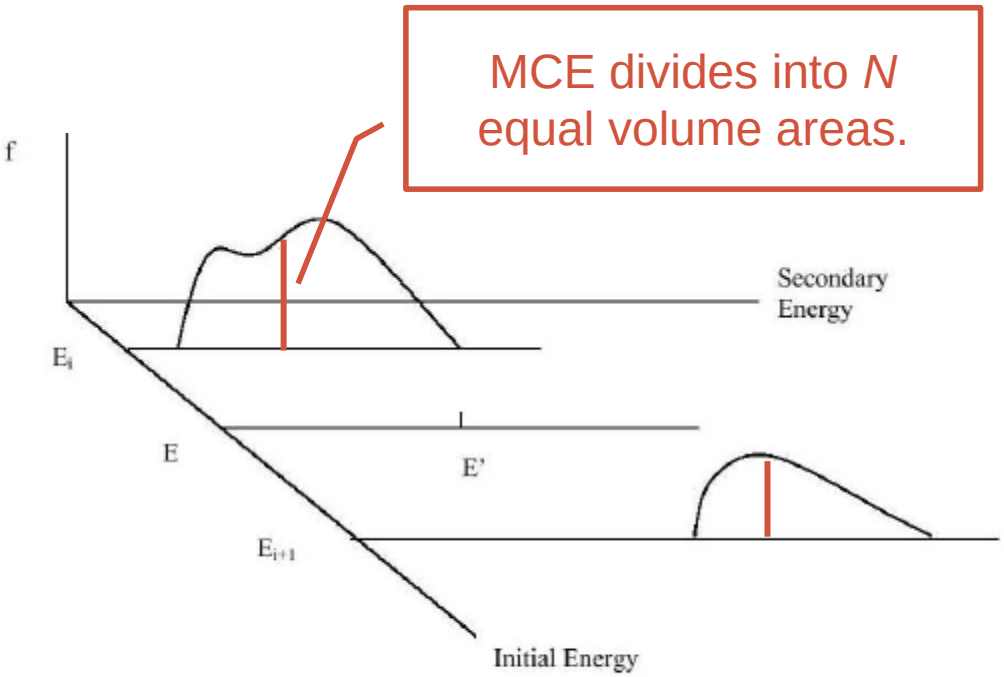


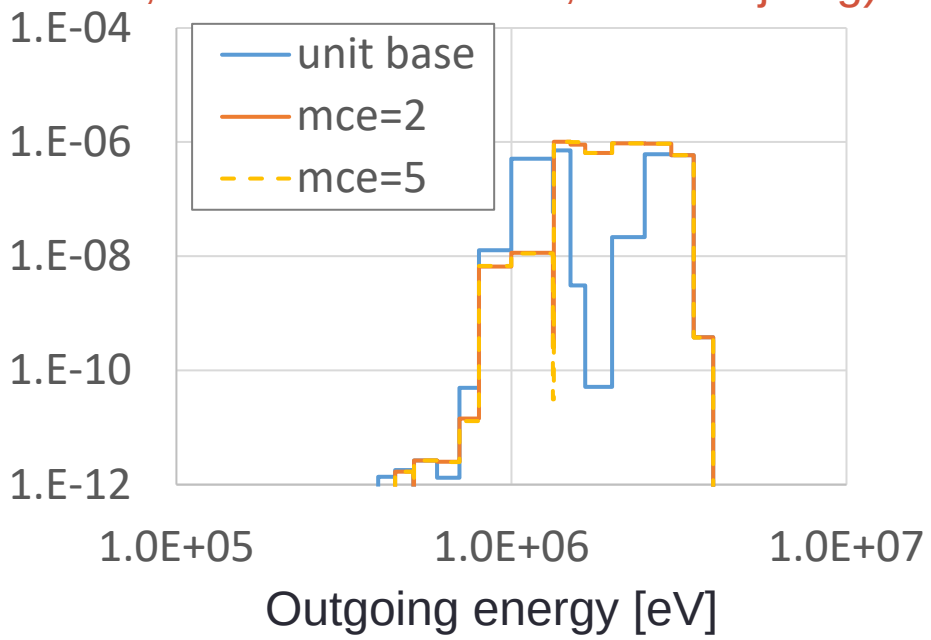
Figure 2: Interpolation between Two-Dimensional Panels.*)

*) A. Trkov et al., "ENDF-6 Format Manual," BNL-203218-2018-INRE. (2018).

Difference of 2D interpolation scheme

- Difference was found in the secondary gamma spectrum between the unit base and MCE.
  - Close to threshold energy.
  - We think that MCE shows a reasonable distribution.
  - Default number of divisions in FRENDY is 2.
    - Gamma spectrum does not change even if the number of divisions is increased.

Secondary gamma spectrum of Fe-56 from J5
(MT=22, Ein=12.5-12.8MeV, vitamin-j 42g)



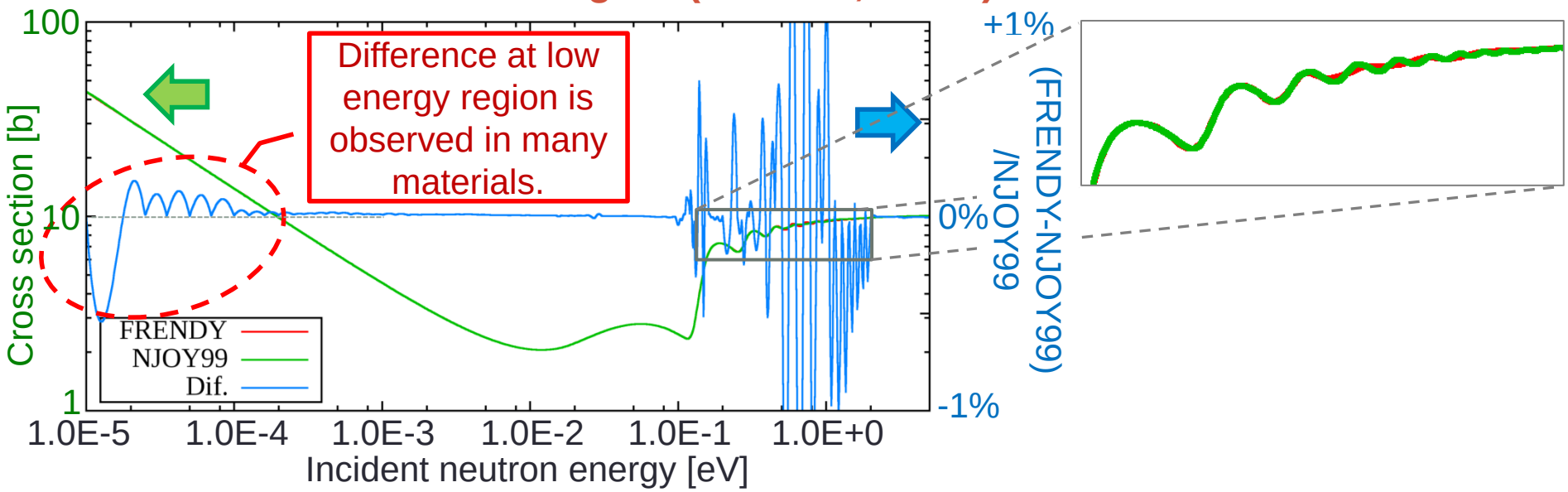
Calculation of thermal neutron scattering cross section

- NJOY uses 118 fixed energy grid points.
  - These fixed energy grid points are insufficient for neutronics calculation.
- FRENDY used the incident energy grid points of the corresponding nuclide.
  - Very large processed data size
- Optimization of the number of incident energy grid points is required to reduce the data size.
  - Linearization function is newly added for thermal scattering law data processing.
  - From FRENDY Ver. 2.02

Comparison of thermal neutron scattering cross section

- NJOY only calculates the incoherent inelastic XS on 118 energy grids.
  - Other energy grids are interpolated using the 5th order Lagrange interpolation.
- The fixed energy grid is not appropriate for a material of which the cross section is oscillated.
  - This difference may have impact on the TRIGA reactor.

<Incoherent inelastic scattering XS (H in ZrH, 400 K)>



Impact of number of energy grids on k-eff

- Investigation of appropriate tolerance value for linearization.
  - Criticality benchmarks which contain H in ZrH were selected.
- Large differences between FRENDY and NJOY were found.
  - The tolerance value for linearization should be less than or equal to 0.05%.
  - FRENDY uses a default tolerance value of **0.02%**.

<Relative difference of k-eff in each criticality benchmark>

	Fixed 118 energy grid	Old FRENDY	Tolerance value 0.10%	0.05%	0.02%
HCM-3-1	*-0.037%*	0.003%	*0.013%*	0.002%	0.002%
ICT-3-132	*0.026%*	-0.002%	*-0.009%*	-0.001%	-0.006%
ICT-3-133	*0.021%*	0.001%	*-0.012%*	-0.004%	-0.005%

Comparison of incident energy grid points

- The number of incident energy grid points is very small even if tolerance value is 0.02%.
  - Incident energy grid points and data size of the ACE file are reduced by more than **80%** for many materials when the tolerance value is 0.02%.

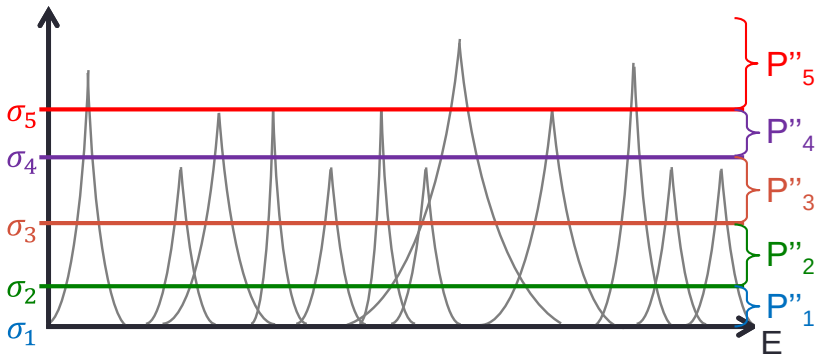
<Comparison of the number of incident neutron energies in each tolerance value>

	Old FRENDY	Tolerance value 0.10%	0.05%	0.02%
Al-27	2,773	173	234	330
Fe-56	9,775	174	238	345
Be in BeO	10,272	186	261	387
D in D_2O	559	166	208	280
H in H_2O	500	157	194	274
H in ZrH	500	297	423	*653*
O in BeO	10,243	185	256	381
O in H_2O	512	152	176	225
O in UO_2	3,958	178	246	352
U in UO_2	4,626	170	230	326
Zr in ZrH	3,378	172	235	336

Uncertainty quantification for probability tables

- FRENDY Ver. 1 requires number of ladders as an input parameter to calculate probability table.
  - An optimal number of ladders has not been investigated.
  - Probability table is important to consider self-shielding effect in unresolved resonance region.
- FRENDY Ver. 2 calculates statistical uncertainty of probability table.
  - Product of probability table and total XS is considered as target of statistical uncertainty of probability table.
- User can generate probability table with optimal number of ladders.
  - This function is also contributed to reduce the total processing time.

<Example of ladder (pseudo resonance structure)>



Calculation time of probability table in each energy grid (U235 from J-40)

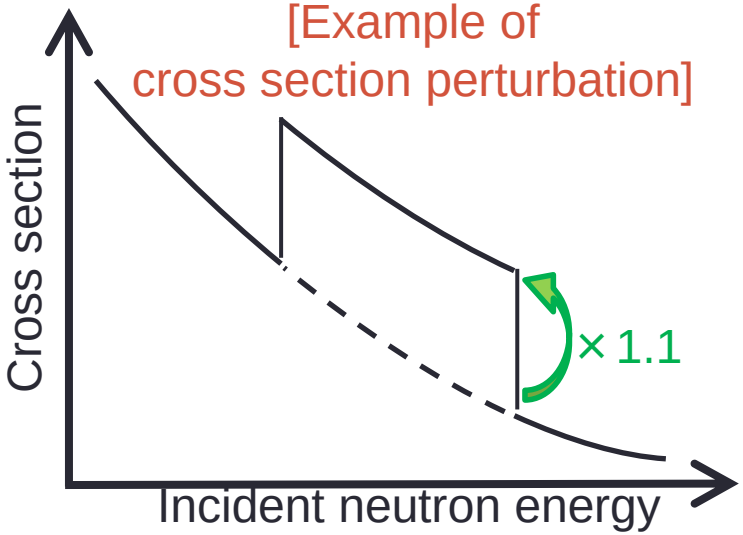
- Optimal number of ladders is different in each energy grid.
  - Criteria of statistical error : **5%** (default value)
- Ladder number optimization effectively reduces generation time of probability table.
  - Number of ladders becomes smaller when incident energy is increased.
  - Calculation time to generate one ladder becomes longer when incident energy is increased.

Incident energy [eV]	Total time [s]	No. of ladders [-]	Time per ladder [ms]
500	4.28	80	53.5
563	3.33	60	55.5
850	3.81	60	63.5
1110	3.52	50	70.4
1300	2.25	30	75.0
4250	3.74	30	124.7
6500	4.53	30	151.0
13000	8.15	40	203.8
26900	16.40	60	273.3
30000	11.50	40	287.5

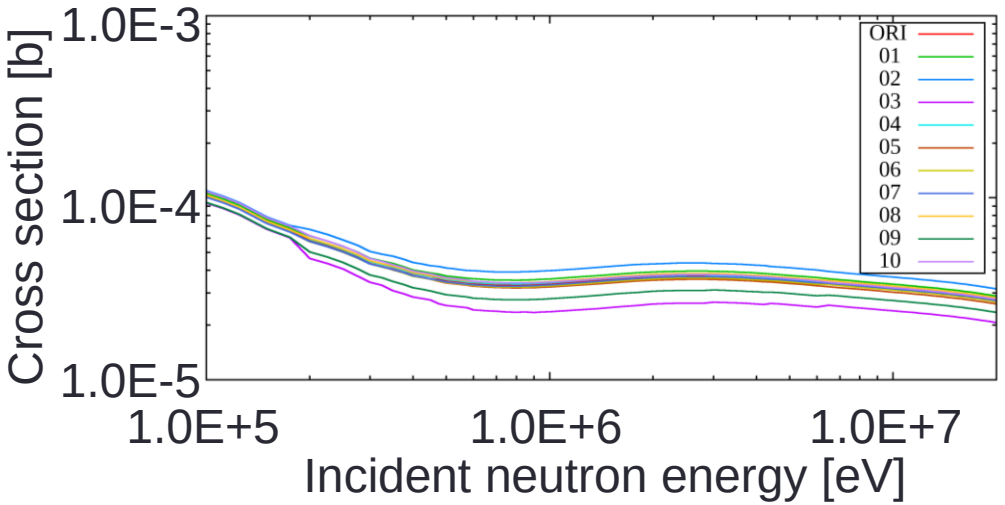
ACE file perturbation tool

- Implementation of a random sampling tool to perturb cross section and fission spectrum of ACE file*).
  - User sets reaction type, energy region, and amount of perturbation.
  - Cross section and fission spectrum are randomly perturbed using random sampling mode.
- This tool is available from FRENDY Ver. 1.01.001.

[Example of cross section perturbation]



[Example of random sampling (^{1}H, (n,γ))]



*) K. Tada, et al., "Development of ACE file perturbation tool using FRENDY," *J. Nucl. Sci. Technol.*, 60, pp.624-631 (2023). https://doi.org/10.1080/00223131.2022.2130463

ENDF modification function

- This function removes, adds, exchanges specified MF/MT data.

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=6

The modified evaluated nuclear data file **must be checked carefully** since FRENDY does not check the new file.

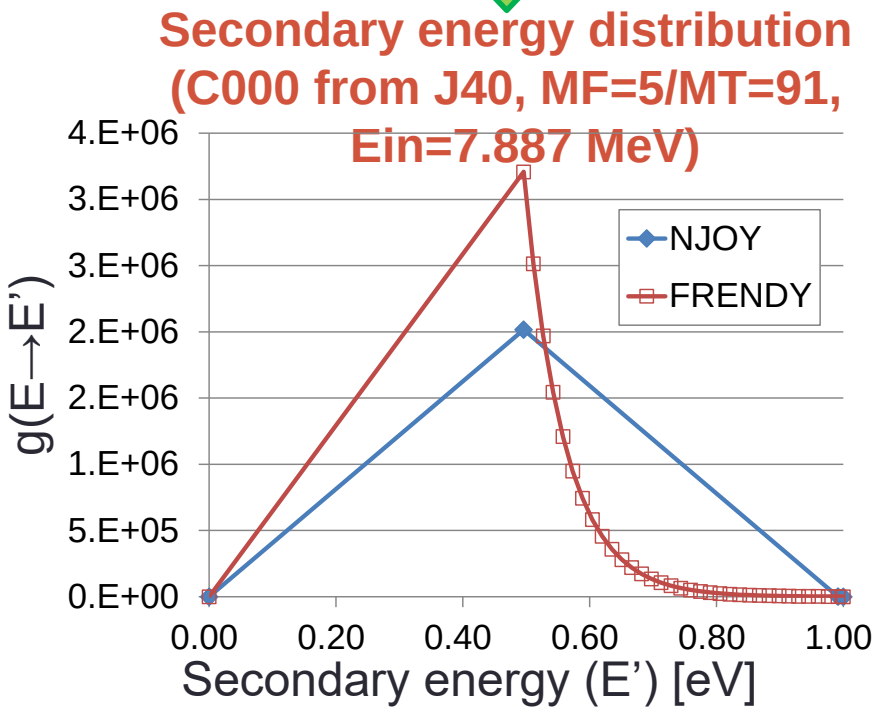
MF=1
MF=2, MT=151
MF=3, MT=1
MF=6

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=3, MT=102
MF=6

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=6

Linearization function of TAB1 data

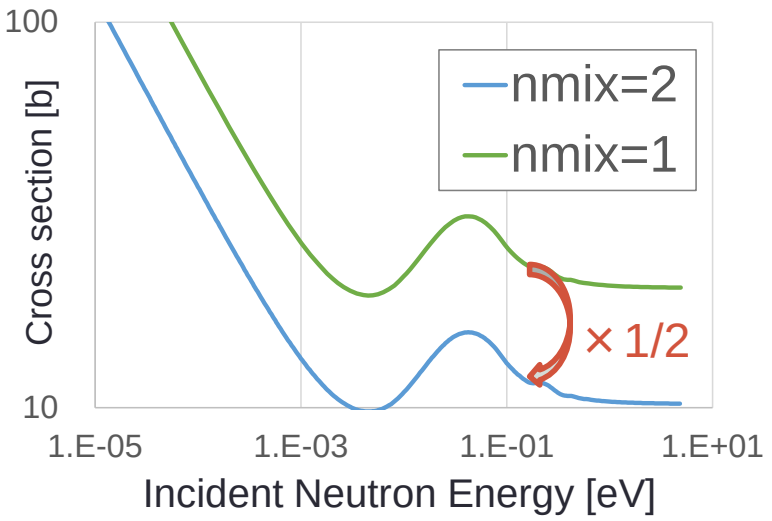
- NJOY uses the first interpolation scheme for multiple interpolation schemes in some MF data.
  - This process is not applicable when multiple interpolation schemes are used in the TAB1 data.
  - FRENDY linearizes TAB1 data to handle multiple interpolation schemes.
    - Differences were found between FRENDY and NJOY.
- Linearization function of TAB1 data was prepared as a tool of FRENDY.
  - Such interpolation problem is solved if the TAB1 data are linearized before the nuclear data processing.



Input checker functions to reduce input errors

- FRENDY automatically checks input parameters and processing results.
  - FRENDY reads nuclear data files and sets recommended values.
    - Input parameters are compared to recommended values.
  - Processing results are also used to verify input parameters.
- These functions help many users to generate correct input file.
  - These functions are also available for NJOY input format.
  - FRENDY is also used as the input checker of NJOY.

< Incoh-Inela XS of H in CH2 >



Input format of FRENDY

Basics of FRENDY input format

- First line **must be** processing mode.
  - ace_fast_mode : Neutron induced ACE file
  - ace_tsl_mode : ACE file of thermal scattering law data
  - ace_dosi_mode : Dosimetry ACE file
  - mg_neutron_mode : Neutron induced multi-group XS file
- Other lines are free format.
  - Setting “input data name” and “input data”
  - Parentheses are used to describe array data, *e.g.*, (1.0 2.0 3.0).
  - Text data is surrounded by single or double quotation mark, *e.g.*, “~” or ‘~’.
    - Multiple lines are available for array data and text data.
- Comment line is similar to C/C++.
  - //~ or /* ~ */

Main input parameters

- Required parameters
  - nucl_file_name : Evaluated nuclear data file name
  - nucl_file_name_tsl : TSL data file name (TSL only)
- Other main input parameters
  - temp : Temperature (K) (Default: 293.6 K)
  - ace_file_name : ACE file name (Default: “nucl_file_name”.ace)
  - ace_dir_file_name : XSDIR file name (Default: “nucl_file_name”.ace.dir)
  - suffix_id : Suffix ID of ACE file (Default: 00)
  - ace_label_data : Comment line of ACE file (one line) (Default: none)
  - thermal_za_id_name : S(α, β) identifier of MCNP (TSL only) (Default: ZA value)
- Additional parameters
  - write_pendf_probability_table : PENDF file name after probability table generation
  - write_pendf_tsl : PENDF file name after TSL data processing (TSL only)
    - PENDF (Point-wise ENDF) file is a processing result of NJOY.
    - These PENDF file can be used as input PENDF of NJOY.

Example of FRENDY input (Neutron induced)

```
ace_fast_mode  // Processing mode
  nucl_file_name        ../lib/U235.dat
  temp /* [K] */        300.0
  ace_file_name         ./ace/U235.ace
  ace_dir_file_name     ./xsd/U235.xsdir
  ace_label_data        “U-235 from JENDL-4.0”
  suffix_id             50
```

First line **must be** set processing mode.

Relative path or absolute path

- Processing conditions of above example
  - Evaluated nuclear data file name : ../lib/U235.dat
  - Temperature : 300.0 [K]
  - ACE file name : ./ace/U235.ace
  - XSDIR file name : ./xsd/U235.xsdir
  - Comment line of ACE file : U-235 from JENDL-4.0
  - Suffix ID : 0.50

Example of FRENDY input (TSL)

```
ace_tsl_mode  // Processing mode
  nucl_file_name          ../lib/H001.dat
  nucl_file_name_tsl      ../lib_sab/01_h_in_h2o.txt
  ace_label_data          "HinH2O from JENDL-4.0"
  temp                    296.0
  ace_file_name           ./ace_sab/lwtr.ace
  ace_dir_file_name       ./xsd_sab/lwtr.xsdir
  suffix_id               50
  thermal_za_id_name      "lwtr"
```

First line **must be** set processing mode.

TSL data file name

Temperature prepared in TSL data file (nucl_file_name_tsl) is **only** available.

S(α, β) identifier of MCNP (Maximum: 6 characters)

- Processing conditions of above example
  - TSL data file name: ../lib_sab/01_h_in_h2o.txt
  - S(α, β) identifier of MCNP : lwtr
    - lwtr : light water
    - This name is used in S(α, β) card of MCNP input.

Input format of multi-group generation

- Input format of multi-group generation is similar to that of ACE file generation.
  - Difference is only processing mode name
  - Multi-group file can be generated from ENDF and ACE files
- Processing of U-235

```
mg_neutron_mode                          //Process mode
   nucl_file_name ( ../lib/U235.dat ) //ENDF file name
```

- Processing of H in H2O

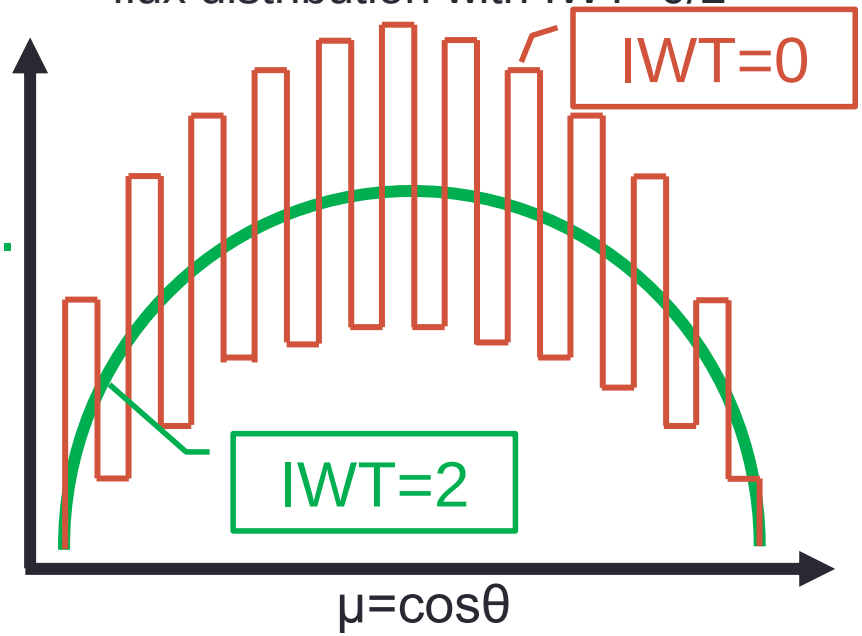
```
mg_neutron_mode                          //Process mode
  nucl_file_name     ( ../lib/H001.dat ) //ENDF file name
  nucl_file_name_tsl ( ../lib/01_h_in_h2o.txt )

  mg_tsl_data_type   (hh2o) //This data type is used for MATXS
```

Difference of IWT options

- IWT option affects the angular neutron flux distribution
  - Angular neutron flux distribution may become jagged when IWT=0 (variable) *).
- Recommend option: IWT=2
  - If users want to accurately calculate the angular neutron flux distribution.
  - IWT must be 2 for the multi-group cross section generation.
- Do not use IWT=1 (constant).
  - This option will affect not only the angular neutron flux distribution but also k-effective value.

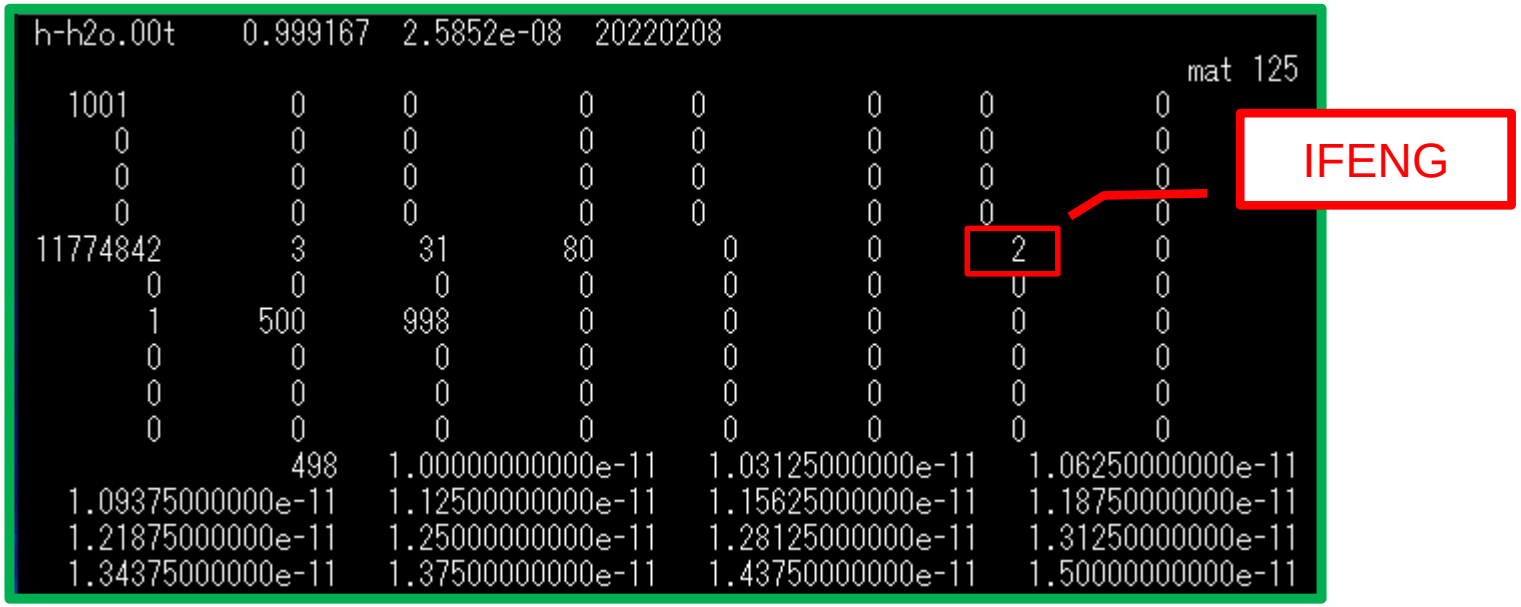
Example of angular neutron flux distribution with IWT=0/2



*) J. L. Conlin, et al., "Continuous-S(α, β) Capability in MCNP, *LA-UR-12-00155*, LANL (2012).

IFENG option and weight_option

- weight_option (0~2) used in FRENDY is identical to iwt option in NJOY/ACER module.
  - iwt=0 (variable), 1 (constant), 2 (tabulated)
- The values of weight_option (iwt) and those of IFENG are different.
  - IFENG=0 (discrete), 1 (skewed), 2 (continuous)

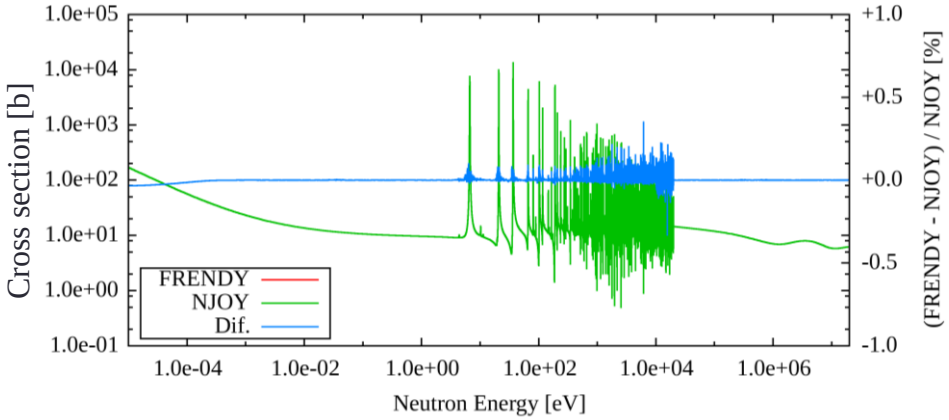


Future work

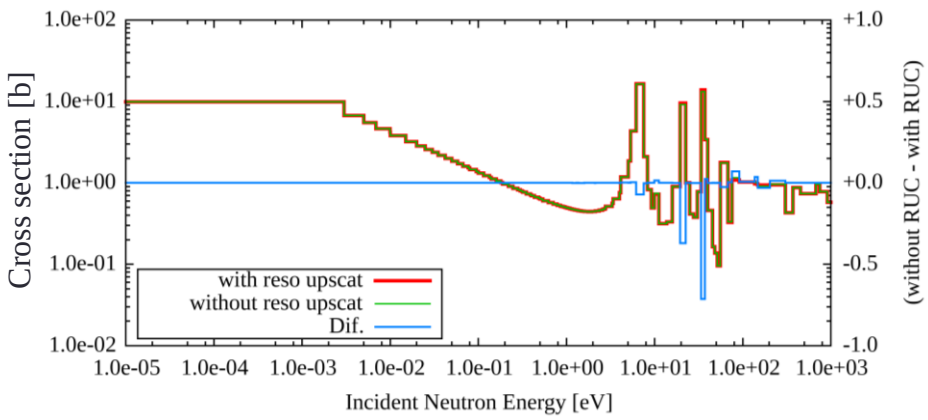
Development of XS output function

- It outputs X-Y data for gnuplot, Matplotlib, and Excel.
  - Cross section data and double differential cross section data from ENDF(PENDF), ACE, and GENDF.
  - Pointwise and multi-group data.
    - Multi-group cross section can be generated from pointwise data.
    - Multi-group cross section generation using flat or 1/E flux.
- This function will be released in next update of FRENDY Ver. 2 (Ver. 2.03).

<Comparison of pointwise XS of U-238>



<Comparison of multi-group XS of U-238>



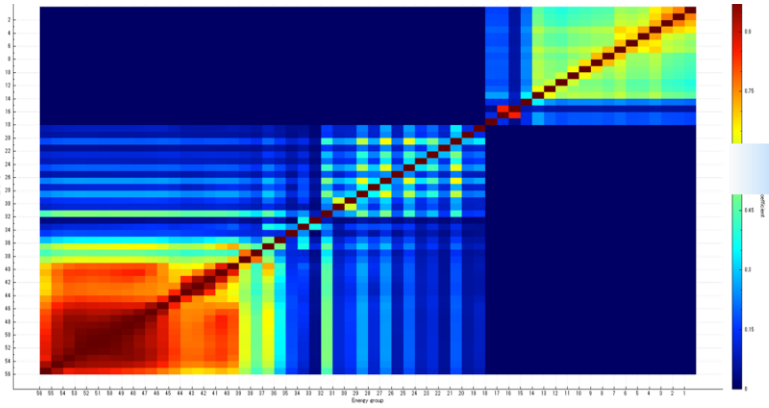
Release of FRENDY Version 3

- FRENDY Ver. 3 will be released including these functions.
  - Calculation function of neutron KERMA factor and DPA cross section (HEATR of NJOY).
    - KERMA: Kinetic Energy Release in Materials
    - DPA: Displacement Per Atom
  - Calculation function of multi-group covariance matrix calculation function (ERRORR of NJOY).
  - Calculation function of multi-group photoatomic cross section, KERMA factors, and group-to-group photon scattering matrix (GAMINR of NJOY).
  - Treatment of the GNDS formatted nuclear data file.
    - Using GIDI+ of LLNL
    - https://github.com/LLNL/gidiplus

Reference Materials

Random sampling

Covariance matrix of nuclear data



inp/Nddd_000x

```
102  2.00E+01  6.43E+00  8.78E-01
102  6.43E+00  4.30E+00  8.67E-01
102  4.30E+00  3.00E+00  8.62E-01
                  . . .
```

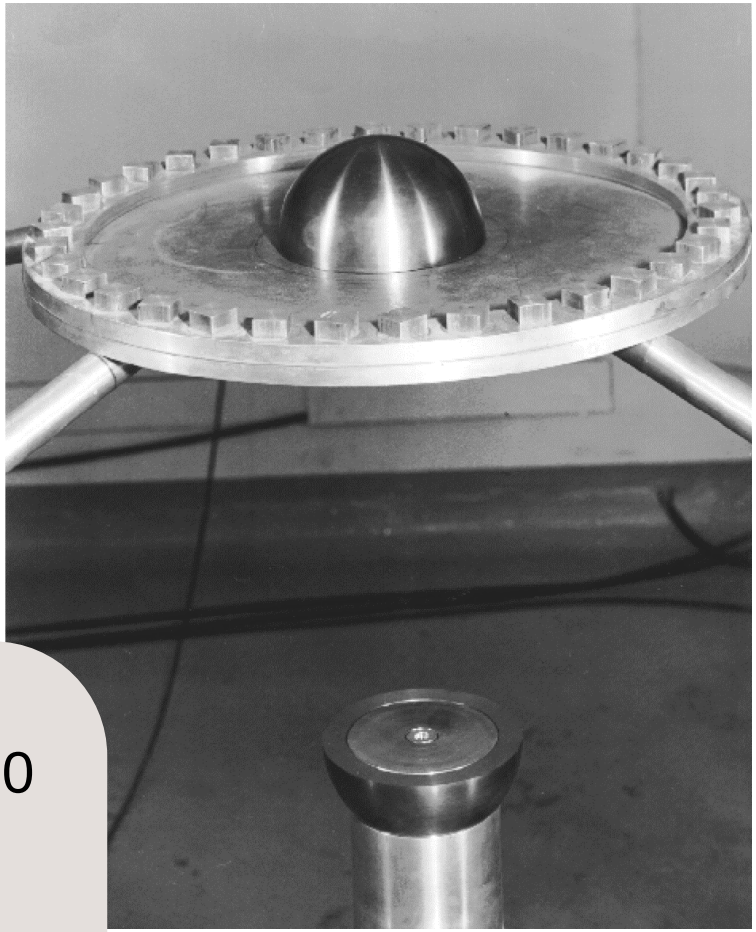
- User has to prepare covariance matrix.
  - We are now developing converter from GENDF file of NJOY/ERROR to input of random sampling tool.
- Generation of perturbation factors using random sampling method
  - See “/frendy_20yymmdd/tools/make_perturbation_factor/sample”

Uncertainty quantification using random sampling method

Godiva (HMF-001)

Geometry	Sphere Radius: 8.7 cm
Composition	U-235: 93.71 wt.% U-238: 5.27 wt.% U-234: 1.02 wt.%
k_{eff}	1.000 ± 0.001

- MCNP6.2
- Number of perturbed ACE file: 100
- Covariance data: 56groupcov7.1 (from SCALE6.2.3)
- MT=2,4,16,18,102,452, and 1018 (MT=452: ν, MT=1018: χ)



Godiva [1]

[1] ICSBEP NEA/NSC/DOC(95)03, Organization for Economic Co-operation and Development-Nuclear Energy Agency (OECD-NEA) (September 2016).

Calculation results (k-effective uncertainty)

k_{eff}-uncertainty due to all nuclides and reactions $\Delta k/k$ [%]

Sensitivity analysis (SA) of MCNP6.2	Random sampling method using perturbation tool
1.11	1.12 [0.98 – 1.24]

Comparison of k_{eff}-uncertainty due to individual nuclide and reaction $\Delta k/k$ [%]

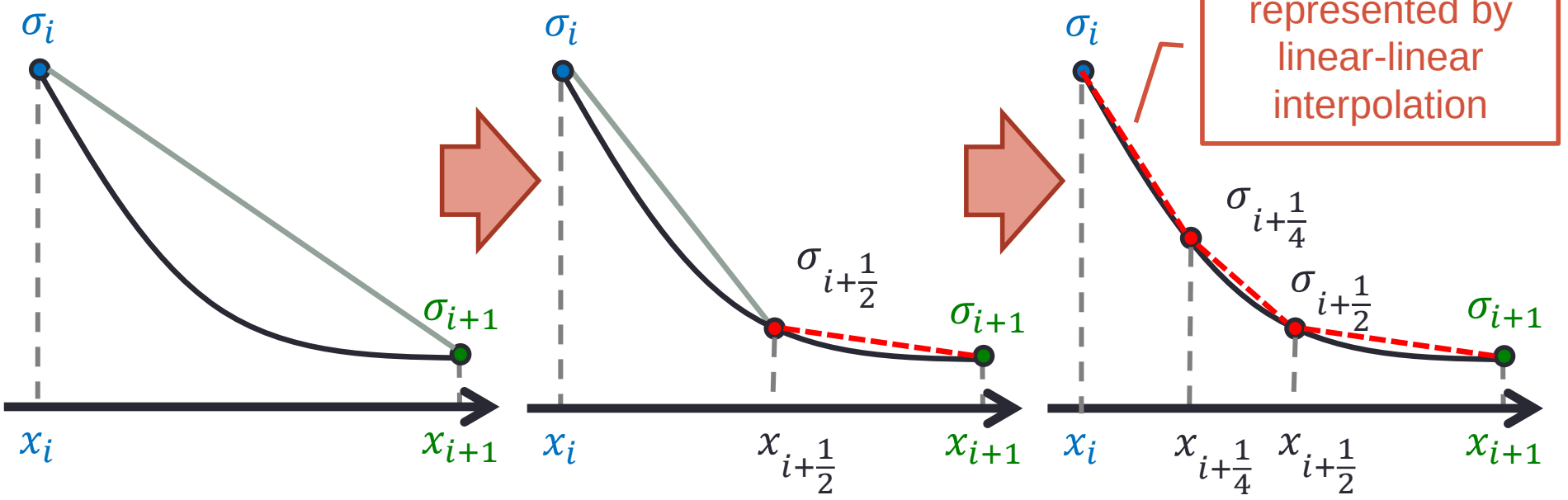
		SA (TSUNAMI-1D)	SA (MCNP6.2)	RS
U-235	(n,γ)	0.880	0.880	0.833
U-235	(n,n')	0.615	0.617	0.664
U-235	Elastic	0.295	0.295	0.305
U-235	Fission	0.269	0.269	0.329
U-235	Fission spectrum	0.253	0.261	0.260
U-234	Fission	0.118	0.118	0.130
U-235	ν_{total}	0.085	0.085	0.093

Appendix

Processing method in FRENDY

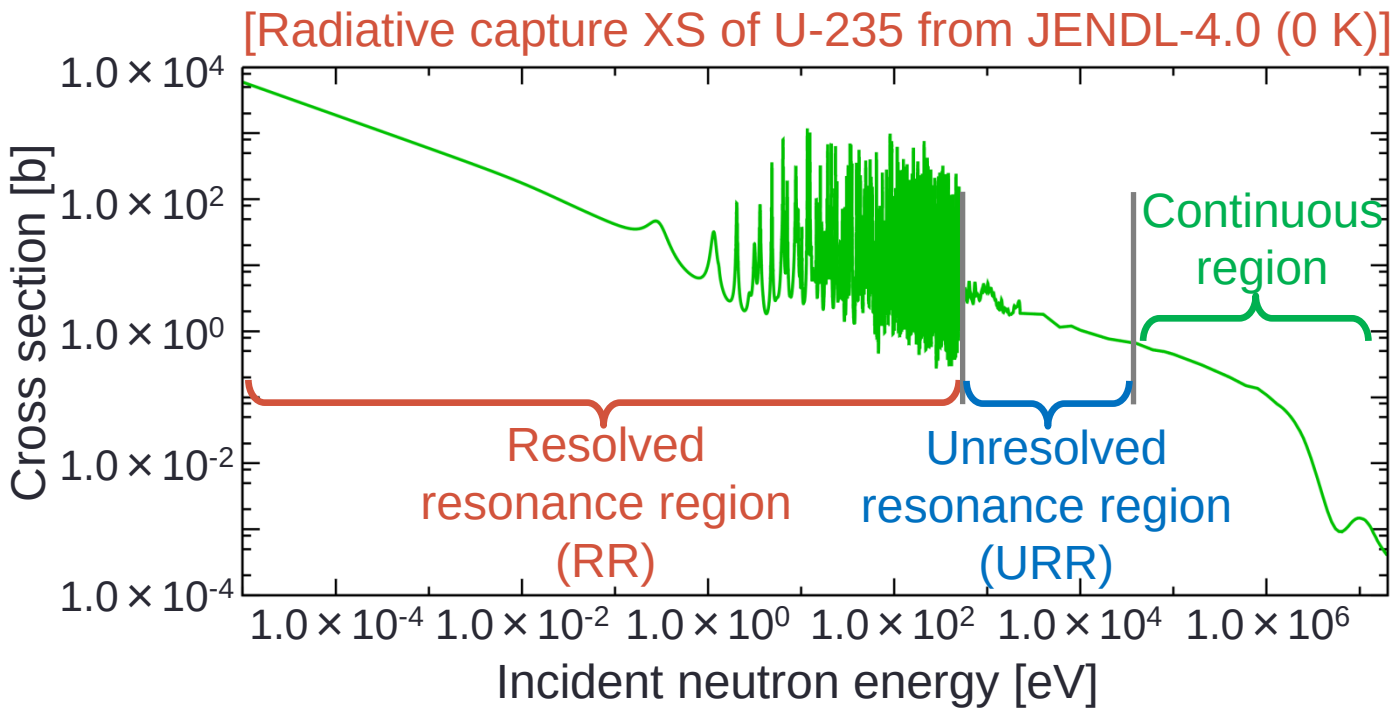
Linearization

- Evaluated nuclear data library describes cross sections with different interpolation scheme.
  - Log-log interpolation, linear-linear interpolation, …
  - Different interpolation schemes are inconvenient.
    - Linearization is required for Doppler broadening.
    - Many nuclear calculation codes use only linear-linear interpolation.



Resonance reconstruction

- XS of resolved and unresolved resonance regions are given as resonance parameters of resonance formula.
  - Calculation of XS in resolved resonance region
  - Calculation of averaged XS in unresolved resonance region
  - XS in continuous region is given in MF=3.



Resonance formulae

- ENDF-6 format arrows to use many resonance formulae
  - Single-Level Breit-Wigner (SLBW)
  - Multi-Level Breit-Wigner (MLBW)
  - Reich-Moore
  - R-Matrix Limited
- These resonance formulae are obtained from calculation of the Schrödinger equation for the multi-particle system.
  - The detail description is found in following papers
    - M. E. Dunn and N. M. Greene, “POLIDENT: A Module for Generating Continuous-Energy Cross Sections from ENDF Resonance Data,” *NUREG/CR-ORNL/TM-2000/035* (2000).
    - A. M. Lane, R. G. Thomas, “R-Matrix Theory of Nuclear Reactions,” *Rev. Mod. Phys.*, **30**, [2], pp.257-353 (1958).
    - N. M. Larson, “Updated Users’ guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes’ Equations,” *ORNL/TM-9179/R8*, *ENDF-364/R2*, p.9 (2008).

Single-Level Breit-Wigner

- Radiative capture cross section of SLBW
  - $\sigma_\gamma = \frac{\pi}{{k_1}^2}\sum_j g_j \sum_{r=1}^{NR_j} \sqrt{\frac{E_1}{E_r}} \frac{\boldsymbol{\Gamma}_{nr}(E_1)\boldsymbol{\Gamma}_{\gamma r}}{(E_r-E_1)^2+{\Gamma_r}^2/4}$
- Elastic scattering cross section of SLBW
  - $\sigma_{sc} = \sigma_p +$
    $\frac{\pi}{{k_1}^2}\sum_j g_j \sum_{r=1}^{NR_j} \frac{\boldsymbol{\Gamma}_{nr}(E_1)^2-2\boldsymbol{\Gamma}_{nr}(E_1)\Gamma_r \sin^2(\phi_l)+2\boldsymbol{\Gamma}_{nr}(E_1)(E_r-E_1)\sin(2\phi_l)}{(E_r-E_1)^2+{\Gamma_r}^2/4}$
  - Evaluated nuclear data file contains many parameters, *e.g.*, neutron width $\boldsymbol{\Gamma}_{nr}$ and Γ_r, spin g_j, resonance energy E_1.
  - Resonance reconstruction calculates cross section at incident energy E_r and linearizes cross section.

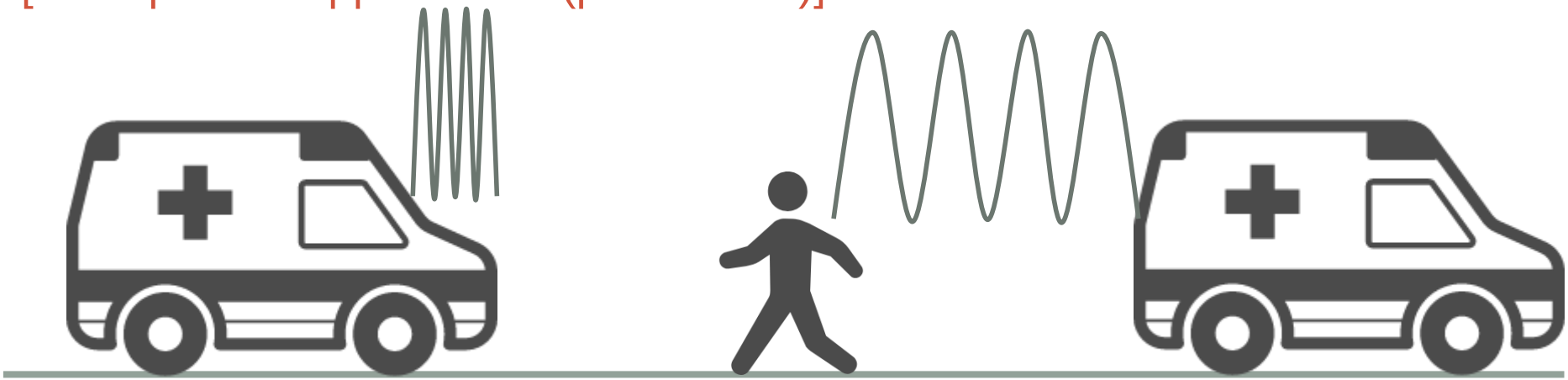
Doppler broadening

- Evaluated nuclear data file contains the data at 0 K.
- Doppler effect must be considered to calculate higher temperature cross section, *i.e.*, Doppler broadened cross section.
  - Nuclear data processing system should generate the temperature-dependent cross section data from the data at 0K.

Doppler effect

- Doppler effect is the change in frequency of a wave.
  - E.g., change of pitch heard when a vehicle sounding a horn approaches and recedes from an observer.
- This effect must be considered in reaction of nucleus and incident particle.
  - Nucleus is at rest when temperature is 0 K.
  - Kinetic energy of nucleus is increased when temperature increases.
    - Relative energy between nucleus and incident particle is changed when temperature changes.

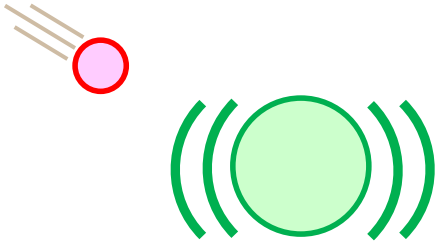
[Example of Doppler effect (pitch heard)]



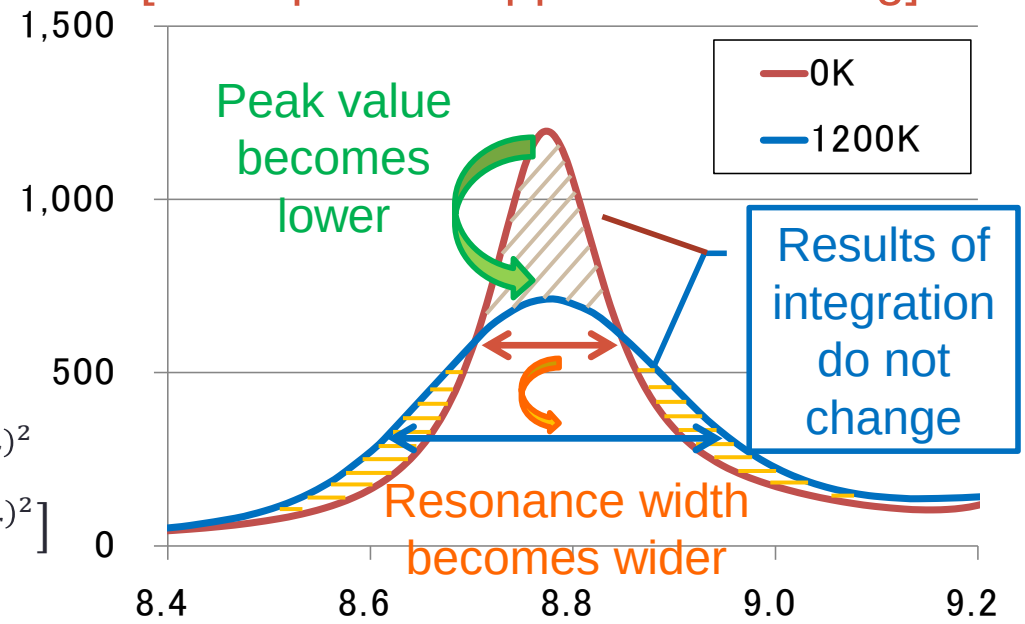
Doppler broadening

- Most of evaluated nuclear data files contain cross sections at 0 K.
  - Nucleus vibration (Doppler broadening) should be considered to calculate cross section at T K.

[Reaction of incident particle and nucleus]



[Example of Doppler broadening]



[Equation of Doppler broadening]

$$\sigma(v,T)=\frac{1}{v^2}\sqrt{\frac{\beta}{\pi}}\int_0^\infty dv_r v_r{}^2\sigma(v_r)\left[e^{-\beta(v-v_r)^2}-e^{-\beta(v+v_r)^2}\right]$$

T: Temperature,

v: velocity of incident particle, v_r: relative velocity

Calculation of Doppler broadened XS

- Linearization is required for easy calculation of Doppler broadened XS.
  - If $\boldsymbol{\sigma(v_r)}$ is not a function of v_r, Doppler broadened XS is obtained using error function.
  - Error function is provided in many programming language as a service routine.

[Calculation formula of Doppler broadened XS]

$$\sigma(v,T) = \frac{1}{v^2}\sqrt{\frac{\beta}{\pi}}\int_0^\infty dv_r {v_r}^2 \boldsymbol{\sigma(v_r)} \left[e^{-\beta(v-v_r)^2} - e^{-\beta(v+v_r)^2}\right]$$

$$\boldsymbol{\sigma(v_r)} = \frac{E-E_k}{E_{k+1}-E_k}\sigma_{k+1} + \frac{E_{k+1}-E}{E_{k+1}-E_k}\sigma_k$$

$$E_r = \frac{1}{2}m{v_r}^2$$

$$\mathrm{F}_n(a) = \frac{1}{\sqrt{\pi}}\int_a^\infty z^n e^{-z^2}\,dz$$

$$= \frac{n-1}{2}\mathrm{F}_{n-2}(a) + a^{n-1}\mathrm{F}_1(a)$$

[Calculation of error function erf(a)]

$$erf(a) = \frac{1}{\sqrt{\pi}}\int_0^a e^{-z^2}\,dz$$

Gas production XS calculation

- Nuclear reactions sometimes yield gases.
  - p(proton: ^{1}H), D(deuteron: ^{2}H), T(triton: ^{3}H), ^{3}He, α(^{4}He)
- Gas generation affects the embrittlement of material and the internal gas pressure in a fuel pin.
  - ENDF-6 format prepares gas production reaction in MT=203-207.
    - MT=203:(z, Xp), MT=204:(z, Xd), MT=205:(z, Xt), MT=206(z, X^{3}He), MT=207(z, Xα)
    - Nuclear data processing system calculates gas production XS even if gas production XS is not found in evaluated nuclear data file.
- Generated nuclide is also considered.
  - For example, ^{12}C(n, n2α)^{4}He reaction generates 3 alpha (^{4}He) particles
    - 2α+^{4}He=3α

Self-shielding effect in URR

- Resonance parameters in URR are averaged ones.
  - Nuclear data processing system cannot reconstruct resonance structure in URR.
  - Consideration of the self-shielding effect in URR is important for accurate neutronics calculations.
    - Self-shielding effect in RR is automatically considered in transport calculation codes using pointwise XS data.
- How to consider the self-shielding effect in URR?
  - NJOY prepares two methods.
    - Deterministic method : UNRESR module
    - Monte Carlo method (probability table method) : PURR module
  - We strongly recommend to use probability table method.
    - "For most purposes, UNRESR has been superseded by PURR."*)
    - "The PURR results may be more reliable at low σ_0 values than UNRESR results."*)

*) R. E. MacFarlane and A. C. Kahler, "Methods for Processing ENDF/B-VII with NJOY," Nuclear Data Sheets, **111**, pp.2739-2890 (2010).

Consideration of self-shielding effect using probability table (NJOY/PURR & FRENDY)

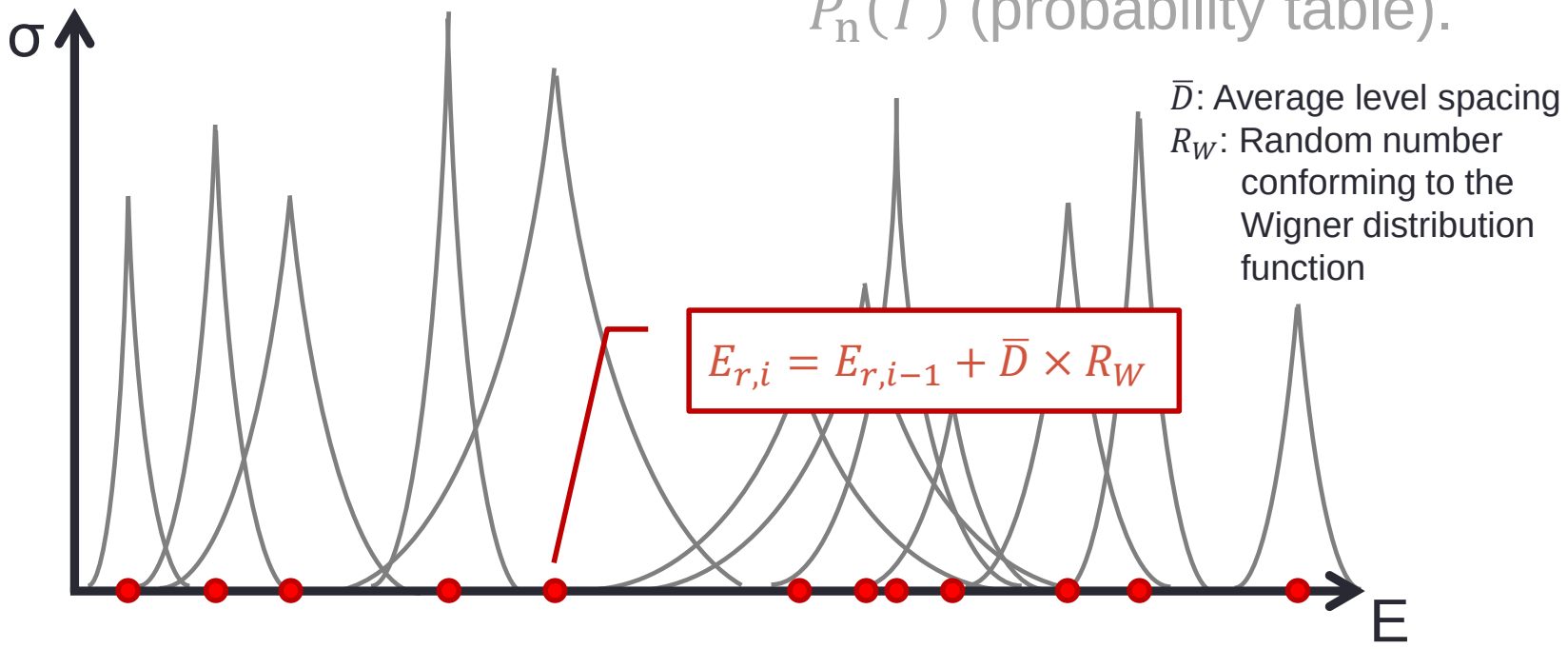
- Bondarenko-type self-shielded XS $\sigma_x(E)$ is used.
  - $\sigma_x(E)$ is obtained by probability table $P_i(E)$.
    - $$\sigma_x(E) = \frac{\sum_{i=1}^{bin} \frac{P_i(E)\sigma_{x,i}(E)}{\sigma_0+\sigma_{t,i}(E)}}{\sum_{i=1}^{bin} \frac{P_i(E)}{\sigma_0+\sigma_{t,i}(E)}}$$
      - x: reaction type $(t, \mathrm{sc}, f, \gamma)$, σ_0: back ground XS
  - Monte Carlo calculation codes directly use $P_i(E)$.

[Example of probability table]

	$\sigma_{x,1}$ (10～16 barn)	$\sigma_{x,2}$ (16～42 barn)	$\sigma_{x,3}$ (42～176 barn)
E=1.2～1.5keV	$P_1 = 0.56$	$P_2 = 0.36$	$P_3 = 0.08$

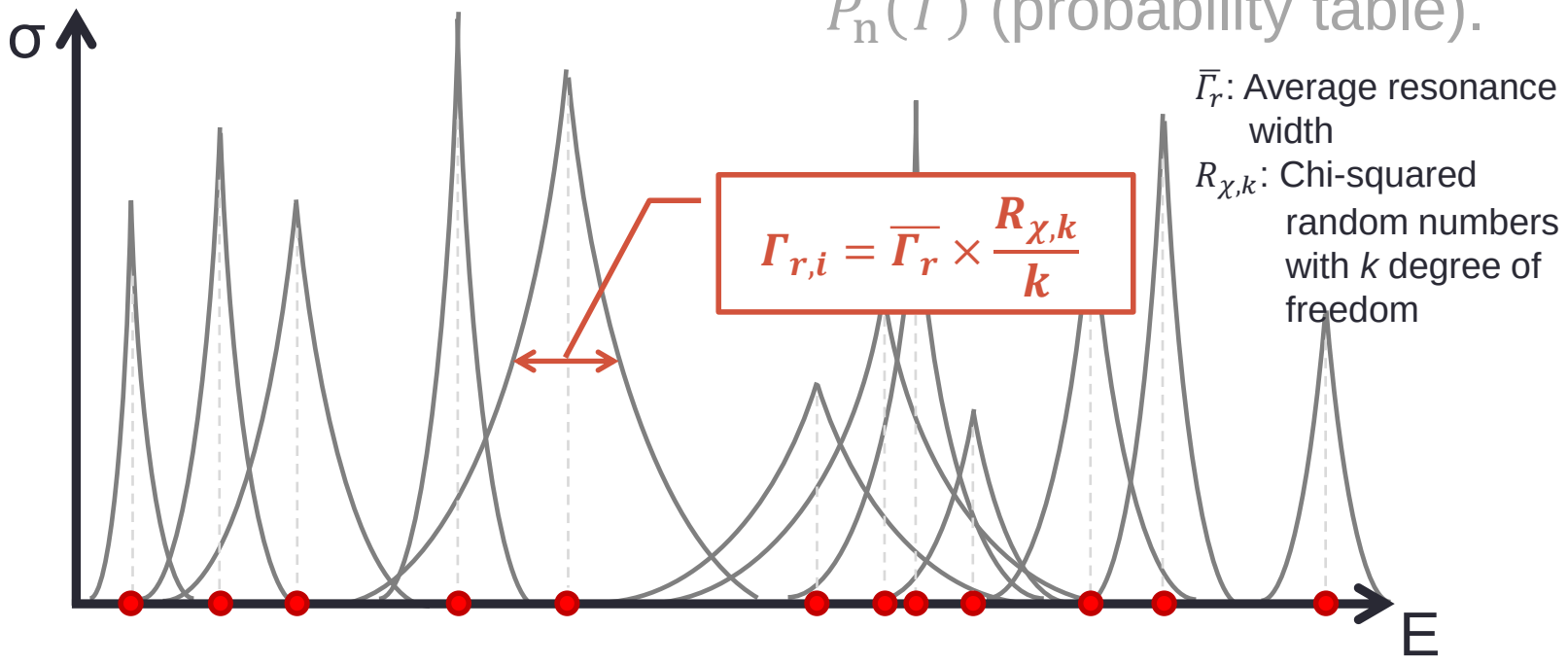
Generation of probability table (1/5)

1. **Determination of resonance energy $E_{r,i}$ using random number**
2. Determination of resonance width using random number
3. Calculation of XS and probability $P_{\mathrm{n}}(T)$ of $\sigma_{n-1} \leq \sigma_{t,j}(E_j, T) < \sigma_n$
4. Continuing generation of pseudo resonance structure (Pseudo resonance structure is called as "ladder")
5. Generation of table bins of average XS $\sigma_{x,n}$ and corresponding probability $P_{\mathrm{n}}(T)$ (probability table).



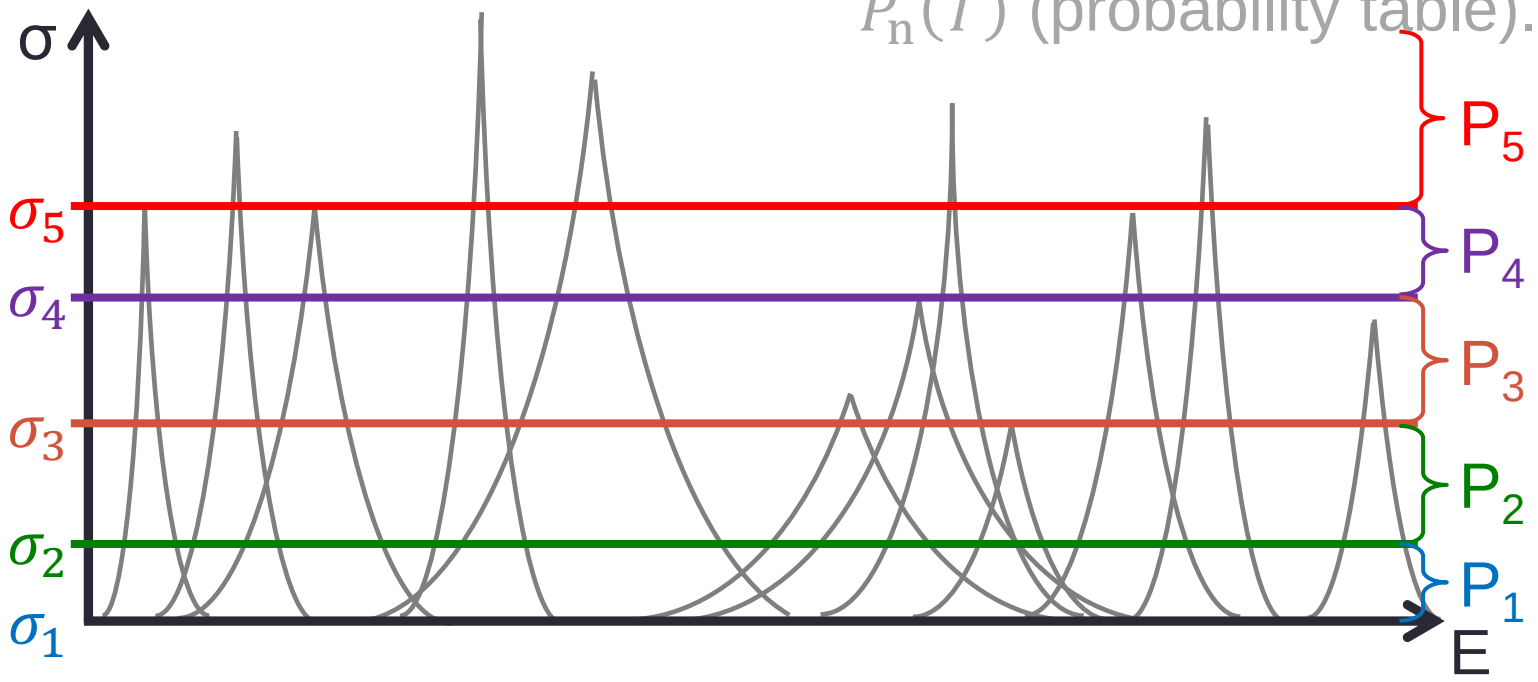
Generation of probability table (2/5)

1. Determination of resonance energy using random number
2. **Determination of resonance width $\Gamma_{r,i}$ using random number**
3. Calculation of XS and probability $P_{\mathrm{n}}(T)$ of $\sigma_{n-1} \leq \sigma_{t,j}(E_j, T) < \sigma_n$
4. Continuing generation of pseudo resonance structure (Pseudo resonance structure is called as "ladder")
5. Generation of table bins of average XS $\sigma_{x,n}$ and corresponding probability $P_{\mathrm{n}}(T)$ (probability table).



Generation of probability table (3/5)

1. Determination of resonance energy using random number
2. Determination of resonance width using random number
3. **Calculation of XS and probability $P_n(T)$ of $\sigma_{n-1} \leq \sigma_{t,j}(E_j, T) < \sigma_n$**
4. Continuing generation of pseudo resonance structure (Pseudo resonance structure is called as "ladder")
5. Generation of table bins of average XS $\sigma_{x,n}$ and corresponding probability $P_n(T)$ (probability table).



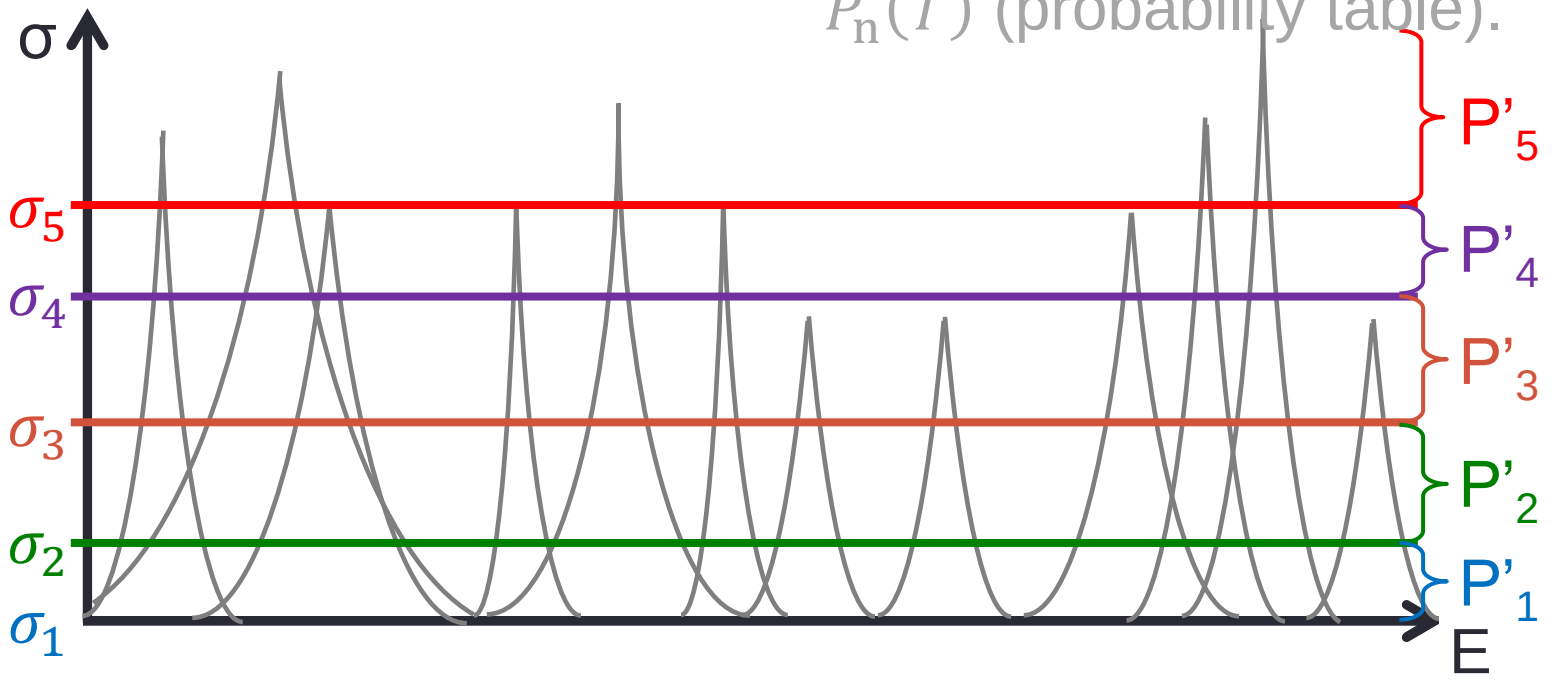
Generation of probability table (4/5)

1. Determination of resonance energy using random number
2. Determination of resonance width using random number
3. Calculation of XS and probability $P_{\mathrm{n}}(T)$ of $\sigma_{n-1} \leq \sigma_{t,j}(E_j, T) < \sigma_n$

4. Continuing generation of pseudo resonance structure

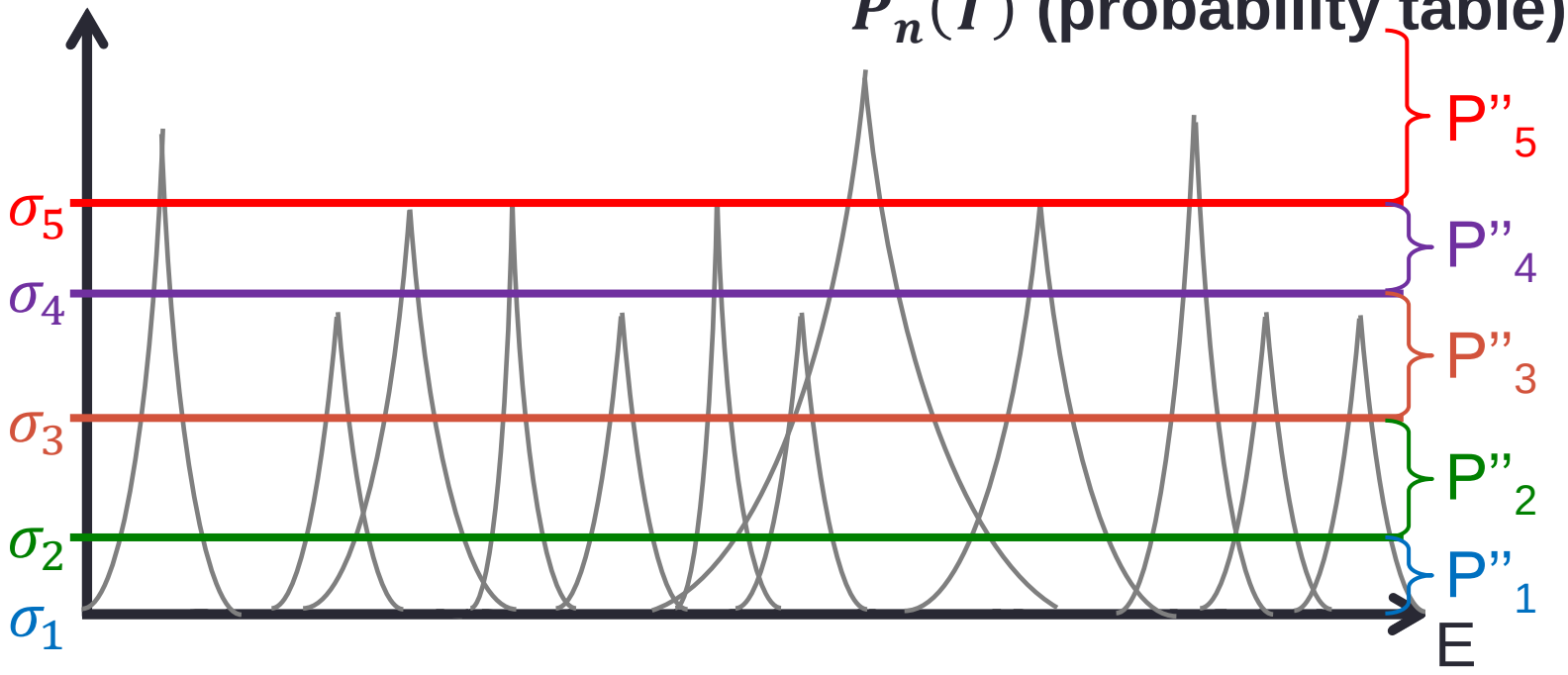
(Pseudo resonance structure is called as “ladder”)

5. Generation of table bins of average XS $\sigma_{x,n}$ and corresponding probability $P_{\mathrm{n}}(T)$ (probability table).



Generation of probability table (5/5)

1. Determination of resonance energy using random number
2. Determination of resonance width using random number
3. Calculation of XS and probability $P_{\mathrm{n}}(T)$ of $\sigma_{n-1} \leq \sigma_{t,j}(E_j, T) < \sigma_n$
4. Continuing generation of pseudo resonance structure (Pseudo resonance structure is called as "ladder")
5. **Generation of table bins of average XS $\sigma_{x,n}$ and corresponding probability $P_n(T)$ (probability table).**



Calculation of Doppler broadened XS in URR

- Single-Level Breit-Wigner (SLBW) resonance formula is used in URR.
- Approximated Doppler broadened XS can be directly obtained using psi-chi method when SLBW is adopted.
  - This approximation method cannot correctly calculate XS at peak and bottom of resonance.
  - This approximation has no large impact on probability table generation.

Radiative capture XS

$$\sigma_c(E,T) \cong \frac{\sigma_1 \Gamma_{\gamma r}}{\Gamma_r} \boldsymbol{\psi(\zeta, x)}$$

Elastic scattering XS

$$\sigma_{sc}(E,T) \cong \frac{\sigma_1 \Gamma_{nr}(E_1)}{\Gamma_r} \boldsymbol{\psi(\zeta, x)} + 2\sigma_1 k_1 a_c \boldsymbol{\chi(\zeta, x)} + \sigma_p$$

$$\psi(\zeta, x) = \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{1+y^2} e^{-\frac{\zeta^2}{4}(x-y)^2} dy$$

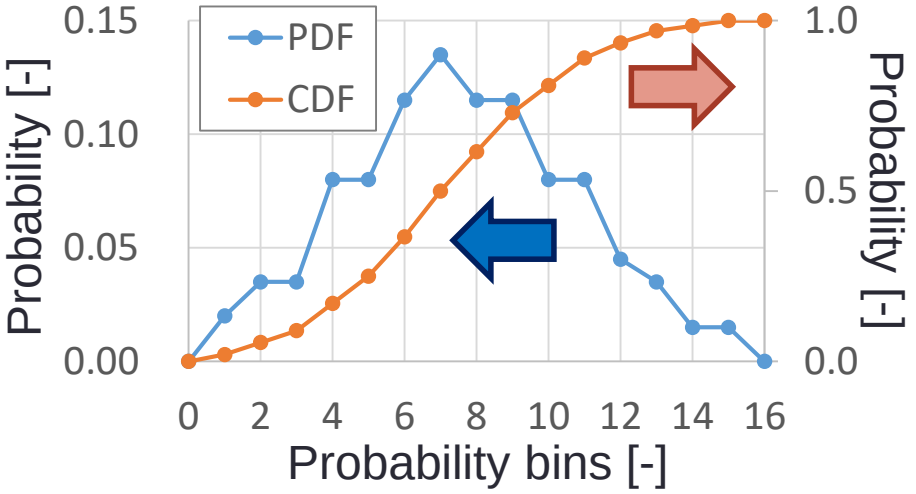
$$\chi(\zeta, x) = \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{y}{1+y^2} e^{-\frac{\zeta^2}{4}(x-y)^2} dy$$

ACE file generation

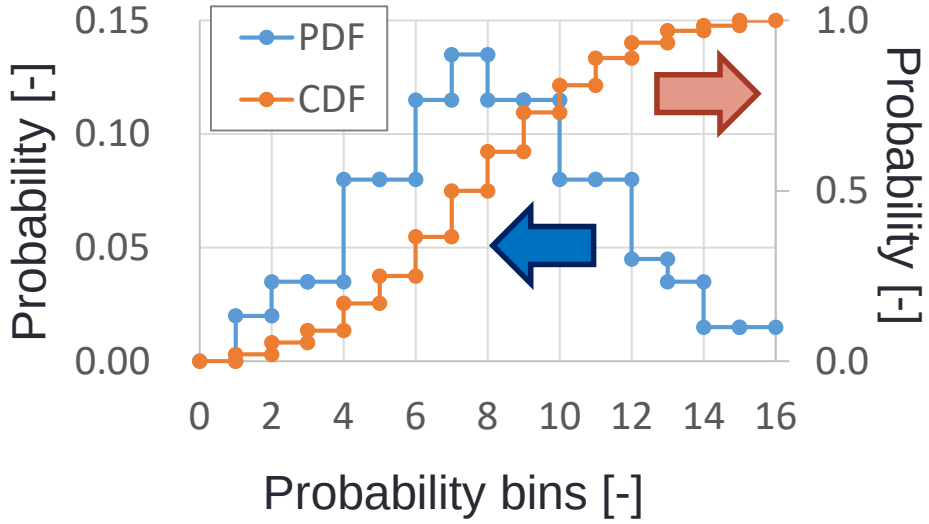
- Continuous energy Monte Carlo calculation codes use cumulative probability distribution (CDF).
  - Angular and energy distributions are converted to cumulative probability distribution.
  - PDF: Probability Density Function
  - CDF : Cumulative Density Function

[Example of PDF and CDF]

From linear-linear to PDF/CDF



From histogram to PDF/CDF



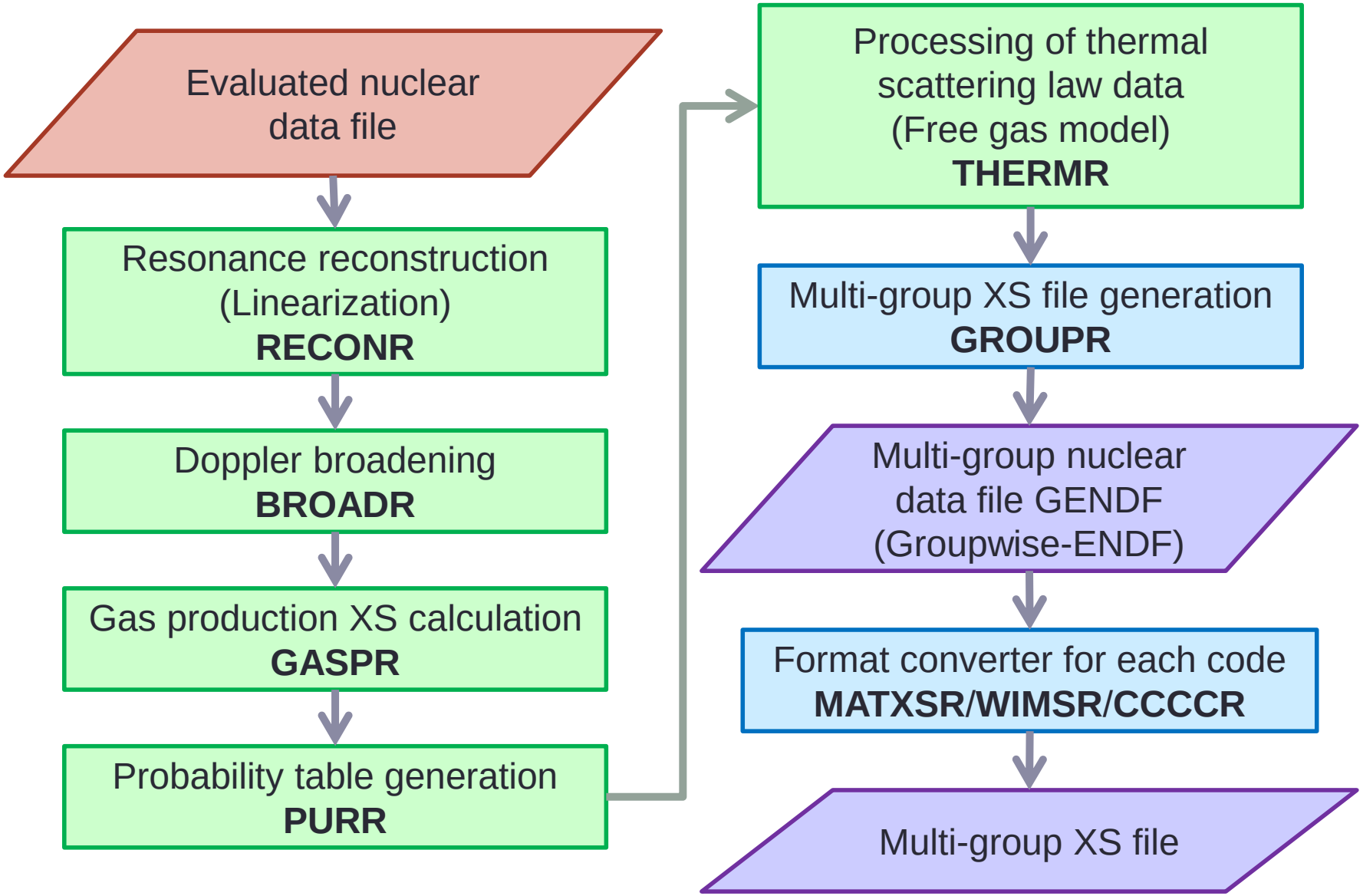
Multi-group XS calculation

- Multi-group XS ${\sigma^i}_{l,g}$ is obtained using continuous XS $\sigma^i(E)$ and weighting flux $\phi_l(E)$.

$$\sigma^i{}_{l,g} = \frac{\int_{E_g}^{E_{g-1}} \sigma^i(E)\phi_l(E)dE}{\int_{E_g}^{E_{g-1}} \phi_l(E)dE}, \quad \sigma^i{}_{l,g\to g'} = \frac{\int_{E_g}^{E_{g-1}} \sigma^i(E)\phi_l(E)dE \times \int_{E_{g'}}^{E_{g'-1}} \int_0^{\pi} f(E\to E',\mu)P_l(\mu)d\mu dE'}{\int_{E_g}^{E_{g-1}} \phi_l(E)dE}$$

  - NJOY uses the following weighting flux $\phi_l(E)$ to consider self-shielding effect.
  - $\phi_l^i(E) = \frac{C(E)}{\left[\sigma_t^i(E)+\sigma_0^i\right]^{l+1}}$
    - $C(E)$ is set by user input, $\sigma_t^i(E)$ is total XS, σ_0^i is background XS.

Multi-group XS file generation using NJOY



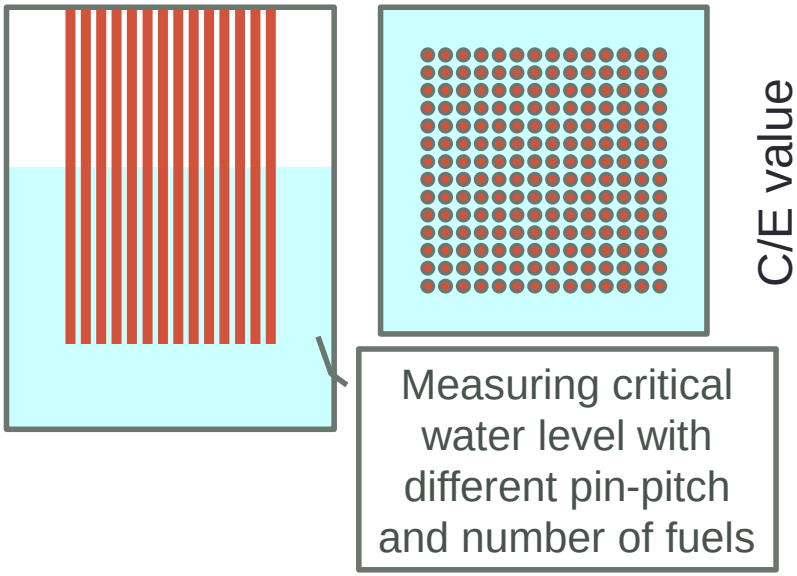
Consideration of TSL data

- Chemical state of material has large impact on thermal neutron scattering property.
  - Crystalline structure and chemical bounding of nuclide
  - H_2O, Polyethylene (CH_2), Graphite, Be, ZrH, …
- Evaluated nuclear data file gives **T**hermal **S**cattering **L**aw data to consider this thermal scattering.
  - Thermal scattering law data S(α, β) is given as a function of α and β.
    - TSL data is also called as "S(α, β)".
    - $\alpha = \left(E' + E - 2\mu\sqrt{EE'}\right)/A_0 k_B T$: dimensionless momentum transfer
    - $\beta = (E' - E)/k_B T$: dimensionless energy transfer

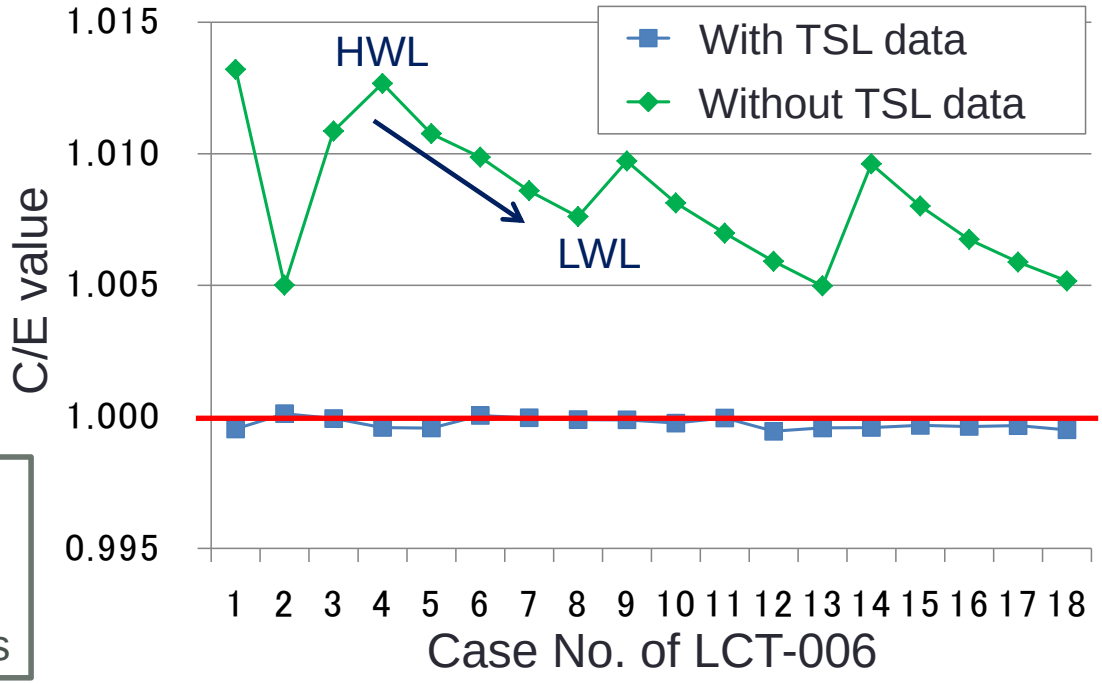
Impact of TSL data on k-effective

- Impact of TSL data on k-effective is evaluated.
  - Calculation geometry : LCT-006 (JAEA/TCA) from ICSBEP benchmark
  - Impart of TSL data on k-effective is 0.5-1.3%Δk
- TSL data is very important for thermal reactor.
  - Users have to use TSL data if TSL data is prepared in XS library.

[LCT-006 (TCA)]



[Impact of TSL data on k-effective]



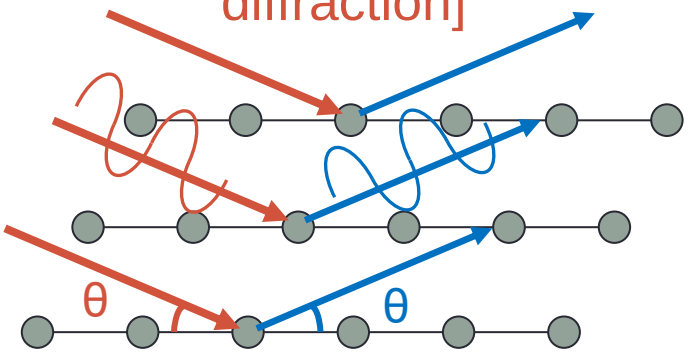
Thermal scattering

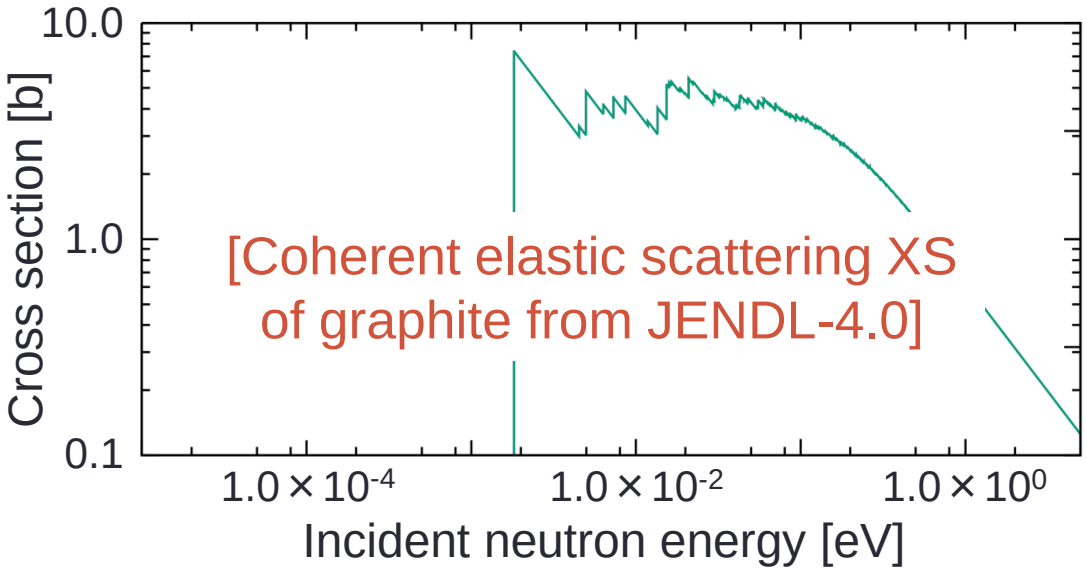
- ENDF-6 format handles three types of thermal scattering in MF=7.
- MF=7/MT=2
  - Coherent elastic scattering for crystalline materials
  - Incoherent elastic scattering for partially ordered materials
- MF=7/MT＝4
  - Incoherent inelastic scattering for non-crystalline materials
    - Represented by S(α, β)

Coherent elastic scattering

- Observed in crystalline materials such as graphite
  - Bragg diffraction
- Evaluated nuclear data file contains number of Bragg edges and its energy.
  - Nuclear data processing systems calculate coherent elastic scattering XS.
    - $\sigma^{coh}(E,E',\mu)=\frac{1}{E}\sum_i^{E_i<E}\sigma_c f_i \mathrm{e}^{-2WE_i}\delta(\mu-\mu_i)\delta(E-E')$

[Example of Bragg diffraction]

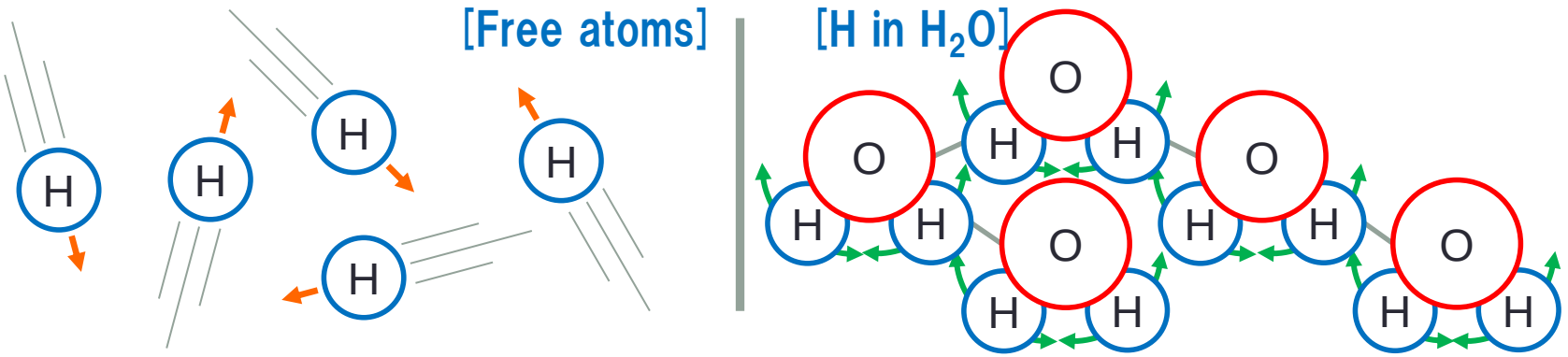




Incoherent inelastic scattering

- Observed in non-crystalline materials such as H_2O, ZrH, and BeO
  - Chemical binding effect of a molecule
  - Non-crystalline materials cannot move like a free atom.
- Thermal scattering law data is used to consider incoherent inelastic scattering.

[Comparison of free atoms and H in H_2O]



Calculation of incoherent inelastic scattering XS

- Incoherent inelastic scattering XS is calculated using $S(\alpha,\beta,T)$
  - $\frac{d^2\sigma}{d\Omega dE'}(E \to E',\mu,T) = \sum_n \frac{M_n \sigma_{bn}}{4\pi k_B T}\sqrt{\frac{E'}{E}}\, e^{-\frac{\beta}{2}} S_n(\alpha,\beta,T)$
  - μ is scattering cosine, M_n is number of atoms
- $S(\alpha,\beta,T)$ is **only available for given temperatures in TSL data**
  - ENDF-6 format gives interpolation law LI.
  - Interpolated $S(\alpha,\beta,T)$ is not correct and many nuclear processing systems, *e.g.*, NJOY and FRENDY, **only process given temperature**.
    - Nuclear data processing system users have to check the given temperature.
    - Given temperature is written in comment line (MF=1/MT=451).

S(α, β) of free gas (free atom)

- Free gas scattering law is required to consider up scattering.
  - S(α, β) of free gas: $S(\alpha,\beta)=\frac{1}{\sqrt{4\pi\alpha}}\exp\left\{-\frac{\alpha^2+\beta^2}{4\alpha}\right\}$
  - Evaluated nuclear data contains 0 K data.
  - Up scattering does not occur at 0 K.
- Continuous energy Monte Carlo codes treat free gas scattering law in their codes.
  - They do not need up scattering XS data in XS libraries.
  - Nuclear data processing systems do not have to process free gas scattering law.
- Multi-group calculation codes need incoherent inelastic scattering XS using free gas scattering law.
  - Nuclear data processing systems have to process free gas scattering law.