FRENDY exercise

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https://rpg.jaea.go.jp/main/en/program_frendy/index.html

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Installation of additional tools for FRENDY exercise

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
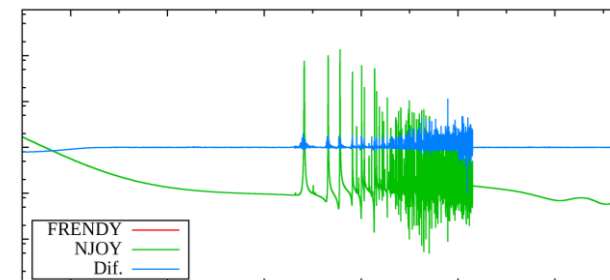 - http://www.njoy21.io/Build/index.html
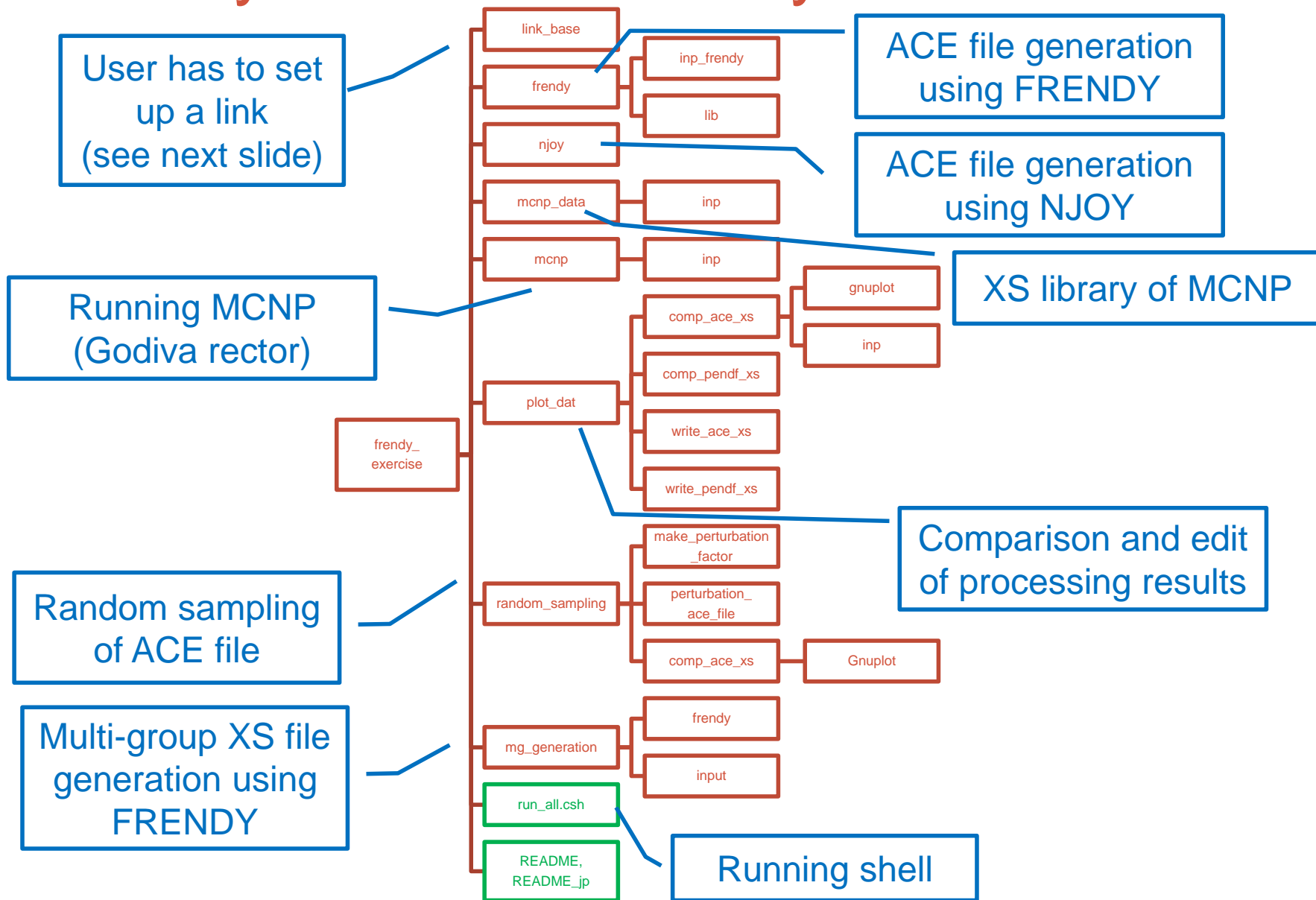
Overview of FRENDY exercise

Content of exercise
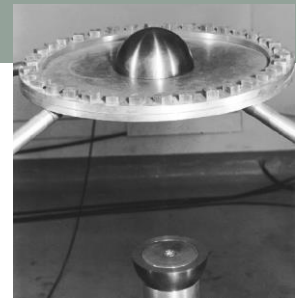
- Calculation of Godiva reactor (HMF-001) using MCNP
  - ACE file generation using FRENDY and NJOY2016
    - U-235, U-238, O-16, and N-14
      - U-234 is removed to reduce processing time.
    - HinH2O is also processed for reference case of TSL data processing.
  - Generation of XS library for MCNP 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

User has to set up a link (see next slide)

ACE file generation using FRENDY

ACE file generation using NJOY

XS library of MCNP

Running MCNP (Godiva rector)

Comparison and edit of processing results

Random sampling of ACE file

Multi-group XS file generation using FRENDY

Running shell

link_base

frendy
- inp_frendy
- lib

njoy

mcnp_data
- inp

mcnp
- inp

plot_dat
- comp_ace_xs
  - gnuplot
  - inp
- comp_pendf_xs
- write_ace_xs
- write_pendf_xs

frendy_exercise

random_sampling
- make_perturbation_factor
- perturbation_ace_file
- comp_ace_xs
  - Gnuplot

mg_generation
- frendy
- input

run_all.csh

README, README_jp

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_xsdir_list/make_xsdir_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]
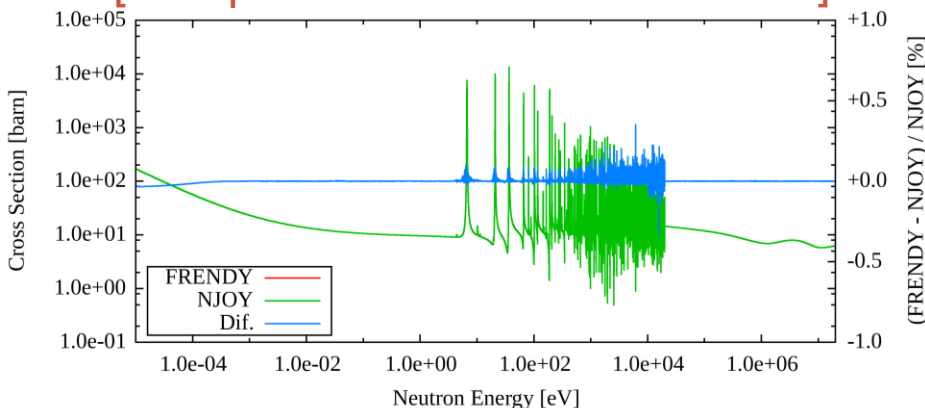
[Comparison of incoherent inelastic scattering XS of Hin H2O]
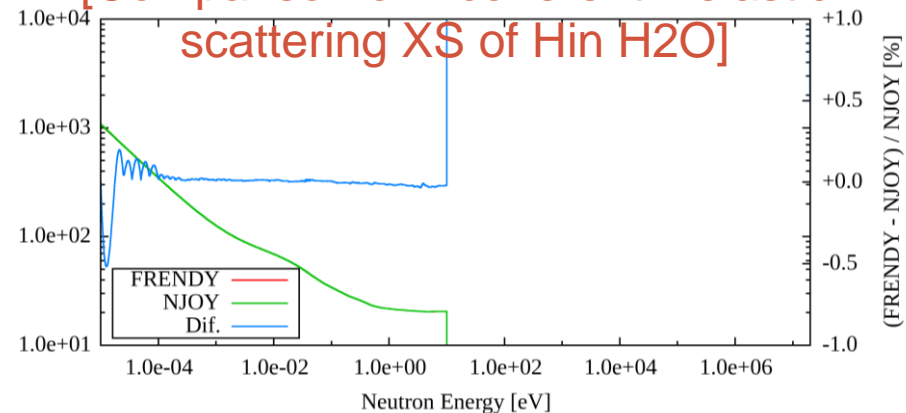
XS edit tool for ACE and PENDF files

- 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

[Total XS of U-235]

[Total XS of O-16]
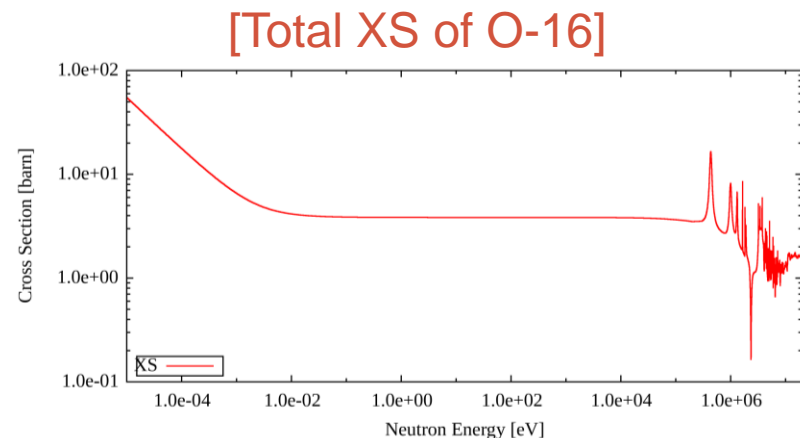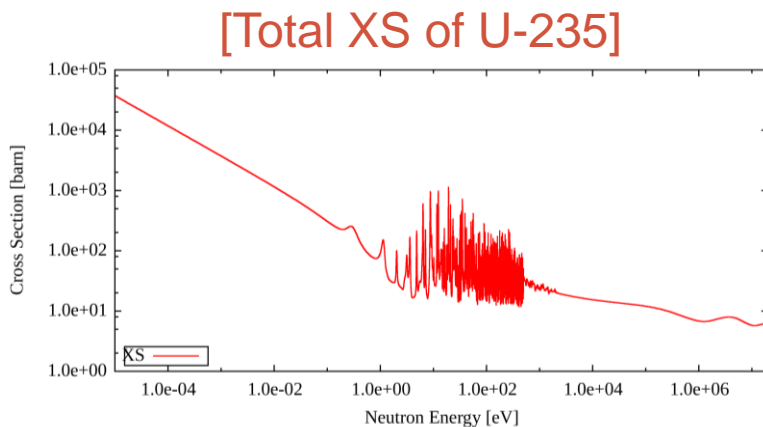
Generation of XS library for MCNP

- 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)
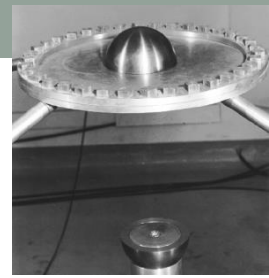
- Working directory: frendy_exercise/mcnp
  - mcnp_data: XS library for MCNP calculation
  - inp: input files
    - hmf001.i: Consideration of self-shielding effect in the unresolved resonance region using probability table
    - hmf001_no_ptable.i: Without probability table
  - run_all.csh: Running 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 befor 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_za_id_name : S(α, β) identifier of MCNP (TSL only)
- Additional parameters
  - Write_pendf_probability_table : PENDF file name after probability table generation
  - Write_pendf_tsl : PENDF file name after TSL data processing (TSL only)
    - PENDF (Point-wise ENDF) file is a processing result of NJOY.
    - These PENDF file can be used as input PENDF of NJOY.

Example of FRENDY input (Neutron induced)

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

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

> Relative path or absolute path

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

Modification of processing conditions (Neutron induced)

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

The answer is next slide.

Modification of processing conditions (Neutron induced)

Input is modified to meet the processing conditions.

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

Text data is surrounded by single or double quotation mark.

Adding PENDF output option

Example of FRENDY input (TSL)

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

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

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

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

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

Modification of processing conditions (TSL)

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

The answer is next slide.

Modification of processing conditions (TSL)

Input is modified to meet the processing conditions.

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

Adding PENDF output option

TSL data generation for MCNP5 and PHITS 3.24

- Three types of ACE format is now available.

  - IFENG=0 (discrete), 1 (skewed), 2 (continuous)

- MCNP5 and PHITS ver.3.24 cannot treat IFENG=2.

  - The default input option of FRENDY version 2 generates IFENG=2.

  - Please add "weight_option" and modify parameter from "tabulated" to "variable".

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