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

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(α, β) 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_za_id_name      "lwtr"
```

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

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

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

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

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.txe
  - 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(α, β) 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

TSL data generation for MCNP5 and PHITS 3.24

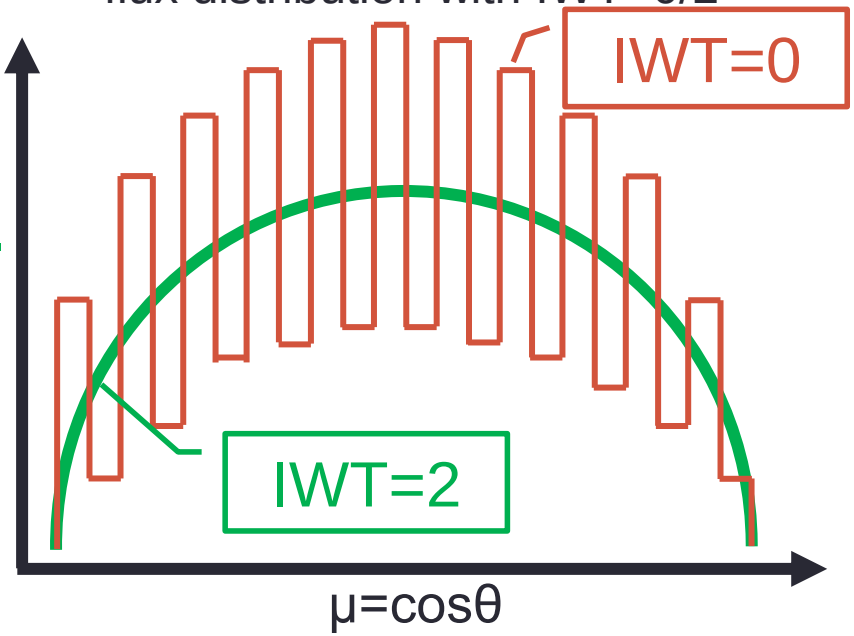
- Three types of ACE format is now available.
  - IFENG=0 (discrete), 1 (skewed), 2 (continuous)
- MCNP5 and PHITS ver.3.24 cannot treat IFENG=2.
  - The default input option of FRENDY version 2 generates IFENG=2.
  - Please add "weight_option" and modify parameter from "tabulated" to "variable".

```
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_za_id_name      "lwtr"
  weight_option           variable
```

Difference of IWT options

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

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



IFENG option and weight_option

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

```
h-h2o.00t    0.999167  2.5852e-08  20220208
                                                                  mat 125
  1001          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
11774842        3      31         80       0          0       2          0
       0        0       0          0       0          0       0          0
       1      500     998          0       0          0       0          0
       0        0       0          0       0          0       0          0
       0        0       0          0       0          0       0          0
       0        0       0          0       0          0       0          0
                498   1.00000000000e-11   1.03125000000e-11   1.06250000000e-11
  1.09375000000e-11   1.12500000000e-11   1.15625000000e-11   1.18750000000e-11
  1.21875000000e-11   1.25000000000e-11   1.28125000000e-11   1.31250000000e-11
  1.34375000000e-11   1.37500000000e-11   1.43750000000e-11   1.50000000000e-11
```

IFENG

FRENDY original input format (Multi-group generation)

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 (1/7): 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 GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  //iwt=3 in GROUPR/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 GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  //iwt=3 in GROUPR/NJOY
```

Input Example (2/7): 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 (3/7): U-235 with specified energy group structure and spectrum

```
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 ( 1.0E-5  0.625  5.0E5  1.0E6  2.0E+7 )  //4-groups
  mg_weighting_spectrum ( 1.0E-5  1.0  2.0E+7  1.0 ) //constant
  legendre_order                3
```

Input Example (4/7): H in H_2O

```
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 GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  //iwt=3 in GROUPR/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 GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  //iwt=3 in GROUPR/NJOY
  mg_tsl_data_type      (hh2o)
```

Input Example (5/7): Graphite

```
mg_neutron_mode                                  //Process mode
  nucl_file_name      ( ../lib/C012.dat )        //ENDF file name
  nucl_file_name_tsl  ( ../lib/31_graphite.txt )  //TSL file name
  mg_edit_option   ( MATXS  GENDF )              //Output format
  mg_file_name        C_in_Graphite              //Output file name
  temperature         293.6 //[K]
  mg_structure ( xmas_nea-lanl_172 )             //ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  //iwt=3 in GROUPR/NJOY
  mg_tsl_data_type      (graph)                  //This data type is used
                                                 //for MATXS file generation
```

Input Example (6/7): UO_2

```
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 GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )                  // iwt=3 in GROUPR/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 (7/7): 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 GROUPR/NJOY
  mg_weighting_spectrum ( iwt03 )        // iwt=3 in GROUPR/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
```

IFENG (weight_option) for TSL data generation

- Please check the IFENG value in the ACE file.
- IFENG=2 (weight_option: tabulated) is strongly recommended to generate multi-group cross section file.
  - The prediction accuracy of transport calculation becomes lower when IFENG=0 or 1.

```
h-h2o.00t    0.999167  2.5852e-08  20220208
                                                                  mat 125
  1001          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
     0          0       0          0       0          0       0          0
11774842        3      31         80       0          0       2          0
       0        0       0          0       0          0       0          0
       1      500     998          0       0          0       0          0
       0        0       0          0       0          0       0          0
       0        0       0          0       0          0       0          0
       0        0       0          0       0          0       0          0
                498   1.00000000000e-11   1.03125000000e-11   1.06250000000e-11
  1.09375000000e-11   1.12500000000e-11   1.15625000000e-11   1.18750000000e-11
  1.21875000000e-11   1.25000000000e-11   1.28125000000e-11   1.31250000000e-11
  1.34375000000e-11   1.37500000000e-11   1.43750000000e-11   1.50000000000e-11
```

IFENG

NJOY compatible input format

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→A＞B, A.ge.B→A≧B, A.lt.B→A＜B, A.le.B→A≦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                    / command
 20  -21                 / nin, nout
```

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

NJOY modules handled in FRENDY

- FRENDY version 2 handles input files of the following NJOY modules.
  - MODER, RECONR, BROADR, GASPR, PURR, UNRESR, THERMR, ACER, GROUPR, and MATXSR.
- 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 THEMR 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 if PURR module even if user sets input file of UNRESR module.

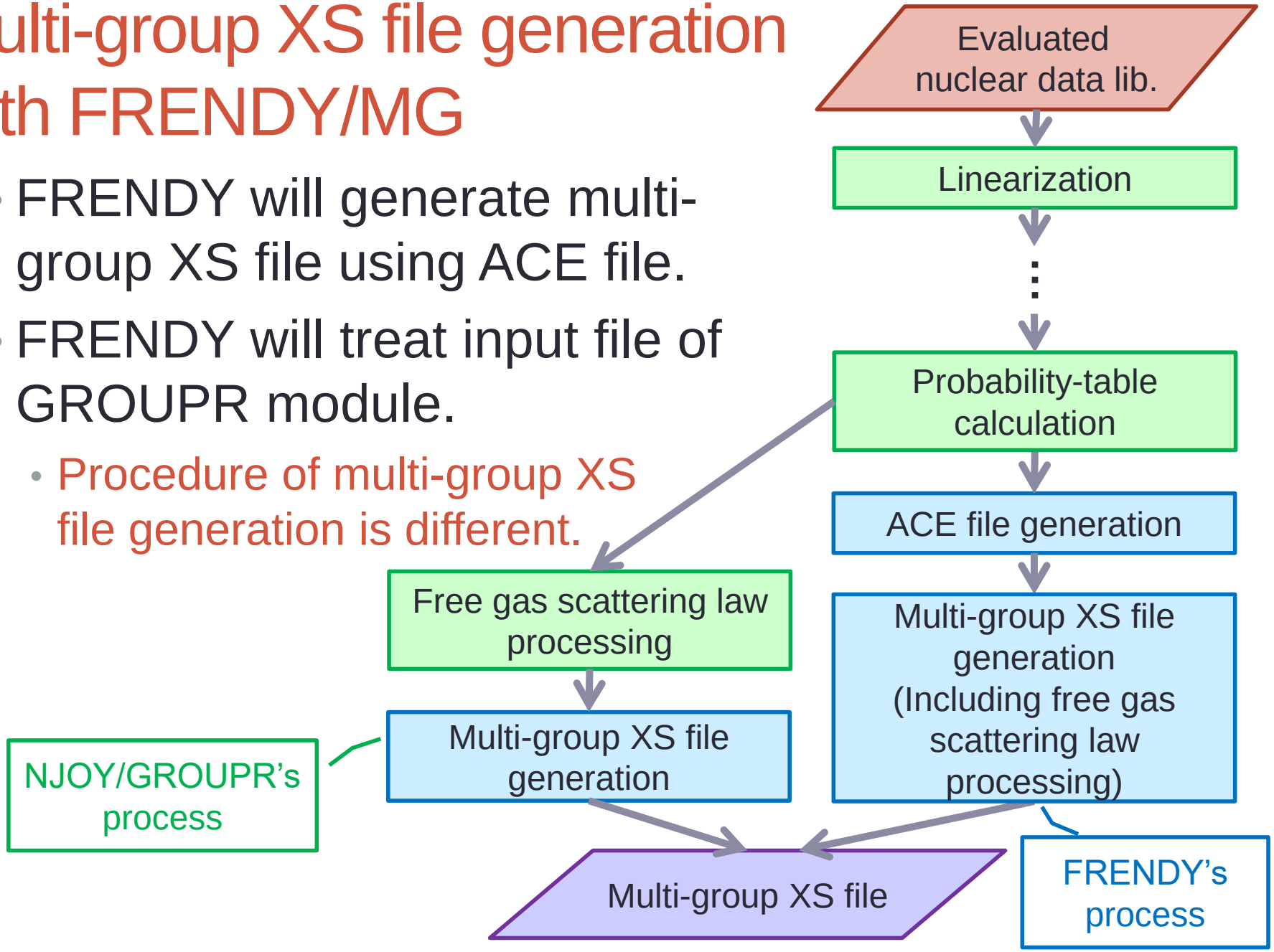
Notes on UNRESR and PURR modules

- 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 σ_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 GROUPR module.
  - Procedure of multi-group XS file generation is different.



NJOY compatible input file generation using FRENDY

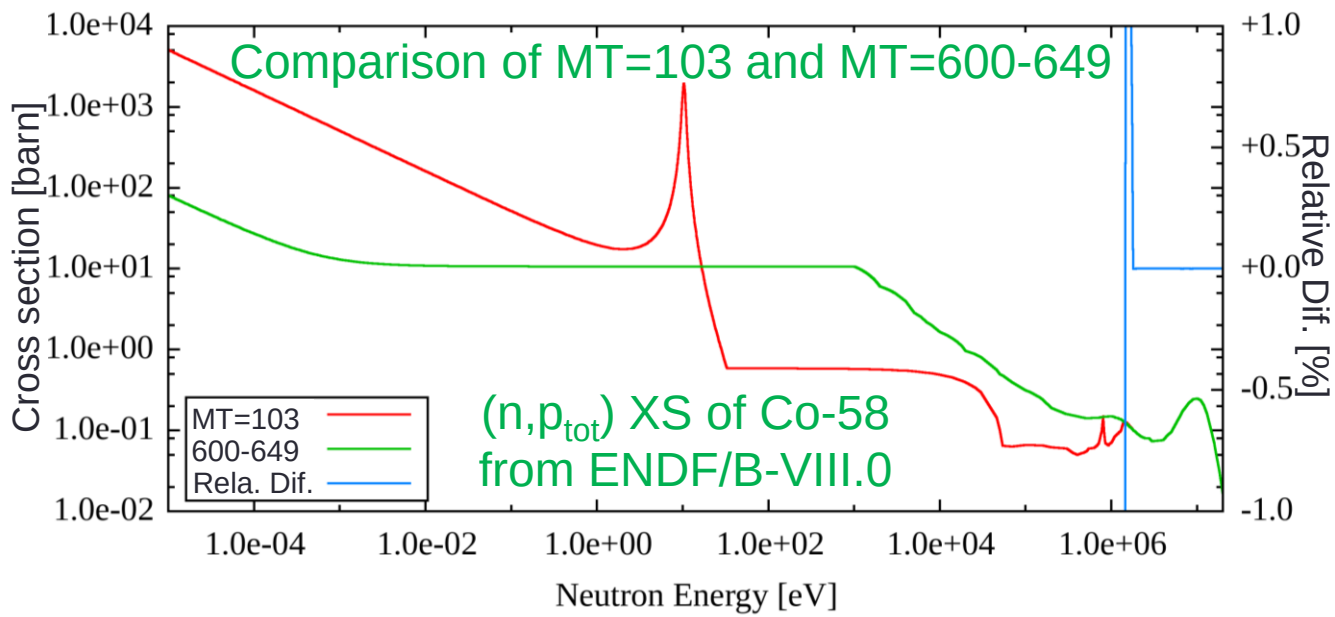
- FRENDY generates NJOY compatible input file using FRENDY input file.
  - Adding "_make_inp" at the end of processing mode
    - ace_fast_mode_make_inp, ace_tsl_mode_make_inp, ace_dosi_mode_make_inp
    - NJOY input file name is "FRENDY input file name".njoy_input.dat.
- We strongly recommend to check 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.*, UO_2, 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

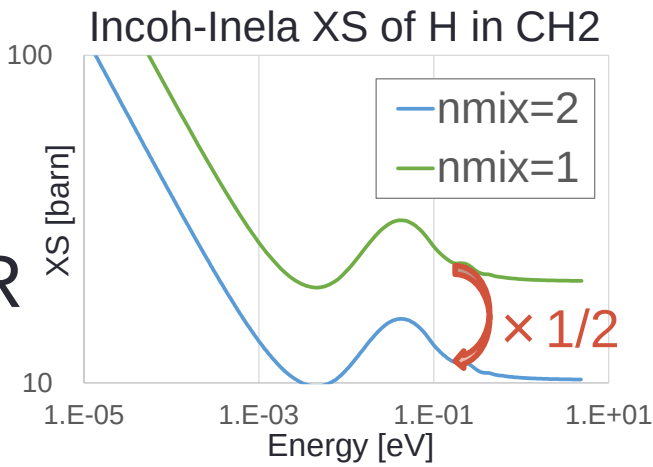
- Several input parameters largely affect processing results.
- FRENDY verifies processing results in each processing step.
  - E.g., linearization and processing of thermal scattering law data
  - This function is available for FRENDY input and NJOY compatible input.
  - This function will be helpful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



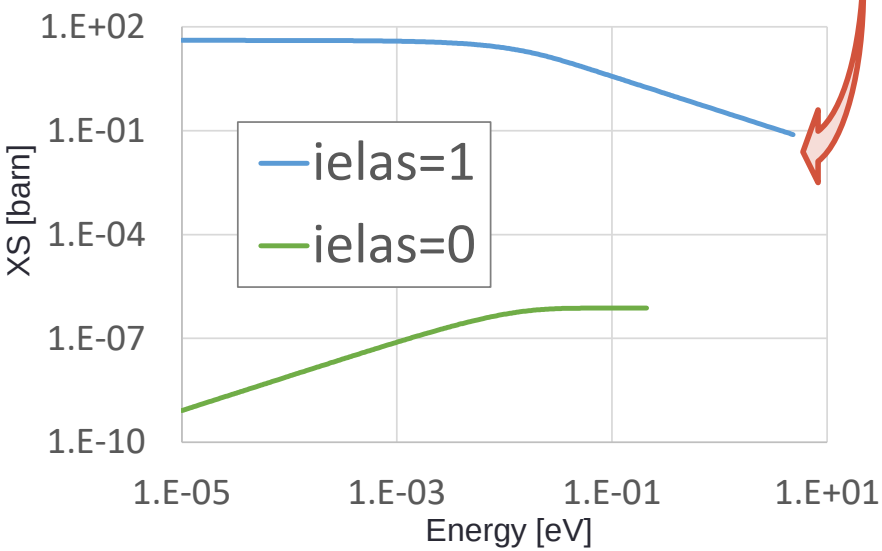
Example of input check function (2/3)



- natom of THEMR 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

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 PEND 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 err＝1.0E-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                                  / command
 20  21                                  / input(tape20), output(tape21)
'pendf tape for JENDL-4 U235'   / identifier for PENDF
 9228                                    / mat
 1.00e-03                                / err
 0                                       /
```

ncards and ngrid are default value. (ncards/ngrid=0)

Last data is mat=0. (Card 3 of 2nd nuclide)

tempr, errmax, and errint are default value.

- 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 istart istrap temp1
  - MAT number, number of temperatures, whether temp1 data is copy to nout or not, whether all temperature data is calculate from tmep1 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 erring of BROADR is identical to err, errmax, and errint of RECONR
- Card 4 : temp2
  - Doppler broadened temperature (temperature number=ntemp2)

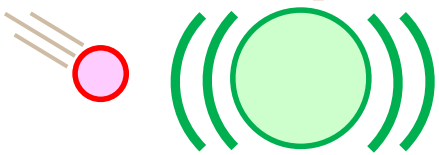
Important point: BROADR

- 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.

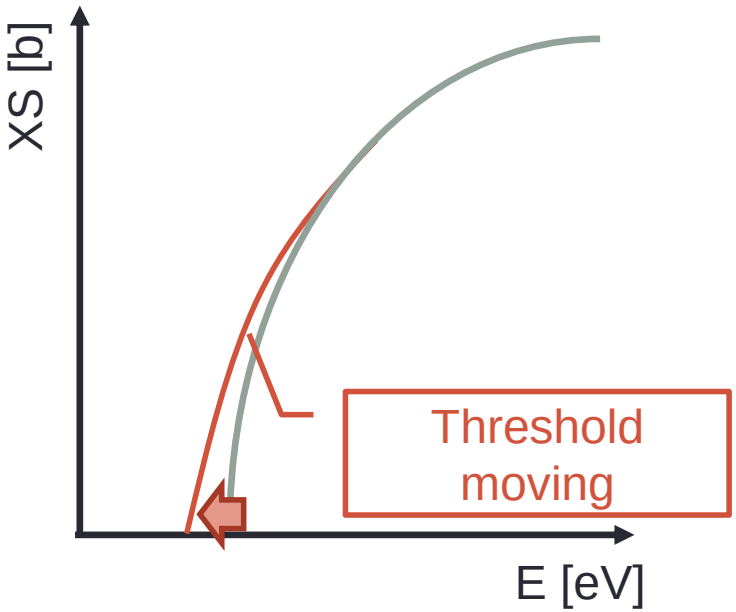
[Reaction of incident particle and nucleus]



[Equation of Doppler broadening]

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

T: Temperature,
v: velocity of incident particle, v_r: relative velocity



Example: BROADR

```
broadr                          / 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                              /
```

Maximum energy is forced to 500 eV.

istart, istrap, and temp1 are default values.

Last data is mat=0. (Card 2 of 2nd 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                    / command
 20  22  23              / endf, pendf(in), pendf(out)
```

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 back-ground 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
  - Bagk-ground XS σ_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

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

This value is considered as inifinite.

nunx is default value.

Last data is mat=0. (Card 2 of 2nd 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 equi-probable 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, HinH2O: natom=2, OinH$_2$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)

Option number is identical!!

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)

Example: THERMR

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

```
thermr                          /command
26 23 27                        /nendf nin nout
1 125 60 1 2 0 0 2 221          /matde matdp nbin ntemp iin icoh
iform natom mtref
293.6                           /tempr
1.0e-03 1.00001e+01             /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(α, β) 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 2nd 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 2nd 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 SiO2 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 SiO2.**
- 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                                  / command
 20  24   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                                    / newfor(yes)
                                      / thin(1), thin(2), thin(3)
stop                                  /
```

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.)