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Manual of FRENDY Version 2

(Preliminary version)

Contents

Contents	2
1 Input Instructions	4
1.1 Input Format.....	4
1.2 FRENDY Original Input Format.....	4
1.2.1 Processing Mode.....	6
1.2.2 Input Parameters	7
1.2.3 Examples of the input file for FRENDY input format.....	56
1.3 NJOY Compatible Format	58
1.4 Sample Input Data for ACE file generation	60
1.4.1 Simplest Input Data.....	60
1.4.2 Input Data to Modify Default Input Parameters.....	61
1.4.3 Input Data to Reproduce NJOY99 Input.....	62
1.5 Sample Input Data for Multi-group Cross-Section generation	69
1.5.1 Sample Input Data to Generate Neutron-Induced Multi-Group Cross-Section File ...	69
1.5.2 Sample Input Data to Generate Multi-Group Cross-Section File of TSL Data.....	71
1.5.3 Sample Input Data to Generate Multi-Nuclide Data.....	73
1.5.4 Sample Input Data to Use Automatic Setting of Background Cross-Sections	75
1.5.5 Sample Input Data to Use Automatic Setting of Energy Group Structure	76
1.6 Input Instruction of ACE File Perturbation Tools	77
1.6.1 Input Instruction of make_perturbation_factor	77
1.6.2 Sample Input of make_perturbation_factor	78
1.6.3 Input Instruction of perturbation_ace_file.....	79
1.7 Input Instruction of ENDF Modification Tool.....	80
1.8 Sample Input of ENDF Modification Tool	81
2 Installation of FRENDY	83
2.1 Directory Structure.....	83
2.2 How to Install FRENDY on Linux, UNIX, or macOS Platforms	83
2.3 How to Execute FRENDY	85
2.4 Test Calculation with Samples	85
2.5 Test Programs for Boost test Library	85
2.6 How to Install FRENDY on VisualStudio2019	86
2.6.1 Installation of Boost library	86
2.6.2 Installation of CLAPACK library	86

2.6.3	Installation of FRENDY	87
2.6.4	Running FRENDY with Bat Files.....	88

1 Input Instructions

1.1 Input Format

FRENDY accepts two types of input formats:

- FRENDY original input format,
- NJOY compatible format.

The original input format requires only the processing mode name and evaluated nuclear data file name at the minimum. FRENDY has default values in the source code for the processing. Users can give the parameters in the input file if they want to change the parameters. The original input format is simple and does not require expert knowledge of nuclear data processing.

FRENDY can also treat the input files for NJOY. Many users process the evaluated nuclear data file with NJOY. FRENDY interprets the input as the NJOY compatible format when the first parameter is the NJOY module name, *e.g.*, MODER and RECONR. The available module is MODER, RECONR, BROADR, PURR, UNRESR, THERMR, ACER, GROUPE, and MATXS. Note that the UNRESR module is not prepared in FRENDY. FRENDY calculates the effective self-shielded cross-sections using the probability table method even if the user selects the UNRESR module. Users can easily use FRENDY without changing the input files for NJOY. They can therefore replace NJOY modules with FRENDY ones as they need. In addition, the modules of FRENDY and NJOY can be used in combination. For example, users can generate the multi-group cross-section data library using the GROUPE module of NJOY with the PENDF file generated by FRENDY.

1.2 FRENDY Original Input Format

In the conventional processing code including NJOY and PREPRO, users must select the running modules and prepare the input parameters for these modules to generate the cross-section data library. FRENDY automatically generates the cross-section data library with the recommended processing flow as shown in Fig. 1.2.1 when users select an appropriate processing mode at least. They do not need to worry about what modules are required to generate the cross-section data library when they use FRENDY original input format. FRENDY also prepares the skip option to manually select the modules to be executed. Using this option, users can skip some modules in the recommended processing flow.

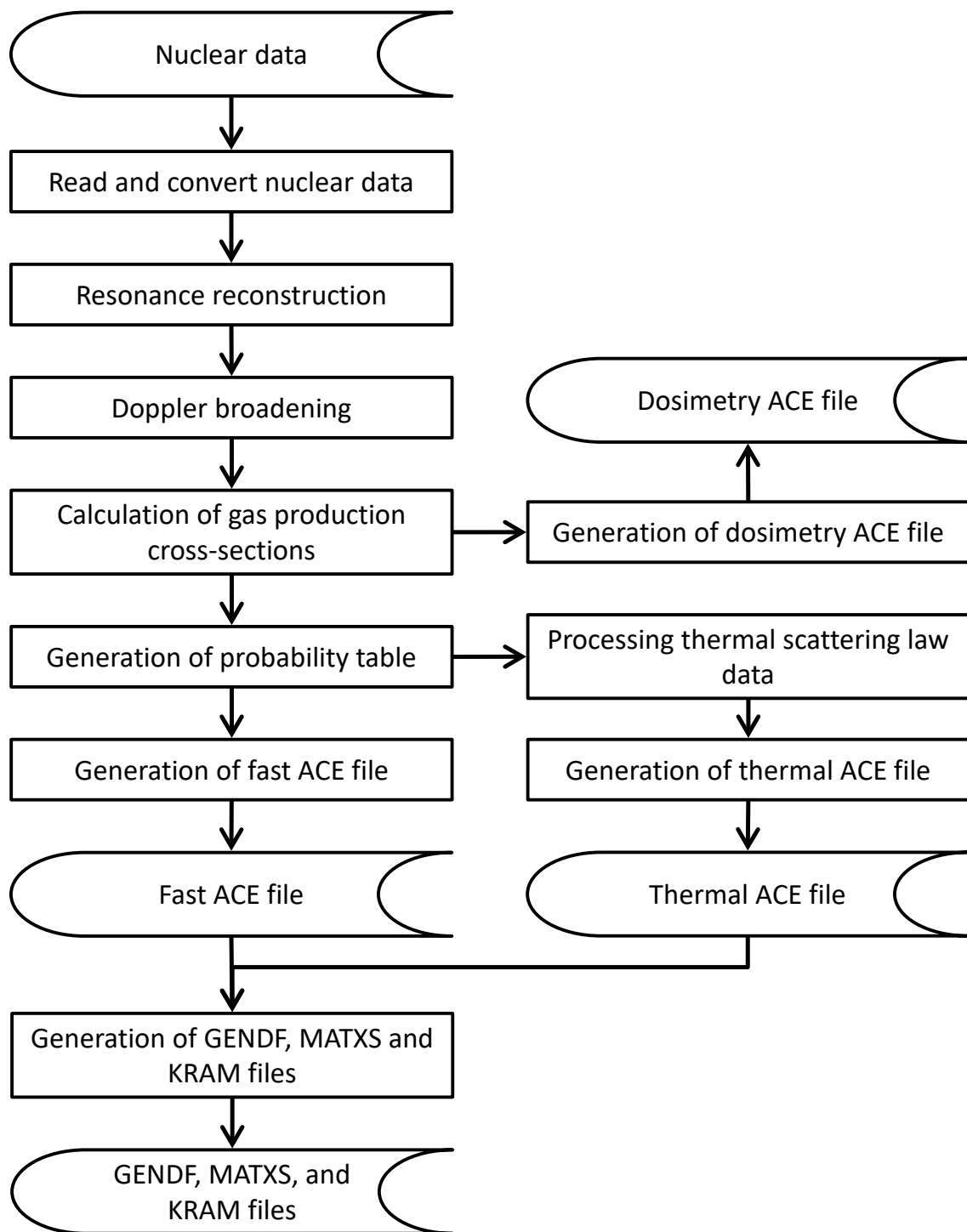


Figure 1.2.1 Processing flow to generate ACE, GENDF, MATXS, and KRAM files

1.2.1 Processing Mode

The order of the input data is free except for the first parameter. Users must set the processing mode as the first parameter. The available processing modes are listed in Table 1.2.1. The representation of the ACE file processing mode is identical to NJOY.

The neutron-induced data and the thermal scattering law data are available to generate the multi-group cross-section file. The multi-group cross-section generation mode is not divided by the processing type since the FRENDY checks the input parameter and judges which type of data is processed.

FRENDY generates the multi-group cross-section file from the ACE file. The input file format is not only the ENDF-6 formatted file but also the ACE formatted file. The start file format does not set in the processing mode. The start file format is set in the input parameter “mg_start_file_mode”.

Table .2.1 Available processing mode

Processing mode name	Description
ace_file_generation_fast_mode ace_fast_mode ace_fast ace_file_generation_normal_mode ace_normal_mode ace_normal	Generation of the particle incident ACE file
ace_file_generation_thermal_scattering_mode ace_file_generation_thermal_scatter_mode ace_therm_mode ace_therm ace_file_generation_tsl_mode ace_tsl_mode ace_tsl	Generation of the ACE file of the thermal scattering law data
ace_file_generation_dosimetry_mode ace_dosi_mode ace_dosi	Generation of the ACE file of the dosimetry data
mg_generation_neutron_mode mg_neutron_mode mg_neutron mg_mode mg	Generation of the neutron-induced multi-group XS file.

<p> endf_file_modification_mode endf_file_modify_mode endf_mod_mode modify_endf_file_mode mod_endf_file_mode mod_endf_mode </p>	<p> Modification of ENDF-6 formatted file. The explanation of the input format is shown in Sec. 1.7. </p>
--	--

1.2.2 Input Parameters

1.2.2.1 General information

The input data except the processing mode consists of “parameter name” and “parameter value”. Users need to set the parameters if they want to modify the default values. FRENDY original input format accepts comment lines. The C++ style comments are available, *i.e.*, “//” for a single line comment and “/* ... */” for multi-line comments. FRENDY can read four types of data, *i.e.*, integer, real, string, and text, and the vector data of integer and real. The available types are as follows:

integer : integer number, *e.g.*, -2, -1, 0, 1, 2,

real : real number, *e.g.*, -1.0, 0.0, 1.0, 1.0E-1, 1.0E+1, 1.0D-1, 1.0D+1, 1.0-1, 1.0+1,

string : character data without space, *e.g.*, nuclide_name, calculation-type,

text : multiple lines character data.

Users have to set the vector data in a bracket when they want to set the vector data of integer and real value. If users want to set three values, *i.e.*, 1.0, 2.0, and 3.0, users write as follows:

(1.0 2.0 3.0).

Since FRENDY can read data specified in multiple lines, the following input style is also acceptable

(**1.0**
 2.0
 3.0 **),**

or

(
 1.0
 2.0

3.0

).

If users want to set the text data, they need to enclose single or double quotation marks. The text data allows multiple lines as follows:

**“92-U-238 from JENDL-4.0
Processed with FRENDY
Processed day: 2017/10/13”**

or

**‘92-U-238 from JENDL-4.0
Processed with FRENDY
Processed day: 2017/10/13’**

If users want to use double quotation marks in the comment line, single quotation marks are used to enclose the text data as follows:

**‘This is the comment line for the PENDF file.
Users can use the “double quotation marks” when the comment line is enclosed by the single quotation marks.’**

If users want to use single quotation marks in the comment line, double quotation marks are used to enclose the text data as follows:

**“This is the comment line for the PENDF file.
Users can use the ‘single quotation marks’ when the comment line is enclosed by the double quotation marks.”**

1.2.2.2 Input parameter name and recommended value for common utilities

nucl_file_name

Data type: string

Default value: This parameter must be required for the processing.

Explanation of this parameter: ENDF file name

Sample of this parameter

nucl_file_name (U235.dat)

pendf_label_data

Data type: string

Default value: none

Explanation of this parameter: Label for new PENDF tape (Max. 66 words)

Sample of this parameter

pendf_label_data ("PENDF file of U235 from JENDL-4.0")

comment_data

Data type: list(string)

Default value: none

Explanation of this parameter: Comment line for the PENDF file.

FRENDY recognizes the comment line that is enclosed by double or single quotation.

If the user wants to use the double/single quotation in the comment line, please use the single/double quotation to enclose the comment.

Sample of this parameter

comment_data

("This is the comment line for the PENDF file.

User can use the 'single quotation mark' when the comment line is enclosed by the double quotation.")

error

Data type: real

Default value: 1.00×10^{-3}

Explanation of this parameter: Tolerance value for linearization.

Sample of this parameter

error 1.0E-3

error_max

Data type: real

Default value: error $\times 10.0$

Explanation of this parameter: Maximum tolerance value for linearization.

Sample of this parameter

error_max 1.0E-2

error_integral

Data type: real

Default value: error/20000.0

Explanation of this parameter: Maximum integral error for linearization.

Sample of this parameter

error_integral 5.0E-8

add_grid_data

Data type: list(real)

Default value: none

Explanation of this parameter: Additional energy grid [eV].

Sample of this parameter

add_grid_data (0.625 1.000 1.0E+6)

temp or temperature

Data type: real

Default value: 293.6 [K]

Explanation of this parameter: Temperature [K].

Sample of this parameter

temp 300.0

max_broadening_ene

Data type: real

Default value: 1.00×10^6 [eV]

Explanation of this parameter: Maximum energy for the Doppler broadening [eV].

If the upper limit of the resolved resonance energy E_h is smaller than max_broadening_ene, the maximum energy for the Doppler broadening is modified to E_h .

Sample of this parameter

max_broadning_ene 1.0E+6

sigma_zero_data

Data type: list(real)

Default value: 1.0×10¹⁰, 1.0×10⁶, 1.0×10⁵, 10000.0, 1000.0, 100.0, 35.0, 10.0, 1.0, 0.1 [barns]

Explanation of this parameter

σ_0 values for the Bondarenko-type self-shielded cross-section in the unresolved resonance region [barns]. Maximum σ_0 is considered as the σ_{inf} value.

The multi-group cross-section generation function can automatically set the background cross-section. The input format for the automatic setting of the background cross-section is as follows:

```
sigma_zero_data ( auto  err  Nmax   $\sigma_{min}$   Target  INT)
```

where,

err: Tolerance value.

N_{max}: Maximum number of the background cross-section.

σ_{min} : Minimum background cross-section [barns]

Target: Target of interpolation. (factor or rr)

INT: Interpolation method (cubic or linear)

factor: self-shielding factor

rr: Interpolation error is estimated for reaction rate

linear: linear interpolation

cubic: monotone cubic interpolation.

Note that the background cross-section of PURR uses the recommended value when the user selects the automatic setting of the background cross-section.

If the upper limit of the resolved resonance energy E_h is smaller than max_broadening_ene, the maximum energy for the Doppler broadening is modified to E_h .

Sample of this parameter

```
sigma_zero_data(1.0E10  1.0E6  1.0E5  10000.0  1000.0  100.0  35.0  10.0  1.0  0.1)
```

```
sigma_zero_data(auto  0.1  50  1.0e-10  rr  linear)
```

probability_bin_no

Data type: integer

Default value: 20

Explanation of this parameter: Number of probability table bins

Sample of this parameter

```
probability_bin_no 20
```

ladder_no

Data type: integer

Default value: 100

Explanation of this parameter: Number of resonance ladders for generating the probability table.

Sample of this parameter

ladder_no 100

err_p_table or err_p_tab or err_ptab

Data type: real

Default value: 5.0e-2

Explanation of this parameter: Tolerance value for probability table generation.

If this parameter is used, the ladder_no parameter is disabled.

Sample of this parameter

err_p_table 0.05

ene_grid_no_par_ladder or ene_grid_par_ladder or ene_no_par_ladder

Data type: integer

Default value: 10000

Explanation of this parameter: Sampling energy grid number for each ladder number.

Sample of this parameter

ene_grid_no_par_ladder 10000

random_seed

Data type: integer

Default value: 12345

Explanation of this parameter: Random number seed for probability table generation.

Sample of this parameter

random_seed 11111

ace_file_name

Data type: string

Default value: "nucl_file_name".ace

Explanation of this parameter: ACE file name.

Sample of this parameter

ace_file_name U235.ace

ace_dir_file_name or ace_dir or mcnp_dir_file_name or mcnp_dir

Data type: string

Default value: "nucl_file_name".ace.dir

Explanation of this parameter: MCNP directory information for the ACE file

When the ace_file_name is set, the default value is "ace_file_name".ace.dir.

Sample of this parameter

ace_dir_file_name U235.xsdir

suffix_id

Data type: real

Default value: .00

Explanation of this parameter: The suffix ID for the ACE file.

Sample of this parameter

suffix_id 0.50

ace_label_data

Data type: string

Default value: none

Explanation of this parameter: Label for the ACE file. (Max. 70 words)

Sample of this parameter

ace_label_data "PENDF file of U235 from JENDL-4.0"

iz_aw_data

Data type: list(real)

Default value: none

Explanation of this parameter: The list of (iz, aw) pairs for the ACE file. (iz= $1000.0 \times Z + A$,
aw=mass)

Sample of this parameter

iz_aw_data (92235.0 2.330250E+2)

cumulative_angle_distribution_format

Data type: string or integer

Default value: string = yes, integer = 1

Explanation of this parameter: Calculation option of whether new cumulative angular
distributions for ACE file generation are used or not.

Available value is use, yes, no, default, 0, and 1 (0=no, 1=use/yes).

where

use, yes, default, 1: Use the new cumulative angular distribution.

no, 0: Do not use the new cumulative angular distribution.

Sample of this parameter

cumulative_angle_distribution_format yes

1.2.2.3 Input parameter name and recommended value which are used only for thermal scattering law data

nucl_file_name_tsl

Data type: string

Default value: This parameter must be required for the processing.

Explanation of this parameter: ENDF file name for thermal scattering law data.

Sample of this parameter

nucl_file_name_tsl (HinH2O.txt)

equi_probable_angle_no

Data type: integer

Default value: 10

Explanation of this parameter: Number of equiprobable angles for thermal scattering law data.

Sample of this parameter

equi_probable_angle_no 10

principal_atom_no

Data type: integer

Default value: FRENDY automatically set from the ENDF file.

Explanation of this parameter: Number of principal atoms for thermal scattering law data.

Sample of this parameter

principal_atom_no 1

atom_type_no

Data type: integer

Default value: FRENDY automatically set from the ENDF file.

Explanation of this parameter: Number of atom types in the mixed moderator.

Sample of this parameter

atom_type_no 1

inelastic_reaction_type_no

Data type: integer

Default value: 221

Explanation of this parameter: Reaction type (MT) number for the inelastic reaction.

Sample of this parameter

inelastic_reaction_type_no 1

max_thermal_ene

Data type: real

Default value: max(10.0, temp/300.0)

Explanation of this parameter: Maximum energy for thermal treatment.

Sample of this parameter

max_thermal_ene 10.0

weight_option

Data type: string of integer

Default value: string = tabulated, integer = 2

Explanation of this parameter: Weighting option for thermal ACE file.

The available value is variable, constant, tabulated , default, or
0-2 (0=variable, 1=constant, 2=tabulated).

Sample of this parameter

Weight_option tabulated

thermal_z_a_id_name

Data type: string

Default value: ZA value of the ENDF file.

Explanation of this parameter: ZA ID name for the thermal ACE file (ZA=1000.0×Z+A, Max. 6 words).

Sample of this parameter

thermal_z_a_id_name lwtr

moderator_z_a_data

Data type: integer

Default value: none

Explanation of this parameter: Moderator component ZA value.

Sample of this parameter

moderator_z_a_data 1001

1.2.2.4 Input parameter name and recommended value which are used only for multi-group cross-section generation

mg_tsl_data_type

Data type: list (string)

Default value: This parameter must be required for the processing of the TSL data.

Explanation of this parameter: The $S(\alpha, \beta)$ type for the MATXS file.

The $S(\alpha, \beta)$ type used in FRENDY is shown in Table 1.2.2. The $S(\alpha, \beta)$ type has no impact on the GENDF file. Please set “free” when the user only generates the GENDF file.

Sample of this parameter

mg_tsl_data_type (hh2o)

mg_tsl_data_type (free)

Table .2.2 $S(\alpha, \beta)$ type name list and corresponding material name

Material name	$S(\alpha, \beta)$ type	Material name	$S(\alpha, \beta)$ type
Al	al	H in YH ₂	hyh2
Be	be	H in ZrH	hzrh
Be in BeO	bebeo	Liquid Methane (CH ₄)	lch4
Benzene	benz	N in UN	nun
C in SiC	csic	O in BeO	obeo
C ₅ O ₂ H ₈	c5o2h8	O in D ₂ O	od2o
D in D ₂ O	dd2o	O in ICE (H ₂ O)	oice
Ortho-D	dortho	O in UO ₂	ouo2
Para-D	dpara	Polyethylene (CH ₂)	poly
Fe	fe	Solid Methane (CH ₄)	sch4
Graphite	graph	Si in SiC	sisic
H in H ₂ O	hh2o	U in UN	uun
H in Ice (H ₂ O)	hice	U in UO ₂	uuo2
Ortho-H	hortho	Y in YH ₂	yyh2
Para-H	hpara	Zr in ZrH	zrzrh

mg_file_name

Data type: string

Default value: input file name

Explanation of this parameter: Multi-group XS file name.

The output file name is as follows:

"mg_file_name"_"mg_file_mode"_"ZAID of the ACE file".mg

Sample of this parameter

mg_file_name "U235"

mg_start_file_mode

Data type: string

Default value: ENDF

Explanation of this parameter: Format of the start file.

FRENDY generates the multi-group cross-section file from the ENDF-6 formatted file and the ACE file. The user selects which data is used to generate the multi-group cross-section file.

The available value is ENDF and ACE.

ENDF: A multi-group cross-section file is generated from the ENDF-6 formatted file.

ACE: A multi-group cross-section file is generated from the ACE file.

Sample of this parameter

mg_start_file_mode ENDF

mg_label_data

Data type: string

Default value: ENDF

Explanation of this parameter: The label of the multi-group cross-section file.

The label is output on the first line of the GENDF file.

Sample of this parameter

mg_label_data "Multi-group XS file of U235"

legendre_order

Data type: integer

Default value: 3

Explanation of this parameter: Maximum Legendre order (P_L order)

Sample of this parameter

legendre_order 3

mg_edit_option or mg_edit_mode or mg_edit_xs

Data type: list(string)

Default value: GENDF

Explanation of this parameter: Output format and output data of the multi-group cross-section generation.

The available output format and output data are as follows:

MATXS, SimpleMATXS, GENDF, FullMATXS, SimpleGENDF, FullGENDF, KRAMXS, 1DXS, 2DXS, NuChi, MGFlux, MGCurrent, UFG, and UFG1DXS.

where

MATXS: Microscopic cross-sections in MATXS format, consistent with NJOY2016.

SimpleMATXS: Microscopic cross-sections in MATXS format, consistent with NJOY99.

FullMATXS: Microscopic cross-sections in MATXS format without truncation of shielded cross-sections. Output file size may be large.

GENDF: Microscopic cross-sections in GENDF format consistent with NJOY2016.

SimpleGENDF: microscopic cross-sections in GENDF format, consistent with NJOY99.

FullGENDF: microscopic cross-sections in GENDF format without truncation of shielded cross-sections. Output file size may be large.

KRAMXS: microscopic cross-sections in KRAM format.

1DXS: One-dimensional cross-sections such as total, fission, radiative capture.

2DXS: Two-dimensional cross-sections such as elastic scattering, inelastic scattering, (n,2n) reaction.

NuChi: Nu-value and fission spectrum.

MGFlux: Multi-group flux (group integrated values).

MGCurrent: Multi-group current (group integrated values).

UFG: Ultra-fine group spectrum, total cross-sections, the slowing down source, total source.

UFG1DXS: One-dimensional ultra-fine group cross-sections such as total, fission, radiative capture.

The user can select the specified MT number when 1DXS, 2DXS, and UFG1DXS options are selected as follows:

"1DXS 1, 2, 4, -50"

The minus value for MT means all MT numbers between the previous MT number.

Sample of this parameter

mg_edit_option "U235"

max_thermal_ene_e_out

Data type: real

Default value: 20.0

Explanation of this parameter: Maximum energy of the thermal treatment for the outgoing particle energy [eV].

Sample of this parameter

max_thermal_ene_e_out 20.0

mg_weighting_spectrum_mode

Data type: string

Default value: 1/E

Explanation of this parameter: Weighting spectrum.

The available output format and output data are 1/E and Fission+1/E+Maxwell.

1/E: 1/E spectrum for the whole energy range.

Fission+1/E+Maxwell: Fission for fast energy range, 1/E for intermediate energy range, Maxwell for the thermal energy range.

The other parameters are required to use "Fission+1/E+Maxwell" option as follows:

mg_weighting_spectrum(Fission+1/E+Maxwell E_h E_l T_{fis} E₁ E₂)

where

E_h: Highest energy [eV],

E_l: Lowest energy [eV],

T_{fis}: Fission temperature [eV],

E₁: Energy boundary between fission and 1/E spectra [eV],

E₂: Energy boundary between 1/E and Maxwell spectra [eV].

The sample of "Fission+1/E+Maxwell" is as follows:

mg_weighting_spectrum(Fission+1/E+Maxwell 2.0e+7 1.0e-5 1.6e+6 1.0e+6 0.625)

The above values are used as the default values if the user does not set these parameters.

Sample of this parameter

mg_weighting_spectrum_mode "1/E"

mg_weighting_spectrum_data or mg_weighting_spectrum

Data type: list (real)

Default value: none

Explanation of this parameter: Weighting spectrum. The user can manually set the weight spectrum.

The format of the weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows:

mg_weighting_spectrum_data(E₁ W₁ E₂ W₂ ... E_{i-1} W_{i-1} E_i W_i)

where

E_i is the ith value of energy [eV],

W_i is the ith value of weight.

NJOY's weight spectrum, *i.e.*, the “iwt” number of the GROUPR module and the weighted spectrum name shown in Table 1.2.3, is also available. The input format to select the NJOY's weight spectrum is as follows:

mg_weighting_spectrum_data(iwtXX)

where XX is the “iwt” number (iwt01 ~ iwt12).

Sample of this parameter

mg_weighting_spectrum_data (1.0E-5 1.0 2.0E7 1.0)

mg_weighting_spectrum_data (iwt06)

Table .2.3 Weighted spectrum name list and corresponding “iwt” number

iwt	Weighting spectrum name		vitamine-e
2	constant	11	vit-e
5	epri-cell-lwr	12	ornl-5505
	epri-cell		vitamine-e-with-t-dependent
	epri		vitamine-e-with-t-depend
9	claw-weight-function		vitamine-e-with-t
10	claw-with-t-dependent		vit-e-with-t-dependent
	claw-with-t-depend		vit-e-with-t-depend
	claw-with-t		vit-e-with-t
	claw-t		

mg_weighting_spectrum_data_int or mg_weighting_spectrum_int

Data type: list (integer)

Default value: 2 (linear-linear)

Explanation of this parameter: Interpolation method of the weight spectrum.

The format of the weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows:

mg_weighting_spectrum_data_int(NBT₁ INT₁ NBT₂ INT₂ ... NBT_{i-1} INT_{i-1} NBT_i INT_i)

where

NBT_i is the value of n separating the i^{th} and $(i+1)^{\text{th}}$ interpolation range,

INT_i is the interpolation scheme identification number used in the i^{th} range.

The available interpolation scheme is 1 (const), 2 (linear-linear), 3 (linear-log), 4 (log-liner), and 5 (log-log).

Sample of this parameter

mg_weighting_spectrum_data_int (2 1) //NBT=2, INT=1 (const)

mg_structure or mg_structure_neutron

Data type: list (real)

Default value: XMAS 172-group structure

Explanation of this parameter: Energy group structure.

The user can manually set the energy group structure [eV].

NJOY's energy group structure, *i.e.*, the “ign” number of the GROUPR module and the energy group structure name shown in Table 10.2.4, is also available. The input format to select the NJOY's energy group structure is as follows:

mg_structure(ignXX)

where XX is the ign number (ign01 ~ ign34).

The energy group structure can be automatically set by the user input.

The input format for the automatic setting of the energy group structure is as follows:

mg_structure (auto E₁ N₁ O₁ E₂ N₂ O₂ ... E_{i-1} N_{i-1} O_{i-1} E_i N_i O_i E_{i+1})

where

E_i: Energy boundary i [eV],

N_i: Number of divisions,

O_i: Option for divisions.

The available option for divisions O_i is as follows:

EL: Divide the energy range by equi-lethargy width,

EE: Divide the energy range by equi-energy width.

Sample of this parameter

```
mg_structure ( ign18 ) //XMAS 172-group structure
mg_structure ( 1.0E-5  0.625  2.0E+7 ) //2-group structure
mg_structure (
    auto
    2.0e+07  3200  EL
    100.0    1      EL
    1.0e-5 )
```

Table .2.4 Energy group structure name list and corresponding “ign” number

ign	Energy group structure name	ign	Energy group structure name	ign	Energy group structure name
2	csewg-239	13	lanl-80	22	xmas-lwpc-172
	csewg	14	eurlib-100		xmas-lwpc
3	lanl-30		eurlib	23	vit-j-lwpc-175
4	anl-27	15	sand-iaa-640		vit-j-lwpc
	anl		sand-iaa	24	shem-cea-281
5	rrd-50		sand-640		shem-cea
	rrd	16	vitamin-e-174	25	shem-epm-295
6	gam-i-68		vitamin-e	26	shem-cea-epm-361
	gam-i		vitamin-174		shem-cea-epm
	gam-68		vit-e-174	27	shem-epm-315
7	gam-ii-100		vit-e	28	rahab-aecl-89
	gam-ii		vit-174		rahab-aecl
	gam-100	17	vitamin-j-175	28	rahab
8	laser-thermos-35		vitamin-j	29	ccfe-660
	laser-thermos		vitamin-175		ccfe
	laser		vit-j-175	30	ukaesa-1025
	laser-35		vit-j	31	ukaesa-1067
9	epri-cpm-69		vit-175	32	ukaesa-1102
	epri-cpm	18	xmas-nea-lanl-172	33	ukaesa-142
	epri		xmas-nea-lanl	34	lanl-618
	epri-69		xmas-lanl		
10	lanl-187		xmas-nea		
11	lanl-70	19	ecco-33		

12	sand-ii-620	20	ecco-1968
	sand-ii	21	tripoli-315
	sand-620		tripoli

mg_ufg_structure or mg_ultra_fine_group_structure

Data type: list (real)

Default value: (2.0e+07 10000 EL
52475.0 56000 EL
9118.8 12000 EL
4307.4 12000 EL
961.12 8000 EL
130.07 12000 EL
0.32242 10000 EL
1.0e-5)

Explanation of this parameter: Energy group structure to generate neutron flux in the ultra-fine group structure.

The format of this parameter is as follows:

mg_ufg_structure(E₁ N₁ O₁ E₂ N₂ O₂ ... E_{i-1} N_{i-1} O_{i-1} E_i N_i O_i E_{i+1})

where

E_i: Energy of ith boundary [eV],

N_i: Number of divisions,

O_i: Option for divisions

The available option for divisions O_i is as follows:

EL: Divide the energy range by equi-lethargy width.

EE: Divide the energy range by equi-energy width.

Sample of this parameter

```
mg_ufg_structure
( 2.0e+07 10000 EL
  52475.0 56000 EL
  9118.8 12000 EL
  4307.4 12000 EL
  961.12 8000 EL
  130.07 12000 EL
  0.32242 10000 EL
  1.0e-5 )
```


mg_number_density

Data type: list (real)

Default value: 1.0 (use only one nuclide)

Explanation of this parameter: Number density of each nuclide [1/barn/cm].

If the user processes the one nuclide data, this parameter can be skipped.

Sample of this parameter

mg_number_density (1.0)

mg_flux_calc_mode

Data type: string

Default value: SLD

Explanation of this parameter: Calculation option at the resonance region.

The available option at the resonance region is as follows:

NR: Use narrow resonance calculation.

SLD: Use ultra-fine group slowing down calculation.

Sample of this parameter

mg_flux_calc_mode SLD

mg_flux_calc_w_eh_el

Data type: list (real)

Default value: W=0.999167, E_h=1.0×10⁴, E_l=1.0

Explanation of this parameter: Calculation condition at the resonance region.

The format of this parameter is as follows:

mg_flux_calc_w_eh_el(W E_h E_l)

where

W: Atomic weight (relative to neutron mass) used for the background moderator nuclide,

E_h: Upper energy to use ultra-fine group slowing down spectrum [eV],

E_l: Lower energy to use ultra-fine group slowing down spectrum [eV].

Sample of this parameter

mg_flux_calc_w_eh_el (0.999167 1.0E4 1.0)

mg_thermal_upscatter_treatment or mg_thermal_xs_treatment

Data type: string

Default value: on

Explanation of this parameter: Option for calculation of the thermal scattering using the free gas model.

Available value is use, on, yes, off, no, default, and def

on, yes, default, def: Calculation of the thermal scattering cross-section

off, no: Skip calculation of the thermal scattering cross-section

Sample of this parameter

mg_thermal_upscatter_treatment on

potential_scatter_xs

Data type: list (real)

Default value: none

Explanation of this parameter: Potential scattering cross-section of each nuclide [barns].

If the user does not set this parameter, FRENDY uses the potential scattering cross-sections obtained by JENDL-4.0, ENDF/B-VIII.0, or JEFF-3.3.

Sample of this parameter

potential_scatter_xs 1.15825E+01 //Potential scattering XS of U-235[barns]

mg_mat_no or mg_mat_list or mg_mat_no_list

Data type: list (integer)

Default value: none

Explanation of this parameter: The MAT number of the GENDF file.

This parameter is only required when the ACE file is used as the start format of the multi-group cross-section generation since the ACE file does not have the MAT number.

Sample of this parameter

mg_mat_no (825 9228 9237) //O16, U235, U238

ace_output_option or ace_edit_option

Data type: string

Default value: on

Explanation of this parameter: Output ACE file option until the multi-group cross-section generation.

Available value is on, output, edit, off, no, skip, default, def.

on, output, edit, default, def: Output the ACE file.

off, no: Do not output the ACE file.

Sample of this parameter

ace_output_option output

1.2.2.5 *Optional input parameter*

print_set_data_resonance_reconstruction or print_set_data_linearize

Data type: string

Default value: on

Explanation of this parameter: Output input information for the resonance reconstruction.

Available value is on, yes print write output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_resonance_reconstruction on

process_resonance_reconstruction or process_linearize

Data type: string

Default value: on

Explanation of this parameter: Processing option for the resonance reconstruction.

Available value is on, yes process, run, off, no, skip, default, and def.

on, yes, process run, default, def: Process the resonance reconstruction.

off, no, skip: Do not process the resonance reconstruction.

Sample of this parameter

process_resonance_reconstruction on

write_pendf_resonance_reconstruction or write_pendf_linearize

Data type: string

Default value: off

Explanation of this parameter: Output PENDF file option for the resonance reconstruction.

Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output: Output the PENDF file of the resonance reconstruction.

on, yes, print, write, output + PENDF file name: Output the PENDF file of the resonance reconstruction with a specific name.

off, no, skip, default, def: Do not output the PENDF file of the resonance reconstruction.

Sample of this parameter

write_pendf_resonance_reconstruction (on "U235_reso.pendf")

pendf_file_name_resonance_reconstruction or pendf_file_name_linearize

Data type: string

Default value: none

Explanation of this parameter: The PENDF file name for the resonance reconstruction.
The write_pendf_linearize parameter is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_resonance_reconstruction ("U235_reso.pendf")

print_set_data_doppler_broadening or print_set_data_dop

Data type: string

Default value: on

Explanation of this parameter: Output input information for the Doppler broadening.
Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_doppler_broadening on

process_doppler_broadening or process_dop

Data type: string

Default value: on

Explanation of this parameter: Processing option for the Doppler broadening.
Available value is on, yes, process, run, off, no, skip, default, and def.

on, yes, process, run, default, def: Process the Doppler broadening.

off, no, skip: Do not process the Doppler broadening.

Sample of this parameter

process_doppler_broadening on

write_pendf_doppler_broadening or write_pendf_dop

Data type: string

Default value: off

Explanation of this parameter: Output PENDF file option for the Doppler broadening.

Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output: Output the PENDF file of the Doppler broadening.

on, yes, print, write, output + PENDF file name: Output the PENDF file of the Doppler broadening with a specific name.

off, no, skip, default, def: Do not output the PENDF file of the Doppler broadening.

Sample of this parameter

write_pendf_doppler_broadening (on "U235_dop.pendf")

pendf_file_name_doppler_broadening or pendf_file_name_dop

Data type: string

Default value: none

Explanation of this parameter: The PENDF file name for the Doppler broadening.

The write_pendf_dop parameter is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_doppler_broadening ("U235_dop.pendf")

print_set_data_gas_production_cross_section or print_set_data_gas_xs

Data type: string

Default value: on

Explanation of this parameter: Output input information for the calculation of the gas production cross-section.

Available value is on, yes print write output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_gas_production_cross_section on

process_gas_production_cross_section or process_gas_xs

Data type: string

Default value: on

Explanation of this parameter: Processing option for the calculation of the gas production cross-section.

Available value is on, yes process, run, off, no, skip, default, and def.

on, yes, process run, default, def: Process the calculation of the gas production cross-section.

off, no, skip: Do not process the calculation of the gas production cross-section.

Sample of this parameter

process_gas_xs on

write PENDF_gas_production_cross_section or write PENDF_gas_xs

Data type: string

Default value: off

Explanation of this parameter: Output PENDF file option for the calculation of the gas production cross-section.

Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output: Output the PENDF file of the calculation of the gas production cross-section.

on, yes, print, write, output + PENDF file name: Output the PENDF file of the calculation of the gas production cross-section with a specific name.

off, no, skip, default, def: Do not output the PENDF file of the calculation of the gas production cross-section.

Sample of this parameter

write PENDF_gas_xs (on "U235_gas_xs.PENDF")

PENDF_file_name_gas_production_cross_section or PENDF_file_name_gas_xs

Data type: string

Default value: none

Explanation of this parameter: The PENDF file name for the calculation of the gas production cross-section.

The write_PENDF_gas_xs is changed from off to on when this parameter is set.

Sample of this parameter

PENDF_file_name_gas_xs ("U235_gas_xs.PENDF")

print_set_data_probability_table or print_set_data_prob_table

Data type: string

Default value: on

Explanation of this parameter: Output input information for the probability table generation.

Available value is on, yes print write output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_probability_table on

process_probability_table or process_prob_table

Data type: string

Default value: on

Explanation of this parameter: Processing option for the probability table generation.

Available value is on, yes process, run, off, no, skip, default, and def.

on, yes, process run, default, def: Process the probability table generation.

off, no, skip: Do not process the probability table generation.

Sample of this parameter

process_probability_table on

write_probability_table or write_pendf_prob_table

Data type: string

Default value: off

Explanation of this parameter: Output PENDF file option for the probability table generation.

Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output: Output the PENDF file of the probability table generation.

on, yes, print, write, output + PENDF file name: Output the PENDF file of the probability table generation with a specific name.

off, no, skip, default, def: Do not output the PENDF file of the probability table generation.

Sample of this parameter

write_pendf_probability_table (on "U235_ptab.pendf")

pendf_file_name_probability_table or pendif_file_name_prob_table

Data type: string

Default value: none

Explanation of this parameter: The PENDF file name for the probability table generation.

The write_pendif_prob_table parameter is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_probability_table ("U235_ptab.pendif")

print_set_data_thermal_scattering_law or print_set_data_tsl

Data type: string

Default value: on

Explanation of this parameter: Output input information for the calculation of the thermal scattering law data.

Available value is on, yes print write output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_thermal_scattering_law on

process_thermal_scattering_law or process_tsl

Data type: string

Default value: on

Explanation of this parameter: Processing option for the calculation of the thermal scattering law data.

Available value is on, yes process, run, off, no, skip, default, and def.

on, yes, process run, default, def: Process the calculation of the thermal scattering law data.

off, no, skip: Do not process the calculation of the thermal scattering law data.

Sample of this parameter

process_thermal_scattering_law on

write_pendf_thermal_scattering_law or write_pendf_tsl

Data type: string

Default value: off

Explanation of this parameter: Output PENDF file option for the calculation of the thermal scattering law data.

Available value is on, yes, print, write, output, off, no, skip, default, and def.

on, yes, print, write, output: Output the PENDF file of the calculation of the thermal scattering law data.

on, yes, print, write, output + PENDF file name: Output the PENDF file of the thermal scattering law data with a specific name.

off, no, skip, default, def: Do not output the PENDF file of the calculation of the thermal scattering law data.

Sample of this parameter

write_pendf_thermal_scattering_law (on "U235_tsl.pendf")

pendf_file_name_thermal_scattering_law or pendl_file_name_tsl

Data type: string

Default value: none

Explanation of this parameter: The PENDF file name for the calculation of the thermal scattering law data.

The write_pendl_tsl is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_thermal_scattering_law ("U235_tsl.pendl")

print_set_data_ace_data_generator or print_set_data_ace

Data type: string

Default value: on

Explanation of this parameter: Output input information for the ACE file generation.

Available value is on, yes print write output, off, no, skip, default, and def.

on, yes, print, write, output, default, def: Output the input information.

off, no, skip: Do not output the input information.

Sample of this parameter

print_set_data_ace_data_generator on

process_ace_data_generator or process_ace

Data type: string

Default value: on

Explanation of this parameter: Processing option for the ACE file generation.

Available value is on, yes process, run, off, no, skip, default, and def.

on, yes, process run, default, def: Process the ACE file generation.

off, no, skip: Do not process the ACE file generation.

Sample of this parameter

process_ace_data_generator on

1.2.2.6 Input parameter name and recommended value list

The input parameter name and its recommended value for the FRENDY original input format are listed in Tables 1.2.5 - 1.2.13. Note the parameters and explanation of them are identical to Sec. 1.2.2.2 - 1.2.2.5.

The parameters shaded in Tables 1.2.5 - 1.2.13 always need input. In the default option, FRENDY does not output the PENDF file and users do not need to select the modules to be executed. Users have to set the print and process flags as listed in Tables 1.2.7 - 1.2.13 when they want to write the PENDF file or skip the modules. FRENDY can recognize synonymous words. For example, FRENDY prepares “ene_grid_no_per_ladder”, “ene_grid_per_ladder”, and “ene_no_per_ladder” as the parameter name to change the number of ladders to generate the probability table and “on”, “yes”, “print”, “write”, and “output” to write the PENDF file.

Table .2.5 Input parameter name and recommended value for common parameter

Parameter name	Type	Recommended value	Description
nucl_file_name	string	-	ENDF file name
pendf_label_data	string	none	Label for new PENDF tape (Max. 66 words)
comment_data	list(string)	none	Descriptive comments for PENDF file (MF=1, MT=451) FRENDY recognize the comment line that is enclosed by double or single quotation. If user wants to use double/single quotation in the comment line, please use single/double quotation to enclose the comment line. Ex) "This is the comment line for the PENDF file. User can use the 'single quotation mark' when the comment line is enclosed by the double quotation."
error	real	1.00×10^{-3}	Tolerance value for linearization
error_max	real	error $\times 10.0$	Maximum tolerance value for linearization
error_integral	real	error/20000.0	Maximum integral error for linearization
add_grid_data	list (real)	none	Additional energy grid [eV]

temp or temperature	real	293.6	Temperature [K]
max_broadening_ene	real	1.00×10^6	Maximum energy for the Doppler broadening [eV]
probability_bin_no	integer	20	Number of probability table bins
ladder_no	integer	100	Number of resonance ladders for generating the probability table
ene_grid_no_par_ladder or ene_grid_par_ladder or ene_no_par_ladder	integer	10000	Sampling energy grid number for each ladder number
random_seed	integer	12345	Random number seed for probability table generation
err_p_table	real	1.00E-02	Tolerance value for probability table generation. If this parameter is used, the ladder_no parameter is disabled.
ace_file_name	string	"nucl_file_name".ace	ACE file name
ace_label_data	string	none	Label for ACE file (Max. 70 words)
iz_aw_data	list (real)	none	list of (iz, aw) pair iz=1000.0×Z+A, aw=mass

sigma_zero_data	list (real)	1.0×10^{10} , 1.0×10^6 , 1.0×10^5 , 10000.0, 1000.0, 100.0, 35.0, 10.0, 1.0, 0.1	<p>σ_0 values for the Bondarenko-type self-shielded cross section in the unresolved resonance region [barns] Maximum σ_0 is considered as the σ_{inf} value.</p> <p>The multi-group cross-section generation function can automatically set the background cross-section. The input format for the automatic setting of the background cross-section is as follows: sigma_zero_data (auto "error" "maximum number of cross-section" "minimum background cross-section [b]" "target of interpolation (factor/rr)" "interpolation method (cubic/linear)") factor: Interpolation error is estimated for self-shielding factor rr: Interpolation error is estimated for reaction rate linear: linear interpolation cubic: monotone cubic interpolation</p> <p>The sample of input is as follows: sigma_zero_data(auto 0.1 50 1.0e-10 rr linear)</p> <p>Note that the background cross-section of PURR uses the recommended value when the user selects the automatic setting of background cross-section.</p>
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ene_grid_no_par_ladder or ene_grid_par_ladder or ene_no_par_ladder	integer	10000	Sampling energy grid number for each ladder number
ace_dir_file_name or ace_dir or mcnp_dir_file_name or mcnp_dir	string	"nucl_file_name".ace.dir or "ace_file_name".ace.dir (When the ace_file_name is changed by user)	MCNP directory information for ACE file
suffix_id	real	.00	Suffix ID for ACE file
cumulative_angle_distribution_format	string or integer	string = yes, integer = 1	Calculation option of whether new cumulative angular distributions for ACE file generation are used or not Available value is use, yes, no, default or 0-1 (0=no, 1=use/yes)

Table .2.6 Input parameter name and recommended value which are used only for thermal scattering law data

Parameter name	Type	Recommended value	Description
nucl_file_name_tsl	string	-	ENDF file name for thermal scattering law data
equi_probable_angle_no	integer	10	Number of equi-probable angles for thermal scattering law data
principal_atom_no	integer	-	Number of principal atoms for thermal scattering law data (If user doesn't set this parameter, FRENDY automatically set from the ENDF file)
inelastic_reaction_type_no	integer	221	Reaction type (MT) number for inelastic reaction. (MT=221-250 only)
max_thermal_ene	real	max(10.0, temp/300.0)	Maximum energy for thermal treatment
thermal_zs_id_name	string	ZA value of ENDF file	ZA ID name for thermal ACE file (ZA=1000.0×Z+A, Max. 6 words)
moderator_zs_data	integer	none	Moderator component ZA value
atom_type_no	integer	-	Number of atom types in mixed moderator (If user doesn't set this, FRENDY automatically set from ENDF file name and so on)
weight_option	string or integer	string = tabulated, integer = 2	Weighting option for thermal ACE file Available value is variable, constant, tabulated, default or 0-2 (0=variable, 1=constant, 2=tabulated)

Table .2.7 Input parameter name and recommended value which are used only for multi-group cross-section generation

Parameter name	Type	Recommended value	Description
mg_tsl_data_type	list (string)	-	S(α,β) type for MATXS file. This parameter must be required when user processes TSL data. S(α,β) type used in FRENDY is shown in Table 1.2.2. S(α,β) type has no impact on GENDF file. Please set “free” when the user only generates GENDF file.
mg_file_name	string	input file name	Multi-group XS file name The output file name is as follows: <i>"mg_file_name"_"mg_file_mode"_"ZAID of the ACE file".mg</i>
mg_start_file_mode	string	ENDF	Format of the start file. FRENDY can generate the multi-group cross-section file from the ENDF-6 formatted file and the ACE file. The available value is ENDF and ACE. ENDF: Multi-group cross-section file is generated from the ENDF-6 formatted file. ACE: Multi-group cross-section file is generated from the ACE file.
mg_label_data	string	-	Label of multi-group cross-section file. The label is output on the first line of the GENDF file.
legendre_order	integer	3	Maximum Legendre order (PL order)
max_thermal_ene_e_out	real	20.0	Maximum energy of thermal treatment for outgoing energy [eV]

mg_edit_option or mg_edit_mode or mg_edit_xs	list (string)	GENDF	<p>Output format and output data of the multi-group cross-section generation.</p> <p>The available output format and output data are MATXS, SimpleMATXS, GENDF, FullMATXS, SimpleGENDF, FullGENDF, KRAMXS, 1DXS, 2DXS, NuChi, MGFlux, MGCurrent, UFG, and UFG1DXS.</p> <p>MATXS: Microscopic cross sections in MATXS format, consistent with NJOY2016.</p> <p>SimpleMATXS: Microscopic cross sections in MATXS format, consistent with NJOY99.</p> <p>FullMATXS: Microscopic cross sections in MATXS format without truncation of shielded cross sections. Output file size may be large.</p> <p>GENDF: Microscopic cross sections in GENDF format consistent with NJOY2016.</p> <p>SimpleGENDF: microscopic cross sections in GENDF format, consistent with NJOY99.</p> <p>FullGENDF: microscopic cross sections in GENDF format without truncation of shielded cross sections. Output file size may be large.</p> <p>KRAMXS: microscopic cross sections in KRAM format.</p> <p>1DXS: 1D cross sections such as total, fission, radiative capture.</p> <p>2DXS: 2D cross sections such as elastic scattering, inelastic scattering, (n,2n) reaction.</p> <p>NuChi: Nu-value and fission spectrum.</p> <p>MGFlux: Multi-group flux (group integrated values).</p> <p>MGCurrent: Multi-group current (group integrated values).</p> <p>UFG: Ultra-fine group spectrum, total cross sections, slowing down source, total source.</p> <p>UFG1DXS: 1D ultra-fine group cross sections such as total, fission, radiative capture.</p> <p>User can select specified MT number when 1DXS, 2DXS, and UFG1DXS options are selected as follows: "1DXS 1, 2, 4, -50"</p> <p>The minus value for MT means all MT number between previous MT number.</p>
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mg_weighting_spectrum_mode	string	1/E	<p>Weighting spectrum.</p> <p>The available output format and output data are 1/E and Fission+1/E+Maxwell.</p> <p>1/E: 1/E spectrum for the whole energy range.</p> <p>Fission+1/E+Maxwell: Fission for fast energy range, 1/E for intermediate energy range, Maxwell for the thermal energy range.</p> <p>The other parameters are required to use "Fission+1/E+Maxwell" option as follows:</p> <p>mg_weighting_spectrum(Fission+1/E+Maxwell E_h E_l T_{fis} E₁ E₂)</p> <p>E_h: Highest energy [eV].</p> <p>E_l: Lowest energy [eV].</p> <p>T_{fis}: Fission temperature [eV].</p> <p>E₁: Energy boundary between fission and 1/E spectra [eV].</p> <p>E₂: Energy boundary between 1/E and Maxwell spectra [eV].</p> <p>The sample of "Fission+1/E+Maxwell" is as follows:</p> <p>mg_weighting_spectrum(Fission+1/E+Maxwell 2.0e+7 1.0e-5 1.6e+6 1.0e+6 0.625)</p> <p>The above values are used as the default values if the user does not set these parameters.</p>
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mg_weighting_spectrum_data or mg_weighting_spectrum	list (real)	-	<p>Weight spectrum.</p> <p>The user can manually set the weight spectrum.</p> <p>The format of weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows:</p> <p>mg_weighting_spectrum_data($E_1 W_1 \quad E_2 W_2 \quad \dots \quad E_{i-1} W_{i-1} \quad E_i W_i$)</p> <p>NJOY's weight spectrum, i.e., iwt of the GROUPT module and the weighted spectrum name shown in Table 1.2.3, is also available. The input format to select the NJOY's weight spectrum is as follows:</p> <p>mg_weighting_spectrum_data(iwtXX)</p> <p>where XX is the iwt number (iwt01 ~ iwt12).</p>
mg_weighting_spectrum_data_int or mg_weighting_spectrum_int	list (integer)	2 (linear-linear)	<p>Interpolation method of the weight spectrum.</p> <p>The format of weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows:</p> <p>mg_weighting_spectrum_data_int($NBT_1 INT_1 \quad NBT_2 INT_2 \dots NBT_{i-1} INT_{i-1} \quad NBT_i INT_i$)</p>

<p>mg_structure or mg_structure_neutron</p>	<p>list (real)</p>	<p>XMAS 172-group structure</p>	<p>Energy group structure. The user can manually set the energy group structure [eV].</p> <p>NJOY's energy group structure, i.e., ign of the GROUPR module and energy group structure name shown in Table 1.2.4, is also available. The input format to select the NJOY's energy group structure is as follows: mg_structure(ignXX) where XX is the ign number (ign01 ~ ign34).</p> <p>The energy group structure can be automatically set by the user input. The input format for the automatic setting of the energy group structure is as follows: mg_structure (auto E₁ N₁ O₁ E₂ N₂ O₂ ... E_{i-1} N_{i-1} O_{i-1} E_i N_i O_i E_{i+1}) E_i: Energy boundary i [eV] N_i: Number of divisions O_i: Option for divisions The available option for divisions is EL and EE. EL: Divide the energy range by equi-lethargy width. EE: Divide the energy range by equi-energy width. The sample of input is as follows: mg_structure (auto 2.0e+07 3200 EL 100.0 1 EL 1.0e-5)</p>
---	--------------------	-------------------------------------	--

mg_ufg_structure or mg_ultra_fine_group_structure	list (real)	(2.0e+07 10000 EL 52475.0 56000 EL 9118.8 12000 EL 4307.4 12000 EL 961.12 8000 EL 130.07 12000 EL 0.32242 10000 EL 1.0e-5)	Energy group structure to generate neutron flux in the ultra-fine group structure. The format of this parameter is as follows: mg_ufg_structure(E ₁ N ₁ O ₁ E ₂ N ₂ O ₂ ... E _{i-1} N _{i-1} O _{i-1} E _i N _i O _i E _{i+1}) E _i : Energy boundary i [eV] N _i : Number of divisions O _i : Option for divisions The available option for divisions is EL and EE. EL: Divide the energy range by equi-lethargy width. EE: Divide the energy range by equi-energy width.
mg_number_density	list (real)	1.0 (use only one nuclide)	Number density of each nuclide [1/barn/cm]. If the user processes the one nuclide data, this parameter can be skipped.
mg_thermal_upscatter_treatment or mg_thermal_xs_treatment	string	on	Option for calculation of the thermal scattering using the free gas model. <Calculation of the thermal scattering cross-section> on/yes/def/default <Skip calculation of the thermal scattering cross-section> off/no
potential_scatter_xs	list (real)	-	Potential scattering cross-section of each nuclide [barns]. If the user does not set this parameter, FREN DY uses the potential scattering cross-sections obtained by JENDL-4.0, ENDF/B-VIII.0, or JEFF-3.3.

mg_flux_calc_mode	string	SLD	<p>Calculation option at the resonance region.</p> <p>NR: Use narrow resonance calculation.</p> <p>SLD: Use ultra-fine group slowing down calculation.</p>
mg_flux_calc_w_eh_el	list (real)	0.999167, 1.0×10 ⁴ , 1.0	<p>Calculation condition at the resonance region.</p> <p>The format of this parameter is as follows: mg_flux_calc_w_eh_el(W Eh El)</p> <p>W: Atomic weight (relative to neutron mass) used for the background moderator nuclide. Eh: Upper energy to use ultra-fine group slowing down spectrum [eV]. El: Lower energy to use ultra-fine group slowing down spectrum [eV].</p>
mg_mat_no or mg_mat_list or mg_mat_no_list	list (integer)	-	<p>The MAT number of the GENDF file.</p> <p>This parameter is only required when the ACE file is used as the start format of the multi-group cross-section generation since the ACE file does not have the MAT number.</p>
ace_output_option or ace_edit_option	string	on	<p>Output ACE file option until multi-group cross-section generation.</p> <p><Writing ACE case> on/output/edit/def/default</p> <p><Skip ACE case> off/no/skip</p>

Table .2.8 Input parameter name and recommended value for resonance reconstruction

Parameter name	Type	Recommended value	Description
print_set_data_resonance_reconstruction or print_set_data_linearize	string	on	Output input information for resonance reconstruction <Writing input information> on/yes/print/write/output/default/def <Skip information> off/no/skip
process_resonance_reconstruction or process_linearize	string	on	Processing option for resonance reconstruction <Running resonance reconstruction case> on/yes/process/run/default/def <Skip resonance reconstruction case> off/no/skip
write_pendf_resonance_reconstruction or write_pendf_linearize	string	off	Output PENDF option for resonance reconstruction <Writing PENDF case> on/yes/print/write/output <Writing PENDF case with specific name> on/yes/print/write/output + PENDF file name <Skip PENDF case> off/no/skip/default/def
pendf_file_name_resonance_reconstruction or pendf_file_name_linearize	string	none	PENDF file name for resonance reconstruction When this parameter is set, write_pendf_linearize parameter is automatically changed from off to on.

Table .2.9 Input parameter name and recommended value for Doppler broadening

Parameter name	Type	Recommended value	Description
print_set_data_doppler_broadening or print_set_data_dop	string	on	Output input information for Doppler broadening <Writing input case> on/yes/print/write/output/default/def <Skip case> off/no/skip
process_doppler_broadening or process_dop	string	on	Processing option for Doppler broadening <Running Doppler broadening case> on/yes/process/run/default/def <Skip Doppler broadening case> off/no/skip
write_pendf_doppler_broadening or write_pendf_dop	string	off	Output PENDF option for Doppler broadening <Writing PENDF case> on/yes/print/write/output <Writing PENDF case with specific name> on/yes/print/write/output + PENDF file name <Skip PENDF case> off/no/skip/default/def
pendf_file_name_doppler_broadening or pendf_file_name_dop	string	none	PENDF file name for Doppler broadening When this parameter is set, write_pendf_dop parameter is automatically changed from off to on.

Table .2.10 Input parameter name and recommended value for gas production cross-section calculation

Parameter name	Type	Recommended value	Description
print_set_data_gas_production_cross_section, print_set_data_gas_production_xs, print_set_data_gas_production, print_set_data_gas_prod_xs, print_set_data_gas_xs, or print_set_data_gas	string	on	Output input information for gas production cross section generation <Writing input case> on/yes/print/write/output/default/def <Skip case> off/no/skip
process_gas_production_cross_section, process_gas_production_xs, process_gas_production, process_gas_prod_xs, process_gas_xs, or process_gas	string	on	Processing option for gas production cross section generation <Gas production cross section generation case> on/yes/process/run/default/def <Skip gas production cross section generation case> off/no/skip

<p>write_pendf_gas_production_cross_section, write_pendf_gas_production_xs, write_pendf_gas_production, write_pendf_gas_prod_xs, write_pendf_gas_xs, or write_pendf_gas</p>	string	off	<p>Output PENDF option for gas production cross section generation</p> <p><Writing PENDF case> on/yes/print/write/output</p> <p><Writing PENDF case with specific name> on/yes/print/write/output + PENDF file name</p> <p><Skip PENDF case> off/no/skip/default/def</p>
<p>pendf_file_name_gas_production_cross_section, pendf_file_name_gas_production_xs, pendf_file_name_gas_production, pendf_file_name_gas_prod_xs, pendf_file_name_gas_xs, or pendf_file_name_gas</p>	string	none	<p>PENDF file name for gas production cross section generation</p> <p>When this parameter is set, write_pendf_gas is automatically changed from off to on.</p>

Table .2.11 Input parameter name and recommended value for probability table generation

Parameter name	Type	Recommended value	Description
print_set_data_probability_table_generator, print_set_data_probability_table, print_set_data_prob_table_generator, print_set_data_prob_table, or print_set_data_unreso_utils	string	on	Output input information for probability table generation <Writing input case> on/yes/print/write/output/default/def <Skip case> off/no/skip
process_probability_table_generator, process_probability_table, process_prob_table_generator, process_prob_table, or process_unreso_utils	string	on	Processing option for probability table generation <Probability table generation case> on/yes/process/run/default/def <Skip probability table generation case> off/no/skip
write_pendf_probability_table_generator, write_pendf_probability_table, write_pendf_prob_table_generator, write_pendf_prob_table, or write_pendf_unreso_utils	string	off	Output PENDF option for probability table generation <Writing PENDF case> on/yes/print/write/output <Writing PENDF case with specific name> on/yes/print/write/output + PENDF file name <Skip PENDF case> off/no/skip/default/def

pendf_file_name_probability_table_generator, pendf_file_name_probability_table, pendf_file_name_prob_table_generator, pendf_file_name_prob_table, or pendf_file_name_unreso_utils	string	none	PENDF file name for probability table generation When this parameter is set, write_pendf_prob_table parameter is automatically changed from off to on.
--	--------	------	---

Table .2.12 Input parameter name and recommended value for thermal scattering law data

Parameter name	Type	Recommended value	Description
print_set_data_thermal_scattering_law, print_set_data_thermal_scattering, print_set_data_tsl	string	on	Output input information for processing thermal scattering law data <Writing input case> on/yes/print/write/output/default/def <Skip case> off/no/skip
process_thermal_scattering_law, process_thermal_scattering, process_tsl	string	on	Processing option for thermal scattering law data <Processing thermal scattering law data case> on/yes/process/run/default/def <Skip thermal scattering law data case> off/no/skip
write_pendf_thermal_scattering_law, write_pendf_thermal_scattering, write_pendf_tsl	string	off	Output PENDF option for thermal scattering law data <Writing PENDF case> on/yes/print/write/output <Writing PENDF case with specific name> on/yes/print/write/output + PENDF file name <Skip PENDF case> off/no/skip/default/def
pendf_file_name_thermal_scattering_law, pendf_file_name_thermal_scattering, pendf_file_name_tsl	string	on	PENDF file name for thermal scattering law data When this parameter is set, write_pendf_tsl parameter is automatically changed from off to on.

Table .2.13 Input parameter name and recommended value for ACE file generation

Parameter name	Type	Recommended value	Description
print_set_data_ace_data_generator or print_set_data_ace	string	on	Output input information for ACE file generation <Writing input case> on/yes/print/write/output/default/def <Skip case> off/no/skip
process_ace_data_generator or process_ace	string	on	Processing option for ACE file generation <ACE file generation case> on/yes/process/run/default/def <Skip ACE file generation case> off/no/skip

1.2.3 Examples of the input file for FRENDY input format

The examples of the input files for the FRENDY original input format are shown in Figs. 1.2.2 - 1.2.6. As shown in Fig. 1.2.2, the “parameter name” and “parameter value” do not need to be placed in the same line. Comment lines can be put among the “parameter name” and the “parameter value”. As shown in Fig. 1.2.4, the minimum input parameters are the processing mode and the evaluated nuclear data file name. FRENDY prepares the recommended values for the other parameters as listed in Tables 1.2.5 - 1.2.13.

```
//Input file of FRENDY for continuous-energy neutron data
ace_fast_mode //processing mode (generate fast ACE file)

//Nuclear data file name
nucl_file_name U235.dat
/* ace file name */
ace_file_name U235.ace
temp 296.0 // temperature [K]
add_grid_data (0.625 4.0) //Additional energy grid point
sigma_zero_data //sigma-infinity is 1.0E10 [b]
(1.0E10 1.0E06 1.0E05 1.0E04 1.0E03 1.0E02
3.5E02 1.0E02 1.0E01 1.0E-1)
```

Figure .2.2 Example of input file for continuous-energy neutron data

```
//Input file of FRENDY for thermal scattering law data
ace_therm_mode //process mode (generate thermal ACE file)

//Nuclear data file name
nucl_file_name
H001.dat
//Nuclear data file name for TSL
nucl_file_name_tsl
H_in_H2O.txt
/* ace file name */
ace_file_name
H_in_H2O.ace
temp /* temperature */ 296.0 //[K]
```

Figure .2.3 Example of input file for continuous-energy thermal scattering law data


```

//Input file of FRENDY for continuous-energy neutron data
ace_dosi_mode //processing mode (generate dosimetry ACE file)

//Nuclear data file name
nucl_file_name U235.dat

```

Figure .2.4 Example of input file for continuous-energy dosimetry data

```

//Input file of FRENDY for multi-group neutron-induced data
mg_neutron_mode //processing mode (generate multi-group XS file)
//Nuclear data file name
nucl_file_name U235.dat
/* multi-group XS file name */
mg_file_name U235
temp 296.0 // temperature [K]
/* Output data type list */
mg_edit_option ( GENDF MATXS )
/* energy group structure */
mg_structure ( ign18 ) // XMAS NEA LANL 172 groups
/* weight spectrum */
mg_weighting_spectrum ( iwt03 ) // 1/e

```

Figure .2.5 Example of input file for multi-group neutron-induced data

```

//Input file of FRENDY for thermal scattering law data
mg_neutron_mode //process mode (generate multi-group XS file)
//Nuclear data file name
nucl_file_name H001.dat
nucl_file_name_tsl H_in_H2O.txt
/* multi-group XS file name */
mg_file_name H_in_H2O
temp /* temperature */ 296.0 // [K]
/* energy group structure */
mg_structure ( xmas_nea-lanl_172 ) // ign=18
/* weight spectrum */
mg_weighting_spectrum ( 1/e ) // iwt=3

```

Figure .2.6 Example of input file for multi-group thermal scattering law data

1.3 NJOY Compatible Format

The input format of NJOY is explained in the source code and manuals of the NJOY code system. Users can consult them for the details of the format. FRENDY can process the evaluated nuclear data file with the input file of the following modules:

MODER, RECONR, BROADR, GASPR, PURR, UNRESR, THERMR, ACER, GROUPR, and MATXSR.

Though FRENDY processes the evaluated nuclear data file using the NJOY compatible format, users should pay attention to the following points.

- FRENDY reads and writes the PENDF file only in the text format.
- FRENDY does not calculate the self-shielding factor in the unresolved resonance region using the deterministic method and the input file of the UNRESR module is automatically converted to that of PURR.
- The “iform” option in the THERMR module and the “ismooth” option in the GROUPR module in NJOY2016 are ignored to treat both NJOY99 and NJOY2016 formats.
- The fast, thermal, and dosimetry ACE file generation functions are only implemented and other functions in ACER are not currently implemented.
- FRENDY cannot generate the MATXS file from the GENDF file. Users must combine the GROUPR and the MATXSR modules to generate MATXS file.
- FRENDY generates multiple MATXS files when the GENDF file or the PENDF file contains the multi-temperature data.

NJOY reads and writes PENDF files in binary format when the input tape number is negative. The PENDF file in the binary format is used to efficiently access the evaluated nuclear data file. It is difficult to perfectly treat the binary file produced by FORTRAN since FRENDY is written in C++. Furthermore, the PENDF file in the binary format is mainly used as a temporary file. FRENDY changes the negative tape number (binary file) to a positive one (text file) when users set a negative tape number.

FRENDY calculates probability tables to treat the self-shielding effect in the unresolved resonance region with the ladder method. NJOY implements the deterministic method to calculate it with the UNRESR module. According to the manual of NJOY, it is not recommended to use the deterministic method. The self-shielding factor generated by the deterministic method sometimes shows inappropriate values, *e.g.*, negative or larger than 1.0. We believe that the calculation time of the ladder method is acceptable on the current computational platforms. Therefore, we do not implement

the deterministic method and FRENDY calculates the self-shielding effect in the unresolved resonance region using the ladder method even if users select the UNRESR module. The input parameters for the ladder method, *e.g.*, the numbers of bins and ladders, are obtained from the recommended value of the FRENDY original input as shown in Table 10.2.2.

The input formats of the THERMR module and the ACER module of NJOY2016 are slightly different from those of NJOY99. Though FRENDY can treat both input formats, the new input parameter prepared in NJOY2016, *i.e.*, the “iform” option in the THERMR module and the “ismooth” option in the GROUPT module are ignored.

As described in Chapter 7, the ACE file generation for the photo-atomic and the photo-nuclear data is not currently implemented. FRENDY terminates with an error message if users select these calculation modes.

FRENDY generates the MATXS file and the GENDF file from the ACE file. FRENDY cannot generate the MATXS file from the GENDF file. FRENDY shows the warning message and terminates the processing when the input of the MATXS module is only found in the input data.

NJOY outputs one MATXS file even if the multi-temperature data is found in the GENDF file. The multi-temperature MATXS file contains the difference data from the base temperature data. The multi-temperature data has some problems, *e.g.*, the number of significant digits is different in each data block. We believe that the multi-temperature MATXS file should be separated in each temperature.

1.4 Sample Input Data for ACE file generation

1.4.1 Simplest Input Data

1.4.1.1 Fast ACE file generation

The simplest input format to generate the neutron incident ACE file requires only the processing mode name and evaluated nuclear data file name.

ace_file_generation_fast_mode		// Processing mode name
nucl_file_name	U235.fast.dat	// Nuclear data file name

The above input data generates the ACE file at a temperature of 293.6 K named “U235.fast.dat.ace” and the directory information file named “U235.fast.dat.ace.dir”. For the other calculation conditions, the default input parameters listed in Tables 1.2.5 - 1.2.13 are used.

1.4.1.2 Thermal ACE file generation

The simplest input format to generate the ACE file of the thermal scattering law data requires only the processing mode name, evaluated nuclear data file name, and thermal scattering law data file name.

ace_file_generation_thermal_scatter_mode		// Processing mode name
nucl_file_name	H001.dat	// Nuclear data file name
nucl_file_name_tsl	HinH2O.dat	// Thermal scattering law data
		// file name

The above input data generates the ACE file at a temperature of 293.6 K named “HinH2O.dat.ace”, and the directory information file named “HinH2O.dat.ace.dir”. For the other calculation conditions, the default input parameters listed in Tables 1.2.5 - 1.2.13 are used.

1.4.1.3 Dosimetry ACE file generation

The simplest input format to generate the ACE file for the dosimetry data requires only the processing mode name and evaluated nuclear data file name.

ace_file_generation_dosimetry_mode		// Processing mode name
nucl_file_name	U235.dosi.dat	// Nuclear data file name

The above input data generates the ACE file at a temperature of 293.6 K named “U235.dosi.dat.ace”, and the directory information file named “U235.dosi.dat.ace.dir”. For the other calculation conditions, the default input parameters listed in Tables 1.2.5 - 1.2.13 are used.

1.4.2 Input Data to Modify Default Input Parameters

As shown in Tables 1.2.5 - 1.2.1 many input parameters are prepared in the FRENDY original format. However, in conventional applications users usually change only 5 parameters, *i.e.*, the temperature, the number of equiprobable angle bins for thermal scattering law data, ACE file name, directory information for the ACE file, and a suffix ID for the ACE file. This section illustrates examples of the input files to change these input parameters.

1.4.2.1 Fast ACE file generation

ace_file_generation_fast_mode		// Processing mode name
nucl_file_name	U235.fast.dat	// Nuclear data file name
temp	600.0	// Temperature [K]
suffix_id	.50	// Suffix ID for ACE file
ace_file_name	U235.fast.ace	// ACE file name
ace_dir_file_name	U235.fast.ace.dir	// MCNP directory information

The above input data generates the ACE file at a temperature of 600.0 K named “U235.fast.ace”, and the directory information file named “U235.fast.ace.dir”. In this input file, the suffix ID of the ACE file is changed from 0.00 to 0.50.

1.4.2.2 Thermal ACE file generation

ace_file_generation_thermal_scatter_mode		// Processing mode name
nucl_file_name	H001.dat	// Nuclear data file name
nucl_file_name_tsl	HinH2O.dat	// TSL data name
temp	600.0	// Temperature [K]
equi_probable_angle_no	30	// Number of equi-probable angles
suffix_id	.50	// Suffix ID for ACE file
ace_file_name	HinH2O.tsl.ace	// ACE file name
ace_dir_file_name	HinH2O.tsl.ace.dir	// MCNP directory information

The above input data generates the ACE file at a temperature of 600.0 K named “HinH2O.tsl.ace”, and the directory information file named “HinH2O.tsl.ace.dir”. In this input file, the number of

equiprobable angles is changed from 10 to 30 and the suffix ID of the ACE file is changed from 0.00 to 0.50.

1.4.2.3 Dosimetry ACE file generation

ace_file_generation_dosimetry_mode		// Processing mode name
nucl_file_name	U235.dosi.dat	// Nuclear data file name
temp	600.0	// Temperature [K]
suffix_id	.50	// Suffix ID for ACE file
ace_file_name	U235.dosi.ace	// ACE file name
ace_dir_file_name	U235.dosi.ace.dir	// MCNP directory information

The above input data generates the ACE file at a temperature of 600.0 K named “U235.dosi.ace”, and the directory information file named “U235.dosi.ace.dir”. In this input file, the suffix ID of the ACE file is changed from 0.00 to 0.50.

1.4.3 Input Data to Reproduce NJOY99 Input

This section illustrates how to make FRENDY input files which is identical to NJOY input files. All the input parameters in the NJOY input files are explicitly set in the FRENDY input files. The processing conditions, PENDF file name, ACE file name, and so on of the FRENDY input files are identical to those of the NJOY input files.

1.4.3.1 Fast ACE file generation

The following input files are typical for the fast ACE file generation. These input files process the evaluated nuclear data file of ²³⁸U at 300.0 K.

< NJOY99 compatible format >

reconr	/ command
20 21	/ input(tape20), output(tape21)
'pendf tape for JENDL-4.0 U-238'	/ identifier for PENDF
9237 3 3	/ mat, ncards, ngrid
1.00e-03 0.00	/ err, temp
'92-U-238 from JENDL-4.0'	/ cards (1)
'Processed with FRENDY'	/ cards (2)
'Processed day: 2017/10/13'	/ cards (3)
0.625 4.0 100.0	/ enode
0	/

```

broadr                                / command
20 21 22                              / input(tape20), pendf(tape21), output(tape22)
9237 1 0 1 0                          / mat, temp_no, restart_opt, bootstrap, temp_initial
1.00E-03 100000                       / err, max_energy
300.0                                 / temp
0                                      /
gaspr                                  / command
20 22 23                              / input(tape20), output(tape23)
0                                      /
purr                                   / command
20 23 25                              / input(tape20), pendf(tape23), output(tape25)
9237 1 7 20 100 1                    / mat, temp_no, sig0_no, bin_no, ladder_no, print_opt
300.0                                 / temp
1.0E10 1.0E4 1.0E3 300.0 100.0 30.0 10.0 / sig0
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 U238'           / descriptive character
9237 300.0                           / mat, temp
1 1                                  / newfor(yes), iopp(yes)
1 1 1                                / thin(1), thin(2), thin(3)
stop                                  /

```

< FRENDY original input format >

```

ace_file_generation_fast_mode         // Processing mode name
nucl_file_name                        tape20

pendf_label_data "pendf tape for JENDL-4.0 U238"
error                                 1.0E-3
temp                                 300.0
add_grid_data                        (0.625 4.0 100.0)
max_broadening_ene                   100000 // 1 MeV
sigma_zero_data (1.0E10 1.0E4 1.0E3 300.0 100.0 30.0 10.0)
probability_bin_no                   20

```

ladder_no	100
ace_file_name	tape30
mcnp_dir_file_name	tape31
ace_label_data	"ACE file for JENDL-4 U238"
suffix_id	0.30
comment_data	

“92-U-238 from JENDL-4.0
Processed with FRENDY
Processed day: 2017/10/13”

// Write PENDF file option for RECONR	
write_pendf_resonance_reconstruction	tape21
// Write PENDF file option for BROADR	
write_pendf_doppler_broadening	tape22
// Write PENDF file option for GASPR	
write_pendf_gas_prod_xs	tape23
// Write PENDF file option for PURR	
write_pendf_prob_table_generator	tape25

// Skip or running RECONR option	
process_resonance_reconstruction	on
// Skip or running BROADR option	
process_doppler_broadening	on
// Skip or running GASPR option	
process_gas_production_cross_section	on
// Skip or running PURR option	
process_probability_table_generator	on
// Skip or running ACER option	
process_ace_data_generator	on

1.4.3.2 Thermal ACE file generation

The following input files are typical for the thermal ACE file generation. These input files process the evaluated nuclear data file of ^9Be in BeO at 300.0 K.

< NJOY99 compatible format >

```

reconr                                / command
  20  21                              / input(tape20), output(tape21)
'pendf tape for JENDL-4.0 Be-009'     / identifier for PENDF
  425                                  / mat
  1.00e-03  0.00                      / err, temp
  0                                    /
broadr                                / command
  20  21  22                          / input(tape20), pendf(tape21), output(tape22)
  425  1  0  1  0                    / mat, temp_no, restart_opt, bootstrap, temp_initial
  1.00E-03 100000.0                  / err, max_energy
  400.0                              / temp
  0                                    /
gaspr                                 / command
  20  22  23                          / input(tape20), pendf(tape22), output(tape23)
  0                                    /
thermr                                / command
  60  23  25                          / input(tape60), pendf(tape23), output(tape25)
  27  425 10 1 4 1 1 221             / natde, matdp, nbin, ntemp, iinc, icof
  400.0                              / temp
  1.00E-2  4.0                      / tolerance, max energy
purr                                  / command
  20  25  26                          / input(tape20), pendf(tape25), output(tape26)
  425  1  7  20  200  1              / mat, temp_no, sig0_no, bin_no, lad_no, print_opt
  400.0                              / temp
  1.0E10  1.0E4  1.0E3  300.0  100.0  30.0  10.0 / sig0
  0                                    /
acer                                  / command
  20  26  0  30  31                  / nendf, npend, ngend, nace, ndir
  2  1  1  0.30                      / iopt(fast), iprint(max), itype, suffix
'ACE file for JENDL-4 BeinBeO'       / descriptive character
  425  400.0 'bebeo'                 / mat, temp

```

```

4009 8016 / iza01, iza02
221 10 222 0 2 4.0 0 / mti, nbint, mte, ielas, nmix, emax, iwt
stop /

```

< FRENDY original input format >

```

ace_file_generation_thermal_scatter_mode // Processing mode name

    nucl_file_name          tape20
    nucl_file_name_tsl      tape60

    pendf_label_data        "pendf tape for JENDL-4.0 Be-009"
    error                   1.0E-3
    temp                   400.0
    max_broadening_ene      100000.0 // 1 MeV
    sigma_zero_data         (1.0E10 1.0E4 1.0E3 300.0 100.0 30.0 10.0)
    probability_bin_no       20
    ladder_no              200
    ace_file_name           tape30_frendy
    mcnp_dir_file_name       tape31_frendy
    ace_label_data          "ACE file for JENDL-4 BeInBeO"
    suffix_id               0.30

//Thermal scattering law data only
    equi_probable_angle_no  10
    principal_atom_no        1 //Be
    inelastic_reaction_type_no 221
    max_thermal_ene          4.0
    thermal_zs_id_name       "bebeo"
    moderator_zs_data        4009
    atom_type_no             2 //Be and O
    weight_option            0 //0 = variable

// Write PENDF file option for RECONR
    write_pendf_resonance_reconstruction    tape21
// Write PENDF file option for BROADR
    write_pendf_doppler_broadening          tape22

```

```

// Write PENDF file option for GASPR
        write_pendf_gas_prod_xs                tape23
// Write PENDF file option for THERMR
        write_pendf_thermal_scattering          tape25
// Write PENDF file option for PURR
        write_pendf_prob_table_generator        tape26

// Skip or running RECONR option
        process_resonance_reconstruction        on
// Skip or running BROADR option
        process_doppler_broadening              on
// Skip or running GASPR option
        process_gas_production_cross_section    on
// Skip or running THERMR option
        process_thermal_scattering_law          on
// Skip or running PURR option
        process_probability_table_generator      on
// Skip or running ACER option
        process_ace_data_generator              on

```

1.4.3.3 Dosimetry ACE file generation

The following input files are typical for the dosimetry ACE file generation. These input files process the evaluated nuclear data file of ^{238}U at 300.0 K.

< NJOY99 compatible format >

```

reconr                                / command
  20  21                              / input(tape20), output(tape21)
'pendf tape for JENDL-4 U238'          / identifier for PENDF
  9237                                / mat
  1.00e-03  0.0                       / err, temp
  0                                    /
broadr                                / command
  20  21  22                          / input(tape20), pendf(tape21), output(tape22)
  9237 1 0  1  0                      / mat, temp_no, restart_opt, bootstrap, temp_initial
  1.00E-03  100000                    / err, max_energy
  300.0                               / temp

```

```

0 /
gaspr / command
20 22 23 / input(tape20), pendf(tape22), output(tape23)
acer / command
20 23 0 30 31 / nendf, npend, ngend, nace, ndir
3 1 1 0.30 / iopt(fast), iprint(max), itype, suffix
'ACE file for JENDL-4 U238' / descriptive character
9237 300.0 / mat, temp
stop

```

< FRENDY original input format >

```

ace_file_generation_dosimetry_mode// Processing mode name
    nucl_file_name          tape20

    pendf_label_data "pendf tape for JENDL-4.0 U-238"
    error              1.0E-3
    temp               300.0
    max_broadening_ene 100000 //1 MeV
    ace_file_name      tape30
    mcnp_dir_file_name tape31
    ace_label_data     "ACE file for JENDL-4 U238"
    suffix_id          0.30

// Write PENDF file option for RECONR
    write_pendf_resonance_reconstruction    tape21
// Write PENDF file option for BROADR
    write_pendf_doppler_broadening          tape22
// Write PENDF file option for GASPR
    write_pendf_gas_prod_xs                 tape23

// Skip or running RECONR option
    process_resonance_reconstruction        on
// Skip or running BROADR option
    process_doppler_broadening              on
// Skip or running GASPR option

```

```

        process_gas_production_cross_section      on
// Skip or running ACER option
        process_ace_data_generator                on

```

1.5 Sample Input Data for Multi-group Cross-Section generation

1.5.1 Sample Input Data to Generate Neutron-Induced Multi-Group Cross-Section File

This section shows the sample input file to generate the neutron-induced multi-group cross-section file from the evaluated nuclear data and the ACE files. The input files in this section process ^1H and ^{235}U at 300.0 K.

< Input file to process ^1H from evaluated nuclear data file >

```

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 ) // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )      // Identical to iwt=3 in GROUPR/NJOY

```

< Input file to process ^{235}U from evaluated nuclear data file >

```

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 ) // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( iwt03 ) // Identical to iwt=3 in GROUPR/NJOY
legendre_order          3

```

< Input file to process ^{235}U from evaluated nuclear data file for fast reactor >

```
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 ( sand-ii-a-640 ) // Identical to ign=15 in GROUPT/NJOY
mg_weighting_spectrum ( iwt08 ) // Identical to iwt=8 in GROUPT/NJOY
legendre_order          3

mg_thermal_upscatter_treatment off //Thermal scattering XS treatment
//Thermal scattering cross-section is not required in fast reactor
```

< Input file to process ^1H 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 ) // Identical to ign=18 in GROUPT/NJOY
mg_weighting_spectrum ( 1/e ) // Identical to iwt=3 in GROUPT/NJOY
```

< Input file to process ^{235}U from ACE file >

```
mg_neutron_mode           //Process mode
ace_file_name ( ../ace/U235.ace ) //ACE 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
```

//MATXS: MATXS format consistent with NJOY2016

< Input file to process ^{235}U from ACE file for fast reactor>

```
mg_thermal_upscatter_treatment  off //Thermal scattering XS treatment
//Thermal scattering cross-section is not required in fast reactor
```

This section shows the sample input file to generate the multi-group cross-section file of the thermal scattering law data from the evaluated nuclear data and the ACE files. The input files in this section process H in H₂O at 293.6 K.

```

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 ) // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( 1/e ) // Identical to iwt=3 in GROUPR/NJOY
mg_tsl_data_type  (hh2o) //This data type is used for MATXS file generation

```

< Input file to process C in Graphite from evaluated nuclear data file >

```

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 ) // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( 1/e ) // Identical to iwt=3 in GROUPR/NJOY
mg_tsl_data_type  (graph) //This data type is used for MATXS file generation

```

< Input file to process H in H₂O 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 ) // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( 1/e ) // Identical to iwt=3 in GROUPR/NJOY
mg_tsl_data_type  (hh2o) //This data type is used for MATXS file generation

```

< Input file to process C in Graphite from ACE file >

```

mg_neutron_mode //Process mode
ace_file_name    ( ../ace/C012.ace ) //ACE file name
ace_file_name_tsl ( ../ace/31_graphite.ace ) //ACE file name (TSL data)
mg_edit_option  ( MATXS  GENDF ) //Output format
mg_file_name    C_in_Graphite //Output file name

```



```

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
mg_tsl_data_type      (graph)        //This data type is used for MATXS file generation

```

1.5.3 Sample Input Data to Generate Multi-Nuclide Data

FRENDY can process multi-nuclide data, e.g., ^{235}U , ^{238}U , and ^{16}O . This section shows the sample input file to process such multi-nuclide data. The input files in this section process ^{235}U , ^{238}U , and ^{16}O at 600.0 K and H in H_2O , D in D_2O , and O in H_2O at 293.6 K.

< Input file to process ^{235}U , ^{238}U , and ^{16}O from evaluated nuclear data file >

```

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

```

```

mg_file_name mix_UO2 //Output file name
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
mg_label_data "This data is UO2 data" //This label is output in the GENDF file
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]

```

< Input file to process H in H_2O , D in D_2O , and O in H_2O from evaluated nuclear data file >

```

mg_neutron_mode //Process mode
nucl_file_name ( ../lib/H001.dat

```

```

        ../lib/H002.dat
        ../lib/O016.dat ) //ENDF file name
nucl_file_name_tsl ( ../lib/01_h_in_h2o.txt
                    ../lib/11_d_in_d2o.txt
                    ../lib/02_o_in_h2o.txt )
mg_edit_option    ( MATXS  GENDF ) //Output format

mg_file_name      mix_H2O      //Output file name
temperature       293.6 //[K]
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
                    //H001    H002    O016
mg_number_density (4.68e-2  7.01e-6  2.34e-2 ) //[1/barn/cm]
mg_tsl_data_type  ( hh2o    dd2o    oh2o    )

```

< Input file to process ²³⁵U, ²³⁸U, and ¹⁶O from ACE file >

```

mg_neutron_mode //Process mode
ace_file_name ( ../ace/O016.ace ../ace/U235.ace ../ace/U238.ace ) //ACE file name
mg_edit_option ( SimpleGENDF SimpleMATXS GENDF MATXS
    "1DXS  1, 2, 4, -50" "2DXS  1, 2, 4, -50" 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
    //"1DXS  1, 2, 4, -50": 1D cross-section data (MT=1, 2, 4 – 50)
    //"2DXS  1, 2, 4, -50": 2D cross-section data (MT=1, 2, 4 – 50)
    //MGFlux: Multi group flux data

mg_file_name  mix_UO2 //Output file name
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

mg_label_data "This data is UO2 data" //This label is output in the GENDF file
legendre_order      3
                    //O016      U235      U238

```

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

< Input file to process H in H₂O, D in D₂O, and O in H₂O from ACE file >

```
mg_neutron_mode //Process mode
ace_file_name ( ../ace/H001.ace ../ace/H002.ace ../ace/O016.ace ) //ACE file name
ace_file_name_tsl ( ../ace/01_h_in_h2o.ace
                    ../ace/11_d_in_d2o.ace
                    ../ace/02_o_in_h2o.ace )
mg_edit_option ( MATXS  GENDF ) //Output format

mg_file_name      mix_H2O      //Output file name
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
                    //H001      H002      O016
mg_number_density      (4.68e-2  7.01e-6  2.34e-2 ) //[1/barn/cm]
mg_tsl_data_type      ( hh2o      dd2o      oh2o      )
```

1.5.4 Sample Input Data to Use Automatic Setting of Background Cross-Sections

This section shows the sample input file to generate the neutron-induced multi-group cross-section file from the evaluated nuclear data and the ACE files. This sample input file automatically set the background cross-sections of multi-group cross-section file. The input files in this section process ²³⁵U at 300.0 K.

< Input file to process ²³⁵U from evaluated nuclear data file >

```
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 ) // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( iwt03 ) // Identical to 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) = rr (reaction rate)
//Interpolation method (cubic / linear) = linear (linear interpolation)

```

< Input file to process ²³⁵U from ACE file >

```

mg_neutron_mode           //Process mode
ace_file_name ( ../ace/U235.ace ) //ACE file name
mg_file_name  U235        //Output file name
mg_edit_option ( GENDF  MATXS )
mg_structure ( ign18 )     // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( iwt03 ) // Identical to iwt=3 in GROUPR/NJOY

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

```

1.5.5 Sample Input Data to Use Automatic Setting of Energy Group Structure

This section shows the sample input file to generate the neutron-induced multi-group cross-section file from the evaluated nuclear data and the ACE files. This sample input file automatically set the energy group structure of multi-group cross-section file. The input files in this section process ²³⁵U at 300.0 K.

< Input file to process ²³⁵U from evaluated nuclear data file >

```

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 ( auto  2.0E+7  100  EL
                1.0E+2  100  EL
                1.0E-5 )
// 2.0E+7 eV – 1.0E+2 eV: Divide 100 energy groups by equi-lethagy width

```

```

// 1.0E+2 eV – 1.0E-5 eV: Divide 100 energy groups by equi-lethagy width
//EL: Divide by equi-lethagy width, EE: Divide by equi-energy width
mg_weighting_spectrum ( iwt03 ) // Identical to iwt=3 in GROUPT/NJOY

```

< Input file to process ²³⁵U from ACE file >

```

mg_neutron_mode           //Process mode
ace_file_name ( ../ace/U235.ace ) //ACE file name
mg_file_name   U235       //Output file name
mg_edit_option ( GENDF  MATXS )
mg_structure ( auto  2.0E+7  100  EL
                1.0E+2  100  EL
                1.0E-5 )
// 2.0E+7 eV – 1.0E+2 eV: Divide 100 energy groups by equi-lethagy width
// 1.0E+2 eV – 1.0E-5 eV: Divide 100 energy groups by equi-lethagy width
//EL: Divide by equi-lethagy width, EE: Divide by equi-energy width
mg_weighting_spectrum ( iwt03 ) // Identical to iwt=3 in GROUPT/NJOY

```

1.6 Input Instruction of ACE File Perturbation Tools

The ACE file perturbation tool contains two tools as follows:

```

tools/make_perturbation_factor/make_perturbation_factor.exe
tools/perturbation_ace_file/perturbation_ace_file.exe

```

The input format of both tools is explained in this section. The installation of these tools is found in the readme file of these tools (tools/README_tools).

1.6.1 Input Instruction of make_perturbation_factor

This tool is the uncertainty analysis tool using the Random Sampling method for the ACE file. This tool generates perturbation factor from the relative covariance matrix of cross-section and outputs the input data of the “perturbation_ace_file.exe”. Note that the license of this tool is not the 2-clause BSD license. The make_perturbation_factor.exe uses the Eigen library. The license of this tool is the MP2L license since the Eigen library is open-source software under the MP2L license.

The tool requires the following input data. In the input file, these terms are required and the user has to enclose by "<>" to set the data of each term.

(1) Sample size (int): <sample_size> *sample_no*

The first parameter is the number of random samplings. The number of random samplings is identical to the number of output files.

(2) Random seed (int): <seed> *seed_val*

The second parameter is the initial random seed.

(3) File name of covariance matrix (string): <relative_covariance> *cov_file_name*

The third parameter is the name of the covariance matrix file.

(4) Energy grid of covariance matrix [MeV] (real): <energy_grid> (*E₁ E₂ E₃ ... E_{g-1} E_g*)

The fourth parameter is the energy group structure. The number of energy grids of the input file must be identical to that of the covariance matrix. The energy group structure is enclosed by the bracket “()”.

(5) Nuclide name of the covariance matrix (string): <nuclide> (*Nucl₁ Nucl₂ ... Nucl_{i-1} Nucl_i*)

The fifth parameter is the energy group structure. The nuclide name is used as the directory name which stores the output files. If the covariance matrix uses the multiple nuclides, the nuclide name is enclosed by the bracket “()”.

(6) Reaction type (MT) of covariance matrix (int): <reaction> (*MT₁ MT₂ MT₃ ... MT_{i-1} MT_i*)

The sixth parameter is the reaction type number. If the covariance matrix uses the multiple reaction type, the reaction type is enclosed by the bracket “()”.

1.6.2 Sample Input of make_perturbation_factor

The sample input file of this tool is as follows:

< Generation of 100 sampling data from U-235 using cov_matrix.csv >

```
<sample_size>          100
<seed>                 20190504
<relative_covariance>  cov_matrix.csv
<energy_grid>          (1.0E-11  6.8E-7  2.0E1)
<nuclide>              (U235)
<reaction>             (2  18  102)
```

In this case, the sample number is 100, the initial random seed is 20190504, the covariance file name

is “cov_matrix.csv”, energy grid number is 2, the energy grid boundary is 1.0E-11 MeV, 6.8E-7 MeV, and 20MeV, the nuclide name is U235, and reaction type (MT number) is MT=2, 18, and 102, respectively.

< Generation of 200 sampling data from U-235 and U-238 using cov_matrix.csv >

```

<sample_size>          200
<seed>                  1
<relative_covariance>  cov_matrix.csv
<energy_grid>          (1.0E-11  6.8E-7  2.0E1)
<nuclide>              (U235  U238)
<reaction>             (2  18  102) (4  16)

```

In this case, the sample number is 200, the initial random seed is 1, the covariance file name is “cov_matrix.csv”, energy grid number is 2, the energy grid boundary is 1.0E-11 MeV, 6.8E-7 MeV, and 20MeV, the nuclide name is U235 and U238, and reaction type (MT number) is MT=2, 18, and 102 for U235 and MT=4 and 16 for U238, respectively.

1.6.3 Input Instruction of perturbation_ace_file

This tool generates the perturbed ACE file when the user sets the ACE file name, reaction type, energy region, and amount of perturbation. This tool can use the output file of the "make_perturbation_factor" tool.

The perturbation tool perturbs the cross-section, the number of neutrons per fission (ν_{total} , ν_{delay} , and ν_{prompt}), and fission spectrum line by line. The input format of this tool is as follows:

“MT number” E_{max} E_{min} f

or

“MT number” E_{min} E_{max} f

where E_{max} is the maximum energy of perturbation [MeV], E_{min} is the minimum energy of perturbation [MeV], and f is the amount of perturbation, respectively. Note that the above data must be set in one line. The number of the perturbed data files is identical to the number of lines. The available reaction type (MT number) is all reaction cross-section type, ν_{total} (MT=452), ν_{delay} (MT=455), ν_{prompt} (MT=456), and fission spectrum (MT=1018).

For example, if the user wants to modify elastic scattering cross-section (MT=2) from 1.0E-11 MeV to 1.0E-10 MeV and fission cross-section (MT=18) from 1.0E-6 eV to 1.0E-5 eV, the perturbation data file is as follows:

```

2  1.0E-10  1.0E-11  1.1
18 1.0E-5   1.0E-6   0.9

```

or

```

2  1.0E-11  1.0E-10  1.1
18 1.0E-6   1.0E-5   0.9

```

The execution command of the perturbation tools is as follows:

`./perturbation_ace_file.exe` “*ACE file name*” “*input file list*”

The perturbation tools developed for the uncertainty analysis tool using the Random Sampling method. The input file list is required to run this tool and the input file name is written in the input file list to perturb a lot of ACE files simultaneously.

This tool is developed to use the output file of "make_perturbation_factor" as the perturbation data file. The input file name must be "AAA_nnnn", where "AAA" is the file name and "nnnn" is 4 numbers. For example, if there are three perturbation data files and the target nuclide is U-235, the input file list is as follows:

```

inp/U235_0001
inp/U235_0020
inp/U235_0300

```

The perturbation tool reads "U235_0001", "U235_0020", and "U235_0300" files in "inp" directory and output three perturbed ACE files. The perturbed ACE file name is automatically set using 4 numbers in the perturbation data file name (the "nnnn" part in the input file name). In this case, the perturbed ACE file name is ace_file.ace_0001, ace_file.ace_0020, and ace_file.ace_0300 when the original ACE file name is "ace_file.ace_0001".

1.7 Input Instruction of ENDF Modification Tool

This tool is involved in the executable of FRENDY. The execution method is identical to the processing of the nuclear data file.

The user must set the processing mode as the first parameter. The processing mode to modify the ENDF-6 formatted file is as follows:

“endf_file_modification_mode”, “endf_file_modify_mode”, “endf_mod_mode”, or

“mod_endf_mode”

The modification tool performs the modifications line by line. If the user wants to remove specified MF/MT data, the user sets the following command:

```
remove MF “MF number” MT “MT number” “Original file name” “Modified file name”
remove MF “MF number” “Original file name” “Modified file name”
remove MT “MT number” “Original file name” “Modified file name”
```

If the user selects both MF and MT numbers, specified MF/MT data is removed from the original file. If the user only selects the MF number, specified MF data is removed. If the user only selects the MT number, specified MT data in all MF data are removed.

If the user wants to replace the specified MF/MT data, the user sets the following command:

```
replace MF “MF number” MT “MT number” “Original file name” “Replaced file name”
“Modified file name”
replace MF “MF number” “Original file name” “Replaced file name” “Modified file name”
replace MT “MT number” “Original file name” “Replaced file name” “Modified file name”
```

The modification tool removes the specified MF/MT data in the original file and copies the specified MF/MT data in the replaced file. The specified MF/MT data in the replaced file is copied even if the original file does not contain the specified MF/MT data

If the user wants to add the specified MF/MT data, the user sets the following command:

```
add MF “MF number” MT “MT number” “Original file name” “Replaced file name”
“Modified file name”
add MF “MF number” “Original file name” “Replaced file name” “Modified file name”
add MT “MT number” “Original file name” “Replaced file name” “Modified file name”
```

The modification tool copies the specified MF/MT data in the replaced file. The specified MF/MT data is replaced if the original file contains the specified MF/MT data.

1.8 Sample Input of ENDF Modification Tool

If the user wants to remove MT=19 from “./j40/Pu239.dat”, replace the MF=2 data with “./b80/n-094_Pu_239.endf”, and add the MF=35/MT=18 data in “./f33/94-Pu-239g.jeff33”, the sample input of modification tools is as follows. Note that after “/” is the comment.

endf_file_modification_mode *//processing mode*

remove MT 19 ./j40/Pu239.dat ./Pu239_mod01.dat

replace MF 2 ./Pu239_mod01.dat ./b80/n-094_Pu_239.endf ./Pu239_mod02.dat

add MF 35 MT 18 ./Pu239_mod02.dat ./f33/94-Pu-239g.jeff33 ./Pu239_mod03.dat

As shown in the sample input file, the user has to modify the original input file name in each line if the user wants to make multiple modifications.

2 Installation of FRENDY

This chapter describes how to install FRENDY on Linux, UNIX, or macOS platforms.

1. A disk space of about 1.2 Gbytes is required to make the executables from the program sources and run all test programs and sample files. A disk space of about 210 Mbytes is required if users make only the executables from the program sources.
2. A C++ compiler, the Boost library, and the LAPACK library are required to compile source programs. The compilation has been confirmed for an Intel compiler (ICC) version 13.1.3 and a GNU compiler (GCC) version 4.4.7 with the Boost library version 1.60.0 and the LAPACK library version 3.8.0.
3. Since FRENDY stores all nuclear data on memory, large memory size is required. More than 1 Gbytes is recommended to run FRENDY.

2.1 Directory Structure

The directory structure is shown in Fig. 2.1.1. The “frendy” directory contains the source files. The “sample” directory contains the input files for the test calculations to generate the fast and thermal ACE files. The “test” directory contains source files to run the Boost.Test library.

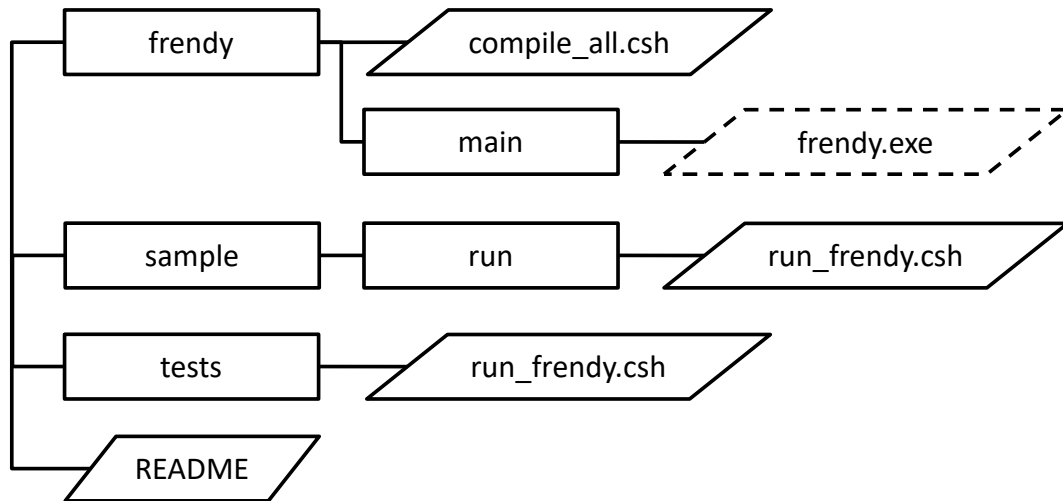


Figure 1.1 Directory structure

2.2 How to Install FRENDY on Linux, UNIX, or macOS Platforms

A shell script of “compile_all.csh” is included in the “frendy” directory to compile FRENDY source codes. The users run only this shell script or issue the “make” command in “frendy/main” directory. If the compiler successfully builds the executable file of FRENDY, the following message

is written on the display.

Completed to make FRENDY

The executable file named “frendy.exe” is generated in “frendy/main” directory.

FRENDY has the NJOY mode which processes the evaluated nuclear data file with the NJOY calculation method. The differences between the NJOY mode and the original mode are as follows:

1. The NJOY mode calculates the unresolved resonance cross-section using cross-section formulae on the fixed energy grid points and other energy grid points are calculated by the interpolation method. The fixed energy grid points are 1.00×10^n , 1.25×10^n , 1.50×10^n , 1.70×10^n , 2.00×10^n , 2.50×10^n , 3.00×10^n , 3.50×10^n , 4.00×10^n , 5.00×10^n , 6.00×10^n , 7.20×10^n , and 8.50×10^n . This difference has an impact on resonance reconstruction.
2. The calculation method of the complex error function which is defined in Eq. (2.3.41) is different. The complex error function is used to calculate the Doppler broadened cross-sections with the Single-Level Breit-Wigner representation. This difference has an impact on resonance reconstruction and probability table generation.
3. The calculation method of the cross-sections at 0 eV is different. The cross-section at 0 eV is required to calculate the Doppler broadened cross-sections at the low energy region. The NJOY mode assumes that the cross-section obeys the $1/v$ law. This approximation is appropriate for many reactions. However, the elastic scattering cross-sections do not obey the $1/v$ law since the elastic scattering cross-section is constant due to the potential scattering cross-section at the low-energy region. In such a case, the linear-linear interpolation is appropriate. The NJOY mode uses the $1/v$ law to reproduce the NJOY results. This difference affects the Doppler broadened elastic scattering cross-sections at the low-energy region.
4. The NJOY mode uses the fixed incident neutron energy grid to calculate the incoherent inelastic scattering cross-section. The number of energy grid points is 117 from 1.0×10^{-5} to 10 eV to calculate the incoherent inelastic scattering cross-section and secondary energy and angular distributions. The incoherent inelastic scattering cross-section at the other energy grid points is interpolated using the fifth-order Lagrange interpolation and secondary energy and angular distributions are not calculated. This difference affects some materials, *e.g.*, H in ZrH, for which the incoherent inelastic scattering cross-section oscillates.
5. The NJOY mode uses discrete random numbers to calculate the chi-squared random numbers with k degrees of freedom $R_{\chi^2}(k)$. This difference has an impact on the probability table

generation.

Users run “compile_all.csh” or “make” command in “frendy/main_njoy_mode” directory if they want to compile with this calculation mode. The executable file named “frendy_njoy_mode.exe” is generated in “frendy/main_njoy_mode” directory.

2.3 How to Execute FRENDY

The execution command is as follow:

frendy.exe “input file name”

The input file name is set as a command-line argument.

2.4 Test Calculation with Samples

The FRENDY suite includes test programs for fast and thermal ACE file generations in the “sample” directory. The “run_frendy.csh” shell script in “sample/run” directory automatically runs all the test programs.

2.5 Test Programs for Boost test Library

For quality assurance, the test programs are included to verify the capabilities. The Boost test library is used for the test programs. Using the Boost test library, comparison of the calculation results and confirmation of the run-time errors are easily done.

The source files for Boost test library are contained in the “test” directory. Users must run the “run_all_class.csh” shell script in the “test” directory if they want to compile and run all the test programs. The source file name and the directory structure correspond to those of FRENDY sources in the “frendy” directory. Users must recompile and run the test programs when they modify the source files.

The test programs start with the following message

Running X test cases...

where X is the number of test cases. If the test programs are successfully finished, the following message is written on the display

***** No errors detected**

If the test programs find errors, the following message is written on the display

***** Y failures detected in test suite "Master Test Suite"**

where Y is the number of errors.

2.6 How to Install FRENDY on VisualStudio2019

This section shows the installation of FRENDY using VisualStudio2019. The author strongly recommends using the Windows Subsystem for Linux to compile FRENDY since the installation of FRENDY using VisualStudio2019 is difficult. The installation of FRENDY using Windows Subsystem for Linux is explained in “FRENDY installation” on the web page of FRENDY training course: https://rpg.jaea.go.jp/main/en/program_frendy/index.html.

2.6.1 Installation of Boost library

Installation of the Boost library is required before the compilation of FRENDY. The installation of the Boost library is as follows:

1. Go to the web page of the Boost library: <https://www.boost.org/doc/>
2. Click “Getting Started”.
3. Click “Next: Getting Started on Microsoft Windows”.
4. Download the latest version of the Boost library.
5. Unzip the downloaded file.
6. Open the x64 native tools command prompt for VS2019. (Windows menu -> Visual Studio 2019 -> x64 Native Tools Command Prompt for VS2019)
7. Move to the unzipped Boost directory.
8. Run “bootstrap”.
9. Run “./b2”

2.6.2 Installation of CLAPACK library

Installation of the CLAPACK library is required before the compilation of FRENDY. The CLAPACK library is only used to treat the resonance parameter written in the R-matrix limited formula. The user can skip this process if the user doesn’t need to treat this resonance parameter.

The installation of the CLAPACK library is as follows:

1. Go to the web page of the CLAPACK library: <http://icl.cs.utk.edu/lapack-for-windows/clapack/>

2. Download the CLAPACK library from the following web page:
<http://icl.cs.utk.edu/lapack-for-windows/clapack/clapack-3.2.1-CMAKE.tgz>
3. Decompress the CLAPACK library.
4. Install the CLAPACK library.
5. Run installed CMake and select the source code directory of the CLAPACK library and the new directory to build.
6. Select Visual Studio 2019.
7. Click the “Finish” button.
8. Select the compiled directory and click the “Configure” button.
9. Click the “Generate” button.
10. Click the “Open Project” button and open the window of the VisualStudio2019.
11. Select the “ALL_BUILD” in the solution explorer and run debug and release.
12. Select the “INSTALL” in the solution explorer and run debug and release.

2.6.3 Installation of FRENDY

The installation of FRENDY is as follows:

1. Download the “msdirent.h” file instead of the “dirent.h” file from the following web page:
<http://svn.apache.org/repos/asf/avro/trunk/lang/c/tests/msdirent.h>
2. Copy the “msdirent.h” file to the “frendy\VisualStudio” directory.
3. Generate project of FRENDY with “Continue without code”.
4. Click File -> New -> Project From Existing Code.
5. Input source directory of FRENDY.
6. Select “Console Application Project”.
7. Click the “Finish” button.
8. Remove main.cpp, main_frendy_njooy_mode.cpp, and main_frendy.cpp.
9. Open property of this project. (Project -> Property).
10. Add include directory of the Boost library, the CLAPACK library and FRENDY.
11. Add additional dependency file as follows:
 For release : lapack.lib;blas.lib;libf2c.lib;
 For debug : lapackd.lib;blasd.lib;libf2cd.lib;
12. Compile FRENDY using release mode.

2.6.4 Running FRENDY with Bat Files

The users can run FRENDY using the following two bat files:

(1) run.bat

```
set INPNAME=inp_JENDL-4_U235
call run_frency.bat
```

(2) run_frency.bat

```
set EXE=frency.exe
rem set EXE= frency.exe
set INP_DIR=.%input
set LIB_DIR=.%lib
```

```
set OUT_DIR=out
set PEN_DIR=pendf
set ACE_DIR =ace
```

```
mkdir %OUT_DIR%
mkdir %PEN_DIR%
mkdir %ACE_DIR_FAST%
mkdir %ACE_DIR_THERM%
```

```
set DIR_DATA=xmdir_list
set LOG=log
```

```
rem del %DIR_DATA%
rem del %LOG%
```

```
set INP=%INP_DIR%¥%INPNAME%.dat
set LIB=%LIB_DIR%¥%LIBNAME%.dat
set LIBK=%LIB_DIR%¥%TSKNAME%.txt
```

```
copy %LIB% tape20
if exist %LIBK% copy %LIBK% tape23
```

```
echo %LIBNAME%
```



```

echo %LIB%
echo %LIBK%
echo %LIBNAME%  >> %LOG%
echo ""          >> %LOG%
%EXE%  %INP%    >> %LOG%
echo ""          >> %LOG%
echo "===== " >> %LOG%
echo ""          >> %LOG%

```

```

copy  output  %OUT_DIR%¥frendy_output_%LIBNAME%%TSKNAME%.dat
copy  tape25  %PEN_DIR%¥frendy_result_%LIBNAME%%TSKNAME%.dat
copy  tape30  %ACE_DIR %¥frendy_acer_%LIBNAME%%TSKNAME%.dat
type  tape31  >> %DIR_DATA%

```

```

del output
del tape20
del tape21
del tape22
del tape23
del tape25
del tape30
del tape31

```

```

rem rmdir /s /q %OUT_DIR%
rem rmdir /s /q %PEN_DIR%
rem rmdir /s /q %ACE_DIR_FAST%
rem rmdir /s /q %ACE_DIR_THERM%

```