ACE file perturbation tool

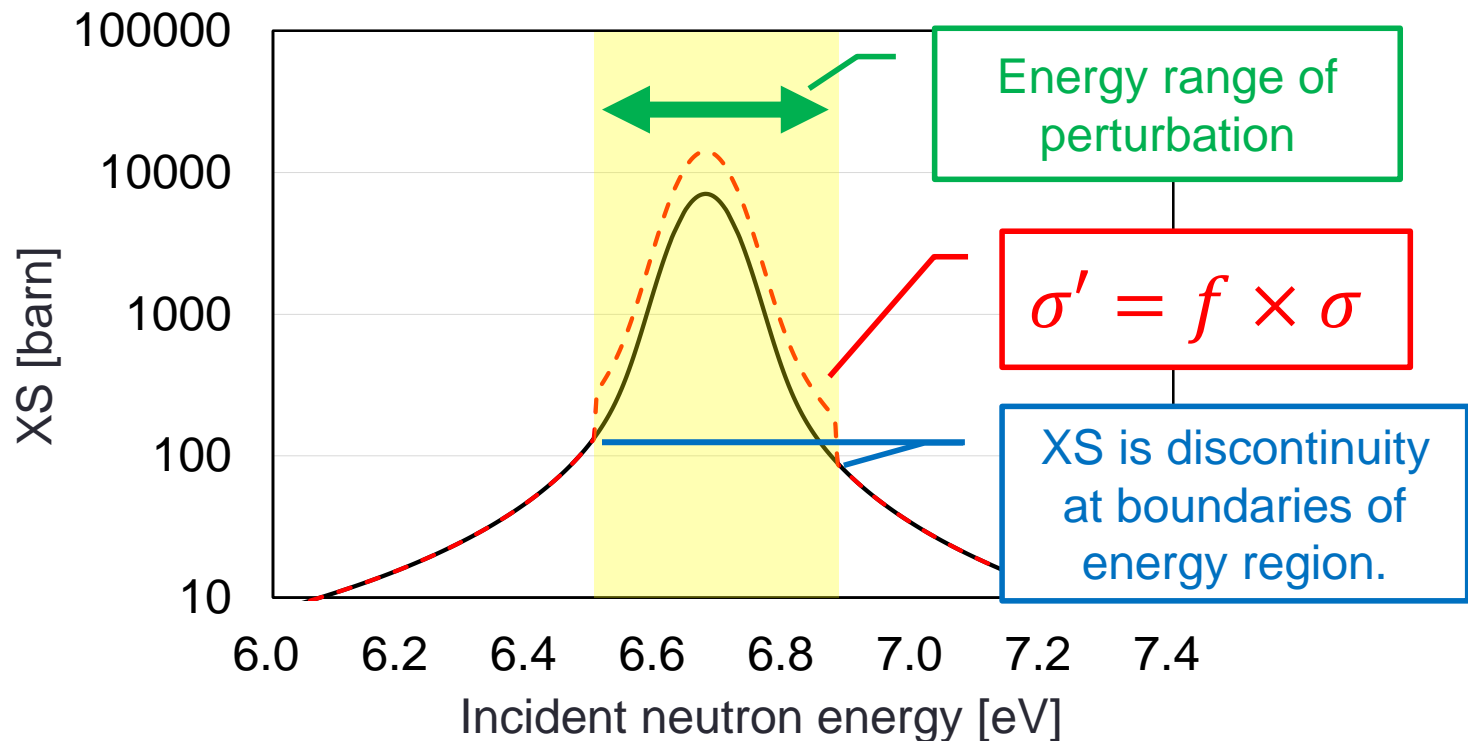Japan Atomic Energy Agency (JAEA)

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Ref: K. Tada, R. Kondo, T. Endo, A. Yamamoto, "Development of ACE file perturbation tool using FRENDY," *J. Nucl. Sci. Technol.*, **60**, pp.624-631 (2023).
https://www.tandfonline.com/doi/full/10.1080/00223131.2022.2130463
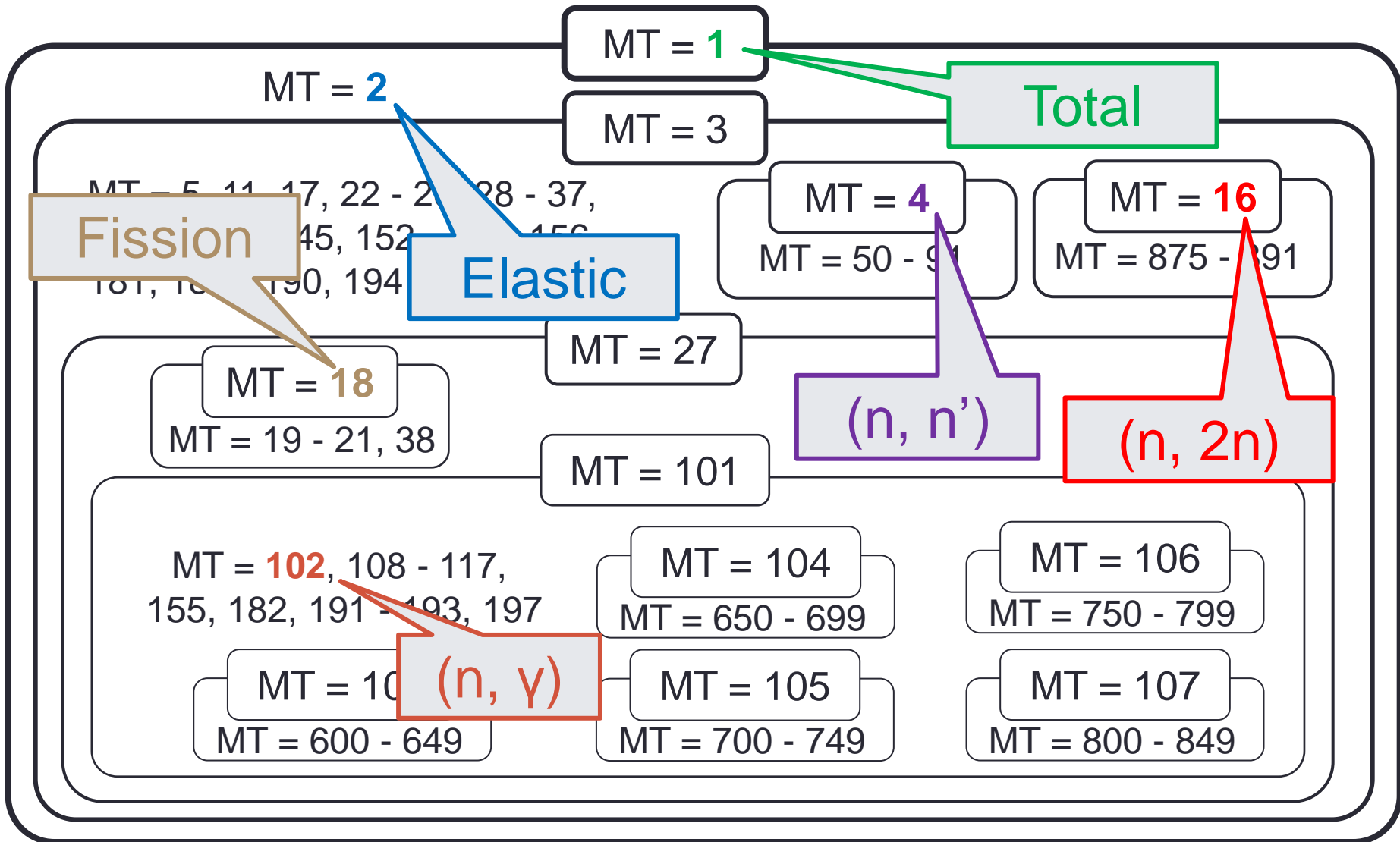
Perturbation of ACE file

- Perturbation tool decreases or increases cross section (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

Energy range of perturbation

$$\sigma' = f \times \sigma$$

XS is discontinuity at boundaries of energy region.

Relations of each reaction type

MT = **1**

Total

MT = **2**

MT = 3

Elastic

MT = 5, 11, 17, 22 - 2 , 28 - 37, 45, 152 - 156 181, 1 190, 194

Fission

MT = 4

MT = 50 - 9

(n, n')

MT = **16**

MT = 875 - 91

(n, 2n)

MT = **18**

MT = 19 - 21, 38

MT = 27

MT = 101

MT = **102**, 108 - 117, 155, 182, 191 - 193, 197

(n, γ)

MT = 10

MT = 600 - 649

MT = 104

MT = 650 - 699

MT = 105

MT = 700 - 749

MT = 106

MT = 750 - 799

MT = 107

MT = 800 - 849

Example of fission XS perturbation

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

MT18 contains MT=19-21 and 38.
MT=19-21 and 38 are also perturbed.
$$\sigma_{19}' = f \times \sigma_{19}, \sigma_{20}' = f \times \sigma_{20},$$
$$\sigma_{21}' = f \times \sigma_{21}, \sigma_{38}' = f \times \sigma_{38}$$
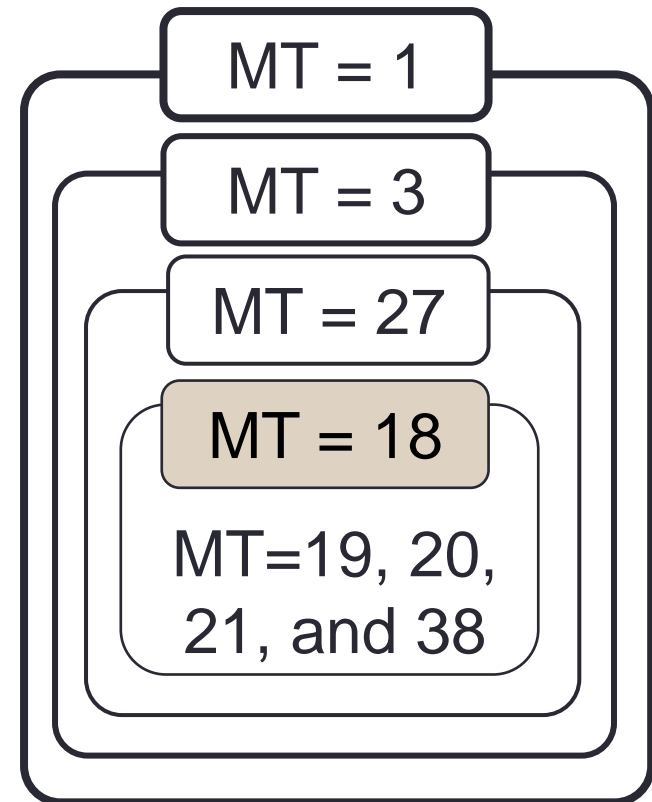
MT=1, 3, and 27 contain MT=18.
XS of MT=1, 3, and 27 are modified.
$$\Delta\sigma_{18} = \sigma_{18}' - \sigma_{18}$$
$$\sigma_1' = \sigma_1 + \Delta\sigma_{18}, \sigma_3' = \sigma_3 + \Delta\sigma_{18}$$
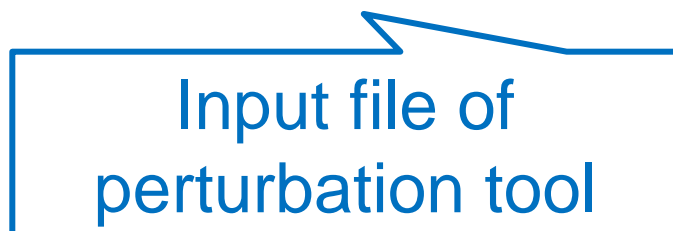$$\sigma_{27}' = \sigma_{27} + \Delta\sigma_{18}$$

MT = 1

MT = 3

MT = 27

MT = 18

MT=19, 20, 21, and 38

How to use perturbation tool

- Compile of perturbation tool
  - Run "make" command on "frendy_20YYMMDD/tools/perturbation_ace_file".
  - Executable file (perturbation_ace_file.exe) is generated.
- Manual of perturbation tool is "frendy_20YYMMDD/tools/README_tools".

./perturbation_ace_file.exe ace_file.ace perturbation_list.inp

Perturbation
ACE file name

Input file of
perturbation tool

Input of perturbation tool

- Following four parameters **must be set in one line**.

  - 1) Reaction type (MT number)

  - 2) Lower energy of perturbed energy range [**MeV**]

  - 3) Upper energy of perturbed energy range [**MeV**]

  - 4) Perturbation factor f ($\sigma' = f \times \sigma$)

ACE file uses MeV for unit of energy.
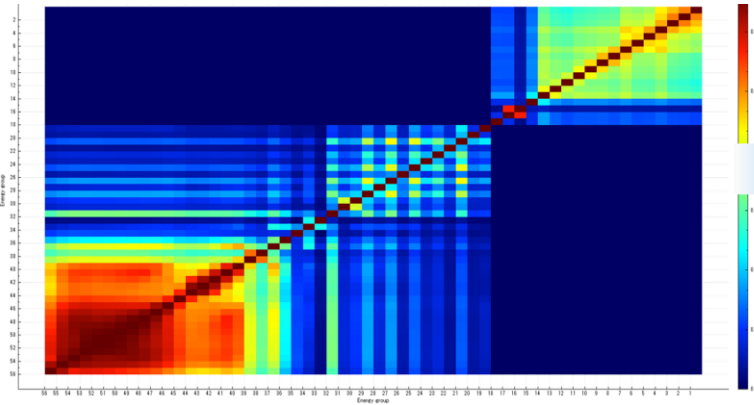
[Example of input of perturbation tool]

```
 2  1.0e-11  1.0e-10  1.1
18  1.0e-6   1.0e-5   0.9
```

Available reaction type

- Cross section data (MF=3)
  - MT=1-999
- Number of neutron per fission (MF=1/MT=452-456)
  - MT=452 (v-tot), 455 (v-d), and 456 (v-p)
- Fission spectrum
  - MT=1018
- Elastic scattering angle distribution
  - MT=251

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

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 [1]

[1] 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