

# ACE file perturbation tool

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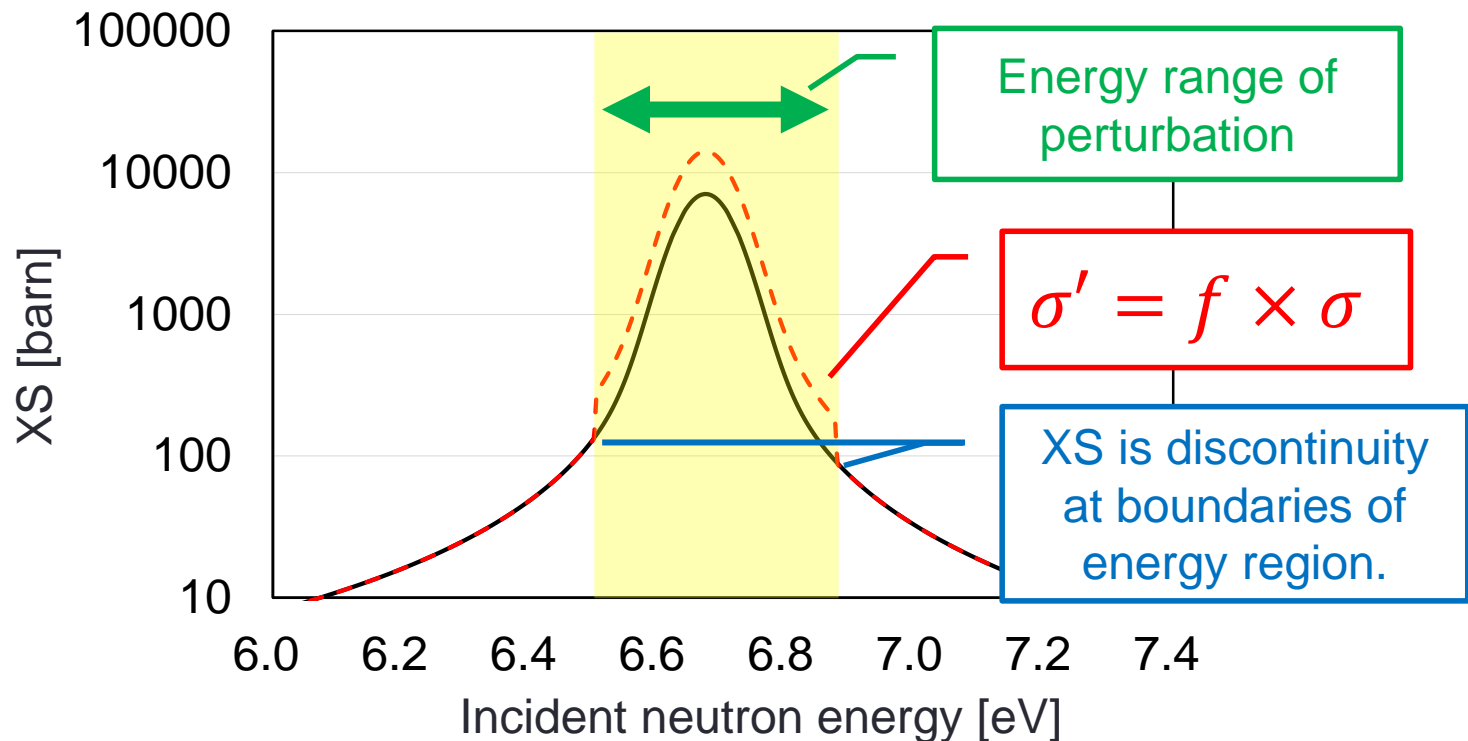
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Ref: K. Tada, R. Kondo, T. Endo, A. Yamamoto, "Development of ACE file perturbation tool using FRENDY," *J. Nucl. Sci. Technol.*, **60**, pp.624-631 (2023).

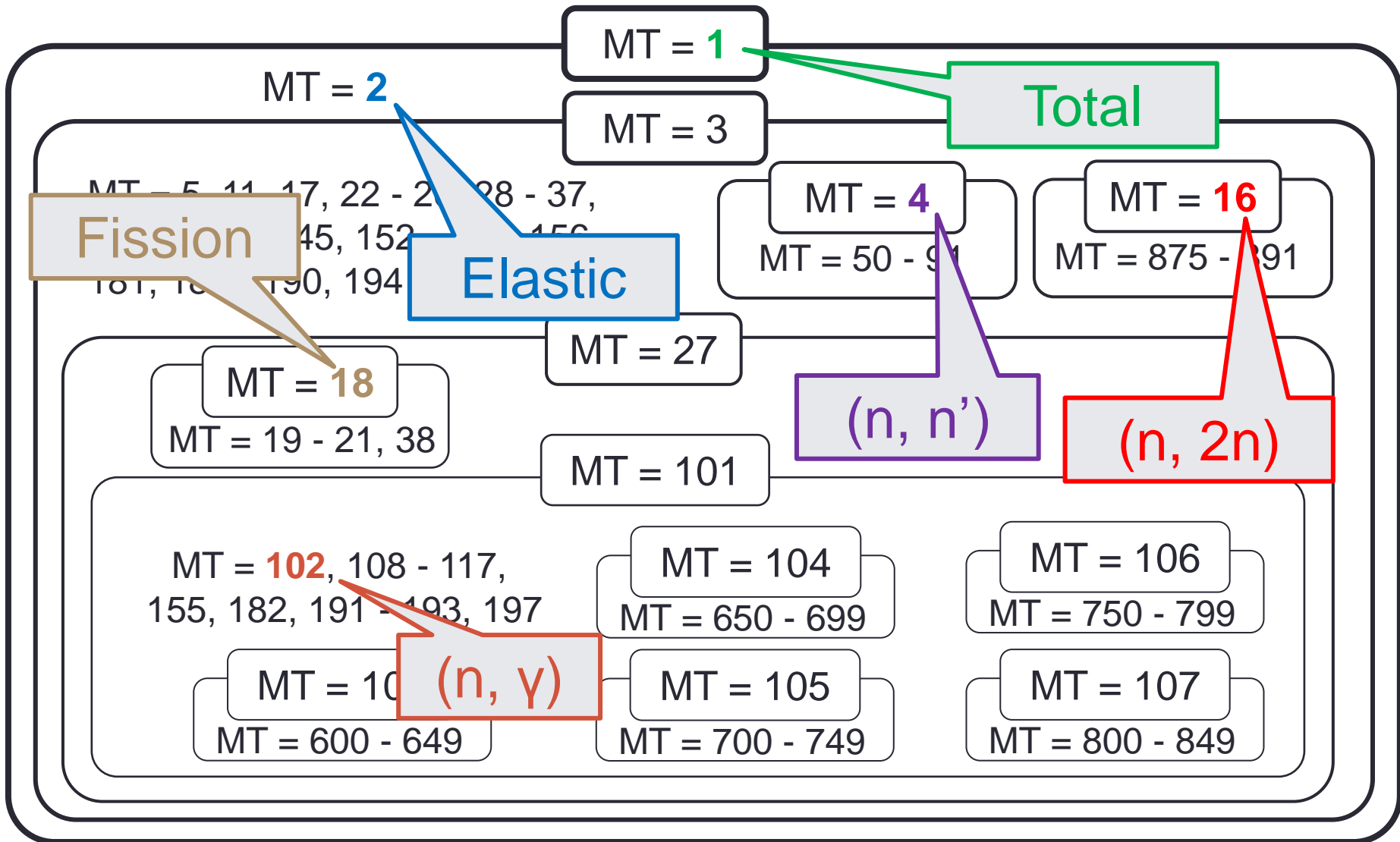
<https://www.tandfonline.com/doi/full/10.1080/00223131.2022.2130463>

# Perturbation of ACE file

- Perturbation tool decreases or increases cross section (XS) or number of neutron per fission ( $\nu$ ) or fission spectrum ( $\chi$ ).
  - XS or  $\chi$  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):  $\sigma_{18}' = f \times \sigma_{18}$  (Perturbation factor:  $f$ )

MT18 contains MT=19-21 and 38.

MT=19-21 and 38 are also perturbed.

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

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

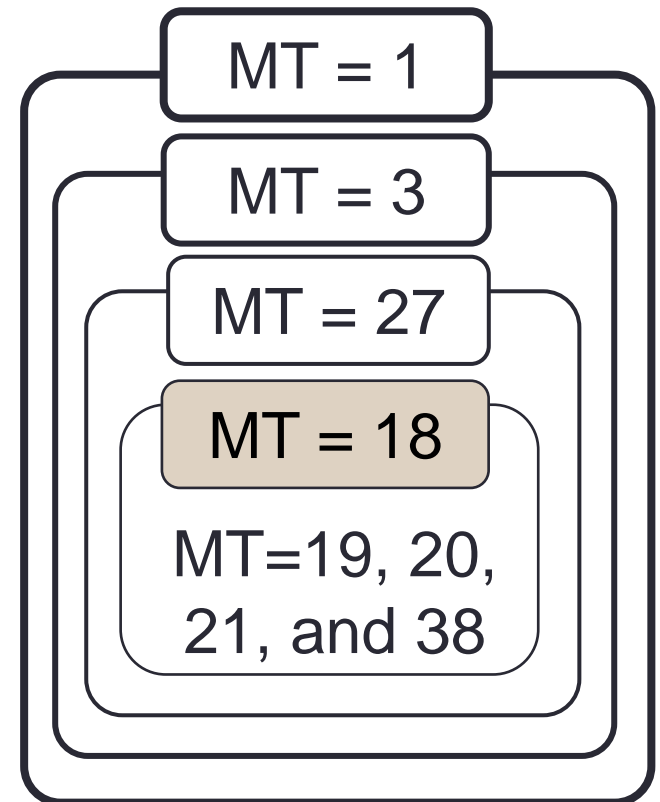
MT=1, 3, and 27 contain MT=18.

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

$$\Delta\sigma_{18} = \sigma_{18}' - \sigma_{18}$$

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

$$\sigma_{27}' = \sigma_{27} + \Delta\sigma_{18}$$



# 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  $f$  ( $\sigma' = f \times \sigma$ )

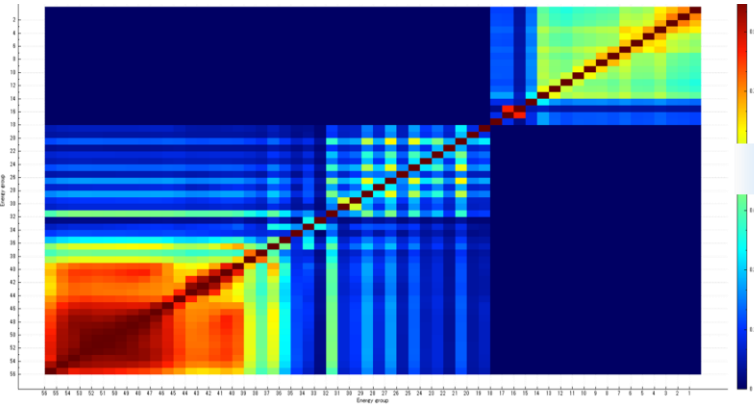
ACE file uses MeV  
for unit of energy.

[Example of input of perturbation tool]

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

# Random sampling

Covariance matrix of nuclear data



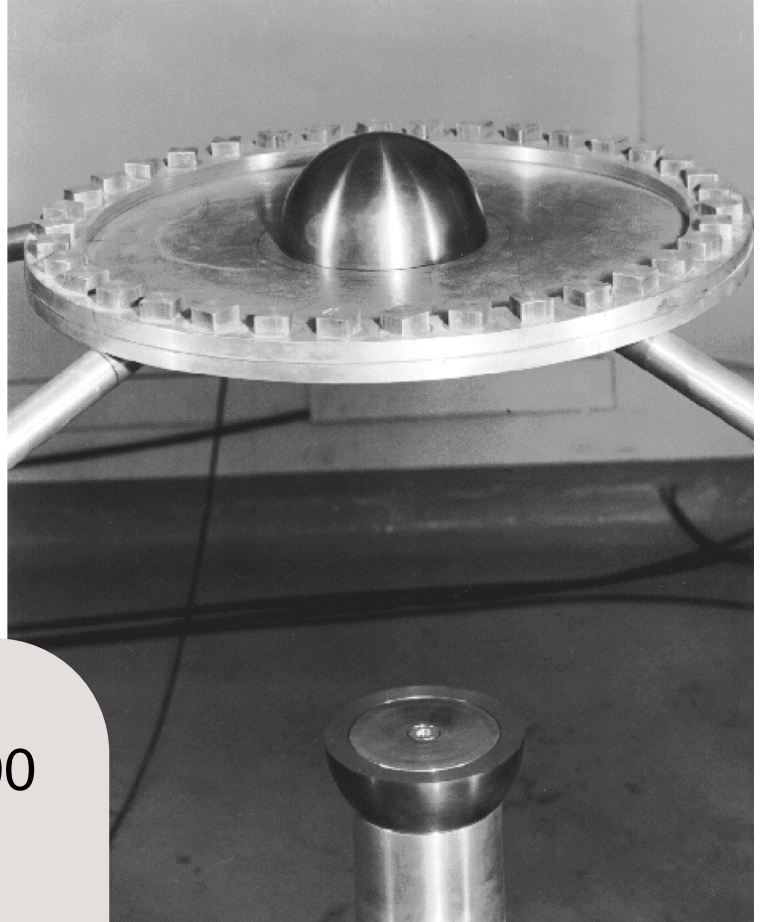
```
inp/Nddd_000x
102 2.00E+01 6.43E+00 8.78E-01
102 6.43E+00 4.30E+00 8.67E-01
102 4.30E+00 3.00E+00 8.62E-01
. . .
```

- 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.%
$k_{eff}$	$1.000 \pm 0.001$



Godiva [1]

- ◆ 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:  $\nu$ , MT=1018:  $\chi$ )

[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)

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

		SA (TSUNAMI-1D)	SA (MCNP6.2)	RS
U-235	(n, $\gamma$ )	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	$\nu_{\text{total}}$	0.085	0.085	0.093