Development of FRENDY Version 2

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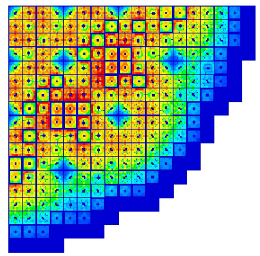
Overview of FRENDY

- 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 Mar. 2022.
  - FRENDY Ver. 2 generates multi-group XS file.

Nuclear data library JENDL → Nuclear data processing system **FRENDY** → Nuclear calculation codes →

k-eff , flux, …



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
- Simple input format
  - Processing mode and nuclear file name is required at minimum.
  - NJOY input format is also available.

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)

Input format of FRENDY

- FRENDY treats two types of the input formats.
  - FRENDY original input format
  - NJOY compatible
- Simple and easy input data
  - The simplest input: Nuclear data file name and processing mode are **only** required for the processing.
    - FRENDY has recommended parameters in the source code.
    - User can also change (override) parameters.

Input format of FRENDY and NJOY

- Input parameters of FRENDY consist of “input data name” and “input data”.
  - Comment line is similar to C/C++.
    - //~ or /* ~ */
- Input format of FRENDY is easy to understand.
  - This input format is suitable for beginners.

[Sample input of FRENDY]

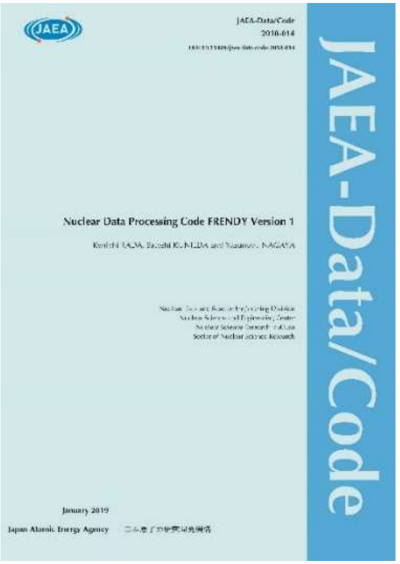
```
ace_fast_mode  // Processing mode
  nucl_file_name  U235.dat
  ace_file_name   U235.ace
  temp            296.0
```

[Sample input of NJOY]

```
reconr                          / command
 20  21                         / input(tape20), output(tape21)
'PENDF file of U235'            / identifier for PENDF
 9228                           / mat
 1.00e-03  0.00                 / err, temp
 0                              /
broadr                          / command
 20  21  22                     / endf, pendf(in), pendf(out)
 9228  1                        / mat, temp no
 1.00e-03  -5.0E+2              / err, thnmax
 296.0                          / temp
 0                              /
gaspr                           / command
 20  22  23                     / endf, pendf(in), pendf(out)
purr                            / command
 20  23  25                     / endf, pendf(in), pendf(out)
 9228  1  10  20  100           / mat, temp no, sig no, bin no, lad no
 296.0                          / temp
 1E10  1E4  1E3  300  100  30  10  1.0  0.1  1.0E-5 / sig zero
 0                              /
acer                            / command
 20  25   0  30  31             / nendf, npend, ngend, nace, ndir
 1   1   1  0.30                / iopt(fast), iprint(max), itype, suffix
 'ACE file of U235'             / descriptive character
 9228  296.0                    / mat, temp
 1                              / newfor(yes)
                                / acer end
stop                            /
```

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

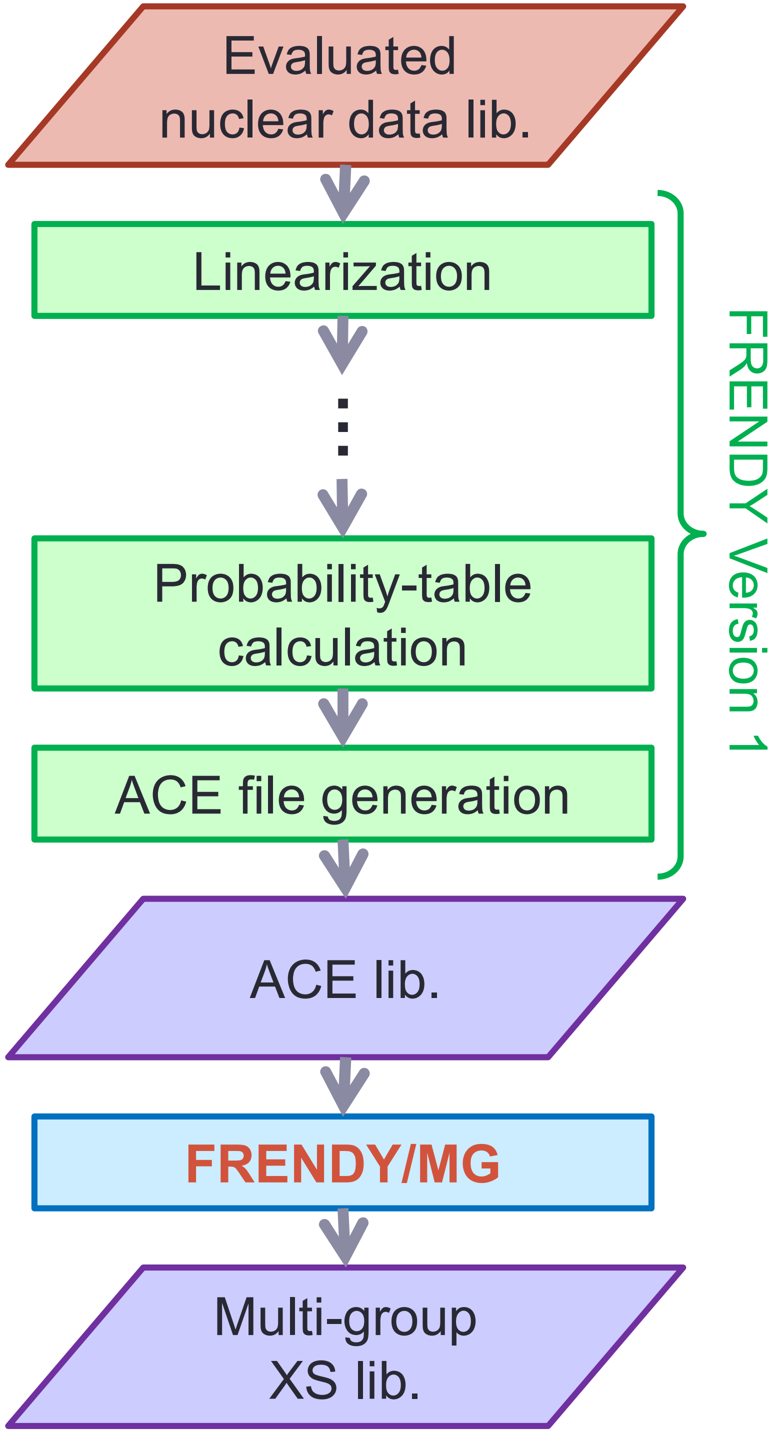
Development of FRENDY Ver. 2

- Many capabilities are prepared after FRENDY Ver. 1.
  - Neutron induced multi-group cross section generation
  - Perturbation of ACE file for uncertainty quantification
    - This function was implemented in FRENDY Ver.1.01.001.
  - Modification of evaluated nuclear data file
  - Uncertainty quantification for probability tables
  - Improvement of input checker to reduce input errors
- FRENDY version 2 will be released including these functions in Mar. 2022.

Multi-group XS generation

- FRENDY/MG*) is used for a multi-group XS files.
  - FRENDY/MG generates multi-group XS files from ACE files.
    - FRENDY/MG can also generate a multi-group XS library from the existing ACE library.
- NJOY input are also available for multi-group XS file generation.
  - Input of GROUPR and MATXSR modules are available.

*) A. Yamamoto, K. Tada, G. Chiba, T. Endo, "Multi-group neutron cross section generation capability for FRENDY nuclear data processing code," J. Nucl. Sci. Technol., 2021.
https://doi.org/10.1080/00223131.2021.1921631



Major capabilities of FRENDY/MG

- Focus on neutron cross section generation.
  - It can treat fast continuous and thermal scattering law data.
- Output format of multi-group cross sections
  - GENDF and MATXS
- Angular/energy distributions
  - LAW=3, 4, 7, 9, 11, 44, 61 66 in ACE file
  - All nuclides in JENDL-4.0, ENDF/B-VII.1, B-VIII.0, JEFF-3.3, and TENDL-2019 are available.
- Scattering matrices
  - It can treat all reactions including anisotropic scattering.
  - $S(\alpha,\beta)$:free gas model, incoherent inelastic, incoherent elastic, coherent elastic

New functions of FRENDY/MG

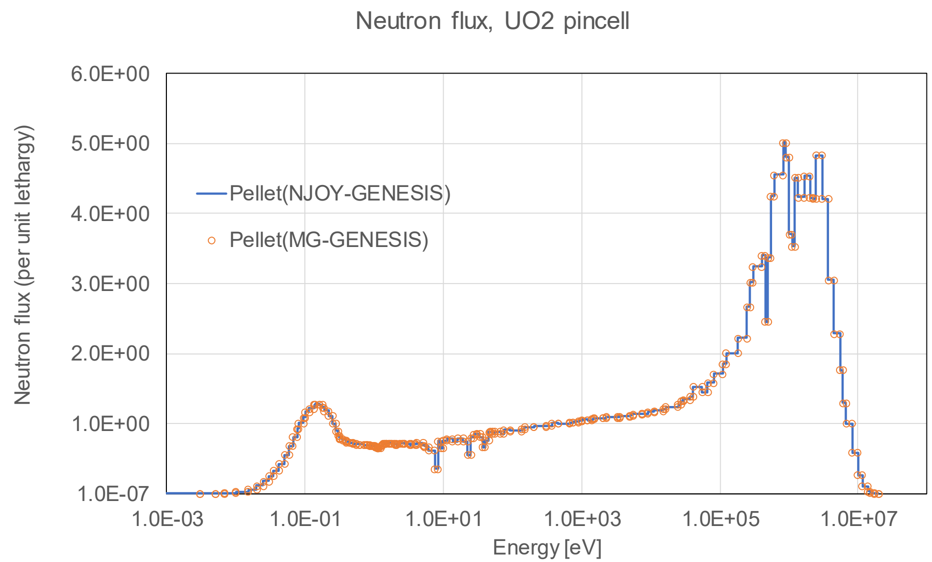
- Back-ground cross-section set can be automatically set with minimum number of background cross-sections*).
- A compound of different isotope can be specified to explicitly consider the resonance interference effect.
  - For example, U-235, U-238, and O-16 in UO_2.
- Current (P_1 flux) weighted total cross-section can be calculated.
- Any energy grid points can be used for ultra-fine group slowing down calculation.

*) A. Yamamoto, T. Endo, K. Tada, “Adaptive setting of background cross sections for generation of effective multi-group cross sections in FRENDY nuclear data processing code,” J. Nucl. Sci. Technol., 2021. https://doi.org/10.1080/00223131.2021.1944930

Verification of FRENDY/MG

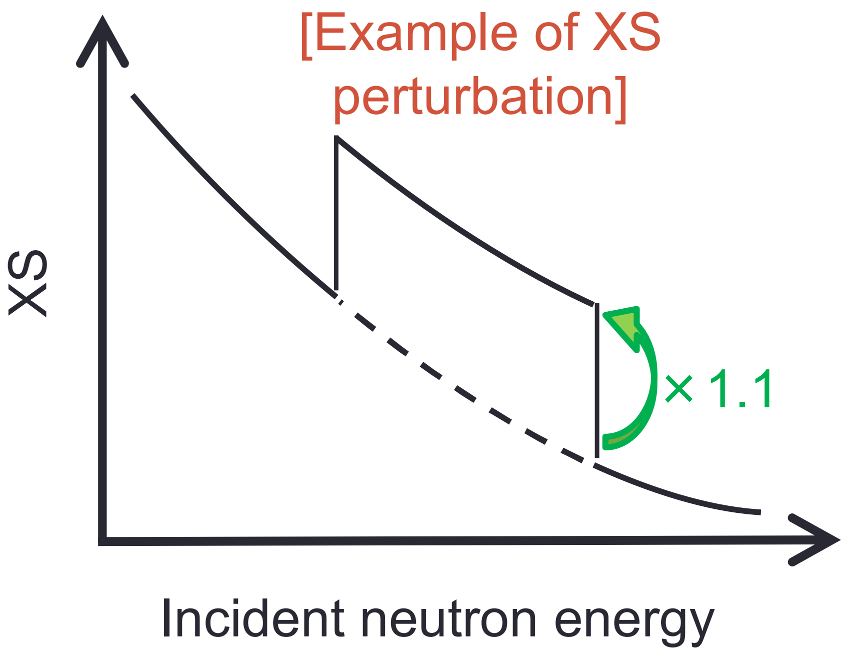
- Comparison of all processing results between FRENDY/MG and NJOY
  - All nuclides in JENDL-4.0, ENDF/B-VII.1, B-VIII.0, and JEFF-3.3
  - The processing results shows good agreement.
- Comparison of neutronics calculations
  - PWR pin-cell (5 wt% UO_2, 600 K)
  - MOC (GENESIS code), 172 gr.
  - $S(\alpha,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

[Comparison of neutron spectrum]



ACE file perturbation tool

- Implementation of a sampling tool to perturb cross section, number of neutrons per fission, and fission spectrum of ACE file*).
  - Reaction type, energy region, and amount of perturbation are required as input parameters.
- This tool is available from FRENDY Ver. 1.01.001.



*) 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).

ENDF modification function

- This function 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

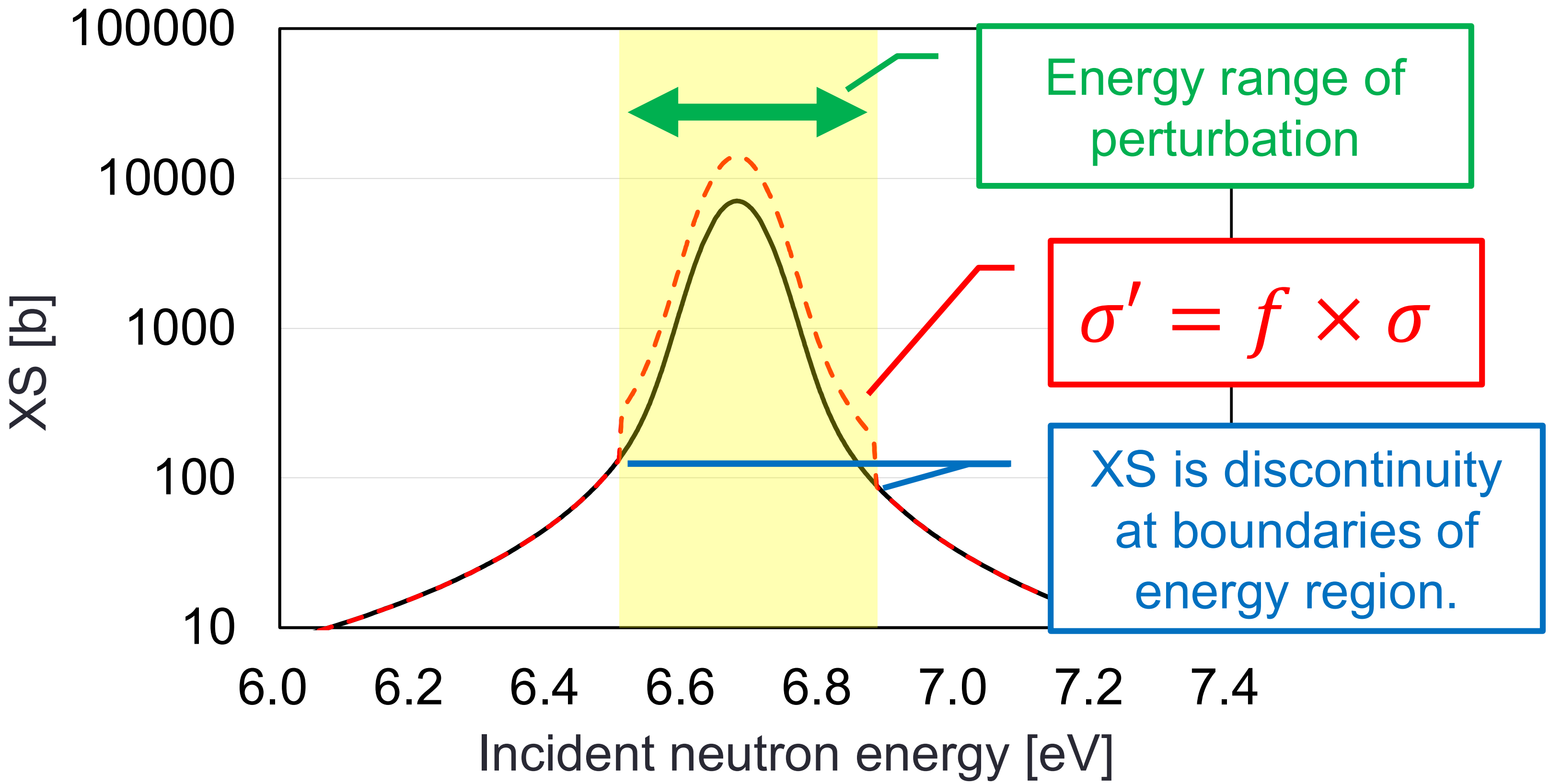
MF=1
MF=2, MT=151
MF=3, MT=1
MF=3, MT=2
MF=6

Conclusions

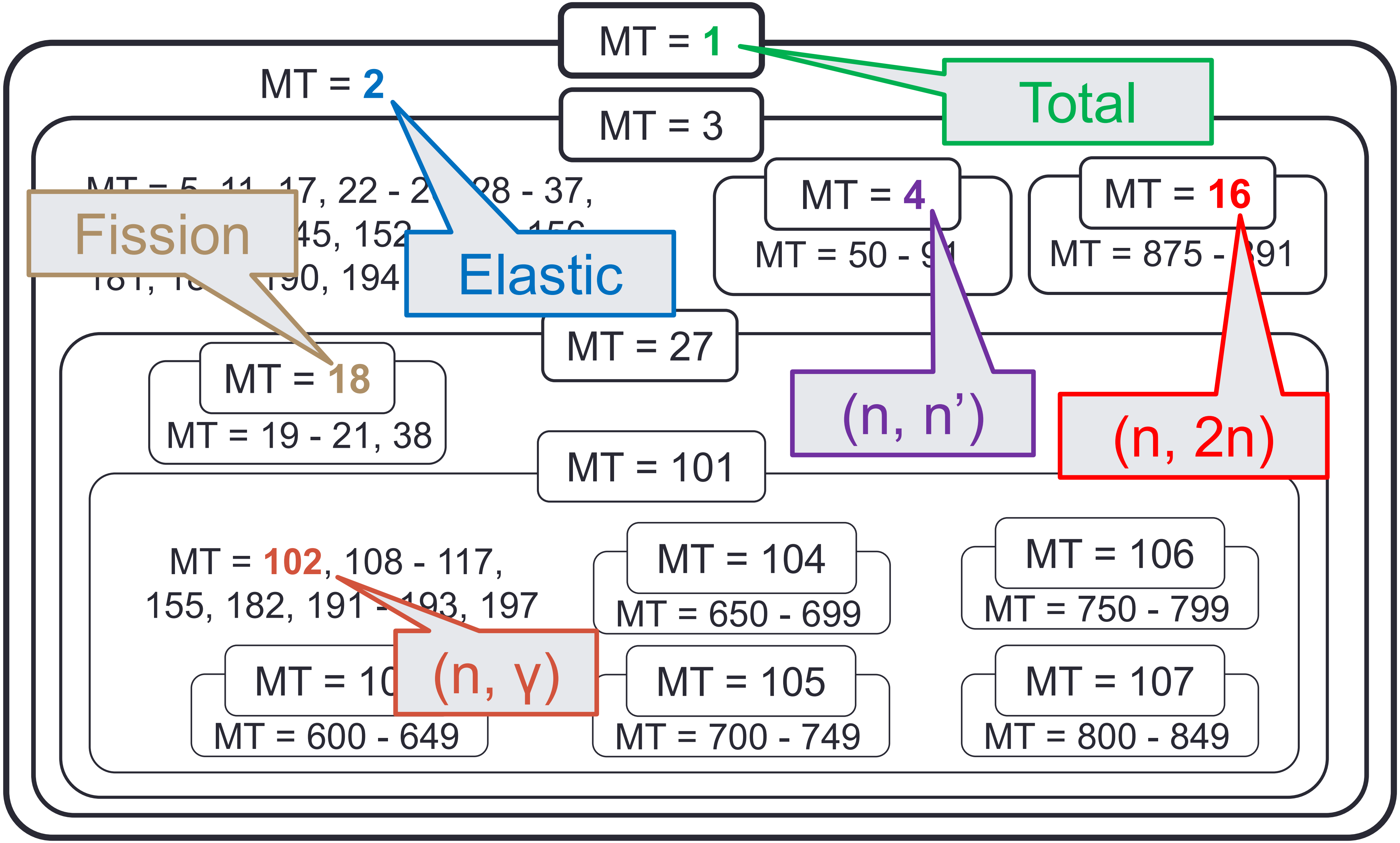
- About FRENDY
  - FRENDY Ver. 1 was released in 2019 as an open-source software.
    - Utilization of modern programming techniques
    - Consideration of maintainability, modularity, and flexibility
    - Simple input format
- New capabilities in FRENDY Ver. 2
  - Neutron induced multi-group cross section generation
  - Perturbation of ACE file for uncertainty quantification
  - Modification of evaluated nuclear data file
- FRENDY Ver. 2 will be released in Mar. 2022.

Perturbation of ACE file

- Perturbation tool decreases or increases XS or number of neutron per fission (ν) or fission spectrum (χ).
  - XS, ν 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

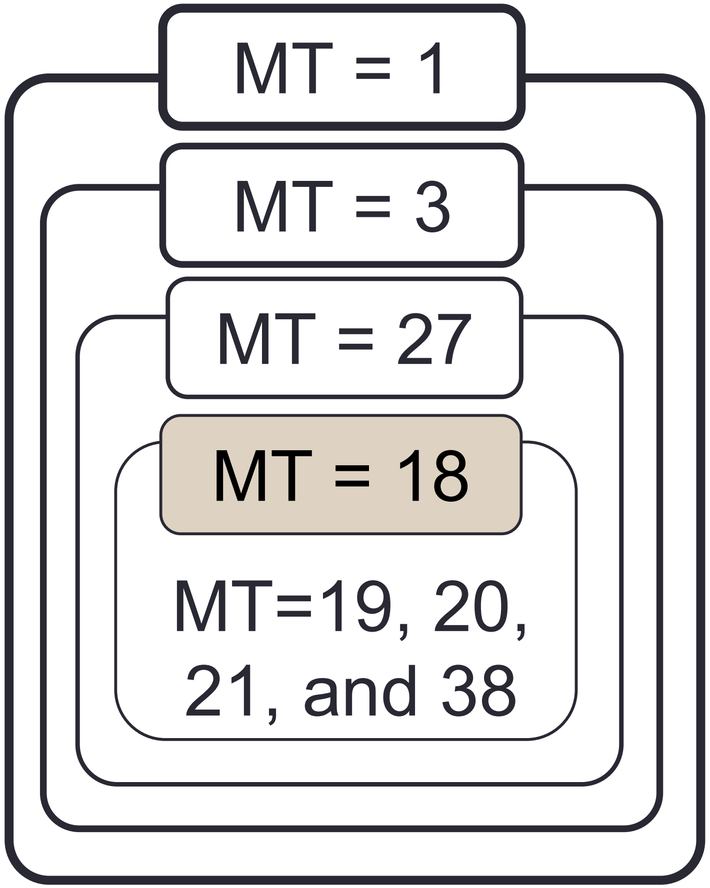
Perturbed fission XS (MT=18): $\sigma_{18}{}' = \boldsymbol{f} \times \sigma_{18}$ (Perturabtion factor: f)

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

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

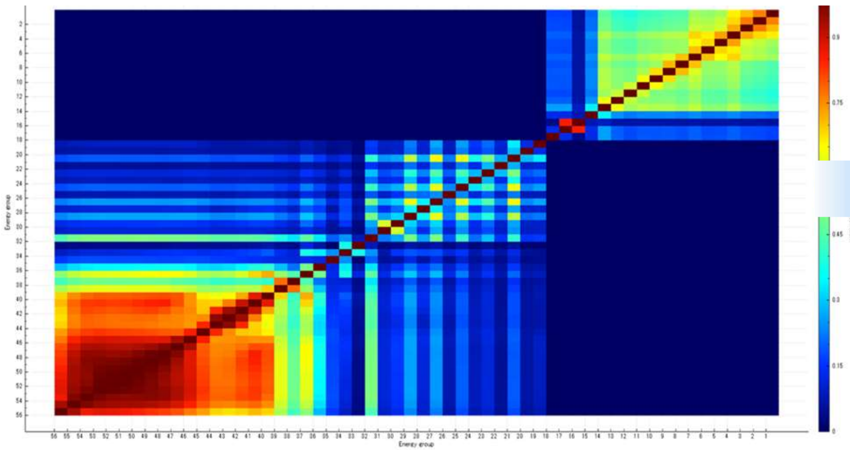
MT=1, 3, and 27 contain MT=18.
XS of MT=1, 3, and 27 are modified.

$$\Delta\sigma_{18} = \sigma_{18}{}' - \sigma_{18}$$
$$\sigma_{1}{}' = \sigma_{1} + \Delta\sigma_{18},\ \sigma_{3}{}' = \sigma_{3} + \Delta\sigma_{18}$$
$$\sigma_{27}{}' = \sigma_{27} + \Delta\sigma_{18}$$



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
. . .
```

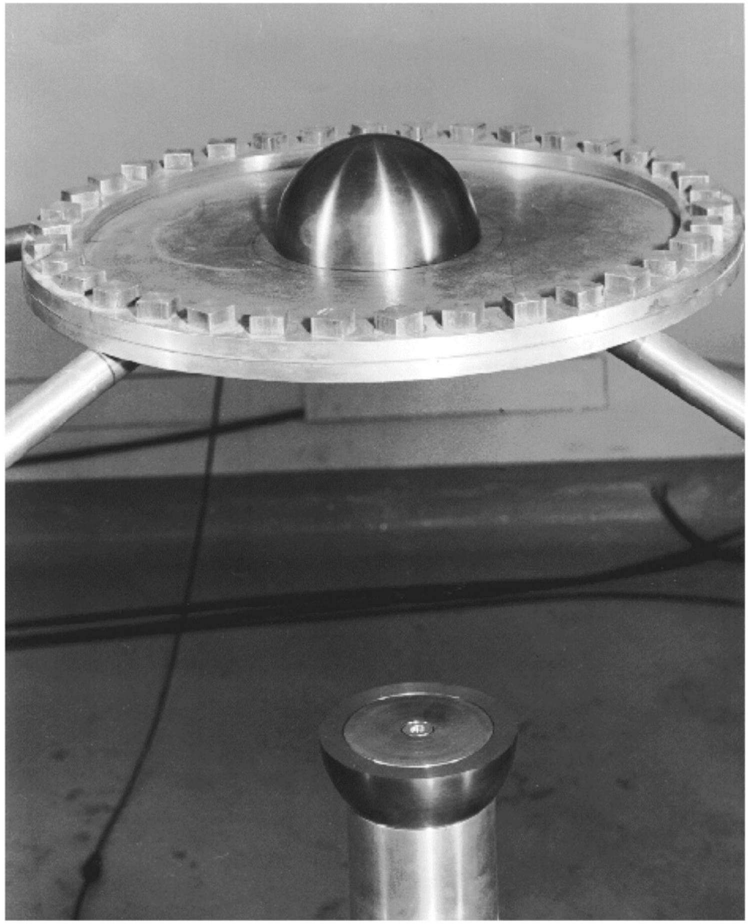
- User must prepare covariance matrix.
  - We are now developing converter from GENDF file of NJOY/ERROR to input of random sampling tool.
- Generation of perturbation factors using random sampling method
  - See “/frendy_20yymmdd/tools/make_perturbation_factor/sample”

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