

# Input format of FRENDY

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# Input format of FRENDY

- FRENDY treats two types of the input formats.
  - FRENDY original input format
  - NJOY compatible
- Simple input format
  - 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 7 20 500 / mat, temp no, sig no, bin no, lad no
296.0 / temp
1E10 1E4 1E3 300 100 30 10 / sig zero
0 /
acer / command
20 25 0 30 31 / nendf, npend, ngend, nace, ndir
1 1 1 0.30 / iopt(fast), iprint(max), itype, suffix
'ACE file for JENDL-4 U235' / descriptive character
9228 296.0 / mat, temp
1 1 / newfor(yes), iopp(yes)
1 1 1 / thin(1), thin(2), thin(3)
stop /
```

# FRENDY original input format

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# Basics of FRENDY input format

- First line **must be** processing mode.
  - ace\_fast\_mode : Neutron induced ACE file
  - ace\_tsl\_mode : ACE file of thermal scattering law data
  - ace\_dosi\_mode: Dosimetry ACE file
- Other lines are free format.
  - Setting “input data name” and “input data”
  - Bracket is used to describe array data, e.g., (1.0 2.0 3.0).
  - Text data is surrounded by single or double quotation mark, e.g., “~” or ‘~’.
    - Multiline is available for array data and text data.
- Comment line is similar to C/C++.
  - //~ or /\* ~ \*/

# Main input parameters

- Required parameters
  - `nucl_file_name` : Evaluated nuclear data file name
  - `nucl_file_name_tsl`: TSL data file name (TSL only)
- Other main input parameters
  - `temp` : Temperature (K) (Default: 293.6 K)
  - `ace_file_name` : ACE file name
  - `ace_dir_file_name`: XSDIR file name
  - `suffix_id` : Suffix ID of ACE file
  - `ace_label_data` : Comment line of ACE file (one line)
  - `thermal_za_id_name`:  $S(\alpha, \beta)$  identifier of MCNP (TSL only)
- Additional parameters
  - `Write_pendf_probability_table`: PENDF file name after probability table generation
  - `Write_pendf_tsl`: PENDF file name after TSL data processing (TSL only)
    - PENDF (Point-wise ENDF) file is a processing result of NJOY.
    - These PENDF file can be used as input PENDF of NJOY.

# Example of FRENDY input (Neutron induced)

```

ace_fast_mode // Processing mode
nucl_file_name    ../lib/U235.dat
temp /* [K] */    300.0
ace_file_name     ./ace/U235.ace
ace_dir_file_name ./xsd/U235.xsdir
ace_label_data    "U-235 from JENDL-4.0"
suffix_id         0.50
  
```

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

Relative path or absolute path

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

# Modification of processing conditions (Neutron induced)

- Please try to modify input file if processing conditions are changed as follows:
  - Evaluated nuclear data file name: `./j40/lib/Fe056.dat`
  - Temperature: `550.0 [K]`
  - ACE file name: `./j40/ace/Fe056.ace`
  - XSDIR file name: `./j40/xsd/Fe056.xsdir`
  - Comment line of ACE file: `Fe-056 from JENDL-4.0`
  - Suffix ID: `0.10`
  - PENDF file name: `./j40/pendf/Fe056.pendf`

The answer is next slide.



# Modification of processing conditions (Neutron induced)

Input is modified to meet the processing conditions.

```

ace_fast_mode // Processing mode
nucl_file_name      ./j40/lib/Fe056.dat
temp /* [K] */      550.0
ace_file_name       ./j40/ace/Fe056.ace
ace_dir_file_name   ./j40/xsd/Fe056.xsdir
ace_label_data      'Fe-056 from JENDL-4.0'
suffix_id           0.10
write PENDF probability table ./j40/PENDF/Fe056.PENDF
    
```

Text data is surrounded by single or double quotation mark.

Adding PENDF output option

# Example of FRENDY input (TSL)

```

ace_tsl_mode // Processing mode
nucl_file_name      ../lib/H001.dat
nucl_file_name_tsl  ../lib_sab/01_h_in_h2o.txt
ace_label_data      "HinH2O from JENDL-4.0"
temp                296.0
ace_file_name        ./ace_sab/lwtr.ace
ace_dir_file_name    ./xsd_sab/lwtr.xsdir
suffix_id            0.50
thermal_zs_id_name  "lwtr"
    
```

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

Temperature prepared in TSL data file (nucl\_file\_name\_tsl) is **only** available.

S( $\alpha$ ,  $\beta$ ) identifier of MCNP (Maximum: 6 characters)

- Processing conditions of above example
  - TSL data file name: ../lib\_sab/01\_h\_in\_h2o.txt
  - S( $\alpha$ ,  $\beta$ ) identifier of MCNP: lwtr
    - lwtr: light water
    - This name is used in S( $\alpha$ ,  $\beta$ ) card of MCNP input.

# Modification of processing conditions (TSL)

- Please try to modify input file if processing conditions are changed as follows:
  - Evaluated nuclear data file name: `./j40/lib/C000.dat`
  - TSL data file name: `./j40/lib/31_graphite.txex`
  - Temperature: `500.0 [K]`
  - ACE file name: `./j40/ace/graphite.ace`
  - XSDIR file name: `./j40/xsd/graphite.xsdir`
  - Comment line of ACE file: `Graphite from JENDL-4.0`
  - Suffix ID: `0.10`
  - S( $\alpha$ ,  $\beta$ ) identifier of MCNP: `grph`
  - PENDF file name: `./j40/pendf/graphite.pendf`

The answer is next slide.

# Modification of processing conditions (TSL)

Input is modified to meet the processing conditions.

```

ace_tsl_mode // Processing mode
nucl_file_name      ./j40/lib/C000.dat
nucl_file_name_tsl  ../lib_sab/31_graphite.txt
temp /* [K] */      500.0
ace_file_name       ./j40/ace/graphite.ace
ace_dir_file_name   ./j40/xsd/graphite.xsdir
ace_label_data      'Graphite from JENDL-4.0'
suffix_id           0.10
thermal_za_id_name  'grph'
write_pendf_tsl     ./j40/pendf/graphite.pendf
    
```

Adding PENDF output option

# FRENDY original input format (Multi-group generation)

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# Input format of multi-group generation

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

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

- Processing of H in H2O

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

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

# Default option of multi-group generation

- Output format: **GENDF**
- Weighting spectrum: **1/E**
- Energy group structure: **XMAS 172-group structure**
- Flux calculation mode: **ultra-fine group slowing down calculation (120,000 groups)**
- Maximum Legendre order: **3 (P3)**

# Input Example (1/6): H-001

mg_neutron_mode		//Process mode
nucl_file_name	( ../lib/H001.dat )	//ENDF file name
mg_file_name	H001	//Output file name
mg_edit_option	( MATXS GENDF )	//Output format
temperature	300.0 // [K]	
mg_structure	( xmas_nea-lanl_172 )	//ign=18 in GROUPT/NJOY
mg_weighting_spectrum	( 1/e )	//iwt=3 in GROUPT/NJOY



Multi-group generation from ACE file

mg_neutron_mode		//Process mode
ace_file_name	( ../ace/H001.ace )	//ACE file name
mg_file_name	H001	//Output file name
mg_edit_option	( MATXS GENDF )	//Output format
mg_structure	( xmas_nea-lanl_172 )	//ign=18 in GROUPT/NJOY
mg_weighting_spectrum	( 1/e )	//iwt=3 in GROUPT/NJOY



# Input Example (2/6): U-235

```

mg_neutron_mode                //Process mode
nucl_file_name ( ../lib/U235.dat ) //ENDF file name
mg_file_name U235                //Output file name
mg_edit_option ( SimpleGENDF SimpleMATXS
                  GENDF MATXS MGFlux )
//SimpleGENDF: MATXS format consistent with NJOY99
//SimpleMATXS: GENDF format consistent with NJOY99
//GENDF: GENDF format consistent with NJOY2016
//MATXS: MATXS format consistent with NJOY2016
temp                300.0 //[K]
mg_structure ( ign18 ) //ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( iwt03 ) // iwt=3 in GROUPR/NJOY
legendre_order      3
  
```

# Input Example (3/6): H in H<sub>2</sub>O

```

mg_neutron_mode           //Process mode
nucl_file_name    ( ../lib/H001.dat )      //ENDF file name
nucl_file_name_tsl ( ../lib/01_h_in_h2o.txt ) //TSL file name
mg_edit_option    ( MATXS GENDF )         //Output format
mg_file_name      H_in_H2O                //Output file name
temperature       293.6 //[K]
mg_structure ( xmas_nea-lanl_172 )        //ign=18 in GROUPT/NJOY
mg_weighting_spectrum ( 1/e )             //iwt=3 in GROUPT/NJOY
mg_tsl_data_type   ( hh2o)
    
```



Multi-group generation from ACE file

```

mg_neutron_mode           //Process mode
ace_file_name    ( ../ace/H001.ace )      //ACE file name
ace_file_name_tsl ( ../ace/01_h_in_h2o.ace ) //ACE file name (TSL data)
mg_edit_option    ( MATXS GENDF )         //Output format
mg_file_name      H_in_H2O                //Output file name
mg_structure ( xmas_nea-lanl_172 )        // ign=18 in GROUPT/NJOY
mg_weighting_spectrum ( 1/e )             //iwt=3 in GROUPT/NJOY
mg_tsl_data_type   ( hh2o)
    
```



# Input Example (5/6): UO<sub>2</sub>

```

mg_neutron_mode                //Process mode
nucl_file_name ( ../lib/O016.dat ../lib/U235.dat ../lib/U238.dat )
mg_edit_option ( SimpleGENDF SimpleMATXS GENDF MATXS
  "1DXS 1, 2, 4, -50" "2DXS 1, 2, 4, -50" MGFlux )
  //"1DXS 1, 2, 4, -50": 1D cross-section data
  //"2DXS 1, 2, 4, -50": 2D cross-section data
  //MGFlux: Multi group flux data

mg_file_name mix_UO2           //Output file name
mg_structure ( xmas_nea-lanl_172 ) //ign=18 in GROUPT/NJOY
mg_weighting_spectrum ( 1/e )   // iwt=3 in GROUPT/NJOY
temp                          600.0 // [K]
legendre_order                 3

                                //O16   U235   U238
mg_number_density              (4.58e-2  7.18e-4  2.22e-2) //[1/barn/cm]
    
```

Atomic number density of each nuclide must be required to process compound of different isotopes.

# Input example (6/6): U-235

## (Automated setting of background XS)

```

mg_neutron_mode           //Process mode
nucl_file_name ( ../lib/U235.dat ) //ENDF file name
mg_file_name U235         //Output file name
mg_edit_option ( GENDF MATXS )
temp                      300.0 //[K]
mg_structure ( ign18 )    //ign=18 in GROUPT/NJOY
mg_weighting_spectrum ( iwt03 ) // iwt=3 in GROUPT/NJOY

sigma_zero_data(auto 0.1 50 1.0e-10 rr linear)
//Tolerance = 0.1 (10%)
//Maximum number of background XS = 50
//Minimum background XS = 1.0E-10 (barn)
//Target of interpolation (factor / rr) = reaction rate)
//Interpolation method (cubic / linear) = linear interpolation
  
```

# NJOY compatible input format

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# Basics of NJOY compatible input format (1/2)

- Each module is independent.
  - RECONR, BROADR, GASPR, PURR, THERMR, ...
  - Input for each module is required.
- Order of module has impact on processing result.
  - RECONR must be set before BROADR.
  - BROADR must be set before PURR and THERMR.
- Comment line is after slash “/”.
  - Input information is written in NJOY manual and source files.
  - Input information uses Fortran language.
    - $A.gt.B \rightarrow A > B$ ,  $A.ge.B \rightarrow A \geq B$ ,  $A.lt.B \rightarrow A < B$ ,  $A.le.B \rightarrow A \leq B$
- Text data is surrounded by single quotation mark.
  - For example, ‘This PENDF file is U-235 from JENDL-4.0’.

# Basics of NJOY compatible input format (2/2)

- Card number of input information is line number.
  - The input parameters written in Card N must be set in one line.
  - If user sets slash, other input data are default values.
    - Third, forth, and fifth data use default values if five data are required in Card N and only two data are set.
  - NJOY needs MAT number to identify nuclide or material.
  - NJOY considers that data of many nuclides are written in one file.
  - NJOY can process data of several nuclides with one input file.
- “tapeNN” is only available for file name.
  - tape20, tape21, tape22, ..., tape99



# MODER module and binary tape file

- Many NJOY sample input files use MODER module before processing.
  - MODER module changes file format (ASCII, binary).
  - NJOY considers that this file is binary data if users set minus value.
    - Binary data is effective to reduce data size and readout time of files.
- FRENDY cannot handle binary data.
  - FRENDY considers that this file is ASCII data even if user sets minus value.

moder 20 -21	/ <i>command</i> / <i>nin, nout</i>
-----------------	--

Original ENDF file name : tape20 Changed file name (binary) : tape21
---

# NJOY modules handled in FRENDY

- FRENDY version 1 handles input files of the following NJOY modules.
  - RECONR, BROADR, GASPR, PURR, UNRESR, THERMR, ACER, MODER.
- Though THERMR input data of NJOY2012 and NJOY2016 are different from those of NJOY99, FRENDY can treat both input data.
  - FRENDY skips new input option “iform” in THERMR of NJOY2016.
  - FRENDY uses “iform=0: MF6 special”.
- Fast, thermal, and dosimetry (iopt=1~3) are only available for ACER module.
- FRENDY considers that this input file is PURR module even if user sets input file of UNRESR module.

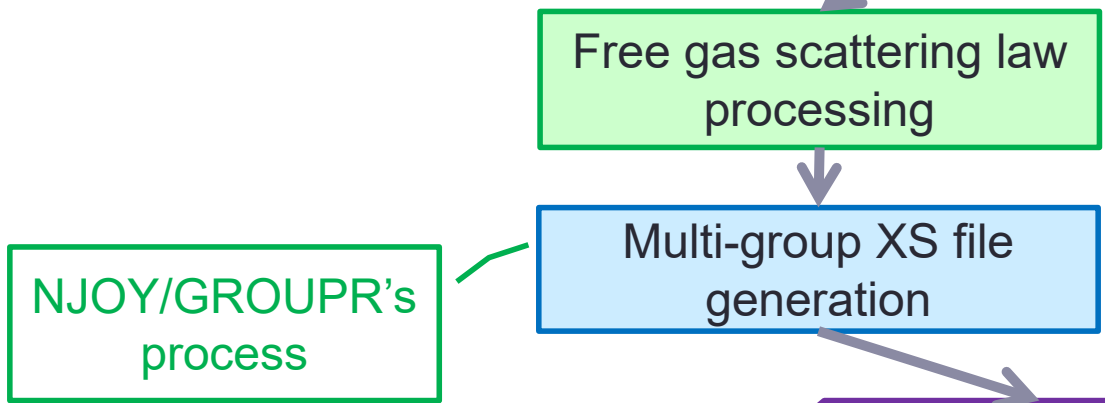
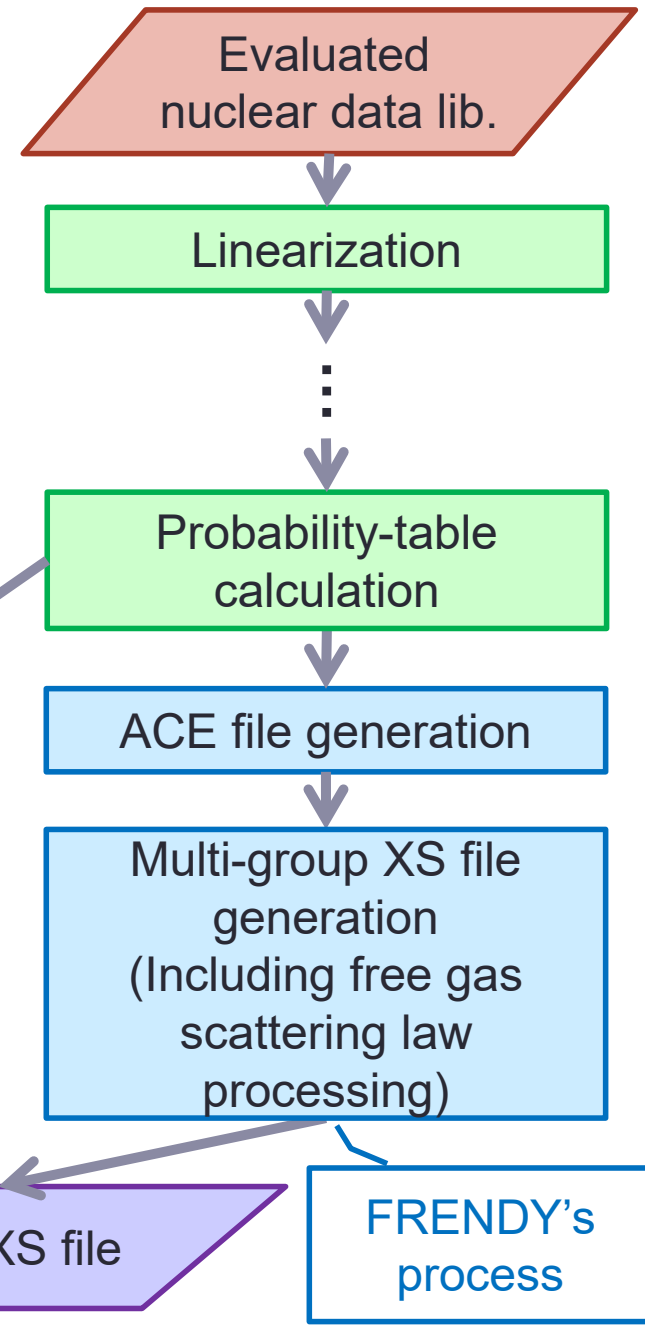
# Notes on UNRESR and PURR modules

- Both modules treat self-shielding effect in the unresolved resonance region.
  - PURR is only available for continuous energy Monte Carlo codes.
  - PURR and UNRESR are available for multi-group calculation codes.
  - Processing time of UNRESR is much shorter than that of PURR.
- NJOY developers do not recommend to use UNRESR.
  - “For most purposes, UNRESR has been superseded by PURR.”\*)
  - “The PURR results may be more reliable at low  $\sigma_0$  values than UNRESR results.”\*)
- FRENDY doesn't have equivalent function of UNRESR.
  - FRENDY uses equivalent function to PURR module even if user uses input of UNRESR module.

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

# Multi-group XS file generation with FRENDY/MG

- FRENDY will generate multi-group XS file using ACE file.
- FRENDY will treat input file of GROUPT module.
  - Procedure of multi-group XS file generation is different.



Multi-group XS file

FRENDY's process

# NJOY compatible input file generation using FRENDY

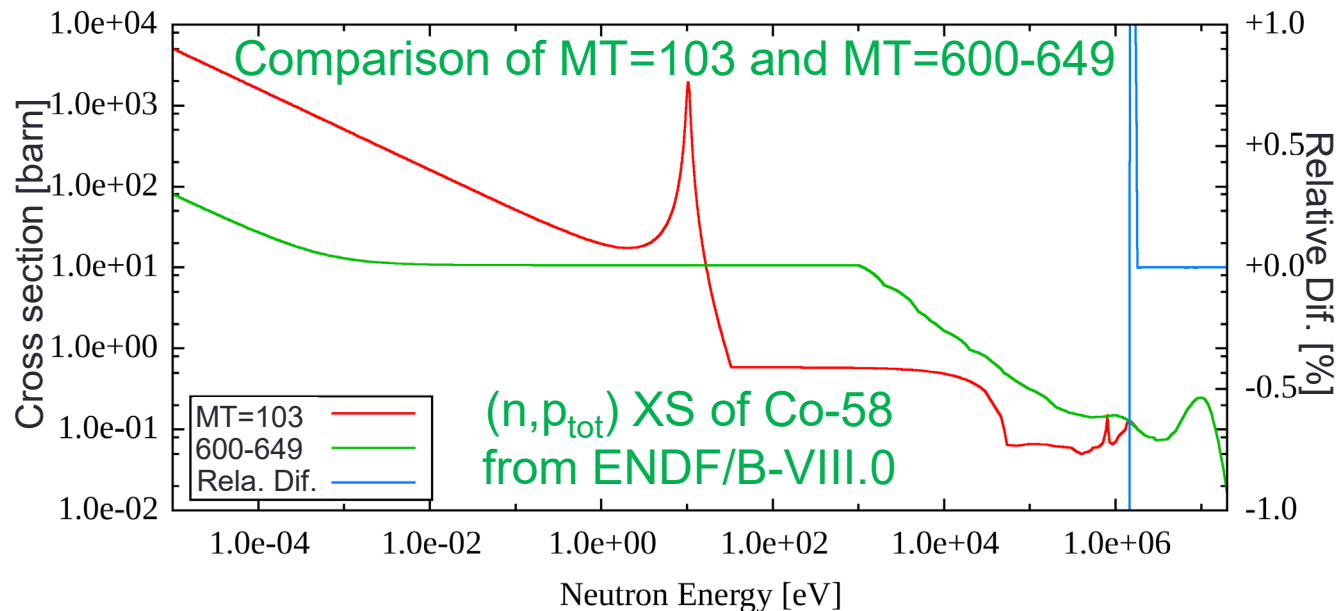
- FRENDY generates NJOY compatible input file using FRENDY input file.
  - Adding ”\_make\_inp” at the end of processing mode
    - ace\_fast\_mode\_make\_inp, ace\_tsl\_mode\_make\_inp, ace\_dosi\_mode\_make\_inp
    - NJOY input file name is “FRENDY input file name”.njoy\_input.dat.
- We strongly recommend to check generated input file.
  - Major nuclides and materials in JENDL-4.0, ENDF/B-VIII.0, JEFF-3.3 have already checked.
  - Other materials, e.g.,  $\text{UO}_2$ ,  $\text{SiO}_2$ , ..., may be incorrect.
    - MAT number of TSL data depends on the evaluated nuclear data library.
    - FRENDY cannot distinguish material data from MAT number.

# Input check function of FRENDY

- Several input parameters largely affect processing results.
- FRENDY verifies processing results in each processing step.
  - E.g., linearization and processing of thermal scattering law data
  - This function is available for FRENDY input and NJOY compatible input.
  - This function will be helpful to make the correct input file.

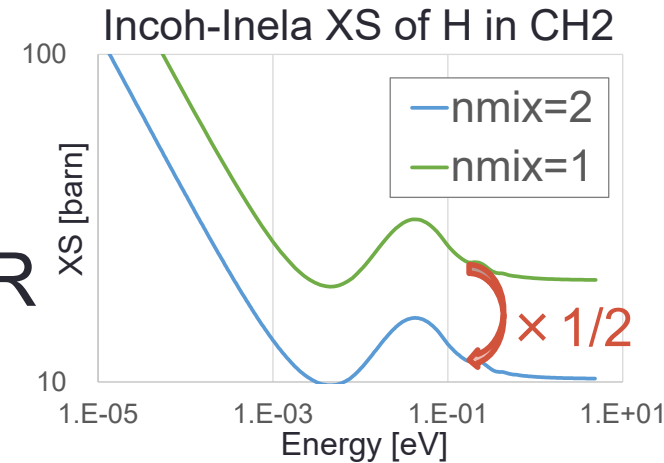
# Example of input check function (1/3)

- ENDF-6 format allows two types of particle production reaction (p, d, t, He-3,  $\alpha$ ).
- Total (MT=103-107) / each excited state (MT=600-849)
  - Total particle production cross section of some nuclides is not identical to sum of each excited state production cross section.
- FRENDY compares total and sum of each excited state XS
  - Output warning message if total XS is different to sum of each excited XS.



# Example of input check function (2/3)

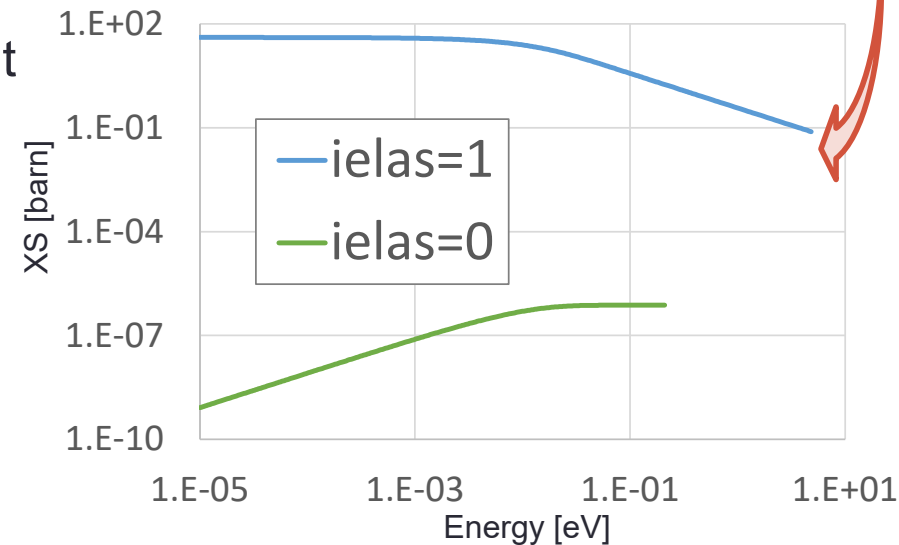
- natom of THEMUR and nmix of ACER affect incoh-inela scattering XS.
  - natom: number of principal atoms
  - nmix: number of atom types in mixed moderator
    - These parameter modifies incoh-inela scattering XS.
- Users have to check XS to verify these parameters.
- **FRENDY automatically checks XS.**
  - Incoh-inela scattering XS is nearly equal to elastic scattering XS at the upper limit of incident energy.
  - FRENDY compares these XSs at the upper energy.
    - Output warning message if the relative difference is larger than 10%.





# Example of input check function (3/3)

- ACER requires elastic scattering type.
  - ielas of ACER : 0=coherent, 1=incoherent
- This parameter has large impact on processing results.
- FRENDY checks elastic scattering type using PENDF file.
  - LCT value of MF=6
    - LCT=7: coherent, LCT=6: incoherent
  - Output warning message if ielas of ACER is different to PENDF data.
- These input check functions will be helpful to make the correct input file.



# Concluding and remarks

- FRENDY treats two types of the input format.
- FRENDY input format
  - First line must be set processing mode.
    - `ace_fast_mode`, `ace_tsl_mode`, `ace_dosi_mode`
  - Other lines are free format.
    - Setting “input data name” and “input data”
    - Bracket is used to describe array data.
    - Text data is surrounded by single or double quotation mark.
    - Comment line is similar to C/C++.
- NJOY compatible input format
  - FRENDY version 1 handles input files of the following NJOY modules.
    - `RECONR`, `BROADR`, `GASPR`, `PURR`, `UNRESR`, `THERMR`, `ACER`, `MODER`.
  - Each module is independent
    - Input for each module is required
    - Order of module has impact on processing result.
  - Comment line is after slash
  - The input parameters written in Card N must be set in one line.
  - If user sets slash, other input data are default values
- Input checker function of FRENDY
  - FRENDY verifies processing results in each processing step.

# [Appendix] Explanation of NJOY input format

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# Input description: RECONR

- Card 1: nendf npend
  - ENDF (input) file name and PENDF (output) file name (20~99)
- Card 2: tlabel
  - Label (one line comment) of PENDF
- Card 3: mat ncards ngrid
  - MAT number, Number of comment lines of PENDF file, Number of additional energy grids
- Card 4: err tempr errmax errint
  - Allowable error of linearization, temperature [K], Maximum error of linearization, Allowable error of linearization (integral value)
- Card 5: cards
  - Comment line of PENDING file (Line number = ncards)
  - ncards=0: Skip this card
- Card 6: enode
  - Additional energy grid (Grid number = ngrid)
  - grid=0: Skip this card

Gray parameters:  
**Recommended to use the default value.**

# Important point: RECONR

- nendf/npendf (card 1)
  - nendf and npendf are only available from 20 to 99.
  - File name of ENDF or PENDF is tapeXX (tape20~tape99).
    - ENDF file name is tape20 if nendf=20.
  - Original ENDF file name: nendf, Output PENDF file name: npendf
- err/errmax/errint (card 4)
  - We recommend to use  $\text{err} = 1.0\text{E-}3$  (0.1%).
  - **Default values should be used for errmax and errint.**
- tempr (card 4)
  - **tempr must be set 0 K.**
  - Single-Level Breit-Wigner resonance formula can directly calculate Doppler broadened XS using psi-chi approximation method.
    - The difference at top and bottom of resonance XS will become larger when psi-chi method is used.
  - **Doppler broadened XS must be calculated in BROADR module.**

# Example: RECONR

reconr	<i>/ command</i>	
20 21	<i>/ input(tape20), output(tape21)</i>	
'pendf tape for JENDL-4 U235'	<i>/ identifier for PENDF</i>	
9228	<i>/ mat</i>	ncards and ngrid are default value. (ncards/ngrid=0)
1.00e-03	<i>/ err</i>	
<b>0</b>	<i>/</i>	tempr, errmax, and errint are default value.

Last data is mat=0. (Card 3 of 2<sup>nd</sup> nuclide)

- NJOY considers that data of many nuclides are written in one file.
  - NJOY processes data of several nuclides with one input file if user repeats Card 3~Card 6.
  - **mat=0 in Card 3 means the end of RECONR module.**

# Input description: BROADR

- Card 1: nendf nin nout
  - ENDF file name, PENDF file name before BROADR (input PENDF), PENDF file name after BROADR (output PENDF)
- Card 2: mat1 ntemp2 istory istryap temp1
  - MAT number, number of temperatures, whether temp1 data is copy to nout or not, whether all temperature data is calculate from temp1 or not, temperature of nin (normally 0 K)
- Card 3: errthn thnmax errmax errint
  - Allowable error of linearization, Maximum energy of Doppler broadening, Maximum error of linearization, Allowable error of linearization (integral value)
    - errthn, errmax, and errint of BROADR is identical to err, errmax, and errint of RECONR
- Card 4: temp2
  - Doppler broadened temperature (temperature number=ntemp2)

# Important point: BROADR

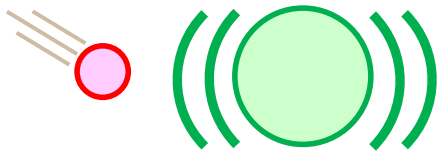
- thnmax (card 3)
  - NJOY considers that thnmax is the lowest of input value, upper boundary of resolved resonance regions, and 1 MeV.
  - Old version of NJOY, *e.g.*, NJOY99 and NJOY2012, uses threshold energy as the thnmax.
    - U-235 in JENDL-4.0 cannot be correctly processed since threshold energies of several reactions are very small.
    - Minus thnmax value must be used to avoid this problem.
      - Input value is forcibly set when user sets minus thnmax value.
  - FRENDY and the current version of NJOY2016 do not check threshold energy.



# Threshold reaction and Doppler broadening

- Doppler broadening considers nucleus vibration.
- Threshold energy will also be moved by nucleus vibration.
  - Current nuclear data processing codes do not consider the moving of threshold energy.

[Reaction of incident particle and nucleus]

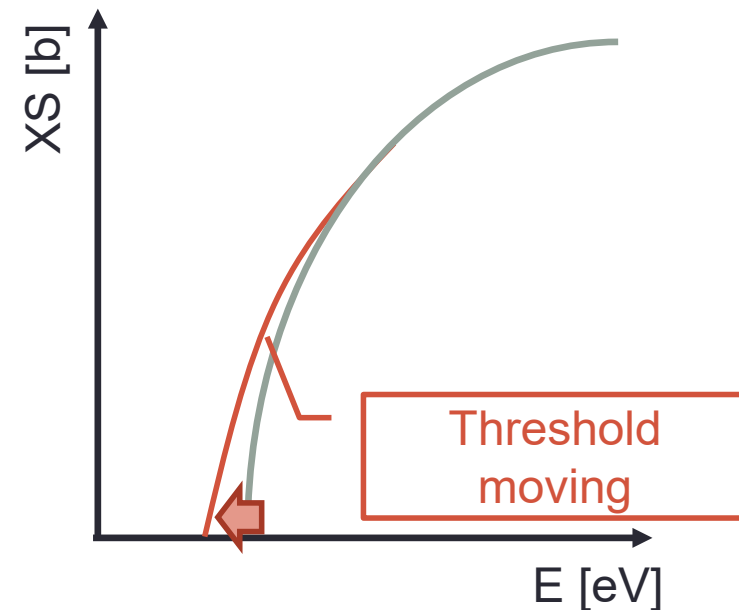


[Equation of Doppler broadening]

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

$T$ : Temperature,

$v$ : velocity of incident particle,  $v_r$ : relative velocity



# Example: BROADR

```

broadr
20 21 22
9228 1
1.00e-03 -5.0E+2
296.0
0
    
```

```

/ command
/ endf, pendf(in), pendf(out)
/ mat, temp no
/ err, thnmax
/ temp
/
    
```

**-5.0E+2**

Maximum energy is forced to 500 eV.

istart, istrap, and temp1 are default values.

Last data is mat=0.  
(Card 2 of 2<sup>nd</sup> nuclide)

errmax and errint are default values.

# Input description: GASPR

- Card 1: nendf nin nout
  - ENDF file name, PENDF file name before GASPR (input PENDF), PENDF file name after GASPR (output PENDF)
- GASPR requires only ENDF/PENDF file names.
  - GASPR can be skipped if user does not need gas production XS (MT=203~207).

## [Example of GASPR]

gaspr	<i>/ command</i>
20 22 23	<i>/ endf, pendf(in), pendf(out)</i>

# Input description: PURR

- Card 1: nendf nin nout
  - ENDF file name, PENDF file name before PURR (input PENDF), PENDF file name after PURR (output PENDF)
- Card 2: matd ntemp nsigz nbin nladr iprint nunx
  - MAT number, number of temperatures, number of background XS, number of probability bins, number of ladders, output option, number of energy grids (0: all)
- Card 3: temp
  - temperature (temperature number = ntemp)
- Card 4: sigz
  - Background XS  $\sigma_0$  (sigz number = nsigz)

# Important point: PURR

- nbin/nladr (card 2)
  - nbin must be larger than or equal to 15.
  - Recommended nladr is larger than or equal to 100.
- iprint (card 2)
  - Probability table information is output in output file if iprint = 1.
- nunx (card 2)
  - Recommended nunx is 0, *i.e.*, processing all energy grids.
  - Considering to current computing performance, the processing time is not so long.
- sigz (card 4)
  - Back-ground XS data **must be descending order.**
  - The first back-ground XS data must set large value, *e.g.*,  $1.0E+10$ .
    - NJOY considers that the first back-ground XS is infinite.
    - FRENDY sorts back-ground XS data.
    - FRENDY considers that the maximum back-ground XS is infinite.

# Example: PURR

purrr		<i>/ command</i>
20 23 24		<i>/ endf, pendf(in), pendf(out)</i>
9228 1 10 20 100 0		<i>/ mat, temp no, sig no, bin no, lad no</i>
296.0		<i>/ temp</i>
1E10 1E4 1E3 300 100 30 10 1 0.1 1.0E-5		<i>/ sig zero</i>
0		<i>/</i>

This value is considered as infinite.

nunx is default value.

Last data is mat=0.  
(Card 2 of 2<sup>nd</sup> nuclide)

# Input description: THERMR

- Card 1: nendf nin nout
  - ENDF file name of TSL data, PENDF file name before THERMR (input PENDF), PENDF file name after THERMR (output PENDF)
- Card 2: matde matdp nbin ntemp iin icoh iform natom mtref iprint
  - MAT number of TSL data, MAT number of nuclide, number of equiprobable angular bins, number of temperatures, inelastic scattering option, elastic scattering option, output format option, number of principal atoms, MT number of inelastic scattering (221~225 only), output option
- Card 3: temp
  - Temperature (temperature number = ntemp)
- Card 4: tol emax
  - Allowable error of linearization, maximum energy to consider thermal scattering
    - tol is identical to err in RECONR.

Green parameters:  
 User have to read TSL data to set these parameters.

# Important point: THERMR (1/3)

- nendf/nin (card 1) & matde/matdp (card 2)
  - nendf and matde are obtained from TSL data.
    - For example, TSL data file name of HinH2O and MAT number
    - nendf and matde are 0 for free gas scattering law processing.
  - nin and matdp are obtained from nuclide data.
    - For example, H-001 for HinH2O.
- iform (card 2)
  - Data format of angular and energy distribution can be changed using this option.
  - This option is added in NJOY2012.
    - NJOY2012/2016 input is incompatible to NJOY99 input.
    - Users have to check whether this input file has iform or not.
    - FRENDY can treat both input format.
- mtref (card 2)
  - MT number of elastic scattering is mtref+1.



# Important point: THERMR (2/3)

- natom (card 2)
  - Number of target nuclides in a molecule.
    - For example, HinH<sub>2</sub>O: natom=2, OinH<sub>2</sub>O: natom=1
- temp (card 3)
  - Temperature is **only available for given temperatures in TSL data.**
  - PENDF file of target nuclide must be broadened in this temperature.
- emax (card 4)
  - Recommended value is the maximum energy of TSL or higher energy, e.g., 10 eV.
  - Short Collision Time (SCT) approximation is used if the energy is higher than the given energy range in TSL data.

# Important point: THERMR (3/3)

- iin (card 2)
  - Meaning of iin value of NJOY2012/2016 is different to NJOY99.
  - User has to check whether TSL data has inelastic scattering data in MF=7/MT=4 or not.
- icof (card 2)
  - User has to check whether TSL data has elastic scattering data in MF=7/MT=2 or not.
  - Elastic scattering XS of graphite is added in output PENDF file if user sets icof=2 and TSL data does not have elastic scattering data.
    - icof=2: compute elastic scattering XS using TSL data or elastic scattering XS of graphite
- iform (card 2)
  - This option is added in NJOY2012.
  - NJOY2012/2016 input is incompatible to NJOY99 input.
  - User have to check whether this input file has iform or not.

# iin/icof options of NJOY99 and NJOY2016

## NJOY99

### iinc inelastic options

- 0 none
- 1 compute as free gas
- 2 reserved
- 3 reserved
- 4 read s(a,b) and compute matrix

### icoh elastic options

- 0 none
- 1 compute using ENDF6 input tape data
- or for pre-ENDF6 input set icoh =
- 1 graphite
- 2 beryllium
- 3 beryllium oxide
- 11 polyethylene
- 12 h(zrh)
- 13 zr(zrh)

## NJOY2016

### iin inelastic options

- 0 none
- 1 compute as free gas
- 2 read s(a,b) and compute matrix

### icoh elastic options

- 0 none
- 1 compute using ENDF6 format data
- or for earlier formats
- 1 graphite
- 2 beryllium
- 3 beryllium oxide
- 11 polyethylene
- 12 h(zrh)
- 13 zr(zrh)

Option number is identical!!

# Example: THERMR

TSL data of HinH2O does not have elastic scattering data.  
(icoh = 0)

```

thermr
26 23 27
1 125 60 1 2 0 0 2 221
iform natom mtref
293.6
1.0e-03 1.00001e+01
    
```

*/command*  
*/nendf nin nout*  
*/matde matdp nbin ntemp iin icoh*  
*/tempr*  
*/tol emax*

Since there is iform option, this is NJOY2012/2016 input data.

# Input description: ACER (common)

- Card 1: nendf npend ngend nace ndir
  - ENDF file name, PENDF file name before ACER (input PENDF), multi-group photon data, ACE file name, XSDIR file name
- Card 2: iopt iprint itype suff nxtra
  - Processing mode, output option, ACE file mode (1=ASCII, 2=binary), suffix ID, number of IZ/AW data
    - **FRENDY can not handle itype=2.**
    - iopt=1: neutron/proton induced, iopt=2: TSL, iopt=3: dosimetry, iopt: 4: photo-atomic, iopt=5: photo-nuclear
- Card 3: hk
  - Label (one line comment) of ACE (Maximum: 70 characters)
- Card 4: iz, aw
  - IZ/AW pair data (number of iz, aw = nxtra)
  - nxtra=0: Skip this card

# Input description: ACER (iopt=1)

- Card 5: matd tempd
  - MAT number, temperature
- Card 6: newfor iopp
  - Whether new angular distribution format (LAW=61) is used or not, whether detailed photon data is used or not
    - Default newfor option is 1 (use LAW=61).
    - MCNP4C and later version of MCNP can handle LAW=61.
- Card 7: thin(1) thin(2) thin(3)
  - Data reduction option
    - User should not enter this option and should skip this card using slash “/”.

# Input description: ACER (iopt=2)

- Card 8:matd tempd tname
  - MAT number of nuclide, temperature,  $S(\alpha, \beta)$  identifier of MCNP, e.g., lwtr (Maximum: 6 characters)
- Card 8a:iza01 iza02 iza03
  - ZA value of target nuclide
- Card 9:mti nbint mte ielas nmix emax iwt
  - MT number of inelastic scattering, number of energy bins of 2<sup>nd</sup> particle, MT number of elastic, whether coherent elastic (ielas=0) or incoherent elastic (ielas=1), number of atom types in mixed moderator, maximum energy to consider thermal scattering, output format of energy of 2<sup>nd</sup> particle
    - mti is 0 or mtref of THERMR, mte is 0 or mtref+1 of THERMR
    - Emax is emax of THERMR
    - iwt=0: skewed, iwt=1:discrete, iwt=2:continuous
      - MCNP6.1 or later version can handle iwt=2.

# Important point: ACER (iopt=2)

- tname (card 8)
  - This name is also used in MCNP input file.
- iza01 iza02 iza03 (card 8a)
  - iza02 and iza03 are normally 0.
  - Target nuclide have several isotopes, e.g., Zr in ZrH, user has to set iza02 and iza03.
- ielas (card 9)
  - User has to check TSL data (MF=7/MT=2) and including data type.
- nmix (card 9)
  - Mainly, Benzene, BeO, and SiO<sub>2</sub> are nmix=2 and others are nmix=1
    - Though BeO from JENDL-4.0 is nmix=2, BeO from ENDF/B-VIII.0 is nmix=1.
    - **Please carefully check TSL data to process Benzene, BeO, and SiO<sub>2</sub>.**
- iwt (card 9)
  - MCNP6.1 or later version of MCNP can handle iwt=2.
  - Recommended iwt value is iwt=0 if user uses PHITS code or previous version of MCNP.
    - The nuclear calculation results using iwt=1 may no be incorrect.



# Example: ACER (iopt=1)

If user does not use photon data, ngend is 0.

acer	<i>/ command</i>
20 24 0 30 31	<i>/ nendf, npend, ngend, nace, ndir</i>
1 1 1 0.00	<i>/ iopt(fast), iprint(max), itype, suffix</i>
'ACE file for JENDL-4 U235'	<i>/ descriptive character</i>
9228 296.0	<i>/ mat, temp</i>
1	<i>/ newfor(yes)</i>
	<i>/ thin(1), thin(2), thin(3)</i>
stop	<i>/</i>

Skip Card 7 (thin(1)~thin(3)).

# Example: ACER (iopt=2)

```
acer /command
26 27 0 30 31 /nendf npend ngend nace ndir
2 1 1 0.0 0 /iopt iprint itype suff nxtra
'ACE file for HinH2O from JENDL-4.0' /hk
125 2.93600e+02 'lwtr' /matd tempd tname
1001 /iza
221 60 0 0 1 1.00001e+01 0 /mti nbint mte ielas nmix emax iwt
```

User considers that 'lwtr' means HinH2O.  
(User has to use 'lwtr' in MCNP input file.)