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Manual of FRENDY Version 2

(Preliminary version)

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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 nuclear data 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, GROUPR, and MATXSR. 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 GROUPR 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.

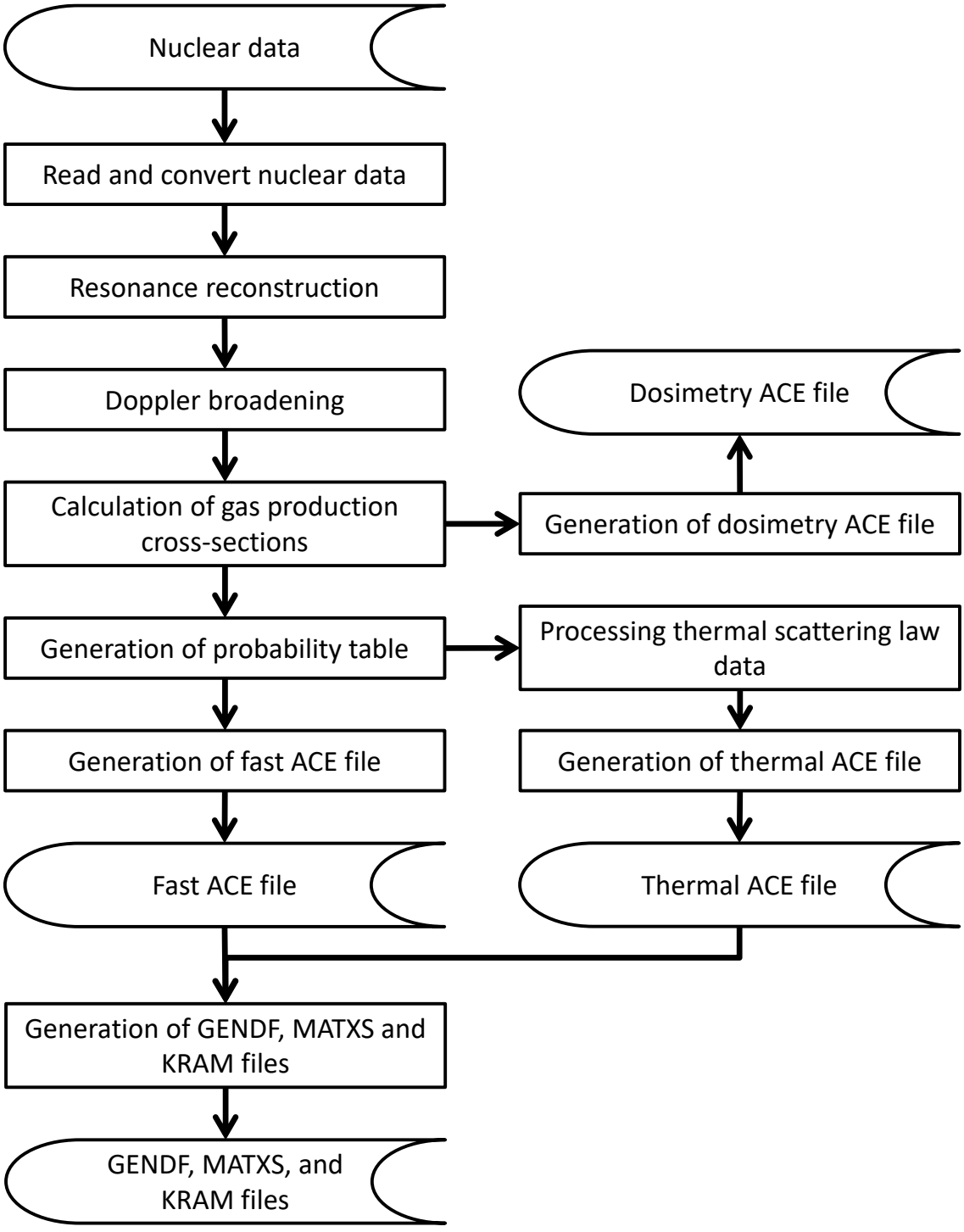

Figure 1.2.1 Processing flow to generate ACE, GENDF, MATXS, and KRAM files

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 1.2.1 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_normale	Generation of the neutron 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 ACE file of the thermal scattering law data
ace_file_generation_dosimetry_mode ace_dosi_mode ace_dosi	Generation of 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.

endf_file_modification_mode endf_file_modify_mode endf_mod_mode modify_endf_file_mode mod_endf_file_mode mod_endf_mode	Modification of ENDF-6 formatted file. The explanation of the input format is shown in Sec. 1.7.
output_xs_mode plot_mode comp_mode	Output 1-D table data from ENDF, GENDF, and ACE formatted file.

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×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_broading_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_broading_ene, the maximum energy for the Doppler broadening is modified to E_h.

Sample of this parameter

max_broadning_ene 1.0E+6

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

sigma_zero_data

Data type: list(real)

Default value: 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 [barns]

Explanation of this parameter

σ0 values for the Bondarenko-type self-shielded cross-section in the unresolved resonance region [barns]. Maximum σ0 is considered as the σinf 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 N_{max} σ_{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: Integerpolation method (cubic or linear)

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_broading_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)

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

err_p_table or **err_p_tab** or **err_ptab**

Data type: real

Default value: 1.0E-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 0.01

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×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

thermal_za_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_za_id_name lwtr

moderator_za_data

Data type: integer

Default value: none

Explanation of this parameter: Moderator component ZA value.

Sample of this parameter

moderator_za_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(α,β) type for the MATXS file.

The S(α,β) type used in FRENDY is shown in Table 1.2.2. The S(α,β) 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 1.2.2 S(α,β) type name list and corresponding material name

Material name	S(α,β) type	Material name	S(α,β) 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
$C_5O_2H_8$	c5o2h8	O in D_2O	od2o
D in D_2O	dd2o	O in ICE (H_2O)	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_2O	hh2o	U in UN	uun
H in Ice (H_2O)	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_edit_mode or mg_edit_option 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, UFG1DXS, and RUC.

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.

RUC: The 0 K scattering cross section data. This data is used for the input file of the resonance upscattering resonance up-scattering correction (reso_upscat).

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_mode "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

max_thermal_ene_e_out

Data type: real

Default value: max_thermal_ene

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 10.0

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} E_1 E_2)

where

E_h: Highest energy [eV],

E_l: Lowest energy [eV],

T_{fis}: Fission temperature [eV],

E_1: Energy boundary between fission and 1/E spectra [eV],

E_2: 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 default value of E_h, E_l, T_{fis}, E_1, and E_2 are 2.0e+7, 1.0e-5, 1.6e+6, 1.0e+6, and 0.0. When E_2 is 0.0, E_2 is automatically set by this program.

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(E_1 W_1 E_2 W_2 … E_{i-1} W_{i-1} E_i W_i)

where

E_i is the i^{th} value of energy [eV],

W_i is the i^{th} 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 (iwt02 ~ iwt12).

Sample of this parameter

mg_weighting_spectrum_data (1.0E-5 1.0 2.0E7 1.0)

mg_weighting_spectrum_data (iwt06)

mg_weighting_spectrum_data (epri-cell-lwr)

Table 1.2.3 Weighted spectrum name list and corresponding "iwt" number

iwt	Weighting spectrum name	iwt	Weighting spectrum name
2	constant	11	vitamine-e
	const		vit-e
3	1/e		ornl-5505
4	fission+1/e+maxwell		vitamine-e-with-t-dependent
5	epri-cell-lwr	12	vitamine-e-with-t-depend
	epri-cell		vitamine-e-with-t
	epri		vit-e-with-t-dependent
9	claw-weight-function		vit-e-with-t-depend
	claw-weight		vit-e-with-t
10	claw-with-t-dependent		vit-e-w-t
	claw-with-t-depend		
	claw-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(NBT_1 INT_1 NBT_2 INT_2 … NBT_{i-1} INT_{i-1} NBT_i INT_i)

where

NBT_i is the value of *n* separating the i^{th} and $(i+1)^{th}$ 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 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 (ign02 ~ ign34, ign101).

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 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})

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 )
```

mg_structure_g or **mg_structure_gam** or **mg_structure_gamma**

Data type: list (real)

Default value: none

Explanation of this parameter: Photon (gamma) production energy group structure.

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

If the user does not set this parameter, the photon production data generation is skipped.

NJOY's energy group structure, *i.e.*, the "igg" number of the GROUPR module and the energy group structure name shown in Table 1.2.5, is also available. The input format to select the NJOY's energy group structure is as follows:

mg_structure(iggXX)

where XX is the igg number (igg02 ~ igg10).

Table 1.2.4 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-iia-640		vit-j-lwpc
	anl		sand-iia	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	ukaea-1025
	laser-35		vit-j	31	ukaea-1067
9	epri-cpm-69		vit-175	32	ukaea-1102
	epri-cpm	18	xmas-nea-lanl-172	33	ukaea-142
	epri		xmas-nea-lanl	34	lanl-618
	epri-69		xmas-lanl	101	vitamin-b6-199
10	lanl-187		xmas-nea		vitamin-199
11	lanl-70	19	ecco-33		vit-b6-199
12	sand-ii-620	20	ecco-1968		vit-199
	sand-ii	21	tripoli-315		
	sand-620		tripoli		

Table 1.2.5 Energy group structure name list and corresponding "igg" number

igg	Energy group structure name	igg	Energy group structure name
2	csewg-94	9	vitamin-e-38
	csewg		vitamin-e
3	lanl-12		vitamin-38
4	steiner-21		vit-e-38
	steiner		vit-e
5	straker-22		vit-38
	straker	10	vitamin-j-42
6	lanl-48		vitamin-j
7	lanl-24		vitamin-42
8	vitamin-c-36		vit-j-42
	vitamin-c		vit-j
	vitamin-36		vit-42
	vit-c-36		
	vit-c		
	vit-36		

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(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})

where

E_i: Energy of i^{th} 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=1.0×10^4, 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

reso_upscat or reso_up_scat or reso_upscat_data or reso_up_scat_data

Data type: list (string)

Default value: none

Explanation of this parameter: The file name list of the 0 K scattering cross section data.

If the user wants to consider the resonance upscattering correction, please use this option. The user has to set the file name of the 0 K scattering cross section data which is generated by the RUC option in mg_edit_option.

Sample of this parameter

reso_upscat (U235_RUC_MT2.mg)

reso_upscat (skip U235_RUC_MT2.mg U238_RUC_MT2.mg)

//Skip means that this nuclide is not considered the resonance upscattering correlation

reso_upscat_mode or reso_up_scat_mode

Data type: string

Default value: ALL

Explanation of this parameter: Calculation option for the resonance up-scattering correction.

ALL: Resonance up-scattering correction is considered not only for 1D effective cross sections but also for the elastic scattering matrix.

XS: Resonance up-scattering correction is considered only for 1D effective cross sections. No resonance up-scattering is considered for the elastic scattering matrix.

Sample of this parameter

reso_upscat_mode (ALL)

potential_scat_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_scat_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 Input parameter name and recommended value which are used only for XS output tool

gendf_ name or **gendf_file_name**

Data type: string

Default value: none

Explanation of this parameter: GENDF formatted file name to output the (x, y) table.

Sample of this parameter

gendf_name ("./gendf/U235.gendf")

output_name or **output_file_name**

Data type: string

Default value: none

Explanation of this parameter: Output file name for XS output tool.

Sample of this parameter

output_name ("./output_xs/xs_data_01")

mat_no or **mat**

Data type: integer

Default value: none

Explanation of this parameter: Specified MAT number to output cross section.

This option is available for ENDF and GENDF formatted files.

Sample of this parameter

mat_no (9228)

mf_list or **mf_data**

Data type: vector<integer>

Default value: 3

Explanation of this parameter: Selection of output MF data.

This option is only available for a GENDF formatted file.

Sample of this parameter

mf_list (3 6)

mt_list or **mt_data_list** or **xs_type_list** or **reaction_type_list**

Data type: vector<integer>

Default value: none (all)

Explanation of this parameter: Selection of output MT data. If the user does not set this option,

this program outputs all cross section data.

Sample of this parameter

mt_list (1 2 102)

mt_list (1 2 50 - 102) //1, 2, 50, 51, 52, 53, …, 99, 100, 101, 102

mt_list (-102) //1, 2, 3, …, 99, 100, 101, 102

mt_list (“all”) //To output all MT data

edit_flag or **edit_mode**

Data type: string

Default value: histogram

Explanation of this parameter: Energy grid data option for multi-group cross section data.

Sample of this parameter

edit_flag("histogram")

If the user selects the non-histogram case, this tool only outputs cross sections at the lowest energy of each energy group, such as (El_i, XS_i), (El_{i+1}, XS_{i+1}). If the user selects the histogram case, this tool outputs cross sections at the lowest and highest energy of each energy group, such as (El_i, XS_i), (Eh_i, XS_i), (El_{i+1}, XS_{i+1}), (Eh_{i+1}, XS_{i+1}). Figure 1.2.2 shows an example of the difference between histogram and non-histogram plots using Excel. The histogram option is useful for plotting the multi-group cross section distribution by an Excel scatter plot.

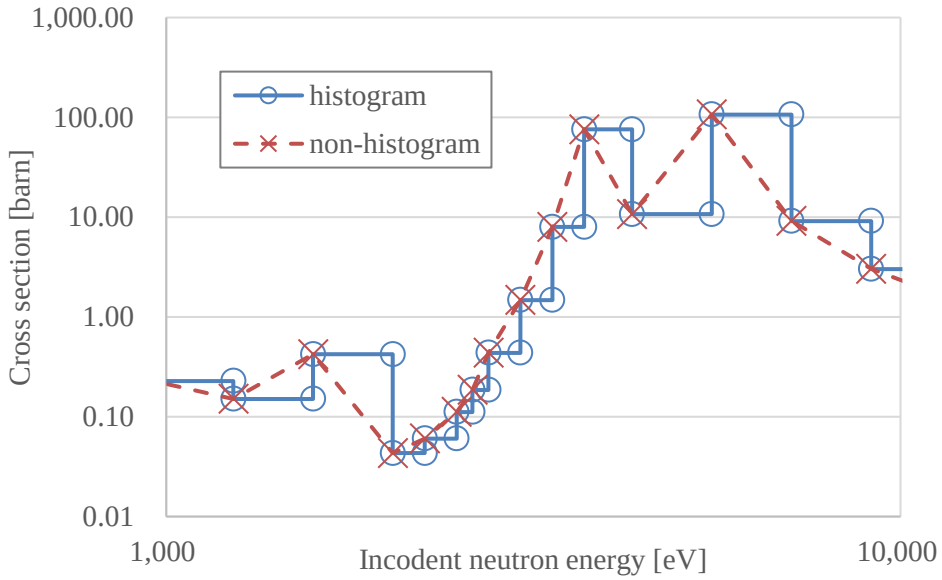

Figure 1.2.2 Difference between histogram and non-histogram plots

1.2.2.6 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_boroadening 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 **pendf_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_pendf_prob_tablle parameter is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_probability_table ("U235_ptab.pendf")

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 **pendf_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_pendf_tsl is changed from off to on when this parameter is set.

Sample of this parameter

pendf_file_name_thermal_scattering_law (“U235_tsl.pendf”)

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

1.2.2.7 Other input parameter

nan_err_mes_opt or **err_mes_nan_opt** or **err_nan_opt** or **nan_opt**

Data type: string

Default value: runtime_error

Explanation of this parameter: Policy for dealing with NaN (Not a Number) when data is output to ENDF, PENDF, and GENDF file.

Available value is runtime, runtime_error, error, caution, warning, default, and def.

runtime, runtime_error, error, default, def: The process is aborted when the "NaN" value is found.

caution, warning: The process is not aborted and the "NaN" value is converted -99999999.0 when the "NaN" value is found.

Sample of this parameter

nan_err_mes_opt runtime_error

1.2.2.8 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 1.2.6 - 1.2.16. Note the parameters and explanation of them are identical to Sections 1.2.2.2 - 1.2.2.7.

The parameters shaded in Tables 1.2.6 - 1.2.15 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 1.2.8 - 1.2.15 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 1.2.16 shows the optional input parameter. The input parameters in Table 1.2.16 are used for debug and checking the processing results.

Table 1.2.6 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×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_broading_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 desabled.
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	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 "error" "maximum number of cross-section" "minimum background cross-section [b]" "target of interpolation (factor/rr)" "interporation 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 The sample of input is as follows: sigma_zero_data(auto 0.1 50 1.0e-10 rr linear) Note that the background cross-section of PURR uses the recommended value when the user selects the automatic setting of background cross-section.

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 1.2.7 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_za_id_name	string	ZA value of ENDF file	ZA ID name for thermal ACE file (ZA=1000.0×Z+A, Max. 6 words)
moderator_za_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 1.2.8 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: "*mg_file_name*"_"*mg_file_mode*"_"*ZAID of the ACE file*".mg
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	max_thermal_ene	Maximum energy of thermal treatment for outgoing energy [eV]

mg_edit_mode or mg_edit_option or mg_edit_xs	list (string)	GENDF	Output format and output data of the multi-group cross-section generation. The available output format and output data are MATXS, SimpleMATXS, GENDF, FullMATXS, SimpleGENDF, FullGENDF, KRAMXS, 1DXS, 2DXS, NuChi, MGFlux, MGCurrent, UFG, UFG1DXS, and URC. 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, slowing down source, total source. UFG1DXS: One-dimensional ultra-fine group cross sections such as total, fission, radiative capture. RUC: The 0 K scattering cross section data. This data is used for the input file of the resonance upscattering resonance up-scattering correction (reso_upscat). User can select 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 number between previous MT number.

mg_weighting_spectrum_mode	string	1/E	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} E_1 E_2) E_h: Highest energy [eV]. E_l: Lowest energy [eV]. T_{fis}: Fission temperature [eV]. E_1: Energy boundary between fission and 1/E spectra [eV]. E_2: 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 default value of E_h, E_l, T_{fis}, E_1, and E_2 are 2.0e+7, 1.0e-5, 1.6e+6, 1.0e+6, and 0.0. When E_2 is 0.0, E_2 is automatically set by this program.

mg_weighting_spectrum_data or mg_weighting_spectrum	list (real)	-	Weight spectrum. The user can manually set the weight spectrum. The format of weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows: mg_weighting_spectrum_data(E_1 W_1 E_2 W_2 … E_{i-1} W_{i-1} E_i W_i) NJOY's weight spectrum, i.e., iwt 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 (iwt02 ~ iwt12).
mg_weighting_spectrum_data_int or mg_weighting_spectrum_int	list (integer)	2 (linear-linear)	Interpolation method of the weight spectrum. The format of weight spectrum is similar to the TAB1 record in the ENDF-6 format as follows: mg_weighting_spectrum_data_int(NBT_1 INT_1 NBT_2 INT_2 … NBT_{i-1} INT_{i-1} NBT_i INT_i)

mg_structure or mg_structure_neutron	list (real)	XMAS 172-group structure	Energy group structure. The user can manually set the energy group structure [eV]. 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 (ign02 ~ ign34, ign101). 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 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. The sample of input is as follows: mg_structure (auto 2.0e+07 3200 EL 100.0 1 EL 1.0e-5)

mg_structure_g or mg_structure_gam or mg_structure_gamm a	list (real)	-	Photon (gamma) production energy group structure. The user can manually set the energy group structure [eV]. If the user does not set this parameter, the photon production data generation is skipped. NJOY's energy group structure, i.e., igg of the GROUPR module and the energy group structure name shown in Table 1.2.5 is also available. The input format to select the NJOY's energy group structure is as follows: mg_structure_gam(iggXX) where XX is the igg number (igg02 ~ igg10).
mg_ufg_structure or mg_ultra_fine_grou p_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
reso_upscat reso_up_scat reso_upscat_data reso_up_scat_data	list (string)	-	The file name list of the 0 K scattering cross section data. If the user wants to consider the resonance upscattering correction, please use this option. The user has to set the file name of the 0 K scattering cross section data which is generated by the RUC option in mg_edit_option.
reso_upscat_mode or reso_up_scat_mode	string	ALL	Calculation option for the resonance up-scattering correction. ALL: Resonance up-scattering correction is considered not only for 1D effective cross sections but also for the elastic scattering matrix. XS: Resonance up-scattering correction is considered only for 1D effective cross sections. No resonance up-scattering is considered for the elastic scattering matrix.
potential_scat_xs	list (real)	-	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.
mg_flux_calc_mode	string	SLD	Calculation option at the resonance region. NR: Use narrow resonance calculation. SLD: Use ultra-fine group slowing down calculation.

mg_flux_calc_w_eh_el	list (real)	0.999167, 1.0×10^4, 1.0	Calculation condition at the resonance region. The format of this parameter is as follows: mg_flux_calc_w_eh_el(W Eh El) 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].
mg_mat_no or mg_mat_list or mg_mat_no_list	list (integer)	-	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.
ace_output_option or ace_edit_option	string	on	Output ACE file option until multi-group cross-section generation. <Writing ACE case> on/output/edit/def/default <Skip ACE case> off/no/skip

Table 1.2.9 Input parameter name and recommended value which are used only for XS output tool

Parameter name	Type	Recommended value	Description
gendf_name or gendf_file_name	string	none	GENDF formatted file name to output the (x, y) table.
output_name or output_file_name	string	none	Output file name for XS output function.
mat_no or mat	integer	none	Specified MAT number to output cross section. This option is available for ENDF and GENDF formatted files.
mf_list or mf_data	vector<Integer>	3	Selection of output MF data. This option is only available for a GENDF formatted file.
mt_list or mt_data_list or xs_type_list or reaction_type_list	vector<Integer>	none (all)	Selection of output MT data. If the user does not set this option, this program outputs all cross section data.

edit_flag or edit_mode	string	histogram	Energy grid data option for multi-group cross section data. If the user selects the non-histogram case, this tool only outputs cross section at the lowest energy of each energy groups, such as (El_i, XS_i), (El_{i+1}, XS_{i+1}). If the user selects the histogram case, this tool outputs cross sections at the lowest and the highest energy of each energy group, such as (El_i, XS_i), (Eh_i, XS_i), (El_{i+1}, XS_{i+1}), (Eh_{i+1}, XS_{i+1}). The histogram option is useful for plotting the multi-group cross section distribution by an Excel scatter plot. <histgram case> histogram/hist/two_point/two <Non histgram case> non_histogram/non_hist/one_point/one

Table 1.2.10 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 1.2.11 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 1.2.12 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

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	string	off	Output PENDF option for gas production cross section 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_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	string	none	PENDF file name for gas production cross section generation When this parameter is set, write_pendf_gas is automatically changed from off to on.

Table 1.2.13 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 1.2.14 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 1.2.15 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

Table 1.2.16 Optional input parameter name and recommended value

Parameter name	Type	Recommended value	Description
nan_err_mes_opt, err_mes_nan_opt, orerr_nan_opt, or nan_opt	string	runtime_error	Policy for dealing with NaN (Not a Number) when data is output to ENDF, PENDF, and GENDF file. <Process is aborted when the “NaN” value is found> runtime/runtime_error/error/default/def <Process is not aborted and the “NaN” value is converted -99999999.0 when the “NaN” value is found > caution/warning

1.2.3 Examples of FRENDY Input Formatted File

The examples of the input files for the FRENDY original input format are shown in Figs. 1.2.3 - 1.2.7. As shown in Fig. 1.2.3, 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. 1.2.5, 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 - 1.2.15.

```
//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
    sigima_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 1.2.3 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 1.2.4 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 1.2.5 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 1.2.6 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 1.2.7 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 1.2.2.

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 GROUPR module are ignored.

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 MATXSR 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 1.2.6 - 1.2.14 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 1.2.6 - 1.2.14 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 1.2.6 - 1.2.14 are used.

1.4.2 Input Data to Modify Default Input Parameters

As shown in Tables 1.2.6 - 1.2.14 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 ^{238}U 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 ^{9}Be 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"
        thermal_za_id_name          "bebeo"
        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_za_id_name              “bebeo”
        moderator_za_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 ^{1}H, and ^{235}U and ^{238}U at 300.0 K. The sample input files to process ^{238}U show the modification of the atomic weight of the moderator in the "mg_flux_calc_w_eh_el" to generate multi-group cross section files for graphite and hydrogen moderators.

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

```
mg_neutron_mode    //Process mode
   mg_edit_option     ( MATXS    GENDF )    //Output format
   nucl_file_name      ( ../lib/H001.dat )        //ENDF file name
   mg_file_name            H001                  //Output file name
   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_mode ( 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

   mg_structure ( ign18 )                // Identical to ign=18 in GROUPR/NJOY
   mg_structure_gam ( vitamin-j-42 ) // Identical to igg=10 in GROUPR/NJOY
   mg_weighting_spectrum ( iwt04 )    // Identical to iwt=4 in GROUPR/NJOY
   temp                           300.0 //[K]
   legendre_order                 3
```

< Input file to process ^{235}U from evaluated nuclear data file using specified energy group structure and weighting spectrum>

```
mg_neutron_mode                    //Process mode
  nucl_file_name ( ../lib/U235.dat )  //ENDF file name
  mg_file_name   U235              //Output file name
  mg_edit_option ( 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 ( 1.0E-5   0.625   5.0E5   1.0E6   2.0E+7 )   //4-groups
  mg_weighting_spectrum ( 1.0E-5   1.0   2.0E+7   1.0 )    //constant
  legendre_order                   3
```

< Input 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-iia-640 )        // Identical to ign=15 in GROUPR/NJOY
  mg_weighting_spectrum ( iwt08 )   // Identical to iwt=8 in GROUPR/NJOY
  legendre_order                   3

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

< Input file to process ^{238}U from evaluated nuclear data file with hydrogen moderator>

```
mg_neutron_mode                    //Process mode
  nucl_file_name ( ../lib/U238.dat )  //ENDF file name
  mg_file_name   U238                 //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 ( xmas_nea-lanl_172 )          // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell )  // Identical to iwt=4 in GROUPR/NJOY
  legendre_order                   3

  sigma_zero_data ( 1.0e+10 3.0e+4 1.0e+4 3.0e+3 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 3.0 )
        // Typical background cross section for U238

  mg_flux_calc_w_eh_el ( 0.999167, 1.0e+4, 1.0 )
        // Atomic weight of moderator (hydrogen, default value)
        // Upper energy [eV] of ultra-fine group slowing down calculation
        // Lower energy [eV] of ultra-fine group slowing down calculation
```

< Input file to process ^{238}U from evaluated nuclear data file with graphite moderator>

```
mg_neutron_mode                    //Process mode
  nucl_file_name ( ../lib/U238.dat )  //ENDF file name
  mg_file_name   U238                 //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 ( xmas_nea-lanl_172 )          // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell )  // Identical to iwt=4 in GROUPR/NJOY
  legendre_order                    3

  sigma_zero_data ( 1.0e+10 3.0e+4 1.0e+4 3.0e+3 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 3.0 )
        // Typical background cross section for U238

  mg_flux_calc_w_eh_el ( 12.0, 1.0e+4, 1.0 )
        // Atomic weight of moderator, (graphite)
        // Upper energy [eV] of ultra-fine group slowing down calculation
        // Lower energy [eV] of ultra-fine group slowing down calculation
```

< Input file to process ^{1}H from ACE file >

```
mg_neutron_mode   //Process mode
  mg_edit_option    ( MATXS   GENDF )   //Output format
  ace_file_name     ( ../ace/H001.ace )     //ACE file name
  mg_file_name        H001                //Output file name
  temperature         300.0 //[K]

  mg_structure ( xmas_nea-lanl_172 )     // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/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_mode ( 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

   mg_structure ( ign18 )                 // Identical to ign=18 in GROUPR/NJOY
   mg_structure_gam ( igg10 )             // Identical to igg=10 in GROUPR/NJOY
   mg_weighting_spectrum ( iwt04 )    // Identical to iwt=4 in GROUPR/NJOY
   temp                                   300.0 //[K]
   legendre_order                         3
```

< Input file to process ^{235}U from ACE file using specified energy group structure and weighting spectrum >

```
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 )
         //SimpleGENDF: MATXS format consistent with NJOY99
         //SimpleMATXS: GENDF format consistent with NJOY99
         //GENDF: GENDF format consistent with NJOY2016
         //MATXS: MATXS format consistent with NJOY2016
   mg_structure ( 1.0E-5    0.625    5.0E5    1.0E6    2.0E+7 )    //4-groups
   mg_weighting_spectrum ( 1.0E-5    1.0    2.0E+7    1.0 )     //constant
   legendre_order                         3
```

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

```
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
         //GENDF: GENDF format consistent with NJOY2016
         //MATXS: MATXS format consistent with NJOY2016

   mg_structure ( ign15 )                 // Identical to ign=15 in GROUPR/NJOY
```

```
   mg_weighting_spectrum ( iwt08 )    // Identical to iwt=8 in GROUPR/NJOY
   legendre_order                3

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

< Input file to process ^{238}U from ACE file with hydrogen moderator>

```
mg_neutron_mode                  //Process mode
   nucl_file_name ( ../ace/U238.ace )    //ACE file name
   mg_file_name    U238             //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 ( xmas_nea-lanl_172 )          // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell )    // Identical to iwt=4 in GROUPR/NJOY
   legendre_order                3

   sigma_zero_data ( 1.0e+10 3.0e+4 1.0e+4 3.0e+3 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 3.0 )
         // Typical background cross section for U238

   mg_flux_calc_w_eh_el ( 0.999167, 1.0e+4, 1.0 )
         // Atomic weight of moderator (hydrogen, default value)
         // Upper energy [eV] of ultra-fine group slowing down calculation
         // Lower energy [eV] of ultra-fine group slowing down calculation
```

< Input file to process ^{238}U from ACE file with graphite moderator>

```
mg_neutron_mode                  //Process mode
   nucl_file_name ( ../ace/U238.ace )    //ENDF file name
   mg_file_name    U238             //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 ( xmas_nea-lanl_172 )              // Identical to ign=18 in GROUPR/NJOY
mg_weighting_spectrum ( fission+1/e+maxwell )   // Identical to iwt=4 in GROUPR/NJOY
legendre_order                      3

sigma_zero_data ( 1.0e+10 3.0e+4 1.0e+4 3.0e+3 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 3.0 )
        // Typical background cross section for U238

mg_flux_calc_w_eh_el ( 12.0, 1.0e+4, 1.0 )
        // Atomic weight of moderator, (graphite)
        // Upper energy [eV] of ultra-fine group slowing down calculation
        // Lower energy [eV] of ultra-fine group slowing down calculation
```

1.5.2 Sample Input Data to Generate Multi-Group Cross-Section File of TSL Data

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 H_2O at 293.6 K and graphite at 293.6 K.

< Input file to process H in H_2O from evaluated nuclear data file >

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( MATXS    GENDF )         //Output format
   nucl_file_name          ( ../lib/H001.dat )          //ENDF file name
   nucl_file_name_tsl    ( ../lib/01_h_in_h2o.txt ) //TSL file name

   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 ( fission+1/e+maxwell ) // Identical to iwt=4 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 H_2O from ACE file >

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( MATXS    GENDF )       //Output format
   ace_file_name          ( ../ace/H001.ace )          //ENDF file name
   ace_file_name_tsl    ( ../ace/01_h_in_h2o.ace ) //TSL file name

   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 ( fission+1/e+maxwell    ) // Identical to iwt=4 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
   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
```

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_file_name    mix_UO2            //Output file name

   mg_edit_mode (
         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_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
   mg_structure_gam ( vitamin-j-42 )        // Identical to igg=10 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 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
                                  //8016.50c     92235.50c    92238.50c
  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
  mg_edit_option     ( MATXS    GENDF )    //Output format

  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_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 ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/NJOY

                                  //1001        1002         8016
  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 H in H_2O, D in D_2O, and O-16 from evaluated nuclear data file >

```
mg_neutron_mode    //Process mode
  mg_edit_option     ( MATXS    GENDF )    //Output format

  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    skip )

  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 ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/NJOY

                                    //1001       1002         8016
  mg_number_density           (4.68e-2    7.01e-6    2.34e-2 ) //[1/barn/cm]
  mg_tsl_data_type            ( hh2o       dd2o      free     )
```

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

```
mg_neutron_mode    //Process mode
  ace_file_name (
        ../ace/O016.ace
        ../ace/U235.ace
        ../ace/U238.ace ) //ACE file name

  mg_file_name    mix_UO2             //Output file name

  mg_edit_mode (
        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_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
  mg_structure_gam ( igg10 )               // Identical to igg=10 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 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
                                    //8016.50c     92235.50c    92238.50c
  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 ACE file >

```
mg_neutron_mode    //Process mode
  mg_edit_option     ( MATXS    GENDF )    //Output format

  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_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 ( fission+1/e+maxwell    ) // Identical to iwt=4 in GROUPR/NJOY

                                    //1001       1002         8016
  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 H in H_2O, D in D_2O, and O-16 from evaluated nuclear data file >

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( MATXS    GENDF )    //Output format

   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    skip )

   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 ( fission+1/e+maxwell    ) // Identical to iwt=4 in GROUPR/NJOY

                                  //1001       1002         8016
   mg_number_density         (4.68e-2    7.01e-6    2.34e-2 ) //[1/barn/cm]
   mg_tsl_data_type          ( hh2o       dd2o       free      )
```

1.5.4 Sample Input Data for 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 ^{235}U at 600.0 K.

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

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( MATXS    GENDF )    //Output format

   nucl_file_name ( ../lib/U235.dat )    //ENDF file name

   mg_file_name              U-235         //Output file name
   temperature               600.0 //[K]
   mg_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/NJOY

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

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

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( MATXS    GENDF )    //Output format

   ace_file_name ( ../ace/U235.ace )    //ENDF file name

   mg_file_name              U-235         //Output file name
   temperature               600.0 //[K]
   mg_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/NJOY
```

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

1.5.5 Sample Input Data for 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 ^{235}U at 300.0 K.

< 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 ( 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 GROUPR/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 ( 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 GROUPR/NJOY
```

1.5.6 Sample Input Data for Resonance Up-Scattering Correction

FRENDY can consider the resonance up-scattering correction. This section shows the sample input file to use this function. The input files in this section process ^{16}O, ^{235}U, and ^{238}U at 600.0 K. The resonance up-scattering correction of ^{16}O is not considered. The scattering cross section data at 0 K is required to consider the resonance up-scattering correction. This section shows two types of input data *i.e.*, generation of the scattering cross section data at 0 K and generation of the multi-group cross section data considering the resonance up-scattering correction.

< Input file to generate scattering cross section data at 0 K (processing ^{235}U from evaluated nuclear data file) >

```
mg_neutron_mode    //Process mode
  mg_edit_option     ( GENDF    RUC )    //Output format
  nucl_file_name ( ../lib/U235.dat )         //ENDF file name

  mg_file_name              U235_RUC      //Output file name
  temperature               0.0 //[K]
  mg_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell    ) // Identical to iwt=4 in GROUPR/NJOY
```

< Input file to generate scattering cross section data at 0 K (processing ^{238}U from evaluated nuclear data file) >

```
mg_neutron_mode    //Process mode
  mg_edit_option     ( GENDF    RUC )    //Output format
  nucl_file_name ( ../lib/U238.dat )         //ENDF file name

  mg_file_name              U238_RUC      //Output file name
  temperature               0.0 //[K]
  mg_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell    ) // Identical to iwt=4 in GROUPR/NJOY
```

< Input file to generate multi-group cross section considering resonance up-scattering correction (processing ^{16}O, ^{235}U, and ^{238}U from evaluated nuclear data file) >

```
mg_neutron_mode    //Process mode
   mg_edit_option      ( GENDF    MATXS )    //Output format
   nucl_file_name ( ../lib/O016.dat    ../lib/U235.dat    ../lib/U238.dat )    //ENDF file name

   mg_file_name              mix_UO2_with_RUC      //Output file name
   temperature               600.0 //[K]
   mg_structure ( xmas_nea-lanl_172 )       // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell ) // Identical to iwt=4 in GROUPR/NJOY

                             //8016.50c      92235.50c    92238.50c
   mg_number_density    (4.58e-2         7.18e-4         2.22e-2)    //[1/barn/cm]
   reso_upscat    ( skip    U235_RUC_92235.00c_MT2.mg    U238_RUC_92238.00c_MT2.mg )
```

1.5.7 Sample Input Data to calculate IR parameter

The IR parameter, which is used to capture the impact of the different atomic mass of moderator nuclides in a slowing down calculation, is calculated by Eq. (1.1).

$$f_{IR} = 1 + \frac{\sigma_1 - \sigma_0}{\frac{\sigma_2 - \sigma_0}{\frac{\sigma_{b1} - \sigma_{b0}}{\sigma_{b0}}}}. \tag{1.1}$$

Here, we consider calculating the IR parameter of ^{16}O for ^{238}U. σ_0 is an effective cross-section of ^{238}U using slowing down calculation using the typical background cross-section of ^{238}U (σ_{b0}) and default mass for the background nuclide (a_0 =0.999167 for light water). σ_1 is an effective cross-section of ^{238}U using slowing down calculation using σ_{b0} and mass of ^{16}O (a_1 =15.8575). σ_2 is an effective cross-section of ^{238}U using slowing down calculation using σ_{b1} (*e.g.*, $\sigma_{b1} = 1.05 \times \sigma_{b0}$) and default mass for the background nuclide (a_0 =0.999167 for light water).

This subsection shows sample input files to calculate σ_0, σ_1, and σ_2. The IR parameters of MT=102 are calculated using these sample files. For example, when we use these input files and evaluated nuclear data files from JENDL-5, σ_0, σ_1, and σ_2 of 88th group (7.52-6.16 eV) are $\sigma_0 = 45.45043$, $\sigma_1 = 42.49696$, $\sigma_2 = 46.30637$. Using Eq. (1.1), the IR parameter 88th group is 0.827.

< Input file to calculate σ_0 for IR parameter >

```
mg_neutron_mode    //Process mode
   nucl_file_name ( ../lib/n_092-U-238.dat ) //ENDF file name
   mg_file_name    U238                //Output file name
   mg_edit_mode ( SimpleGENDF    SimpleMATXS
                  "1DXS    102"
                  "MGFlux" )

   mg_structure ( xmas_nea-lanl_172 )                  // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell )    // Identical to iwt=4 in GROUPR/NJOY

   temp                            300.0 //[K]
   legendre_order                  3

   sigma_zero_data ( 1.0e+10 50.0 )
         // 50.0 barn corresponds to a typical background cross section for U238 in an LWR lattice

   mg_flux_calc_w_eh_el ( 0.999167, 1.0e+4, 1.0 )
         // Atomic weight of moderator (hydrogen)
         // Upper energy [eV] of ultra-fine group slowing down calculation
         // Lower energy [eV] of ultra-fine group slowing down calculation
```

< Input file to calculate σ_1 for IR parameter >

```
mg_neutron_mode    //Process mode
   nucl_file_name ( ../lib/n_092-U-238.dat ) //ENDF file name
   mg_file_name    U238                //Output file name
   mg_edit_mode ( SimpleGENDF    SimpleMATXS
                  "1DXS    102"
                  "MGFlux" )

   mg_structure ( xmas_nea-lanl_172 )                  // Identical to ign=18 in GROUPR/NJOY
   mg_weighting_spectrum ( fission+1/e+maxwell )    // Identical to iwt=4 in GROUPR/NJOY

   temp                            300.0 //[K]
   legendre_order                  3
```

```
  sigma_zero_data ( 1.0e+10 50.0 )
        // 50.0 barn corresponds to a typical background cross section for U238 in an LWR lattice

  mg_flux_calc_w_eh_el ( 15.8575, 1.0e+4, 1.0 )
        // Atomic weight of moderator (oxygen in UO2)
        // Upper energy [eV] of ultra-fine group slowing down calculation
        // Lower energy [eV] of ultra-fine group slowing down calculation
```

< Input file to calculate σ_2 for IR parameter >

```
mg_neutron_mode    //Process mode
  nucl_file_name ( ../lib/n_092-U-238.dat ) //ENDF file name
  mg_file_name    U238              //Output file name
  mg_edit_mode ( SimpleGENDF    SimpleMATXS
                 "1DXS    102"
                 "MGFlux" )

  mg_structure ( xmas_nea-lanl_172 )                  // Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( fission+1/e+maxwell )    // Identical to iwt=4 in GROUPR/NJOY

  temp                          300.0 //[K]
  legendre_order                3

  sigma_zero_data ( 1.0e+10 52.5 ) // sigma_0*1.05 = 50.0*1.05=52.5

  mg_flux_calc_w_eh_el ( 0.999167, 1.0e+4, 1.0 )
        // Atomic weight of moderator (hydrogen)
        // Upper energy [eV] of ultra-fine group slowing down calculation
        // Lower energy [eV] of ultra-fine group slowing down calculation
```

1.6 Input Instruction of ACE File Perturbation Tools

The ACE file perturbation tool contains two tools as follows:

tools/make_perturbation_factor/make_perturation_factor.exe

tools/perturation_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_perturation_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 covaiance matrix file.

(4) Energy grid of covariance matrix [MeV] (real): <energy_grid > (E_1 E_2 E_3 ... 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 > ($Nucl_1$ $Nucl_2$ ... $Nucl_{i-1}$ $Nucl_i$)

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 > (MT_1 MT_2 MT_3 ... 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 is1, 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.

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

linearize MF “*MF number*” MT “*MT number*” “*Original file name*” “*Modified file name*”
linearize MF “*MF number*” “*Original file name*” “*Modified file name*”

The linearization of the data is only available for the specified MF or MF/MT data.

1.8 Sample Input of ENDF Modification Tool

When the user wants to linearize MF=4, 5, and 6 data of “./j40/Pu239.dat”, the sample input of modification tools is as follows.

endf_file_modification_mode ***//processing mode***
linearize MF 4 ./j40/Pu239.dat ./Pu239_mod01.dat
linearize MF 5 ./Pu239_mod01.dat ./Pu239_mod02.dat
linearize MF 6 ./Pu239_mod02.dat ./Pu239_mod03.dat

In this sample input, the modified file name is “./Pu239_mod03.dat”.

This tool can linearize some evaluated nuclear data files in one input file. When the user wants to linearize MF=4 and MF=5/MT=18 of “./j40/U235.dat”, “./j40/U238.dat”, and “./j40/Pu239.dat”, the sample input of modification tools is as follows.

endf_file_modification_mode ***//processing mode***

```
linearize   MF   4              ./j40/U235.dat          ./U235_mod01.dat
linearize   MF   5   MT   18    ./U235_mod01.dat        ./U235_mod02.dat
linearize   MF   4              ./j40/U238.dat          ./U238_mod01.dat
linearize   MF   5   MT   18    ./U238_mod01.dat        ./U238_mod02.dat
linearize   MF   4              ./j40/Pu239.dat         ./Pu239_mod01.dat
linearize   MF   5   MT   18    ./Pu239_mod01.dat       ./Pu239_mod02.dat
```

In this sample input, the modified file name is "./U235_mod02.dat", "./U238_mod02.dat", and "./Pu239_mod02.dat", respectively.

The user can also set the tolerance of the linearization. The default tolerance value is 1.0E-3, *i.e.*, 0.1%. When the user wants to linearize a small tolerance value, the sample input is as follows:

endf_file_modification_mode ***//processing mode***

```
tolerance   1.0E-4
linearize   MF   4              ./j40/U235.dat          ./U235_mod01.dat
linearize   MF   5   MT   18    ./U235_mod01.dat        ./U235_mod02.dat
```

In this sample input, the tolerance value is changed from 1.0E-3 to 1.0E-4.

1.9 Sample Input of XS Output Tool

This tool outputs (x, y) tables from ENDF (PENDF), ACE, and GENDF formatted files. FRENDY does not prepare the plot function. This tool only outputs the (x, y) table and the user has to plot the graph using gnuplot, Matplotlib, Excel, and so on. The unit of energy is eV. Though the ACE file uses MeV for energy, this tool changes from MeV to eV. The calculation conditions, *e.g.*, nuclear data file name, temperature, and MT number, are written in the head of the output file.

The available input parameter of this tool is as follows:

For output the (x, y) table:

"nucl_file_name", "ace_file_name", "gendf_file_name", "error", "error_max", "temp", "output_name", "edit_flag", "mf_list", "mt_list", and "mat_no"

For multi-group cross section generation from the continuous cross section data in the ENDF and the ACE formatted files:

"mg_structure", "mg_weighting_spectrum_data", "mg_weighting_spectrum_data_int", and "mg_weighting_spectrum_mode"

This tool outputs the (x, y) table of a nuclear data file and comparison results (cross sections and relative differences) for comparing differences between the nuclear data libraries.

This tool processes resonance reconstruction, the Doppler broadening, and the multi-group cross section generation. There are some differences between nuclear data processing and this tool. The major differences are as follows:

- The default torelance value of the linearization for the resonance reconstruction and the Doppler broadening is changed from 0.001 (0.1%) to 0.01 (1%) to reduce the processing time and data size.
- The maximum Doppler broadening energy is fixed at 1 MeV. In nuclear data processing, the default Doppler broadening energy is the maximum energy of the resolved resonance region.
- The “Fission+1/E+Maxwell” option which is the weighting spectrum for the multi-group cross section generation is not available in this tool.
- This tool cannot process the thermal scattering law data. The user has to prepare the PENDF file or the ACE file to output the cross section of thermal scattering law data.

1.9.1 Sample Input Data to Output Continuous Energy Cross Section Data from an ENDF Formatted File

The sample input to output MT=1 (total), 2 (elastic), 18 (fission), and 102 (radiative capture) cross section from the ENDF formatted file is as follows:

```
plot_mode //processing mode
  nucl_file_name ( "../lib/U235.dat " )
  output_name ( "./output_xs/U235" )
  mt_list ( 1   2   18   102 )
```

In this sample input, the output data file name is “./output_xs/U235_MT.dat”.

The sample input to change the temperature is follows:

```
plot_mode //processing mode
  nucl_file_name ( "../lib/U235.dat " )
  output_name ( "./output_xs/U235" )
  temp ( 300.0 ) //Temperature [K]
  mt_list ( 1   2   18 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

This tool checks the nuclear data temperature. If the nuclear data temperature is smaller than the input temperature, it calculates Doppler broadening cross sections. This tool outputs an error message if the nuclear data temperature is larger than the input temperature,

If the user wants to output consecutive MT numbers, please use "-", *e.g.*, 18-102, 18 - 102, or 18 -102. The sample input file outputs MT=1, 2, 18, 19, 20, …, 99, 100, 101, and 102.

The default torelance value for the linearization (error option) process, *i.e.*, resonance reconstruction and Doppler broadening, is 0.01. This value is 10 times larger than the ACE file generation to reduce the processing time. The sample input to obtain a more detailed distribution., *i.e.*, to change the torelance value, is as follows:

```
plot_mode //processing mode
   nucl_file_name ( "../lib/U235.dat " )
   output_name ( "./output_xs/U235" )
   temp    300.0
   error    1.0E-3 //1 % -> 0.1 %
   mt_list ( 1    2    18 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

If the user wants to output all reaction type data, please remove the "mt_list" option as follows:

```
plot_mode //processing mode
   nucl_file_name ( "../lib/U235.dat " )
   output_name ( "./output_xs/U235" )
   temp    300.0
   error    1.0E-3 //1 % -> 0.1 %
```

1.9.2 Sample Input Data to Output Multi-Group Cross Section Data from an ENDF Formatted File

The sample input file to output multi-group cross section data from the ENDF formatted file is as follows:

```
plot_mode //processing mode
   endf_file_name ( "../lib/U235.dat " )
   output_name ( "./output_xs/U235" )
   temp            300.0
   error           1.0E-3 //1 % -> 0.1 %
```

mt_list (1 2 18 - 102) ***//MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102***
mg_structure (xmas_nea-lanl_172) ***//Identical to ign=18 in GROUPR/NJOY***
mg_weighting_spectrum (1/e) ***//Identical to iwt=3 in GROUPR/NJOY***
edit_flag("histogram")

The available multi-group cross section generation option is “mg_structure”, “mg_weighting_spectrum_data”, “mg_weighting_spectrum_data_int”, and “mg_weighting_spectrum_mode”. Note that “Fission+1/E+Maxwell” option cannot be used in this function.

The sample input file to output the non-histogram cross section data, *i.e.*, to change the “edit_flag” option from “histogram” to “non-histogram”, is as follows:

plot_mode ***//processing mode***
endf_file_name ("../lib/U235.dat ")
output_name ("./output_xs/U235")
temp 300.0
error 1.0E-3 ***//1 % -> 0.1 %***
mt_list (1 2 18 - 102) ***//MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102***
mg_structure (xmas_nea-lanl_172) ***//Identical to ign=18 in GROUPR/NJOY***
mg_weighting_spectrum (1/e) ***//Identical to iwt=3 in GROUPR/NJOY***
edit_flag("non-histogram")

The difference between histogram and non-histogram is shown in Fig. 1.2.2.

1.9.3 Sample Input Data to Output Continuous Energy Cross Section Data from an ACE Formatted File

The sample input file to output continuous energy cross section data from the ACE formatted file is as follows:

plot_mode ***//processing mode***
ace_file_name ("../ace/U235.ace")
output_name ("./output_xs/U235")
temp (300.0)
mt_list (1 2 18 - 102) ***//MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102***

This tool outputs the specified temperature data using the Doppler broadening calculation.

This tool treats the thermal scattering law data. The sample input files to output the thermal scattering law data are as follows:

plot_mode ***//processing mode***
ace_file_name ("../ace/HinH2O.ace ")
output_name ("./output_xs/HinH2O")

plot_mode ***//processing mode***
ace_file_name_tsl ("../ace/HinH2O.ace ")
output_name ("./output_xs/HinH2O")

Note that the Doppler broadening calculation is not carried out when the user selects the thermal scattering law data. As described in Section 1.9, this tool cannot process the thermal scattering law data. The user has to prepare the PENDF file or the ACE file to output the cross section of thermal scattering law data.

1.9.4 Sample Input Data to Output Multi-Group Cross Section Data from an ACE Formatted File

The sample input file to output multi-group cross section file from the ACE formatted file is as follows:

plot_mode ***//processing mode***
endf_file_name ("../lib/U235.dat ")
output_name ("./output_xs/U235")
temp 300.0
error 1.0E-3 ***//1 % -> 0.1 %***
mt_list (1 2 18 - 102) ***//MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102***
mg_structure (xmas_nea-lanl_172) ***//Identical to ign=18 in GROUPR/NJOY***
mg_weighting_spectrum (1/e) ***//Identical to iwt=3 in GROUPR/NJOY***
edit_flag("histogram")

The sample input file to output the multi-group cross section of thermal scattering law data is as follows:

plot_mode ***//processing mode***
ace_file_name ("../ace/HinH2O.ace ")

```
  output_name ( "./output_xs/HinH2O" )
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )        //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )
```

1.9.5 Sample Input Data to Output Multi-Group Data from a GENDF Formatted File

The sample input file to output multi-group cross section file from the GENDF formatted file is as follows:

```
plot_mode //processing mode
  gendf_file_name ( "../gendf/U235.gendf" )
  output_name ( "./output_xs/U235" )
  mf_list ( 3    6 )
  mt_list ( 1    2    18 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
  edit_flag(    histogram    )
```

1.9.6 Sample Input Data to Output Comparison Results of Continuous Energy Cross Section Data from ENDF/ACE Formatted Files

The sample input file to compare the ENDF formatted files is as follows:

```
plot_mode //processing mode
  endf_file_name ( "../lib/U235.dat"
                   "../pendf/U235.pendf" )
                   //Reference      : ../lib/U235.dat
                   //Comparison : ../pendf/U235.pendf
                   //Relative difference : (comp – ref) / ref
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1    2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

The sample input file to compare the ENDF and the ACE formatted files is as follows:

```
plot_mode //processing mode
  endf_file_name ( "../lib/U235.dat" )    //Reference
  ace_file_name ( "../ace/U235.ace" )    //Comparison
                   //Relative difference : (comp – ref) / ref
```

```
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1    2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

The sample input file to compare the ACE formatted files is as follows:

```
plot_mode //processing mode
  ace_file_name ( "../ace/U235_J40.ace"
                  "../ace/U235_J50.ace" )
                  //Reference     : ../ace/U235_J40.ace
                  //Comparison : ../ace/U235_J50.ace
                  //Relative difference : (comp – ref) / ref
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1    2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
```

The sample input files to compare the thermal scattering law data are as follows:

```
plot_mode //processing mode
  ace_file_name ( "../ace/HinH2O_J40.ace"    "../ace_HinH2O_J50.ace" )
                  //Reference     : ../ace/HinH2O_J40.ace
                  //Comparison : ../ace/HinH2O_J50.ace
                  //Relative difference : (comp – ref) / ref
  output_name ( "./comp/HinH2O_comp" )

plot_mode //processing mode
  nucl_file_name ( "../pendf/HinH2O_J40.pendf")
  ace_file_name (    "../ace_HinH2O_J50.ace" )
                  //Reference     : ../pendf/HinH2O_J40.pendf
                  //Comparison : ../ace/HinH2O_J50.ace
                  //Relative difference : (comp – ref) / ref
  output_name ( "./comp/HinH2O_comp" )
```

1.9.7 Sample Input Data to Output Comparison Results of Multi-Group Cross Section Data from ENDF/ACE Formatted Files

The sample input file to compare the ENDF formatted files is as follows:

```
plot_mode //processing mode
  endf_file_name ( "../lib/U235.dat"
                   "../pendf/U235.pendf" )
                   //Reference     : ../lib/U235.dat
                   //Comparison : ../pendf/U235.pendf
                   //Relative difference : (comp – ref) / ref
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1   2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )       //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )
```

The sample input file to compare the ENDF and the ACE formatted files is as follows:

```
plot_mode //processing mode
  endf_file_name ( "../lib/U235.dat" )   //Reference
  ace_file_name ( "../ace/U235.ace" )   //Comparison
                   //Relative difference : (comp – ref) / ref
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1   2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )       //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )
```

The sample input file to compare the ACE formatted files is as follows:

```
plot_mode //processing mode
  ace_file_name ( "../ace/U235_J40.ace"
                   "../ace/U235_J50.ace" )
                   //Reference     : ../ace/U235_J40.ace
```

```
                    //Comparison : ../ace/U235_J50.ace
                    //Relative difference : (comp – ref) / ref
  output_name ( "./comp/U235_comp" )
  temp ( 300.0 )
  mt_list ( 1    2 - 102 ) //MT=1, 2, 18, 19, 20, ..., 99, 100, 101, and 102
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )       //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )
```

The sample input files to compare the thermal scattering law data are as follows:

```
plot_mode //processing mode
  ace_file_name ( "../ace/HinH2O_J40.ace"    "../ace_HinH2O_J50.ace" )
                    //Reference     : ../ace/HinH2O_J40.ace
                    //Comparison : ../ace/HinH2O_J50.ace
                    //Relative difference : (comp – ref) / ref
  output_name ( "./comp/HinH2O_comp" )
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )       //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )

plot_mode //processing mode
  nucl_file_name ( "../pendf/HinH2O_J40.pendf")
  ace_file_name (    "../ace_HinH2O_J50.ace" )
                    //Reference     : ../pendf/HinH2O_J40.pendf
                    //Comparison : ../ace/HinH2O_J50.ace
                    //Relative difference : (comp – ref) / ref
  output_name ( "./comp/HinH2O_comp" )
  mg_structure ( xmas_nea-lanl_172 ) //Identical to ign=18 in GROUPR/NJOY
  mg_weighting_spectrum ( 1/e )       //Identical to iwt=3 in GROUPR/NJOY
  edit_flag( "histogram" )
```

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, a 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.

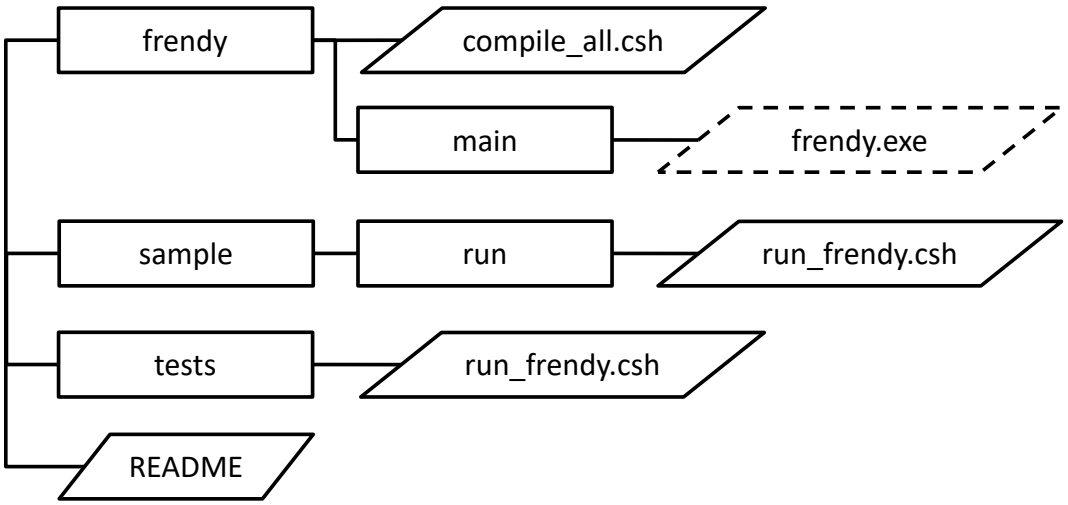

Figure 2.1 Directory structure of FRENDY

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

frendy.exe "input file name"

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

2.4 Test Calculation with Samples

The sample input files are located in the "sample/input" directory. The sample input files which are listed in this manual in Sec. 10 are used as the sample calculations. All nuclides and thermal scattering law data are copied from JENDL-4.0. The "run_all.csh" shell script in the "sample/run" directory automatically runs all the sample input files.

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 Visual Studio 2019

This section shows the installation of FRENDY using Visual Studio 2019. The author strongly recommends using the Windows Subsystem for Linux to compile FRENDY since the installation of FRENDY using Visual Studio 2019 is difficult. The installation of FRENDY using Windows Subsystem for Linux is explained in "FRENDY installation" on the web page of the 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 Visual Studio 2019.
11. Select "ALL_BUILD" in the solution explorer and run debug and release.
12. Select "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 a 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_frrendy.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_frendy.bat
```

(2) run_frendy.bat

```
set EXE=frendy.exe
rem set EXE= frendy.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=xsdir_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%
```