Handling the evaluated nuclear data format and ACE format in FRENDY

Japan Atomic Energy Agency
Kenichi TADA
Nagoya University
Akio YAMAMOTO and Tomohiro ENDO

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Development of nuclear data processing system FRENDY

- JAEA started developing a new nuclear data processing system FRENDY in 2013.
  - **FR**om **E**valuated **N**uclear **D**ata librar**Y** to any application
  - To process nuclear data library by JAEA's nuclear application code users **with simple input file**.
- FRENDY Version 1 was released in 2019.
  - FRENDY Ver. 1 only generates ACE files.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
- FRENDY Version 2 will be released in the near future.
  - FRENDY Ver. 2 generates multi-group XS file.

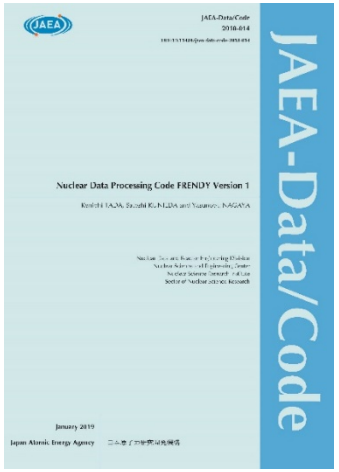
Features of FRENDY

- Utilization of modern programming techniques
  - C++, BoostTest library, Git
  - Improvement of quality and reliability
- Consideration of maintainability, modularity, and flexibility
  - Encapsulate all classes
  - Minimize the function of module
  - Maintain the independence of each module
- Processing methods of FRENDY are similar to NJOY.

Ref. K. Tada, et. al., “Development and verification of a new nuclear data processing system FRENDY,” *J. Nucl. Sci. Technol.*, **54** [7], pp.806-817 (2017). (http://www.tandfonline.com/doi/abs/10.1080/00223131.2017.1309306)

Release of FRENDY Ver. 1

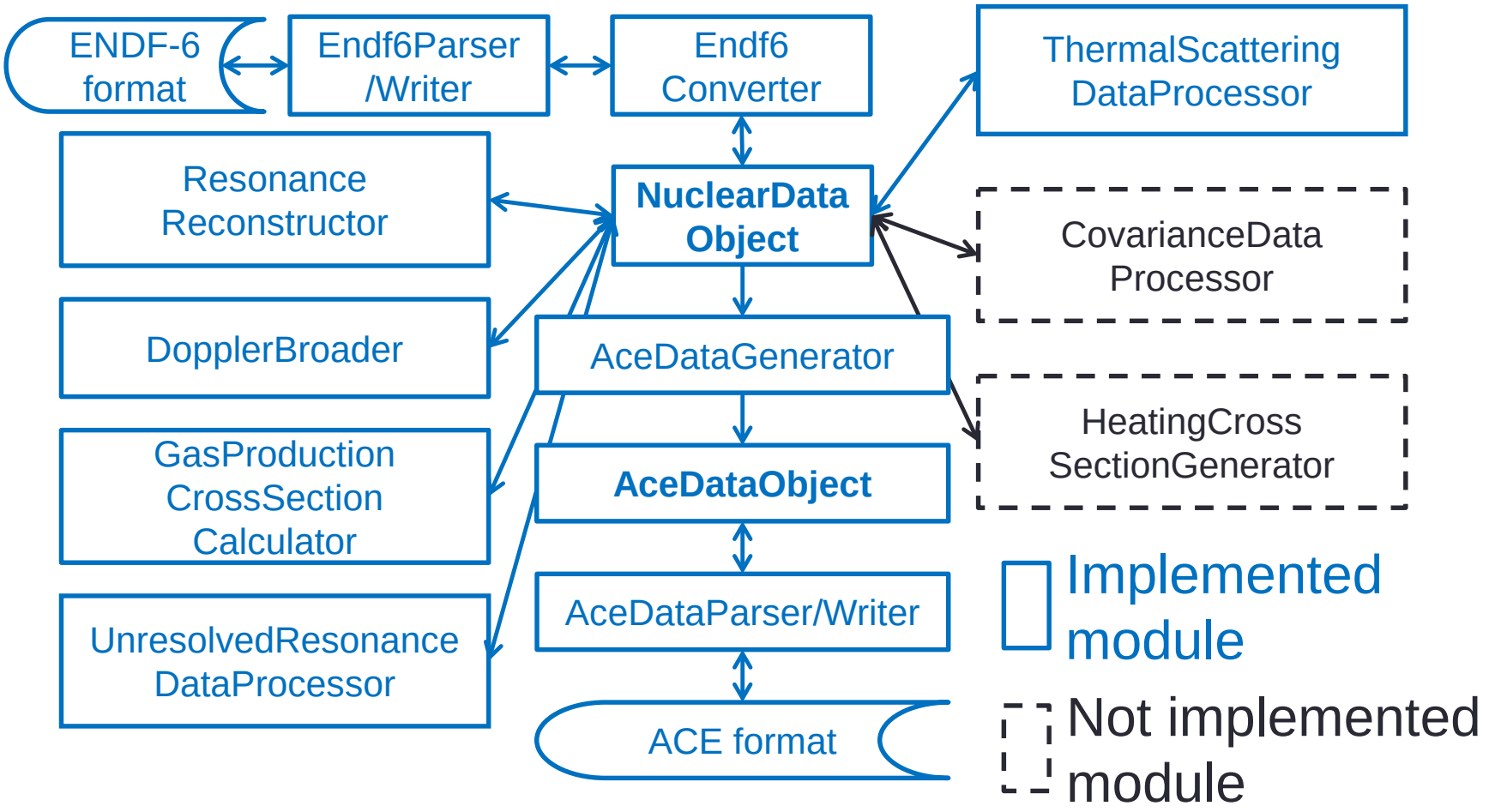
- FRENDY Ver.1 was released from our website.
  - https://rpg.jaea.go.jp/main/en/program_frendy/
  - Only generates ACE files.
    - Generation of multi-group cross section will be implemented soon.
  - Open source software
    - 2-Clause BSD license
  - Presentations of FRENDY training course and exercise are also found in this website
- Manual of FRENDY Ver. 1
  - JAEA-Data/Code 2018-014
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2018-014.pdf



Treatment of GNDS (plan)

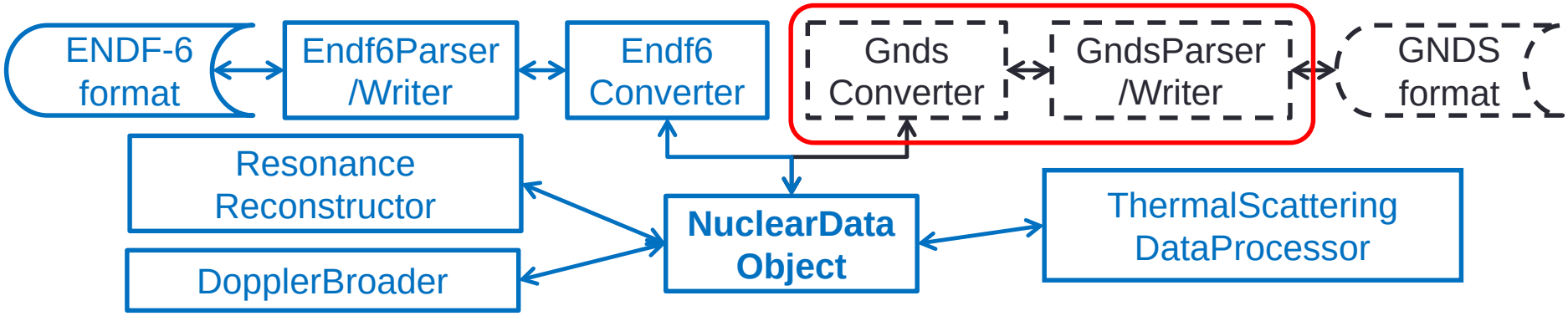
Structure of FRENDY

- Modularity is carefully considered.
  - Modules of FRENDY can be used other calculation codes by adding only a few lines.



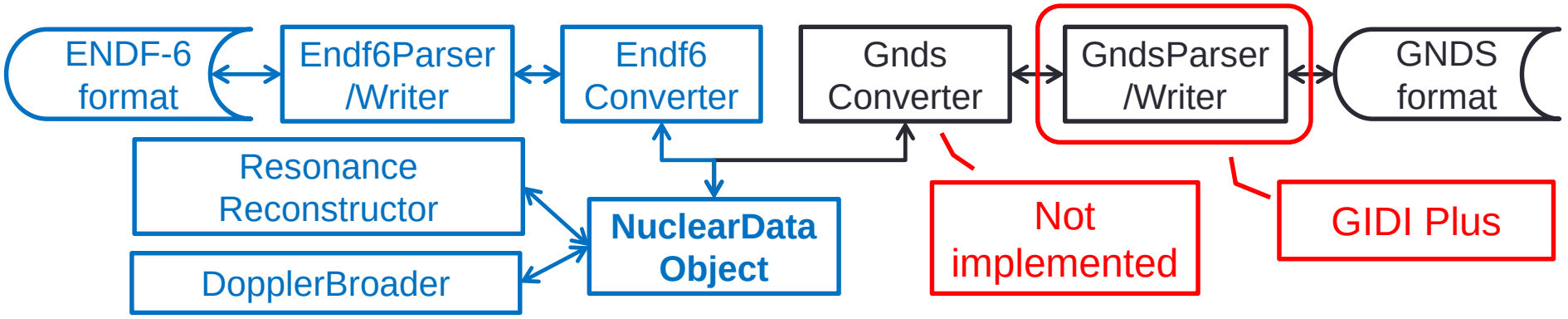
Advantage for using the FRENDY's original nuclear data object

- FRENDY has original format of the nuclear data for efficient management.
  - NuclearDataObject class
- Minimizing the impact by the change of nuclear data format
  - Developer and users are not necessary to consider the nuclear data format.
  - Consideration of a new data format GNDS
    - GNDS format can be addressed if another set of parser, writer and converter classes are implemented.



Treatment of GNDS (plan)

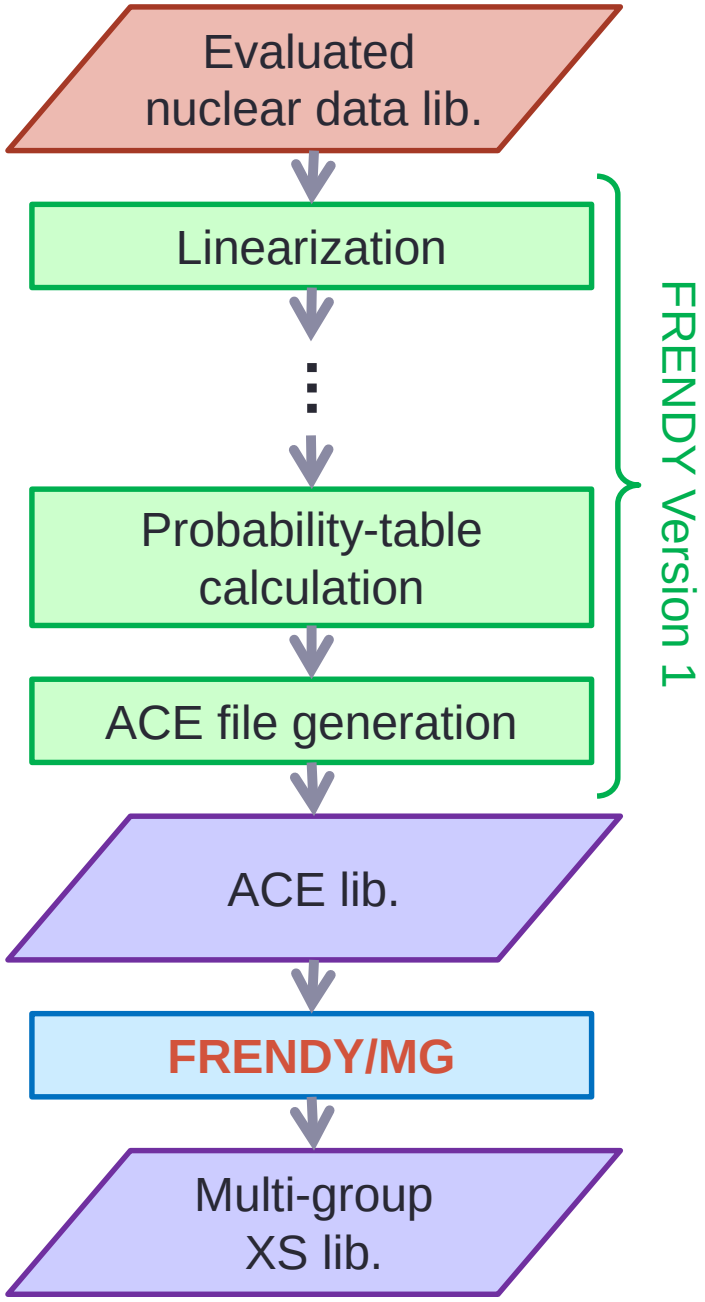
- FRENDY will use GIDI plus of LLNL for accessing GNDS.
  - We will implement a converter class to copy the nuclear data from GIDI plus to FRENDY (NuclearDataObject).
- We are now focusing on development multi-group generation and processing covariance data.
  - Treatment of GNDS will be considered after these work is completed.



Multi-group XS file generation from ACE file

Development of FRENDY/MG*)

- FRENDY/MG is a multi-group cross section generator from ACE file.
  - Multi-group XS file is generated from combination of FRENDY Version 1 and FRENDY/MG.
  - FRENDY/MG can generate multi-group XS file from the existing ACE file.
    - FRENDY/MG will be released as a function of FRENDY Version 2 in the near future.



*) A. Yamamoto et al., Trans. Am. Nucl. Soc., 122, pp.714-717 (2020). https://doi.org/10.13182/T122-32047

Major capabilities and features of FRENDY/MG (1/2)

- Focus on neutron cross section generation
  - Can treat fast continuous and thermal scattering law data
- Output format of multi-group cross sections
  - MATXS
  - GENDF (to be implemented)
- Weighting spectrum
  - 1/E, Fission+1/E+Maxwell (arbitral cutoff, temperature), or User input
- Ultra-fine group spectrum
  - Direct slowing down calculation or narrow resonance approximation
  - Automated ultra-fine energy grid refinement using ACE pointwise energy grid
  - Can treat a material including arbitrary number of isotopes; allows explicit consideration of resonance interference effect
  - Arbitrary mass weight of background moderator nuclide for evaluation of IR parameters

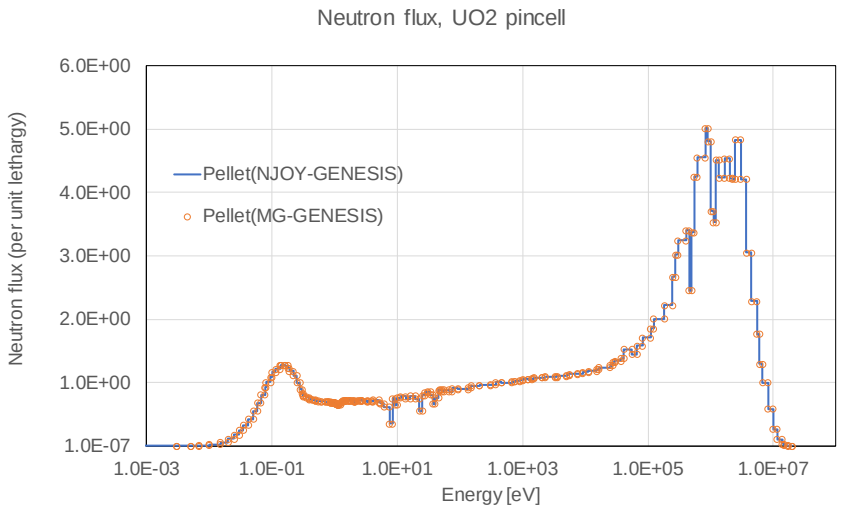
Major capabilities and features of FRENDY/MG (2/2)

- Angular/energy distribution
  - Can treat LAW=3, 4, 7, 9, 11, 44, 61 66 in an ACE file
  - Can treat all nuclides in JENDL-4.0, ENDF/B-VII.0, VII.1, B-VIII.0, JEFF-3.3, and TENDL-2019 (without Pu-238)
- Scattering matrices
  - Can treat all reactions including anisotropic scattering
  - $S(\alpha,\beta)$: free gas model, incoherent inelastic, incoherent elastic, coherent elastic
- Self-shielding for unresolved resonance region using probability table
- Fission spectrum, ν values
  - Prompt, Delayed (each group), Prompt + Delayed
- Arbitral multi-group energy structure
- Arbitral thermal cutoff

Verification of FRENDY/MG

- Comparison of all processing results between FRENDY/MG and NJOY
  - All nuclides in JENDL-4.0, ENDF/B-VII.1, B-VIII.0, and JEFF-3.3
  - The processing results shows good agreement.
- Comparison of neutronics calculations
  - PWR pin-cell (5 wt% UO_2, 600 K)
  - MOC (GENESIS code), 172 gr.
  - $S(\alpha,\beta)$:free gas
- K-effective
  - NJOY :1.4089250
  - FRENDY/MG :1.4089277

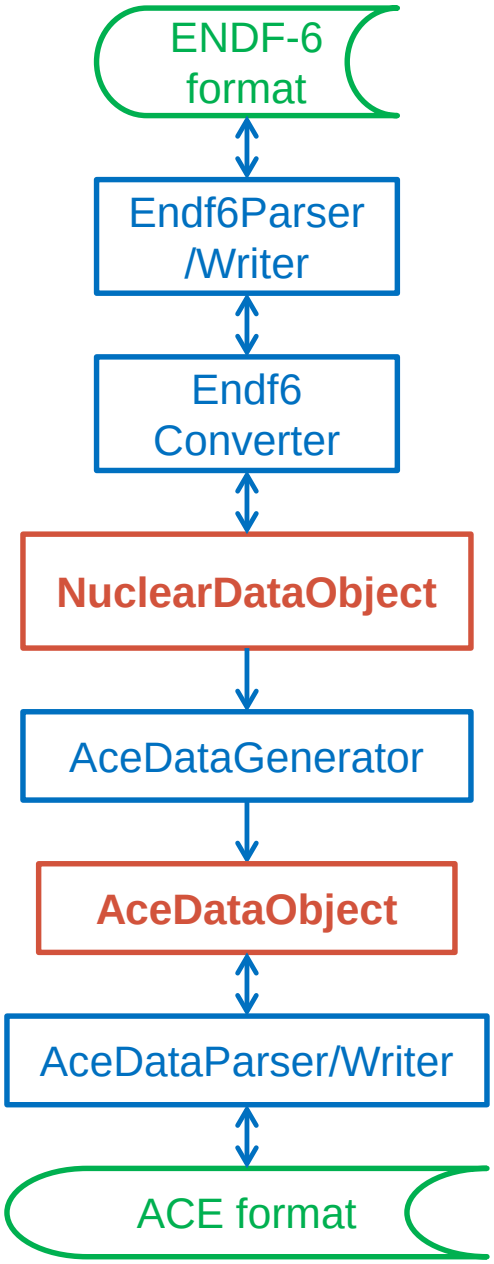
[Comparison of neutron spectrum]



Other tools to handle ENDF and ACE files

Handling ENDF/ACE files

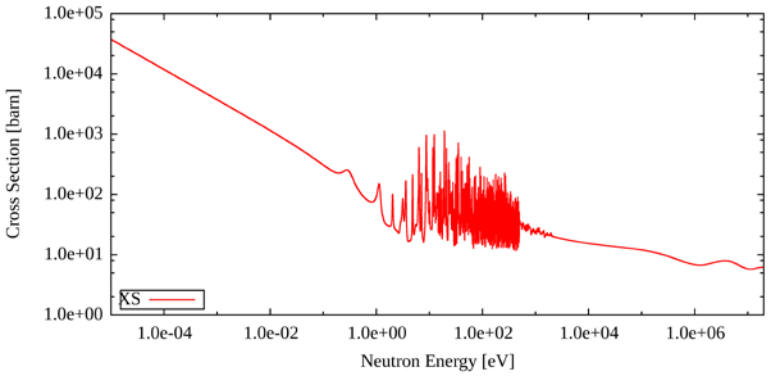
- FRENDY has data object for ENDF and ACE files.
  - User can plot or modify the data in ENDF and ACE files **without** knowledge of data format.
- We prepared functions to plotting or modify ENDF/ACE files.
  - XS plotting tool for ENDF/ACE files
  - ENDF/ACE modification function
  - ACE file perturbation tool
    - For sensitivity analysis and uncertainty quantification using random sampling method



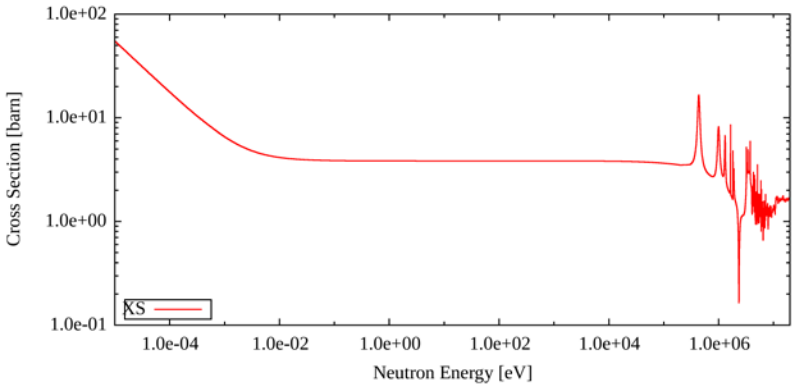
XS plotting tool for ENDF and ACE files

- This tool plots XS in ACE and ENDF files.
  - This tool contained in frendy_exercise.
    - ACE file plotting tool: frendy_exercise/write_ace_xs
    - ENDF file plotting tool: frendy_exercise/write_pendf_xs
  - This tool output one-dimensional table data.
    - GNUPLOT is used to plot the graph from this table data.

[Total XS of U-235]



[Total XS of O-16]



ENDF/PENDF modification tool

- This tool removes, adds, exchanges specified MF/MT data.

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=6

The modified evaluated nuclear data file **must be checked carefully** since FRENDY does not check the new file.

remove

MF=1
MF=2, MT=151
MF=3, MT=1
MF=6

add

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=3, MT=102
MF=6

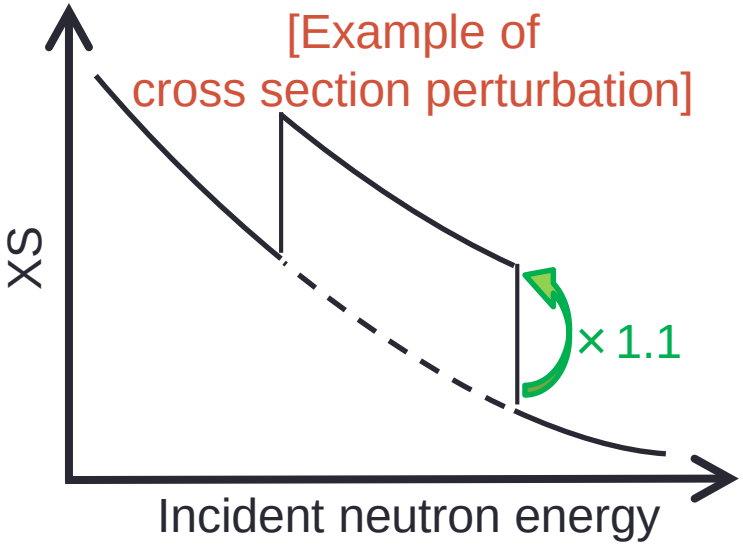
exchange

MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=6

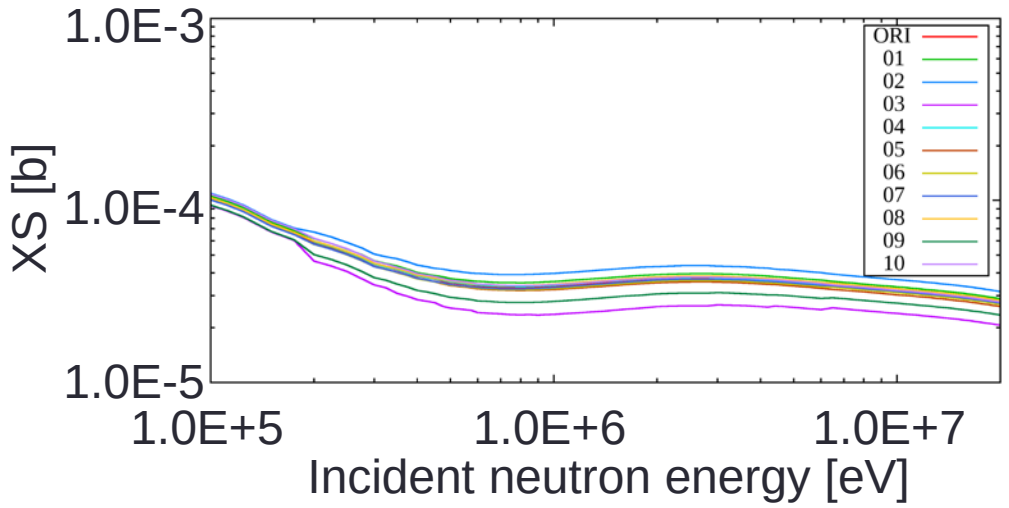
ACE file perturbation tool

- Implementation of a random sampling tool to perturb cross section and fission spectrum of ACE file*).
  - User sets reaction type, energy region, and amount of perturbation.
  - Cross section and fission spectrum are randomly perturbed using random sampling mode.
- This tool is available from FRENDY Ver. 1.01.001.

[Example of cross section perturbation]



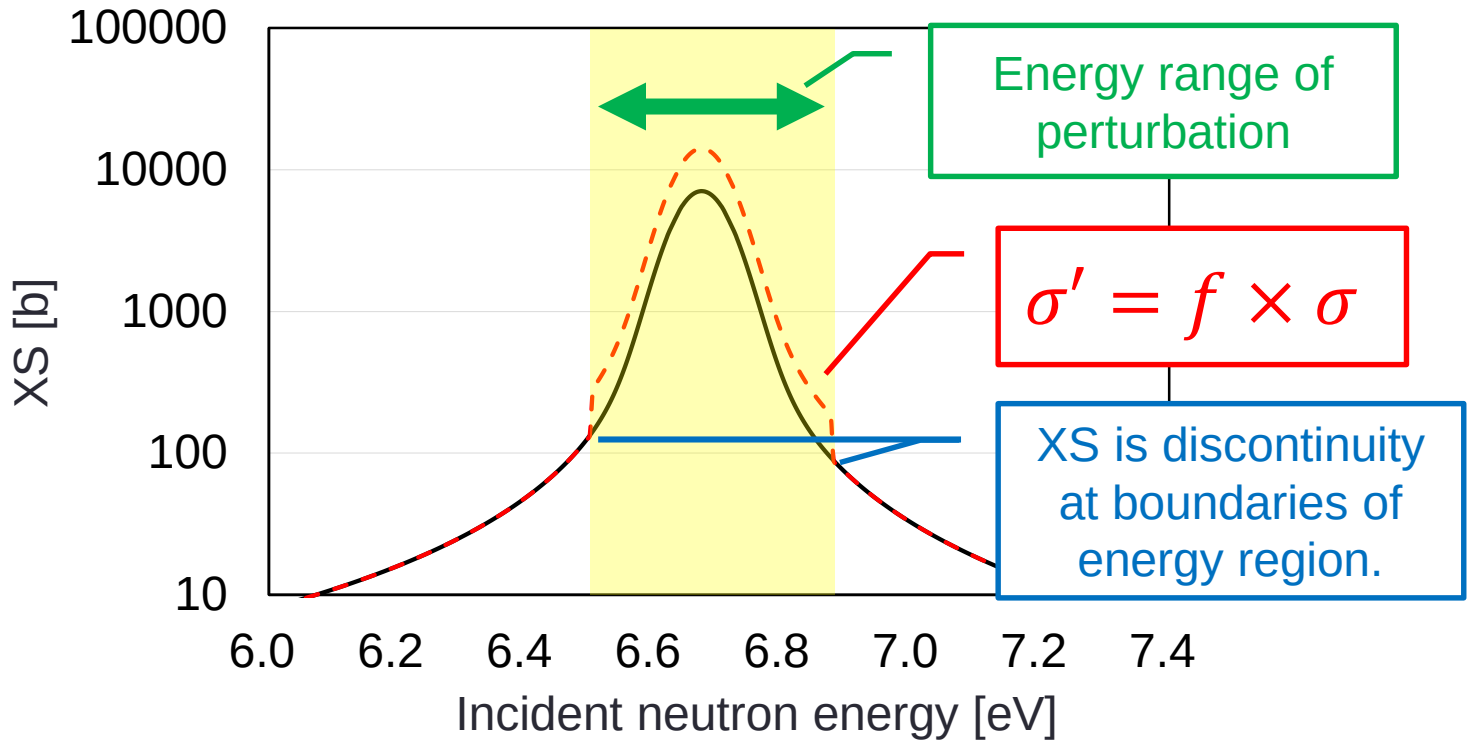
[Example of random sampling (^{1}H, (n,γ))]



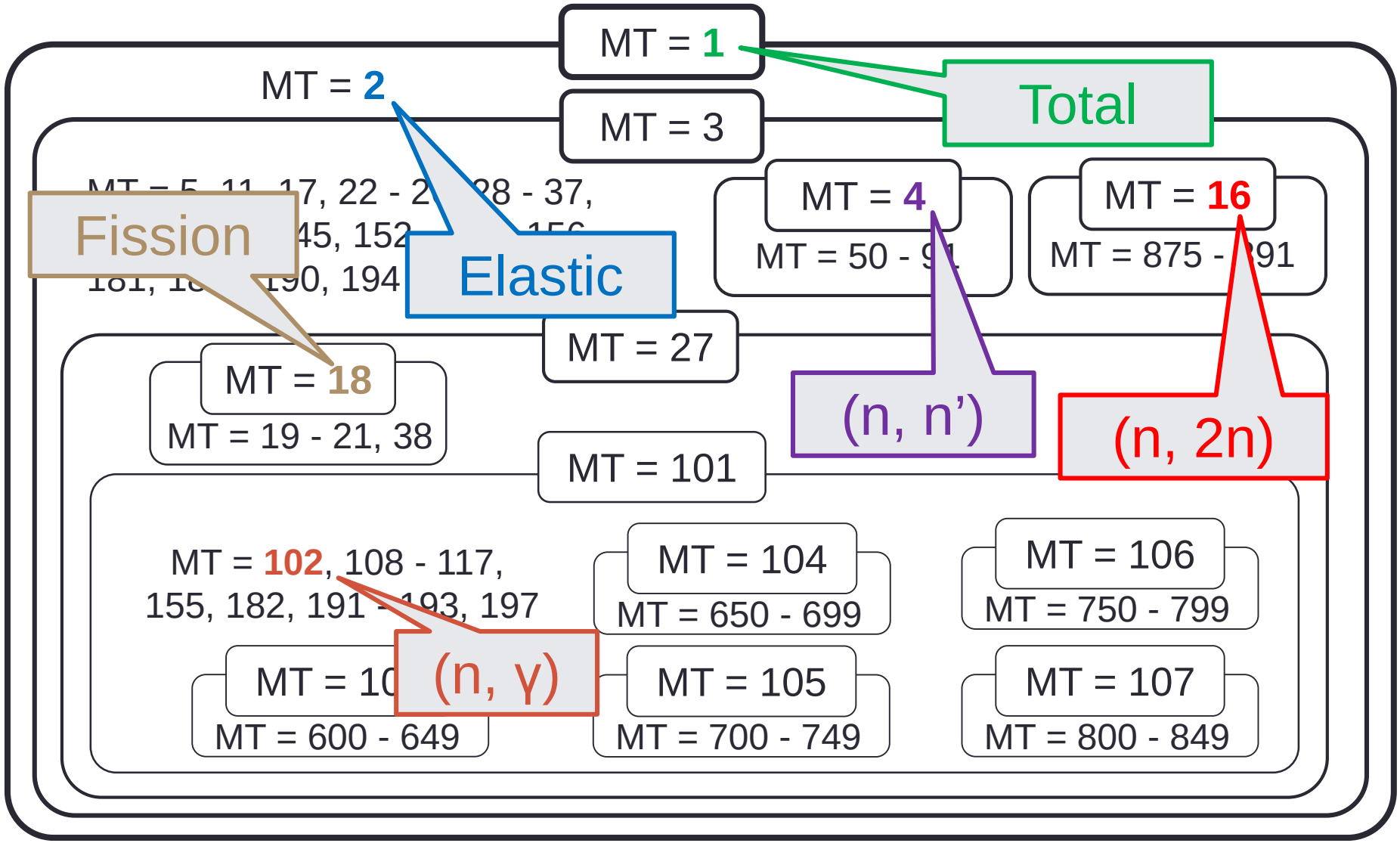
*) R. Kondo, et al., "Implementation of random sampling for ACE-format cross sections using FRENDY and application to uncertainty reduction," *Proc. M&C2019*, Aug. 25-29 (2019).

Perturbation of ACE file

- Perturbation tool decreases or increases XS or number of neutron per fission (ν) or fission spectrum (χ).
  - XS or χ is multiplied by perturbation factor f within arbitrary energy range.
- This tools can be adopted to two analyses.
  - Sensitivity analysis with direct perturbation method
  - Uncertainty analysis with random sampling method



Relations of each reaction type



Example of fission XS perturbation

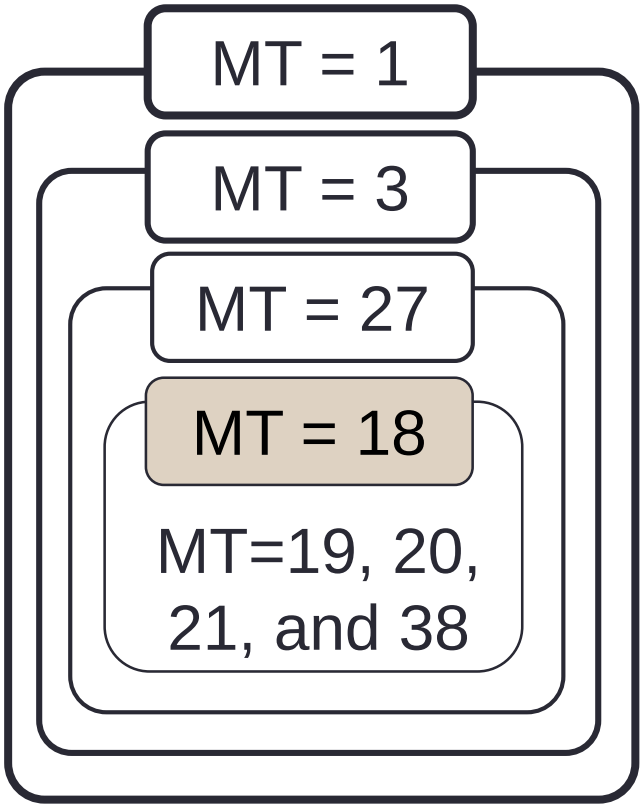
Perturbed fission XS (MT=18): $\sigma_{18}' = \boldsymbol{f} \times \sigma_{18}$ (Perturabtion factor: f)

MT18 contains MT=19-21 and 38.
MT=19-21 and 38 are also perturbed.

$$\sigma_{19}' = \boldsymbol{f} \times \sigma_{19},\ \sigma_{20}' = \boldsymbol{f} \times \sigma_{20},$$
$$\sigma_{21}' = \boldsymbol{f} \times \sigma_{21},\ \sigma_{38}' = \boldsymbol{f} \times \sigma_{38}$$

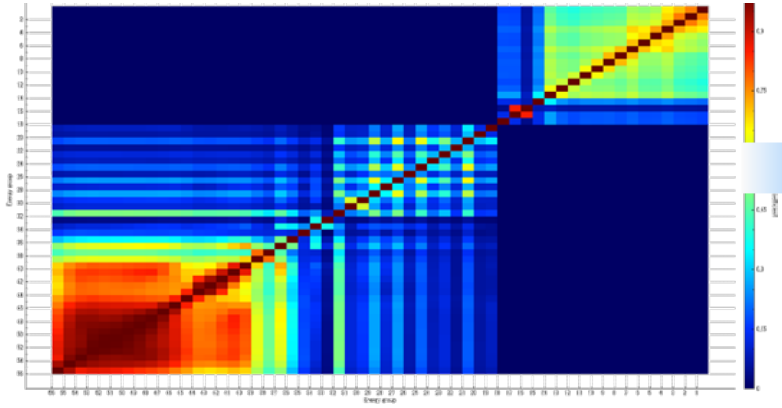
MT=1, 3, and 27 contain MT=18.
XS of MT=1, 3, and 27 are modified.

$$\Delta\sigma_{18} = \sigma_{18}' - \sigma_{18}$$
$$\sigma_1' = \sigma_1 + \Delta\sigma_{18},\ \sigma_3' = \sigma_3 + \Delta\sigma_{18}$$
$$\sigma_{27}' = \sigma_{27} + \Delta\sigma_{18}$$



Random sampling

Covariance matrix of nuclear data



inp/Nddd_000x

```
102 2.00E+01 6.43E+00 8.78E-01
102 6.43E+00 4.30E+00 8.67E-01
102 4.30E+00 3.00E+00 8.62E-01
                 . . .
```

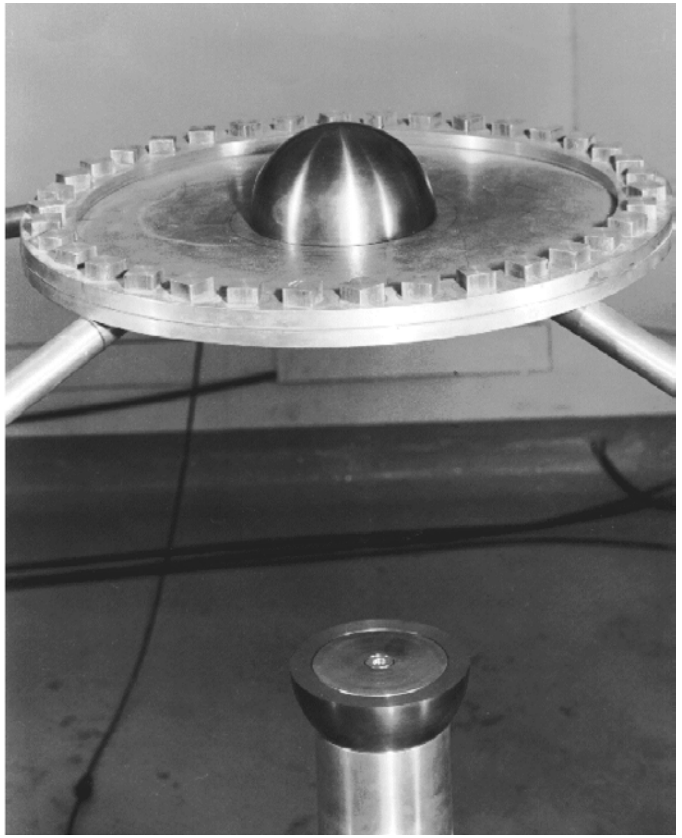
- User has to prepare covariance matrix.
  - We are now developing converter from GENDF file of NJOY/ERROR to input of random sampling tool.
- Generation of perturbation factors using random sampling method
  - See “/frendy_20yymmdd/tools/make_perturbation_factor/sample”

Uncertainty quantification using random sampling method [1]

Godiva (HMF-001)

Geometry	Sphere Radius: 8.7 cm
Composition	U-235: 93.71 wt.% U-238: 5.27 wt.% U-234: 1.02 wt.%
k_{eff}	1.000 ± 0.001

- MCNP6.2
- Number of perturbed ACE file: 100
- Covariance data: 56groupcov7.1 (from SCALE6.2.3)
- MT=2,4,16,18,102,452, and 1018 (MT=452: ν, MT=1018: χ)



Godiva [2]

[1] R. Kondo, et al., "Implementation of random sampling for ACE-format cross sections using FRENDY and application to uncertainty reduction," Proc. M&C2019, Aug. 25-29, Portland, USA (2019).
[2] ICSBEP NEA/NSC/DOC(95)03, Organization for Economic Co-operation and Development-Nuclear Energy Agency (OECD-NEA) (September 2016).

Calculation results (k-effective uncertainty)

k_{eff}-uncertainty due to all nuclides and reactions $\Delta k/k$ [%]

Sensitivity analysis (SA) of MCNP6.2	Random sampling method using perturbation tool
1.11	1.12 [0.98 – 1.24]

Comparison of k_{eff}-uncertainty due to individual nuclide and reaction $\Delta k/k$ [%]

		SA (TSUNAMI-1D)	SA (MCNP6.2)	RS
U-235	(n,γ)	0.880	0.880	0.833
U-235	(n,n')	0.615	0.617	0.664
U-235	Elastic	0.295	0.295	0.305
U-235	Fission	0.269	0.269	0.329
U-235	Fission spectrum	0.253	0.261	0.260
U-234	Fission	0.118	0.118	0.130
U-235	ν_{total}	0.085	0.085	0.093

Conclusions

- FRENDY Version 2 will be released in the near future.
  - FRENDY Ver. 2 generates multi-group XS file.
    - ACE file is used to generate multi-group XS file.
  - Treatment of GNDS format will be considered.
- We prepared many tools to plot or modify ENDF/ACE files using FRENDY.
  - XS plotting tool for ENDF/ACE files
  - ENDF/ACE modification tool
  - ACE file perturbation tool