Overview of Evaluated Nuclear Data and Processing

Japan Atomic Energy Agency (JAEA)
Kenichi TADA

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

tada.kenichi@jaea.go.jp

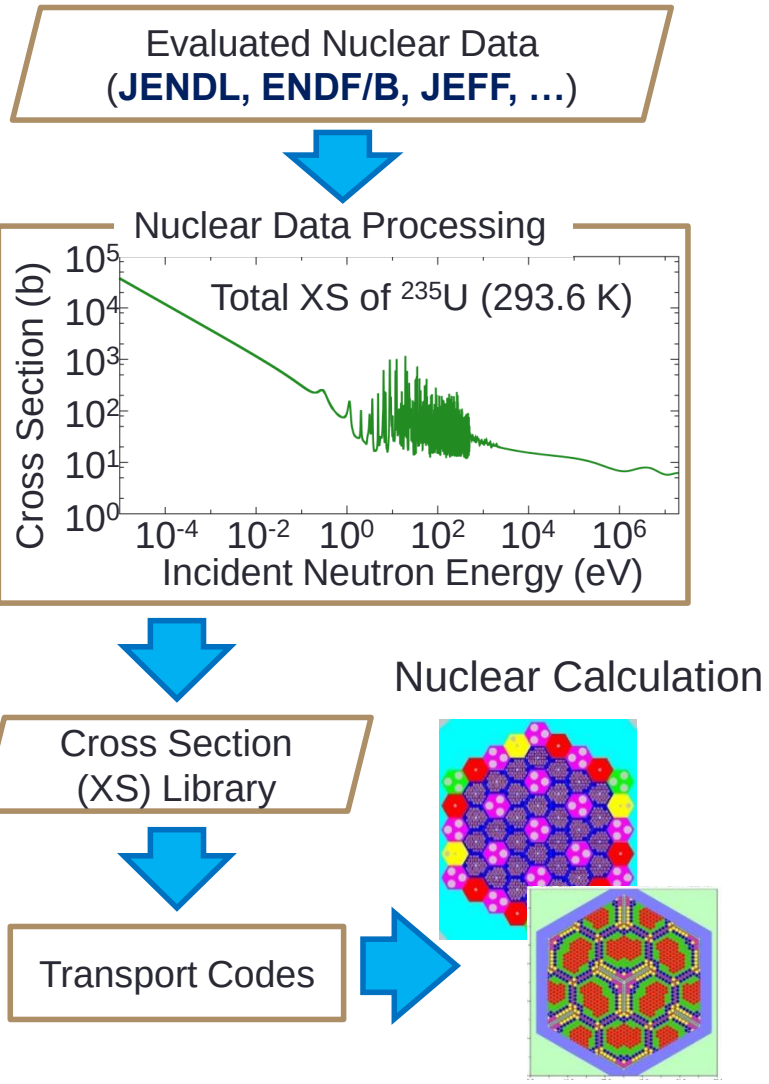
Outline

- Introduction of evaluated nuclear data library
  - MF & MT number
  - How to read evaluated nuclear data?
  - New nuclear data format GNDS
- Overview of nuclear data processing
  - Processing flow from evaluated nuclear data file to continuous energy / multi-group cross section (XS) file
  - Overview of each processing step
- Characteristics of nuclear data processing code FRENDY

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.

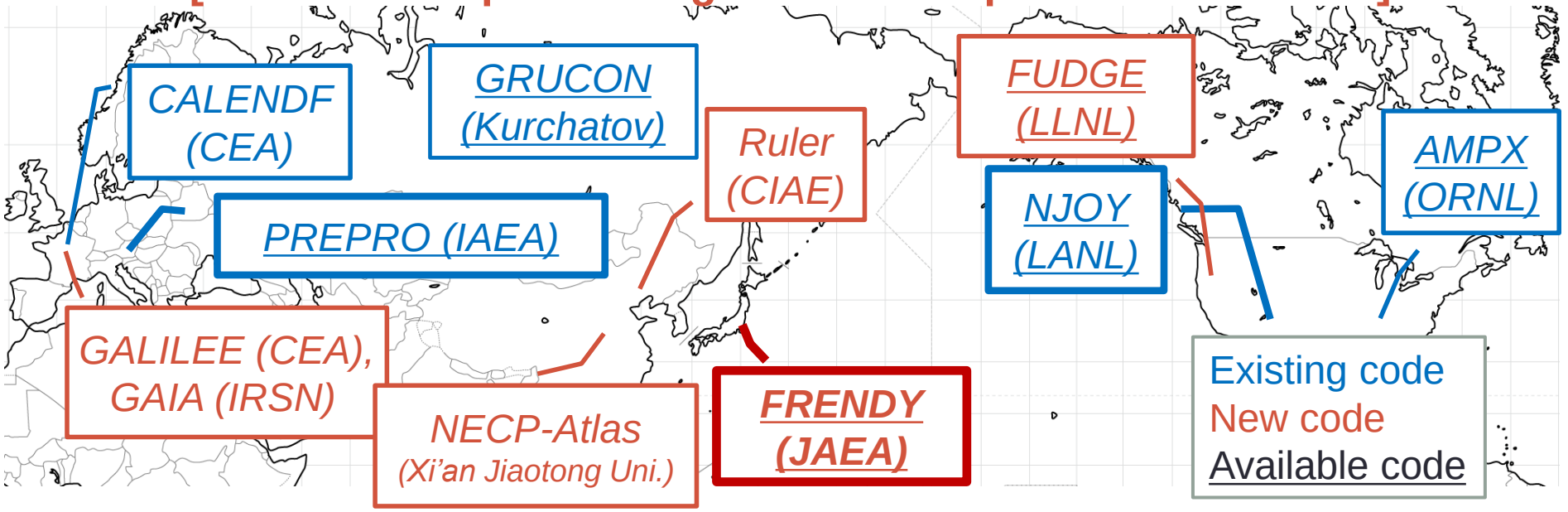
[Example of processing]



Status of nuclear data processing code development

- Development of nuclear data processing code has been started in many institutes.
  - To process their own nuclear data library
  - To handle new nuclear data format GNDS

[Nuclear data processing code development in the world]



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

What is evaluated nuclear data library?

- Evaluated nuclear data library contains many physical values.
  - Cross sections, energy and angular distributions of 2nd particle, fission yield, fission spectrum, …
- Well-known libraries
  - JENDL (Japan/JAEA)
    - **J**apanese **E**valuated **N**uclear **D**ata **L**ibrary
  - ENDF/B (USA/CSEWG)
    - **E**valuated **N**uclear **D**ata **F**ile
  - JEFF (Europe, OECD/NEA)
    - **J**oint **E**valuated **F**ission and **F**usion File
  - TENDL (PSI, IAEA)
    - **T**ALYS **E**valuated **N**uclear **D**ata **L**ibrary
    - By-product of TALYS
      - Automatically generated by TALYS
  - Others: BROND (Russia), CENDL (China)

What is “B” in ENDF/B?

- ENDF/B means ENDF Version B
- ENDF/A (ENDF Version A) is formed in 1965 (BNL-8381).
  - Update version of UKNDL (United Kingdom Nuclear Data Library)
  - ENDF/A is not completed and it cannot be used for nuclear calculation.
- ENDF/B grew out of ENDF/A in 1966 (BNL-50066)
  - The latest version is ENDF-6 format.
    - ENDF/B-VI, -VII, and -VIII libraries use ENDF-6 format.
      - ENDF-6: format name
      - ENDF/B-VI, -VII, and -VIII: library name

Ref. : https://www.nndc.bnl.gov/endf/history.html

Physical values contained in nuclear data

Mainly used for neutron transport calculation

- Cross section
  - Probability that a nuclear reaction will occur
- Angular distribution of 2nd particle
- Energy spectrum of 2nd particle
- Resolved and unresolved resonance parameters
- Number of neutrons per fission
- Fission spectrum
- Thermal scattering law data (S(α,β))

Mainly used for burnup calculation

- Fission product yield
- Radioactive decay data
  - $T_{1/2}$ (hal-life) and transition probability
- γ ray data (Transition probability, intensity, energy, …)
- Nuclear structure data (Level energy, spin, parity, …)
- Mass, abundance, …

Typical use of evaluated nuclear data

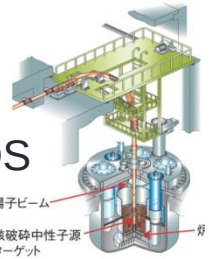
Energy use

LWR

HTGR

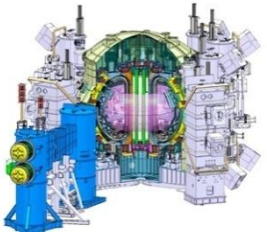
FBR

ADS



Reprocessing

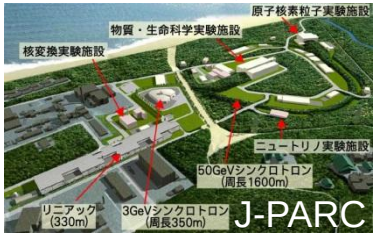
Fusion



Evaluated nuclear data library

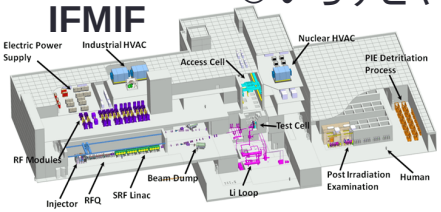
Space technology

Medical

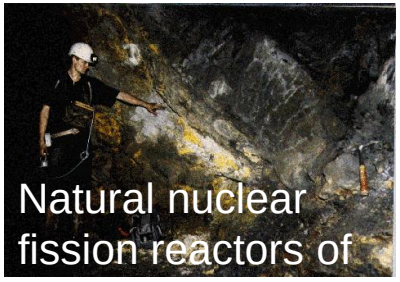


© いらすとや

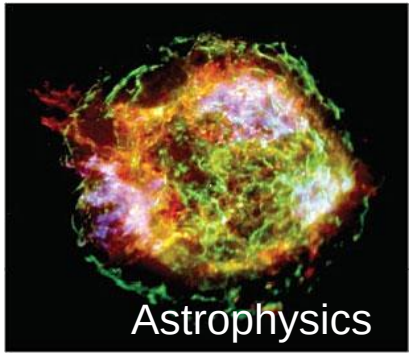
IFMIF



Non-Energy use



Natural nuclear fission reactors of Oklo



Astrophysics

© NASA

Others

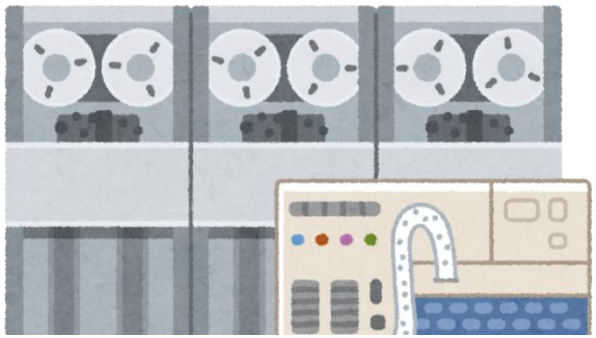
ENDF-6 format

- ENDF-6 format is a de facto standard.
  - Prepared for ENDF/B library
  - Managed by CSEWG in USA
    - Cross Section Evaluation Working Group
- OECD/NEA/NSC/WPEC/SG-38 formed new nuclear data format GNDS.
  - GNDS: **G**eneralized **N**uclear **D**ata **S**tructure
    - Serializable in any nested hierarchical meta-language (XML/HDF5/JSON)
    - Easy to read
  - Reference (GNDS format manual)
    - Specifications for the Generalized Nuclear Database Structure (GNDS)
    - https://www.oecd-nea.org/science/wpec/documents/7519-GNDS.pdf

Data structure of ENDF-6 format

- Construction of data; four structures
- tape > material > file > section
  - tape : One or more material data
  - material : One nuclide or matrial (H_2O, ZrH, …)
    Subdivided by MAT number
  - file : Data block
    (XS, angular and energy distribution, …)
    Subdivided by MF number
  - section : Reaction data
    Subdivided by MT number
- Latest evaluated nuclear data library contains one material data in each file.
  - “Tape” is a relic of the past.

[Example of tape]



MAT number

- MAT : Proton number "**ZZ**" + isotope number "**NN**"
  - Significant digits of MAT number are 4 : MAT=ZZNN.
  - The lightest stable isotope is assigned 25.
    - If there is no stable isotope, *e.g.*, Technetium and Uranium, the lightest naturally-occurring isotope number is assigned 25.
  - If atomic mass number increases/decreases **1**, isotope number increases/decreases **3**.
    - One ground state and two metastable states, *e.g.*, ^{156}Tb, ^{156m1}Tb, and ^{156m2}Tb, are available.
  - Transuranic elements are set by other rule.
- Natural elements use "**00**" for isotope number
  - JENDL-4.0 contains natural carbon as MAT=600.
- Example of MAT number
  - ^{1}H:125, ^{2}H:128, ^{156}Tb:6516, ^{156m1}Tb:6517, ^{156m2}Tb:6518
  - ^{230}U:9213, ^{235}U:9228, ^{238}U:9237
  - ^{242}Am:9546, ^{242m}Am:9547

Ref : BNL-203218-2018-INRE

Important MF numbers for neutronics calculations

- **MF= 1**: General information, comment, number of neutrons per fission
- **MF= 2**: Resonance parameters
- **MF= 3**: Cross sections
- **MF= 4**: Angular distribution
- **MF= 5**: Energy distribution
- **MF= 6**: Angular and energy distribution
- **MF= 7**: Thermal scattering law data
- **MF= 8**: Decay and fission product yields
- **MF= 9**: Multiplicities of radioactive products
- **MF=10**: Production XS for radionuclides
- **MF=11**: General comments on photon production
- **MF=12-15**: Photon production data
- **MF=30-40**: Covariance data

BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
SVN Commit: Revision 215

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown
With contributions from
N. Holden and G. Hedstrom

February 1, 2018

National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973-5000
www.nndc.bnl.gov

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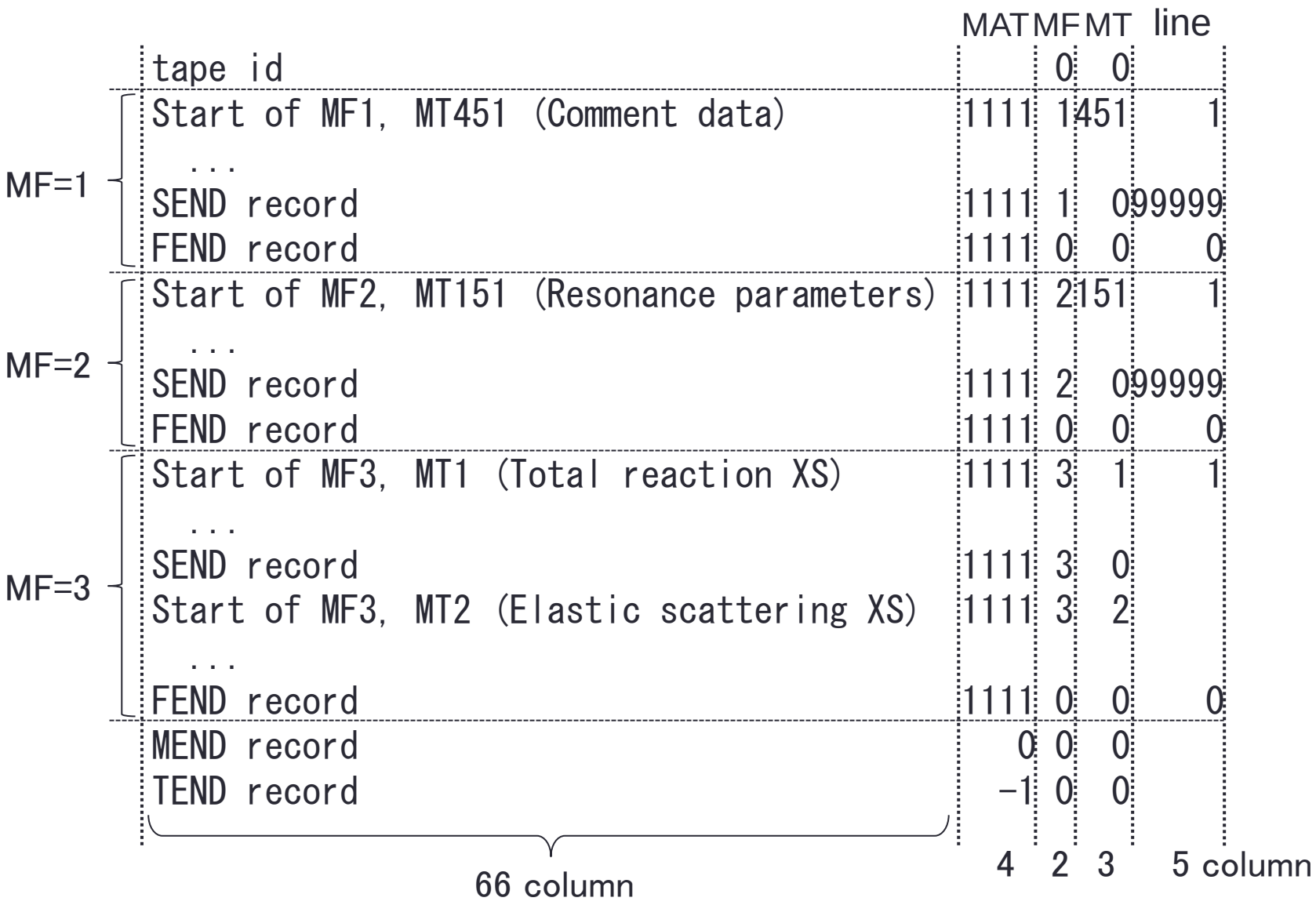
Ref : BNL-203218-2018-INRE

Important MT numbers for neutronics calculations

- **MT= 1** : (n, total)
- **MT= 2** : (z, elastic)
- **MT= 3** : (z, nonelastic)
- **MT= 16** : (z, 2n)
- **MT= 18** : (z, fission)
- **MT=51-90**: (z, n_x)
- **MT= 91** : (z, n_c)
- **MT=102** : (z, γ)
- **MT=151** : Resonance parameters (MF=2)
- **MT=452** : Number of neutrons per fission $\bar{\nu}_T$ (MF=1)

Ref : BNL-203218-2018-INRE, Appendix B

Data structure of ENDF-6 format



Example of ENDF-6 format

(n,2n) cross section of Fe-56 from JENDL-4.0

MF
MAT ↓ MT

2.605600+4	5.545440+1	0	0	0	0	2631	3	16	1
−1.120270+7	−1.120270+7	0	0	1	11	2631	3	16	2
11	2	0	0	0	0	2631	3	16	3
1.140470+7	0.000000+0	1.170000+7	1.622410−2	1.200000+7	4.800450−2	2631	3	16	4
1.300000+7	2.138200−1	1.400000+7	3.891650−1	1.500000+7	5.134000−1	2631	3	16	5
1.600000+7	5.817500−1	1.700000+7	6.107500−1	1.800000+7	6.118000−1	2631	3	16	6
1.900000+7	5.977000−1	2.000000+7	5.759000−1			2631	3	16	7
						2631	3	0	99999

11 column × 6

All numbers are given in fields of 11 columns.

- ±1.234567±*n*
- ±1.23456±*nn* (*nn*≦38)
- ±1.23456789

Single precision (32 bit)

Example of XS data (MF=3)

(n,2n) cross section of Fe-56 from JENDL-4.0

						MAT	MF	MT		
2.605600+4	5.545440+1	0	0	0	0	2631	3	16	1	HEAD
−1.120270+7	−1.120270+7	0	0	1	11	2631	3	16	2	TAB1
11	2	0	0	0	0	2631	3	16	3	
1.140470+7	0.000000+0	1.170000+7	1.622410−2	1.200000+7	4.800450−2	2631	3	16	4	
1.300000+7	2.138200−1	1.400000+7	3.891650−1	1.500000+7	5.134000−1	2631	3	16	5	
1.600000+7	5.817500−1	1.700000+7	6.107500−1	1.800000+7	6.118000−1	2631	3	16	6	
1.900000+7	5.977000−1	2.000000+7	5.759000−1			2631	3	16	7	
						2631	3	099999		SEND

[MAT, 3, MT/ ZA, AWR, 0, 0, 0, 0] HEAD
[MAT, 3, MT/ QM, QI, 0, LR, NR, NP/ Eint/ σ(E)] TAB1
[MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

ZA, AWR : 1000.0 × Z + A, mass quantities for materials
QM : Mass-difference Q value (eV)
QI : Reaction Q value
LR : Complex or “breakup” reaction flag

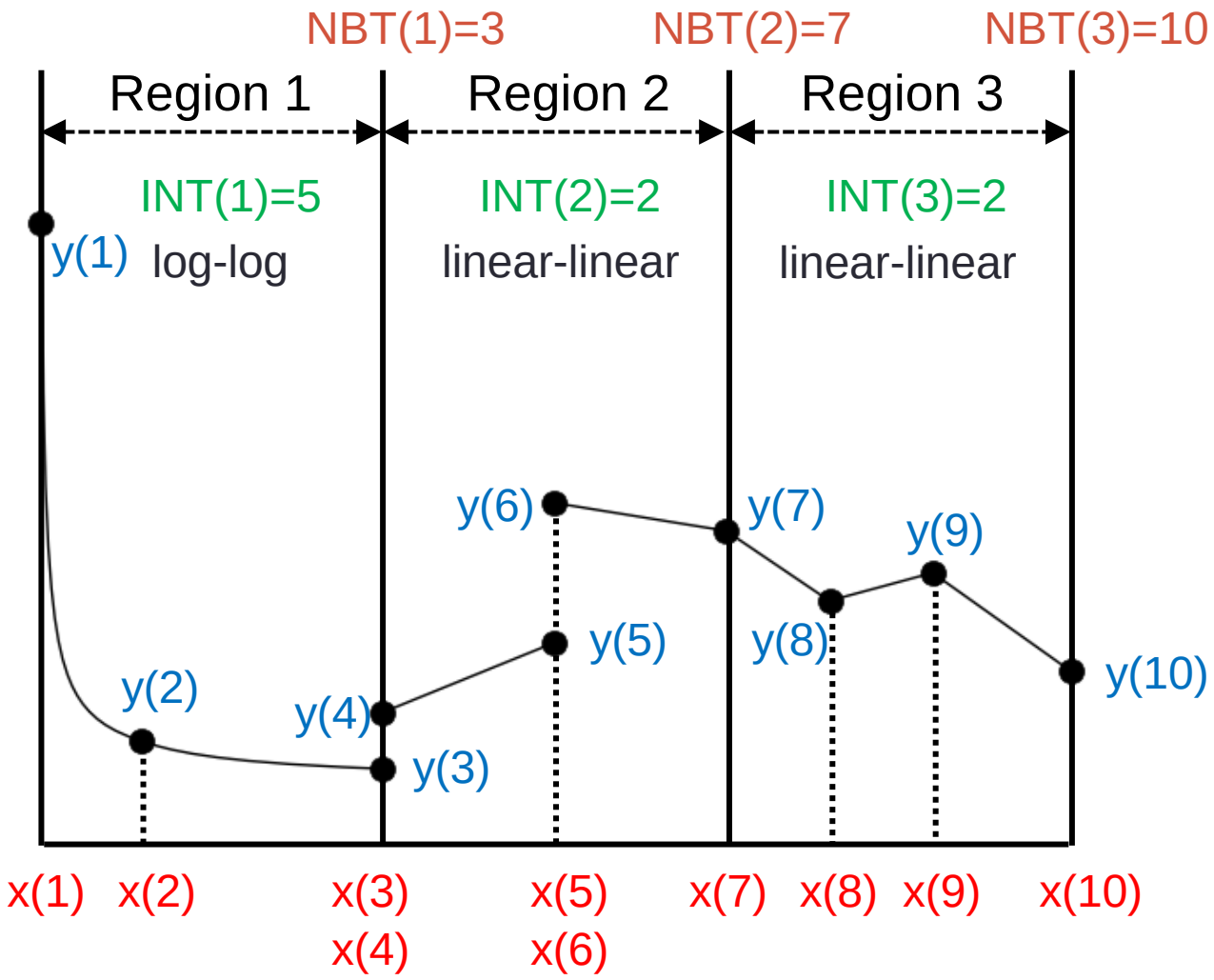
Data form of ENDF-6 format

- Given as a table
  - 1-D or 2-D array : $(E_1, \sigma_1), (E_2, \sigma_2), \cdots$
  - Cross section data, angular and energy distribution, …
- Given as a parameters of a function
  - Resonance formula, Legendre polynomial, …

Interpolation of tabulated 1-D array

NR = 3
Number of regions
(NBT and INT)

NP = 10
Number of data
(X and Y)



Tabulated data gives (X, Y) data and interpolation.

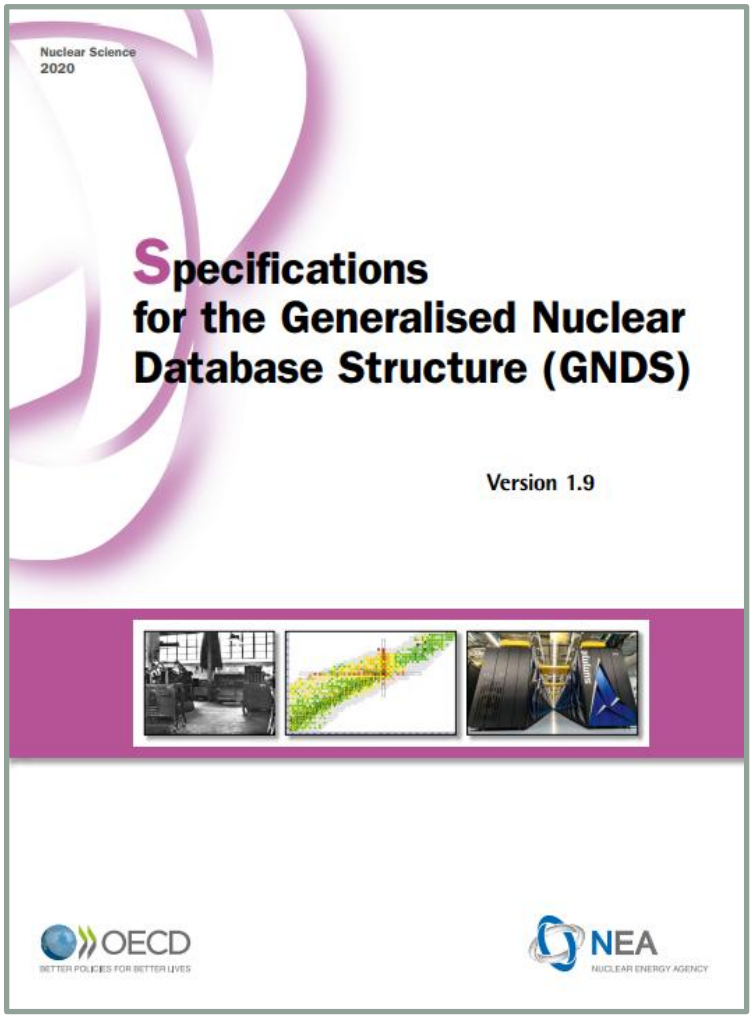
Interpolation types used in ENDF-6 format

- **INT=1:** histogram, constant
- **INT=2:** linear-linear
- **INT=3:** y - ln(x) (linear-log）
- **INT=4:** ln(y) - x（log-linear）
- **INT=5:** ln(y) - ln(x)（log-log）
- **INT=6:** Special 1-D law, used for charged particle XS
- **INT=11-15:** method of corresponding points （2-D array）
- **INT=21-25:** Unit base interpolation (2-D array）

$$\sigma(E) = \frac{A}{E} e^{-\frac{B}{\sqrt{E-T}}}$$

New nuclear data format : GNDS

- Formed by OECD/NEA WPEC/SG-38
  - Managed by WPEC/EG-GNDS
  - **G**eneralized **N**uclear **D**ata **S**tructure
  - **W**orking **P**arty on international nuclear data **E**valuation **C**o-operation
- LLNL develops FUDGE and GIDI plus to handle GNDS.
  - FUDGE is nuclear data processing code for LLNL neutronics codes.
  - FUDGE can convert from ENDF-6 format to GNDS format.



Ref : https://www.oecd-nea.org/science/wpec/documents/7519-GNDS.pdf

Example of GNDS format (XML form)

(n,2n) XS of Fe-56 from JENDL-4.0

(n,2n) reaction

Reaction

```
<reaction label="29" outputChannel="n[multiplicity:'2']
  + Fe55 + gamma" date="1987-03-01" ENDF_MT="16">
  <crossSection nativeData="linear">
    <linear xData="XYs" length="11" accuracy="0.001">
      <axes>
        <axis index="0" label="energy_in" unit="eV"
          interpolation="linear,linear" frame="lab"/>
        <axis index="1" label="crossSection" unit="b"
          frame="lab"/></axes>
      <data> 1.14e7 0.00000 1.17e7 0.0162241 1.20e7 0.0480045
             1.30e7 0.21382 1.40e7 0.3891650 1.50e7 0.5134000
             1.60e7 0.58175 1.70e7 0.6107500 1.80e7 0.6118000
             1.90e7 0.59770 2.00e7 0.5759000 </data></linear>
  </crossSection>
  <outputChannel genre="NBody" Q="-11202700 eV">
    <product name="n" label="n" multiplicity="2"
      ENDFconversionFlag="MF6">
      <distributions nativeData="Legendre">
        <Legendre nativeData="LegendrePointwise">
```

XS

Interpolation

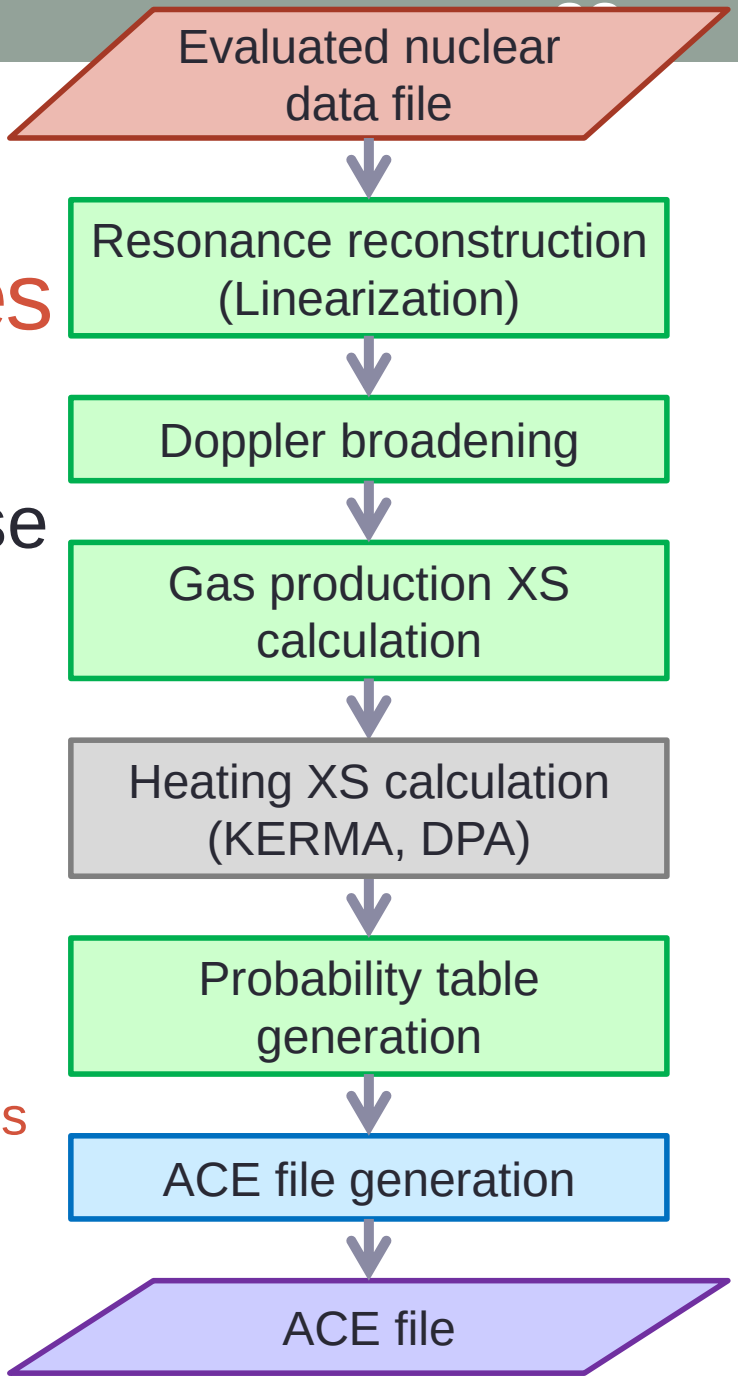
XS data

Angular and energy distribution of 2nd particle

Overview of nuclear data processing

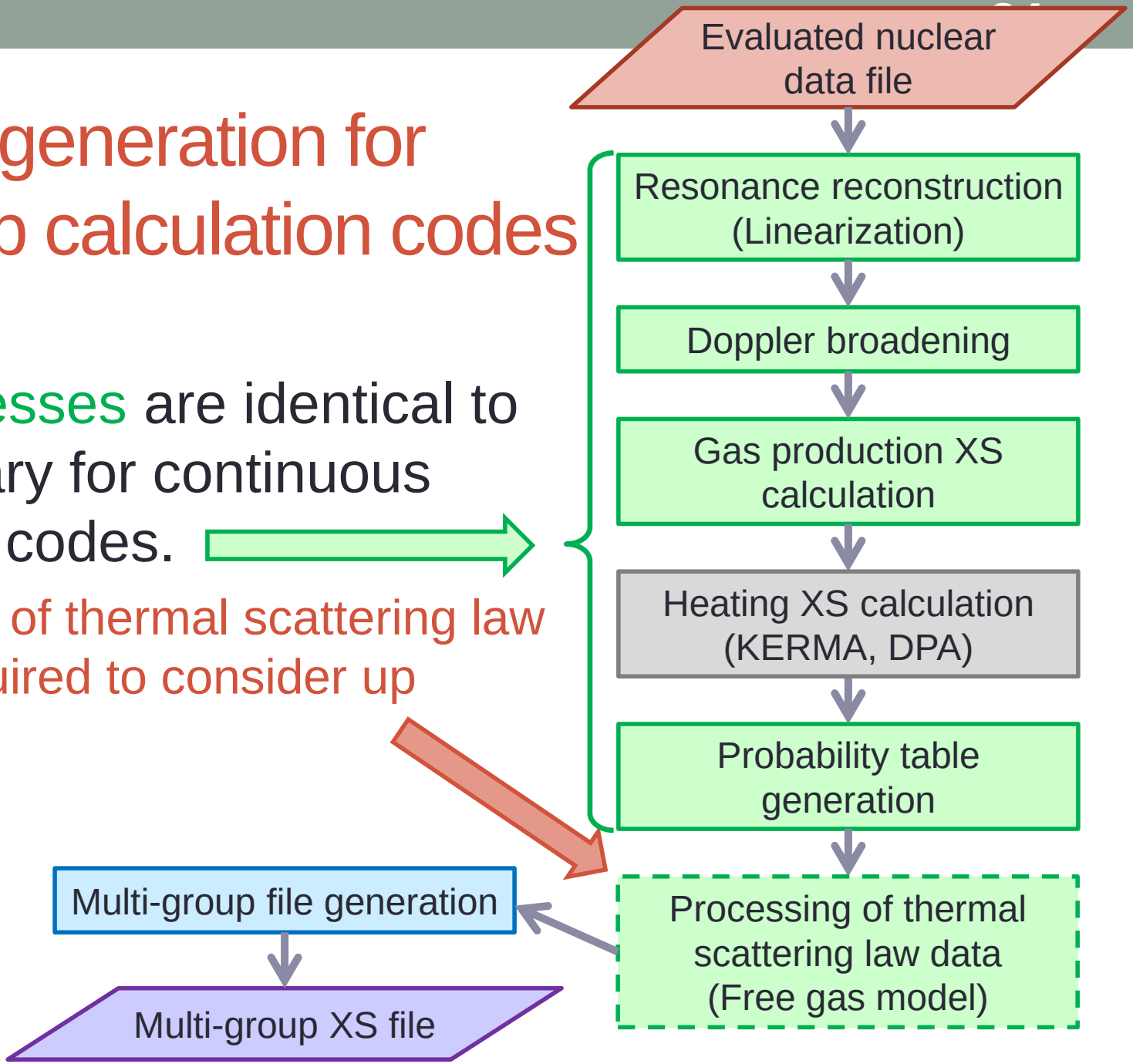
XS library generation for continuous energy MC codes

- 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



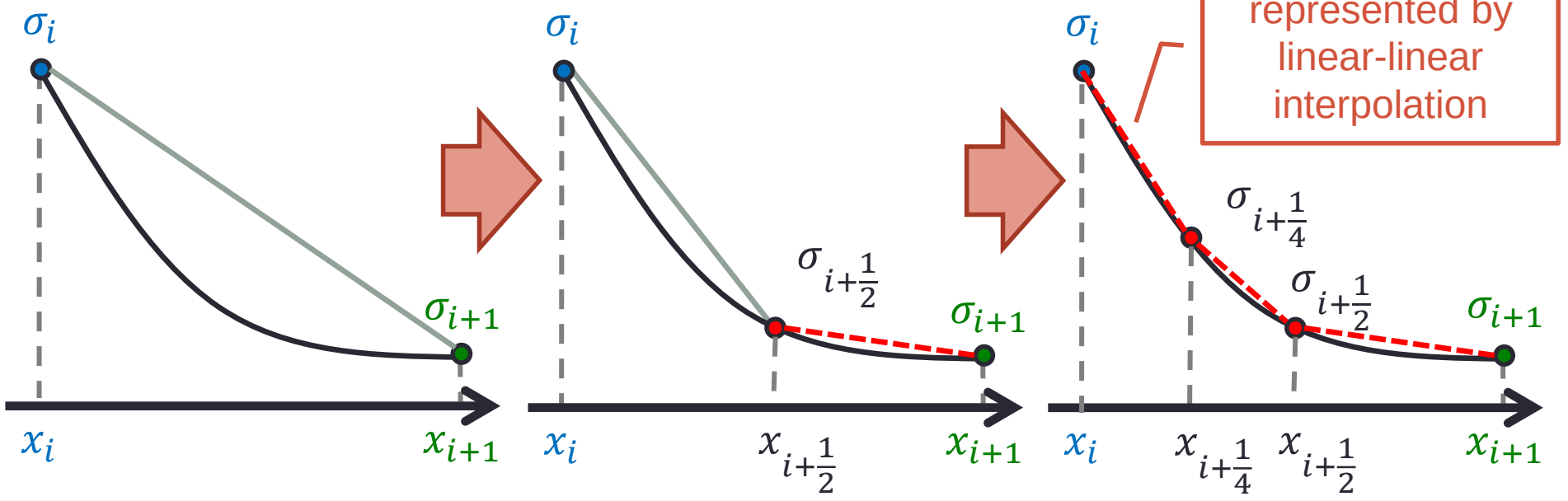
XS library generation for multi-group calculation codes

- 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.



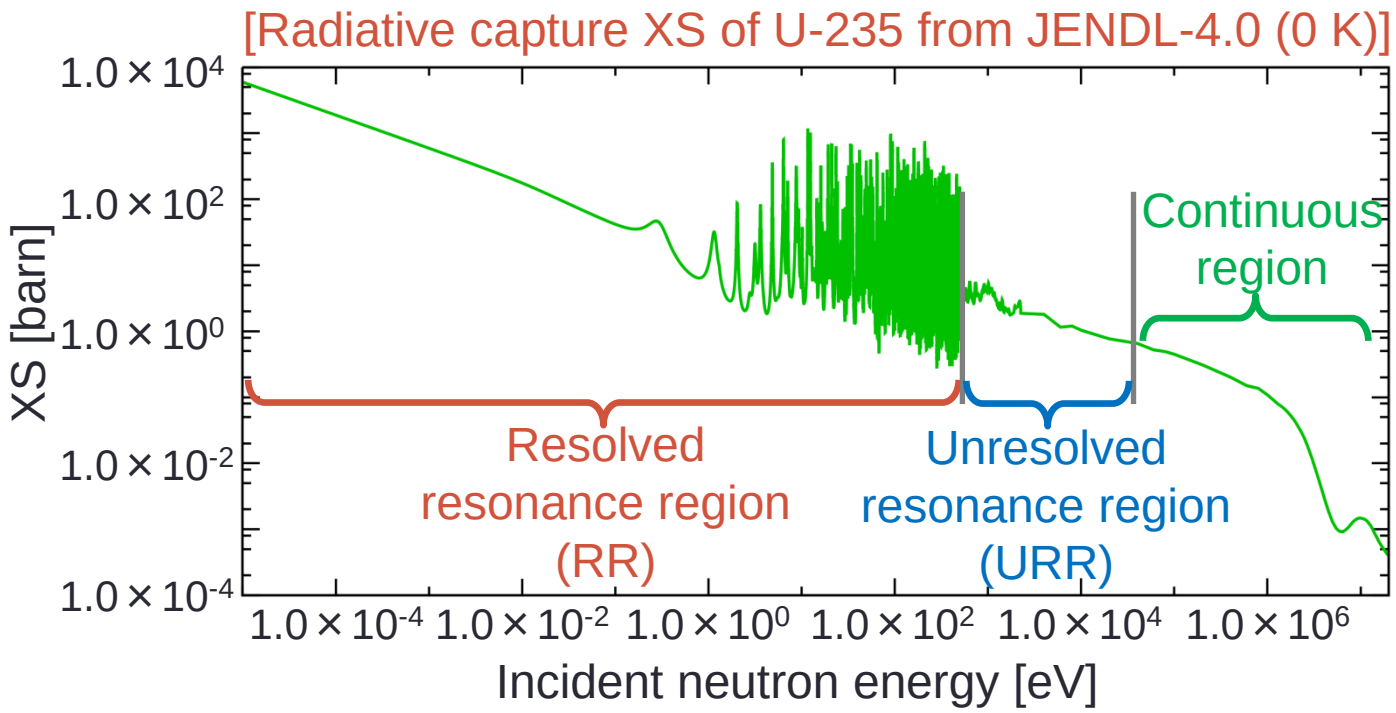
Linearization

- 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

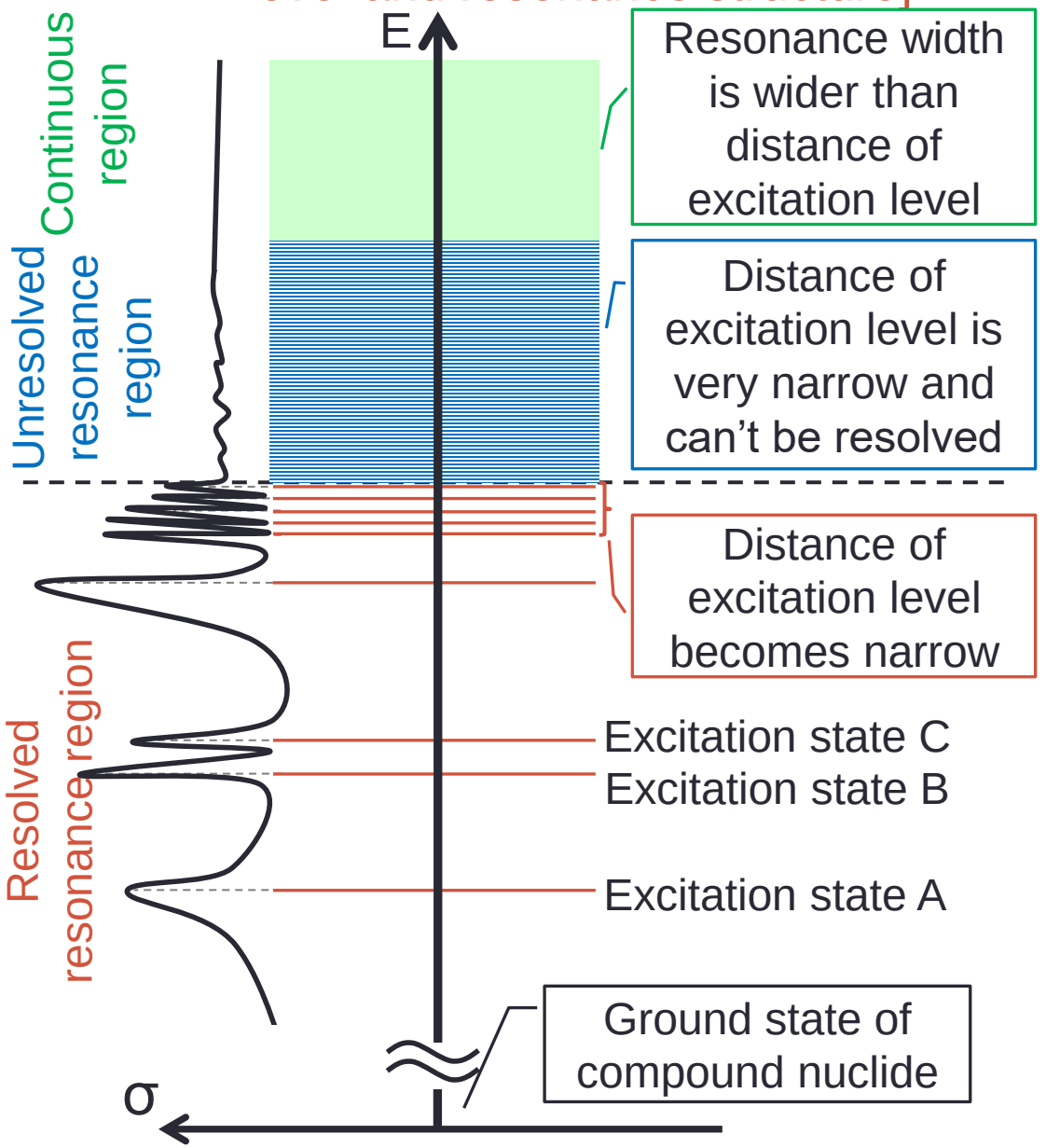
- XS of resolved and unresolved resonance regions are given as resonance parameters of resonance formula.
  - Calculation of XS in resolved resonance region
  - Calculation of averaged XS in unresolved resonance region
  - XS in continuous region is given in MF=3.



What is resonance?

- XS becomes larger.
  - When sum of induced energy and binding energy is equal to excitation level of compound nuclide.
- Resonance energy is identical to the excitation level.

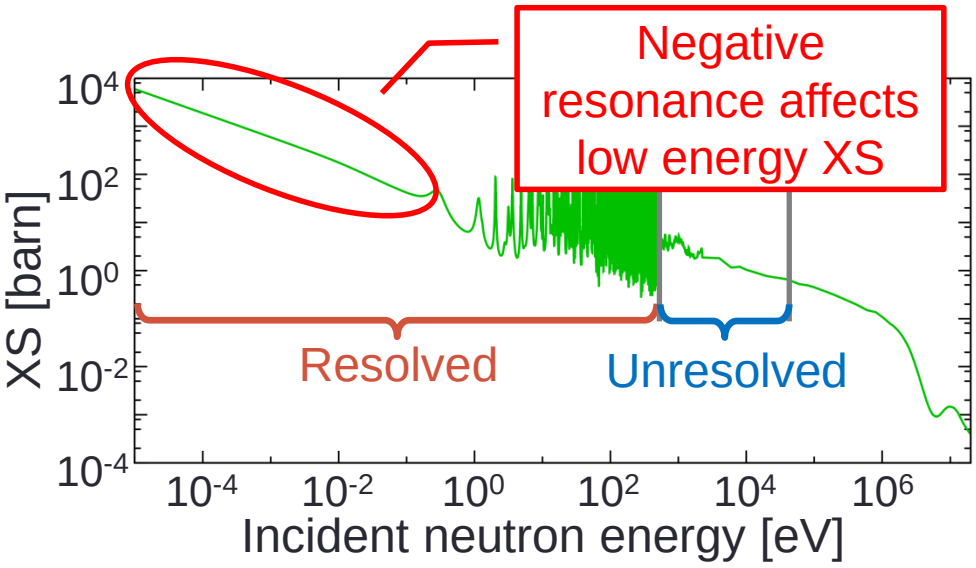
[Relationship between excitation level and resonance structure]



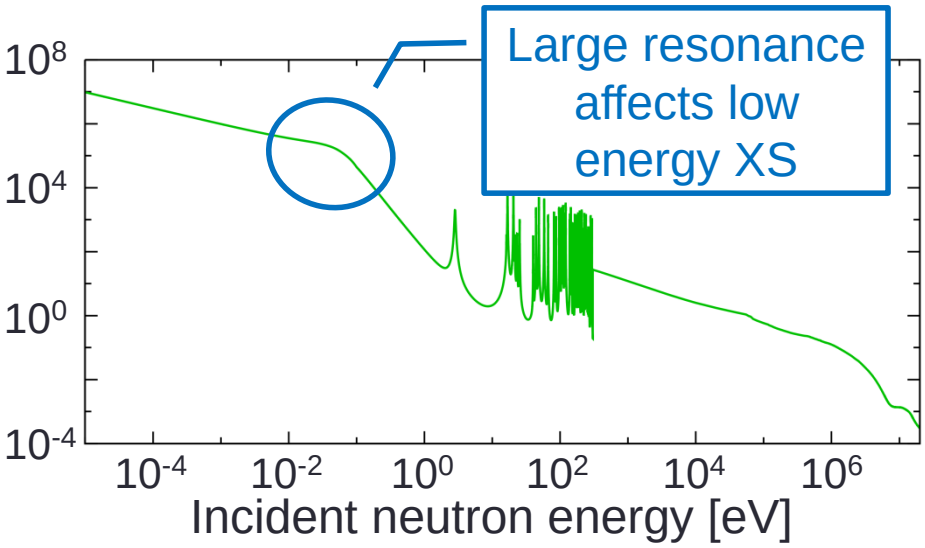
Cross section in low energy region

- XS in low energy region can be approximated by 1/v low.
  - The difference between actual XS and 1/v low is effect of negative resonance.
    - Several nuclides, *e.g.*, Gd-157, have large resonance in low energy region and its also affect XS in low energy region.

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

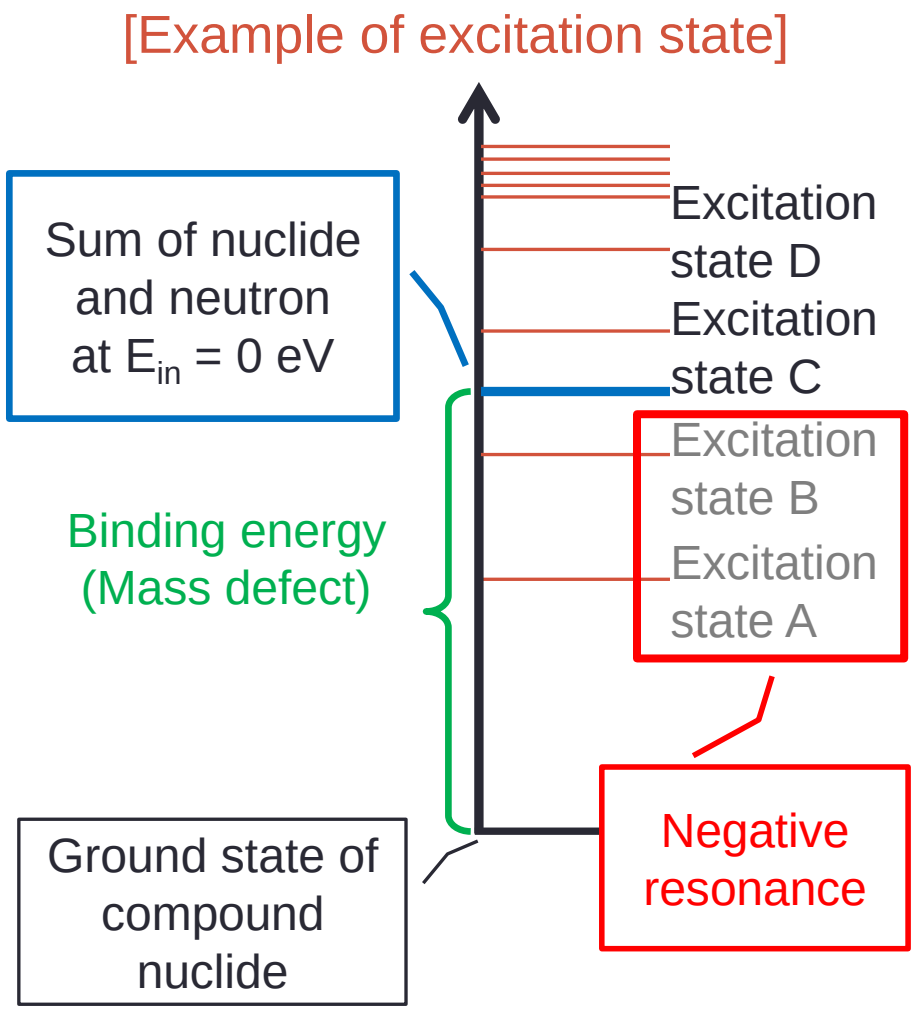


[Radiative capture XS of Gd-157 from JENDL-4.0 (0 K)]



What is negative resonance?

- Resonance of excitation state lower than sum of nuclide and neutron energy at E_{in} = 0 eV .
  - Compound nuclide is not grand state when 0 eV neutron is captured.
  - Binding energy should be considered.



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.

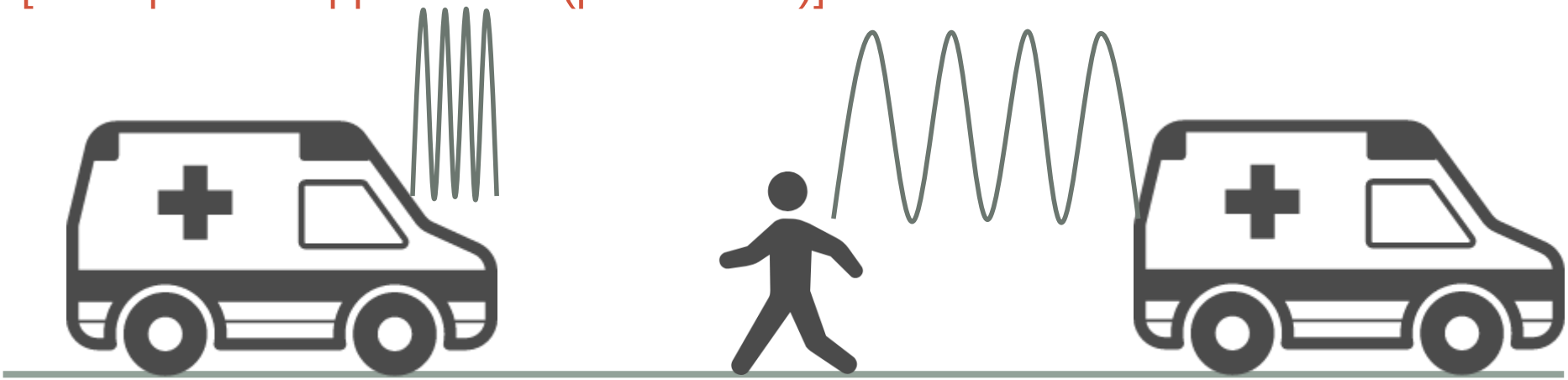
Doppler broadening

- 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 code 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.

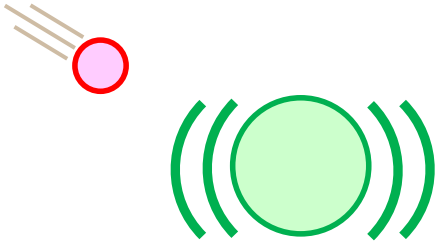
[Example of Doppler effect (pitch heard)]



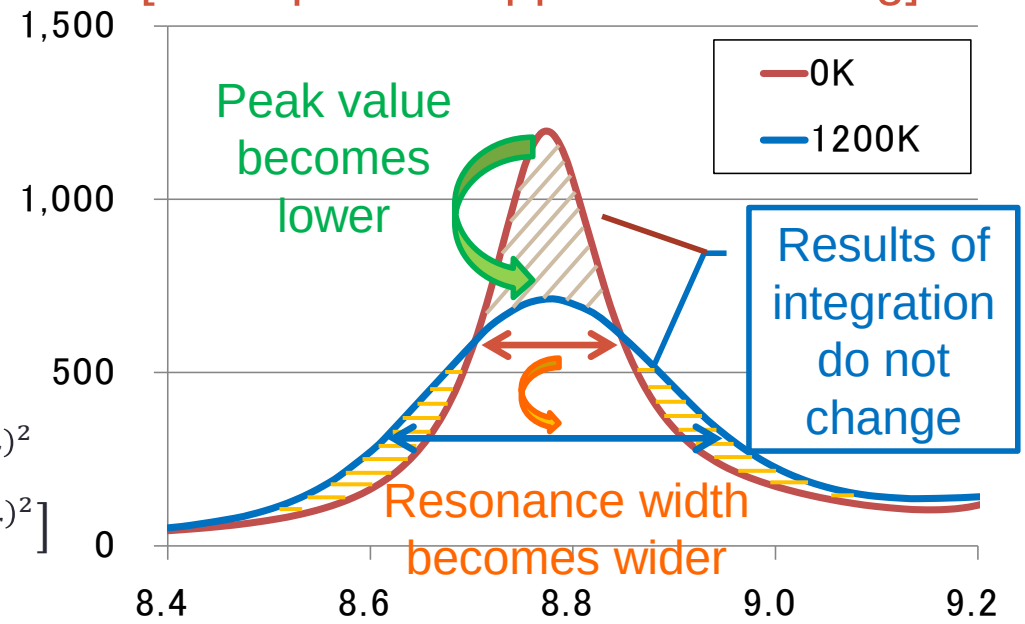
Doppler broadening

- 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 code 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 code 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)

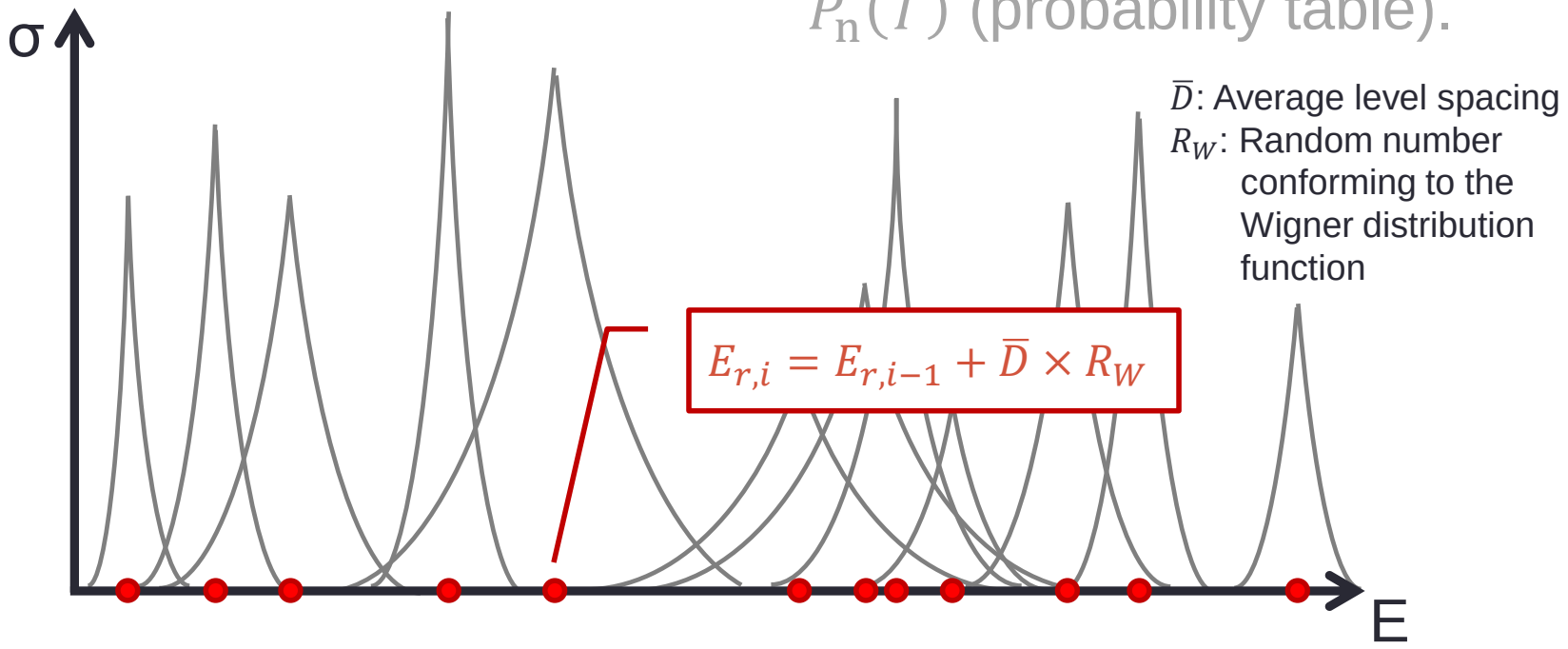
- Bondarenko-type self-shielded XS $\sigma_x(E)$ is used.
  - $\sigma_x(E)$ is obtained by probability table $P_i(E)$.
    - $$\sigma_x(E) = \frac{\sum_{i=1}^{bin} \frac{P_i(E)\sigma_{x,i}(E)}{\sigma_0+\sigma_{t,i}(E)}}{\sum_{i=1}^{bin} \frac{P_i(E)}{\sigma_0+\sigma_{t,i}(E)}}$$
      - x: reaction type $(t, \mathrm{sc}, f, \gamma)$, 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	$P_1 = 0.56$	$P_2 = 0.36$	$P_3 = 0.08$

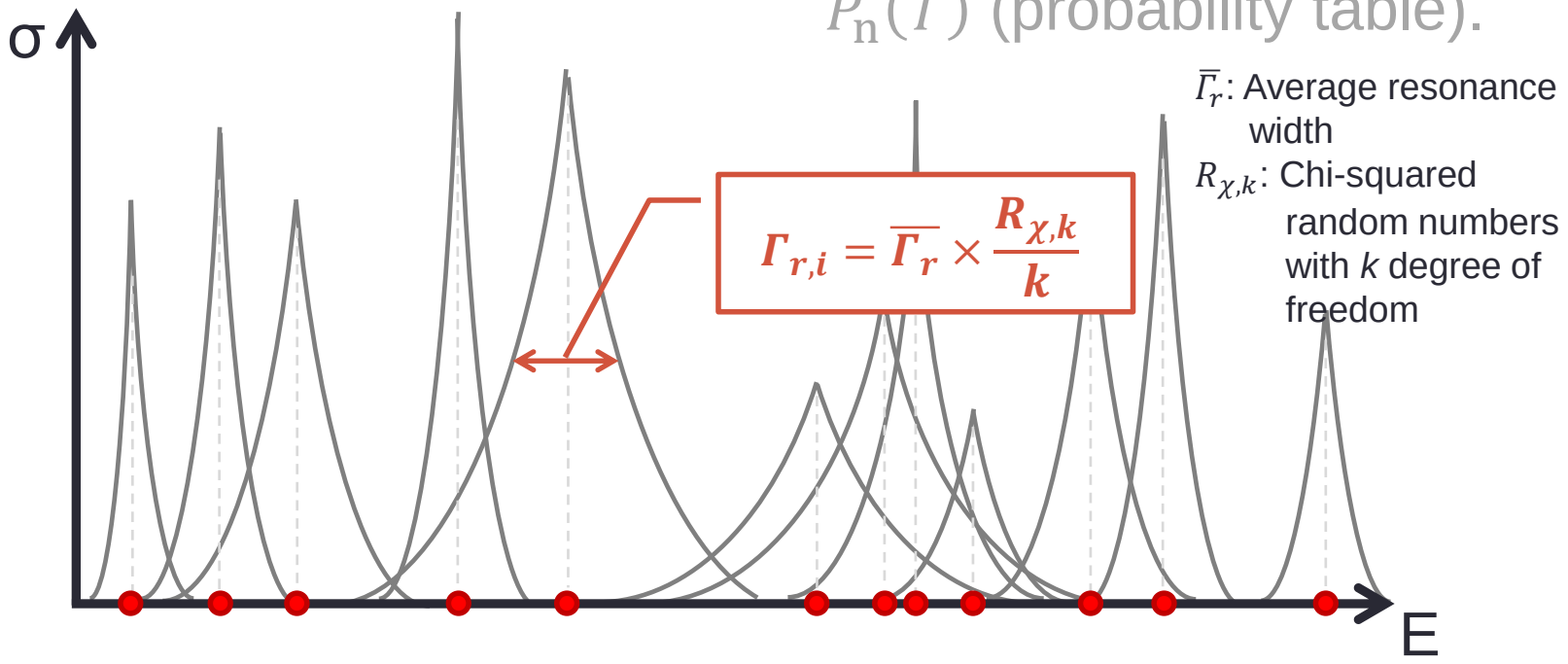
Generation of probability table (1/5)

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).



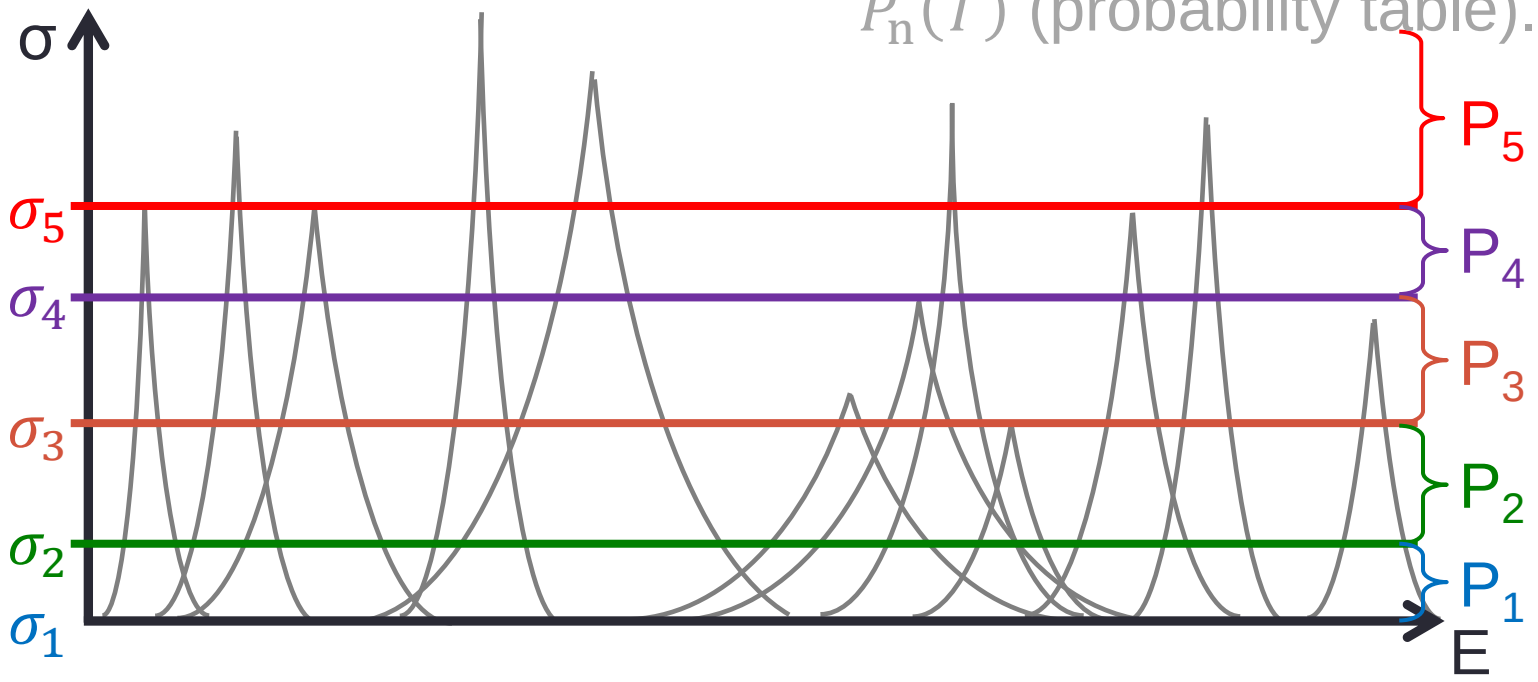
Generation of probability table (2/5)

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).



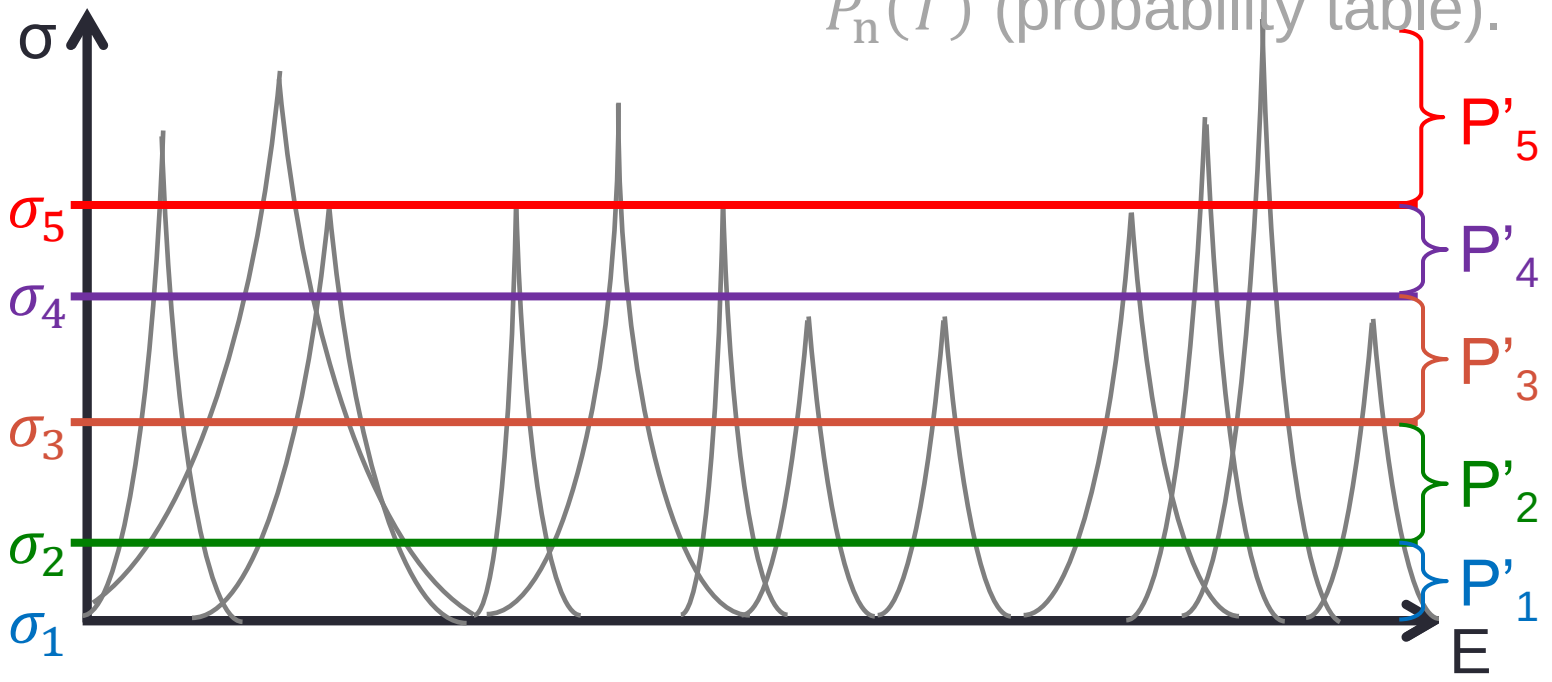
Generation of probability table (4/5)

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

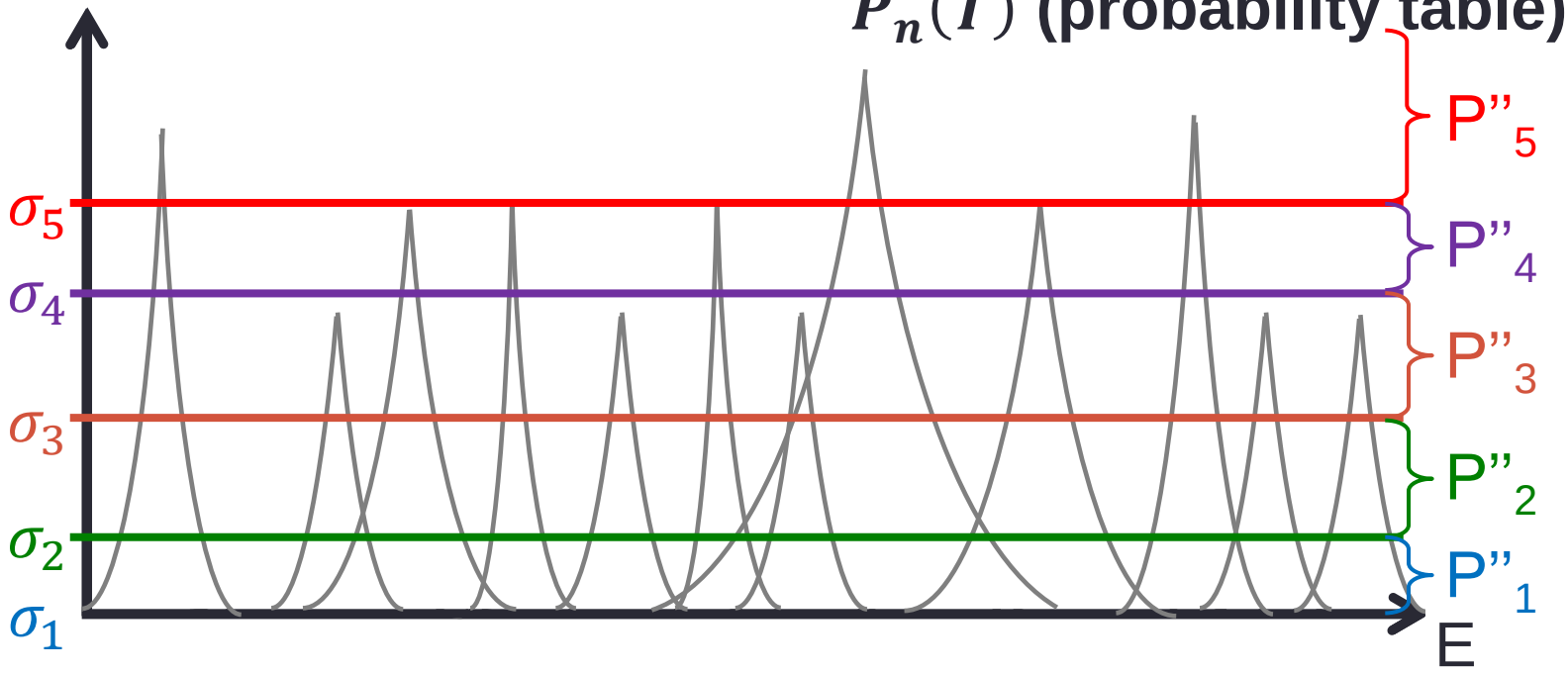
(Pseudo resonance structure is called as “ladder”)

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

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

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

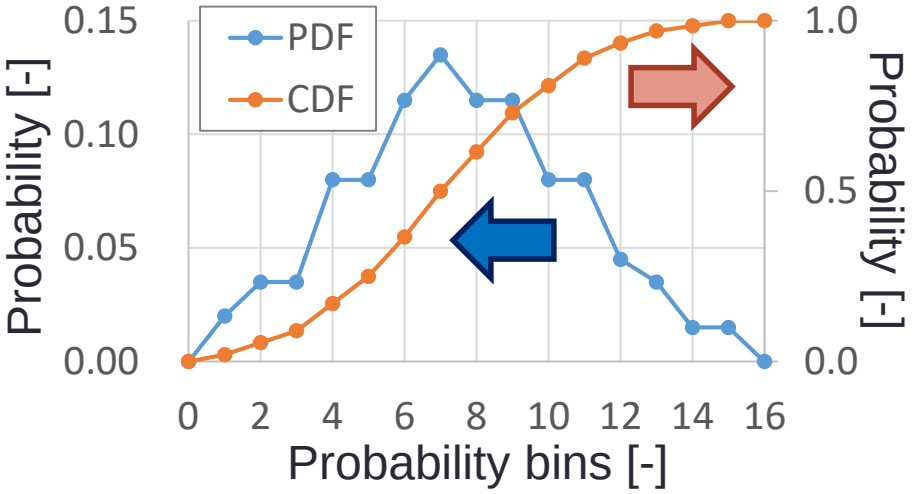
$$\chi(\zeta, x) = \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{y}{1+y^2} e^{-\frac{\zeta^2}{4}(x-y)^2} dy$$

ACE file generation

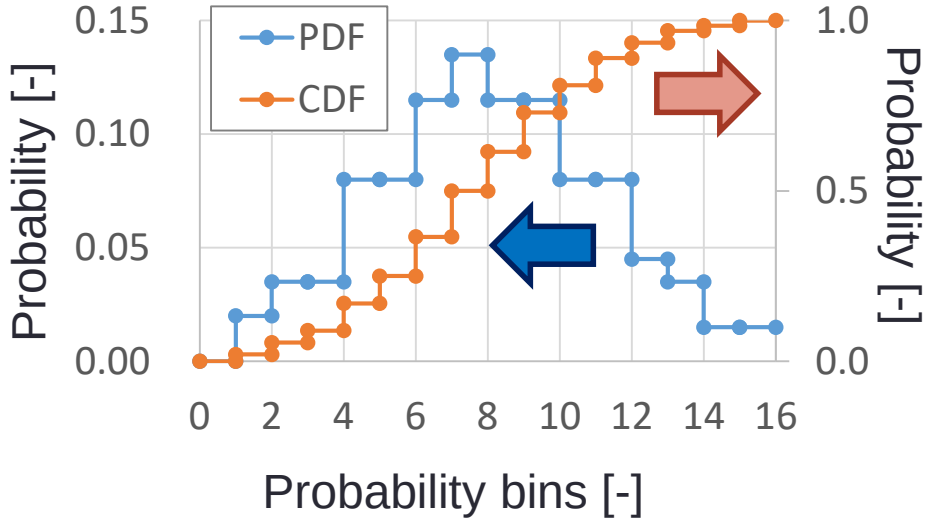
- Continuous energy Monte Carlo calculation codes use cumulative probability distribution (CDF).
  - Angular and energy distributions are converted to cumulative probability distribution.
  - PDF: Probability Density Function
  - CDF : Cumulative Density Function

[Example of PDF and CDF]

From linear-linear to PDF/CDF



From histogram to PDF/CDF



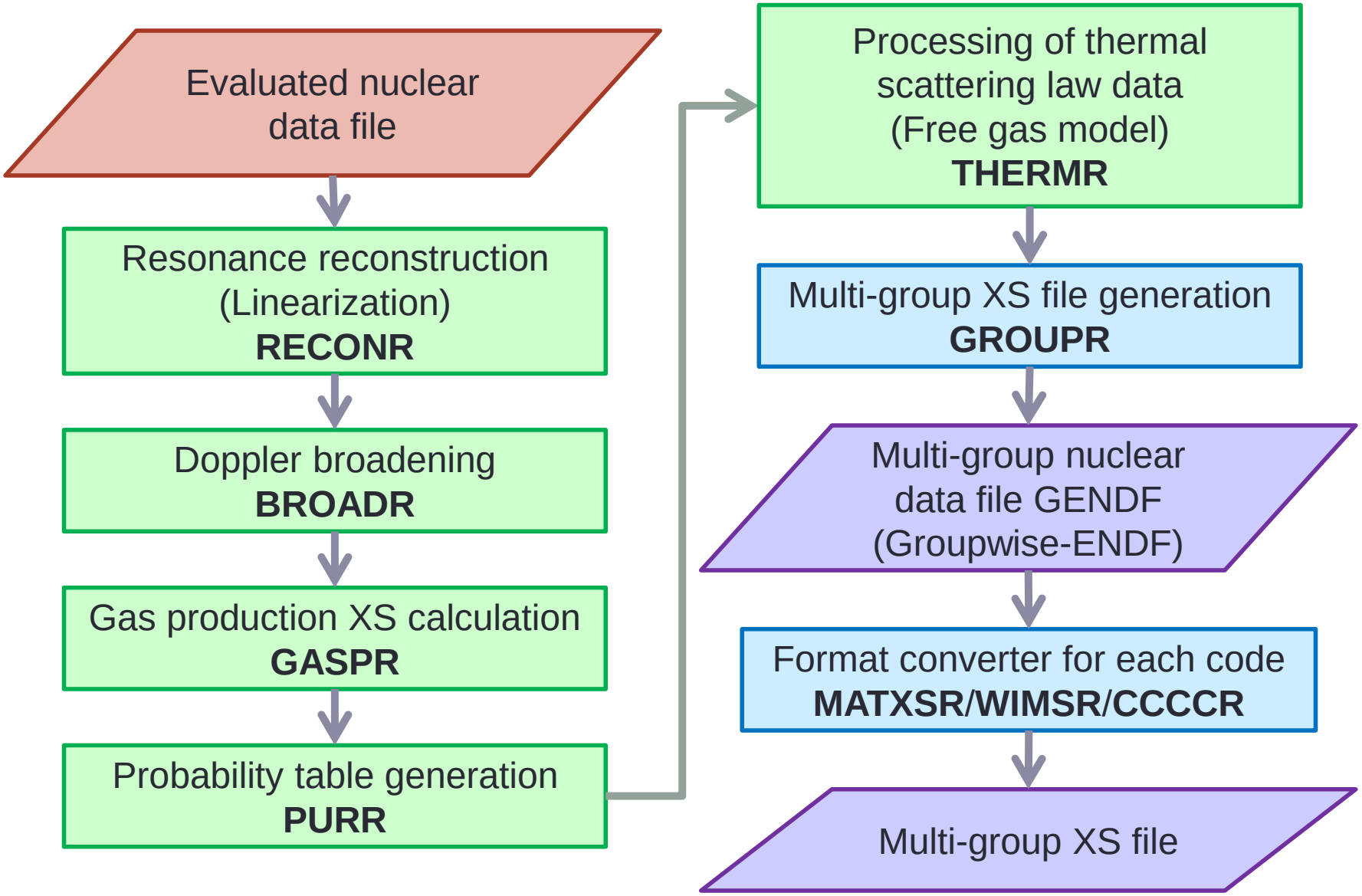
Multi-group XS calculation

- 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.
- $\phi_l^i(E) = \frac{C(E)}{[\sigma_t^i(E)+\sigma_0^i]^{l+1}}$
  - $C(E)$ 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



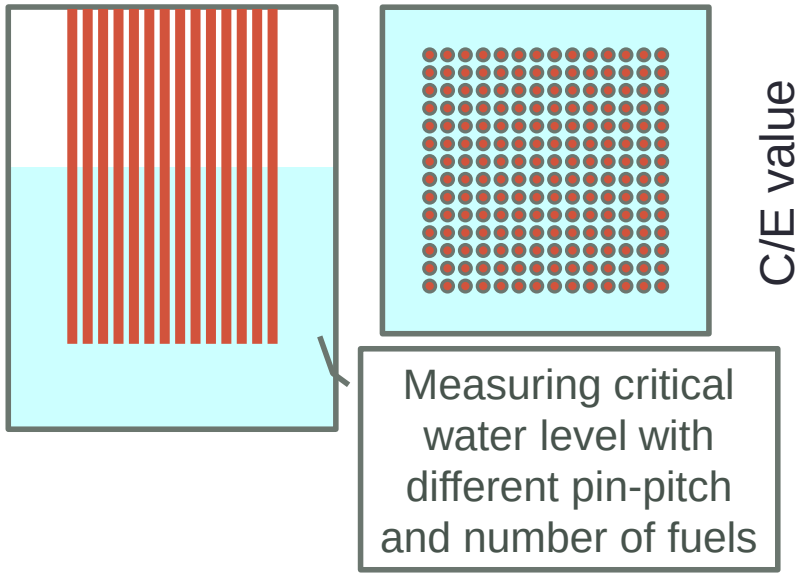
Consideration of TSL data

- 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

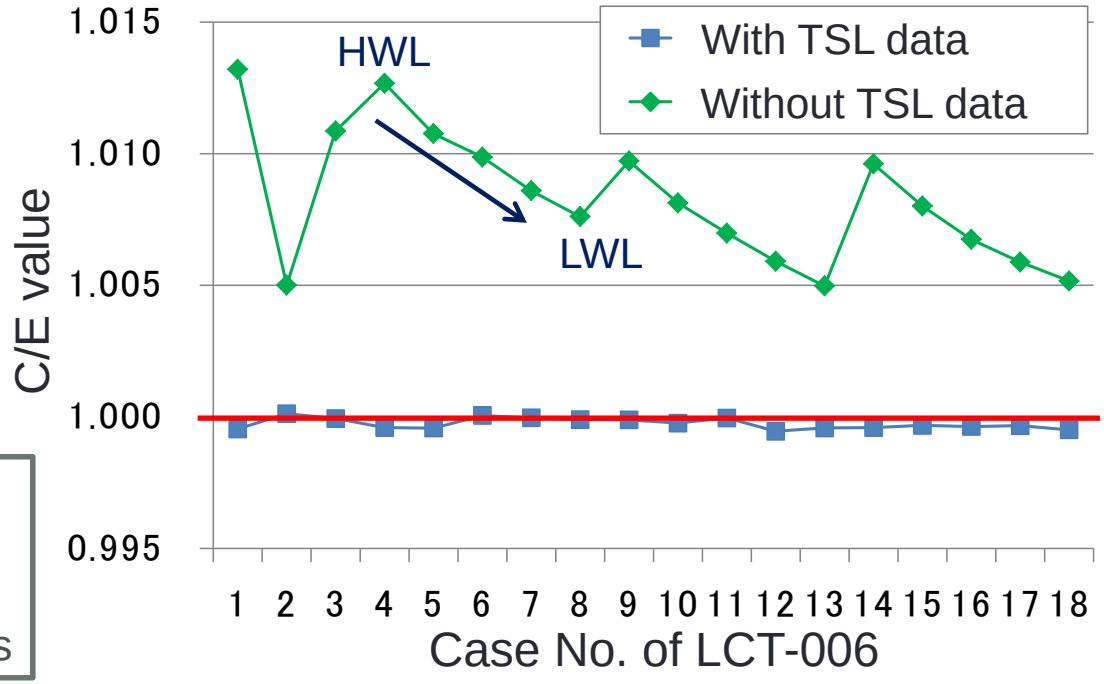
Impact of TSL data on k-effective

- 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]



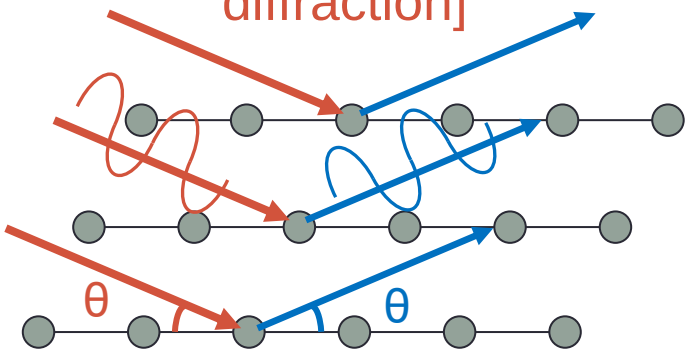
Thermal scattering

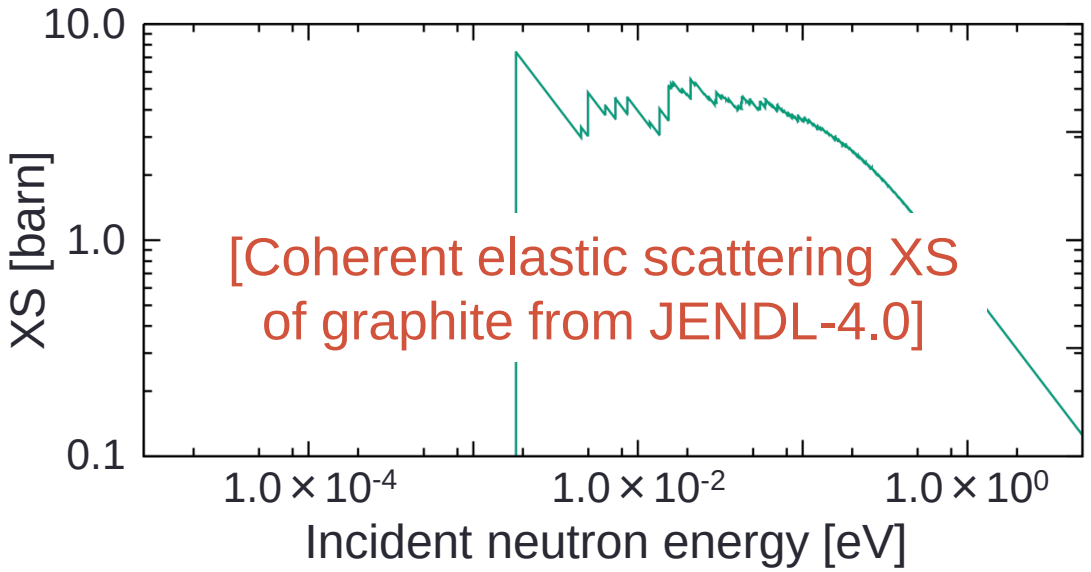
- ENDF-6 format handles three types of thermal scattering in MF=7.
- MF=7/MT=2
  - Coherent elastic scattering for crystalline materials
  - Incoherent elastic scattering for partially ordered materials
- MF=7/MT＝4
  - Incoherent inelastic scattering for non-crystalline materials
    - Represented by 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 codes 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]

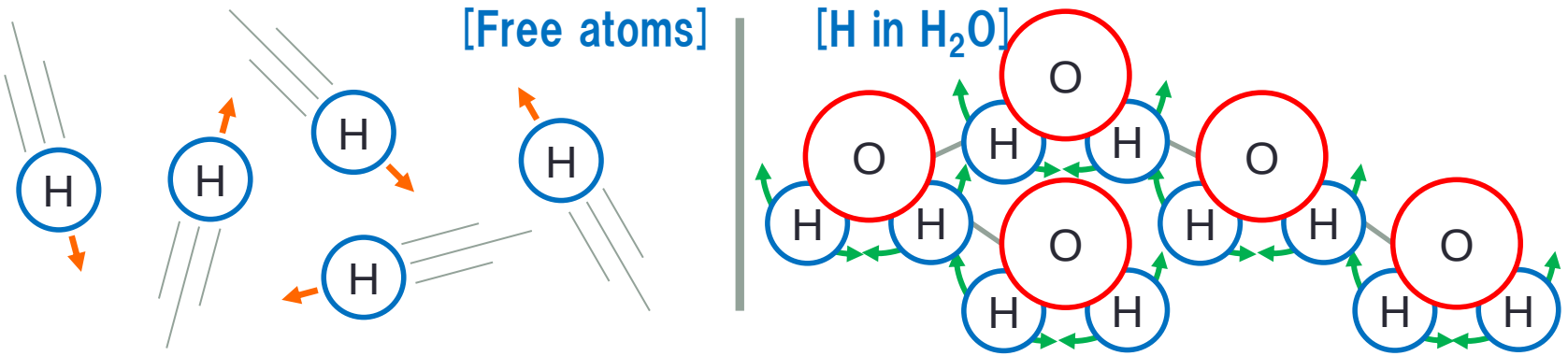




Incoherent inelastic scattering

- 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 codes, *e.g.*, NJOY and FRENDY, **only process given temperature**.
    - Nuclear data processing code 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 codes 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 codes have to process free gas scattering law.

Open nuclear data processing code

- FRENDY (JAEA): https://rpg.jaea.go.jp/main/en/program_frendy/
  - C++
  - FRENDY Version 1 can generate ACE file.
  - Development of multi-group XS file generation function is now under going.
- NJOY2016 (LANL): https://github.com/njoy
  - De facto standard code
  - NJOY2016: Fotran90 / NJOY21: C++
- PREPRO (IAEA): https://www-nds.iaea.org/public/endf/prepro/
  - FORTRAN 77
  - Widely used in the world.
- FUDGE (LLNL): https://github.com/LLNL/fudge
  - Python
  - FUDGE can also convert from ENDF-6 format to GNDS format
- AMPX-6 (ORNL)
  - Nuclear data processing system for SCALE
- GRUCON (Russia): https://www-nds.iaea.org/grucon/

Characteristics of FRENDY

Development of nuclear data processing code FRENDY

- JAEA started developing a new nuclear data processing code 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 1 was released in 2019.
  - FRENDY Ver. 1 only generates ACE files.
  - https://rpg.jaea.go.jp/main/en/program_frendy/

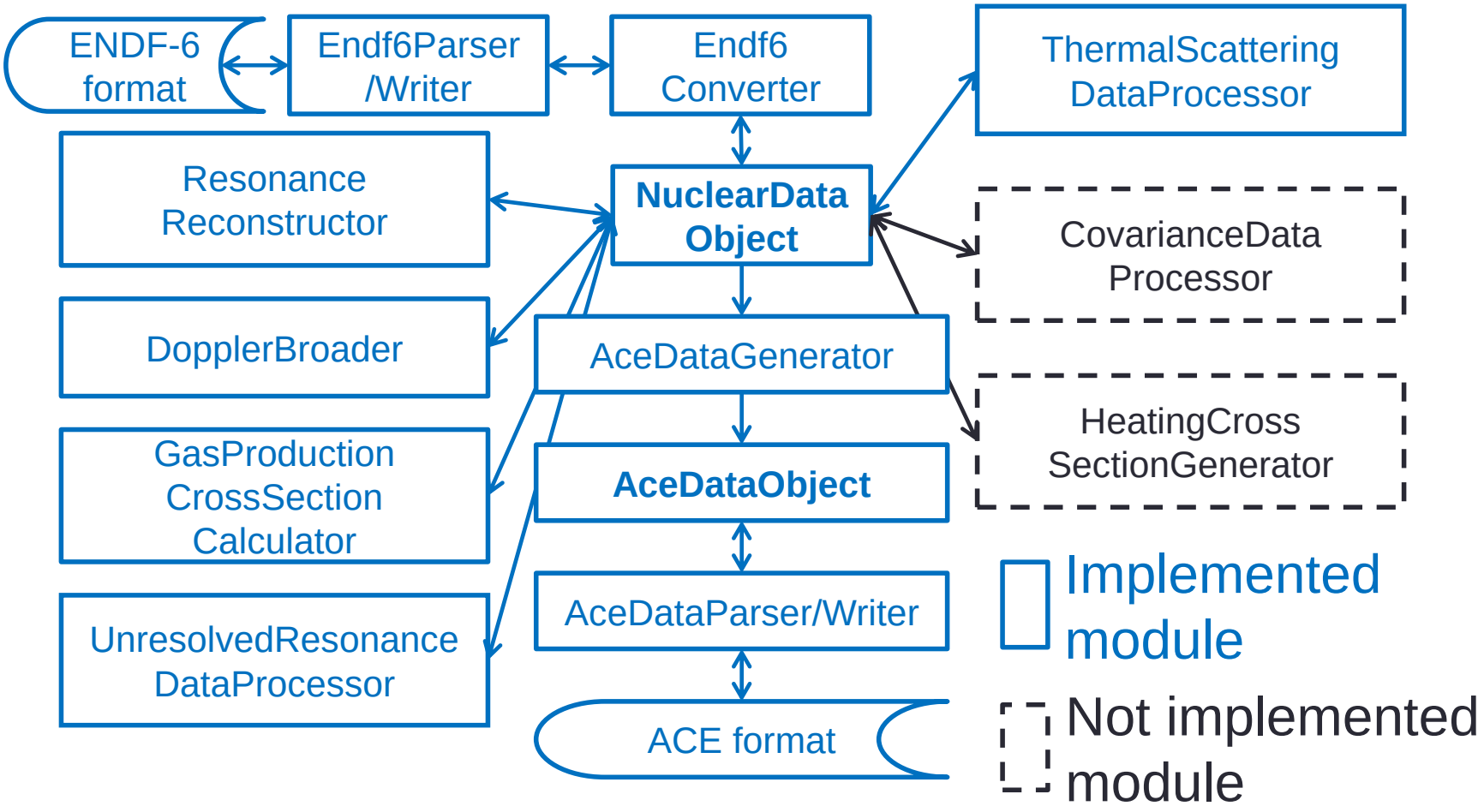
Features of FRENDY

- 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 and verification of a new nuclear data processing system FRENDY,” *J. Nucl. Sci. Technol.*, **54** [7], pp.806-817 (2017). (http://www.tandfonline.com/doi/abs/10.1080/00223131.2017.1309306)

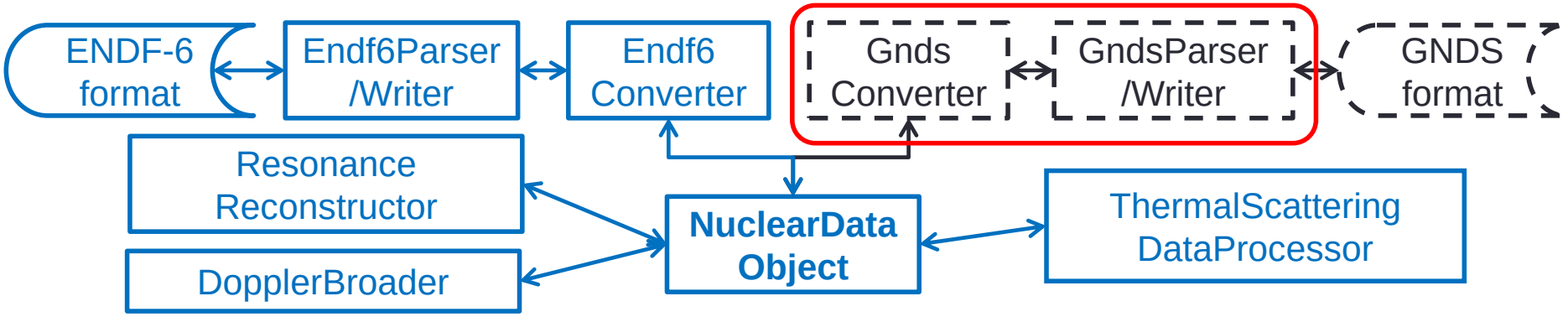
Structure of FRENDY

- 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.

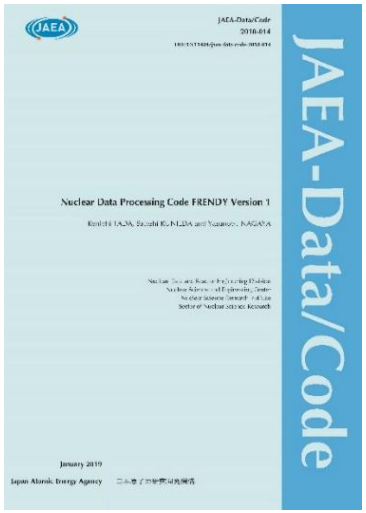


Difference of FRENDY and NJOY

- FRENDY uses the same processing method adopted in NJOY.
- Several processing methods are improved.
  - The details of these differences are described in Sec. 9.2 of FRENDY manual (JAEA-Data/Code 2018-014).
  - Treatment of 0 eV XS to calculate Doppler broadened XS
    - NJOY uses 1/v law / FRENDY uses linear interpolation.
  - Number of energy grids to process TSL data
    - NJOY uses fixed energy grid points (118 from 1.0E-5 to 10 eV).
  - Determination of resonance width using random number in probability table generation
    - NJOY uses discrete random numbers to calculate chi-squared random numbers $R_{\chi,k}$.

Release of FRENDY Ver. 1

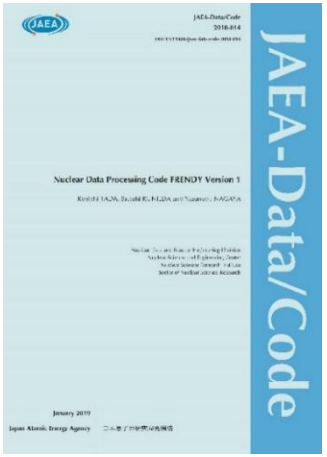
- FRENDY Ver.1 was released from our website.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
  - Only generates ACE files.
    - Generation of multi-group cross section will be implemented soon.
  - Open-source software
    - 2-Clause BSD license
  - Presentations of FRENDY training course and exercise are also found in this website.
- Manual of FRENDY Ver. 1
  - JAEA-Data/Code 2018-014
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2018-014.pdf



Development of FRENDY Ver. 2

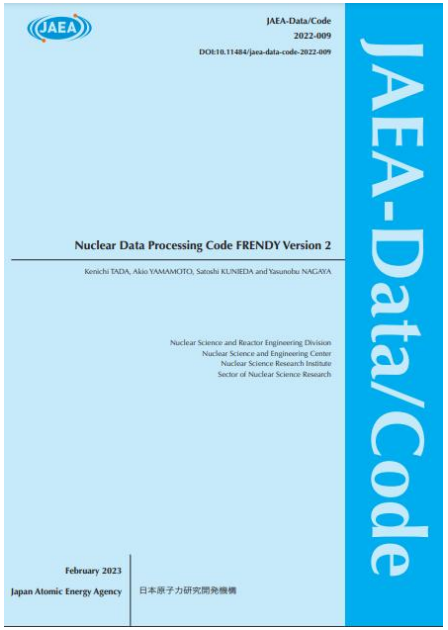
- Many capabilities are prepared after FRENDY Ver. 1.
  - Neutron induced multi-group cross section generation
  - Perturbation of ACE file for uncertainty quantification
    - This function was implemented in FRENDY Ver.1.01.001.
  - Modification of evaluated nuclear data file
  - Uncertainty quantification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

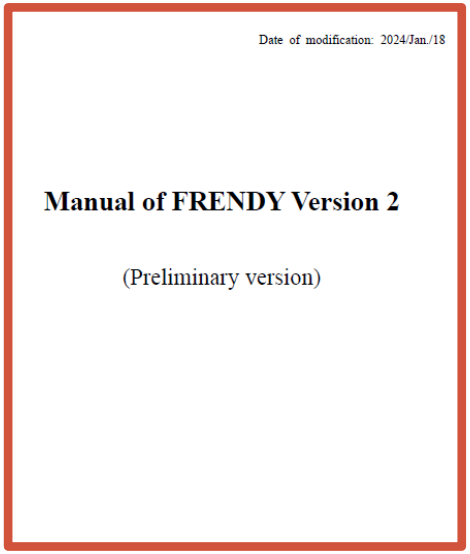
- FRENDY version 2 was released including these functions in Jan. 2022.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
- Manual of FRENDY Ver. 2
  - JAEA-Data/Code 2022-009
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2022-009.pdf



Manual of FRENDY

- Latest manual of FRENDY
  - JAEA-Data/Code 2022-009
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2022-009.pdf
  - There are many sample inputs in this manual.
- FRENDY package has simple input manual.
  - It also has many sample inputs.




Date of modification: 2024/Jan./18

Manual of FRENDY Version 2

(Preliminary version)

Input format of FRENDY

- FRENDY treats two types of the input formats.
  - FRENDY original input format
  - NJOY compatible
- 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
```

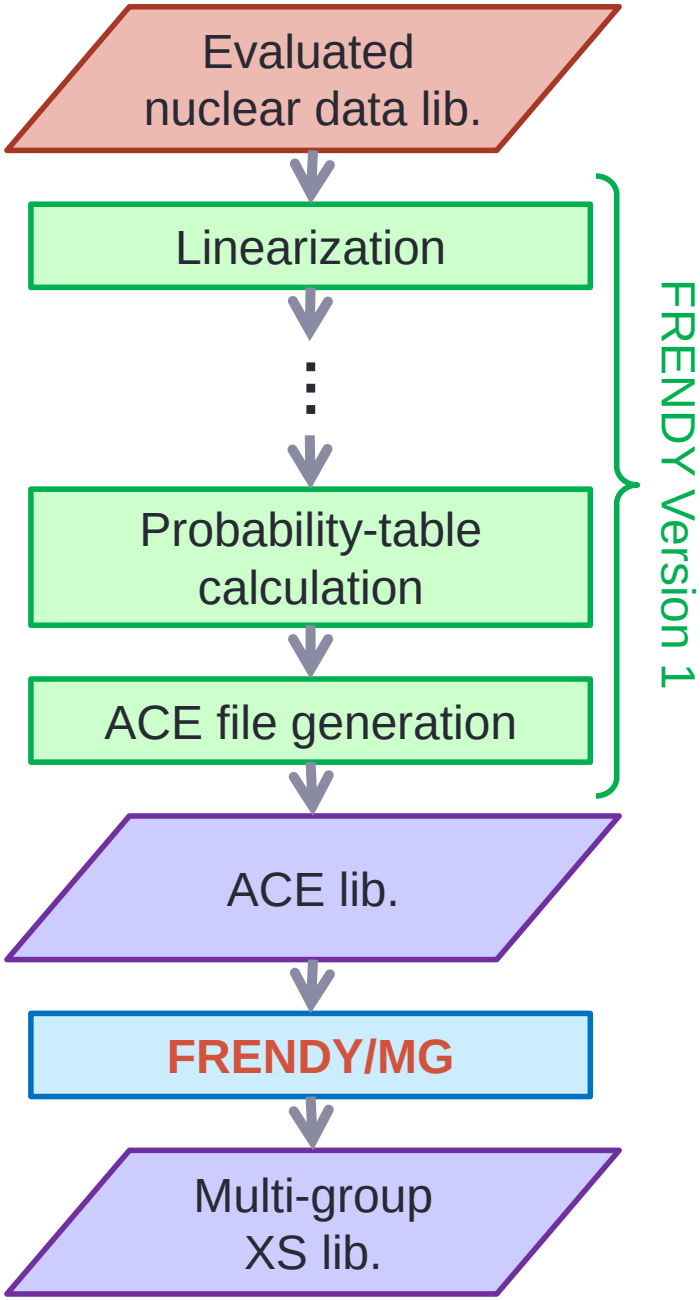
[Sample input of NJOY]

```
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  1E4  1E3  300  100  30  10  1.0  0.1   1.0E-5  / sig zero
 0                                  /
acer                                / command
 20  25   0  30  31                 / nendf, npend, ngend, nace, ndir
 1   1   1  0.00                    / 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                                /
```

Characteristics of 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 are 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 FRENDY/MG

- Focus on neutron cross section generation.
  - It can treat fast continuous and thermal scattering law data.
- Output format of multi-group cross sections
  - GENDF and MATXS
- Angular/energy distributions
  - LAW=3, 4, 7, 9, 11, 44, 61 66 in ACE file
  - All nuclides in JENDL-4.0, ENDF/B-VII.1, B-VIII.0, JEFF-3.3, and TENDL-2019 are available.

New functions of FRENDY/MG

- 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)

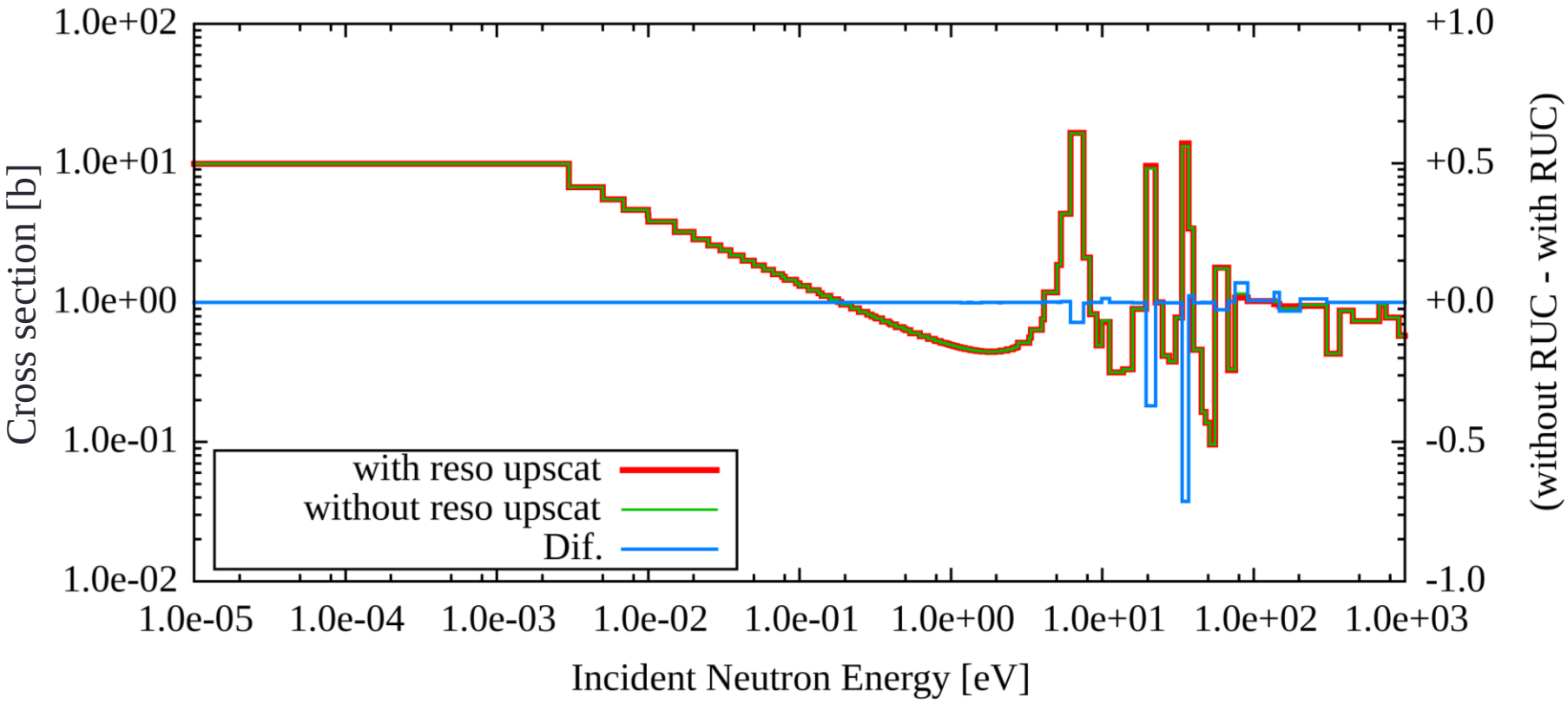
- Calculation of elastic scattering cross section and scattering kernel using 0 K scattering cross section data generated by FRENDY.
  - Mixed nuclide is also available to explicitly consider the resonance interference effect.
    - For example, U-235 with RUC, U-238 with RUC, and O-16 without RUC in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

A. Yamamoto et al., "Implementation of Resonance Upscattering Treatment in FRENDY Nuclear Data Processing Systems," Nucl. Sci. Eng., 196, pp.1267-1279 (2022).
https://www.tandfonline.com/doi/full/10.1080/00295639.2022.2087833

Comparison of XS with and without RUC

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

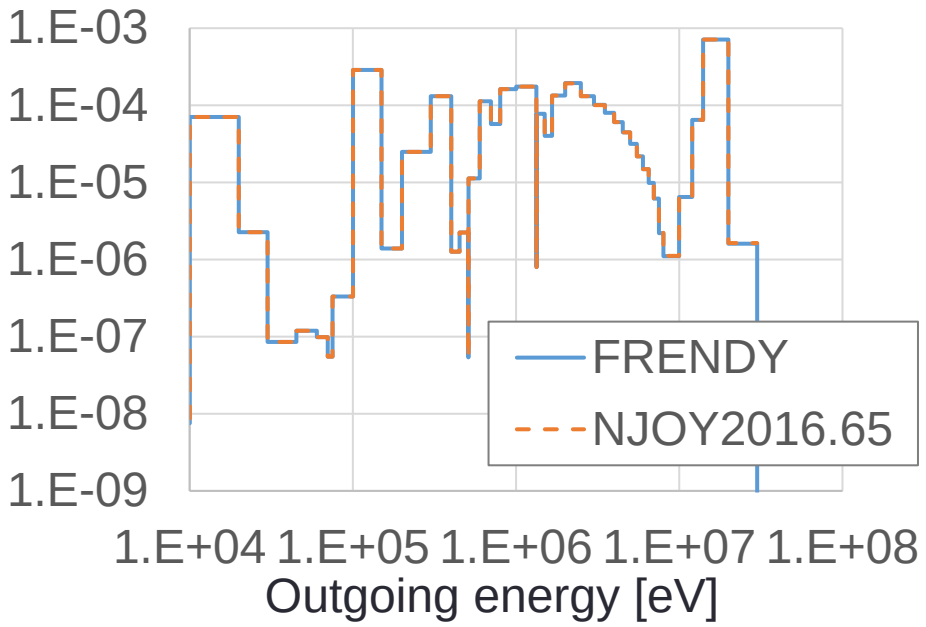
<Comparison of cross section with and without RUC (U-238, MT=102)>



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.

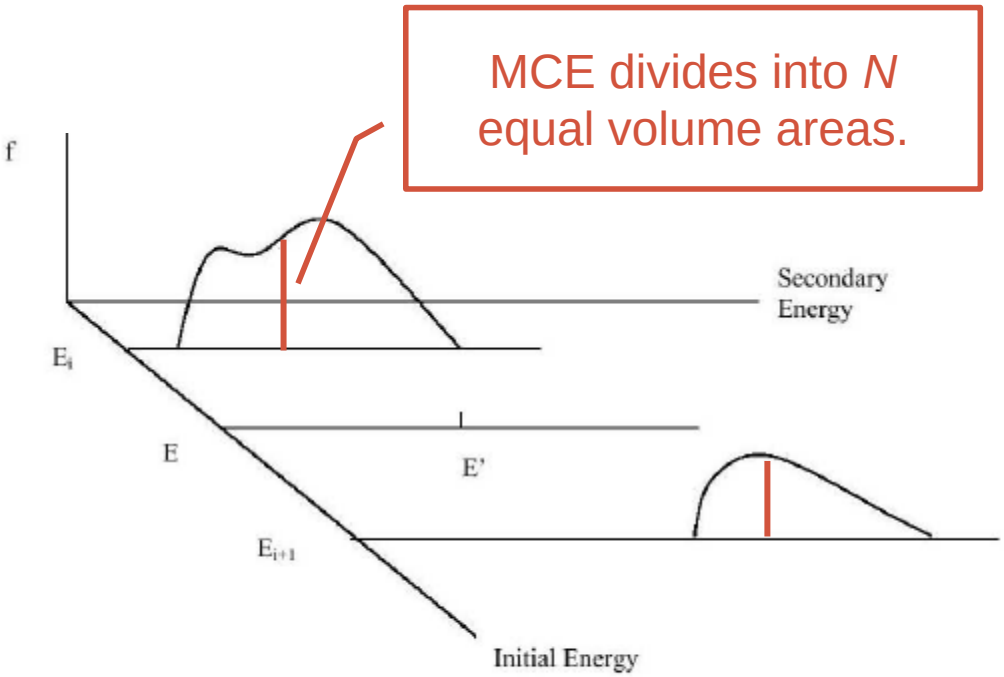


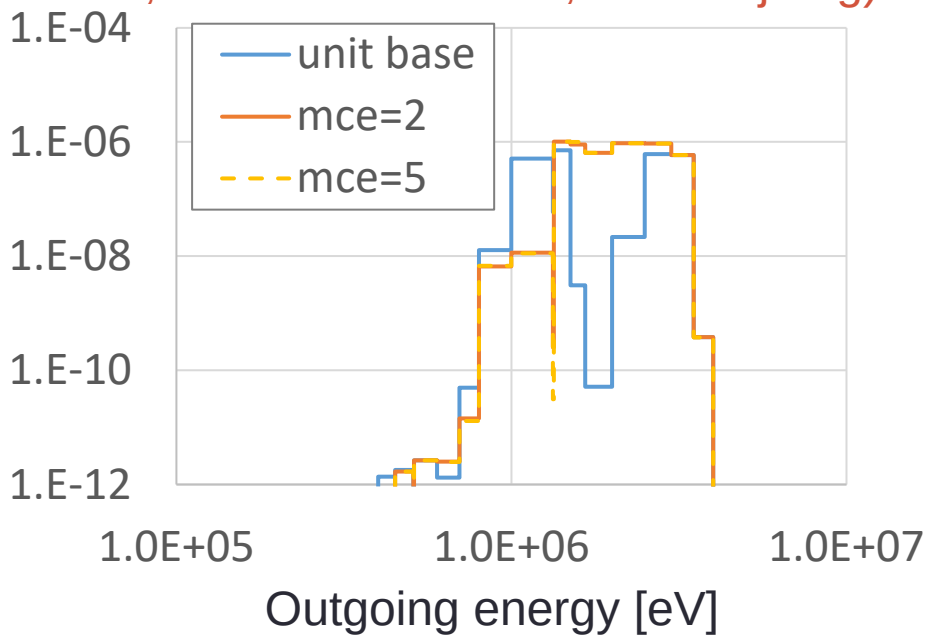
Figure 2: Interpolation between Two-Dimensional Panels.*)

*) 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

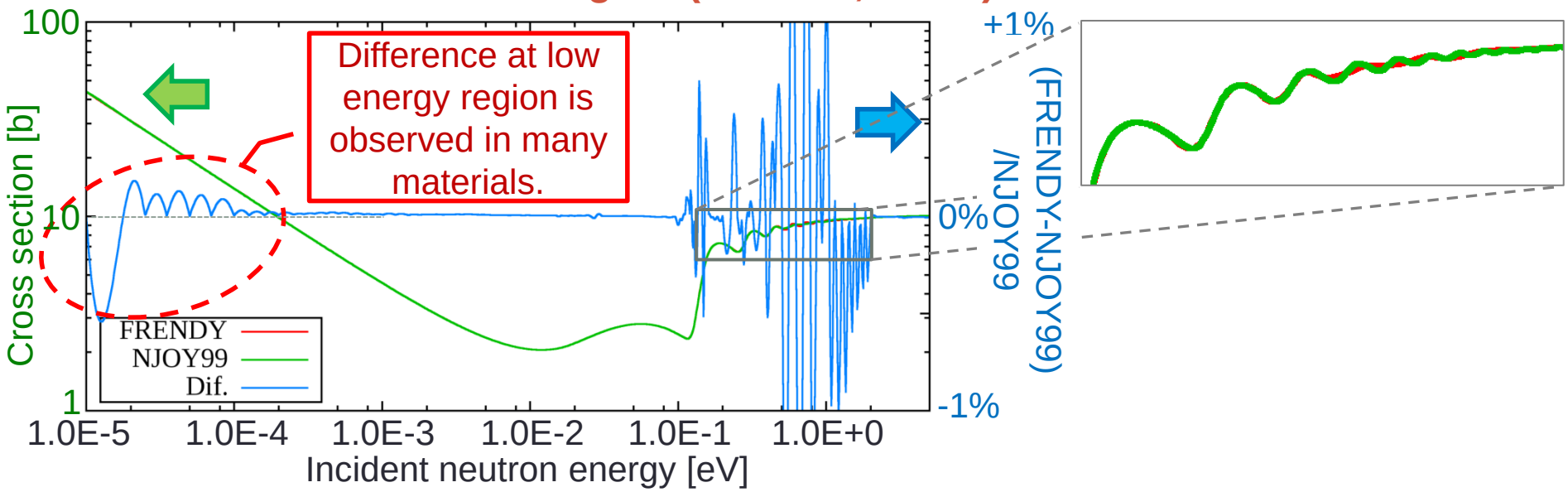
- NJOY uses 118 fixed energy grid points.
  - These fixed energy grid points are insufficient for neutronics calculation.
- FRENDY used the incident energy grid points of the corresponding nuclide.
  - Very large processed data size
- Optimization of the number of incident energy grid points is required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

*) K. Tada, “Linearization of Thermal Neutron Scattering Cross Section to Optimize the Number of Energy Grid Points," Proc. ICNC2023, (2023).

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

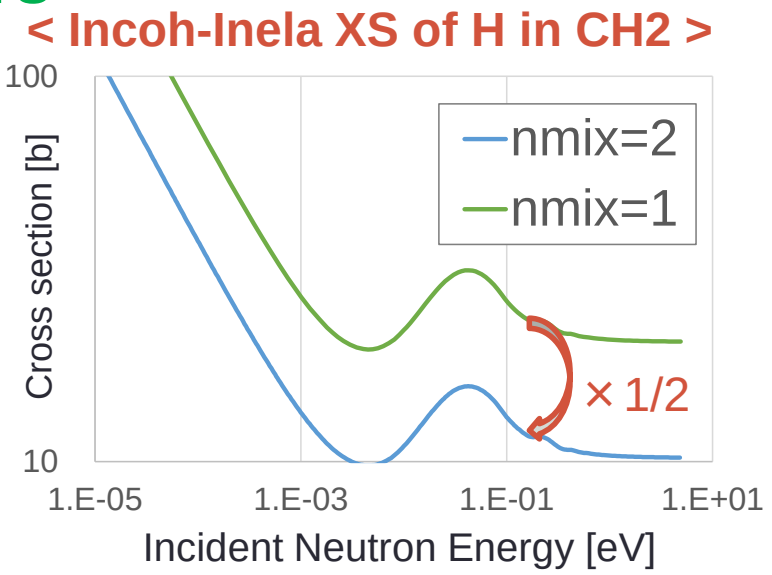
- The number of incident energy grid points is very small even if tolerance value is 0.02%.
  - Incident energy grid points and data size of the ACE file are reduced by more than **80%** for many materials when the tolerance value is 0.02%.

<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

Input checker functions to reduce input errors

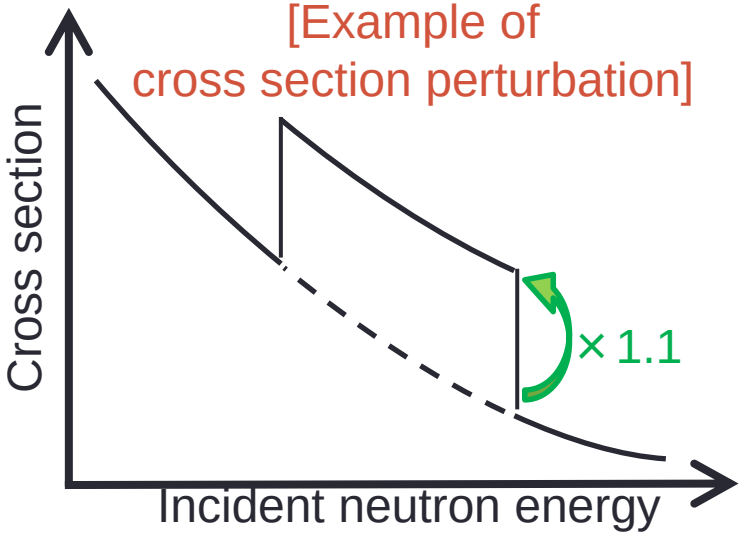
- FRENDY automatically checks input parameters and processing results.
  - FRENDY reads nuclear data files and sets recommended values.
    - Input parameters are compared to recommended values.
  - Processing results are also used to verify input parameters.
- These functions help many users to generate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



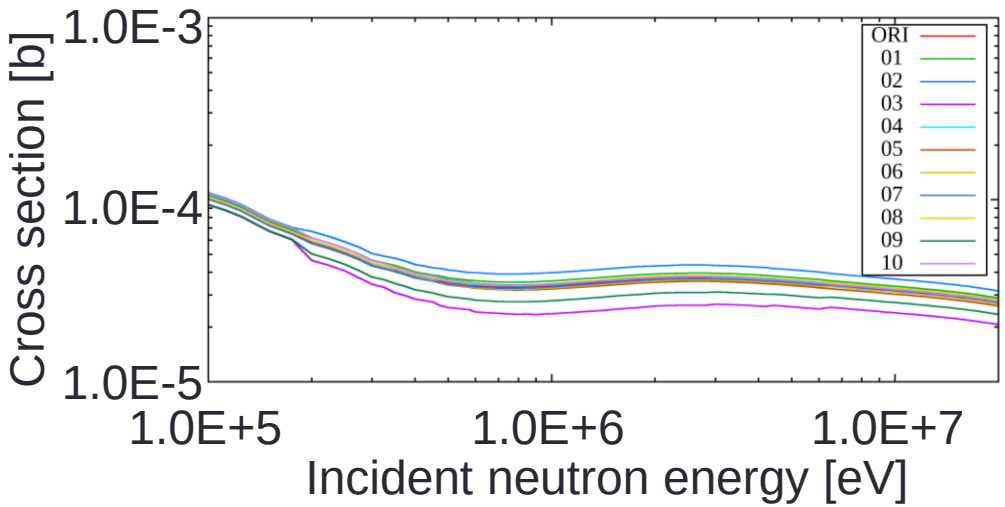
ACE file perturbation tool

- 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.

[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

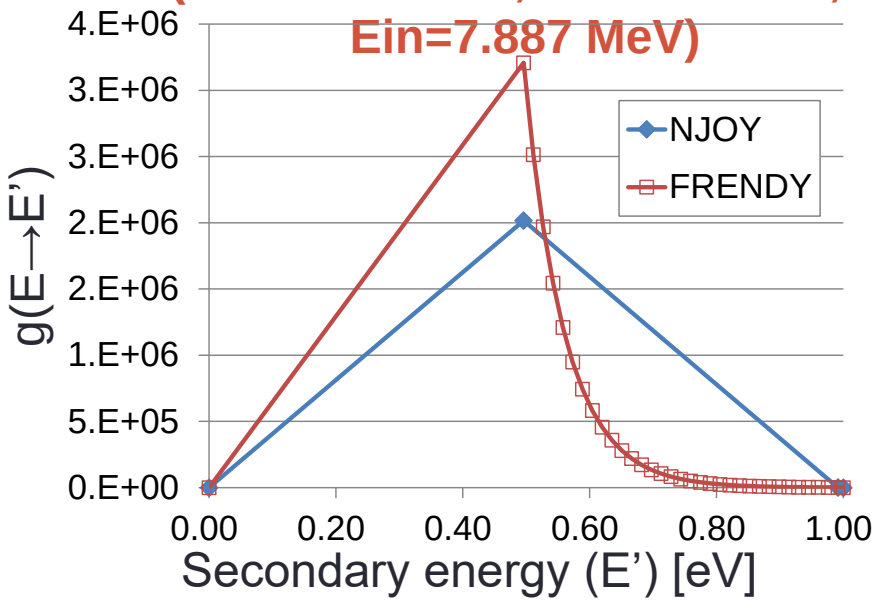
MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=3, MT=102
MF=6

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.

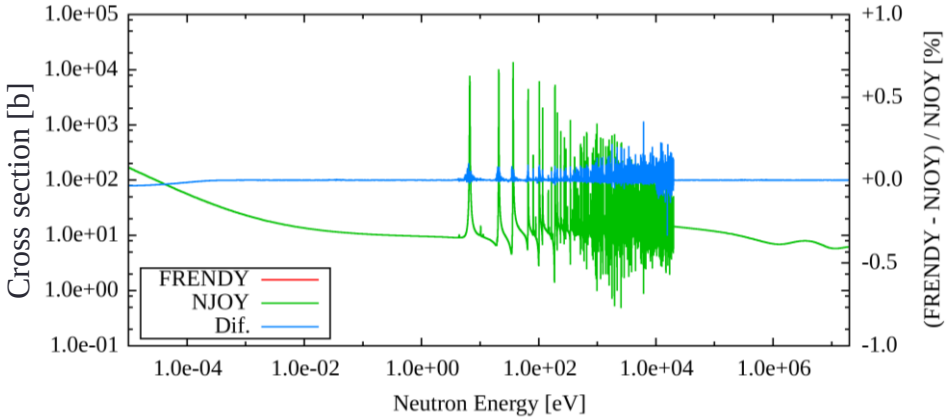
Secondary energy distribution (C000 from J40, MF=5/MT=91, Ein=7.887 MeV)



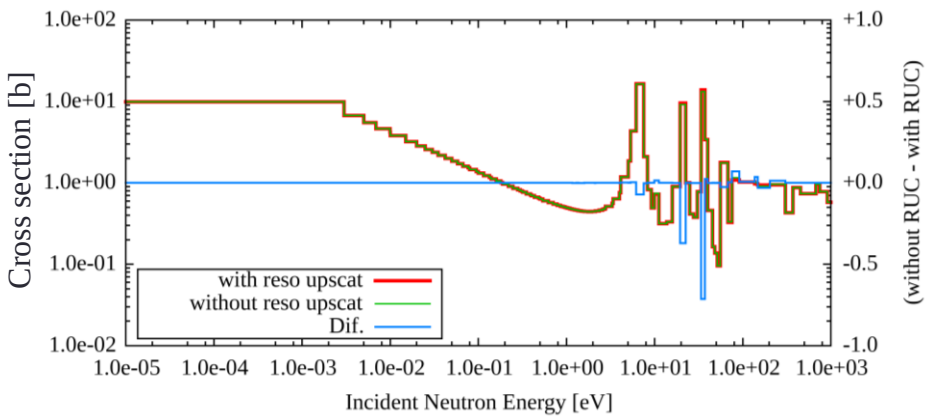
XS output function

- 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 the specified weighting function such as flat and 1/E flux.
  - From FRENDY Ver. 2.03.

<Comparison of pointwise XS of U-238>



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



Available format

- ENDF(PENDF), ACE, and GENDF format
  - ENDF and ACE (fast and tsl)
    - It outputs 1-D data or comparison results (1-D data and relative difference)
    - It automatically processes the linearization and resonance reconstruction if the ENDF file does not linearized.
    - It automatically calculates the Doppler broadened cross section if the specified temperature is higher.
    - It generates multi-group cross section using specified weighting function.
  - GENDF
    - It outputs 1-D data.
    - It outputs all Legendre order data.
    - It outputs double differential cross section in the MF=5, 6, and 16.

Changing default values for output 1D data

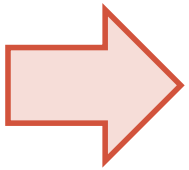
- Tolerance value for resonance reconstruction, linearization, and Doppler broadening
  - Nuclear data processing: 0.1%
  - Output function: 1%
    - To reduce processing time and data size.
    - User can change tolerance value using “error” parameter.
- Maximum energy of Doppler broadening
  - Nuclear data processing: top of resolved resonance region
  - Output function: 1 MeV
- IWT=4 (fission+1/E+Maxwell) is not available for the weighting function.

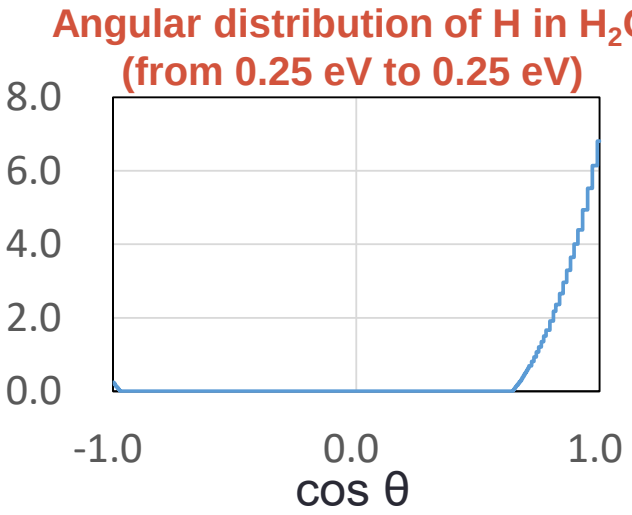
Available X-Y data for ENDF and ACE files

- For ENDF and ACE files
  - Cross section data (MF=3)
    - MT=1-999
  - Number of neutron per fission (MF=1/MT=452-456)
    - MT=1452 (v-tot), 1455 (v-d), and 1456 (v-p)
  - Multiplicities of radioactive products (MF=9)
    - MT=9001-9999 (MF=9/MT1-MF=9/MT=999)
  - Production cross sections for radioactive nuclides (MF=10)
    - MT=10001-10999 (MF=10/MT1-MF=10/MT=999)
- For ACE file
  - Fission spectrum
    - MT=1018

Available X-Y data for GENDF files

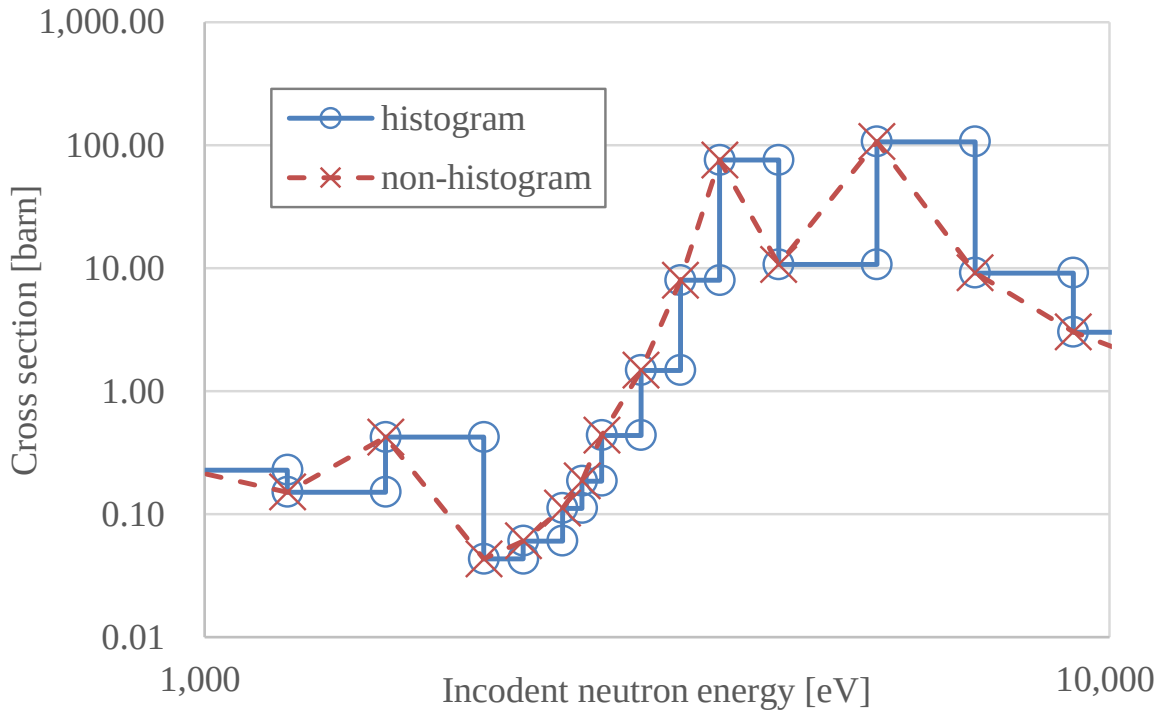
- Cross section data (MF=3 and 13)
  - MT=1-999, 1452 (v-tot), 1455 (v-d), and 1456 (v-p)
  - FRENDY outputs cross section data in all Legendre polynomial and background cross sections.
- Double differential cross section data
  - MF=5, 6, and 16
  - FRENDY can reconstruct X-Y data from Legendre polynomial coefficients.





Multi-group plot of FRENDY

- FRENDY has two plot mode (Histogram and Non-histogram)
  - Histogram outputs two energy grid points for each energy group.
    - Maximum and minimum energy grid of each energy group.
    - This is used for drawing graph on a scatter plot in Excel.
  - Non-histogram outputs minimum energy grid of each energy group.
    - This is used for drawing graph on histogram plot in GNUPLOT.



Outputs file of X-Y data

- Processing conditions are written in the head of X-Y data file.
  - File name, temperature, MT number
  - The header is treated as comments by gnuplot.

<Example of X-Y data>

```
# endf/pendf/ace file name     : ../lib/n_001-H-001.dat
# Temperature [K] (inp / nucl) :  300.000 /  0.00000
# MT (reaction type)           : 1
#
# energy [eV] / data
1.0000100000e-05  3.9452647507e+02
2.9999990000e-03  3.9452647507e+02
```

<Example of X-Y data (for comparison)>

```
# endf/pendf/ace file name (ref)       : ../lib/n_092-U-235.dat
# endf/pendf/ace file name (comp)   : ../ace/n_092-U-235.ace
# Temperature [K] (ref / comp)       :  0.00000 /  300.000
# MT (reaction type)                 : 1
#
# energy [eV] / ref data / comp data / relative dif (comp - ref)/ref
1.0000100000e-05  1.2155372817e+04  1.2123152889e+04  -2.6506738090e-03
2.9999990000e-03  1.2155372817e+04  1.2123152889e+04  -2.6506738090e-03
```

Sample input for X-Y data generation (ENDF)

- Input for X-Y data generation is similar to that for nuclear data processing.
  - Nuclear data file name, output case name, temperature, and MT number list.
  - Temperature and MT number list are optional.
    - If users do not set temperature, FRENDY skips doppler broadening.
    - If users do not set MT number list, FRENDY outputs all cross section data in MF=3.
    - If users use minus “-” in the MT number list, such as “A - B", FRENDY generates all MT numbers from A to B.

```
plot_mode //processing mode
  nucl_file_name ( "../lib/U235.dat " )
  output_name ( "./output_xs/U235" )
  temp ( 300.0 ) //Temperature [K]
  mt_list ( 1  2  18 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

Sample input for X-Y data generation (ACE)

- Users use ACE file name (ace_file_name) instead of nuclear data file name (nucl_file_name).
  - FRENDY handles neutron induced data (fast), thermal scattering law data, and dosimetry data

```
plot_mode //processing mode
  ace_file_name ( ../ace/tsl_HinH2O_0300.00K.ace )
  output_name   ( ./out/tsl_HinH2O_300k_ace/tsl_HinH2O )
```

```
plot_mode //processing
  ace_file_name ( ../ace/n_092-U-235.ace )
  output_name ( ./out/n_092-U-235_600k_ace/n_092-U-235 )
  temp ( 600.0 ) //Temperature [K]
  mt_list ( 1  2  18  102 )
```

Sample input for X-Y data generation (Multi-group)

- Users have to add multi-group structure, weighting spectrum, and editing option to generate multi-group cross section from ENDF or ACE file.
  - Multi-group structure name and weighting function name are found in the manual of FRENDY in the FRENDY package.

```
plot_mode //processing
  nucl_file_name ( ../lib/n_092-U-235.dat )
  temp  300.0  //Temperature [K]
  mt_list ( 1  2  18  102  1452 - 1456 ) //1452=nu-tot, 1455=nu-d, 1456=nu-p
  output_name ( ./out/n_092-U-235_300k_endf_mg_hist/n_092-U-235 )

  //For multi-group generation
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )      //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( histogram )             //histogram or non-histogram
```

Sample input for X-Y data generation (GENDF)

- Users use GENDF file name (gendf_file_name) instead of nuclear data file name (nucl_file_name).
  - If users set the temperature and/or material number (mat_no), FRENDY search the input temperature and/or material number data from the GENDF file.
  - If users do not set the temperature and/or material number, the first data in the GENDF file is used for X-Y data generation.

```
plot_mode //processing mode
  gendf_file_name ( "../lib/U235.dat " )
  temp ( 300.0 )              //Temperature [K]
  mat_no ( 9228 )             //Material number
  output_name ( "./output_xs/U235_gendf" )
  mf_list ( 3 )               //MF=3
  mt_list ( 1  2  18 - 102 )  //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

Sample input for nuclear data comparison

- Users must set two data file name.
  - The other input parameters of nuclear data comparison are the same as those of X-Y data generation.

<Comparison of nuclear data file and ACE file>

```
plot_mode //processing mode
  nucl_file_name ( ../lib/n_092-U-235.dat )
  ace_file_name ( ../ace/n_092-U-235.ace )
  mt_list ( 1  2  18 - 102 1452 - 1456 )
  output_name ( ./out/comp_mg/n_092-U-235 )

  //For multi-group generation
  mg_structure ( xmas_nea-lanl_172 )
  mg_weighting_spectrum ( 1/e )
  edit_flag( histogram )
```

<Comparison of nuclear data files>

```
plot_mode //processing mode
  nucl_file_name ( ../j50/n_092-U-235.dat
                   ../f33/92-U-235g.jeff33 )
  mt_list ( 1  2  18 - 102  1452 - 1456 )
  output_name ( ./out/comp_ce/n_092-U-235 )
```

Multitasking tool

- FRENDY Ver. 2.05 provides multitasking tool.
  - tools/frendy_parallel/frendy_parallel.exe
  - It automatically generates FRENDY input files and generates ACE or multi-group cross section files.
  - Users only makes input parameters list and input templates.
    - Temperature set, background cross section set, directory and file name, and so on

<Example of input templates>

```
mg_neutron_mode
  mg_structure                ( xmas_nea-lanl_172 )
  mg_weighting_spectrum ( fission+1/e+maxwell )

  max_thermal_ene             10.0
  max_thermal_ene_e_out    15.0
```

Sample input of multitasking tool (1/2)

```
<TEMP_SET>    //Tempeature set
  DEFAULT  293  600  900  1200  1500
  TEMP2    293  400  450  500  550  600  650
  TEMP3    293  450  600  750  900  1050  1200  1350  1500
  TEMP4    293

<BGXS_SET>    //Background cross section data set
  DEFAULT  auto
  BGXS1    1.0e+10 1.0e+4 1.0e+3 3.0e+2 1.0e+2 3.0e+1
1.0e+1 1.0e+0 1.0e-1 1.0e-5
  BGXS2    1.0e+10

<FRENDY_INPUT_TEMPLATE>  //FRENDY input template
  DEFAULT   FRENDY_TEMPLATE_INPUT1.txt
  FRENDY2   FRENDY_TEMPLATE_INPUT2.txt

<FRENDY_MODULE>    //FRENDY execution module
  /home/code/frendy/main/frendy.exe
```

```
<ENDF_DIR>     //ENDF file directory (neutron induced)
  /home/data/nucl/jendl/JENDL-5

<TSL_DIR>      //ENDF file directory (TSL data)
  /home/data/nucl/jendl/JENDL-5_sab

<OUTPUT_DIR>  //Output directory.
//Users must make these directories before processing.
  /home/data/proc/out/frendy_inp  //FRENDY input file directory
  /home/data/proc/out/frendy_log  //FRENDY log file directory

<OUTPUT_DIR_MG>  //Multi-group cross section file directory
  /home/data/proc/out/mg

<OUTPUT_DIR_ACE>  //ACE file directory
  /home/data/proc/out/ace

<RESTART>      //Restart option
  restart            //restart or no_restart

<THREAD_NO>    //Number of threads
  30
```

Sample input of multitasking tool (2/2)

- Input of this tool consists of four parts.
  - Processing condition, Nuclear data directory, parallel calculation condition, and nuclear data file and control region

```
<INP_LIST>
//If users skipped data, the DEFAULT value was used.
//ENDF file name,  Temp,       Background XS, FRENDY input template
 n_001-H-001.dat   DEFAULT  DEFAULT         DEFAULT
 n_001-H-002.dat
 n_001-H-003.dat   TEMP2      BGXS2
 n_002-He-003.dat
//ENDF file name, TSL file name          TSL type, TEMP,     BGXS,  input template
 n_001-H-001.dat   tsl_HinH2O.dat            hh2o    TEMP2  BGXS2  DEFAULT
 n_001-H-001.dat   tsl_HinZrH.dat            hzrh    TEMP2  BGXS2  DEFAULT
 n_001-H-002.dat   tsl_DinD2O.dat            dd2o    TEMP2  BGXS2  DEFAULT
 n_006-C-012.dat   tsl_reactor-graphite.dat  graph   ALL    BGXS2  FRENDY2
```

References

Nuclear data processing

- Nuclear data processing
  - D. E. Cullen, “4 Nuclear Data Preparation,” Handbook of Nuclear Engineering, Springer (2010).
  - R. E. MacFarlane and A. C. Kahler, “Methods for Processing ENDF/B-VII with NJOY,” Nuclear Data Sheets, **111**, pp.2739-2890 (2010).
- Resonance formulae
  - 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).

Nuclear data format

- ENDF-6 format
  - A. Trkov, et. al, “ENDF-6 Formats Manual,” CSEWG Document ENDF-102, BNL-203218-2018-INRE (2018).
  - “Introduction to ENDF format,” LA-UR-98-1779 (1998).
    - http://t2.lanl.gov/nis/endf/
- GNDS
  - C. M. Mattoon, et.al, “Generalized Nuclear Data: a New Structure (with Supporting Infrastructure) for Handling Nuclear Data, Nuclear Data Sheets, **113**, pp.3145-3171 (2012).
  - GNDS＆FUDGE
    - https://ndclx4.bnl.gov/gf/project/gnd/

NJOY

- NJOY99
  - R. E. MacFarlane, “The NJOY Nuclear Data Processing System Version 91,” LA-12740-M (1994).
  - http://t2.lanl.gov/nis/codes/njoy99/
- NJOY2012
  - A. C. Kahler, “The NJOY Nuclear Data Processing System, Version 2012,” LA-UR-12-27079 (2012).
  - http://t2.lanl.gov/nis/codes/NJOY12/
- NJOY2016 / NJOY21
  - A. C. Kahler, “The NJOY Nuclear Data Processing System, Version 2016,” LA-UR-17-20093 (2016).
  - https://njoy.github.io/

Other processing code

- FRENDY
  - K. Tada, et. al, "Development and verification of nuclear data processing code FRENDY version 2," *J. Nucl. Sci. Technol.* (2023).
- FUDGE (LLNL)
  - https://github.com/LLNL/fudge
- PREPRO (IAEA)
  - https://www-nds.iaea.org/public/endf/prepro/
- AMPX (ORNL)
  - D. Wiarda, “AMPX-6: A Modular Code System for Processing ENDF/B,” ORNL/TM-2016/43 (2016).
- GRUCON (Russia)
  - https://www-nds.iaea.org/grucon/

Nuclear data utilization tool

- Evaluated Nuclear Data File (ENDF)
  - Plotting cross section data in each evaluated nuclear data library
  - https://www-nds.iaea.org/exfor/endf.htm
- Sigma
  - Plotting cross section data in each evaluated nuclear data library
  - http://www.nndc.bnl.gov/sigma/