

# Manual of FRENDY Parallel

## 1. Overview of FRENDY Parallel

FRENDY Parallel is a multitasking tool that automatically generates cross section files from ENDF-6 formatted files or ACE formatted files. The main characteristics of FRENDY Parallel are as follows:

- It generates a large number of ACE files or multi-group cross section files (GENDF and MATXS formatted files) using FRENDY from a simple input file and FRENDY input templates.
- It uses FRENDY internally or executable files to process nuclear data files. If this tool uses FRENDY internally, users do not need to set the executable file name. In this case, all processing will stop if an unexpected abnormal termination occurs during the nuclear data processing.
- It supports parallel processing using OpenMP. The number of parallel processes can be set by the input file.
- It outputs a list of nuclear data file names for which processing has not been completed to make it easier to check which nuclides have stopped. It has a restart mode. It checks the log file and only processes the nuclear data files that have not been completed if restart mode is used.
- Same to FRENDY, it accepts comment lines. The C++ style comments are available, *i.e.*, “//” for a single-line comment and “/\* ... \*/” for multi-line comments.

## 2. Input parameters

The available input parameters are as follows:

<TEMP>	Temperature data list
<BG_XS>	Background cross section data list
<FRENDY_INPUT>	FRENDY input file template
<ENDF_DIR>	ENDF file directory (neutron-induced file)
<ACE_DIR>	ACE file directory (neutron-induced file) (option)
<TSL_DIR>	ENDF of ACE file directory (TSL: thermal scattering law data)
<OUT_DIR>	Generated FRENDY input file and log file directories
<OUT_DIR_ACE>	Generated ACE file directory (option)

<OUT_DIR_MG>	Generated multi-group cross section file directory (option)
<FRENDY_EXE>	FRENDY executable file name (option)
<RESTART>	Restart option (option)
<THREAD_NO>	Number of parallels (option)
<INP_LIST>	Input data list

This tool can treat the above input parameter in either uppercase or lowercase and either hyphen “-” or underscore “\_”. For example, <OUT\_MG>, <out-mg>, <out-MG>, and <Out\_mG> are the same in this tool.

### <TEMP>

**Data type:** string (case name) vector<Real> temperature [K]

**Default value:** None

This parameter sets the temperature data list. Users have to set temperature case names, such as “DEFAULT”, “TEMP1”, and “TEMP-TSL01”, and temperature [K].

#### Sample of this parameter

```
<TEMP_SET> //Temperature set
  DEFAULT 293 600 900 1200 1500
  TEMP1   293 400 450 500 550 600 650
  TEMP2   293 450 600 750 900 1050 1200 1350 1500
  TEMP3   293
```

### <BG\_XS>

**Data type:** string (case name) vector<string> background cross section

**Default value:** None

This parameter sets the background cross section data list. This tool simply copies one line after the background cross section name to the FRENDY input parameter “sigma\_zero\_data”. Users can set all data formats available in “sigma\_zero\_data”.

#### Sample of this parameter

```
<BGXS_SET> //Background cross section data set
  DEFAULT auto
  BGXS1    1.0e+10 1.0e+4 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 1.0e+0 1.0e-1 1.0e-5
```

BGXS2 1.0e+10

### <FRENDY\_INPUT>

**Data type:** string (case name) string (FRENDY input template file name)

**Default value:** None

This parameter sets the FRENDY input template file name. This tool automatically generates some input parameters, such as temperature, background cross section options, and output file name. However, the other input parameters, such as processing mode, energy group structure, and weighting function, are required to generate cross section files. Users have to prepare input template files and set file names (absolute or relative path).

#### Sample of this parameter

```
<FRENDY_INPUT > //FRENDY input template
  DEFAULT  FRENDY_inp_template_def.txt
  FRENDY1  FRENDY_inp_template_01.txt
  FRENDY2  FRENDY_inp_template_02.txt
```

### <ENDF\_DIR>

**Data type:** string (directory name)

**Default value:** None

This parameter sets the neutron-induced ENDF-6 formatted nuclear data file directory. The nuclear data file name is “directory name/nuclear data file name”. The “nuclear data file name” is set in the <INP\_LIST> parameter. If users want to generate multi-group cross section files from the ACE file, users must not use this parameter and use <ACE\_DIR>.

This tool does not consider whether the directory separator “/” is found at the end of the directory. This tool removes the directory separator if the last character is “/”. For example, “/home/data/nucl/jendl/JENDL-5” and “/home/data/nucl/jendl/JENDL-5/” are the same in this tool.

#### Sample of this parameter

```
<ENDF_DIR> //ENDF file directory (neutron-induced)
/home/data/nucl/jendl/JENDL-5
```

### <ACE\_DIR>

**Data type:** string (directory name)

**Default value:** None

This parameter sets the neutron-induced ACE file directory to generate multi-group cross section files. The ACE file name is “directory name/ACE file name”. The “ACE file name” is set in the <INP\_LIST> parameter. If users want to generate multi-group cross section files from the ENDF-6 formatted file, users must not use this parameter and use <ENDF\_DIR>.

**Sample of this parameter**

```
<ACE_DIR> //ACE file directory (neutron-induced)
/home/data/ace/jendl/JENDL-5
```

**<TSL\_DIR>**

**Data type:** string (directory name)

**Default value:** None

This parameter sets the thermal scattering law (TSL) data file directory. The nuclear data file name is “directory name/thermal scattering law data file name”. The “thermal scattering law data file name” is set in the <INP\_LIST> parameter. If users use <ENDF\_DIR> for the neutron-induced directory name, users have to set the ENDF-6 formatted TSL data file directory. If users use <ACE\_DIR>, users have to set the ACE formatted TSL data file directory.

**Sample of this parameter**

```
<TSL_DIR> //ENDF file directory (TSL data)
/home/ data/nucl/jendl/JENDL-5_sab
```

**<OUT\_DIR>**

**Data type:** string (FRENDY input file directory name) string (FRENDY log file directory)

**Default value:** None

This parameter sets the input file directory and the log file directory of FRENDY. The former string data is set as the input file directory and the latter string data is set as the log file directory. Users have to make these directories before processing.

**Sample of this parameter**

```
<OUT_DIR> //Output directory.
/home/data/proc/out/frendy_inp //FRENDY input file directory
```

/home/data/proc/out/frendy\_log //FRENDY log file directory

### <OUT\_DIR\_ACE>

**Data type:** string (Generated ACE file directory name)

**Default value:** None

This parameter sets the generated ACE directory. If users set this parameter in the multi-group cross section file generation, this tool outputs ACE and multi-group cross section files. Users have to make these directories before processing.

#### Sample of this parameter

```
<OUT_DIR_ACE> //ACE file directory
/home/data/proc/out/ace
```

### <OUT\_DIR\_MG>

**Data type:** string (Generated multi-group cross section file directory name)

**Default value:** None

This parameter sets the generated multi-group cross section directory. Even if users want to generate GENDF and MATXS files, users only set one directory name. This tool copies GENDF and MATXS files in this directory. Users have to make these directories before processing.

#### Sample of this parameter

```
<OUT_DIR_MG> //Multi-group cross section file directory
/home/data/proc/out/mg
```

### <FRENDY\_EXE>

**Data type:** string (FRENDY executable file name)

**Default value:** None

This parameter sets the FRENDY executable file name. If users do not set this parameter, this tool internally runs FRENDY. In this case, all processing will stop if an unexpected abnormal termination occurs during the nuclear data processing.

#### Sample of this parameter

```
<FRENDY_EXE> //FRENDY executable file name
```

/home/code/frendy/main/frendy.exe

## <RESTART>

**Data type:** string (restart or no\_restart)

**Default value:** no\_restart

This parameter sets the restart option. If users select restart, this tool checks the log file and skips the process if the log file has completed all processes.

This tool confirms whether “FRENDY CALCULATION STATUS: NORMAL TERMINATION” is found in the log file or not. If the above words are found in the log file, it considers the process complete.

### Sample of this parameter

```
<RESTART> //Restart option
restart //restart or no_restart
```

## <THREAD\_NO>

**Data type:** Real (number of parallels)

**Default value:** 1

This parameter sets the number of threads for cross section file generation. If the number of threads is zero, minus, or larger than the number of processes, this parameter is changed to the number of processes.

### Sample of this parameter

```
<THREAD_NO> //Number of threads
30
```

## <INP\_LIST>

### Data type

#### For neutron-induced data

string (neutron-induced file name) string (temp case) string (Background (BG) cross section (XS) case) string (template case)

#### For TSL data

string (neutron-induced file name) string (TSL file name) string (TSL type) string (temp case) string (BG XS case) string (template case)

**Default value:** None

This parameter sets the processing conditions for each nuclide, i.e., nuclear data file name, temperature data case name set by the <TEMP> parameter, background cross section case name set by the <BGXS> parameter, and FRENDY input template case name set by the <FRENDY\_INPUT> parameter. If users want to generate TSL data, users have to set the TSL data file name and TSL data type before the temperature data case name. This tool distinguishes the processing data type, i.e., neutron-induced or TSL, by the second data name. If the second data is the TSL data file name, this tool recognizes that this line is thermal scattering law data processing.

Though the TSL data type is only used in the MATXS generation, this parameter is required for all processing cases. The typical TSL data types are listed in “mg\_tsl\_data\_type” in the FRENDY input manual. If users do not want to generate MATXS files, i.e., they want to generate ACE and/or GENDF files, the recommended TSL data type is “free”.

Each nuclide information should be set in one line. If the users omit the temperature case name, background cross section case name, or input template case name, this tool automatically sets the first case.

“ALL” in the temperature case name is only used for processing the thermal scattering law data. If users set “ALL” as the temperature case name, it processes the nuclear data file in all temperatures listed in the thermal scattering law data.

### Sample of this parameter

<INP\_LIST>

//If users skipped data, the first value was used.

//ENDF file name, Temp, BG XS, input template

n\_001-H-001.dat DEFAULT DEFAULT DEFAULT

n\_001-H-002.dat TEMP1 BGXS1 RENDY1

n\_001-H-003.dat TEMP2 BGXS2

n\_002-He-003.dat

//ENDF file name, TSL file name, TSL type, Temp, BG XS, input template

n\_001-H-001.dat tsl\_HinH2O.dat hh2o TEMP2 BGXS2 DEFAULT

n\_001-H-001.dat tsl\_HinZrH.dat hzrh TEMP2 BGXS2 DEFAULT

n\_001-H-002.dat tsl\_DinD2O.dat dd2o ALL BGXS2 FRENDY1

### 3. Sample inputs of FRENDY parallel

#### 3.1. Multi-group cross section generation from ENDF-6 formatted files

```
<TEMP_SET>    //Temperature set
  DEFAULT  293  600  900  1200  1500
  TEMP2    293  400  450  500  550  600  650
  TEMP3    293  450  600  750  900  1050  1200  1350  1500
  TEMP4    293

<BGXS_SET>    //Background cross section data set
  DEFAULT  auto
  BGXS1    1.0e+10 1.0e+4 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 1.0e+0 1.0e-1 1.0e-5
  BGXS2    1.0e+10

<FRENDY_INPUT> //FRENDY input template
  DEFAULT  FRENDY_inp_template_def.txt
  FRENDY1  FRENDY_inp_template_01.txt
  FRENDY2  FRENDY_inp_template_02.txt

<ENDF_DIR>    //ENDF file directory (neutron induced)
  /home/data/nucl/jendl/JENDL-5

<TSL_DIR>    //ENDF file directory (TSL data)
  /home/data/nucl/jendl/JENDL-5_sab

<OUT_DIR>    //Output directory.
//Users must make these directories before processing.
  /home/data/proc/out/frendy_inp //FRENDY input file directory
  /home/data/proc/out/frendy_log //FRENDY log file directory

<OUT_DIR_ACE> //ACE file directory
  /home/data/proc/out/ace

<OUT_DIR_MG> //Multi-group cross section file directory
```

/home/data/proc/out/mg

<FRENDY\_EXE> //FRENDY executable file name

/home/code/frendy/main/frendy.exe

<RESTART> //Restart option

restart //restart or no\_restart

<THREAD\_NO> //Number of threads

30

<INP\_LIST>

//If users skipped data, the first value was used.

//ENDF file name, Temp, BG XS, input template

n\_001-H-001.dat DEFAULT DEFAULT DEFAULT

n\_001-H-002.dat TEMP1 BGXS1 FRENDY1

n\_001-H-003.dat TEMP2 BGXS2

n\_002-He-003.dat

//ENDF file name, TSL file name, TSL type, Temp, BG XS, input template

n\_001-H-001.dat tsl\_HinH2O.dat hh2o TEMP2 BGXS2 DEFAULT

n\_001-H-001.dat tsl\_HinZrH.dat hzrh TEMP2 BGXS2 DEFAULT

n\_001-H-002.dat tsl\_DinD2O.dat dd2o ALL BGXS2 FRENDY1

### 3.2. Multi-group cross section generation from ACE files

<TEMP\_SET> //Temperature set

DEFAULT 293 600 900 1200 1500

TEMP2 293 400 450 500 550 600 650

TEMP3 293 450 600 750 900 1050 1200 1350 1500

TEMP4 293

<BGXS\_SET> //Background cross section data set

DEFAULT auto

BGXS1 1.0e+10 1.0e+4 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 1.0e+0 1.0e-1 1.0e-5

BGXS2 1.0e+10

```

<FRENDY_INPUT> //FRENDY input template
  DEFAULT   FRENDY_inp_template_def.txt
  FRENDY1   FRENDY_inp_template_01.txt
  FRENDY2   FRENDY_inp_template_02.txt

<ACE_DIR>      //ACE file directory (neutron induced)
  /home/data/ace/jendl/JENDL-5

<TSL_DIR>      //ENDF file directory (TSL data)
  /home/data/nucl/jendl/JENDL-5_sab

<OUT_DIR>     //Output directory.
//Users must make these directories before processing.
  /home/data/proc/out/frendy_inp //FRENDY input file directory
  /home/data/proc/out/frendy_log //FRENDY log file directory

<OUT_DIR_MG>  //Multi-group cross section file directory
  /home/data/proc/out/mg

<FRENDY_EXE>  //FRENDY executable file name
  /home/code/frendy/main/frendy.exe

<RESTART>     //Restart option
  no_restart  //restart or no_restart

<THREAD_NO>   //Number of threads
  30

<INP_LIST>
  //If users skipped data, the first value was used.
  //ACE file name, Temp, BG XS, input template
  n_001-H-001.ace  DEFAULT  DEFAULT  DEFAULT
  n_001-H-002.ace  TEMP1    BGXS1   FRENDY1
  n_001-H-003.ace  TEMP2    BGXS2
  n_002-He-003.ace

```

//ACE file name,	TSL file name,	TSL type,	Temp,	BG XS,	input template
n_001-H-001.ace	tsl_HinH2O.ace	hh2o	TEMP2	BGXS2	DEFAULT
n_001-H-001.ace	tsl_HinZrH.ace	hzrh	TEMP2	BGXS2	DEFAULT
n_001-H-002.ace	tsl_DinD2O.ace	dd2o	ALL	BGXS2	FRENDY1

### 3.3. ACE file generation from ENDF-6 formatted files

```

<TEMP_SET>    //Temperature set
  DEFAULT  293  600  900  1200  1500
  TEMP2    293  400  450  500  550  600  650
  TEMP3    293  450  600  750  900  1050  1200  1350  1500
  TEMP4    293

<BGXS_SET>    //Background cross section data set
  DEFAULT  auto
  BGXS1    1.0e+10 1.0e+4 1.0e+3 3.0e+2 1.0e+2 3.0e+1 1.0e+1 1.0e+0 1.0e-1 1.0e-5
  BGXS2    1.0e+10

<FRENDY_INPUT> //FRENDY input template
  DEFAULT  FRENDY_inp_template_def.txt
  FRENDY1  FRENDY_inp_template_01.txt
  FRENDY2  FRENDY_inp_template_02.txt

<ENDF_DIR>    //ENDF file directory (neutron induced)
  /home/data/nucl/jendl/JENDL-5

<TSL_DIR>    //ENDF file directory (TSL data)
  /home/data/nucl/jendl/JENDL-5_sab

<OUT_DIR>    //Output directory.
//Users must make these directories before processing.
  /home/data/proc/out/frendy_inp //FRENDY input file directory
  /home/data/proc/out/frendy_log //FRENDY log file directory

<OUT_DIR_ACE> //ACE file directory
  /home/data/proc/out/ace

```

<FRENDY\_EXE> //FRENDY executable file name  
/home/code/frendy/main/frendy.exe

<RESTART> //Restart option  
restart //restart or no\_restart

<THREAD\_NO> //Number of threads  
30

<INP\_LIST>

//If users skipped data, the first value was used.

//ENDF file name,	Temp,	BG XS,	input template
n_001-H-001.dat	DEFAULT	DEFAULT	DEFAULT
n_001-H-002.dat	TEMP1	BGXS1	FRENDY1
n_001-H-003.dat	TEMP2	BGXS2	
n_002-He-003.dat			

//ENDF file name,	TSL file name,	TSL type,	Temp,	BG XS,	input template
n_001-H-001.dat	tsl_HinH2O.dat	hh2o	ALL	BGXS2	DEFAULT
n_001-H-001.dat	tsl_HinZrH.dat	hzrh	ALL	BGXS2	DEFAULT
n_001-H-002.dat	tsl_DinD2O.dat	dd2o	ALL	BGXS2	FRENDY1

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## **4. Sample inputs of FRENDY input templates**

### **4.1. Multi-group cross section generation (1)**

```
mg_neutron_mode
mg_structure          ( xmas_nea-lanl_172 )
mg_weighting_spectrum ( fission+1/e+maxwell )
```

### **4.2. Multi-group cross section generation (2)**

```
mg_neutron_mode
mg_structure ( xmas_nea-lanl_172 )
mg_weighting_spectrum ( fission+1/e+maxwell )
max_thermal_ene      30.0
max_thermal_ene_e_out 40.0
```

### **4.3. ACE file generation (neutron-induced)**

```
ace_fast_mode
```

### **4.4. ACE file generation (TSL)**

```
ace_tsl_mode
```

## **5. Installation of FRENDY Parallel**

To generate the executable file (tools/frendy\_parallel/frendy\_parallel.exe), run “compile\_all.csh” in the “tools” directory or run the make command in the “tools/frendy\_parallel” directory. This tool uses all object files in FRENDY since it calls FRENDY internally. If users do not generate the FRENDY executable file in the “frendy/main” directory, it will take a long time to compile all object files in the “frendy” directory.