Current status of nuclear data processing code NECP-Atlas

Tiejun Zu
tiejun@mail.xjtu.edu.cn
NECP Lab., Xi'an Jiaotong University
2022.07.25

15th International Conference on Nuclear Data for Science and Technology (ND2022)
24-29 July, 2022

Contents

1. Overview

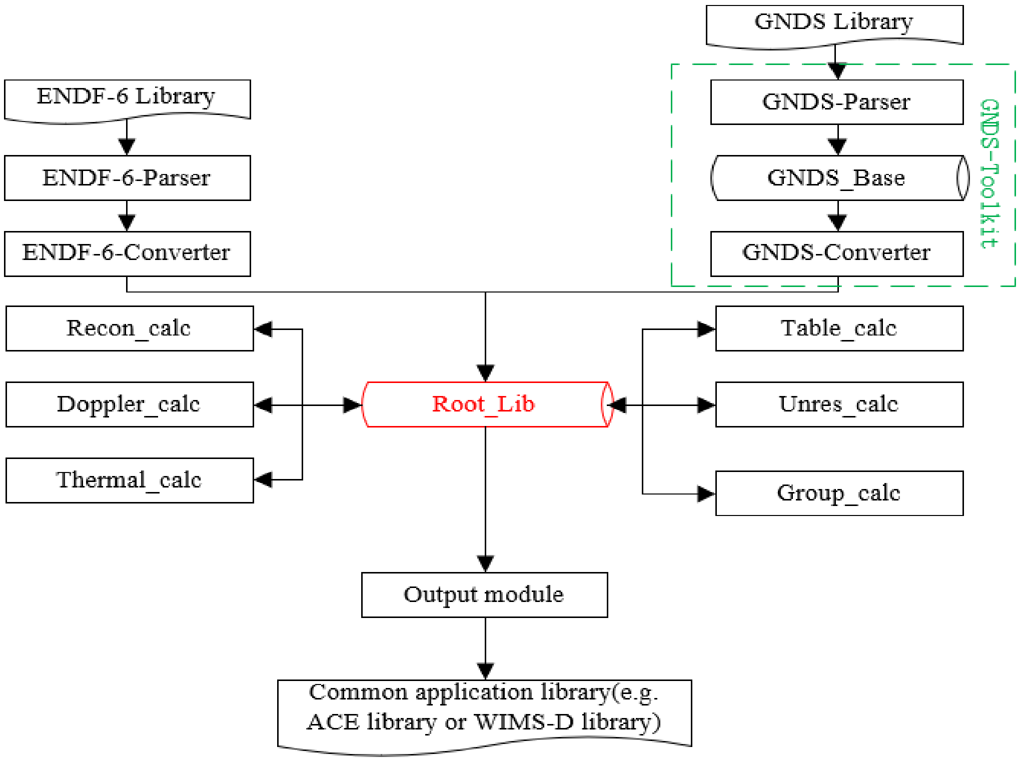
- The development of NECP-Atlas was started in 2015.
- In ND2019, the basic functions for generating the neutron cross section libraries were reported.

□ In the past three years:

- Tested against several newly released evaluations
  - CENDL-3.2, JENDL-5.0, TENDL-2021, FENDL-3.2
- Verified with various benchmarks, and operated commercial PWRs.
- New capability for processing the GNDS format evaluations
- New processing functions:
  - Treatment of resonance elastic scattering
  - Thermal scattering law data
  - Photon related data
  - Damage production data caused by neutron, electron, photon
  - Multigroup covariance for reaction cross sections; covariance for fission yields

2. Processing of GNDS format evaluations

- Version 1.9 for GNDS format was released by OECD/NEA, in 2020
- NECP-Atlas was updated to process the GNDS format evaluations.
- A Fortran derived data type named Root_Lib is designed to store the evaluated data in ENDF-6 and GNDS formats, and transfer data among various functional modules.



Publication: Y. Huang, T. Zu*, et al., Progress in Nuclear Energy, 150 (2022) 104293

2. Processing of GNDS format evaluations

- The data structure of Root_Lib keeps ENDF-6 format, due to the fact it was originally designed according to the hierarchy of ENDF-6 format.
- A module called GNDS-Toolkit is developed to read, parse and convert the GNDS/XML format into Root_Lib.

```
type Root_Lib
    real                          ::  target_mass
    integer                       ::  target_ZA
    real                          ::  projectile_mass
    real                          ::  projectile_ZA
    integer                       ::  number_temperature
    real                          ::  AWR
    type(root_type),allocatable   :: datas(:)
end type Root_Lib
```

```
type root_type
    real                                 :: temperature
    integer                              :: number_reaction
    type(hash_map_type)                  :: mftp_map
    type(data_base_type),allocatable     :: mftp(:)
end type root_type
```

```
type data_base_type
    integer                          :: mf
    integer                          :: mt
    type(head_type),allocatable      :: head(:)
    type(cont_type),allocatable      :: cont(:)
    type(list_type),allocatable      :: list(:)
    type(tab1_type),allocatable      :: tab1(:)
    type(tab2_type),allocatable      :: tab2(:)
end type data_base_type
```

Data records

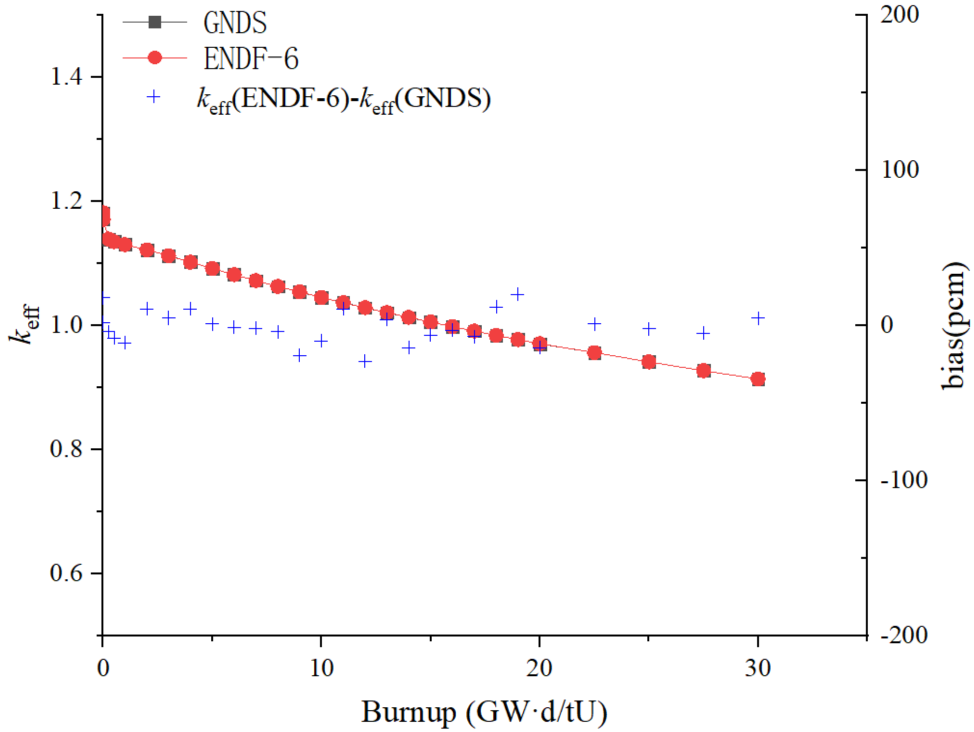
- A Hash map is constructed to store the mapping information of the reactions.
- The key for a certain reaction is defined as:

$$key = MF \times 1000 + MT$$

- For the non-ENDF allowed reactions, it can be assigned with an artificial MF and MT.

2. Processing of GNDS format evaluations

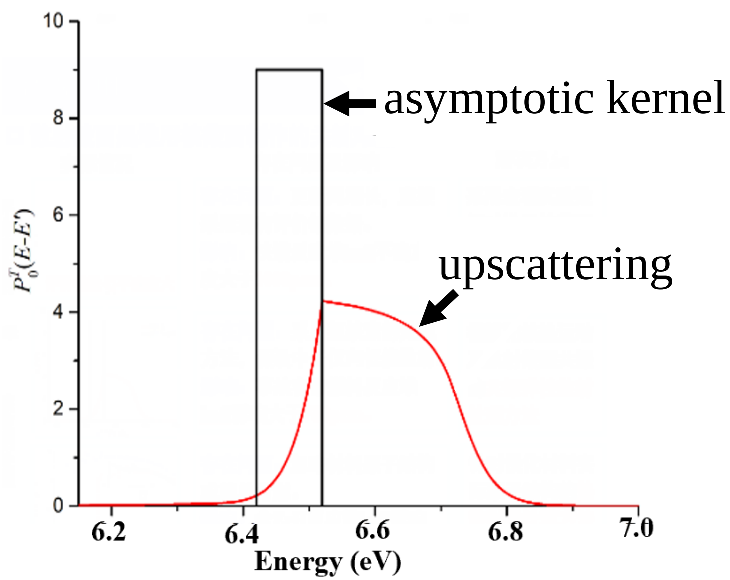
- The new capability is verified with various benchmarks
- The following is the result for VERA-1B benchmark
  - ENDF-B/VIII.0; ACE format Library
  - Calculation tool: Monte Carlo code NECP-MCX
  - 220 fission products + 28 heavy nuclides
- The results between ENDF-6 and GNDS libraries are in good agreement.



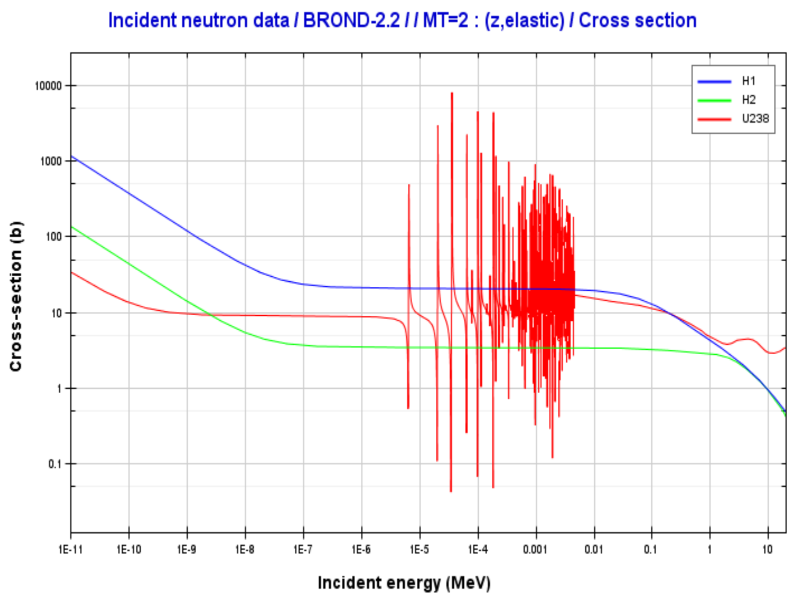
k_{eff} changing with burnup

3. Treatment of resonance elastic scattering

- Among 4eV~250eV, the thermal agitation of the target nuclides will cause the neutron upscattering.
- Monte Carlo codes use the Doppler Broadened Rejection Correction (DBRC) method to simulate the exact secondary energy distributions.
- As for the multi-group cross section calculations in the nuclear data processing codes:
  - the free gas model assume the scattering cross section is constant
  - the asymptotic kernel is usually used to calculate the weighting function



Secondary energy distribution for incident neutron of 6.52eV



Elastic scattering cross section of different nuclides

3. Treatment of resonance elastic scattering

- Implement the Doppler broadening for the resonance elastic scattering kernel (RESK) to calculate the secondary energy distribution

$$\sigma_{sn}^{T}(E \to E') = \frac{\beta^{5/2}}{4E} \exp(E / k_B T) \int_0^\infty t \sigma_s\left(\frac{\beta k_B T}{A} t^2\right) \times \exp(-t^2 / A) \psi_n(t) dt \Rightarrow P_n^T(E \to E') = \frac{\sigma_{sn}^{T}(E \to E')}{\sigma_{sn}^{T}(E)}$$

- Based on the RESK, the $S(\alpha, \beta)$ table is generated for Monte Carlo codes to simulate the upscattering, avoiding to use the DBRC model.

- To get the weighting function for the multi-group cross section calculation:
  - Hyper-fine group slowing-down equation is established with RESK model.
  - Gauss-Seidel iteration strategy is adopted to solve the hyper-fine group neutron slowing-down equation.

- *The above method has been implemented into NJOY2012 by Prof. Alain Hébert of Polytechnique Montréal, Canada. He will report the work in the poster session in ND-2022.*

Publication: J. Xu, T. Zu*, et al., Progress in Nuclear Energy, 110 (2019) 301-310.

3. Treatment of resonance elastic scattering

- The results Mosteller UOX fuel benchmark at 900 K
  - The results based on the S(α, β) table agree well with those from DBRC model.
  - The effect of the upscattering on the keff can reach about 200pcm.

UO_2 (wt. %)	no S(α, β) table	DBRC	S(α, β) table	Diff. / pcm (S(α, β) table – DBRC)	Diff. (S(α, β) table – no S(α, β) table)
0.71	0.66050 ± 5	0.65956 ± 5	0.65939 ± 5	-17	-111
1.60	0.95352 ± 7	0.95194 ± 7	0.95199 ± 7	5	-153
2.40	1.09077 ± 8	1.08889 ± 8	1.08902 ± 8	13	-175
3.10	1.16828 ± 8	1.16637 ± 7	1.16645 ± 8	8	-183
3.90	1.23044 ± 8	1.22867 ± 8	1.22856 ± 8	-11	-188
4.50	1.26583 ± 7	1.26381 ± 7	1.26384 ± 7	3	-199
5.00	1.28996 ± 8	1.28799 ± 8	1.28799 ± 8	0	-197

4. Generation of thermal scattering law

- The codes capable of calculating thermal scattering law (TSL) data are limited around the world.
- A module named sab_calc is developed in NECP-Atlas to calculate TSL, based on
  - phonon expansion model
  - trajectory data obtained by using molecular dynamics (MD) simulation (on going)

- The double differential scattering cross section under phonon expansion:

$$\frac{d^2\sigma}{d\mu dE'} = \frac{1}{4\pi}\frac{1}{k_B T}\sqrt{\frac{E'}{E}}\left[\sigma_{\mathrm{coh}}\left(S_s + S_d\right) + \sigma_{\mathrm{inc}} S_s\right]$$

$$= \frac{1}{4\pi}\frac{1}{k_B T}\sqrt{\frac{E'}{E}}\left[\sigma_{\mathrm{coh}}\left(\sum_{n=0}^{\infty} S_s^n + \sum_{n=0}^{\infty} S_d^n\right) + \sigma_{\mathrm{inc}}\sum_{n=0}^{\infty} S_s^n\right]$$

Phonon expansion

- Some techniques are adopted to relax the approximations in the phonon expansion model:
  - Incoherent approximation for inelastic scattering
  - Cubic approximation and atom site approximation for coherent elastic scattering

Publication: Y. Tang, T. Zu*, et al., Annals of Nuclear Energy, 153 (2021) 108044.

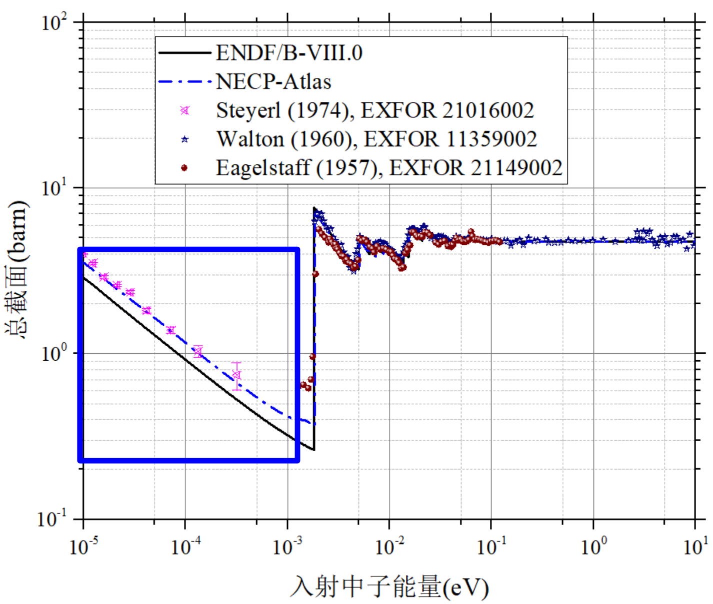
4. Generation of thermal scattering law

- The incoherent approximation for inelastic scattering assumes: S_d=0

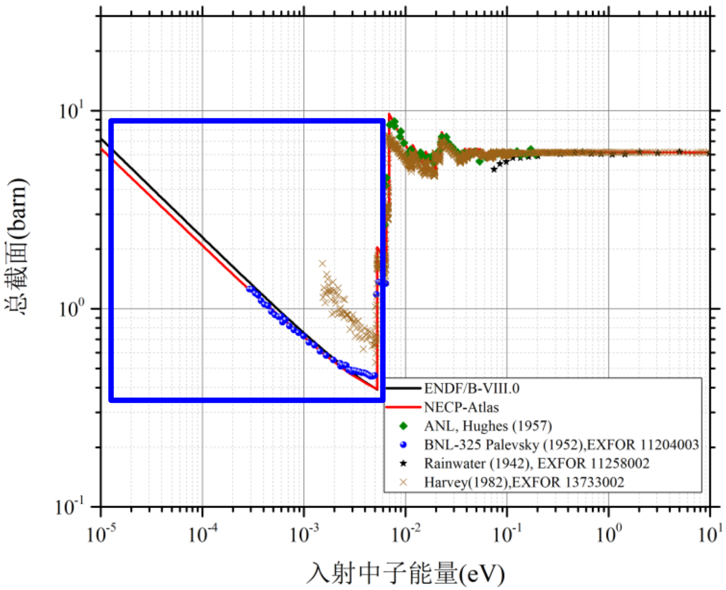
$$\sigma_{ine}(E \to E', \mu) = \frac{\sigma_b}{2k_B T}\sqrt{\frac{E'}{E}} S_s(\alpha, \beta)$$

- In the present work, this approximation is relaxed by using the first order phonon expansion:

$$\sigma_{ine}(E \to E', \mu) = \frac{\sigma_b}{2k_B T}\sqrt{\frac{E'}{E}} \times \left(\sum_{n=2}^{\infty} S_s^n(\alpha, \beta) + \frac{\sigma_{coh}}{\sigma_b} S^1(\alpha, \beta) + \frac{\sigma_{inc}}{\sigma_b} S_s^1(\alpha, \beta) \right)$$



Thermal scattering cross section for graphite



Thermal scattering cross section for Be metal

4. Generation of thermal scattering law

- The cubic and atom site approximations for coherent elastic scattering assume isotropic atomic interaction forces in a crystal, ignoring anisotropic forces and the correlation of forces from different directions.

$$W(|\vec{\tau}|) = \frac{\hbar^2 \tau^2}{4M_\mu k_B T} \int_0^\infty \frac{\rho(\beta)}{\beta} \coth\left(\frac{\beta}{2}\right) d\beta$$

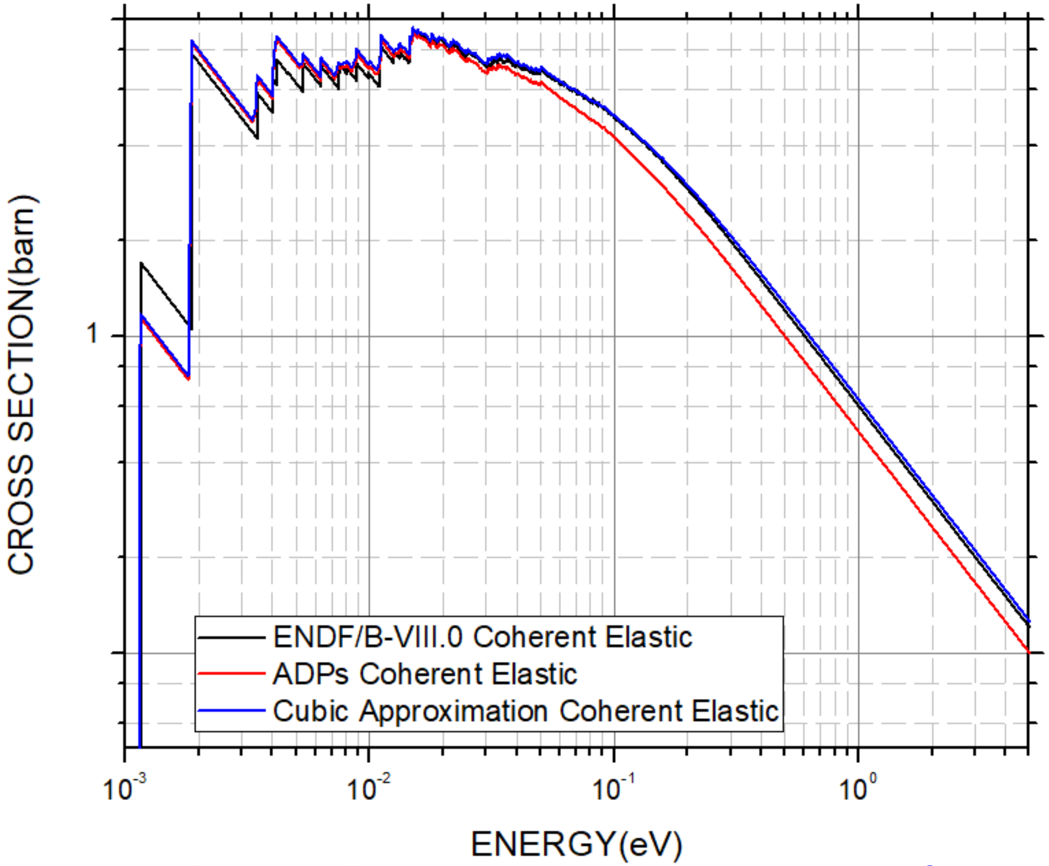
A universal phonon DOS

- In the present work, a method named anisotropic displacement parameters (ADP) is developed to correctly describe the forces of atoms in crystal.

$$W_j(\vec{\boldsymbol{\tau}}) = 2\pi^2 \vec{\boldsymbol{\tau}}^{\mathrm{T}} \boldsymbol{U}^j \vec{\boldsymbol{\tau}}$$

where

$$\vec{\boldsymbol{\tau}}^{\mathrm{T}} \boldsymbol{U}^j \vec{\boldsymbol{\tau}} = \frac{\begin{pmatrix} U_{11}\frac{h^2}{a^2}\sin^2\alpha + U_{22}\frac{k^2}{b^2}\sin^2\beta + U_{33}\frac{l^2}{c^2}\sin^2\gamma \\ +U_{23}\frac{2kl}{bc}(\cos\beta\cos\gamma - \cos\alpha) \\ U_{13}\frac{2hl}{ac}(\cos\alpha\cos\gamma - \cos\beta) + U_{12}\frac{2hk}{ab}(\cos\alpha\cos\beta - \cos\gamma) \end{pmatrix}}{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$



Coherent elastic scattering cross section for SiO_2.

The difference between the ADP model and cubic approximation reach about 17%. The result is consistent with the work in FLASSH code developed by North Carolina State University, USA.

5. Photon related data

- In the conventional nuclear data processing code, only the prompt gamma emitted during reactions is considered. But the delayed gamma emitted by decay of the unstable nuclides (for example the fission products) can not be taken into account.

- In the fast reactor, gamma heating can contribute more than 90% to the total heating; and the delayed gamma contributes roughly 30% to the total gamma heating.

- In NECP-Atlas, we develop the functions to generate photon related data as conventional nuclear data processing codes, including prompt gamma production data, phonon-atom reaction cross section, and the KERMA factor.

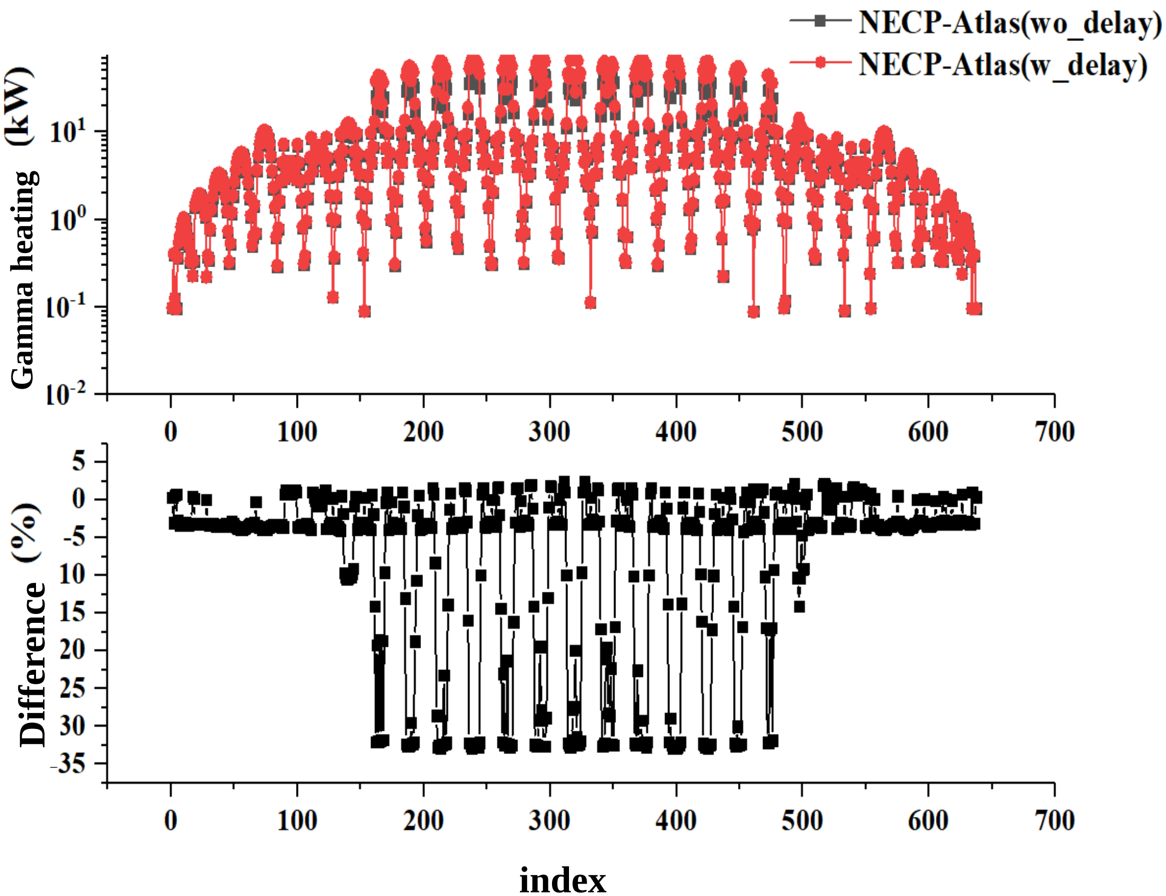
- The delayed gamma production data are calculated based on equilibrium condition as ERANOS code and MC^2 code.

Reference:

1. *A. Luthi, et al., Nuclear Science and Engineering, 138, 233-255, 2001*
2. *P. Deng, et al., Nuclear Science and Engineering, 193, 1310-1338, 2019.*

5. Photon related data

- The above implementation is used to generate photon related data for the home-developed fast reactor simulation code NECP-SARAX.
- Ignoring the delayed gamma will underestimate the gamma heating by about 30% for some assemblies.



Gamma heating of the assemblies in a fast reactor.

6. Summary

- The evaluated nuclear data for neutron reaction in GNDS format can be processed by NECP-Atlas.

- Several new processing functions are developed in NECP-Atlas, such as:
  - Treatment of resonance elastic scattering
  - Calculation of thermal scattering law
  - Generation of photon related data

Thanks for your listening!