Nuclear Data Editing Functions of FRENDY

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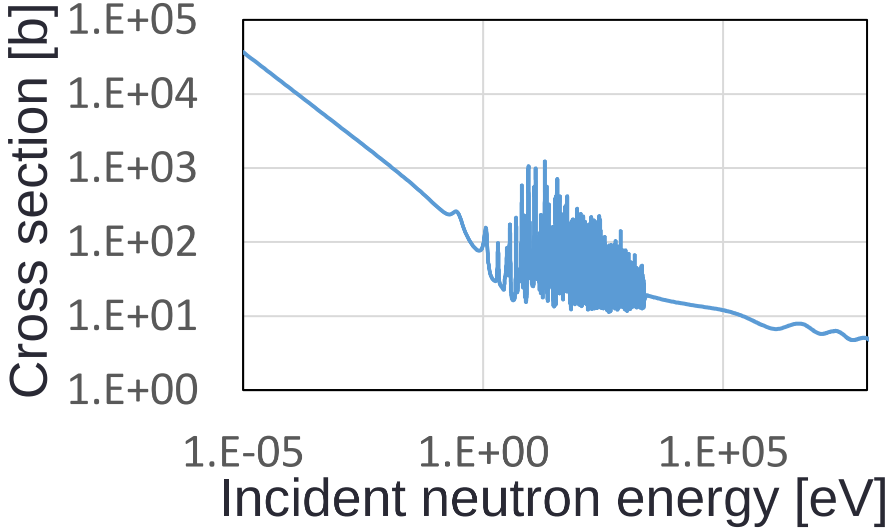
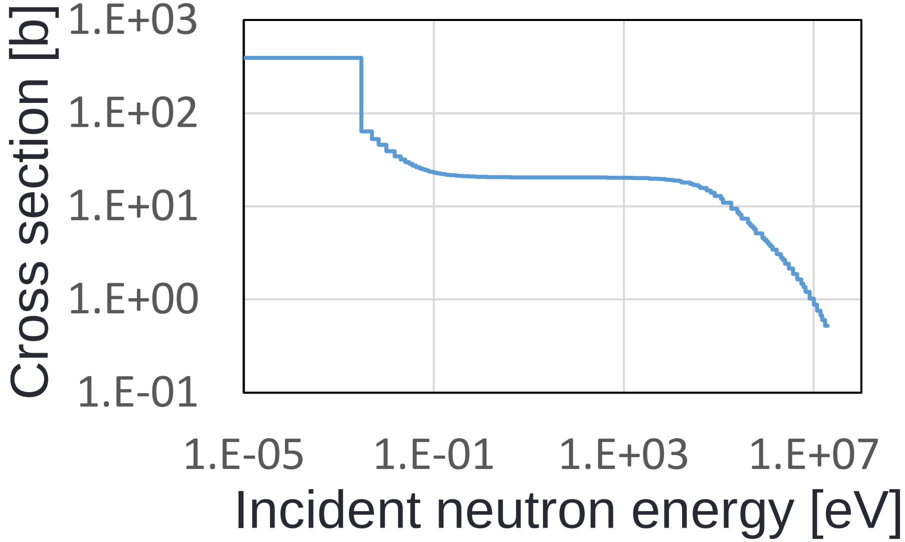
<Continuous energy XS of U-235>



<Multi-group XS of H-001>



About FRENDY

- FRENDY is a nuclear data processing code.
  - **FR**om **E**valuated **N**uclear **D**ata librar**Y** to any application
  - FRENDY is an open-source software under 2-clause BSD license.
  - Everyone can download FRENDY from following website:
    - https://rpg.jaea.go.jp/main/en/program_frendy/index.html
  - Presentation and exercise materials can be found on this website.
- The main purpose of FRENDY is generating cross section files for nuclear application codes.
  - ACE formatted files for MCNP, PHITS, Serpent, and so on.
  - Multi-group cross section files (GENDF/MATXS) for deterministic codes.
- We are now modifying FRENDY to handle ENDF/B-VIII.1.

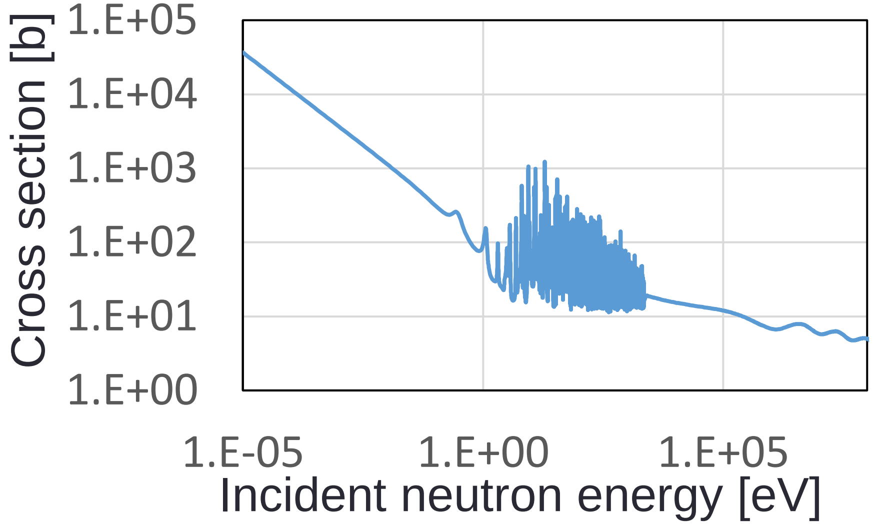
Nuclear data editing functions of FRENDY

- FRENDY has editing functions to modify nuclear data files and to confirm processing results.
  - Modifying nuclear data files
    - It removes, adds, and/or exchanges specified MF/MT data.
  - Confirming processing results
    - FRENDY generates 1D data (X-Y data) from ENDF, ACE, and GENDF files.
      - It outputs X-Y data for gnuplot, Matplotlib, and Excel.
    - It also outputs comparison results.
      - Difference of libraries, difference of processing codes, and difference of processing conditions.

```
# endf/pendf/ace file name     : ../lib/n_092-U-235.dat
# Temperature [K] (inp / nucl) :  300.000 /  0.00000
# MT (reaction type)           : 1
#
# energy [eV] / data
1.0000000000e-05  3.6739375500e+04
1.1250000000e-05  3.4638406900e+04
1.2500000000e-05  3.2861060200e+04
```

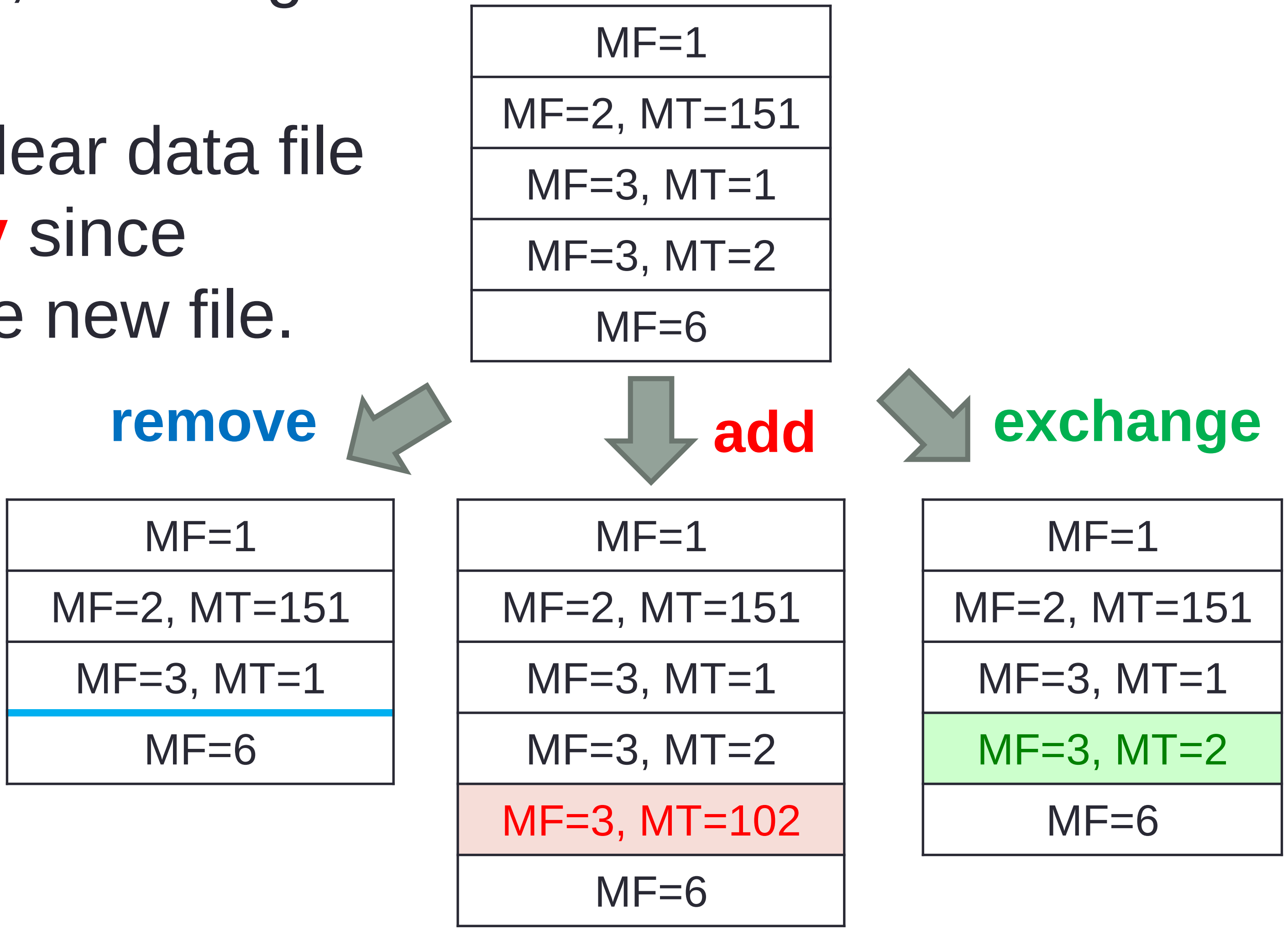
Example of X-Y data

Plotting with Excel



ENDF modification function

- This function removes, adds, exchanges specified MF/MT data.
- The modified evaluated nuclear data file **must be checked carefully** since FRENDY does not check the new file.



Sample input for ENDF modification function

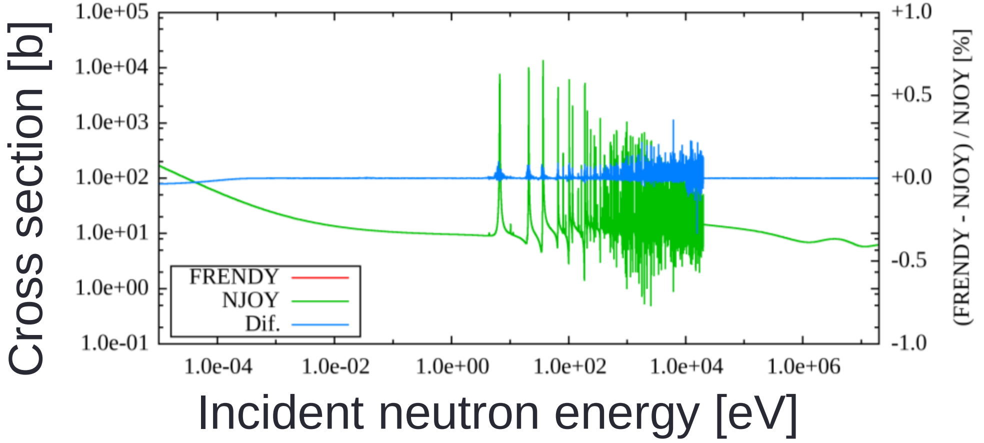
- This function performs the modifications line by line.
  - replace MF “MF number” MT “MT number” “Original file name” “Replaced file name” “Modified file name”
  - remove MF “MF number” MT “MT number” “Original file name” “Modified file name”
  - add MF “MF number” MT “MT number” “Original file name” “Replaced file name” “Modified file name”
    - If the users only select the MF number, specified MF data are modified.
    - If the users only select the MT number, specified MT data in all MF data are modified.

```
endf_file_modification_mode //processing mode
  replace  MF  2   MT 151  ./j40/Pu239.dat        ./B80/n-094_Pu_239.endf   ./Pu239_mod01.dat
  remove   MF  33          ./Pu239_mod01.dat                                ./Pu239_mod02.dat
  add      MF  14  MT 18   ./Pu239_mod02.dat  ./ B80/n-094_Pu_239.endf ./Pu239_mod03.dat
```

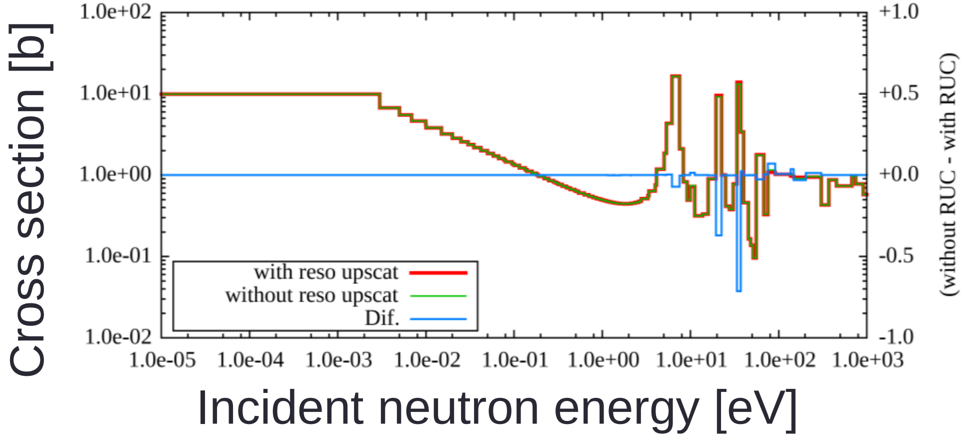
1D data (X-Y data) generation function

- This function outputs X-Y data for gnuplot, Matplotlib, Excel, and so on.
  - Cross section data and double differential cross section data from ENDF (PENDF), ACE, and GENDF.
  - Pointwise and multi-group data.
    - Multi-group cross section data were generated from pointwise data with a specified weighting function such as flat and 1/E flux.
  - From FRENDY Version 2.03.

<Comparison of pointwise XS of U-238>



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



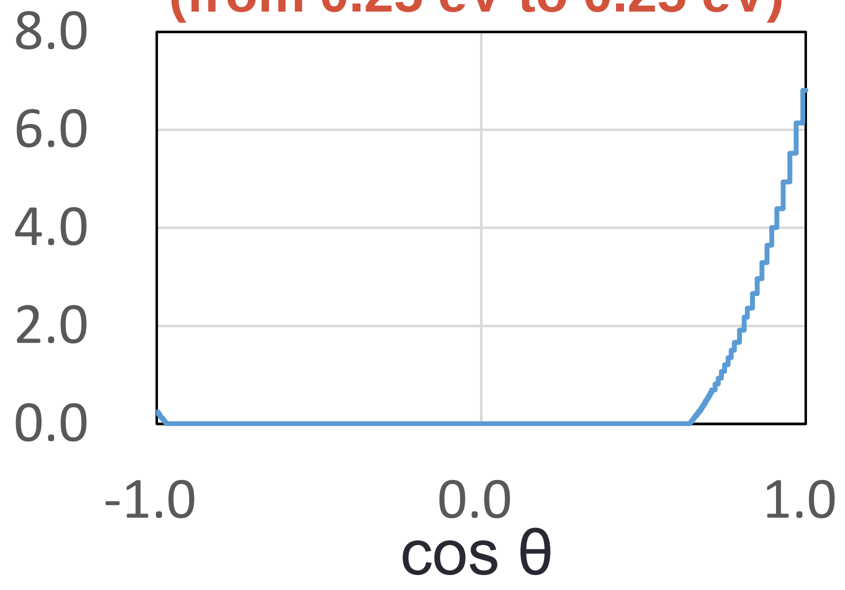
Available X-Y data for ENDF and ACE files

- 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 (ν-tot), 1455 (ν-d), and 1456 (ν-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 (ν-tot), 1455 (ν-d), and 1456 (ν-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.

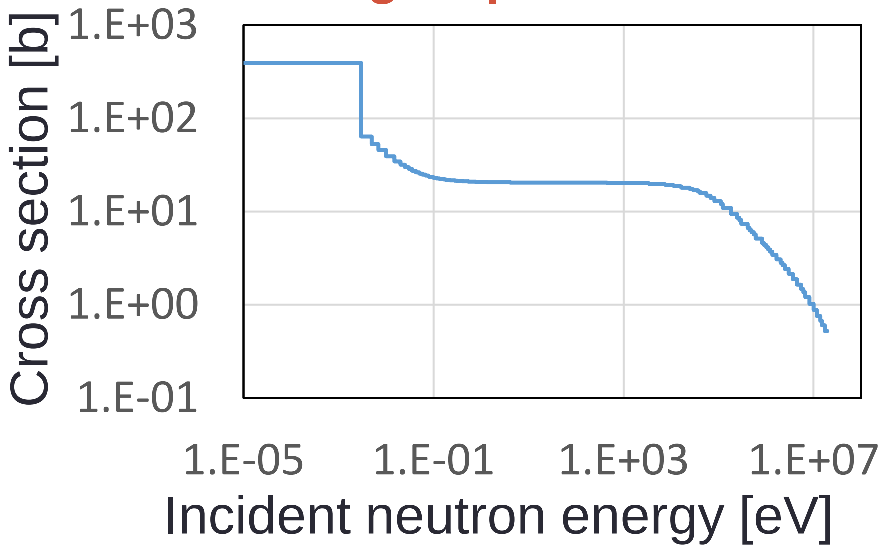
Angular distribution of H in H_2O (from 0.25 eV to 0.25 eV)



Nuclear data processing before X-Y data generation

- FRENDY reconstructs resonance formula and linearize TAB1 data if users use original nuclear data (ENDF file).
- FRENDY calculates doppler broadened cross section if the input temperature is higher than that of input ENDF or ACE files.
- FRENDY can generates multi-group cross section data from ENDF or ACE files.

<Multi-group XS of H-001>



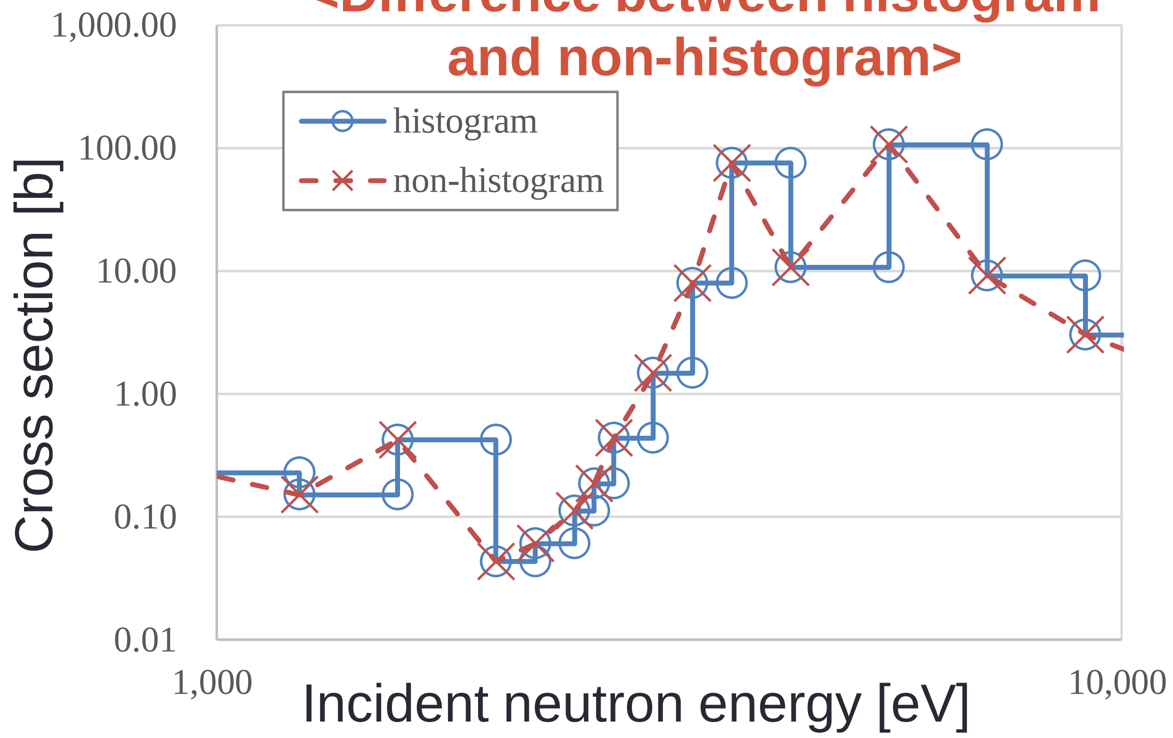
Processing conditions for X-Y data generation

- Tolerance value for resonance reconstruction, linearization, and Doppler broadening is changed from 0.1% to 1.0%.
  - To reduce processing time and data size.
  - Users can change tolerance value using “error” option.
- Maximum energy of Doppler broadening is changed from top of resolved resonance region to 1 MeV.
- In the multi-group cross section generation, IWT=4 is not available for the weighting function.
  - IWT=4: fission+1/E+Maxwell

Multi-group plotting option

- FRENDY has two plot options (Histogram and Non-histogram)
  - Histogram outputs two energy grid points for each energy group.
    - Maximum and minimum energy grids 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.
  - Users can easily change plot option using “edit_flag” option.

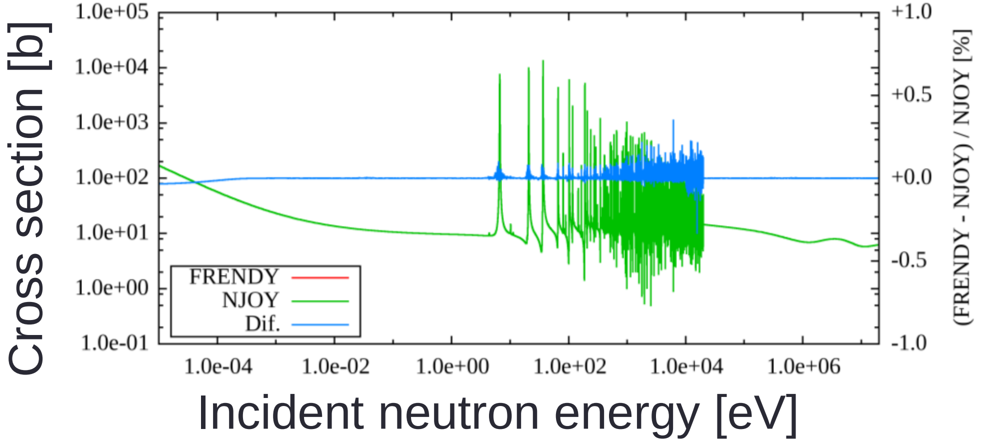
<Difference between histogram and non-histogram>



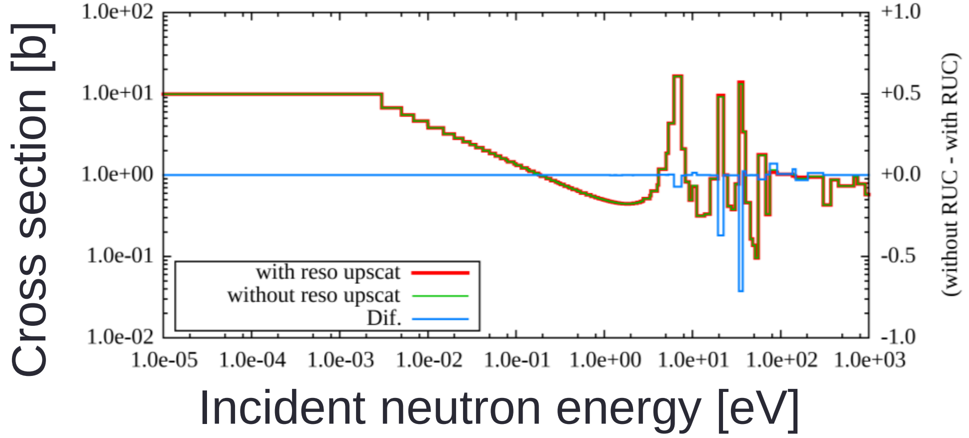
Comparison of nuclear data (1/2)

- FRENDY outputs relative difference of two nuclear data.
  - For comparison of processing results, nuclear data, and so on.
- FRENDY calculates all energy grids for both data.
  - Energy grids of data 1: 1.0E-5, 1.0E-3, 1.0E-1, 1.0E+1
  - Energy grids of data 2: 1.0E-4, 1.0E-2, 1.0E-0, 1.0E+2
  - Energy grids of plotting file: 1.0E-5, 1.0E-4, 1.0E-3, 1.0E-2, 1.0E-1, …, 1.0E+2

<Comparison of pointwise XS of U-238>



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



Comparison of nuclear data (2/2)

- FRENDY automatically processes resonance reconstruction and doppler broadening before comparison.
- If users do not set temperature, FRENDY does not check the temperature in the ENDF or ACE file.
- Comparison of different format, *i.e.*, ENDF-6 formatted file and ACE formatted file, is possible.
  - Users can confirm the ACE file generation.

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 have to 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 )
```

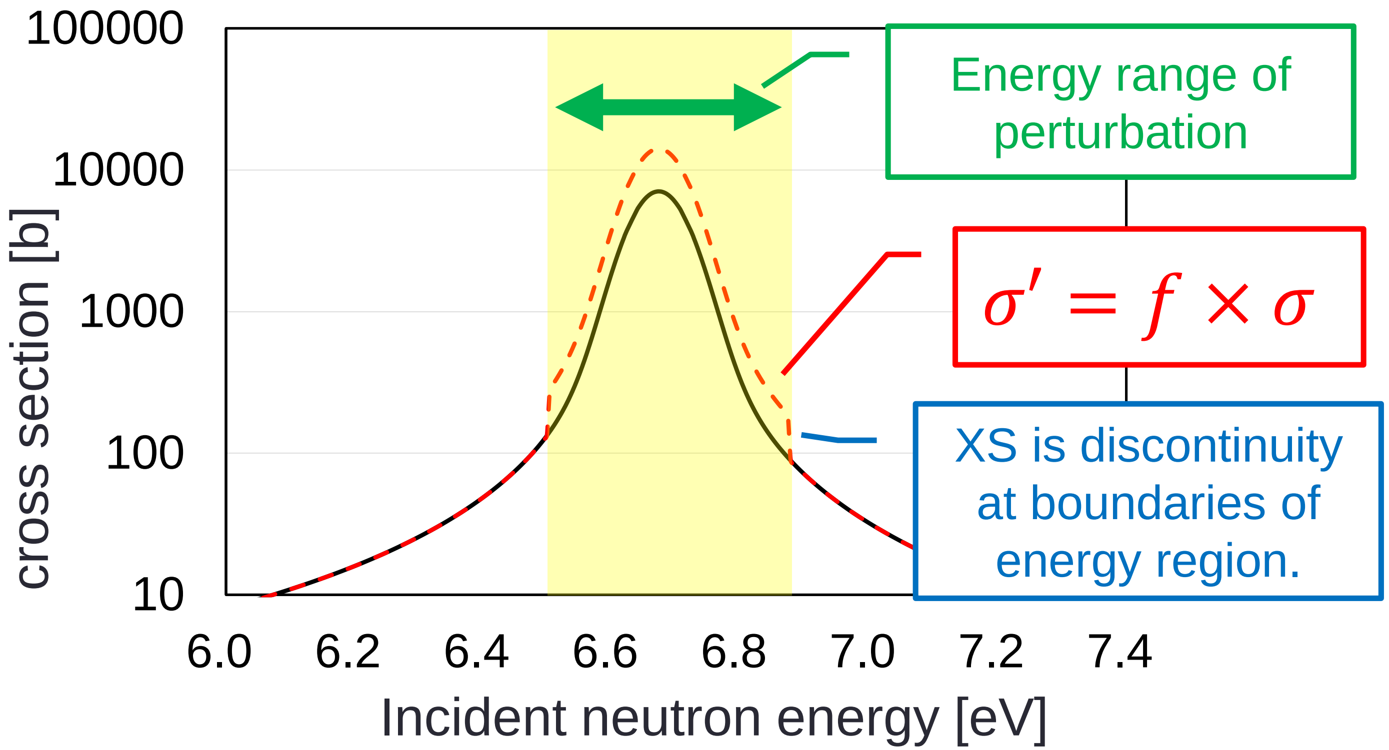
<Comparison of nuclear data files>

```
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 )
```

Other functions without nuclear data processing

- ACE file perturbation tool
  - For sensitivity analysis with direct perturbation method and uncertainty analysis with random sampling method.
  - New version can perturb elastic scattering angular distribution.
- NJOY input file generation function
  - This function generates NJOY input file from FRENDY input file.

<Example of perturbation>



NJOY input file generation function

- This function generates NJOY input file from FRENDY input file.
  - Only change the mode name from XXX to XXX_make_inp.
    - For example, ace_fast_mode_make_inp, ace_tsl_mode_make_inp, mg_mode_make_inp
  - Available module of NJOY is RECONR, BROADR, GASPR, PURR, THERMR, ACER, GROUPR, and MATXSR.
  - NJOY input file name is "FRENDY input file name".njoy_input.dat.
    - When FRENDY input file name is "U235.inp", NJOY input file name is "U235.inp.njoy_input.dat".
- This option will be useful to check NJOY input file prepared by users.

Sample of NJOY input file generation function

```
ace_file_generation_fast_mode_make_inp
nucl_file_name          tape20
  temp                  293.6
  ace_file_name         tape30
  mcnp_dir_file_name    tape31
  ace_label_data
        "ACE file for ENDF8.1 n-092_U_235"
  suffix_id             0.20
```

```
reconr                          /reconr start
20 21                           /card01: nendf npend
'no label data'                 /card02: tlabel
9228                            /card03: mat
1.00000e-03                     /card04: err
0                               /reconr end
broadr                          /broadr start
20 21 22                        /card01: nendf nin nout
9228 1                          /card02: nmat1 ntemp2
1.00e-03 -2.250e+03             /card03: errthn thnmax
2.93600e+02                     /card04: temp2
0                               /broadr end
gaspr                           /gaspr start
20 22 23                        /card01: nendf nin nout
purr                            /purr start
20 23 24                        /card01: nendf nin nout
9228 1 10 20 100 0              /card02: matd ntemp nsigz nbin nladr iprint
2.93600e+02                     /card03: temp
1.00e+10 1.00e+04 1.00e+03 3.00e+02 1.00e+02 3.00e+01 1.00e+01
1.00e+00 1.00e-01 1.00e-05 /card04: sigz
0                               /purr end
acer                            /acer start
20 24 0 30 31                   /card01: nendf npend ngend nace ndir
1 1 1 2.00000e-01 0             /card02: iopt iprint itype suff nxtra
'ACE file for ENDF8.1 n-092_U_235' /card03: hk
9228 2.93600e+02                /card05: matd tempd
1                               /card06: newfor
                                /acer end
stop                            /
```

Other functions related nuclear data processing

- Multi-nuclear data processing tool
  - The latest version of FRENDY 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 <u>input templates</u>.
    - 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
```

Conclusions

- Many functions were developed to easily handle nuclear data and cross section data files.
  - ENDF modification function
  - 1D data (X-Y data) generation
  - ACE file perturbation tool
- FRENDY also has some tools for efficient nuclear data processing.
  - NJOY input file generation function
  - Multitasking tool