New capability of FRENDY for multi-group neutron cross section processing

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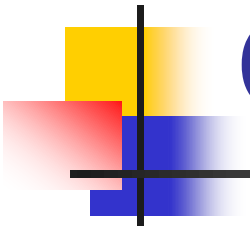
Manual: https://doi.org/10.11484/jaea-data-code-2022-009
Download: https://rpg.jaea.go.jp/main/ja/program_frendy/



Outline

- Background
- Outline of FRENDY V1 (ACE file generation)
- Multi-group generation capability of FRENDY
  - Outline
  - Theory
  - Verifications

Background

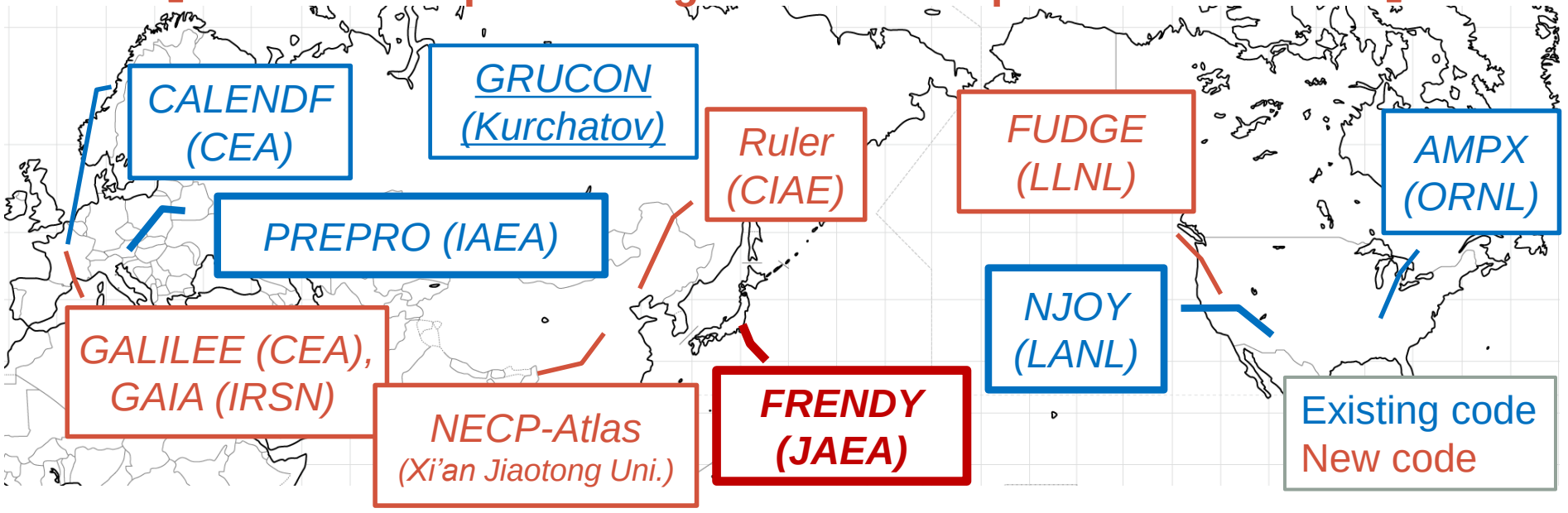
- NJOY has been widely used to generate multi-group cross sections for deterministic core analysis codes
- Independent efforts to develop nuclear data processing codes have been carried out
- A nuclear data processing code, FRENDY, is being developed in JAEA (Japan Atomic Energy Agency)
- Generation capability of ACE pointwise cross section has been implemented and released (FRENDY V1)
- Generation capability of multi-group cross section is implemented and released as FRENDY V2

Outline of FRENDY V1 nuclear data processing code

Present status of nuclear data processing code developments

- Development of nuclear data processing code is started in many institute
  - To process their own nuclear data library
  - To handle new nuclear data format GNDS

【Nuclear data processing codes development in the world】



Ref. D. Brown, "The New Evaluated Nuclear Data File Processing Capabilities," *INDC(NDS)-0695*.

Development of nuclear data processing code FRENDY

- JAEA started developing a new nuclear data processing code FRENDY in 2013
  - **FR**om **E**valuated **N**uclear **D**ata librar**Y** to any application
  - To process the nuclear data library **with simple input file**

- The **first goal** is processing the nuclear data for continuous energy Monte Carlo codes
  - For MVP, PHITS of JAEA and MCNP of LANL

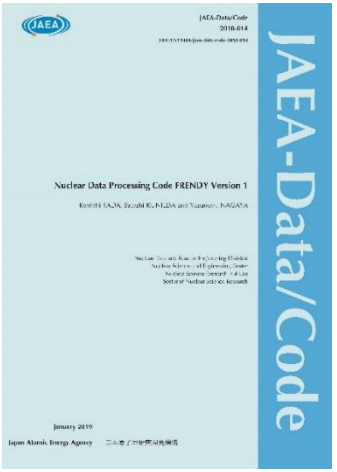
Features of FRENDY

- Utilization of modern programming techniques
  - C++, BoostTest library, Git
  - Improvement of quality and reliability
- Consideration of maintainability, modularity, portability and flexibility
  - Encapsulate all classes
  - Minimize the function
  - Maintain the independence of each module
- Processing methods of FRENDY is similar to NJOY99
- Incorporating requests from users of nuclear data processing codes
  - Development of FRENDY is supported by many organizations and companies in Japan

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 JAEA website
  - https://rpg.jaea.go.jp/main/en/program_frendy/
  - FRENDY Ver.1 generates ACE files
  - FRENDY Ver.1 is open source software
    - 2-Clause BSD license
- Manual of FRENDY Ver. 1 is published from JAEA
  - JAEA-Data/Code 2018-014
    - https://jopss.jaea.go.jp/pdfdata/JAEA-Data-Code-2018-014.pdf
  - The input instructions and the details of processing method are described



Outline and features of multi-group generation capability of FRENDY V2

Concepts for developments of MG XS generation capability

- Use ACE files as input cross section rather than original ENDF files
  - FRENDY V1 can generate ACE files
  - Processing corresponding to RECONR-BROADR-UNRESR(PURR)-THERMR in NJOY has been done in ACE cross sections
  - Highly accurate
  - Versatile cross section data including delayed neutron information
  - Formal document for ACE format
  - Adopted in many continuous energy Monte-Carlo codes; familiar in reactor physics community
- Focus on neutron cross sections. Processing of photon cross section will be a future extension
- Developed as a class library of c++ using namespace considering integration to FRENDY.

Major capabilities and features

- Weighting spectrum
  - 1/E
  - Fission + 1/E + Maxwell (arbitrary cutoff, temperature)
  - User input
- Ultra-fine group spectrum
  - Direct slowing down calculation or narrow resonance approximation
  - Automated correction of ultra-fine energy grid 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
  - Arbitrary number of background cross sections

Major capabilities and features

- Self-shielding for unresolved resonance region using probability table
- Automated background cross section settings
- Resonance up-scattering treatment
- Treatment of angle/energy distributions
  - Can treat LAW=3, 4, 7, 9, 44, 61, and 66 in an ACE file
  - Can treat all nuclides in B-VII.1, B-VIII.0, JEFF-3.3, TENDL-2019, 2021, JENDL4.0, and JENDL5
- Scattering matrices
  - Can treat all reactions with secondary neutron(s) including self-shielding and anisotropic scattering
  - $S(\alpha,\beta)$: free gas model, short collision time approximation, incoherent inelastic, incoherent elastic, and coherent elastic.

Major capabilities and features

- Fission spectrum, ν values
  - Prompt
  - Delayed (each group)
  - Prompt + Delayed
  - Any number of delayed neutron groups
- Arbitrary thermal cutoff
- Arbitrary multi-group energy structure up to a few thousands
- Output format of multi-group cross sections
  - FRENDY V2 original format (readable output list)
  - MATXS
  - GENDF

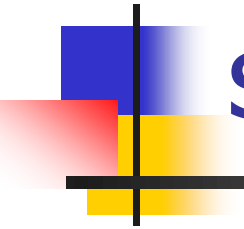
Example of input data(UO2)

```
mg_neutron_mode                          //Process mode

  mg_edit_option          MATXS

  nucl_file_name        (
      n_008-O-016.dat
      n_092-U-235.dat
      n_092-U-238.dat)

  mg_file_name          mix_UO2         //Output file name
  mg_structure ( xmas-nea-lanl-172 )

  temp                     600.0
  legendre_order           3
  sigma_zero_data         (auto)

                         //8016.50c     92235.50c    92238.50c
  mg_number_density       (4.0e-2       1.0e-3       2.0e-2)
```

Example of input data (H in H2O)

```
mg_neutron_mode                                  //Processing mode

  mg_edit_option       (MATXS  GENDF)

  nucl_file_name       H001.dat
  nucl_file_name_tsl   01_h_in_h2o.txt

  mg_file_name         lwtr_from_endf

  legendre_order            3
  mg_label_data            "HinH2O from JENDL"
  temp                      300.0
  sigma_zero_data          (1.0E+10  1000.0 1.0)

  mg_number_density         1.0
  mg_tsl_data_type          hh2o

  mg_flux_calc_mode         NR
```

Theories for multi-group cross section generation



Calculation of multi-group constants

1D cross sections

- 1D cross sections are collapsed by:

$$\sigma_{g,x,l} = \frac{\int_{E \in E_g} \sigma_x(E)\phi_l(E)dE}{\int_{E \in E_g} \phi_l(E)dE}$$

where g, x, l, $\sigma_x(E)$, $\phi_l(E)$, E_g, and E are energy group index, reaction type, Legendre order of angular flux moment, pointwise cross section of reaction x, l-th order angular flux moment, energy range for energy group g, and incident energy, respectively.

2D cross sections

- 2D cross sections are collapsed by:

$$\sigma_{g,g',x,l} = \frac{\int_{E\in E_g}\int_{E'\in E_{g'}} \sigma_{x,l}(E,E')\phi_l(E)dE'\,dE}{\int_{E\in E_g}\phi_l(E)dE}$$

where g, g', x, l, $\sigma_x(E)$, $\phi_l(E)$, E_g, $E_{g'}$, and E are incident energy group index, outgoing energy group index, reaction type, Legendre order of angular flux moment, l-th order angular flux moment, energy range for energy group g, energy range for energy group g', and incident energy, respectively.

- Legendre moments are calculated by:

$$\sigma_{x,l}(E,E') = \frac{\int_{-1}^{1}\sigma_x(E,E',\mu)P_l(\mu)d\mu}{\int_{-1}^{1}P_l(\mu)d\mu}$$

where $\sigma_x(E,E',\mu)$, μ, and $P_l(\mu)$ are the double differential cross section of incident energy E, outgoing energy E', scattering angle μ, scattering angle (direction cosine), l-th Legendre polynomial.

Treatment of MTs

- All types of cross sections for neutrons in an ACE file are automatically considered in FRENDY V2 and their multi-group cross sections are generated
- Some of (missing) MTs are automatically generated:

Automatically generated mt number if not exist in an ACE file	Summed mt numbers
4 (inelastic)	51-91
18 (fission)	19, 20, 21, 38
103 (n,p)	600-649
104 (n,d)	650-699
105 (n,t)	700-749
106 (n, ^{3}He)	750-799
107 (n, a)	800-849

Ultra-fine group spectrum calculation

- Two options can be used for ultra-fine group spectrum to collapse pointwise cross sections
  - Narrow resonance (NR) approximation
  - Ultra-fine group slowing down calculation
- Spectrum by the NR approximation

$$\phi_l(E) = \frac{W(E)}{(\sigma_t(E) + \sigma_b)^{l+1}}$$

$$\phi_l(E) = \frac{W(E)}{\left(\sum_k \sigma_{t,k}(E) N_k + \sigma_b \sum_k N_k\right)^{l+1}}$$

where $l, \phi_l(E), W(E), \sigma_t(E), \sigma_{t,k}(E), \sigma_b$, and N_k, are order of Legendre moment, neutron spectrum (P_l flux), weight, total microscopic cross section (of k-th nuclide), microscopic background cross section, and, number density of k-th nuclide, respectively.

Ultra-fine group spectrum calculation

- Weight can be chosen from
  - 1/E
  - Fission + 1/E + Maxwell
  - User input
- 1/E

$$W(E) = \frac{1}{E}$$

- Fission + 1/E + Maxwell

$$W(E) = \sqrt{E}\,\mathrm{e}^{-\frac{E}{T_f}} \quad (E \geq E_f)$$

$$W(E) = \frac{1}{E} \quad (E_f > E > E_t)$$

$$W(E) = E e^{-\frac{E}{T_m B}} \quad (E_t \geq E)$$

where E, T_f, T_m, B, E_f, and E_t are incident energy [eV], fission temperature [eV], Maxwell temperature [K], Boltzmann constant [eV/K], energy boundary between fission and $1/E$ spectra, and energy boundary between $1/E$ and thermal Maxwell spectra, respectively.

Ultra-fine group spectrum calculation

- The NR spectrum may not be accurate for wide resonances of heavy nuclides (e.g., 6.8eV large resonance of U238)
- Slowing down calculation provides more accurate results
- Slowing down equation

$$\Sigma_t(E)\phi(E) = S^{fission}(E) + \int_{E'>E} \sum_k \left(N_k \sigma_{s,k}(E')\right) \phi(E') \frac{dE'}{(1-\alpha_k)E'}$$

where E, $\Sigma_t(E)$, $\phi(E)$, $S^{fission}(E)$, N_k, $\sigma_{s,k}(E)$, and α_k are energy at the LAB system, total cross section, scalar flux, fission source, number density of k-th nuclide, elastic scattering cross section of k-th nuclide, and $\alpha_k = \frac{(A_k-1)^2}{(A_k+1)^2}$ (A_k is the relative mass of k-th nuclide to neutron).

- Assumptions
  - Inelastic scattering is neglected
  - A fictitious background (moderator) nuclide having a constant scattering cross section (σb)
  - Zero absorption cross section for moderator fictitious moderator nuclide

Ultra-fine group spectrum calculation

- In numerical calculation:

$$\Sigma_{t,g}\phi_g = S_g^{fission} + \sum_{g'=1}^{g-1}\sum_k \left(N_k\sigma_{S,k,g'}\right)\phi_{g'}\frac{dE_{g'}}{(1-\alpha_k)E_{g'}}$$

where g and $dE_{g'}$ are the index of ultra-fine energy group and energy width of g'-th ultra-fine energy group.

- The above equation is numerically solved by the recurrent formula proposed by Kier.
  - Details are described in "Handbook of Nuclear Engineering" Chap.9, Lattice Physics Computation.

Ultra-fine group spectrum calculation

- The NR spectrum and slowing down spectrum are combined even if slowing down calculations are carried out since slowing down calculation cannot accurately consider:
  - Fast spectrum shape due to fission spectrum
  - Thermal Maxwell spectrum shape
- The NR spectrum is used for $E > E_{high}$, $E < E_{low}$
- Slowing down spectrum is used for $E_{high} \geq E \geq E_{low}$
- E_{high} and E_{low} are user specified parameters, e.g., $E_{high} = 10^4$ eV, $E_{low} = 1$ eV.
- For multi-group P0/P1 flux, the NR spectrum is used for whole energy range to avoid discontinuity between NR/slowing down spectra

Ultra-fine group spectrum calculation

- Slowing down calculation can be carried out considering multiple nuclides
- Total cross section is calculated by:

$$\Sigma_t(E) = \sum_k \sigma_{t,k}(E) N_k + \sigma_b \sum_k N_k \,.$$

- Note that the background cross section is multiplied by $\sum_k N_k$ in this calculation. Namely, a mixture is considered as a "fictitious resonance nuclide".

Ultra-fine group spectrum calculation

- Choice of background cross section and its mass
  - Infinite dilute background cross section is always necessary (10^{10} barn)
  - Smaller background cross sections representing shielded conditions should be appropriately provided by input. Number and point of background cross sections depend on the behavior and interpolation scheme of self-shielding factor.
- Mass of the background nuclide can be specified
  - Mass is defined by the relative mass to the neutron
  - Default: hydrogen, 0.999167
  - Can consider heavier nuclide such as oxygen.
  - Can be used for intermediate resonance (IR) parameter estimation

Ultra-fine group spectrum calculation

- Example of IR estimation procedure (O16 & U238)

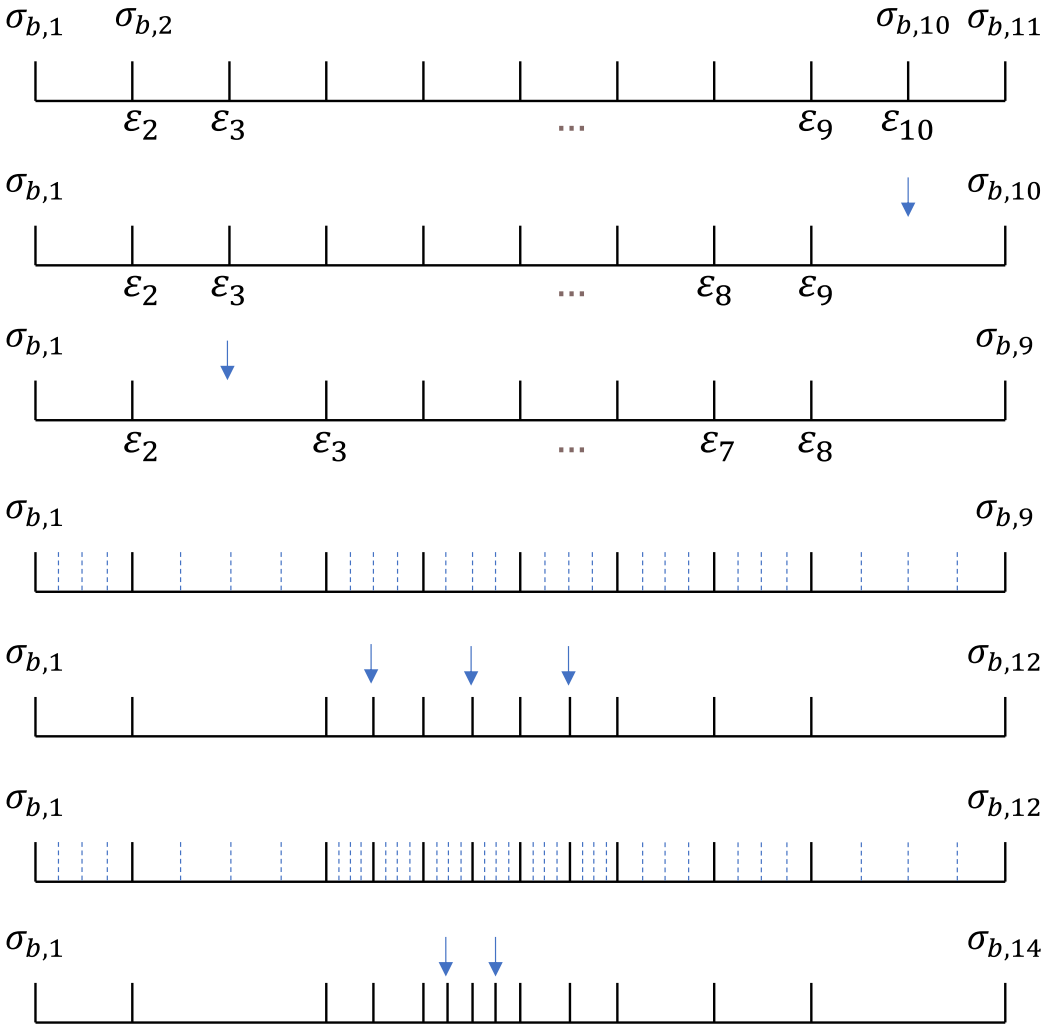
1) Generate effective cross section of U238 using slowing down calculation. The background cross section of σ_{b0} and default mass (a_0 =0.999167) for the background nuclide are used. The generated microscopic cross section is σ_0.
2) Generate effective cross section of U238 using slowing down calculation. The background cross section of σ_{b0} and mass of oxygen (a_1 =15.8575) for the background nuclide are used. The generated microscopic cross section is σ_1.
3) Generate effective cross section of U238 using slowing down calculation. The background cross section of σ_{b1} (e.g., $\sigma_{b1} = 1.05 \times \sigma_{b0}$) and default mass ($a_0$ =0.999167) for the background nuclide are used. The generated microscopic cross section is σ_2.
4) The IR parameter is calculated by:

$$f_{IR} = 1 + \frac{\sigma_1 - \sigma_0}{\frac{\sigma_2 - \sigma_0}{\frac{\sigma_{b1} - \sigma_{b0}}{\sigma_{b0}}}}$$

Automated background XS settings

- Choice of background cross section in slowing down calculation requires experience and knowledge
- An automated sequence to choose appropriate background XS is implemented in FRENDY V2.
  - Minimize interpolation error and number of background cross sections
  - Adaptively add/eliminate background cross sections
  - Interpolation error is measured by self-shielding factor or reaction rate

Automated background XS settings



Steps (1) - (4)

Steps (5), (6), (7)

Steps (5), (6), (7)

Steps (8) - (12)

Steps (13) - (16)

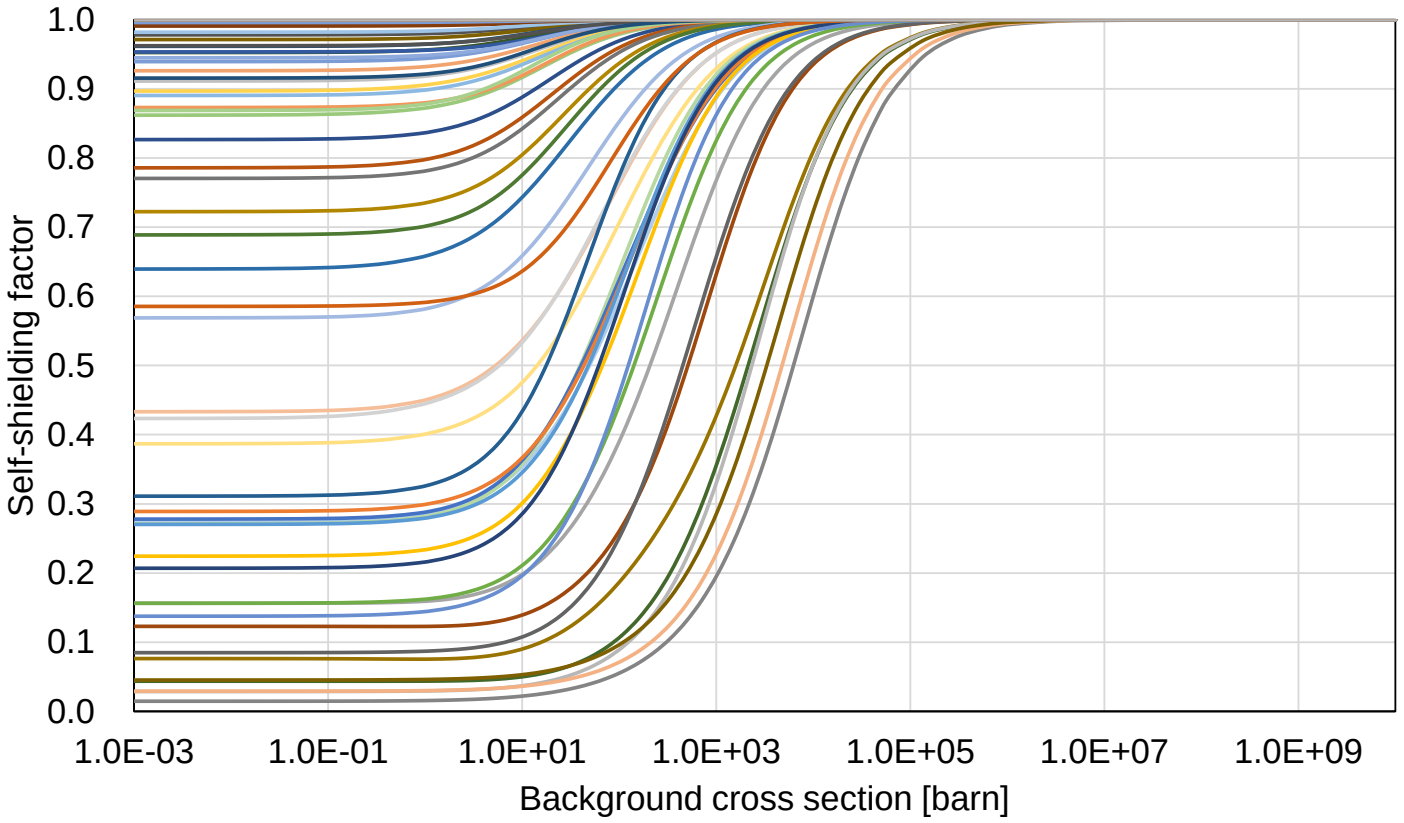
Steps (13) - (16)

Steps (13) - (16)

- https://doi.org/10.1080/00223131.2021.1944930

Automated background XS settings

- Example of self-shielding factor (U-238, capture cross section, XMAS 172 energy groups, >1.0eV, 300 K).



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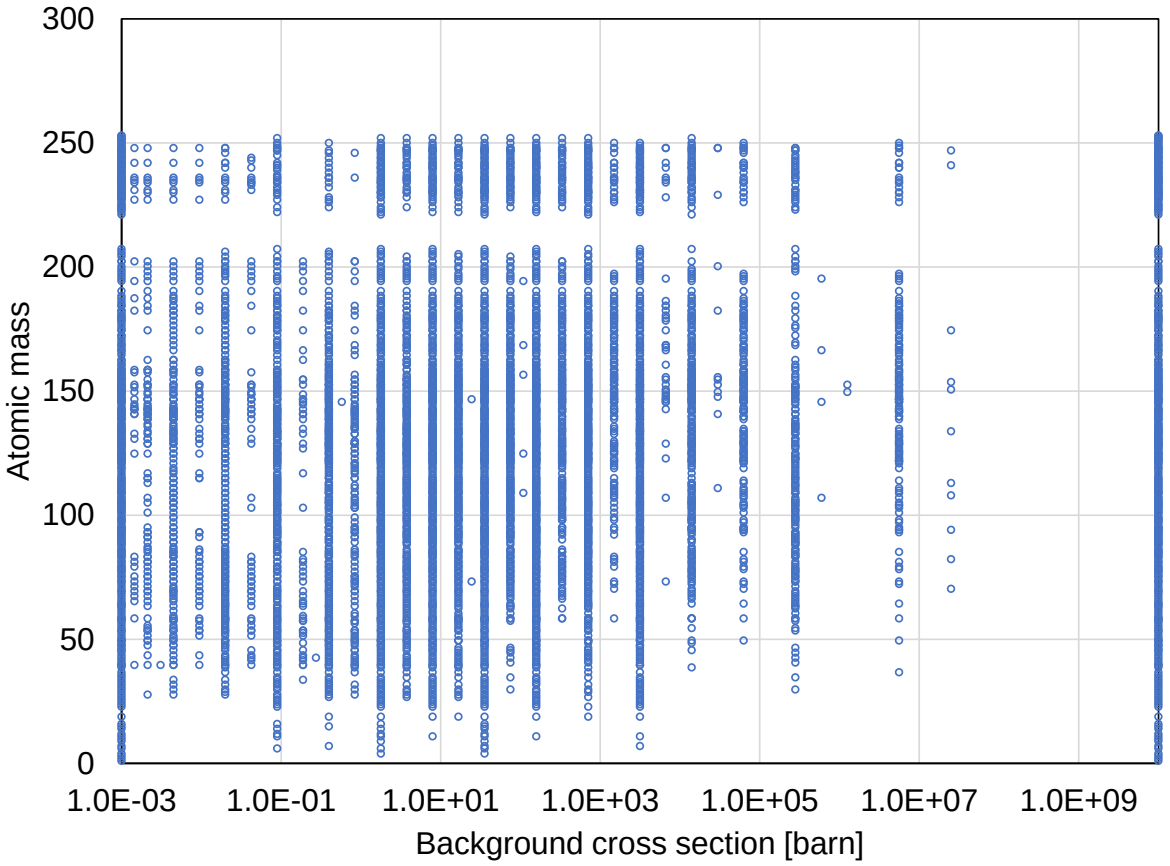
Automated background XS settings

- Adaptively set background cross sections for all nuclides in JENDL-4.0 or -4.0u.



•https://doi.org/10.1080/00223131.2021.1944930

Resonance up-scattering treatment

- In the epi-thermal energy range, neutron scattering is usually treated as the asymptotic kernel:

$$K_{as,i}(E \to E') = \begin{cases} \dfrac{1}{(1-\alpha_i)E} & (\alpha_i E \le E' \le E) \\ 0 & (E', < \alpha_i E \; E' > E) \end{cases}$$

where $\alpha_i = (A_i - 1)^2/(A_i + 1)^2$ and A_i is the relative mass of target nuclide i to a neutron. In the asymptotic kernel, transfer probability takes a constant value for $\alpha_i E \le E' \le E$.

Resonance up-scattering treatment

- However, especially for heavy nuclides, up-scattering due to thermal motion of nucleus may no be neglected in epi-thermal energy range:

$$K_{ru,i,l}(E \to E')$$

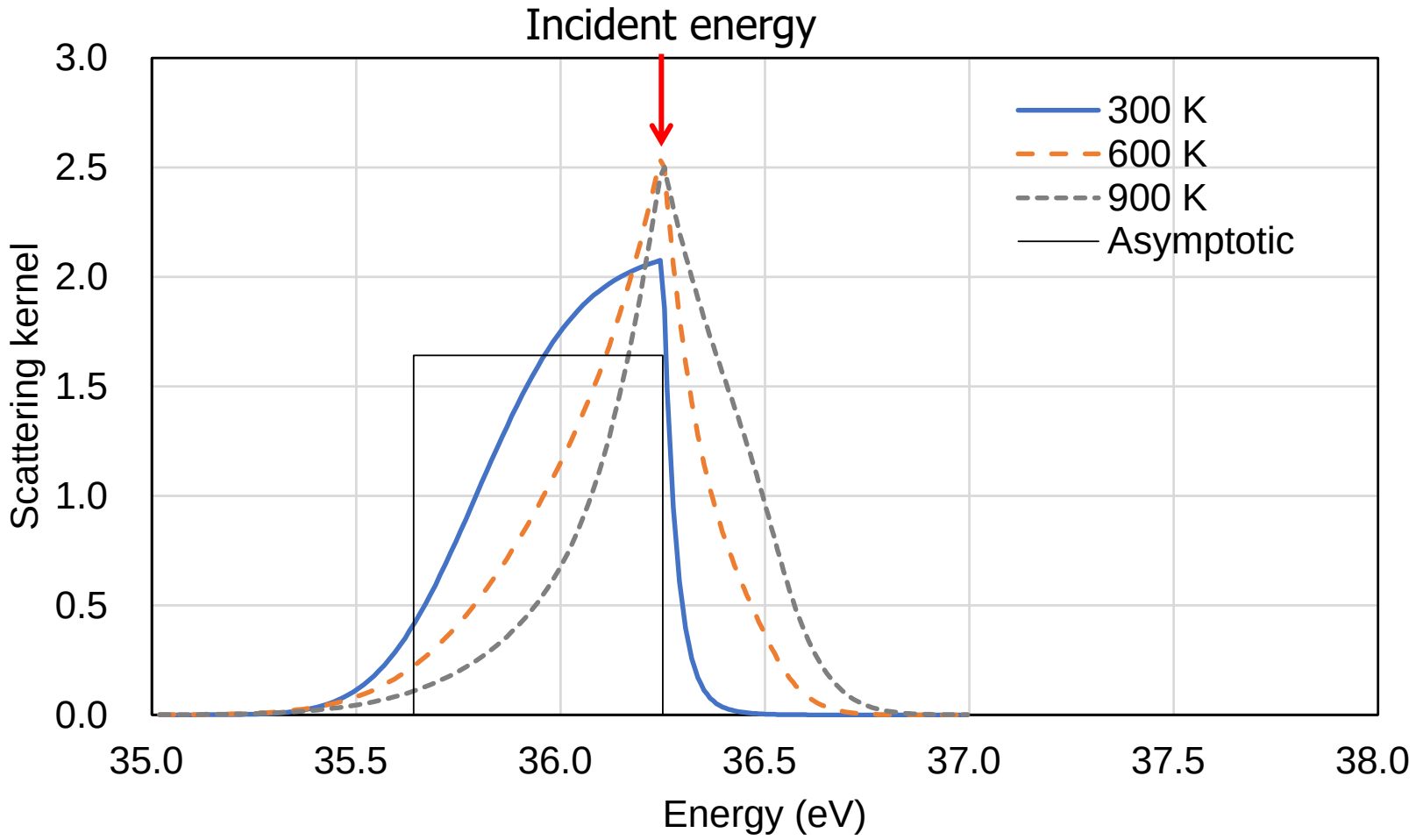
$$= \frac{1}{\sigma_{s,i,l}(E)} \frac{\beta_i^{\frac{5}{2}}}{4E} \int_0^\infty t\sigma_{s,i}\left(\beta_i \frac{kT}{A_i} t^2\right) \exp\left(\frac{E}{kT} - \frac{t^2}{A_i}\right) \Psi_l(t) dt$$

where $\sigma_{s,i,l}(E)$, $\sigma_{s,i}(E)$, β_i, k, and T are the l-th order total elastic scattering cross section at T K, the total elastic scattering at 0 K of nuclide i at incident energy E, $\beta_i = (A_i + 1)/A_i$, the Boltzmann constant, and temperature, respectively.

$$\Psi_0(t) = H(t_+ - t)H(t - t_-)[\mathrm{erf}(t + \varepsilon_{min}) - \mathrm{erf}(\varepsilon_{max} - t)] + H(t - t_+)[\mathrm{erf}(t + \varepsilon_{min}) - \mathrm{erf}(t - \varepsilon_{min})]$$

where H and erf represent the Heaviside and error functions, respectively, and $\varepsilon_{min} = \sqrt{\min(E, E')(A_i + 1)/kT}$, $\varepsilon_{max} = \sqrt{\max(E, E')(A_i + 1)/kT}$, $t_\pm = (\varepsilon_{max} \pm \varepsilon_{min})/2$.

Resonance up-scattering treatment



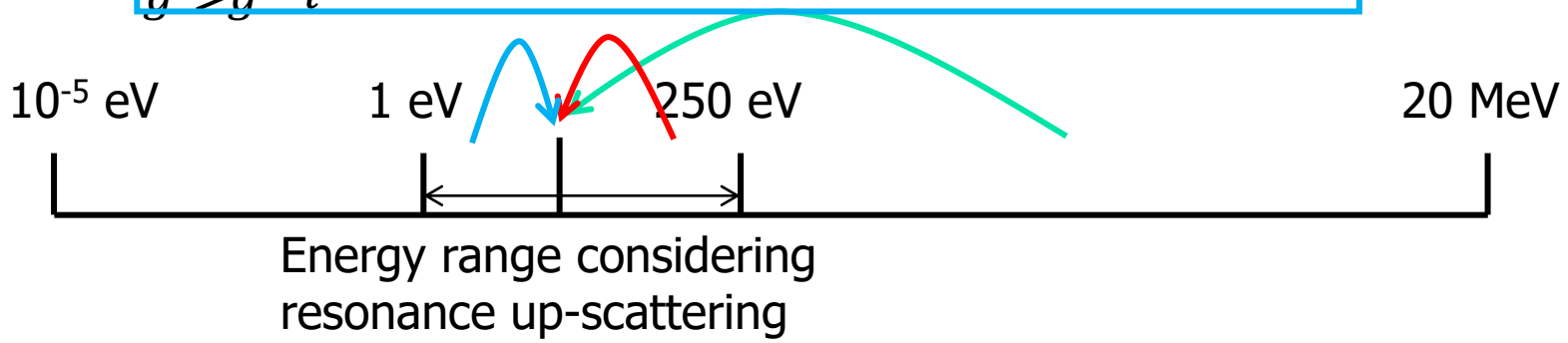
Resonance up-scattering treatment

$$\sum_i N_i \sigma_{t,i,g}\, \phi_g^{(n+1)} \Delta E_g$$

$$= \sum_{g' < g_{250eV}} \sum_i K_{ru,i,0,g' \to g} N_i \sigma_{s,i,g'}\, \phi_{g'}^{(0)} \Delta E_{g'}$$

$$+ \sum_{g_{250eV} \le g' < g} \sum_i K_{ru,i,0,g' \to g} N_i \sigma_{s,i,g'}\, \phi_{g'}^{(n+1)} \Delta E_{g'}$$

$$+ \sum_{g' > g} \sum_i K_{ru,i,0,g' \to g} N_i \sigma_{s,i,g'}\, \phi_{g'}^{(n)} \Delta E_{g'}$$



Resonance up-scattering treatment

- Mosteller benchmark results

	Method	Asymptotic kernel			RUSK			FTC Diff. (%)
		HZP	HFP	FTC	HZP	HFP	FTC	
Lee, et al. (2008)	CASMO-5	1.29990	1.28907	-2.15	1.29878	1.28696	-2.36	9.4
Xu, et al., (2019)	EPRI-CPM 69G	1.29831	1.28719	-2.22	1.29790	1.28569	-2.44	10.0
Ouisloumen, et al., (2015)	PARAGON	1.29964	1.28952	-2.01	1.29902	1.28803	-2.19	8.8
FRENDY V2	CBZ/XMAS 172G	1.28392	1.27232	-2.37	1.28258	1.26995	-2.58	9.2
	CBZ/SHEM 361G	1.29643	1.28614	-2.06	1.29564	1.28444	-2.24	9.1

Unresolved Resonance treatment

- Self-shielding factor for unresolved resonance region is calculated using the probability table
- "Self-shielded" point-wise cross sections in the unresolved resonance region are used for ultra-fine group calculation and successive processing
- Two options for the probability table in an ACE file
  - IFF=0, probability table for cross section
  - IFF=1, probability table for self-shielding factor
- For IFF=0, effective cross section is once generated and then converted to self-shielding factor
- Cross section/self-shielding factor is calculated by:

$$\sigma_x = \frac{\sum_i \frac{w_i \sigma_{x,i}}{\sigma_b + \sigma_{t,i}}}{\sum_i \frac{w_i}{\sigma_b + \sigma_{t,i}}}$$

where σ_x, $\sigma_{x,i}$, σ_b, $\sigma_{t,i}$, and w_i are the effective cross section of reaction x, the i-th band cross section of reaction x, background cross section, i-th band total cross section, and the band probability (weight).

Unresolved Resonance treatment

- P1 weighted total cross section is calculated by:

$$\sigma_t^{P1} = \frac{\sum_i \frac{w_i \sigma_{t,i}}{\left(\sigma_b + \sigma_{t,i}\right)^2}}{\sum_i \frac{w_i}{\left(\sigma_b + \sigma_{t,i}\right)^2}}$$

- Note on infinite dilute cross sections for total cross section
  - Two different definition of infinite dilute cross sections: point-wise total cross section, average total cross section obtained by the resonance ladder calculation in a probability table calculation
  - These two values are different
  - In FRENDY V2, point-wise total cross section is used for the infinite-dilute total cross section.
  - In the case of IFF=1, $\sigma_{t,i}$ is calculated by the point-wise total cross section in FRENDY (MG generation) while the average total cross section obtained in a ladder calculation is used in FRENDY (ACE generation)
  - The above inconsistency is the cause of difference of shielded cross section between FRENDY(ACE) and FRENDY(MG)

Cross sections with emitting neutrons

- Following LAWs in an ACE file can be treated

LAW	Angular distribution	Energy distribution
None (Elastic scattering, mt=2)	AND block	Analytically calculated from angular distribution
3 (Inelastic scattering, mt=51-90)	AND block	Analytically calculated from angular distribution and parameter from DLW block
4, 7, 9, 11, 66 (Fission, (n,2n) reactions, etc.)	AND block	DLW block
44, 61 (Continuum inelastic scattering, mt=91)	DLW block	DLW block

Cross sections with emitting neutrons (Elastic scattering)

- In the elastic scattering, only angular distribution for an incident energy is given since outgoing energy is analytically calculated
- The multi-group elastic scattering cross section is calculated by:

$$\sigma_{s,l,g\to g'} = \frac{\int_{E\in g} \phi_l(E)\sigma_{s,l,E\to g'}dE}{\int_{E\in g} \phi_l(E)dE}$$

$$\sigma_{s,l,E\to g'} = \int_{E'\in g'} \sigma_s\big(E,E',\mu(E,E')\big)P_l\big(\mu(E,E')\big)dE'$$

$$= \int_{E'\in g'} \sigma_s\big(E,E',\mu(E,E')\big)P_l\big(\mu(E,E')\big)\frac{1}{\frac{d\mu(E,E')}{dE'}}d\mu$$

where E, E', $\sigma_{s,l,g\to g'}$, $\phi_l(E)$, $\sigma_s(E,E',\mu)$, and $P_l(\mu)$ are the incident energy (LAB), outgoing energy (LAB), multi-group scattering cross section (l-th order anisotropic), l-th order angular flux moment (P_l flux), scattering cross section from E to E', scattering angle μ, and l-th order Legendre polynomial $P_l(\mu)$.

Cross sections with emitting neutrons (Elastic scattering)

- The following relations are used for numerical integration:

$$\mu'_{CM} = \frac{\left(2 \times \frac{E'}{E} - (1+\alpha)\right)}{(1-\alpha)},$$

$$\alpha = \frac{(1-A)^2}{(1+A)^2}$$

$$\mu_{CM} = \begin{cases} -1 \left(\mu'_{CM} < -1\right) \\ \mu'_{CM} \left(-1 \le \mu'_{CM} \le 1\right) \\ 1 \left(\mu'_{CM} > 1\right) \end{cases}.$$

$$\mu_{LAB} = \frac{1 + A\mu_{CM}}{\sqrt{1 + A^2 + 2A\mu_{CM}}}$$

$$pdf_{LAB,i} = pdf_{CM,i} \times \frac{\left(A^2 + 2A\mu_{LAB,i,average} + 1\right)^{\frac{3}{2}}}{A^2\left(A + \mu_{LAB,i,average}\right)}$$

$$\sigma_{s,l,E\to g'} = \sum_{i=0}^{n-1} pdf_{LAB,i} \times P_l\left(\mu_{LAB,i,average}\right) \times \left(\mu_{LAB,i,upper} - \mu_{LAB,i,lower}\right)$$

Cross sections with emitting neutrons (LAW=3, level scattering)

- In the inelastic scattering(LAW=3), only angular distribution for an incident energy is given since outgoing energy is analytically calculated:

$$E_C^{out} = \left(\frac{A}{A+1}\right)^2 \times \left(E_L^{in} - \left(\frac{A+1}{A}\right)|Q|\right)$$

where
E_C^{out}: outgoing energy of a neutron in the CM system,
E_L^{in}: incident energy of a neutron in the LAB system,
A: relative atomic mass of target nuclide to a neutron,
$|Q|$: Q-value of inelastic scattering where $Q < 0$. The values of $\left(\frac{A}{A+1}\right)^2$ and $\left(\frac{A+1}{A}\right)|Q|$ are given in the DLW block of an ACE file.

$$E_L^{out} = E_C^{out} + \frac{E_L^{in} + 2\mu_C(A+1)\sqrt{E_L^{in}E_C^{out}}}{(A+1)^2}$$

μ_C: direction cosine in the CM system.

Cross sections with emitting neutrons (LAW=3)

- Legendre coefficients are calculated by the following equation when angular distribution is given in the laboratory system:

$$p_{L,l,g'}\left(E_L^{in}\right) = \int_{+\mu_{L,g',lower}}^{+\mu_{L,g',upper}} p_L\left(E_L^{in}, \mu_L\right) P_l(\mu_L) d\mu_L$$

where

$p_{L,l,g'}\left(E_L^{in}\right)$: Legendre coefficient for incident energy E_L^{in} and outgoing energy for g',

$p_L\left(E_L^{in}, \mu_L\right)$: probability density in the LAB system.

$\mu_{L,g',upper}$: upper value of direction cosine in the LAB system corresponding outgoing energy group g',

$\mu_{L,g',lower}$: lower value of direction cosine in the LAB system corresponding outgoing energy group g'.

Cross sections with emitting neutrons (LAW=3)

- Legendre coefficients are calculated by the following equation when angular distribution is given in the center of mass system

$$p_{L,l,g'}\left(E_L^{in}\right) = \int_{+\mu_{L,g',lower}}^{+\mu_{L,g',upper}} p_C\left(E_L^{in},\mu_C\right) J\left(E_L^{in},\mu_C\right) P_l(\mu_L) d\mu_L$$

where $p_C\left(E_L^{in},\mu_C\right)$ and $J\left(E_L^{in},\mu_C\right)$ is the probability density in the CM system and the Jacobian, respectively.

$$\mu_C = \frac{(A+1)^2 E_L^{out} - E_L^{in}(1+R^2)}{2RE_L^{in}},$$

$$\mu_L = \frac{1+R\mu_C}{\sqrt{1+R^2+2R\mu_C}}$$

$$R = A\sqrt{1-\frac{(A+1)(-Q)}{AE_L^{in}}}$$

$$J\left(E_L^{in},\mu_C\right) = \frac{d\mu_C}{d\mu_L} = \frac{(1+R^2+2R\mu_C)^{\frac{3}{2}}}{R^2(R+\mu_C)}$$

Cross sections with emitting neutrons (LAW=44/61, Kalbach-87 etc.)

- LAW=44/61 is used for mt=91 (continuum inelastic scattering)
- Coupled angular and energy distribution is given
- Legendre coefficients are calculated by the following equation when angular distribution is given in the LAB system:

$$p_{L,l}\left(E_L^{in}, E_L^{out}\right) = \int_{-1}^{+1} p_L\left(E_L^{in}, E_L^{out}, \mu_L\right) P_l(\mu_L) d\mu_L ,$$

where
$p_{L,l}\left(E_L^{in}, E_L^{out}\right)$: Legendre coefficient,
$p_L\left(E_L^{in}, E_L^{out}, \mu_L\right)$: probability density in the LAB system,
E_L^{in}: incident energy in the LAB system,
E_L^{out}: outgoing energy in the LAB system,
μ_L: direction cosine in the LAB system,
$P_l(\mu_L)$: Legendre polynomial of the *l*-th order.

Cross sections with emitting neutrons (LAW=41/61)

- Legendre coefficients are calculated by the following equation when angular distribution is given in the CM system:

$$p_{L,l}\left(E_L^{in}, E_L^{out}\right) = \int_{\mu_L^{min}}^{+1} p_C\left(E_L^{in}, E_C^{out}, \mu_C\right) J\, P_l(\mu_L) d\mu_L$$

where
$p_C\left(E_L^{in}, E_C^{out}, \mu_C\right)$: probability density distribution in the CM system,
E_C^{out}: outgoing energy in the CM system,
μ_C: direction cosine in the CM system,
$J = \frac{dE_C^{out}}{dE_L^{out}} \frac{d\mu_C}{d\mu_L}$: Jacobian.

Cross sections with emitting neutrons (LAW=41/61)

- The following relations are used for numerical integration

$$E_L^{out,max} = E_L^{in}\left(\sqrt{\frac{E_C^{out,max}}{E_L^{in}}} + \frac{1}{A+1}\right)^2$$

$$\mu_L^{min} = \frac{1}{2c}\left(1 + c^2 - \frac{E_C^{out,max}}{E_L^{out}}\right)$$

$$J = \sqrt{\frac{E_L^{out}}{E_C^{out}}} = \frac{1}{\sqrt{1 + c^2 - 2c\mu_L}},$$

$$c = \frac{1}{A+1}\sqrt{\frac{E_L^{in}}{E_L^{out}}} = \frac{1}{A+1}\frac{v_L^{in}}{v_L^{out}} = \frac{v_L^{in}}{A+1}\frac{1}{v_L^{out}} = v_{cm}\frac{1}{v_L^{out}} = \frac{v_{cm}}{v_L^{out}},$$

$$\mu_C = J(\mu_L - c),$$

Cross sections with emitting neutrons (other reactions)

- LAW=4 (continuous tabular)
  - The outgoing energy distribution is given in a tabulated form for each incident energy grid.
  - The table is interpolated based on the option specified by INTT (1/2=histogram/linear-linear).
  - The incident and outgoing energies are specified in the laboratory system.
- LAW=7 (simple Maxwellian fission spectrum)
  - The incident and outgoing energies are specified in the laboratory system.

$$f(E \to E') = \frac{\sqrt{E'}}{I} \exp\left(-\frac{E'}{\theta(E)}\right), 0 \le E' \le (E - U)$$

where

I: normalization factor to make $\int_0^{E-U} f(E \to E')dE' = 1$,

$\theta(E)$: effective temperature as a function of incident energy,

U: a constant to define the upper limit of outgoing energy.

Cross sections with emitting neutrons (other reactions)

- LAW=9 (evaporation spectrum)
  - The incident and outgoing energies are specified in the laboratory system.

$$f(E \to E') = \frac{E'}{I} \exp\left(-\frac{E'}{\theta(E)}\right), 0 \le E' \le (E - U)$$

where

I: normalization factor so that $\int_0^{E-U} f(E \to E')dE' = 1$,

$\theta(E)$: effective temperature as a function of incident energy,

U: a constant to define the upper limit of outgoing energy.

- LAW=11 (energy dependent Watt spectrum)
  - The incident and outgoing energies are specified in the laboratory system.

$$f(E \to E') = \frac{\exp\left(-\frac{E'}{a}\right)}{I} \sinh\left(\sqrt{bE'}\right), 0 \le E' \le (E - U)$$

where

I: normalization factor so that $\int_0^{E-U} f(E \to E')dE' = 1$,

a, b: parameters as a function of incident energy,

U: a constant to define the upper limit of outgoing energy.

Cross sections with emitting neutrons (other reactions)

- Definition of ENDF for LAW=66 (n-body phase space distribution), e.g., D2O evaluation of B7.1

$$f(E_C \rightarrow E'_C, \mu_C) = C_n \sqrt{E'_C}(E_C^{max} - E'_C),$$

$$C_3 = \frac{4}{\pi (E_C^{max})^2},$$

$$C_4 = \frac{105}{32 (E_C^{max})^{\frac{7}{2}}},$$

$$C_5 = \frac{256}{14\pi (E_C^{max})^5},$$

where

n: number of bodies in phase space, defined in an ACE file,

E_C^{max}: maximum possible outgoing energy in the CM system,

E_C: incident energy in the CM system,

E'_C: outgoing energy in the CM system,

μ_C: scattering angle (cosine direction) in the CM system.

Cross sections with emitting neutrons (other reactions)

- In FRENDY V2, following relation is used for LAW=66:

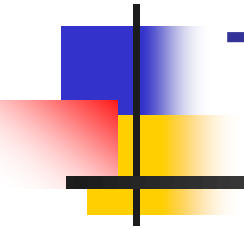
$$f(E_L \to E'_L, \mu_L) = C_n \sqrt{E'_L} \left(E_C^{max} - \left(E_L^* + E'_L - \mu_L \sqrt{E_L^* E'_L} \right) \right)^{\left(\frac{3n}{2}\right)-4},$$

$$E_L^* = \frac{E_L}{(A+1)^2},$$

where
E_L: incident energy in the LAB system,
E'_L: outgoing energy in the LAB system,
μ_L: scattering angle (cosine direction) in the LAB system.

$$f_l(E \to g') = \int_{E_{g'l}}^{E_{g'u}} \int_{-1}^{1} f(E_L \to E'_L, \mu_L) P_l(\mu_L) d\mu_L \, dE'_L$$

where
$E_{g'u}$: upper energy boundary of g'-th energy group,
$E_{g'l}$: lower energy boundary of g'-th energy group.



Thermal cross sections

Thermal cross sections

- Three different reactions are considered
  - Incoherent inelastic
    - Free gas model
    - Short collision time (SCT) approximation
    - $S(\alpha,\beta)$ data in an ACE file
  - Incoherent elastic
    - $S(\alpha,\beta)$ data in an ACE file
  - Coherent elastic
    - $S(\alpha,\beta)$ data in an ACE file

Free gas model

- The thermal incoherent inelastic scattering for free gas (unbounded atom) is given by

$$\sigma^{inc,inela}(E,E',\mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\frac{1}{\sqrt{4\pi\alpha}}\exp\left(-\frac{(\alpha+\beta)^2}{4\alpha}\right),$$

$$\alpha = \frac{E'+E-2\mu\sqrt{EE'}}{AkT},$$

$$\beta = \frac{E'-E}{kT},$$

where

$\sigma_b = \sigma_{free}\frac{(A+1)^2}{A^2}$: the incoherent inelastic scattering cross section for the bounded state,

σ_{free} : elastic scattering cross section for unbounded (free) state obtained by pointwise elastic scattering cross section,

A: relative mass of a nucleus to a neutron,

k: Boltzmann constant [eV/K],

T: Temperature [K],

E: incident energy in the LAB system,

E': outgoing energy in the LAB system,

μ: scattering cosine angle in the LAB system.

Free gas model

- The Legendre moments can be calculated by

$$\sigma_l^{inc,inela}(E,E') = \int_{-1}^{1} \sigma^{inc}(E,E',\mu) P_l(\mu) d\mu ,$$

where
$P_l(\mu)$: Legendre polynomial of l-th order.

- The above numerical integration is difficult since $\sigma^{inc}(E,E',\mu)$ shows steep variation on μ since α can be zero when $E \approx E'$.
- NJOY uses adaptive numerical integration (discretization is changed on-the-fly based on the behavior of $\sigma^{inc}(E,E',\mu)$)

Free gas model

- FRENDY/MG utilize the following relation to avoid numerical difficulty:

$$\sigma_l^{inc,inela}(E,E') = \int_{\sqrt{a-b}}^{\sqrt{a+b}} \frac{2c}{b} \exp\left(-\frac{1}{4}\left(u+\frac{\beta}{u}\right)^2\right) P_l\left(\frac{a-u^2}{b}\right) du\,,$$

$$a = \frac{E'+E}{AkT},$$

$$b = \frac{\sqrt{EE'}}{AkT},$$

$$c = \frac{\sigma_b}{4kT}\frac{1}{\sqrt{4\pi}}\sqrt{\frac{E'}{E}},$$

$$u^2 = \alpha$$

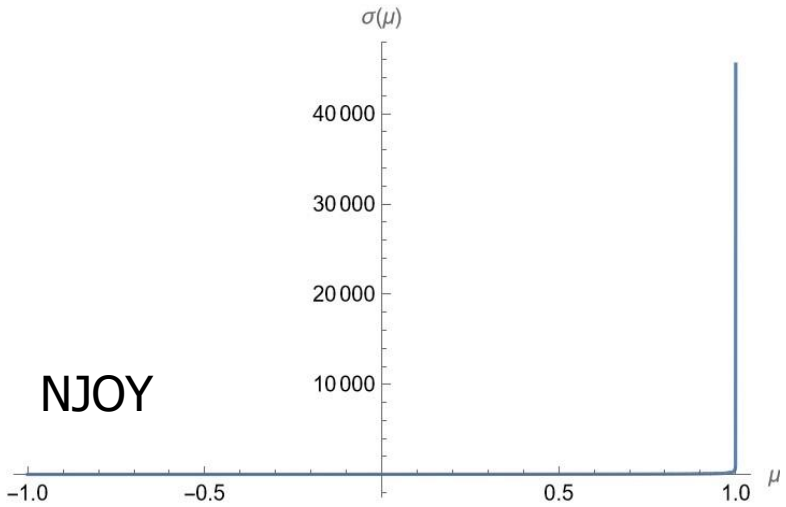
- Adaptive numerical integration with the Simpson formula is used

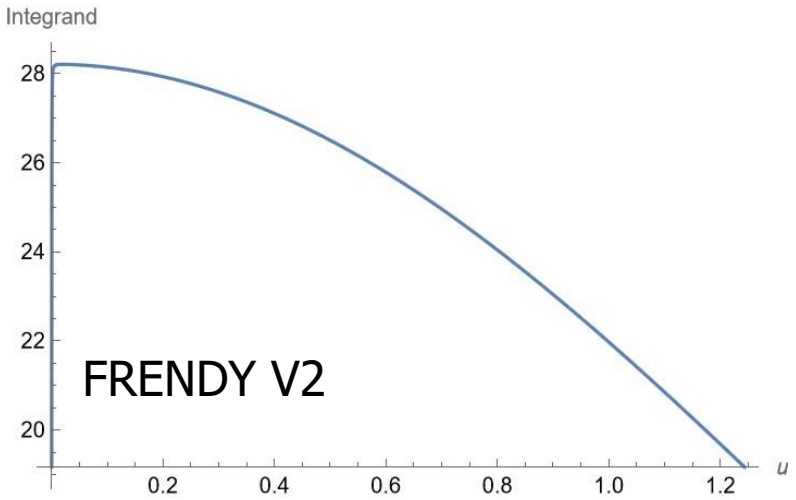
Free gas model

- Comparison of integrand

$$\sigma^{inc,inela}(E,E',\mu)=\frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\frac{1}{\sqrt{4\pi\alpha}}\exp\left(-\frac{(\alpha+\beta)^2}{4\alpha}\right),$$

$$\frac{2c}{b}\exp\left(-\frac{1}{4}\left(u+\frac{\beta}{u}\right)^2\right)$$





E=0.01 [eV], E'=0.00999 [eV], A=1, T=300 [K], σ_b=1.0

Free gas model

- Numerical integration on μ still gives some discretization error even if adaptive numerical integration is used
- To reduce the numerical integration error, the analytic solution is used. The analytic solution for P0 component is:

$$\sigma_{0,ana}^{inc,inela}(E,E') = \frac{\sigma_f}{E}\frac{\eta^2}{2}\left[\exp\left(\frac{E}{kT}-\frac{E'}{kT}\right)\left\{\operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}}-\rho\sqrt{\frac{E'}{kT}}\right)\pm\operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}}+\rho\sqrt{\frac{E'}{kT}}\right)\right\}\right.$$
$$\left.+\left\{\operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}}-\rho\sqrt{\frac{E}{kT}}\right)\mp\operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}}+\rho\sqrt{\frac{E}{kT}}\right)\right\}\right]$$

where erf is the error function, $\eta=\frac{A+1}{2\sqrt{A}}$, $\rho=\frac{A-1}{2\sqrt{A}}$, and upper/lower signs correspond to $E<E'$ or $E'<E$, respectively.

Free gas model

- Multi-group scattering matrix is obtained by:

$$\sigma_{l,g\to g'}^{inc,inela} = \frac{\int_{E_g^{lower}}^{E_g^{upper}} \phi_l(E) \int_{E_{g'}^{lower}}^{E_{g'}^{upper}} \sigma_l^{inc,inela}(E,E')dE'\,dE}{\int_{E_g^{lower}}^{E_g^{upper}} \phi_l(E)dE}$$

$$= \frac{\sum_{E_i\in g} \Delta E_i\, \phi_l(E_i) \sum_{E_j\in g'} \sigma_l^{inc,inela}\left(E_i, E'_j\right)\Delta E'_j}{\sum_{E_i\in g} \Delta E_i\, \phi_l(E_i)},$$

- Then normalized by analytic solution as:

$$\hat{\sigma}_{l,g\to g'}^{inc,inela} = \sigma_{l,g\to g'}^{inc,inela} \frac{\sigma_{0,g\to g',ana}^{inc,inela}}{\sigma_{0,g\to g'}^{inc,inela}}$$

Short collision time (SCT) approximation

- When the energy transfer is large in the thermal energy range, the short time collision (SCT) approximation gives better results
- In FRENDY V2, the SCT approximation can used with $S(\alpha,\beta)$ treatment. Namely, scattering outside the energy range of $S(\alpha,\beta)$ is treated by the SCT approximation when UseSCT option is used.
- The SCT approximation is not used with the free gas model.
- In the SCT approximation, cross section is given by:

$$\sigma^{inc,inela}(E,E',\mu)=\frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\frac{1}{\sqrt{4\pi\alpha}}\sqrt{\frac{T}{T_{eff}}}\exp\left(-\frac{(\alpha-|\beta|)^2}{4\alpha}\frac{T}{T_{eff}}-\frac{\beta+|\beta|}{2}\right)$$

where T and T_{eff} are temperature and the effective temperature in [K].

Short collision time (SCT) approximation

- The SCT approximation can be formulated as:

$$\sigma_l^{inc,inela}(E,E') = \int_{\sqrt{a-b}}^{\sqrt{a+b}} \frac{2c}{b} \exp\left(-\frac{1}{4}\left(u+\frac{\beta}{u}\right)^2\right) \times \sqrt{\frac{T}{T_{eff}}} \exp\left(\frac{1}{4}\left(1-\frac{T}{T_{eff}}\right)\left(u-\frac{|\beta|}{u}\right)^2\right) P_l\left(\frac{a-u^2}{b}\right) du$$

- The difference between the free gas model and SCT is the following factor in integration

$$\sqrt{\frac{T}{T_{eff}}} \exp\left(\frac{1}{4}\left(1-\frac{T}{T_{eff}}\right)\left(u-\frac{|\beta|}{u}\right)^2\right)$$

- Identical numerical integration scheme can be used with the free gas treatment
- Normalization by the analytic solution is not applied

$S(\alpha,\beta)$ data in ACE file (incoherent inelastic)

- The $S(\alpha,\beta)$ data except for the free gas model and the SCT approximation are stored in the thermal scattering block of a thermal ACE file.
- In the case of incoherent inelastic scattering, the following data exist in an ACE file
  - Cross sections for incident energy grid points. (ITIE block)
  - Energy/angle distribution table for each incident energy grid points (ITXE block)
- Cross section is given by:

$$\sigma_l^{inc,inela}(E,E') = \sum_{i=1}^{N_\mu} \sigma^{inc,inela}(E,E') \frac{1}{N_\mu} P_l(\mu_i)$$

where

$\sigma^{inc}(E,E')$: incoherent inelastic scattering cross section given in ITIE block, and outgoing energies are given by the LAB system,

N_μ: number of equi-probable cosine bins,

μ_i: direction cosine of i-th bin in the LAB system.

$S(\alpha,\beta)$ data in ACE file (incoherent inelastic)

- To describe the energy transfer probability, one of the following three options are used in an ACE file:
  - 1) Equally distributed energy grid points (ifeng=0 in ACE file, iwt=1 in ACER)
  - 2) Skewed distribution of energy grid points (ifeng=1 in ACE file, iwt=0 in ACER)
  - 3) Continuous distribution energy grid points (ifeng=2 in ACE file, iwt=2 in ACER)
- Most precise option is 3). However, this option can be used in MCNP6.2 or later.
- Option 2) is the default of FRENDY (ACE generation).
- FRENDY V2 can treat all options. However, use of option 3) is recommended from the viewpoint of accuracy.
- Use of option 2) may affect the shape of thermal spectrum (as well as MCNP).

$S(\alpha,\beta)$ data in ACE file (incoherent inelastic)

- To reduce the energy discretization error of option 1) and 2), the following energy dependencies are assumed in FRENDY V2

$$\sigma^{inc,inela}(E,E') = \begin{cases} \sigma^{inc,inela}(E) f_i \exp\left(-\dfrac{E'}{kT}\right), E < E' \\ \sigma^{inc,inela}(E) f_i \operatorname{erf}\left(\sqrt{\dfrac{E'}{kT}}\right), E > E' \end{cases}$$

$$f_i = \begin{cases} \dfrac{w_i}{\int_{E_{i,l}}^{E_{i,u}} \exp\left(-\dfrac{E'}{kT}\right) dE'}, E < E' \\ \dfrac{w_i}{\int_{E_{i,l}}^{E_{i,u}} \operatorname{erf}\left(\sqrt{\dfrac{E'}{kT}}\right) dE'}, E > E' \end{cases}$$

w_i:weight for i-th energy interval, which is specified by iwt,
$E_{i,l}$: lower energy boundary of i-th outgoing energy interval,
$E_{i,u}$: upper energy boundary of i-th outgoing energy interval.

$S(\alpha,\beta)$ data in ACE file (coherent elastic)

- Coherent elastic scattering occurs due to interference of scattering by crystalline solids, e.g., graphite. Sharp Bragg-edges are observed in scattering cross sections. No energy change occurred (only self-scattering). Only flight direction of neutron is changed.
- Angular dependence of coherent elastic scattering cross section is given by:

$$\sigma^{coh,ela}(E,\mu) = \sum_{i\in(\mu_i\geq -1)} \frac{b_i}{E}\delta(\mu-\mu_i)$$

$$\mu_i = 1 - 2\frac{E_i}{E}$$

$$E\sigma^{coh,ela}(E) = \sum_{i\in(\mu_i\geq -1)} b_i$$

where

b_i: size of step, defined later,

E_i: the energy of i-th Bragg edge.

$S(\alpha,\beta)$ data in ACE file (coherent elastic)

- Coherent elastic scattering cross section is given by:

$$\sigma^{coh,ela}(E) = \frac{P(i)}{E}\ , E_{ela}(i) \le E < E_{ela}(i+1),$$
$$\sigma^{coh,ela}(E) = 0, E < E_{ela}(1),$$
$$\sigma^{coh,ela}(E) = \frac{P(N_{ela})}{E}, E_{ela}(N_{ela}) < E$$

where
$P(i)$: constant given in an ACE file for the interval between i-th and (i+1)-th Bragg edges,
$E_{ela}(i)$: energy of i-th Bragg edge,
N_{ela}: total number of Bragg edges.

- Legendre component is calculated by:

$$\sigma_l^{coh,ela}(E) = \int_{-1}^{1} \sigma^{coh,ela}(E,\mu)d\mu = \sum_{i\in(\mu_i\ge -1)} \int_{-1}^{1} \frac{b_i}{E} P_l(\mu_i)\delta(\mu-\mu_i)d\mu = \sum_{i\in(\mu_i\ge -1)} \frac{b_i}{E} P_l(\mu_i)$$

$S(\alpha,\beta)$ data in ACE file (incoherent elastic)

- Scattering with no energy change is occurred in hydrogenous solids due to zero phonon term, e.g, H in ZrH.
- Cross section is given by:

$$\sigma_l^{incoh,ela}(E) = \sigma^{incoh,ela}(E)\frac{1}{N}\sum_{i=1}^{N} P_l(\mu_i)$$

where
N: total number of discrete cosine directions,
μ_i: the i-th discrete cosine direction given in an ACE file.

- $\sigma^{incoh,ela}(E)$ and μ_i is tabulated as function of incident energy in ACE file.

$S(\alpha,\beta)$データ (B-VIII.0)

FRENDY	Description
al	Al
be	Be
bebeo	Be in BeO
benz	Benzene (caution: not implemented in FRENDY V2)
csic	C in SiC
c5o2h8	C5O2H8 (caution: not implemented in FRENDY V2)
dd2o	D in D2O
dortho	D in Ortho-D
dpara	D in Para-D
fe	Fe
graph	Graphite
poly	Polyethylene
hh2o	H in H2O
hice	H in Ice (H2O)
hortho	H in Ortho-H
hpara	H in Para-H
hyh2	H in YH2
hzrh	H in ZrH
lch4	Liquid CH4 (Methane)
nun	N in UN
obeo	O in BeO
od2o	O in D2O
oice	O in Ice (H2O)
ouo2	O in UO2
sch4	Solid CH4 (Methane)
sisic	Si in SiC
uun	U in UN
uuo2	U in UO2
yyh2	Y in YH2
zrzrh	Zr in ZrH

Fission spectrum, Nu-value, fission cross sections

Fission spectrum

- In an ACE file, energy distributions for prompt and delayed neutrons are given in the DLW block.
- The fission spectrum for delayed neutron is calculated by

$$\chi_{D,i}(g \to g') = \frac{\int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E) \int_{E'\in g'} f_{Di}(E \to E')dE'\,dE}{\int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E)dE}$$

$$\nu_{D,i}(E) = \nu_D(E)g_i(E)$$

where

$\chi_{D,i}(g \to g')$: delayed neutron spectrum for delayed group i, from group g to g',

$\nu_D(E)$: delayed neutron nu-value,

$\nu_{D,i}(E)$: delayed neutron nu-value for delayed group i,

$g_i(E)$: fraction of neutron for delayed group i,

$\sigma_f(E)$: fission cross section,

$\phi(E)$: neutron spectrum (scalar flux),

$f_{Di}(E \to E')$: energy distribution of delayed neutron group i, from incident energy E to outgoing energy E', where $\int f_{Di}(E \to E')dE' = 1$.

Fission spectrum

- Total delayed neutron spectrum is calculated by

$$\chi_D(g \to g') = \frac{\sum_i \int_{E \in g} \nu_{D,i}(E)\sigma_f(E)\phi(E) \int_{E' \in g'} f_i(E \to E')dE'\,dE}{\sum_i \int_{E \in g} \nu_{D,i}(E)\sigma_f(E)\phi(E)dE}$$

- The fission spectrum for prompt neutrons is calculated by

$$\chi_P(g \to g') = \frac{\int_{E \in g} \nu_P(E)\sigma_f(E)\phi(E) \int_{E' \in g'} f_P(E \to E')dE'\,dE}{\int_{E \in g} \nu_P(E)\sigma_f(E)\phi(E)dE}$$

where

$\nu_P(E)$: prompt neutron nu-value,

$f_P(E \to E')$: energy distribution of prompt neutron, from incident energy E to outgoing energy E', where $\int f_P(E \to E')dE' = 1$.

Fission spectrum

- The fission spectrum for total (prompt+delayed) neutrons is calculated by

$$\chi(g \to g') = \frac{\int_{E\in g} \nu_P(E)\sigma_f(E)\phi(E) \int_{E'\in g'} f_P(E \to E')dE'\,dE + \sum_i \int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E) \int_{E'\in g'} f_i(E \to E')dE'\,dE}{\int_{E\in g} \nu_P(E)\sigma_f(E)\phi(E)dE + \sum_i \int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E)dE}$$

Nu-values

- The total and/or delayed nu-values are given in an ACE file.
- In FRENDY MG generation, the prompt nu-values are not used even if they are given in the ACE file.
- The prompt nu-value is evaluated by subtracting the delayed nu-value from the total nu-value.
- Any number of delayed neutron groups can be used in FRENDY V2.

$$\nu_T(g) = \frac{\int_{E\in g} \nu_T(E)\sigma_f(E)\phi(E)dE}{\int_{E\in g} \sigma_f(E)\phi(E)dE},$$

$$\nu_D(g) = \frac{\int_{E\in g} \nu_D(E)\sigma_f(E)\phi(E)dE}{\int_{E\in g} \sigma_f(E)\phi(E)dE},$$

$$\nu_P(g) = \nu_T(g) - \nu_D(g).$$

where
$\nu_T(g)$: total nu-value for group g,
$\nu_D(g)$: delayed nu-value for group g,
$\nu_P(g)$: prompt nu-value for group g.

Delayed neutron constants

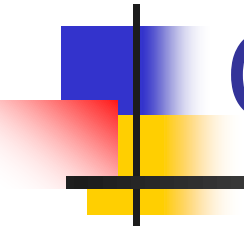
- The delayed neutron fraction of each group is calculated by:

$$r_{D,i} = \frac{\int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E)dE}{\sum_i \int_{E\in g} \nu_{D,i}(E)\sigma_f(E)\phi(E)dE}$$

where

$r_{D,i}$: delayed neutron fraction of group i, normalized as $\sum_i r_{D,i} = 1$.

- The delayed neutron decay constant of each group is edited from ACE file



Outputs/Edits

Outputs/Edits

- FRENDY/MG has the following outputs
  - Edit files: self-explanatory and readable
    - 1D multi-group cross sections
    - 2D multi-group cross sections
    - Nu-values for total, prompt, and delayed neutrons
    - Fission spectra for total, prompt, and delayed neutrons
    - Multi-group scalar flux (P0 flux) used for weighting
    - Multi-group current (P1 flux) used for weighting
    - Ultra-fine group scalar flux
    - Ultra-fine group 1D cross sections
    - KRAM format multi-group cross sections
    - MATXS format multi-group cross sections
    - Debug output
  - Cross sections in the KRAM cross section format
  - MATXS format
  - GENDF format
- Can be controlled by input

KRAM format

- The KRAM format was used in the KRAM code, which is a MOC transport solver.
- The cross sections generated in the KRAM format is suitable for ordinary transport calculations since various cross sections are processed to be consistent with common transport solvers.

$$\sigma_{t,g} = \sigma_{1,g}$$

$$\sigma_{f,g} = \sigma_{18,g}$$

$$\nu_g = \frac{\sum_{g'} \sigma_{18,g\to g'}}{\sigma_{18,g}} + \nu_{D,g}$$

$$\sigma_{a,g} = \sigma_{18,g} + \sum_{i=102}^{117} \sigma_{i,g} + (1 - n_{5,g})\sigma_{5,g} - (\sigma_{16,g} + \sigma_{24,g} + \sigma_{30,g} + \sigma_{41,g}) - 2(\sigma_{17,g} + \sigma_{25,g} + \sigma_{42,g}) - 3\sigma_{37,g}$$

$$\sigma_{s,g\to g'} = \sum_{\substack{i=2,5,16,17,24,\\ 25,30,37,41,42}} \sigma_{i,g\to g'} + \sum_{j=51}^{91} \sigma_{j,g\to g'}$$

$$\chi_g = \frac{\left(\sum_{g'} \sigma_{18,g'\to g}\phi_{g'} + \chi_{D,g} \sum_{g'} \nu_{D,g'}\sigma_{18,g'}\phi_{g'}\right)}{\left(\sum_{g} \sum_{g'} \sigma_{18,g'\to g}\phi_{g'} + \sum_{g'} \nu_{D,g'}\sigma_{18,g'}\phi_{g'}\right)}$$

where $\sigma_{i,g}$, $\sigma_{i,g\to g'}$, $n_{5,g}$, subscript D show 1D microscopic cross section for mt=i, 2D microscopic cross section for mt=i from energy group g to g', the number of released neutron for g-th energy group for mt=5, and delayed neutron parameters, respectively.

KRAM format

- Following relations are used to calculate mt=18, 103-107 when mt=18, 103-107 do not exist but the following reactions exist in an ACE file.

$$\sigma_{18,g} = \sum_{i=19,20,21,38}^{649} \sigma_{i,g}$$

$$\sigma_{103,g} = \sum_{i=600}^{699} \sigma_{i,g}$$

$$\sigma_{104,g} = \sum_{i=650}^{749} \sigma_{i,g}$$

$$\sigma_{105,g} = \sum_{i=700}^{799} \sigma_{i,g}$$

$$\sigma_{106,g} = \sum_{i=750}^{849} \sigma_{i,g}$$

$$\sigma_{107,g} = \sum_{i=800} \sigma_{i,g}$$

MATXS format

- The MATXS is a versatile cross section format for multi-group cross sections.
- The FRENDY/MG code can output the generated multi-group cross sections in the MATXS format.
- The output cross sections are chosen to be consistent with GROUPR/MATXSR in the NJOY code.
- Part of the edited cross sections in FRENDY/MG are not used in the cross section in the MATXS format.
- For example, though self-shielded cross sections are generated for all reactions with energy transfer in FRENDY/MG, only the elastic scattering and fission matrix cross sections are output as the self-shielded cross sections in the MATXS format
- In FRENDY/MG, full shielded cross sections (1D/2D) without truncation can be output in the MATXS format by input data (FullMATXS) though file size is larger.

MATXS format

- 1D cross sections
  - All reaction types having 1D cross section is output in the MATXS file.
  - In addition to the cross section, the following quantities are also output:
    - P0 multi-group flux
    - P1 multi-group flux (current)
    - Group averaged inverse velocity (mt259)
    - Lethargy width (mt258)
    - Average direction cosine (mu-bar) (mt251)

$$\frac{1}{v_g} = \frac{\int_{E\in g} \frac{1}{v(E)} \phi(E) dE}{\int_{E\in g} \phi(E) dE},$$

$$\Delta u_g = ln\left(\frac{E_{g,upper}}{E_{g,lower}}\right),$$

$$\bar{\mu} = \frac{\Sigma_{s1,g}}{\Sigma_{s0,g}} = \frac{\sum_{g'} \Sigma_{s1,g\to g'}}{\sum_{g'} \Sigma_{s0,g\to g'}}.$$

MATXS format

- All 1D cross sections are output for the infinite-dilute condition
- The following cross sections and parameters are output for shielded conditions:
  - P0 multi-group flux
  - P1 multi-group flux (current)
  - P0 weighted total cross section
  - P1 weighted total cross section
  - Elastic scattering
  - Fission cross sections (mt=18, or 19, 20, 21, 38), if exist
  - Inelastic scattering (mt=51)
  - Capture cross section (mt=102)
- All 2D cross sections with energy transfer are output in the infinite-dilute condition.
- For the shielded conditions, only the elastic scattering and fission matrix (nftot, mt=18) cross sections are output in the MATXS cross section file.

MATXS format

- Three options available for MATXS file
- Ordinary MATXS (option MATXS)
  - Compatible with MATXS file generated by NJOY2016
- Simple MATXS format
  - Compatible with MATXS file generated by NJOY99
- Full MATXS format
  - All shielded cross sections (including anisotropic scattering)

MATXS format

```
 0v   matxs *frendy/mg        *     1
 1d         1     2     9     1  5000    90
 2d
92238.51c : generated by frendy/mg at 2023/03/02 08:58:21
 3d     n        nscat   ntherm  u238
   172     1     1     1     1     3     0
 4d          1.96403e+07 1.73325e+07 1.49182e+07 1.38403e+07 1.16183e+07
 1.00000e+07 8.18731e+06 6.70320e+06 6.06531e+06 5.48812e+06 4.49329e+06
 3.67879e+06 3.01194e+06 2.46597e+06 2.23130e+06 2.01896e+06 1.65299e+06
 1.35335e+06 1.22456e+06 1.10803e+06 1.00259e+06 9.07180e+05 8.20850e+05
 6.08101e+05 5.50232e+05 4.97871e+05 4.50492e+05 4.07622e+05 3.01974e+05
Skip
 1.50000e-02 1.00000e-02 6.90000e-03 5.00000e-03 3.00000e-03 1.00001e-05
 5d u238     2.36006e+02
 6.00000e+02 1.00000e+10     1    46    33     0
 6.00000e+02 5.20000e+01     1     8     2    75
 6.00000e+02 1.00000e+10     2     1     1    86
 6d     nwt0    nwt1    ntot0   ntot1   nelas   ninel   n2n     n3n
nftot   n4n     n01     n02     n03     n04     n05     n06     n07
n08     n09     n10     n11     n12     n13     n14     n15     n16
n17     n18     n19     n20     n21     n22     n23     n24     n25
n26     n27     ncn     ng      mt258   invel   mubar   nutot   nudel
chid    nupmt
Data follows
```

GENDF format

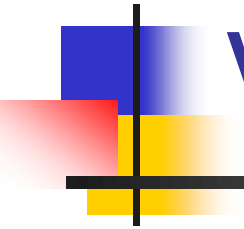
- The GENDF format is used as the output file of the GROUPR module of NJOY.
- It is also used as an interface file format among several modules, such as DTFR, CCCCR, MATXSR, POWR, and WIMSR.
- In FRENDY V2, the GENDF output in text (ASCII) format is implemented.
- The GENDF format utilizes a similar format with that of ENDF.
- The major structure of the GENDF format is as follows:
  - General information, background cross section, energy group structure (mf=1, mt=451)
  - One-dimensional cross sections, nu-value, flux (mf=3)
  - Decay constant of delayed neutron, delayed neutron spectrum, if exist (mf=5)
  - Two-dimensional cross sections (mf=6)

GENDF format

- Three options available for GENDF file
- Ordinary GENDF (option GENDF)
  - Compatible with MATXS file generated by NJOY2016
- Simple GENDF format
  - Compatible with MATXS file generated by NJOY99
- Full GENDF format
  - All shielded cross sections (including anisotropic scattering)

GENDF format

```
92235.60c : frendy/mg at 2021/04/01 09:17:24                          0 0  0    0
 9.223500+4 2.330250+2          0          3         -1          19228 1451    1
 2.936059+2 0.000000+0        172          0        178          09228 1451    2
 0.000000+0 1.00000+10 1.000000+3 1.000000+0 1.000010-5 3.000000-39228 1451    3
 5.000000-3 6.900000-3 1.000000-2 1.500000-2 2.000000-2 2.500000-29228 1451    4
Skip
 6.065307+6 6.703200+6 8.187308+6 1.000000+7 1.161834+7 1.384031+79228 1451   31
 1.491825+7 1.733253+7 1.964033+7 0.000000+0                   9228 1451   32
                                                               9228 0  0    0
 9.223500+4 2.330250+2          2          3          0        1729228 3  1    1
 2.936059+2 0.000000+0          2          1         12          19228 3  1    2
 2.015037-1 2.015035-1 3.397897-2 6.815823-3 7.842878-4 2.197617-69228 3  1    3
 1.235639+4 1.235639+4 7.042329+3 4.546633+3 6.523738+3 4.067116+39228 3  1    4
 2.936059+2 0.000000+0          2          1         12          29228 3  1    5
 1.804654-2 1.804655-2 8.497675-3 3.290681-3 2.441188-4 1.490679-69228 3  1    6
 1.887062+3 1.887062+3 1.880066+3 1.873107+3 1.876361+3 1.865753+39228 3  1    7
Data follows
```

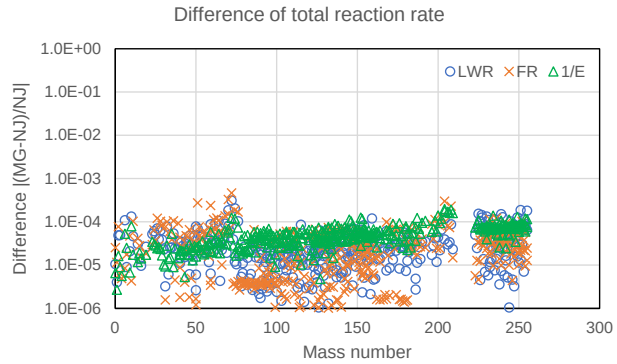


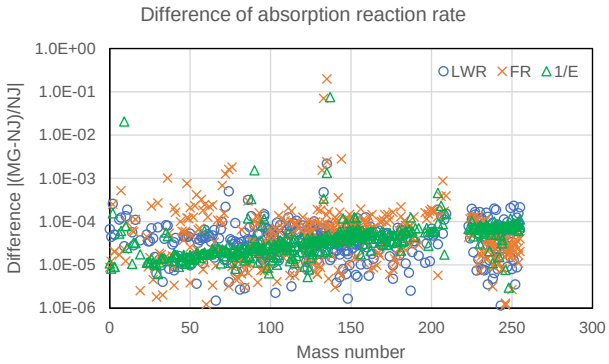
Verifications

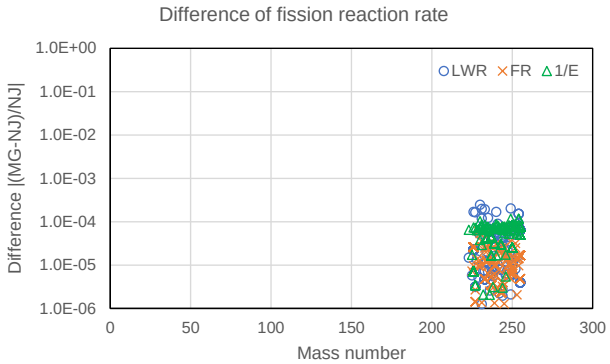
Comparison of microscopic reaction rate

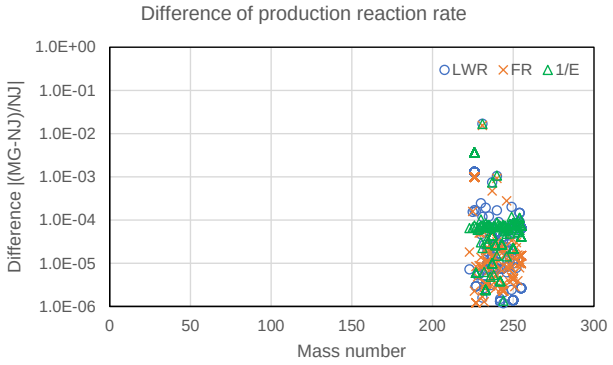
- 172 group microscopic cross sections obtained by NJOY2016 and FRENDY/MG are multiplied by LWR, small fast reactor, 1/E spectra to obtain 1-group reaction rates
- All nuclides in JENDL-4 -4u, 5, ENDF-B7.1, -8.0, JEFF-3.3, TENDL-2021
- 300K
- 10^{10}, 1 barn
- Compared reaction
  - Total
  - Absorption
  - Fission
  - Production
  - Scattering (P0, P1)

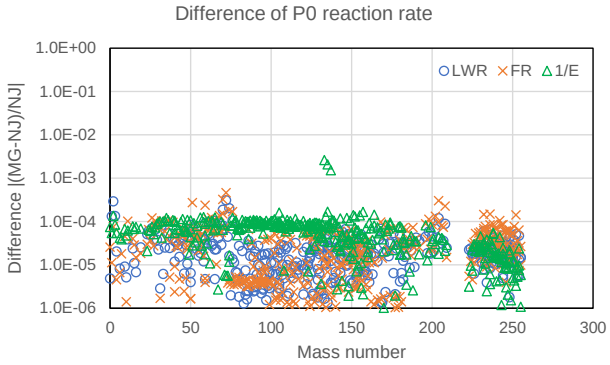
JENDL4, 300K, 10^{10} barn

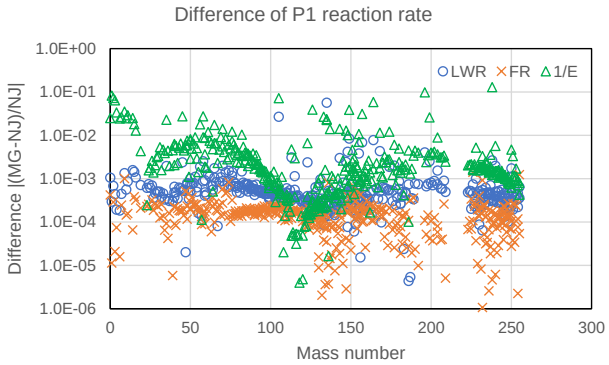




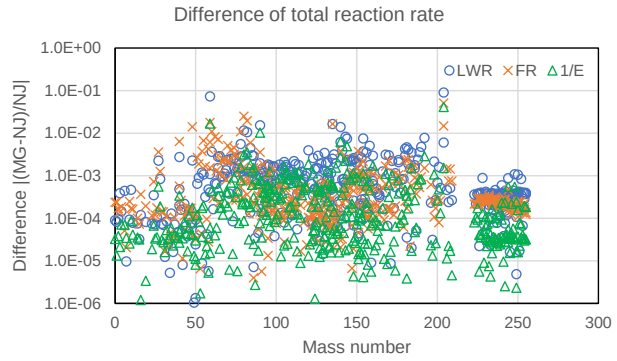


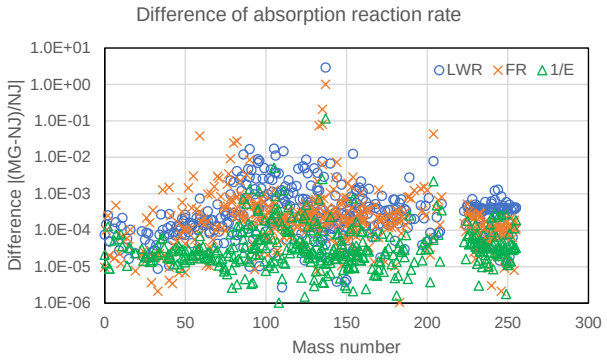


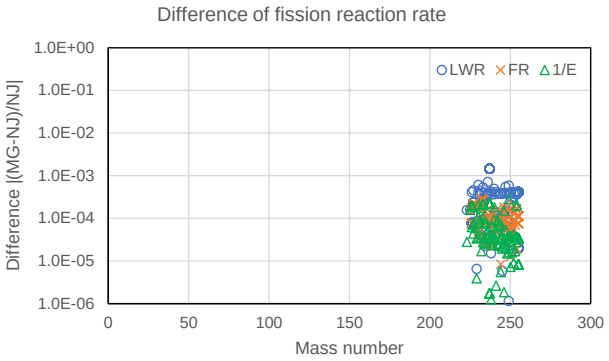


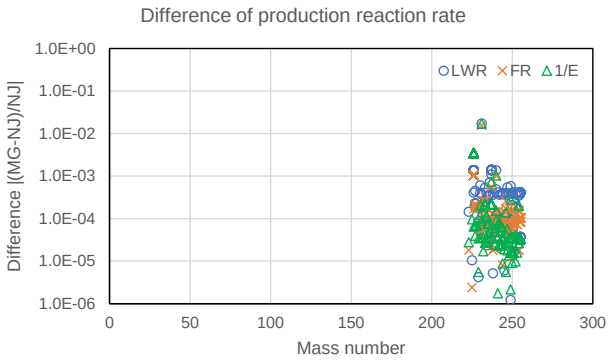


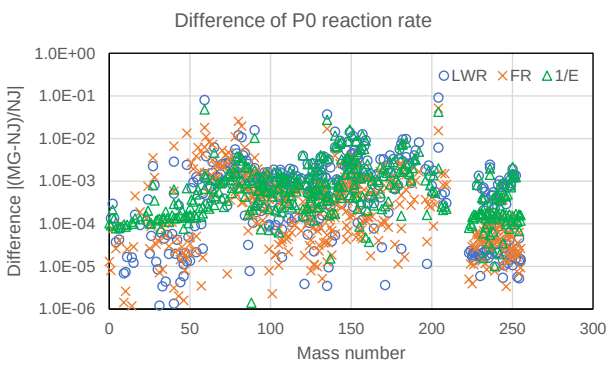
JENDL4, 300K, 1 barn

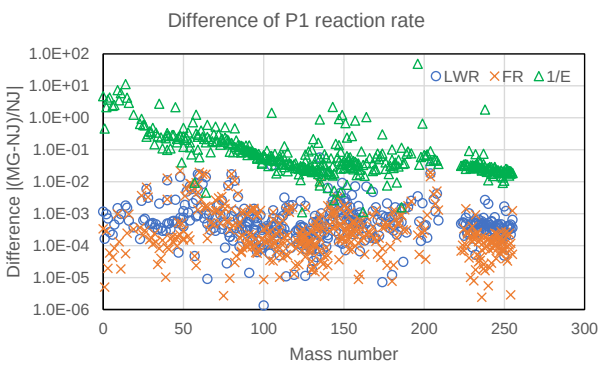




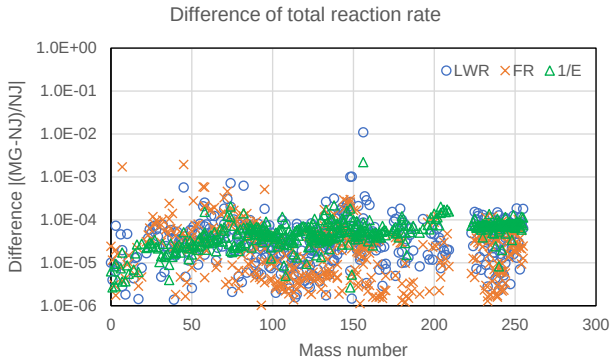


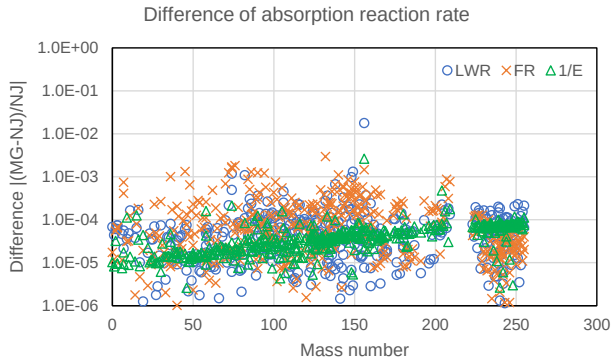


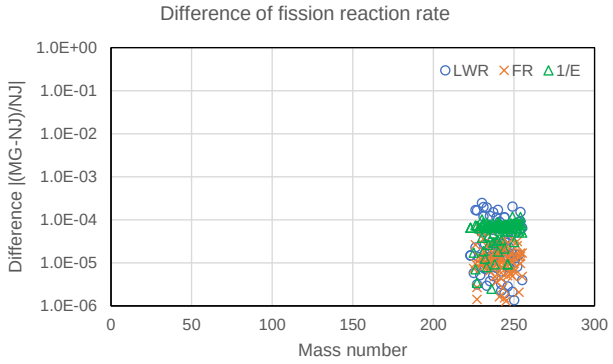


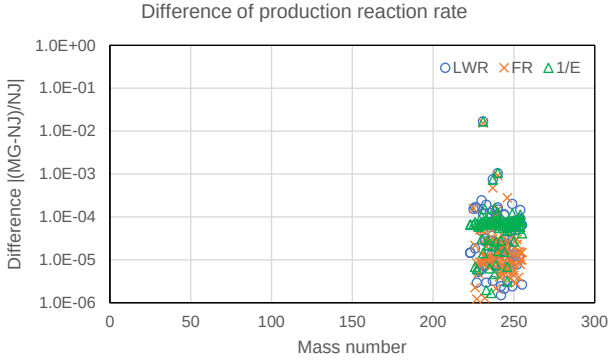


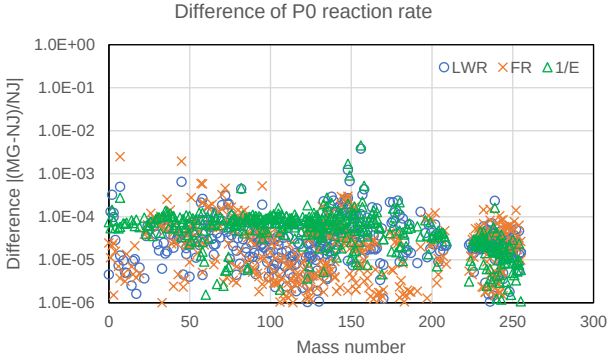
B7.1, 300K, 10^{10} barn

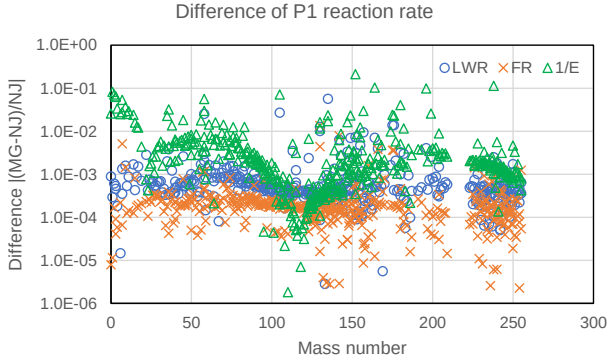




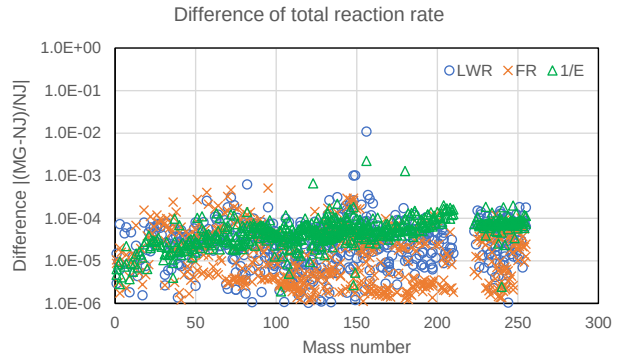


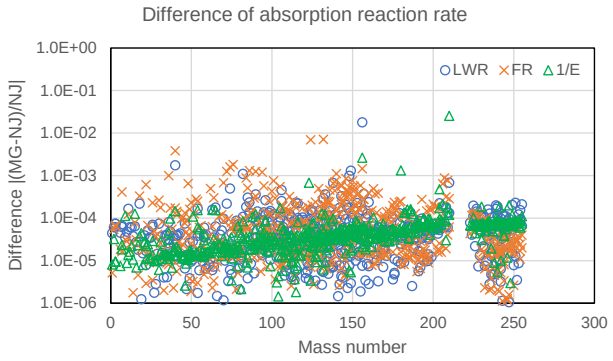


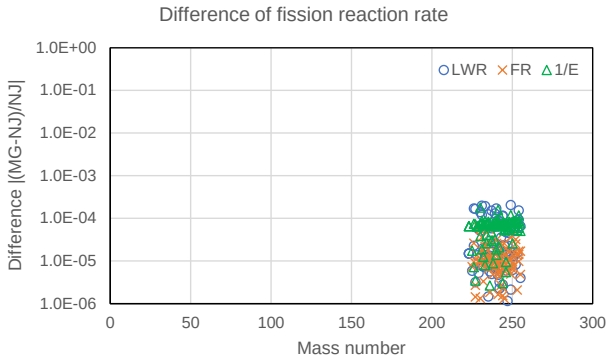


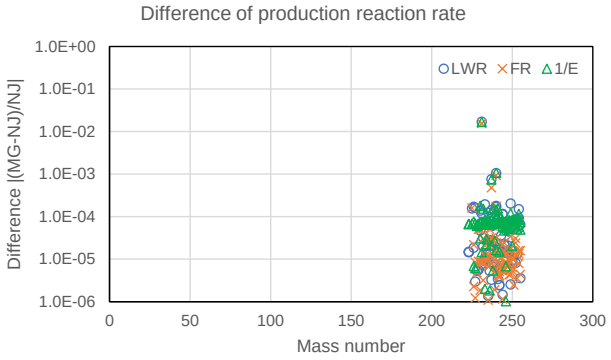


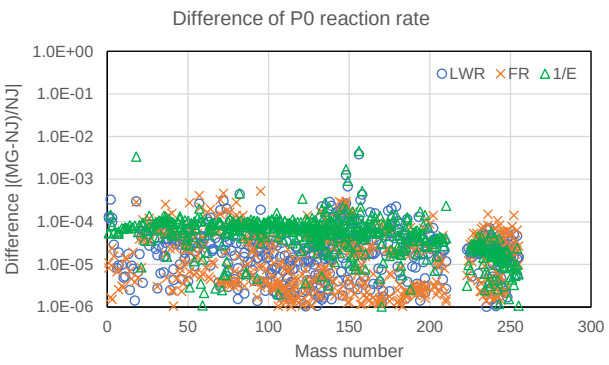
B8.0, 300K, 10^{10} barn

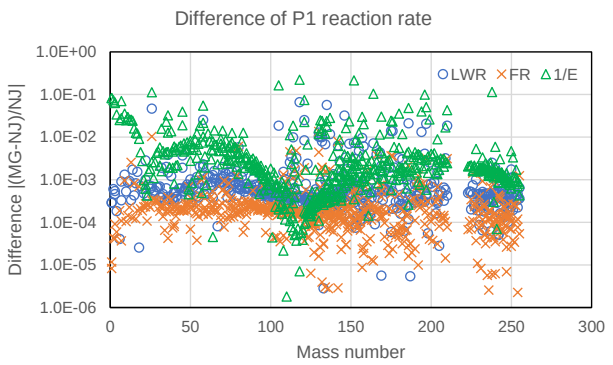




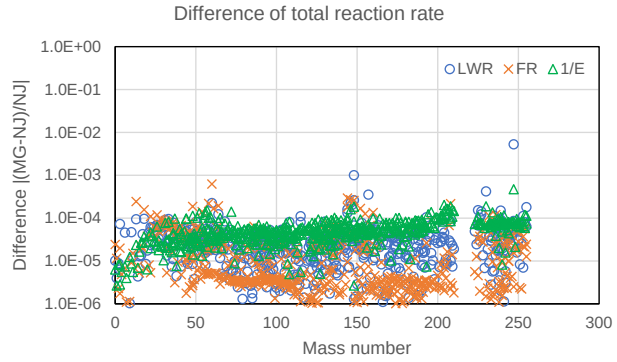


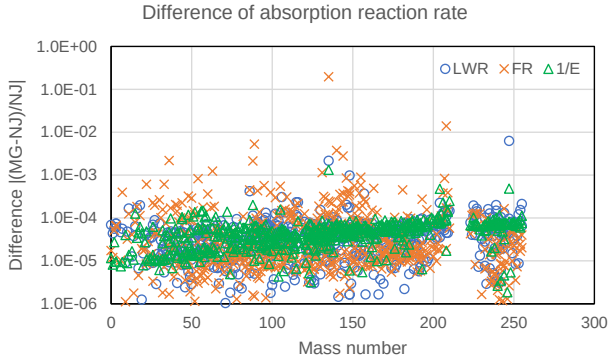


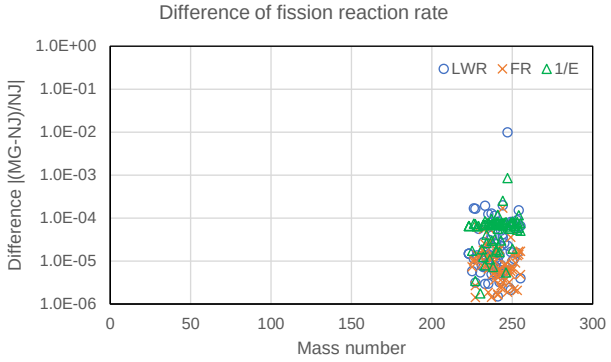


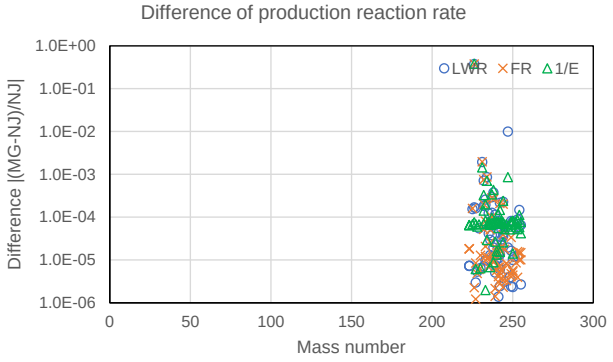


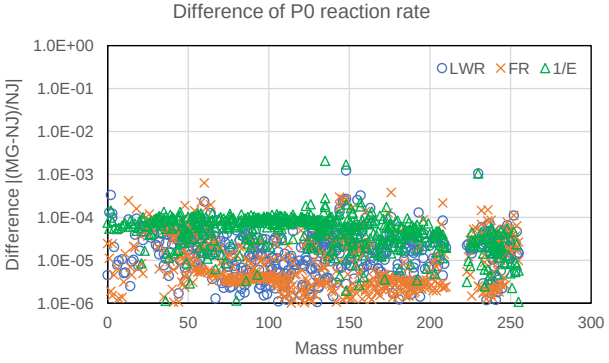
JEFF3.3, 300K, 10^{10} barn

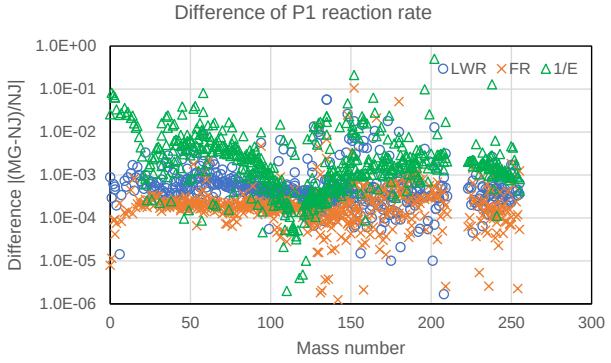




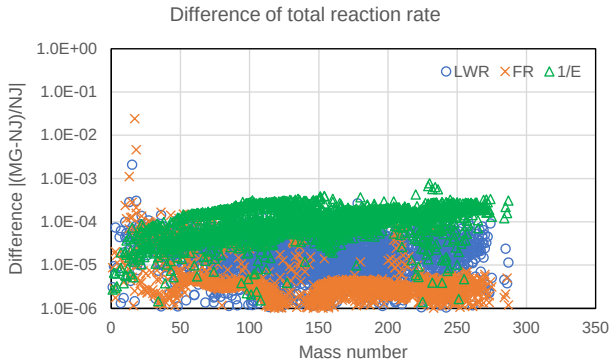


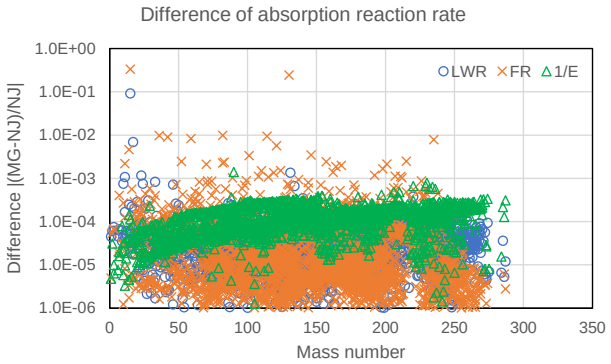


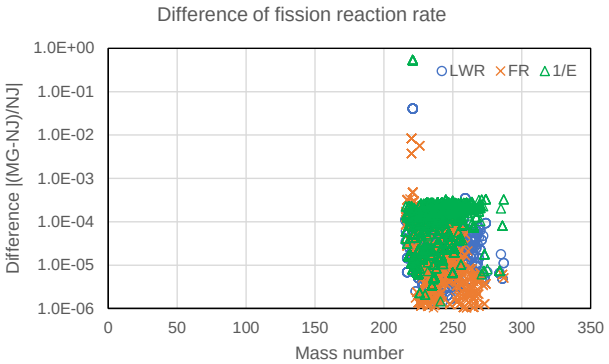


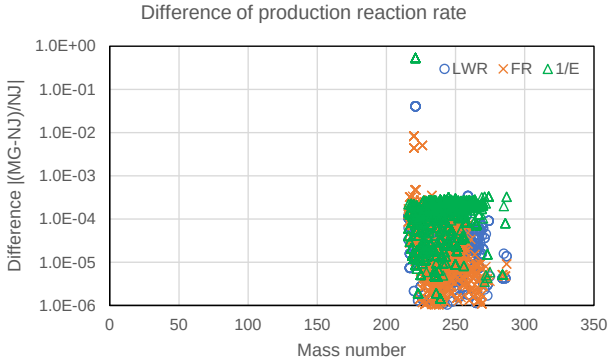


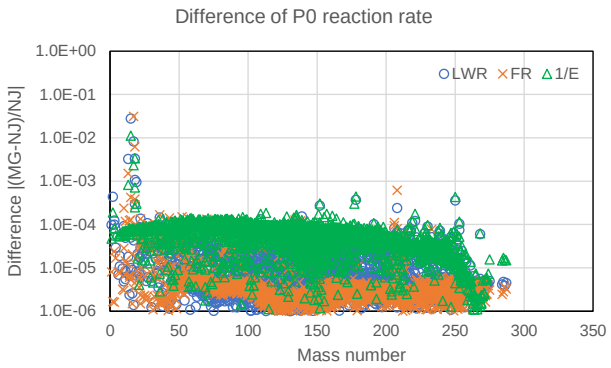
TENDL2021, 300K, 10^{10} barn

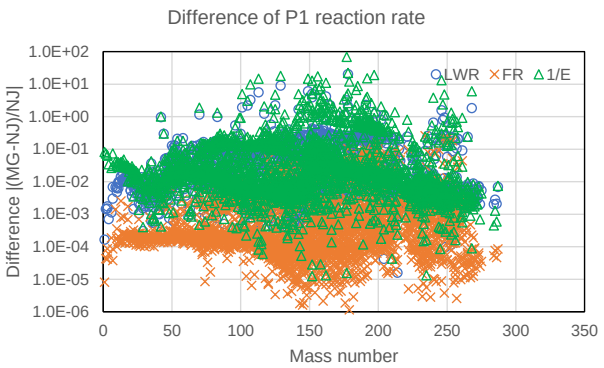




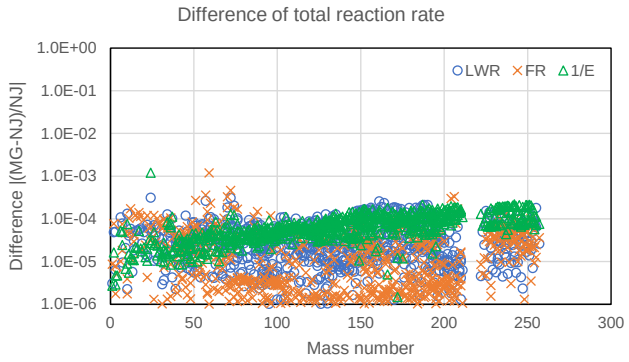


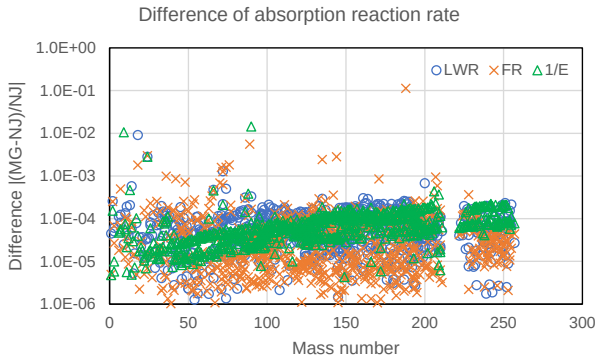


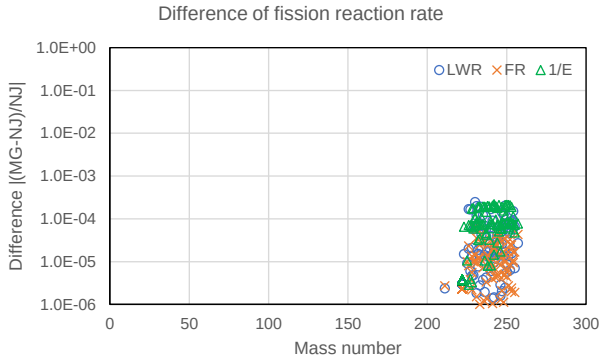


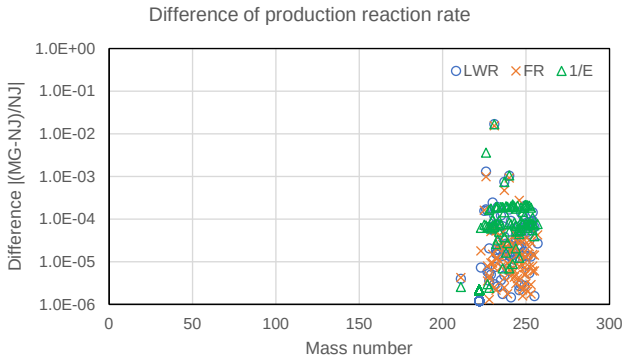


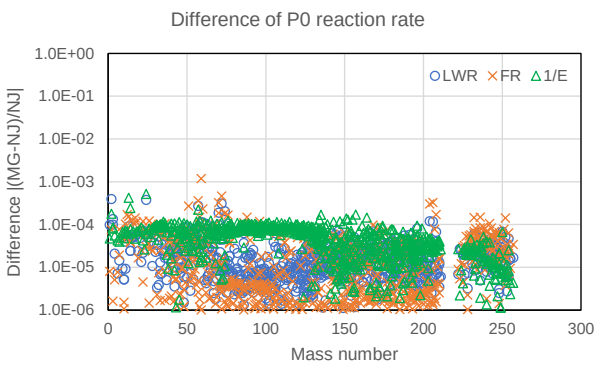
JENDL5, 300K, 10^{10} barn

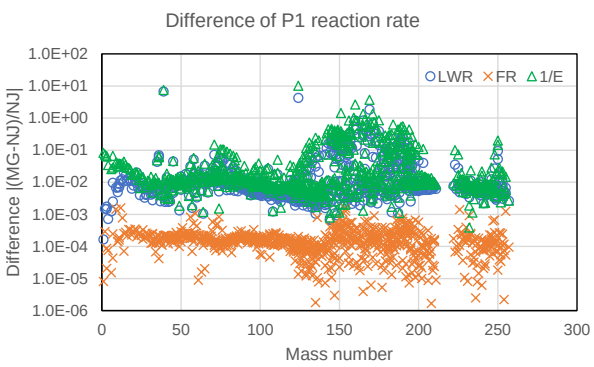












Note on processing

- FRENDY V2
  - All nuclides are processed without errors, except for Pu238 of TENDL-2021 (inconsistent nuclear data for number of delayed neutron groups).
- NJOY2016 (latest at 2020/12) :
  - All nuclides are processed without errors by increasing dimension size (next page)
  - Compilation for 64-bit execution module may be necessary (using Visual C++)

Note on processing

```
===================================================
acefc.f90
27c27
<     integer,parameter::nxcmax=600
---
 >    integer,parameter::nxcmax=500
86c86
<     integer,parameter::nxss=100000000
---
 >    integer,parameter::nxss=20000000
8004,8005c8004,8005
<     integer,parameter::nwscr=20000
<     integer,parameter::ndise=20000
---
 >    integer,parameter::nwscr=5000
 >    integer,parameter::ndise=5000
8019c8019
<     nwords=10*ntrp
---
 >    nwords=5*ntrp
===================================================
purr.f90
44c44
<     integer,parameter::jx=100000
---
 >    integer,parameter::jx=10000
133c133
<     nermax=5000
---
 >    nermax=1000
150c150
<     maxscr=1000000
---
 >    maxscr=20000
1094c1094
<     nthr=300
---
 >    nthr=140
1854c1854
<     dmin= 150000
---
 >    dmin= 100000
===================================================
```

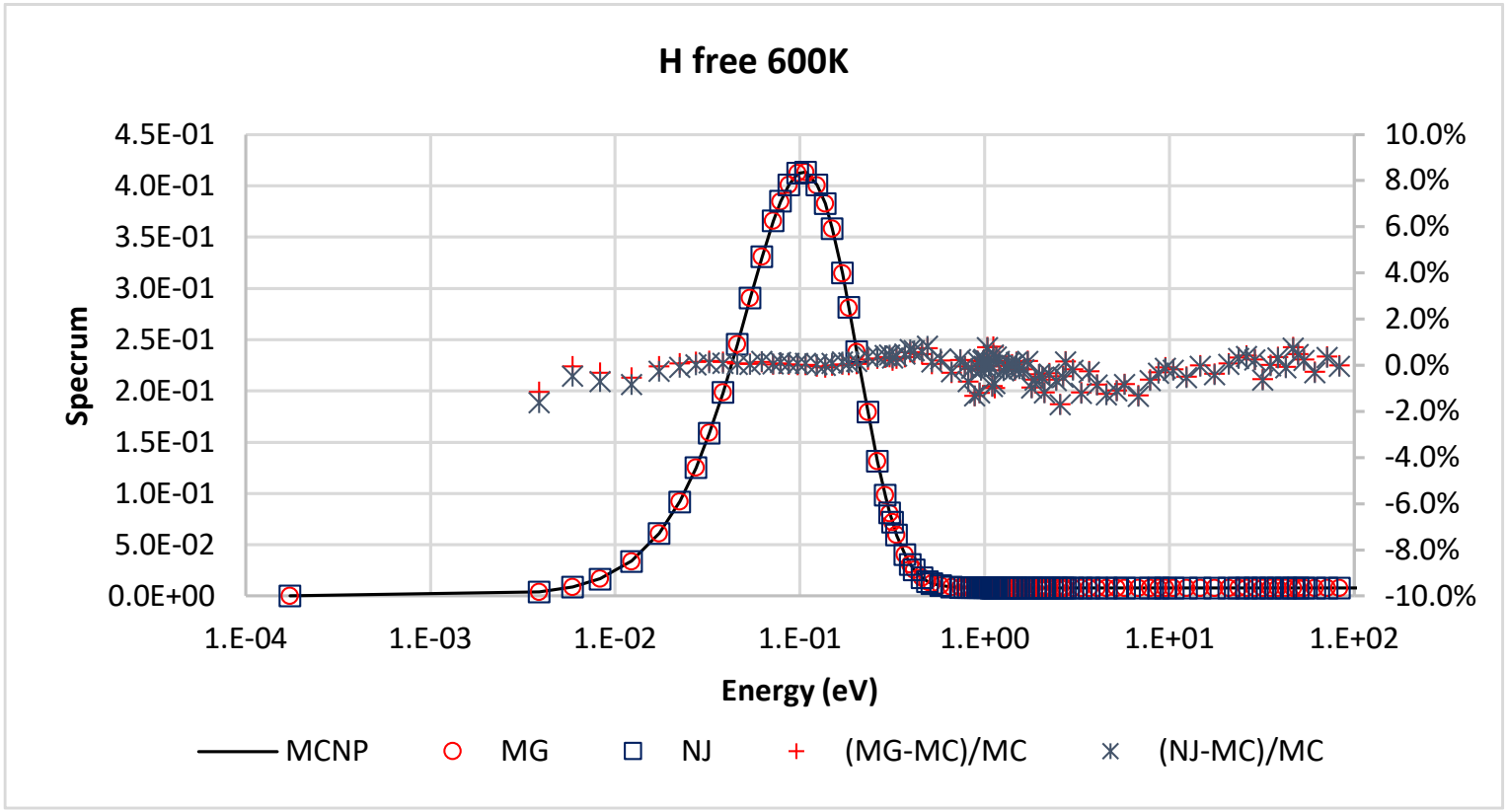
Modification of NJOY2016

- When multiple temperatures or background cross sections are specified, 10d block of matxs file is not correct.
- To avoid this issue, treatment by 10d block is bypassed.
- In groupr.f90, subroutine getff add statement with yellow marked. (start – end)

```
   ! find group where e-dependence begins
   ngn1=ngn+1
   do ig=1,ngn1
      if (econst.gt.egn(ig)*(1+small)) jconst=ig-1
   enddo
   econst=egn(jconst+1)
   if (jconst.le.2) econst=0
!do not use constant spectrum start
  econst = 0
  jconst = 0
!do not use constant spectrum end
   return
```

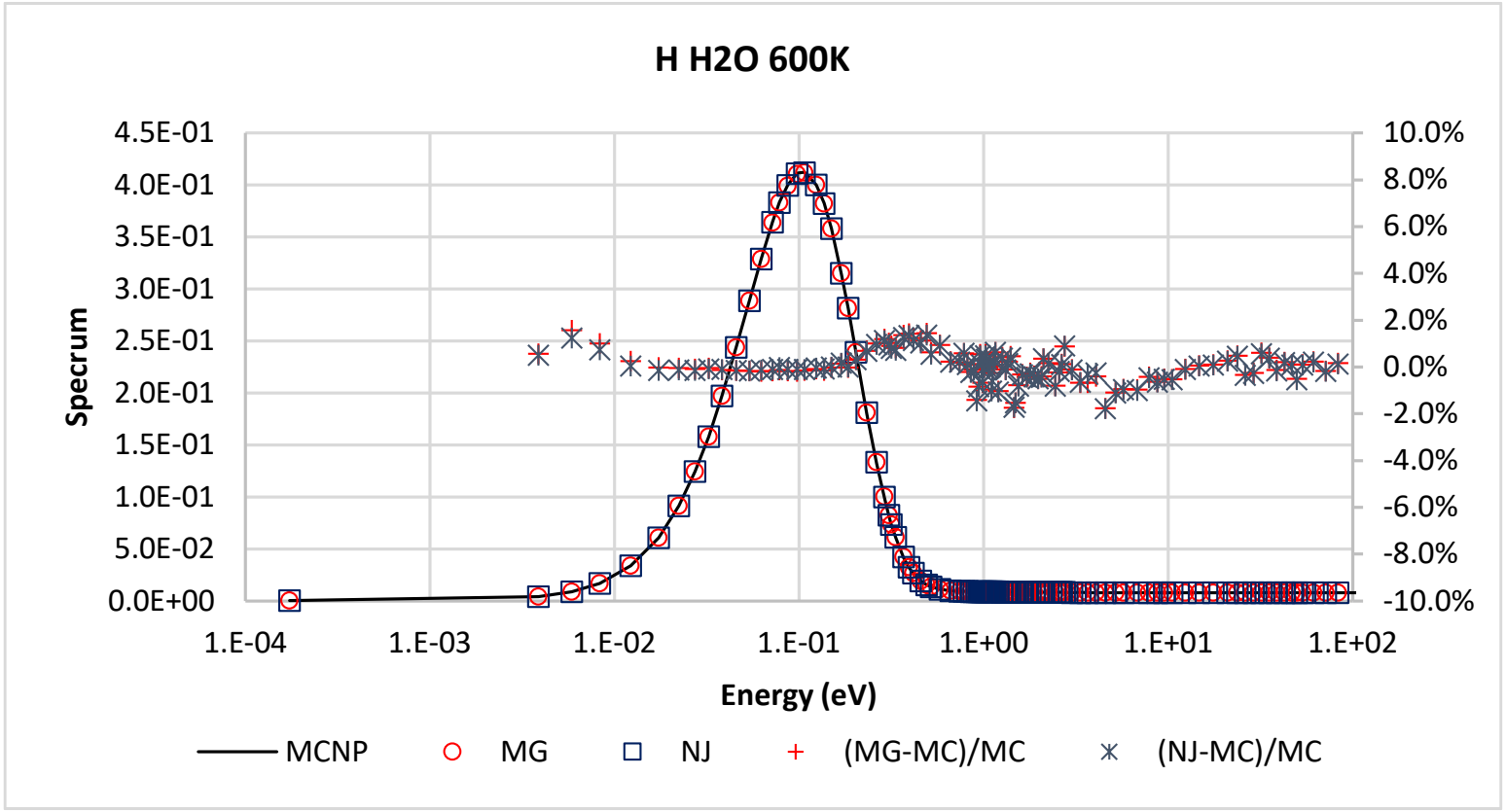
Thermal spectrum in homogeneous medium (H-free gas)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 600K



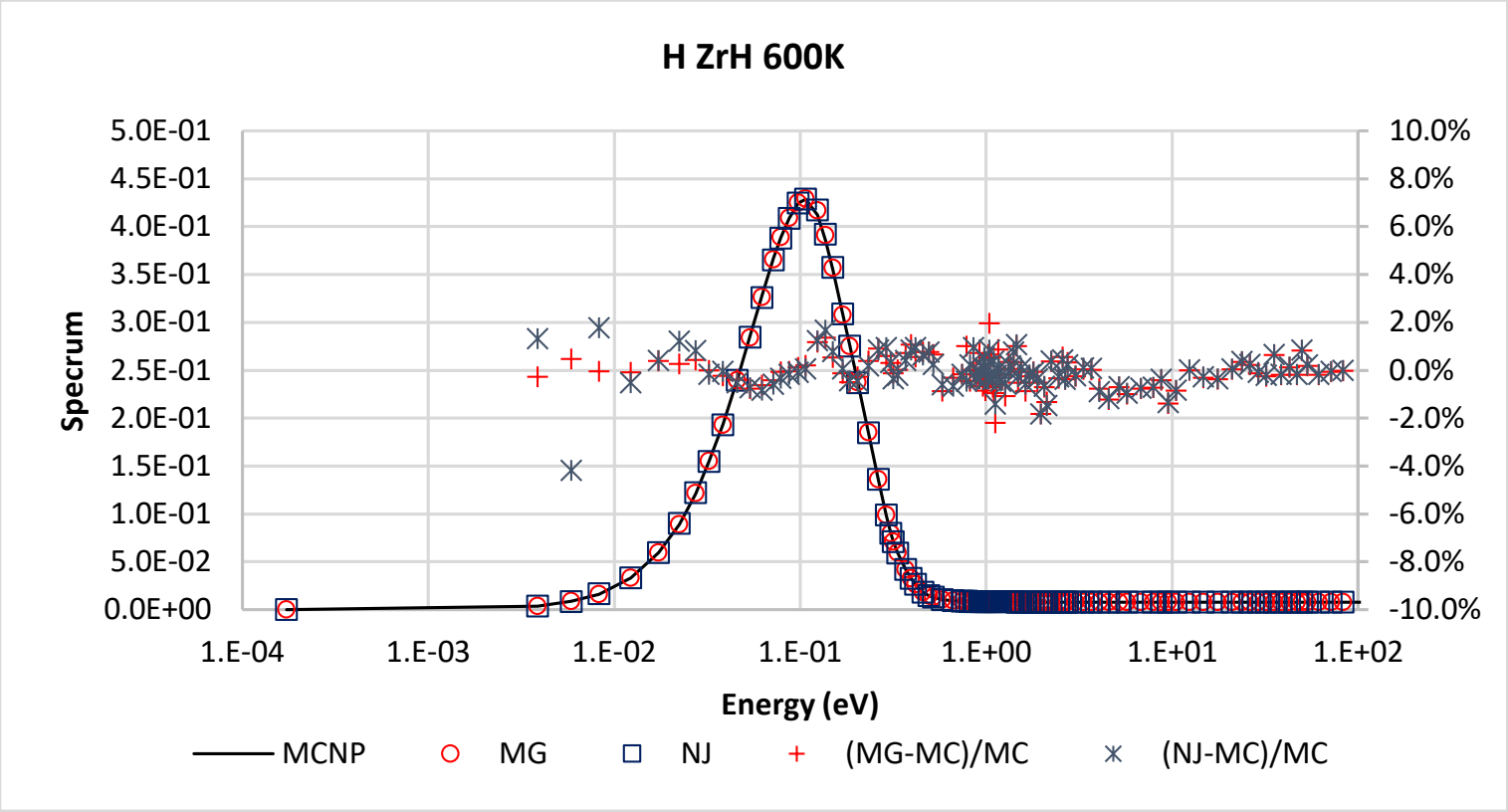
Thermal spectrum in homogeneous medium (H-H2O)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 600K



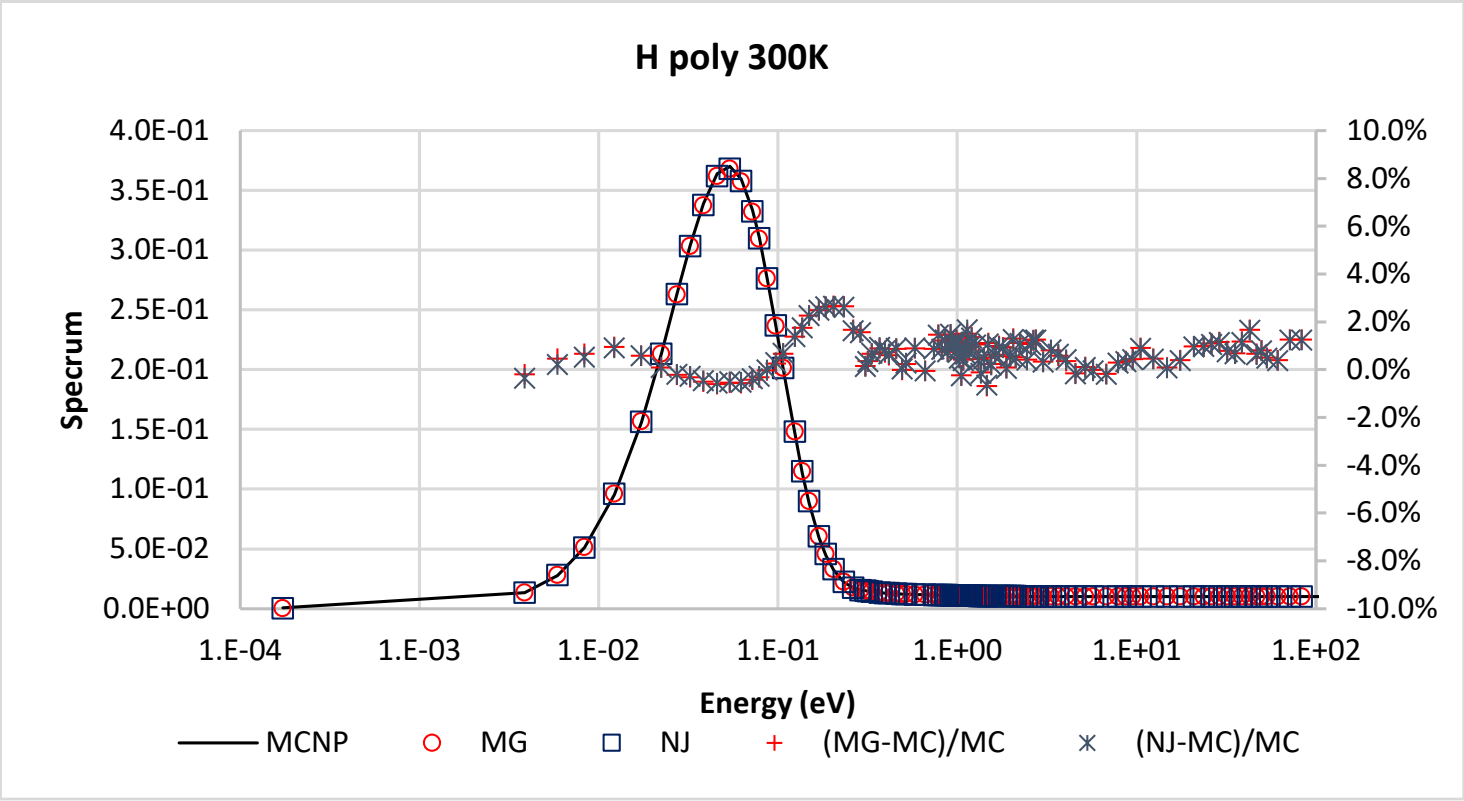
Thermal spectrum in homogeneous medium (H-ZrH)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 600K



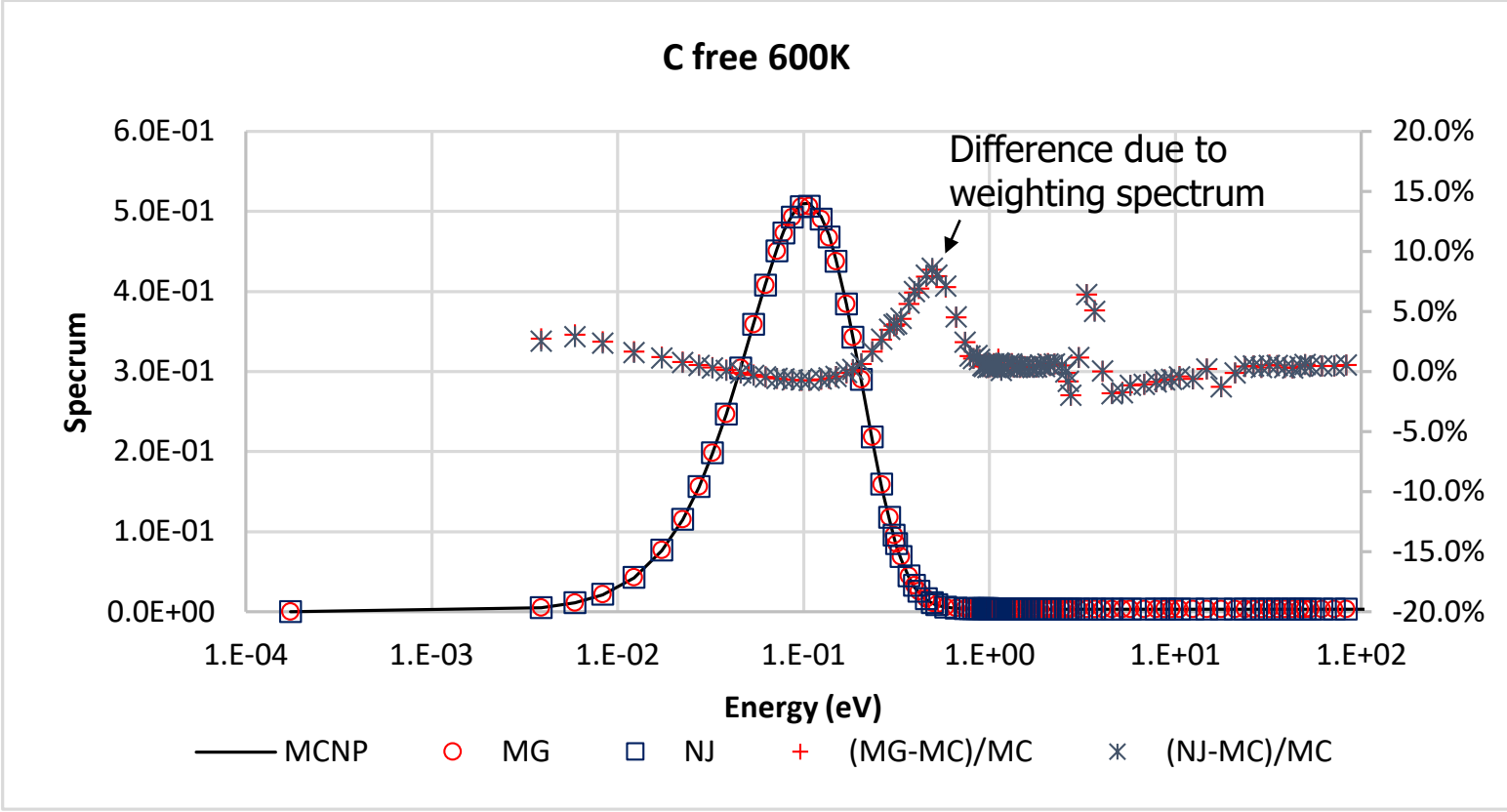
Thermal spectrum in homogeneous medium (H-Polyethylene)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 300K



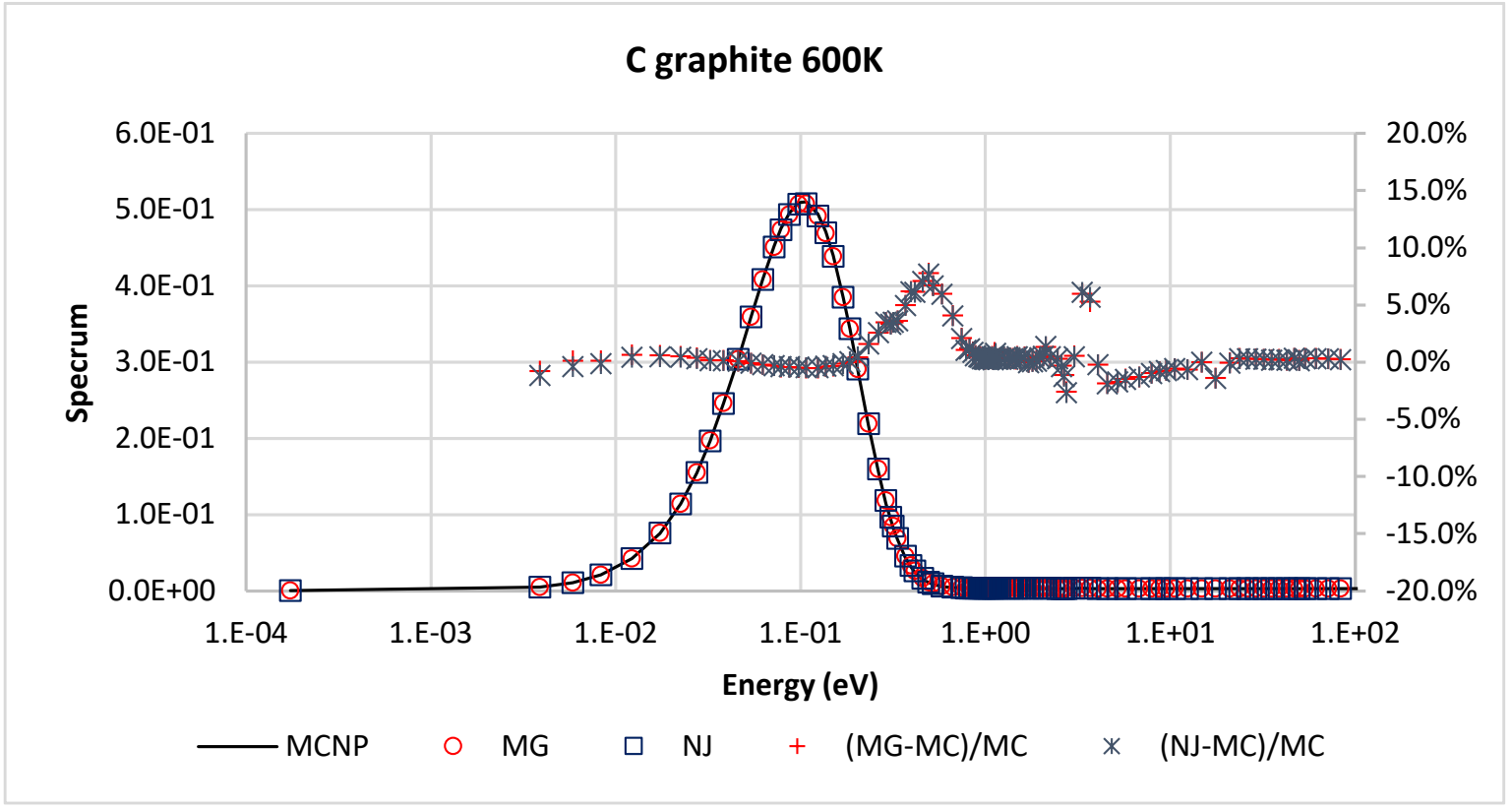
Thermal spectrum in homogeneous medium (C-Free)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 600K



Thermal spectrum in homogeneous medium (C-Graphite)

- MCNP6.2, FRENGY/ACE/MG-GENESIS(MG), NJOY(99.364)-GENESIS(NJ)
- JENDL4.0, 600K



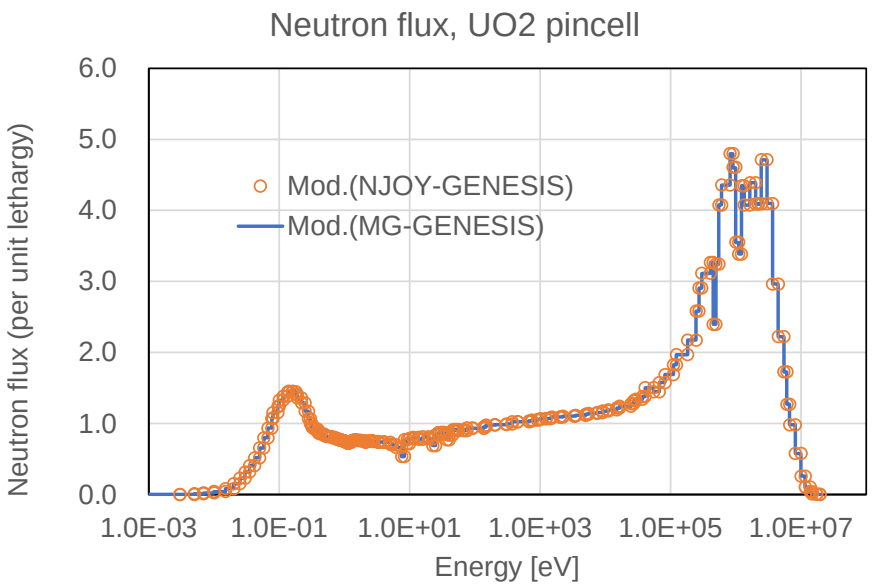
k-effective of UO2 pincell

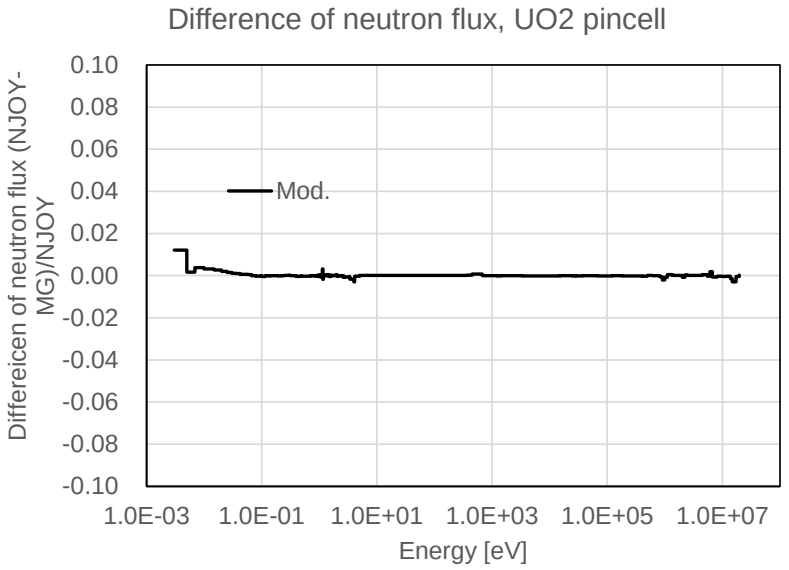
- 5wt% UO2, 600K, PWR pincell
- GENESIS (MOC), 172gr., P3
- $S(\alpha,\beta)$: H-free gas, H-H2O, H-ZrH, H-Polyethylene
- Summary of k-effective

H-temp.	S(a,b)	FRENDY/MG	NJOY99	Difference (MG-NJ)/NJ
600K	Free gas	1.4089470	1.4089180	0.002%
	H2O	1.4075497	1.4075113	0.003%
	H-Zrh	1.4075781	1.4075327	0.003%
300K	Free gas	1.4125241	1.4125083	0.001%
	Poly	1.4102028	1.4101741	0.002%

Neutron spectrum in pincell

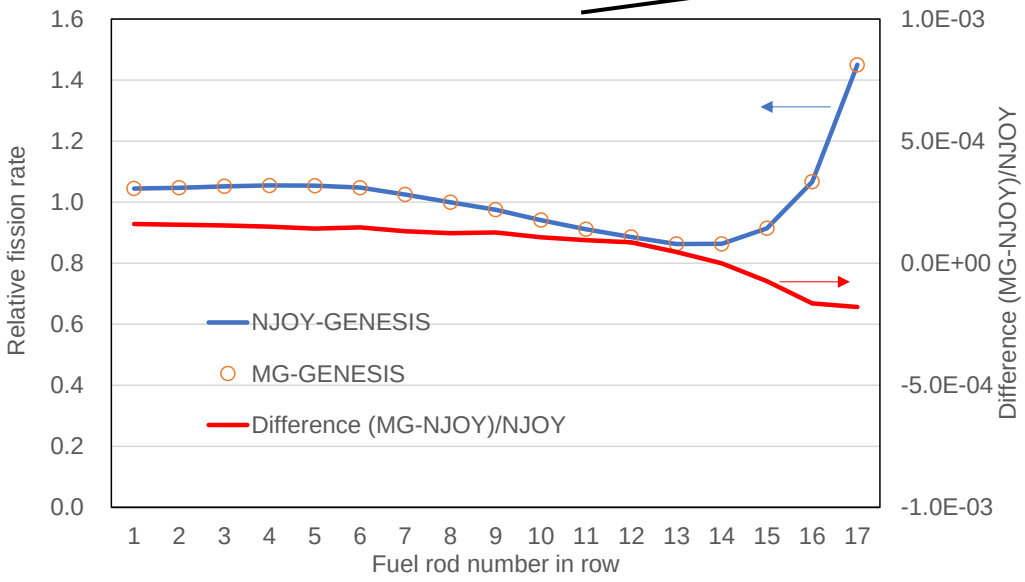
- Spectrum in H2O

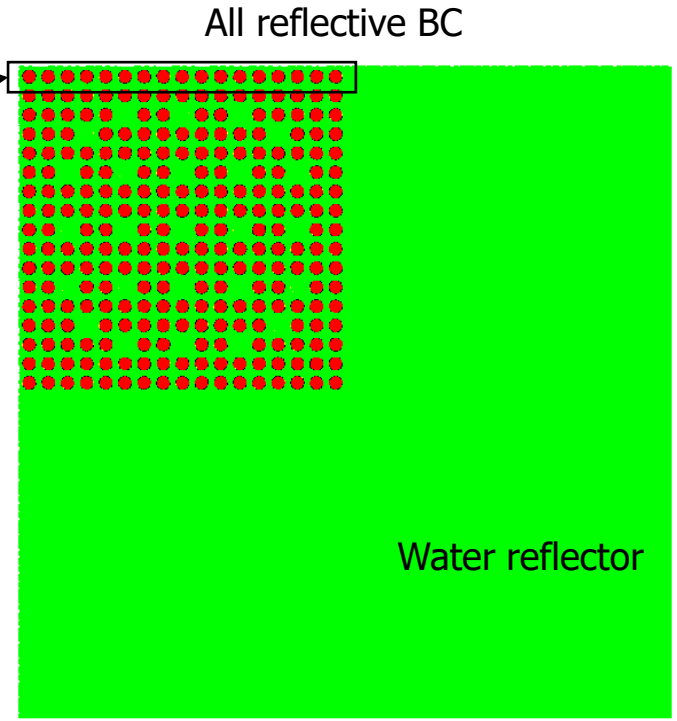




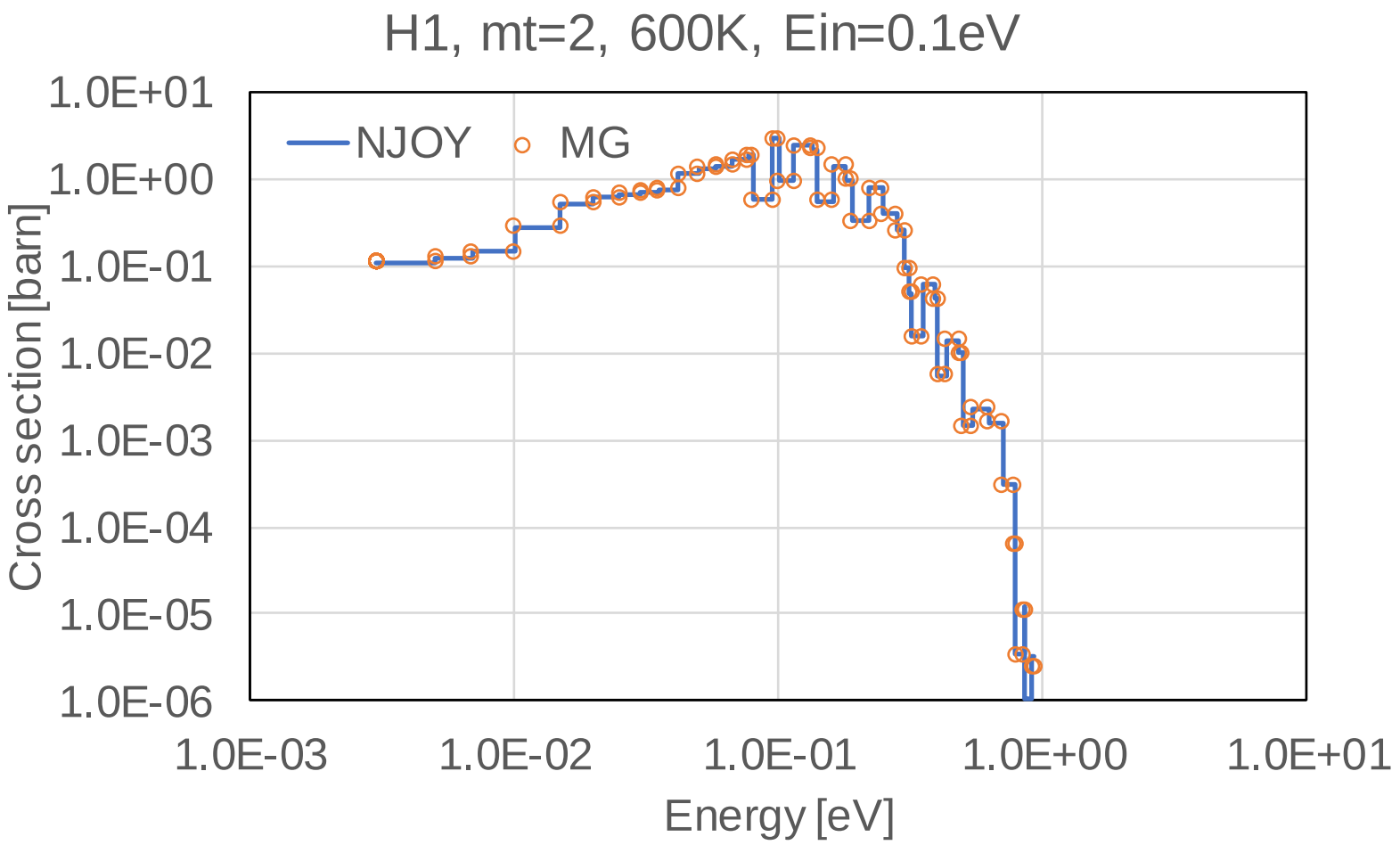
UO2 assembly+reflector

- 5wt% UO2, 600K, PWR fuel assembly
- GENESIS, 172 gr., P3, $S(\alpha,\beta)$: free gas
- K-effective
  - NJOY-GENESIS : 1.12372
  - MG-GENESIS : 1.12368
- Fission rate distribution



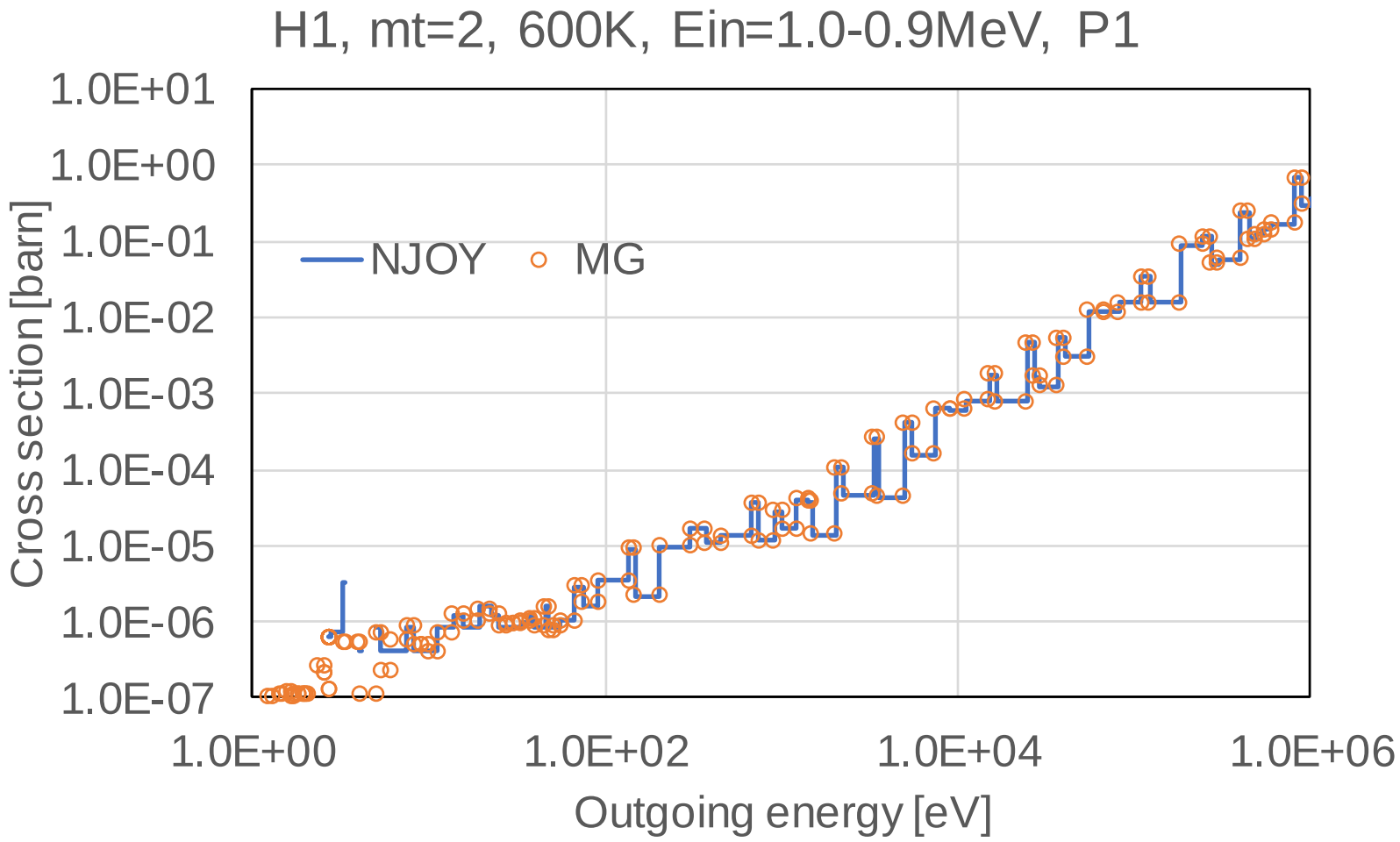


Comparison of cross sections H1 Thermal free gas scattering



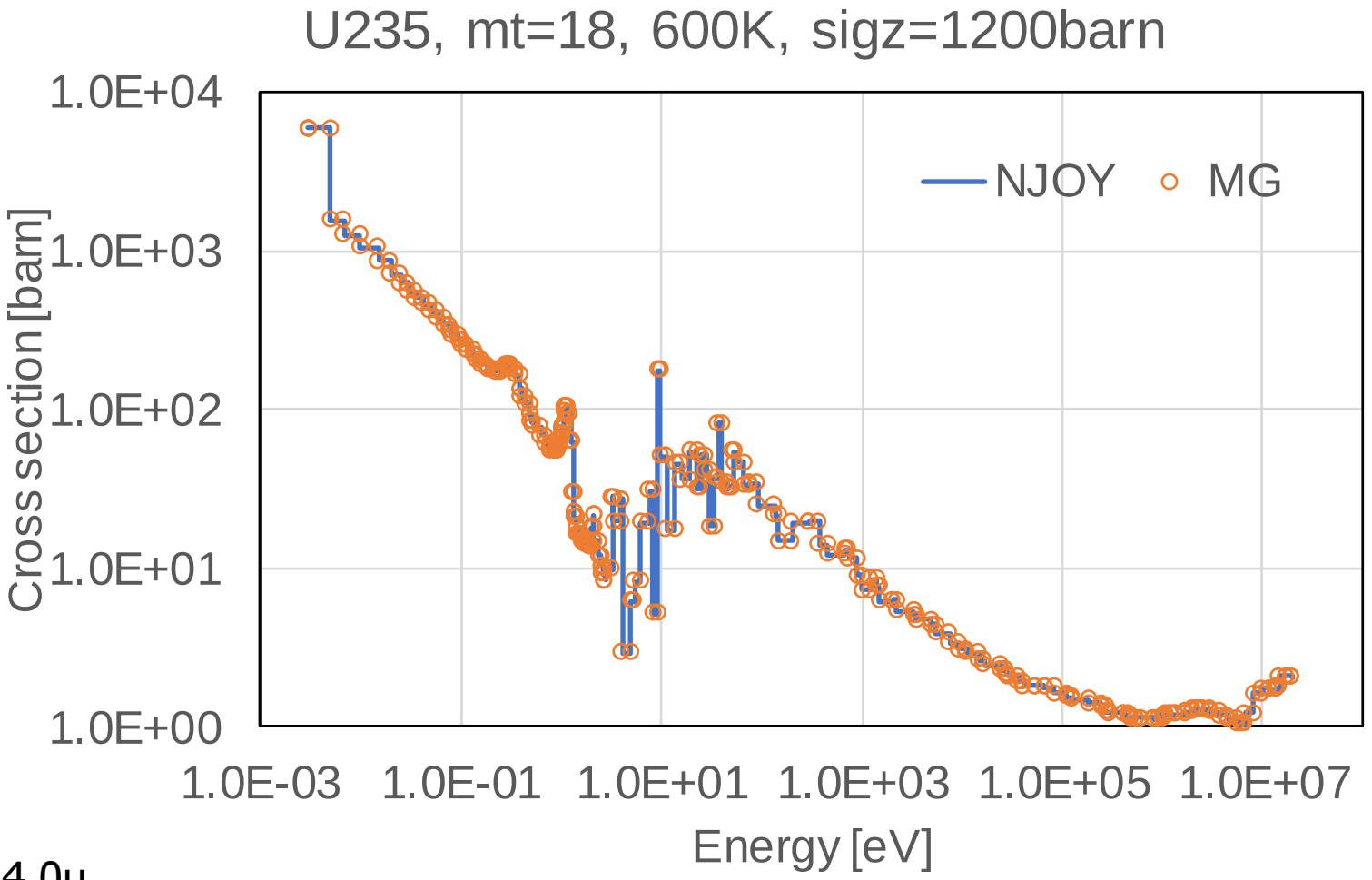
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section H1 elastic scattering (P1)



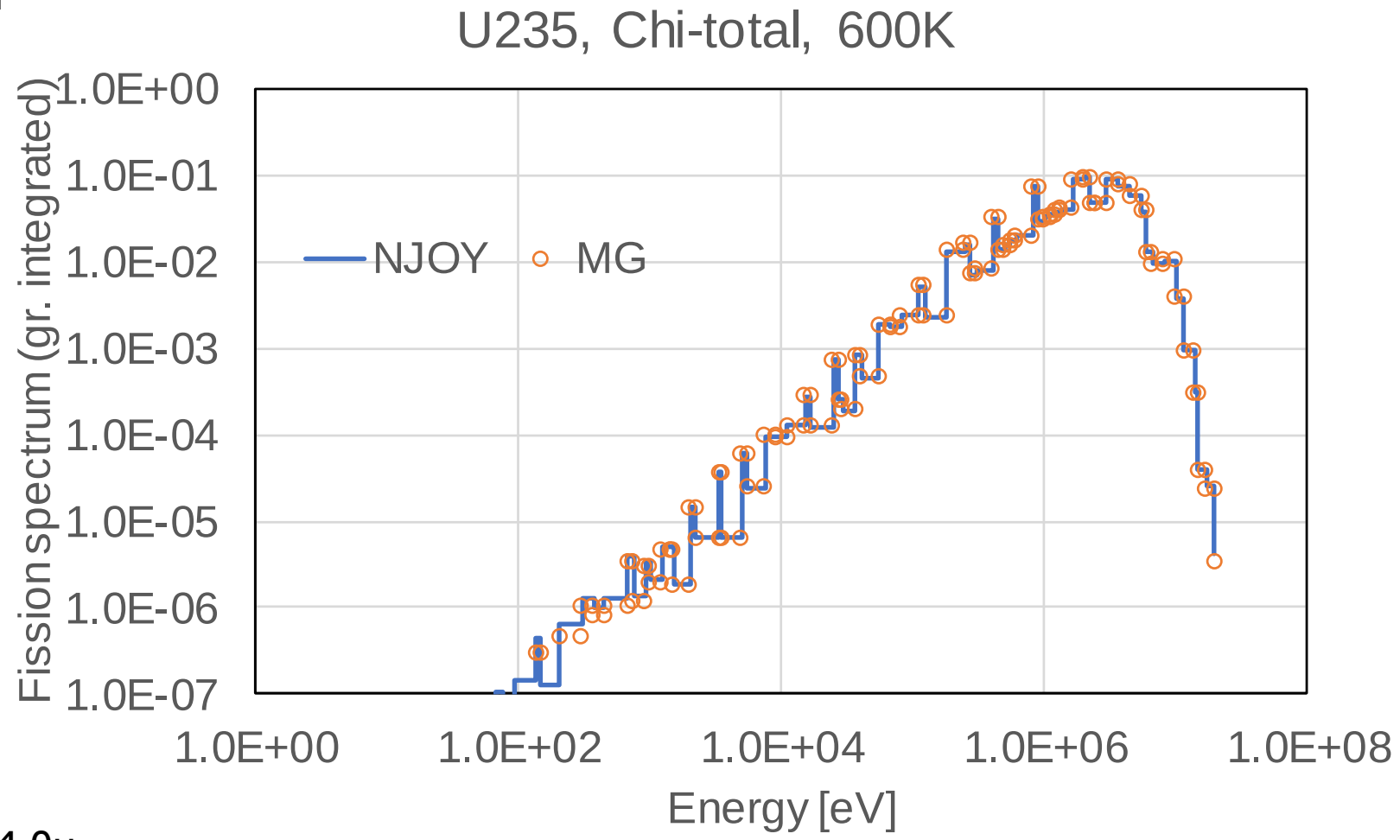
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section U235 fission



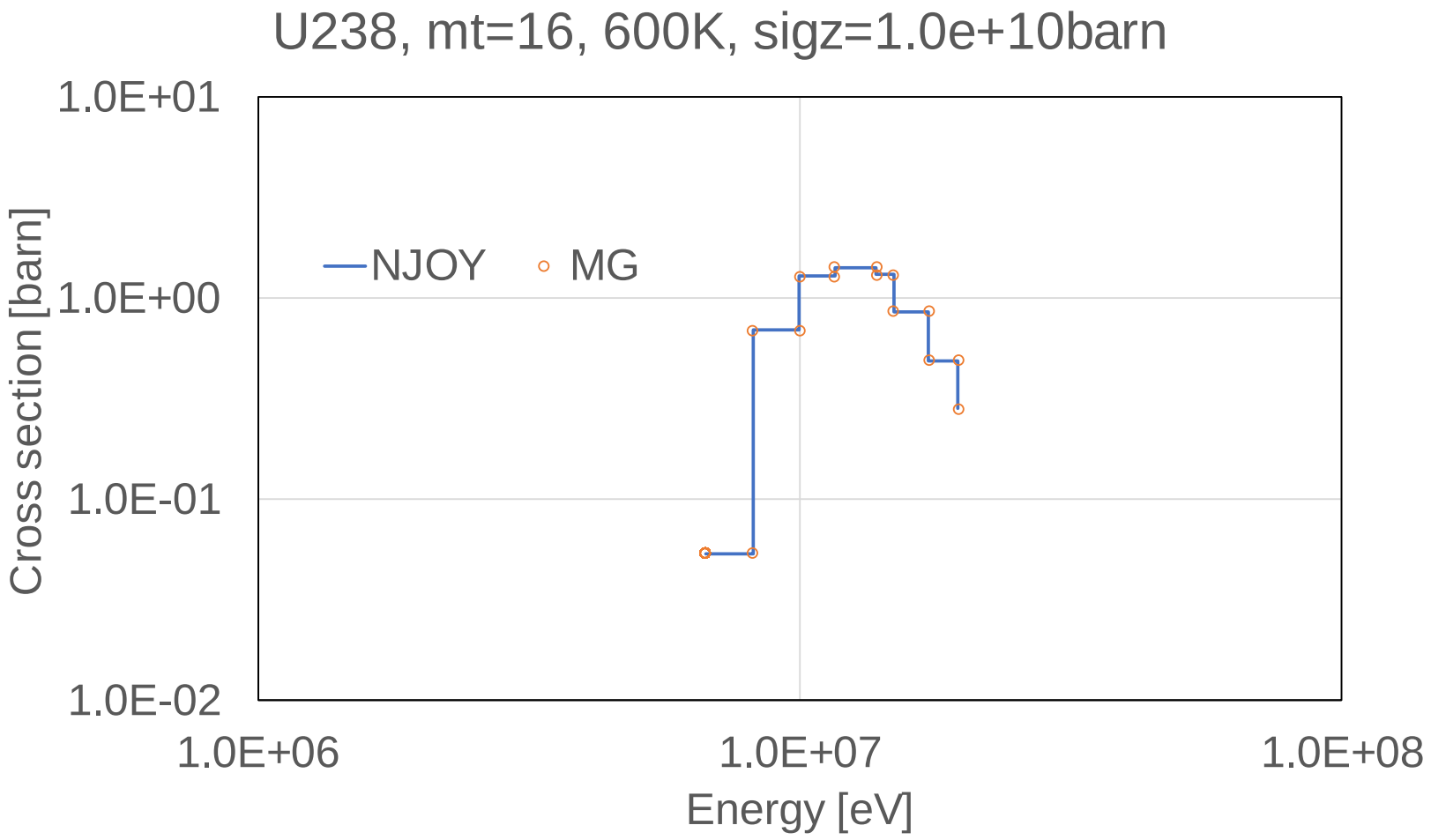
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section
U235 fission spectrum (prompt+delayed)



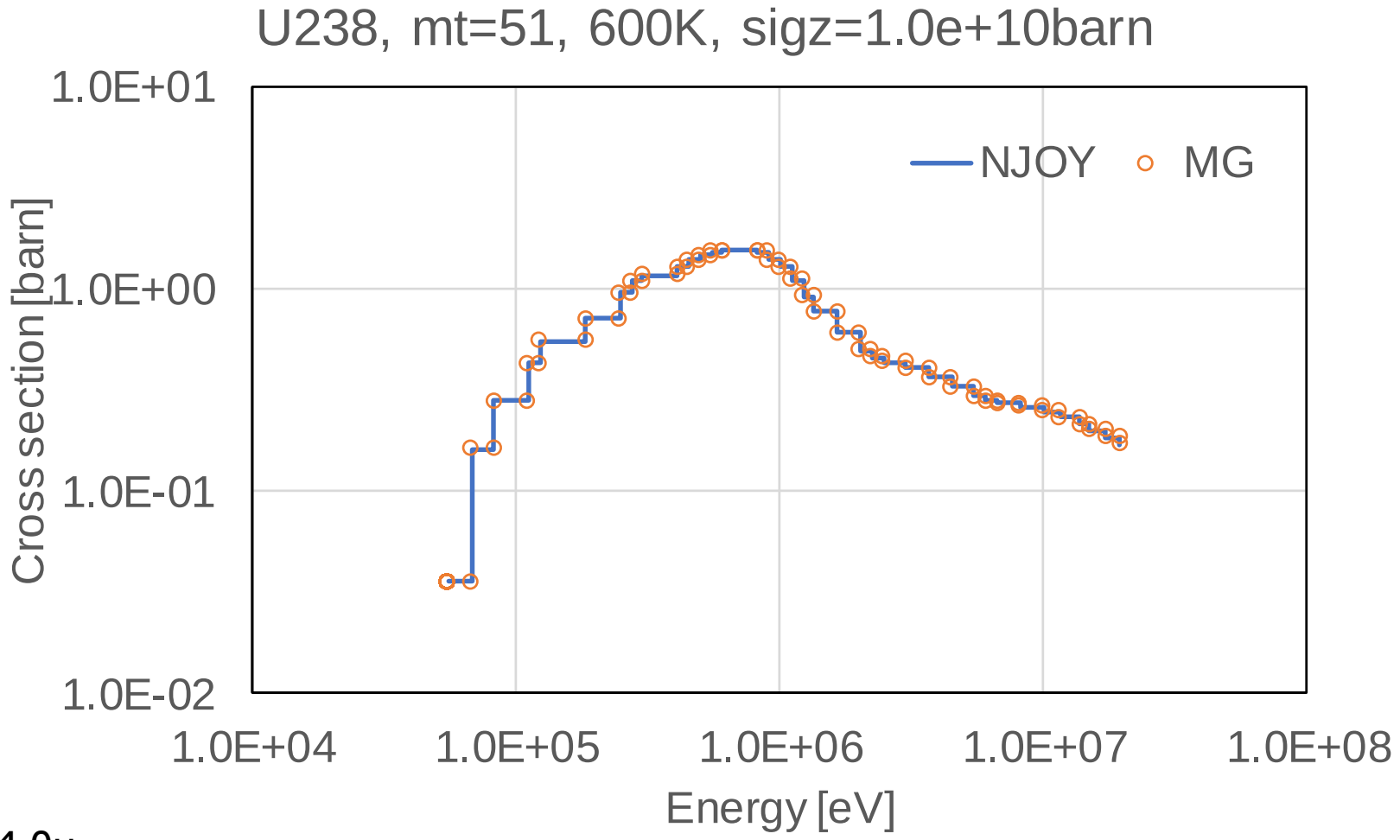
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section U238 (n,2n)



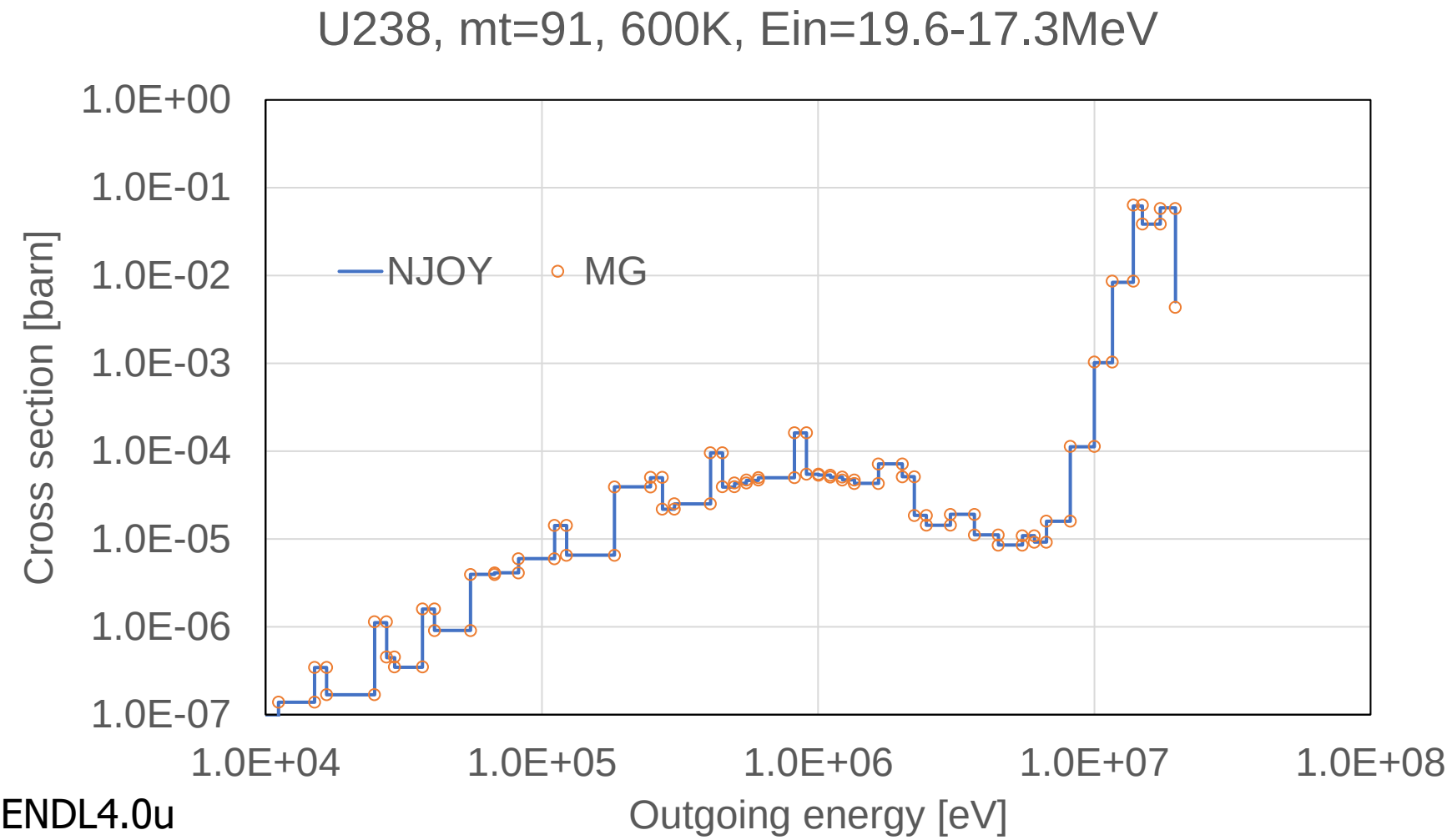
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section U238 inelastic scattering (mt=51)



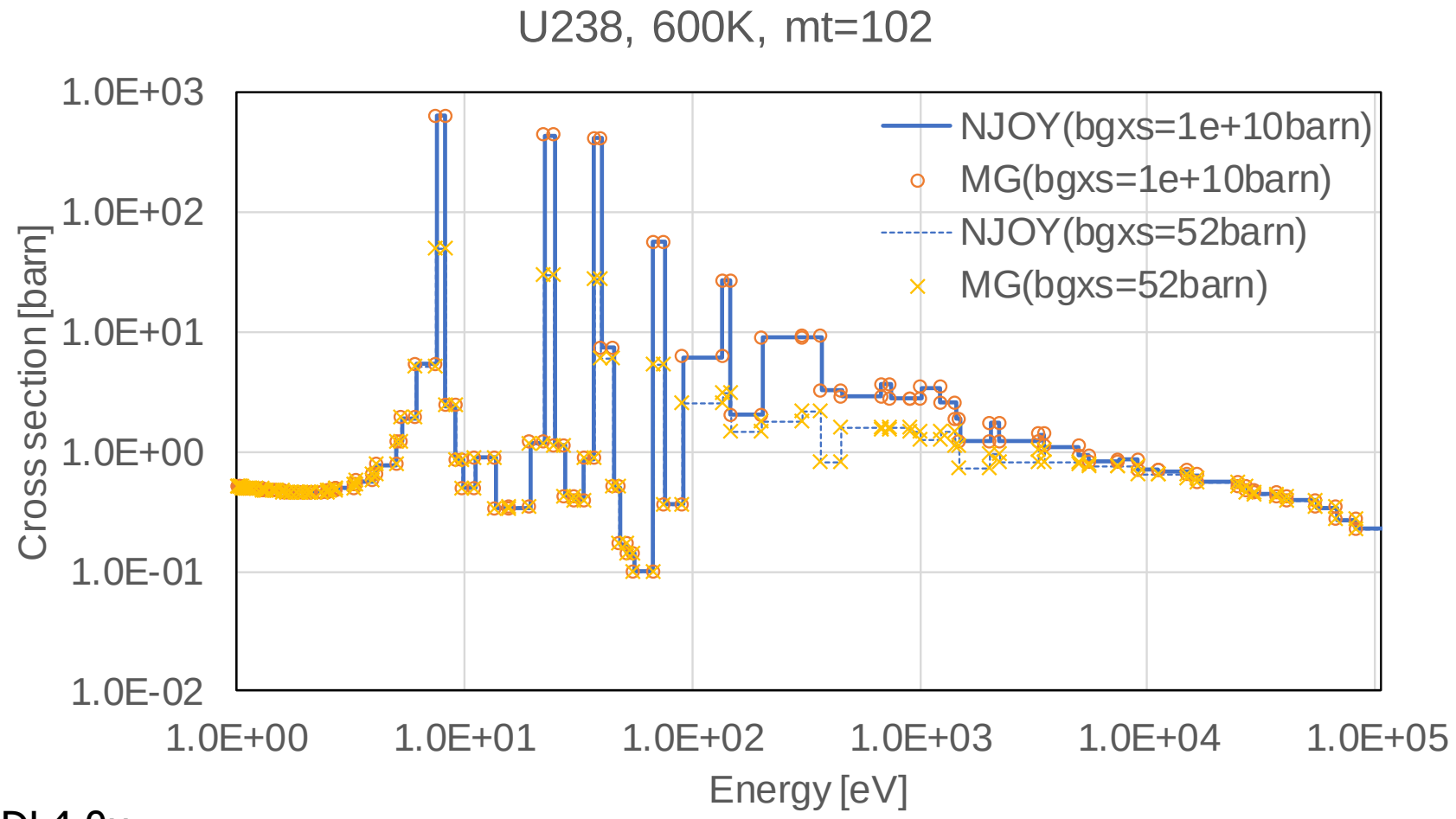
JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section U238 inelastic scattering (mt=91)

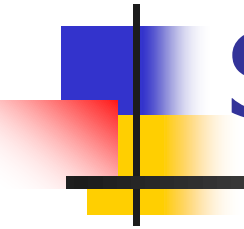


JENDL4.0u
1/E spectrum, NR approximation

Comparison of cross section U238 capture



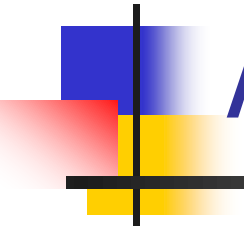
JENDL4.0u
1/E spectrum, NR approximation



Summary and future works

Summary

- Generation capability of multi-group cross sections in FRENDY V2 is described.
- FRENDY V2 can be downloaded from:
  - https://rpg.jaea.go.jp/main/en/program_frendy/
- Reference of FRENDY V2
  - K. Tada, Y. Nagaya, S. Kunieda, K. Suyama, T. Fukahori, "Development and verification of a new nuclear data processing system FRENDY," J. Nucl. Sci. Technol., 54, pp.806-817 (2017).
  - https://www.tandfonline.com/doi/abs/10.1080/00223131.2017.1309306
  - 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., 58, pp.1165-1183 (2021).
  - https://www.tandfonline.com/doi/full/10.1080/00223131.2021.1921631
  - K. Tada, R. Kondo, T. Endo, A. Yamamoto, "Development of ACE file perturbation tool using FRENDY," J. Nucl. Sci. Technol. (2022).
  - https://www.tandfonline.com/doi/full/10.1080/00223131.2022.2130463



Appendix

Potential issues of NJOY2016

- Difference of absorption reaction in Cs137 of JENDL4.0: Due to inconsistency for mt=30, which provides zero cross sections at mf=3 in nuclear data. In the 7d section of the MATXS file, zero cross sections are automatically eliminated, but not in 6d in the NJOY processing. FRENDY/ACE/MG avoids this issue by bypassing 1d cross section processing whose all elements are zero.
  - Issue of NJOY, MATXSR.
- In NJOY, self-shielding factors are calculated only for total, fission, capture, and elastic scattering. However, some nuclides have large resonances in other reactions. For example, in the case of C000 (J4) and Ni059 (J4), self-shielding in mt=107 is not negligible in the high energy region. However, infinite dilute cross sections are used in the GROUPR of NJOY. FRENDY/MG explicitly considers self-shielding for all reactions.
  - Issue of NJOY. In GROUPR, self-shielding is calculated only for mt=1, 2, 18, 102. For 2d cross section, only for mt=2. Therefore, even if GENDF is used, this issue will not be resolved.
- Eu156 of B7.1, 8.0: Some difference is observed in all reactions. Smooth cross sections for 1 - 7eV show difference due to different interpolation scheme
  - Issue of NJOY. Log-log in NJOY using limited energy points, FRENDY/ACE does not perform interpolation - direct calculation at all energy points.

Potential issues of NJOY2016

- Pm148g of JEFF3.3: Some difference is observed in all reactions. Smooth cross sections for 1.5 – 10 eV show difference due to different interpolation scheme.
  - Same as above.
- Cm247 of JEFF3.3: Some difference is observed in all reactions. Smooth cross sections for 50 – 500 eV show difference.
  - Same as above.
- Ca040 of B8.0: peak value of mt=600 around 1 MeV is not appropriately reconstructed in NJOY due to numerical issue of the Coulomb function.
  - Issue of NJOY
- Cs135 in JEFF3.3: inconsistent definition of mt=30 for mf=3 (zero) and mf=6 (nonzero small value). FRENDY/ACE/MG sets zero values for mt=30, but NJOY21 provides some value, which seems to be incorrect. The same issue exists for Cs135 and Cs137 of JENDL4.0.
  - Issue of NJOY, MATXSR

Potential issues of NJOY2016

- Ra226 of JEFF-3.3: nu-value is incorrect in NJOY.
- Be7 of ENDF-7.1: mt=1 of the 7th group in XMAS 172 energy group is zero
- P1 reaction rates: Differences are generally larger than those of the P0 reaction rate. These differences mainly come from insufficient numerical integration accuracy of NJOY in the thermal energy region.
  - Deficiency of NJOY
- F017, Ne019 of TENDL2019: reconstructed pointwise cross sections by NJOY2016 are not accurate (due to zero cross section at the upper energy of resonance range in nuclear data file)
- Sc45 (mt=1) in B7.1, Sn124 (mt=102), Po210 (mt=102) in B8.0: Boundary between unresolved/resolved energy range is not appropriately set in NJOY.
- O018 of TENDL2019: scattering matrix of mt=91 is half of the appropriate values
- O018 of TENDL2019: pointwise cross section reconstruction for mt=102 is inaccurate
- Reaction name in MATXS file correspond to mt=749 is “tcd” in NJOY2016, while “tcn” is correct.

Potential issues of nuclear data

- Zero cross sections between resolved/unresolved resonance
  - TENDL-2019, C011 mt=2, F017 mt=1, Ne019 mt=2
- Sum of prompt and delayed nu-values is not consistent with total nu-value
  - Th231, ENDF-7.1, 8.0
  - Pa231, Cm247, JEFF-3.3
- Some metastable nuclides in B8.0: Differences of P0 reaction rate are observed. Elastic cross section (mt=2) is not adequately processed in the MATXS file of NJOY.
  - Issue of nuclear data (Q-value of mt=2 is not zero in B8.0)
  - Al26m, Ag118m, Sn121m, Te121m, Te131m, I132m, Ce137m, Re186m, Ir197m, Hg197m, Bi210m
- Delayed nu-value for mf=1 mt=451 exists but mf=5 mt=455 does not exist. No delayed nu-value is given in the ACE file (both of FRENDY and NJOY).