FRENDY exercise

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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

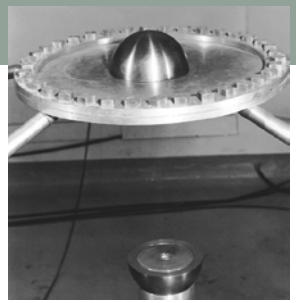
Installation of NJOY2016 (1/2)

- 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)

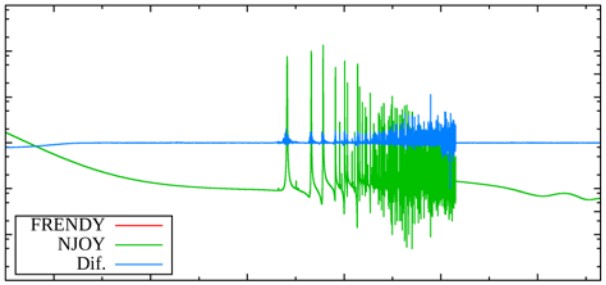
- Compilation of NJOY
  - cd NJOY2016 (Move to cloned “NJOY2016” directory.)
  - Mkdir bin (Make “bin” directory.)
  - cd bin (Move to “bin” directory)
  - cmake ../ (Run CMake in “bin” directory)
    - Please use CMake3 when CMake cannot generate make file of NJOY2016.
      - cmake3 ../
    - Linux 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

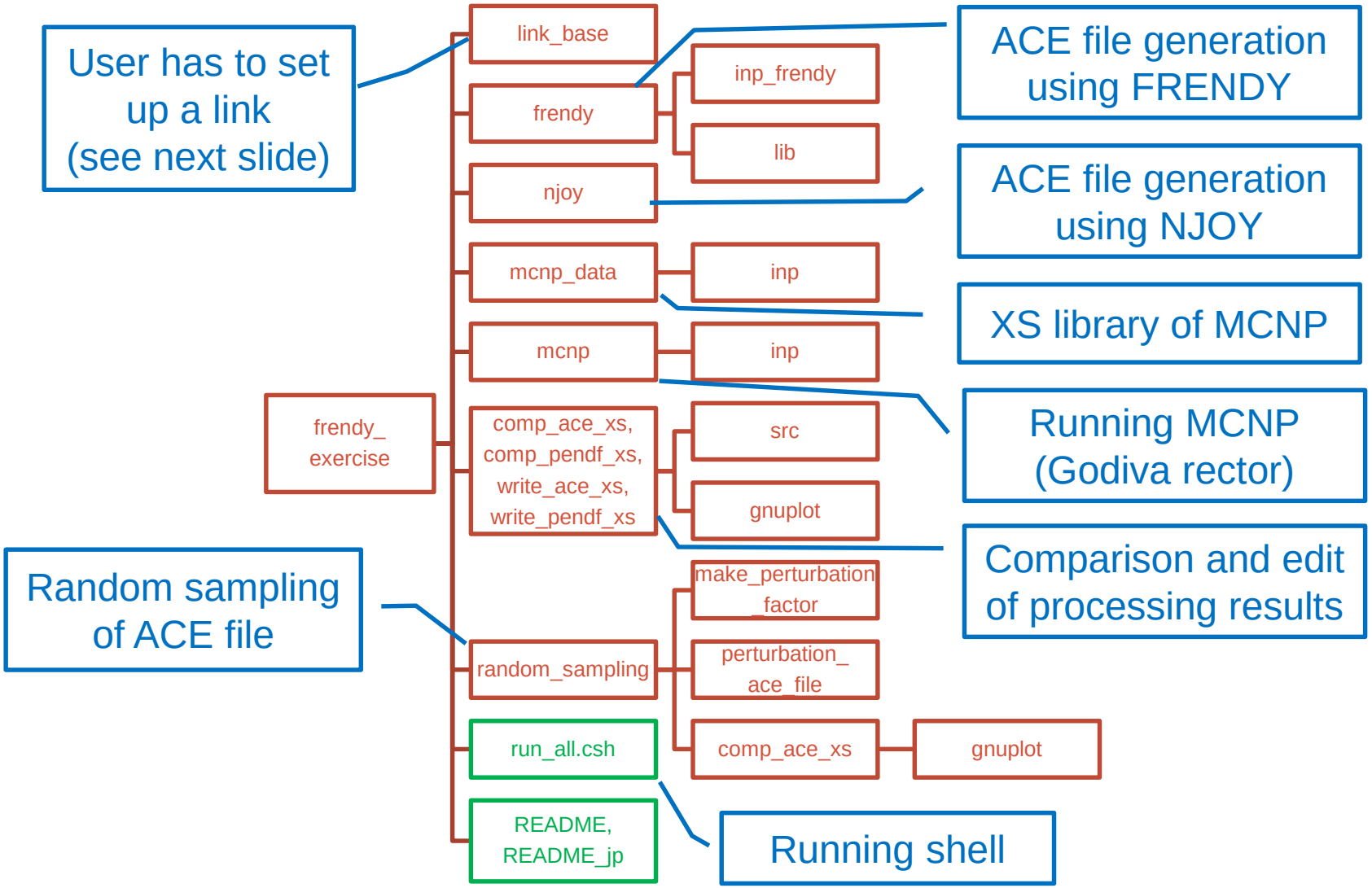


Content of exercise

- 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



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 (sample/sample/ace_data_collector.exe)
    - cd sample/tool
    - csh ./compile_all.csh
  - ACE file random sampling tool (tools/make_perturbation_factor/make_perturbation_factor.exe)
    - cd tools/make_perturbation_factor
    - make
  - ACE file perturbation tool (tools/perturbation_ace_file/perturbation_ace_file.exe)
    - cd tools/perturbation_ace_file
    - make

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

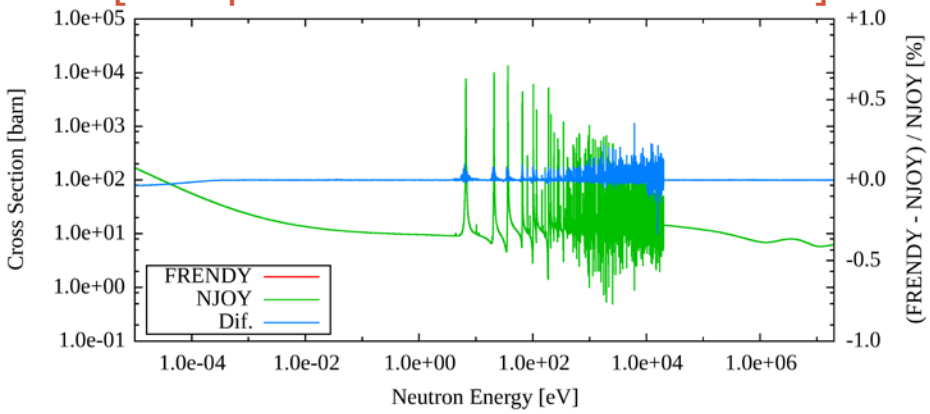
ACE file generation using NJOY

- 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

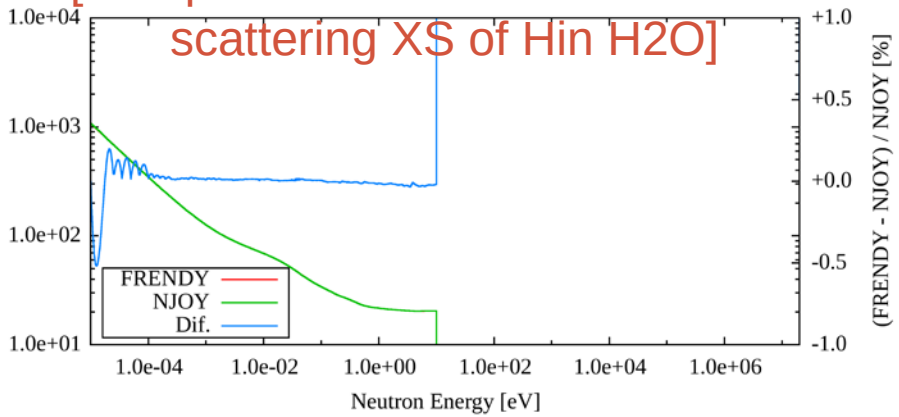
Comparison of processing results

- 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]



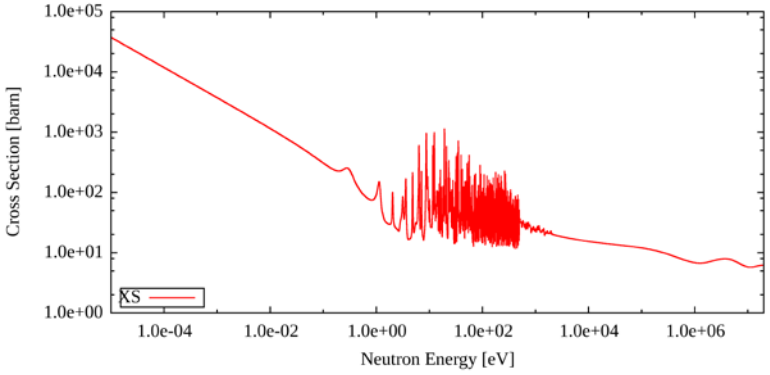
[Comparison of incoherent inelastic scattering XS of Hin H2O]



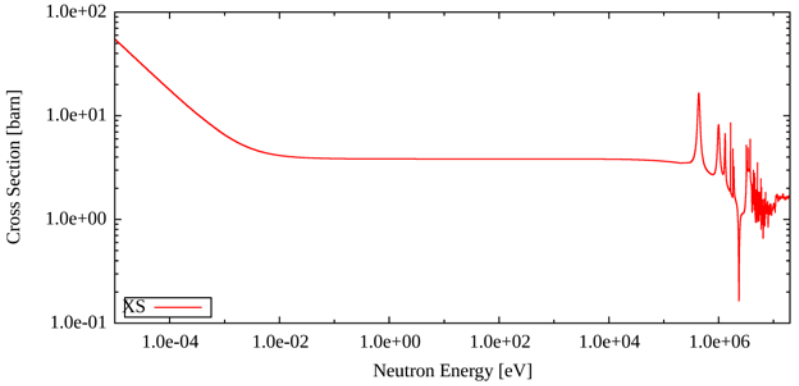
XS edit tool for ACE and PENDF files

- 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]



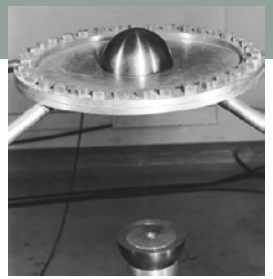
[Total XS of O-16]



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.mod : XSDIR file
  - Generated by NJOY
    - ace_n/j40a00na : Collected ACE files
    - xsdir.j40a00n.mod : 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.