

# FRENDY exercise

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[https://rpg.jaea.go.jp/main/en/program\\_frendy/index.html](https://rpg.jaea.go.jp/main/en/program_frendy/index.html)

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# Installation of additional tools for FRENDY exercise

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# Installation environment

- Ubuntu (Ubuntu 20.04.1 LTS) on WSL
  - WSL: Windows subsystem for Linux
- **Green letters** mean Ubuntu command.
- **Please ask the administrator before installing these tools.**

# Installation of gnuplot

- FRENDY exercise plots figures using gnuplot to compare the processing results (XS data)
- Installation of gnuplot
  - `sudo apt-get install gnuplot`
  - Wait about 10 minutes.
    - For CentOS: `sudo yum install gnuplot`
- Try to run the following command if gnuplot does not plot figures and shows the following warning message.
  - Warning message
    - gnuplot: error while loading shared libraries: libQt5Core.so.5: cannot open shared object file: No such file or directory
  - Command to resolve this problem
    - `sudo strip --remove-section=.note.ABI-tag /usr/lib/x86_64-linux-gnu/libQt5Core.so.5`

# Installation of NJOY2016 (1/2)

- FRENDY exercise uses NJOY2016 to compare the processing results.
- NJOY2016 compilation requires Cmake.
  - gcc version 7, gfortran, and python are also required
    - Default gcc version of CentOS may not compile NJOY2016.
    - In this case, devtoolset should be used to install higher version of gcc.
      - 1) `sudo yum install centos-release-scl`
      - 2) `sudo yum install devtoolset-9`
      - 3) `scl enable devtoolset-9 bash`
  - Installation of CMake
    - `sudo apt-get install cmake`
      - Please install CMake3 when CMake cannot generate make file of NJOY2016.
        - `sudo apt-get install cmake3`
- Get NJOY2016 from github
  - `git clone` <https://github.com/njoy/NJOY2016.git>
  - Installation of Git is required if git command is not available.
    - `sudo apt-get install git`

# Installation of NJOY2016 (2/2)

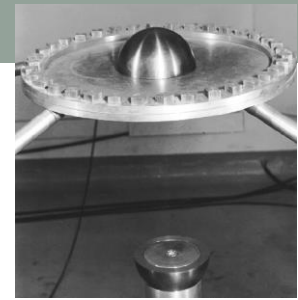
- Compilation of NJOY
  - `cd NJOY2016` (Move to cloned “NJOY2016” directory.)
  - `mkdir bin` (Make “bin” directory.)
  - `cd bin` (Move to “bin” directory)
  - `cmake ../` (Run CMake in “bin” directory)
    - Please use CMake3 when CMake cannot generate make file of NJOY2016.
      - `cmake3 ../`
    - Linux OS may not have f95 and make file of NJOY2016 may not be generated.
    - User has to set up a link to f95.
      - `ln -s /usr/bin/gfortran /usr/bin/f95`
    - For CentOS using devtoolset (Please change version number of devtoolset.)
      - `ln -s /opt/rh/devtoolset-9/root/usr/bin/gfortran /opt/rh/devtoolset-9/root/usr/bin/f95`
  - `make` (Compile NJOY2016)
  - Executable file of NJOY2016 (njoy) in “bin” directory
- References for NJOY2016 compilation
  - <https://github.com/njoy/NJOY2016>
  - <http://www.njoy21.io/Build/index.html>

# Overview of FRENDY exercise

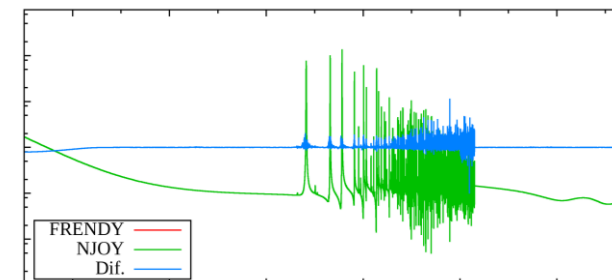
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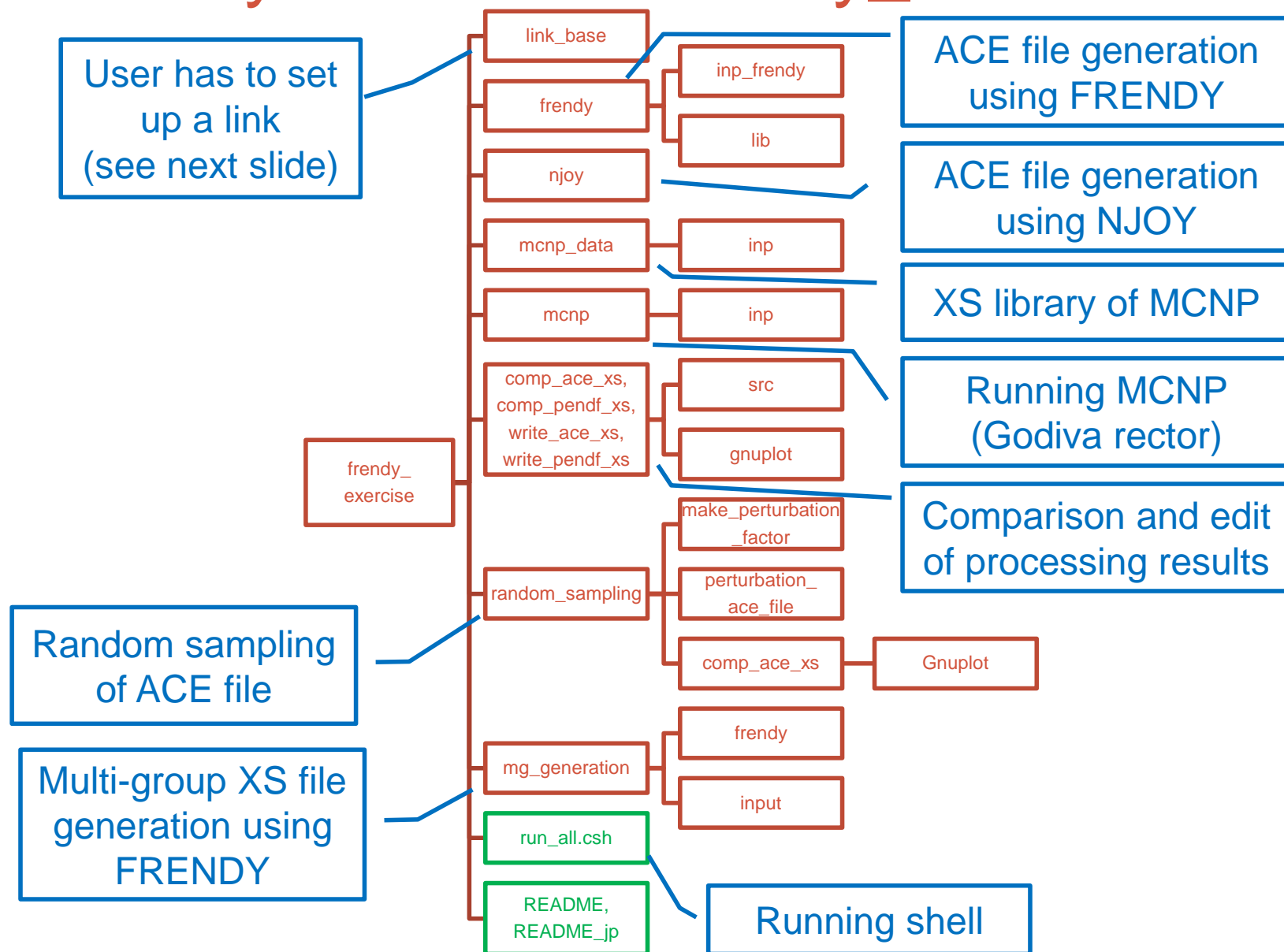
# Content of exercise



- Calculation of Godiva reactor (HMF-001) using MCNP
  - ACE file generation using FRENDY and NJOY2016
    - U-235, U-238, O-16, and N-14
      - U-234 is removed to reduce processing time.
    - HinH2O is also processed for reference case of TSL data processing.
  - Generation of XS library for MCNP calculation using above ACE files
- Application example of FRENDY's modules
  - Comparison and edit of XS using FRENDY modules
    - Plotting comparison results using gnuplot
  - Perturbation of ACE file
    - Random sampling of ACE file
- Total calculation time: about 2 hours



# Directory structure of frendy\_exercise



# Preparation of exercise (1/2)

- FRENDY exercise uses FRENDY, NJOY2016, and MCNP
- User has to set up a link at “frendy\_exercise/link\_base”
  - frendy\_dir
    - Top directory of FRENDY (frendy\_YYYYMMDD)
      - YYYYMMDD means release date
  - njoy
    - Executable file of NJOY2016
  - mcnp6
    - Executable file of MCNP

# Preparation of exercise (2/2)

- Compilation of FRENDY and some tools
  - Executable of FRENDY (frendy/main/frendy.exe)
    - `cd frendy/main`
    - `make`
  - Collection of ACE file tool, ACE file random sampling tool, and ACE file perturbation tool
    - `tools/make_xmdir_list/make_xmdir_list.exe`
    - `tools/make_perturbation_factor/make_perturbation_factor.exe`
    - `tools/perturbation_ace_file/perturbation_ace_file.exe`
  - `cd tools`
  - `csh ./compile_all.csh`

# ACE file generation using FRENDY

- Working directory: frendy\_exercise/frendy
  - inp\_frendy: Input files of FRENDY
    - “~.dat”: Input for FRENDY to generate ACE file
    - “~.n”: Input for FRENDY to generate NJOY input file (see next slide)
    - Input format is explained in “02.Input\_format\_of\_FRENDY”.
  - lib: Evaluated nuclear data files
  - run\_frendy.csh: Running shell
- Generated directories
  - ace: ACE files generated by FRENDY
  - pendf: PENDF files generated by FRENDY
    - After probability table generation

# NJOY input file generation using FRENDY

- Working directory: frendy\_exercise/frendy
  - inp\_frendy: input files of FRENDY
    - “~.n” is input for FRENDY to generate NJOY input file
  - lib: Evaluated nuclear data files
  - make\_njoy\_input.csh: Running shell
- Generated directory
  - inp\_njoy: Input files for NJOY

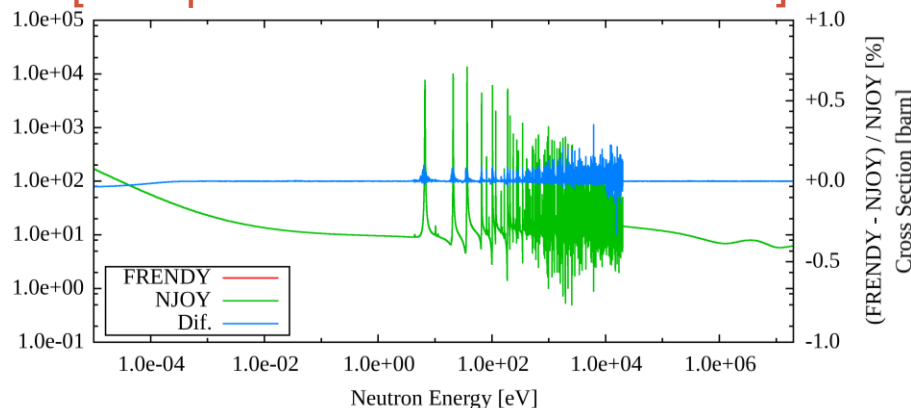
# ACE file generation using NJOY

- Working directory: frendy\_exercise/njoy
  - Input files of NJOY are generated by FRENDY
    - frendy\_exercise/frendy/inp\_njoy: Input files of NJOY
  - run\_njoy.csh: Running shell
- Generated directories
  - ace: ACE files generated by NJOY
  - pendf: PENDF files generated by NJOY
    - After probability table generation
  - out: Output files of NJOY

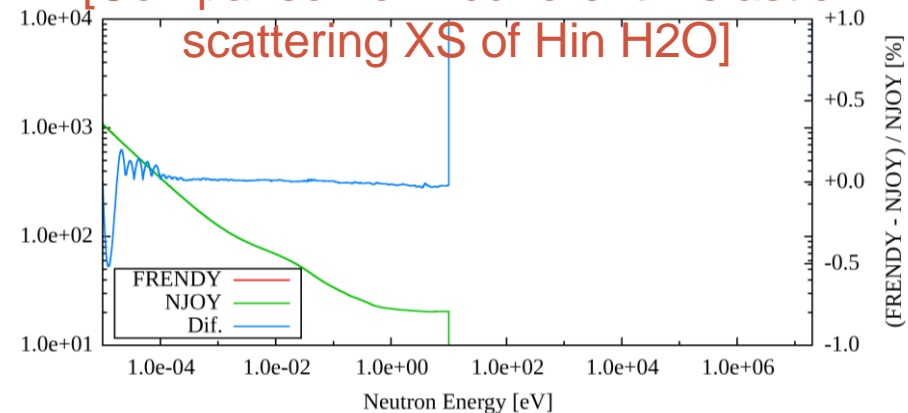
# Comparison of processing results

- Comparison of XS processed by FRENDY and NJOY
  - frendy\_exercise/comp\_ace\_xs
    - Comparison of all XS data in ACE file and plotting using gnuplot.
  - frendy\_exercise/comp\_pendf\_xs
    - Comparison of all XS data in PENDF file and plotting using gnuplot.
- Source files are set in “src” directories.
  - frendy\_exercise/comp\_ace\_xs/src,  
frendy\_exercise/comp\_pendf\_xs/src
- Running shells
  - run\_comp\_ace.csh, run\_comp\_pendf.csh

[Comparison of total XS of U-238]



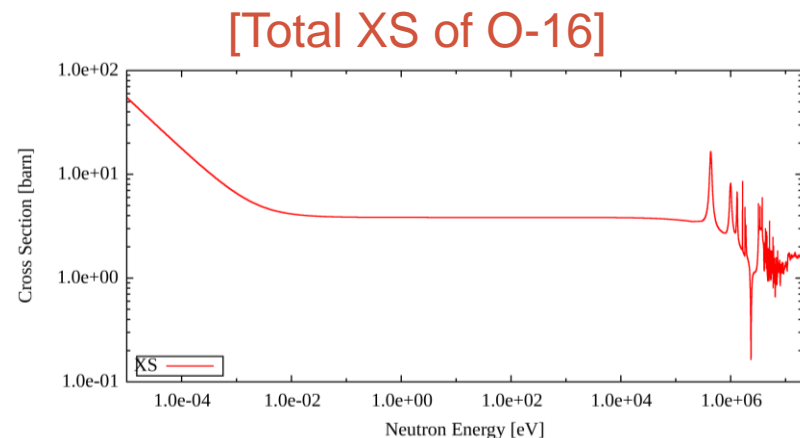
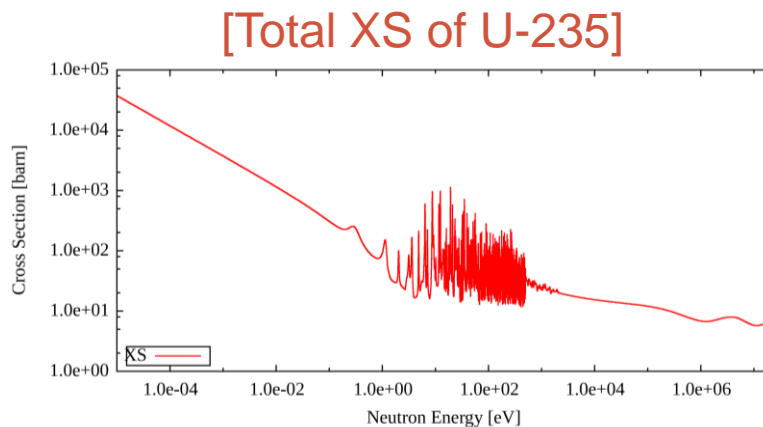
[Comparison of incoherent inelastic scattering XS of H in H2O]





# XS edit tool for ACE and PENDF files

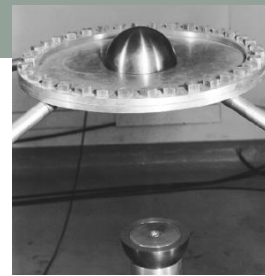
- This tool is a sample to make edit tool for ACE and ENDF files by users.
  - frendy\_exercise/write\_ace\_xs
    - Extraction of all cross sections in ACE file and plotting using gnuplot.
  - frendy\_exercise/write\_pendf\_xs
    - Extraction of all cross sections in PENDF file and plotting using gnuplot.
- Source files are set in “src” directories.
  - frendy\_exercise/write\_ace\_xs/src, frendy\_exercise/write\_pendf\_xs/src
- Running shells
  - run\_write\_ace\_xs.csh、run\_write\_pendf\_xs.csh



# Generation of XS library for MCNP

- Working directory: frendy\_exercise/mcnp\_data
  - Collect ACE files generated by FRENDY and NJOY
  - Modification of XSDIR file
    - Add atomic weight ratio and modify directory information
  - inp: input files
  - run\_ace\_data\_collector.csh: Running shell
- Generated files
  - Generated by FRENDY
    - ace\_f/j40a00fa : Collected ACE files
    - xsdir.j40a00f : XSDIR file
  - Generated by NJOY
    - ace\_n/j40a00na : Collected ACE files
    - xsdir.j40a00n : XSDIR file

# MCNP calculation (Godiva)



- Working directory: frendy\_exercise/mcnp
  - mcnp\_data: XS library for MCNP calculation
  - inp: input files
    - hmf001.i: Consideration of self-shielding effect in the unresolved resonance region using probability table
    - hmf001\_no\_ptable.i: Without probability table
  - run\_all.csh: Running shell
    - Running MCNP calculation and copying k-eff to result\_keff.log
- Generated directory
  - out: output files
    - “~\_f~.out”: Calculation result using ACE files processed by FRENDY
    - “~\_n~.out”: Calculation result using ACE files processed by NJOY

# Perturbation of ACE file

- This exercise is identical to sample in FRENDY
- Working directory:  
frendy\_exercise/random\_sampling
  - Random sampling of ACE file
    - make\_perturbation\_factor
    - Generation of perturbation factor using covariance data “1001\_MT\_102\_2.csv”.
  - Perturbation of ACE file
    - perturbation\_ace\_file
    - Perturbation factor is generated in “make\_perturbation\_factor” directory
  - Perturbed XS is compared to the original data and plotted by gnuplot

# Automatic execution of all calculations

- Running run\_all.csh in “frendy\_exercise” directory
  - `csh ./run_all.csh`
- Running remove\_all.csh in “frendy\_exercise” directory if user wants to remove all generated directories and files.
  - `csh ./remove_all.csh`
  - run\_all.csh shell runs remove\_all.csh shell before execution of all calculations to remove previous calculation results.

# Input format of FRENDY

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# Basics of FRENDY input format

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

# Main input parameters

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



# Example of FRENDY input (Neutron induced)

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

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

Relative path or  
absolute path

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

# Modification of processing conditions (Neutron induced)

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

The answer is next slide.

# Modification of processing conditions (Neutron induced)

Input is modified to meet the processing conditions.

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

Text data is surrounded by single or double quotation mark.

Adding PENDF output option

# Example of FRENDY input (TSL)

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

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

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

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

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

# Modification of processing conditions (TSL)

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

The answer is next slide.

# Modification of processing conditions (TSL)

Input is modified to meet the processing conditions.

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

Adding PENDF output option

# TSL data generation for MCNP5 and PHITS 3.24

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

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