Generation of thermal neutron scattering cross section from evaluated nuclear data

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Outline

- Overview of evaluated nuclear data library
- Thermal neutron scattering data in evaluated nuclear data
  - Coherent elastic scattering
    - For crystalline materials（Bragg diffraction)
  - Incoherent elastic scattering
    - For non-crystalline materials
  - Incoherent inelastic scattering
    - Using thermal scattering law data : S(α, β)
- Processing flow to generate cross section (XS) libraries
  - Overview of nuclear data processing
  - Processing of thermal neutron scattering data
  - Generation of XS library

Evaluated nuclear data

- Containing many physical quantities for nucleus
  - Cross section, energy and angular distribution of emitted particle, fission yield, half-life, …

- Major evaluated nuclear data library
  - JENDL (JAEA, Japan)
    - **J**apanese **E**valuated **N**uclear **D**ata **L**ibrary
  - ENDF/B (CSEWG, USA)
    - **E**valuated **N**uclear **D**ata **F**ile
  - JEFF (OECD/NEA)
    - **J**oint **E**valuated **F**ission and **F**usion File
  - Others
    - TENDL (PSI, IAEA), BROND (Russia), CENDL (China)

Physical quantities in evaluated nuclear data

For neutronics calculation

- Resonance parameter
- Number of neutrons per fission
- Fission spectrum
- Cross section
- Angular distribution of emitted particle
- Energy distribution of emitted particle
- Thermal neutron scattering data
- Fission yield
- Decay data （half-life, transition probability）
- γ-ray data （Intensity, Energy）

⋮

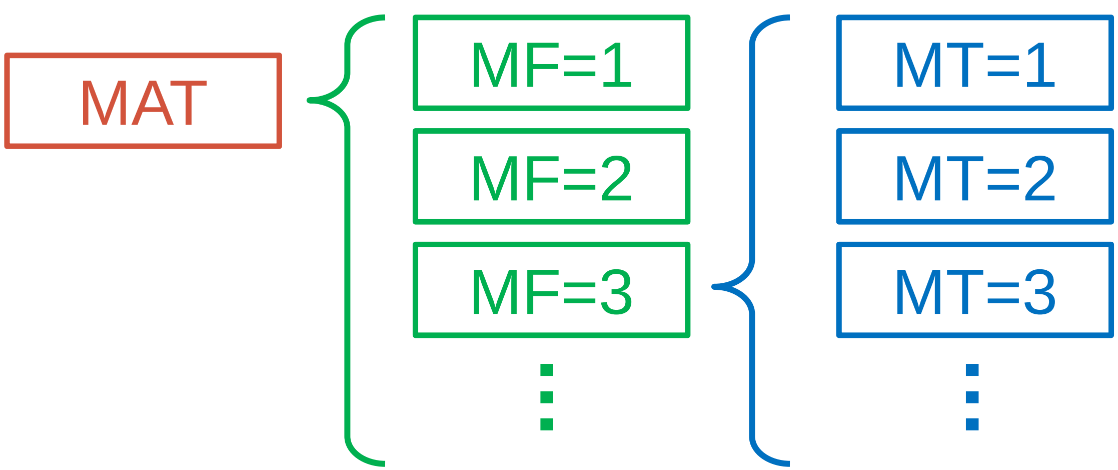
For thermal neutron scattering

Data format for evaluated nuclear data

- The current format is ENDF-6 format
  - Formatted for ENDF/B library
  - Maintained by the cross section evaluation working group (CSEWG) in USA
    - Ref: A. Trkov, et. al., “ENDF-6 Format Manual,” BNL-203218-2018-INRE
- The new format GNDS is defined in OECD/NEA
  - GNDS : **G**eneralized **N**uclear **D**ata **S**tructure
    - XML format
    - The format manual will be released in 2019
    - Ref: Nuclear Data Sheets, **113**, pp.3145-3171, (2012).

Data structure of ENDF-6 format

- ENDF-6 format consists mainly three stages
  - material : One nucleus or material
    Distinguished by MAT number
  - file : Physical quantities (XS, energy and angular distributions, …)
    Distinguished by MF number
  - section : Reaction type and data type
    Distinguished by MT number



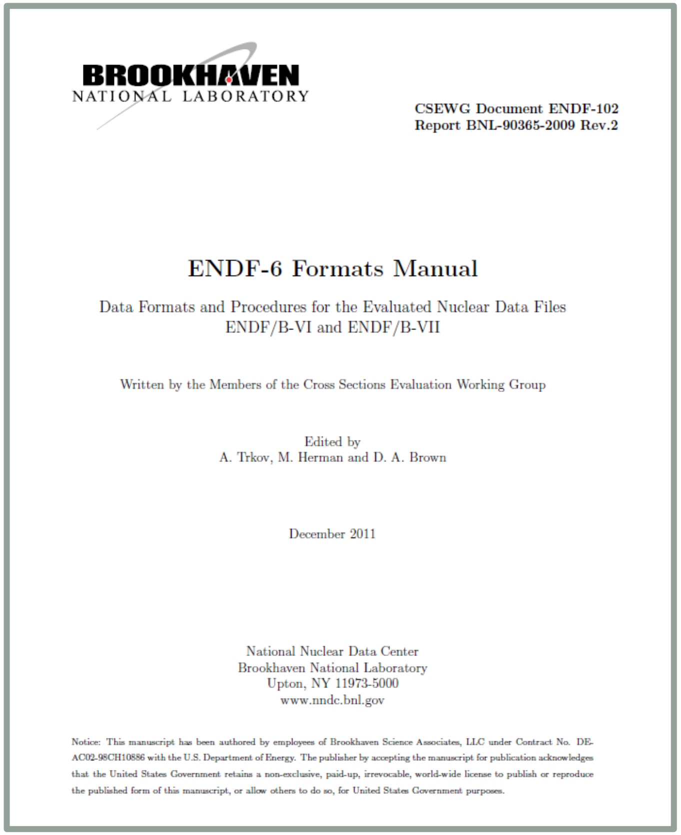
Data representation of ENDF-6 format

- One or two dimensional tabulated functions
  - Tabulated pairs of x(n) and y(n) are provided
    - $(E_1, \sigma_1), (E_2, \sigma_2), (E_3, \sigma_3), \cdots, (E_n, \sigma_n)$
  - Available interpolation scheme
    - Constant (histogram), linear-linear, linear-log, log-linear, log-log
- Parameters of function
  - Ex) resonance formula, polynomial representation, Legendre polynomials, …

Typical file (MF) number

- **MF= 1**: Comments, number of neutrons per fission
- **MF= 2**: Resonance parameters
- **MF= 3**: Reaction cross sections
- **MF= 4**: Angular distributions of emitted particle
- **MF= 5**: Energy distributions of emitted particle
- **MF= 6**: Angular and energy distributions of emitted particle
- **MF= 7**: Thermal neutron scattering data
- **MF= 8**: Fission yield and decay data
- **MF= 9**: Multiplicities of radioactive products
- **MF=10**: Production cross sections for radio nuclides
- **MF=11-15**: Photon production
- **MF=30-40**: Covariance data

Important for thermal neutron scattering



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CSEWG Document ENDF-102
Report BNL-90365-2009 Rev.2

ENDF-6 Formats Manual

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

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
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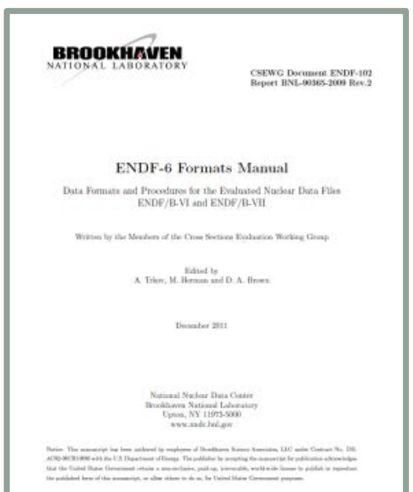
Ref: BNL-203218-2018-INRE

Example of evaluated nuclear data

(n,2n) XS of Fe−56 from JENDL−4.0

```
                                                                  MF
                                                            MAT   ↓ MT
 2.605600+4 5.545440+1          0          0          0          02631 3 16    1 } HEAD
-1.120270+7-1.120270+7          0          0          1         112631 3 16    2 ]
         11          2          0          0          0          02631 3 16    3 |
 1.140470+7 0.000000+0 1.170000+7 1.622410-2 1.200000+7 4.800450-22631 3 16    4 |
 1.300000+7 2.138200-1 1.400000+7 3.891650-1 1.500000+7 5.134000-12631 3 16    5 | TAB1
 1.600000+7 5.817500-1 1.700000+7 6.107500-1 1.800000+7 6.118000-12631 3 16    6 |
 1.900000+7 5.977000-1 2.000000+7 5.759000-1                       2631 3 16    7 ]
                                                                  2631 3  099999 } SEND
```

66 letters (11 data) | 4 2 3 5 letters



[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

Thermal neutron scattering data in nuclear data

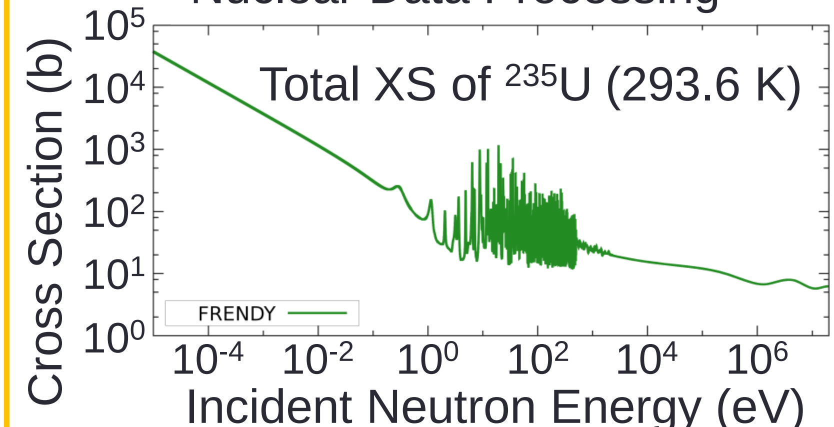
- Evaluated nuclear data library contained in MF=7
- Three scattering reactions are available
  - Coherent elastic scattering (MF=7, MT=2)
    - For crystalline materials（Bragg diffraction)
  - Incoherent elastic scattering (MF=7, MT=2)
    - For non-crystalline materials
  - Incoherent inelastic scattering (MF=7, MT=4)
    - Using thermal scattering law data : S(α, β)
  - ENDF-6 format cannot contain both the parameters of coherent and incoherent elastic scattering cross sections
    - The new nuclear data format GNDS will be able to contain both cross sections
    - Covariance data of thermal neutron scattering is not formatted and it will be formatted in GNDS

Overview of nuclear data processing

- Generating cross section (XS) library from evaluated nuclear data library
  - Not just a converter
  - Many processes, *e.g.*, linearization and Doppler broadening, are required
- NJOY of LANL is widely used in the world
  - Development of domestic nuclear data processing code was required
  - We started to develop a new nuclear data processing code **FRENDY** in 2013

Evaluated Nuclear Data File
(**JENDL、ENDF、JEFF**)

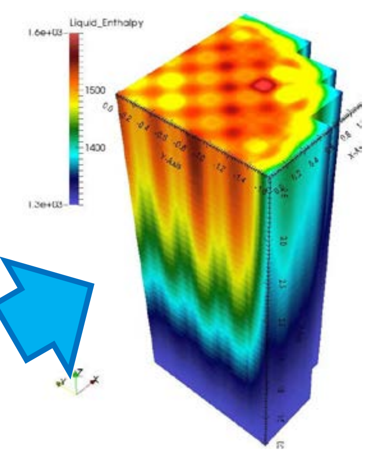
Nuclear Data Processing



Cross Section library

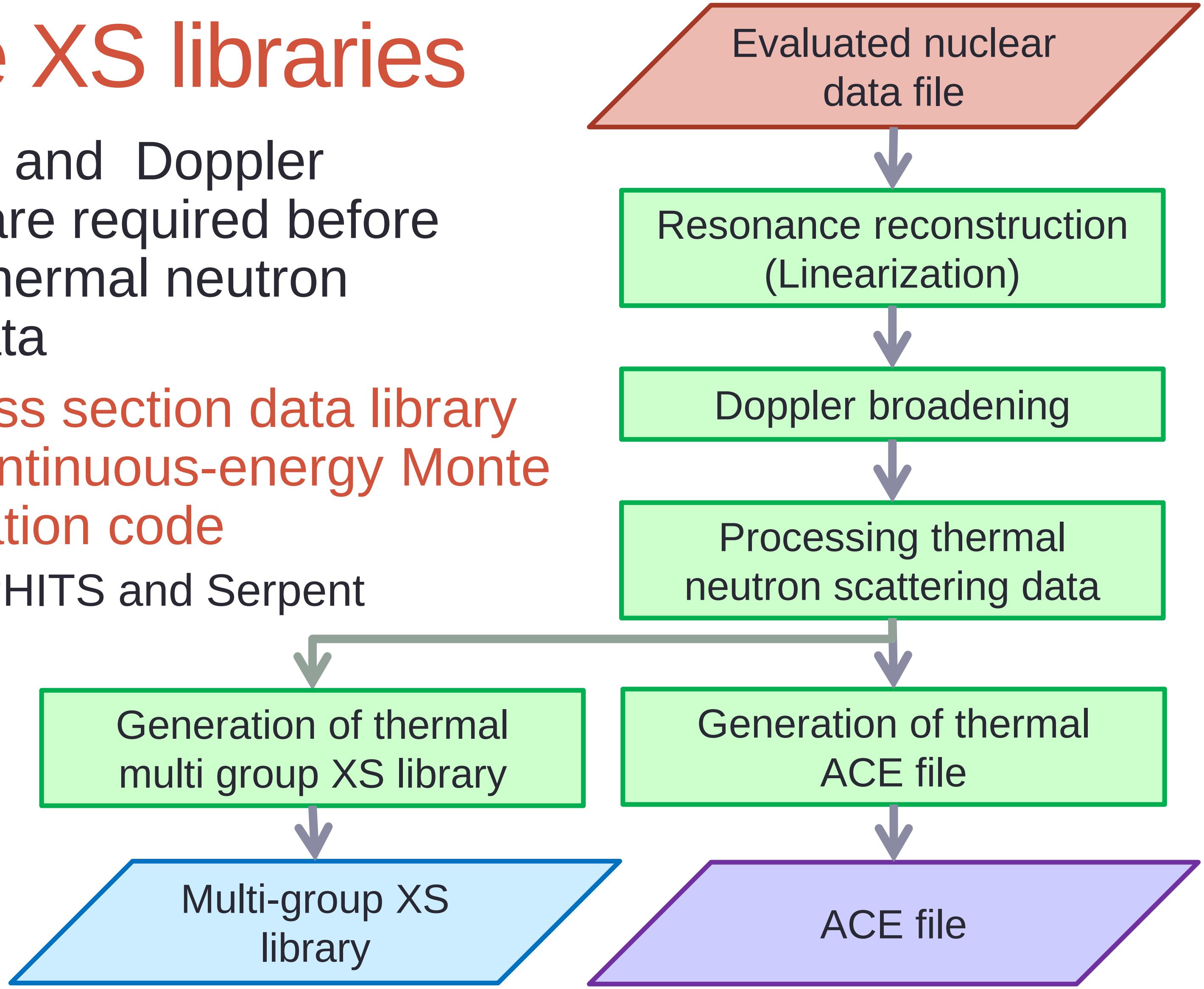
Transport codes
MVP, PHITS, MCNP

Flux Distribution



Processing flow to generate XS libraries

- Linearization and Doppler broadening are required before processing thermal neutron scattering data
- ACE is a cross section data library format for continuous-energy Monte Carlo calculation code
  - For MCNP, PHITS and Serpent



Sample input of NJOY (H in H_2O)

- Input file of NJOY is so difficult
  - Input data cannot be made if user cannot read the evaluated nuclear data file
- FRENDY can easily generate ACE file with simple input
  - Evaluated nuclear data file name and temperature are only required

```
reconr                          / command
 20  21                         / input(tape20), output(tape21)
'pendf tape for JENDL-4.0 H001'  / identifier for PENDF
 125                            / mat
 1.00e-03  0.00                 / err, temp
 0                              /
broadr                          / command
 20  21  22                     / input(tape20), output(tape21)
 125   1                        / mat
 1.00e-03                       / err
 296.0                          / temp
 0                              /
thermr                          / command
 23  22  25                     / endf, pendf(in), pendf(out)
 1 125 8 1 4 1 2 229 0          / mat_e, mat_p, bin no, temp no,
                                  inela opt, ela opt, principal atom no,
                                  mtref, pri opt
 296.0                          / temp
 1.0E-3  5.0                    / err, max ene
acer                            / command
 23  25   0  30  31             / nendf, npend, ngend, nace, ndir
  2   1   1  0.20               / iopt(fast), iprint(max), itype, suffix
 'ACE file for 01_h_in_h2o'     / identifier for ACE file
 125  296.0   'lwtr'            / matd, tempd, tname
 1001  0  0                     / moderator component za value
 229  64  230  0  1  1000.0  0  / mti, nbint, mte, ielas,
                                  nmix, emax, iwt
stop                            /
```

Sample input of FRENDY (H in H_2O)

- Simple input file
  - Nuclear data file name (^1H and H_2O), ACE file name and temperature are only required
- Comment line is similar to C/C++
  - //~ or /* ~ */

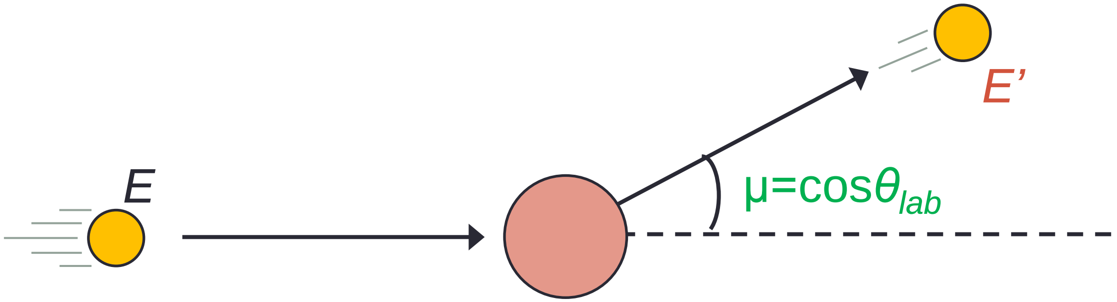
< Sample input of FRENDY (H in H_2O) >

```
ace_therm_mode  //process TSL data
  nucl_file_name        H001.dat
  nucl_file_name_tsl    H_in_H2O.txt
  ace_file_name         H_in_H2O.ace
  temp  /* temp data */  296.0 // [K]
```

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).
K. Tada, "Comparison of the processing results between FRENDY and NJOY", Technical Meeting on the Nuclear Data Processing (2017).
(https://www-nds.iaea.org/index-meeting-crp/TM_NDP/)

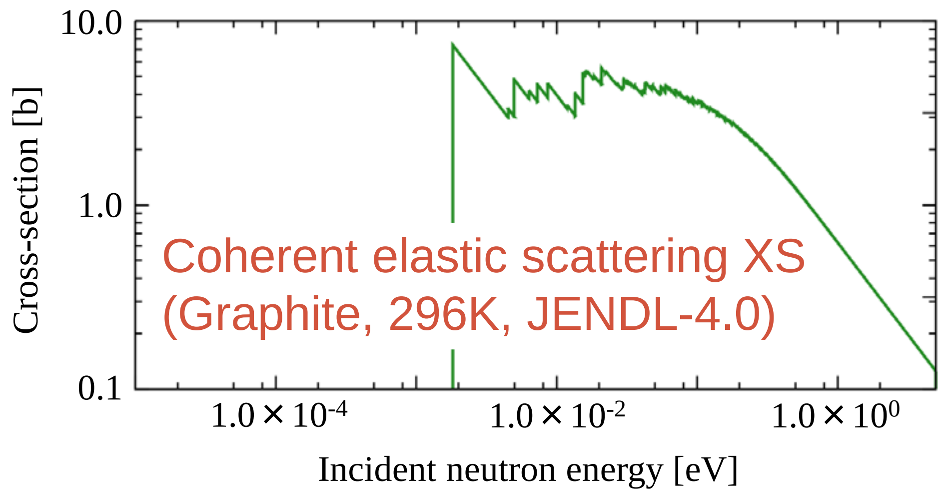
Processing of thermal neutron scattering data

- Calculates scattering cross sections and angular and energy distributions for secondary neutron
  - Neutronics calculation codes cannot treat the parameters of thermal neutron scattering data
    - Converting MF=7 into MF=3 (cross section) and MF=6 (angular and energy distributions of emitted particle) is required
  - To reduce the data size of evaluated nuclear data file, parameters of thermal neutron scattering data are contained
    - The large amount of data size is required to storage XS and angular and energy distributions for secondary neutron



Evaluated nuclear data (coherent elastic)

- Temperature
- Number of Bragg edge
- Bragg edges and structure factors

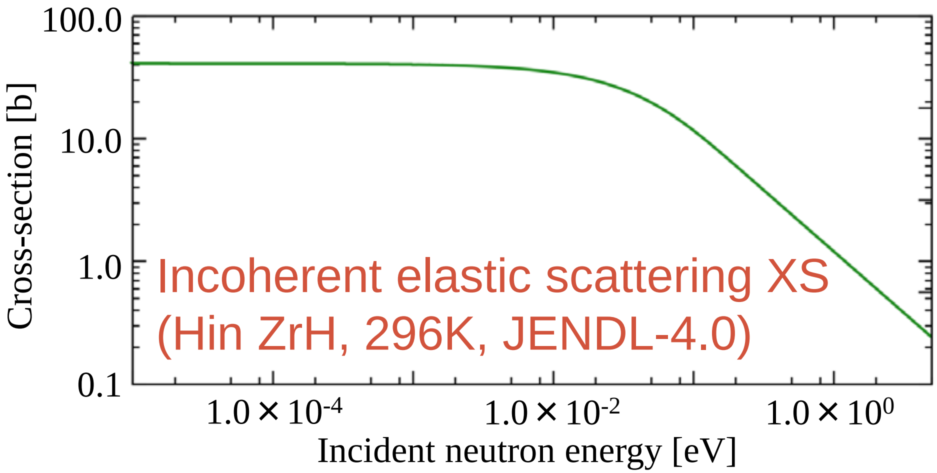


$$\sigma^{coh}(E,E',\mu) = \frac{1}{E}\sum_{i}^{E_i<E} s_i \delta(\mu-\mu_i)\delta(E-E')$$

- s_i : structure factors
- E_i : energy of Bragg edge
- E : incident energy
- μ : scattering cosine in laboratory system

Evaluated nuclear data (incoherent elastic)

- Temperature
- Bound scattering XS
- Debye-Waller factor

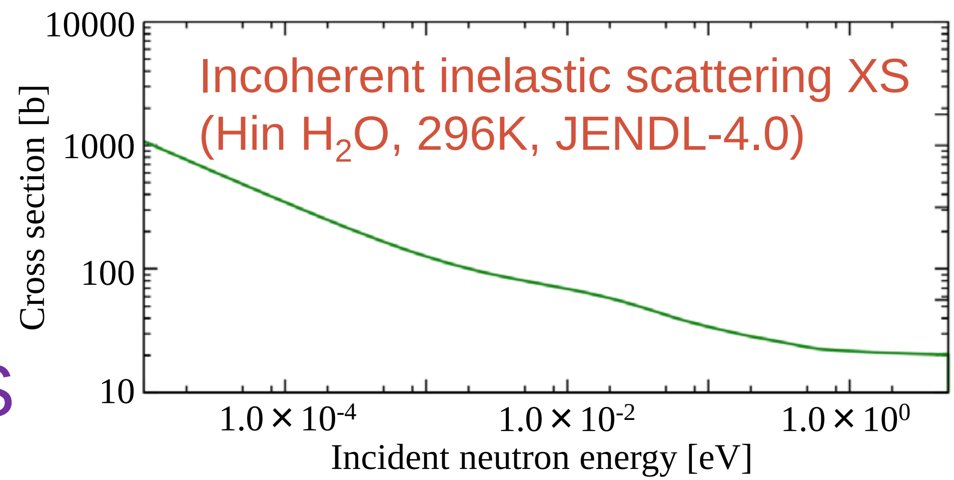


$$\sigma^{iel}(E,E',\mu) = \frac{\sigma_b}{2} e^{-2WE(1-\mu)} \delta(E - E')$$

- σ_b : Characteristics bound scattering XS
- W : Debye-Waller integral divided by the atomic mass (eV^{-1}) as a function of temperature (K)

Evaluated nuclear data (incoherent inelastic)

- Number of atoms
- Temperature
- S(α,β), α, and β
- Free atom scattering XS



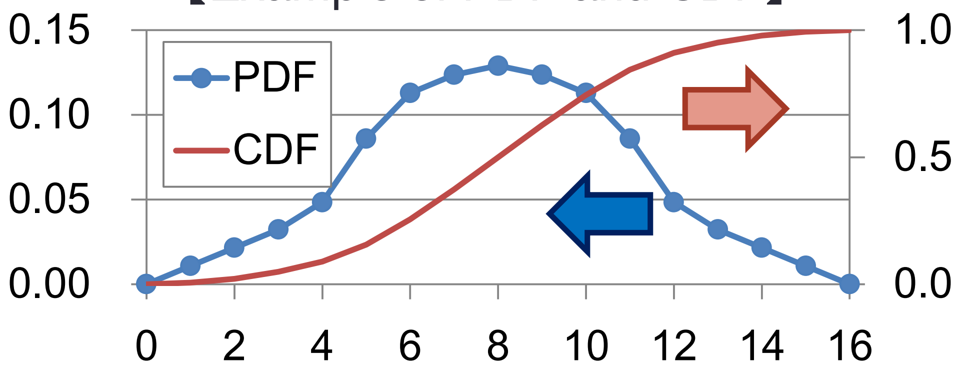
$$\sigma^{inc}(E,E',\mu)=\sum_{n=0}^{N_s}\frac{M_n}{2\mathrm{k_B}T}\sigma_{fn}\left(\frac{A_n+1}{A_n}\right)^2\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S_n(\alpha_n,\beta)$$

- N_s : Number of non-principal scattering atom types
- M_n: Number of *n*-th type atoms
- σ_{fn}: Characteristics free atom scattering cross section

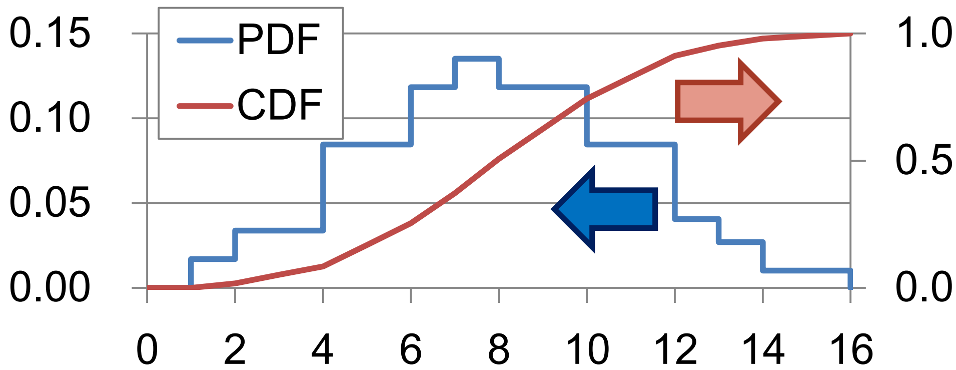
Generation of ACE file

- Continuous energy Monte Carlo calculation codes use cumulative probability distribution (PDF/CDF)
  - Cross section, angular and energy distributions are converted to cumulative probability distribution
  - PDF: Probability Density Function
  - CDF : Cumulative Density Function

【Example of PDF and CDF】



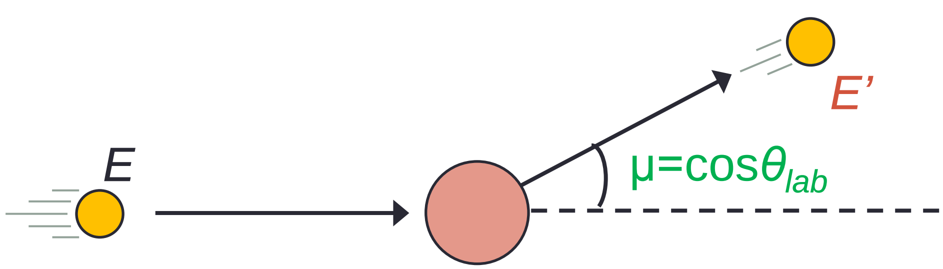
From linear-linear to PDF/CDF

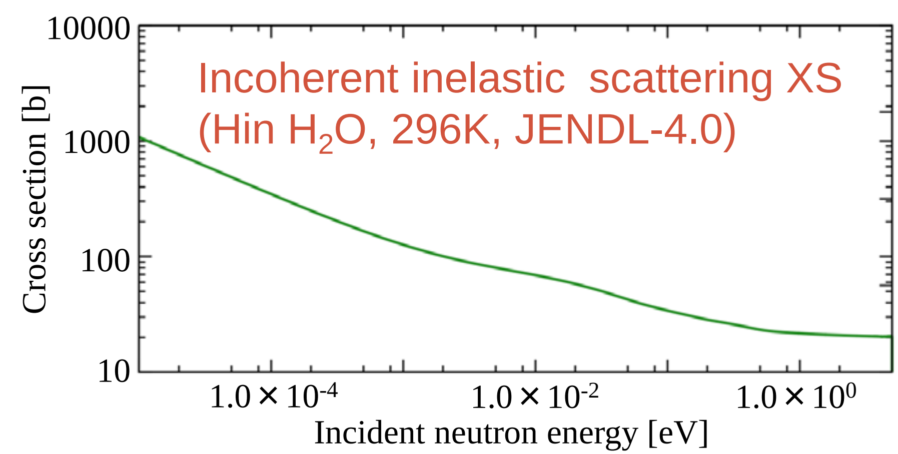


From histogram to PDF/CDF

Required data to generate XS library

- Two types of data are available to generate ACE file
  - Parameters of thermal neutron scattering data (MF=7)
  - Scattering cross section (MF=3) and angular and energy distributions for secondary neutron (MF=6)
    - The unified energy grid is used to generate ACE file
    - These data must be calculated in specified incident energy (10^{-5} ~ 10 eV) using linear-linear, linear-log, log-linear or log-log interpolation
- If users generate XS library from the latter type, modification of nuclear data processing code is required
  - FRENDY is a good tool to generate XS library from it!!





Conclusions

- Overview of evaluated nuclear data library
- Thermal neutron scattering data in evaluated nuclear data
  - Coherent and incoherent elastic scattering
  - Incoherent inelastic scattering
- Processing flow to generate XS libraries
  - Two types of data are available to generate ACE file
    - Parameters of thermal neutron scattering data
    - Scattering cross section and angular and energy distributions for secondary neutron
  - FRENDY is a good tool to generate XS library from these data