XI'AN JIAOTONG UNIVERSITY

5th UPM/CEIDEN Workshop on "Impact of recent nuclear data evaluations on energy and non-energy nuclear applications"

Uncertainty Quantification Comparisons in Different Evaluated Libraries Based on the ENDF-6 Formatted Sampling Method

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Nuclear Engineering Computational Physics

Content

- Introduction
- Method
- Results
- Conclusions and Next Plan

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➢ Methods of sensitivity and uncertainty analysis

S&U Analysis

Deterministic Method

- Sensitivity:

$$S_{R,\sigma_{x,g}} = \frac{\sigma_{x,g}}{R}\frac{\partial R}{\partial \sigma_{x,g}}$$

- Uncertainty:

$$\frac{\sigma^2(R)}{R^2} = \mathbf{S}_{R,\alpha_i}\mathbf{\Sigma}_{\alpha_i\alpha_j}\mathbf{S}^T_{R,\alpha_j}$$

Perturbation Theory

$$S_{k_{eff},\sigma} = \frac{\delta k_{eff}/k_{eff}}{\delta\sigma/\sigma} = \frac{\sigma}{k_{eff}}\frac{\partial k_{eff}}{\partial\sigma} = -\frac{\sigma}{k_{eff}}\frac{\left\langle \phi^*, \frac{\partial \boldsymbol{L}}{\partial\sigma} - \frac{1}{k_{eff}}\frac{\partial \boldsymbol{F}}{\partial\sigma}\phi \right\rangle}{\left\langle \phi^*, \frac{1}{k_{eff}^2}\boldsymbol{F}\phi \right\rangle}$$

Directly Numerical Perturbation Method

$$S_{R_k,\sigma_{x,g}} = \frac{\sigma_{x,g}}{R_k}\frac{\partial R_k}{\partial\sigma_{x,g}} = \frac{1}{R_k}\frac{R_k((1+\delta^+_{x,g})\sigma_{x,g}) - R_k((1+\delta^-_{x,g})\sigma_{x,g})}{\delta^+_{x,g} - \delta^-_{x,g}}$$

Sampling Method

Deterministic method: $$Cov(A) \approx \sum_{i,j} \underbrace{\frac{\partial A}{\partial\alpha_i}\frac{\partial A}{\partial\alpha_j}}_{\text{Sensitivities}} \underbrace{Cov(\alpha_i,\alpha_j)}_{\text{Nuclear Data Covariances}}$$

Deterministic method calculate uncertainties based on sensitivities and nuclear data covariances, called sandwich rules.

Sampling method: $$Cov(A) \approx \frac{N}{N-1}\left[\frac{1}{N}\sum_{i=1}^{N}A(\vec{\alpha}(i))^2 - \left(\frac{1}{N}\sum_{i=1}^{N}A(\vec{\alpha}(i))\right)^2\right]$$

Sampling method generate samples based on nuclear data covariances, and uses statistical method to calculate uncertainties

Introduction

- **Why we do uncertainty analysis based on ENDF-6 format and sampling method?**
  - More accuracy
    - 1. **reduce the approximation** in covariance calculation method
    - 2. consider the fluence of **nuclear data processing code**
  - More covariances
    - 1. consider the covariance of different Legendre orders of **angular distributions**
    - 2. consider the covariance between **cross sections and distributions**
    - 3. consider the covariance of **TSL data, fission yield data, decay data** (**in the future**)
  - Generalized
    - 1. **ACE libraries or multi-libraries can both be generated**, and it can be used in any neutronics transport code
    - 2. **No need to modify neutronics transport code**.

For the above motivations, we developed an ENDF-6 files sampling code, named NECP-SOUL

Content

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- Method
- Results
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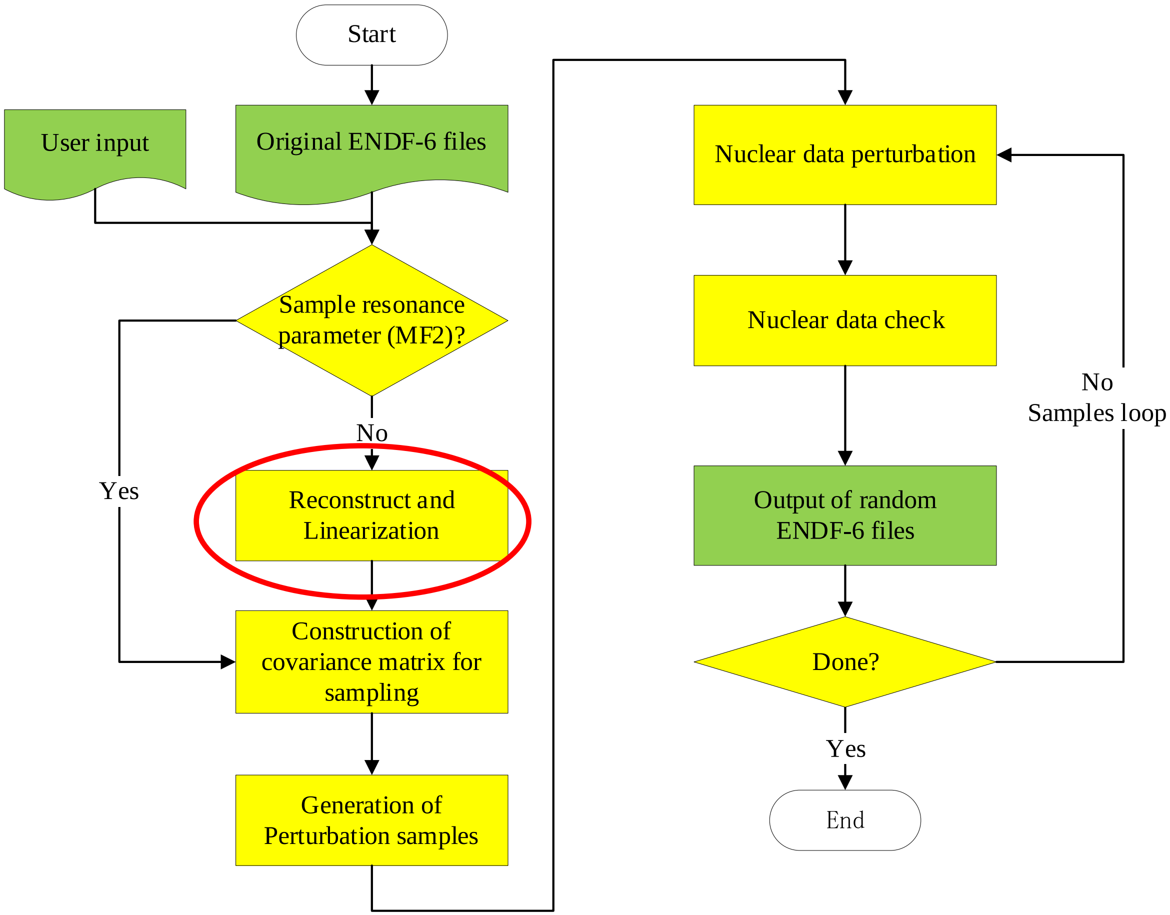
Flowchart of the NECP-SOUL code



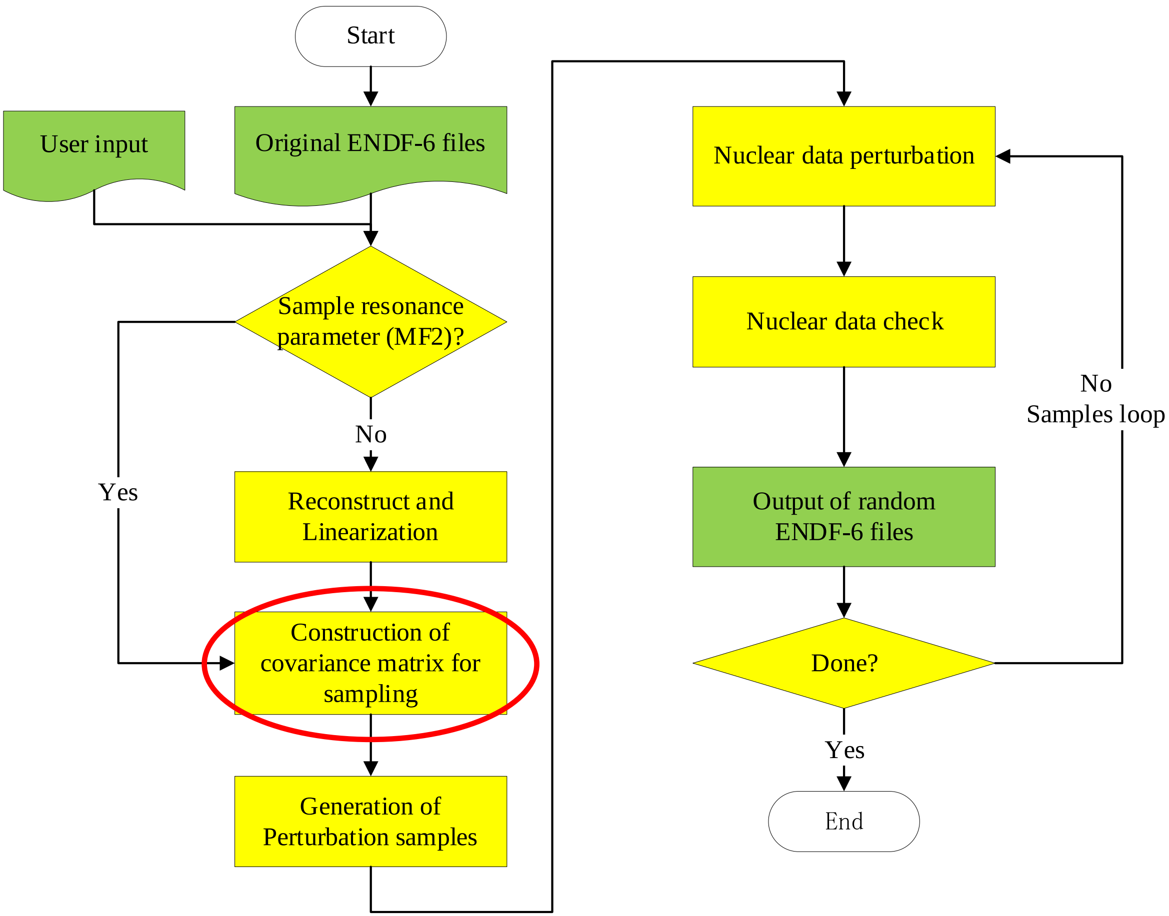
1. Reconstruct and Linearization

In original ENDF-6 library, only the background cross sections of **the resonance reactions** are given, and resonance parameter is provided, so the cross sections **must be reconstructed** according to resonance parameters.

In original ENDF-6 library, the interpolation method of cross sections may not be **lin-lin (INT≠2)**, it **must be linearized**.

Methods

Flowchart of the NECP-SOUL code



2.Construction of covariance matrix for sampling

In NECP-SOUL, As for cross sections, **relative covariances** are used in sampling method

According to ENDF-6 format, Flag **LB=0** means that **absolute covariances** are stored in ENDF-6 file, **relative covariances are calculated :**

$\boxed{\text{LB=0}}$ $$\mathrm{rcov}\left(\sigma_{xI},\sigma_{yJ}\right)_n=\frac{\mathrm{cov}\left(\sigma_x,\sigma_y\right)_n}{\sigma_{xI}\sigma_{yJ}}$$

- Flag **LB=[1,6]** means that **relative covariances** are stored in ENDF-6 file, relative covariance are used directly

$\boxed{1\text{<=LB<=}6}$ $$\mathrm{rcov}\left(\sigma_{xI},\sigma_{yJ}\right)_n=\mathrm{rcov}\left(\sigma_x,\sigma_y\right)_n$$

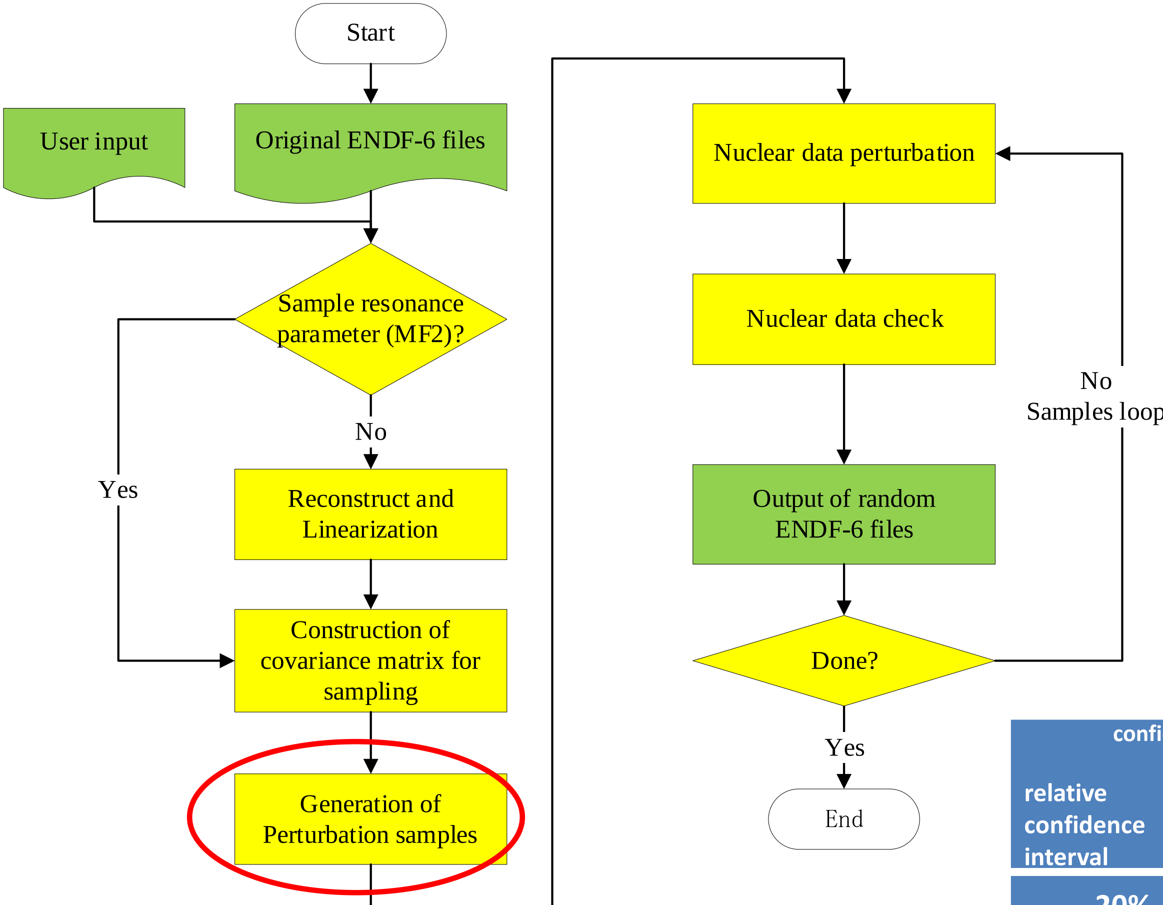
- Finally equation:

$$\mathrm{rcov}\left(\sigma_{xI},\sigma_{yJ}\right)=\sum_{n(\mathrm{LB}=0)}\frac{\mathrm{cov}\left(\sigma_{xI},\sigma_{yJ}\right)_n}{\sigma_{xI}\sigma_{yJ}}+\sum_{n(\mathrm{LB}=1\sim6)}\mathrm{rcov}\left(\sigma_x,\sigma_y\right)_n$$

Note: Only **NI-type covariances** are used for **sampling**, **NC-type covariances** are only used for **nuclear data check** module

Methods

Flowchart of the NECP-SOUL code



3. Generation of Perturbation samples

Latin Hypercube Sampling method (**LHS**) is used to generate samples.

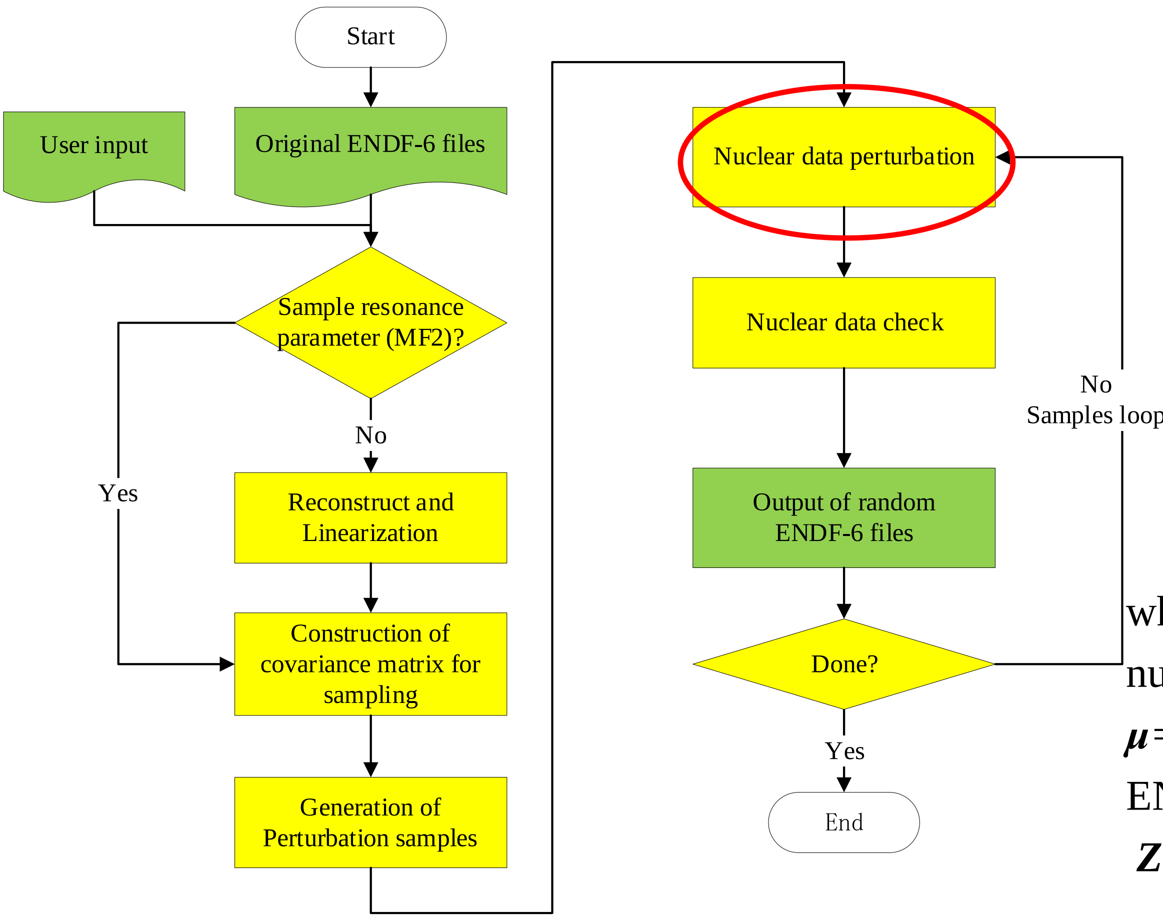
The number of samples can **be specified by the user**, or calculated according to **the confidence and relative confidence interval** requirements:

relative confidence interval \ confidence 1-α	0.90	0.95	0.99
20%	142	201	345
10%	548	777	1340
5%	1436	3084	5329
1%	54132	76852	132836

The detail steps of LHS sampling method can be find in our previous work:

Zu, T., Wan, C., Cao, L., et al., 2016, Total Uncertainty Analysis for PWR Assembly Based on the Statistical Sampling Method. Nuclear Science and Engineering 183. https://doi.org/10.13182/nse15-96.

Flowchart of the NECP-SOUL code



4. Nuclear Data Perturbation

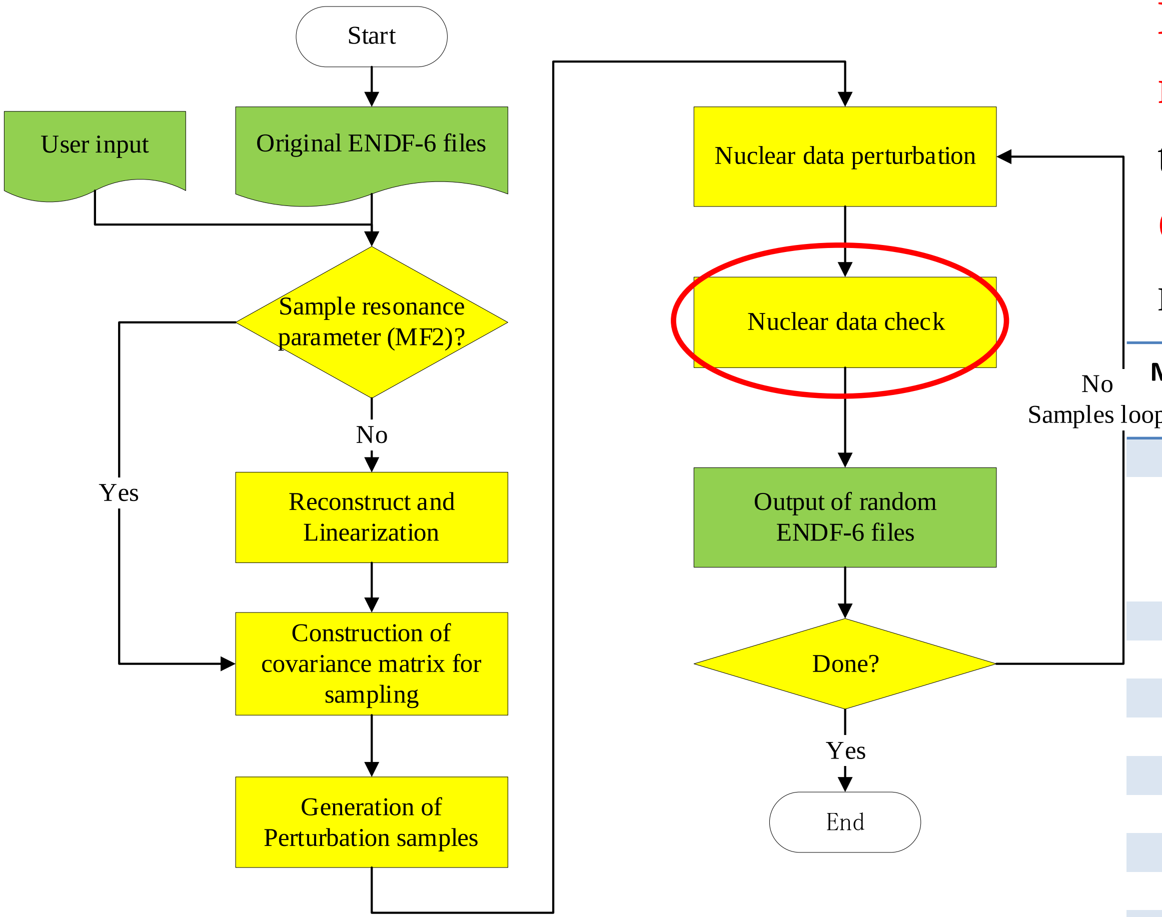
For cross sections, **the relative covariance** is used to generate perturbance factors, and the Equation of generate random cross sections can be described as:

$$\boldsymbol{X}_i = \boldsymbol{\mu}\left(\vec{\mathbf{1}} + \boldsymbol{Z}_i\right)$$

where $\boldsymbol{X}_i$ is the i-th output of the random nuclear data (**cross sections** in this example), $\boldsymbol{\mu}=[\mu_1, \mu_2, \ldots, \mu_m]^T$ is the best-estimates in ENDF-6 files

$\boldsymbol{Z}_i$ is the i-th column of perturbation factors.

Flowchart of the NECP-SOUL code

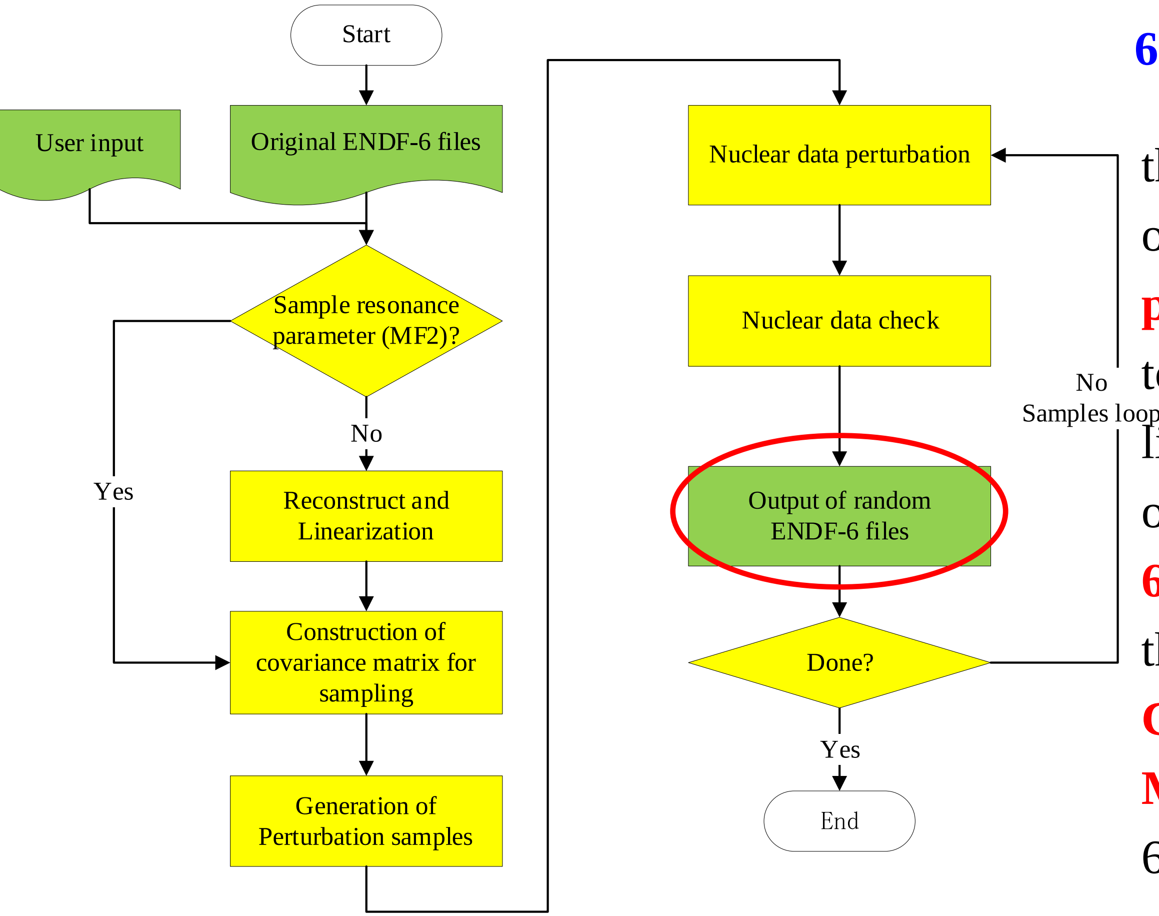


5. Nuclear Data Check

NC-type covariances are used to **recalculate cross sections** according to the Equation given in ENDF-6 file. **Other no covariances reactions** are recalculated based on ENDF-6 rules.

MT number of redundant reaction	MT number of constituting reactions
1	2,3
3	4-5,11,16-17,22-37,41-42,44-45, 152-154,156-181,183-190,194-196,198-200
4	50-91
16	875-891
18	19-21,38
27	18,101
101	102-117,155,182,191-193,197
103	600-649
104	650-699
105	700-749
106	750-799
107	800-849

Flowchart of the NECP-SOUL code

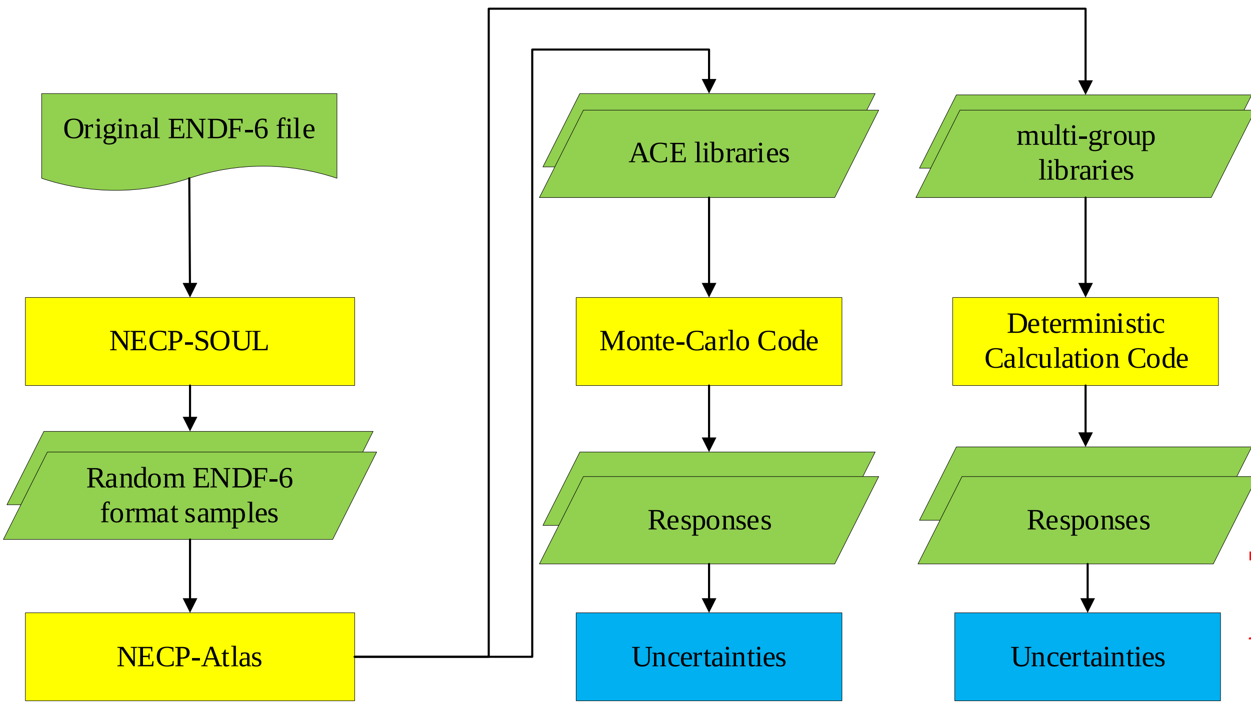


6.Output of random ENDF-6 files

the **reconstructed cross sections** are output in **MF 3,** and the **LRP parameter in MF 1 is modified to 2** to indicate the reconstruction and linearization has completed. Other output nuclear data (**MF 4, MF 5, MF 6, MF12, MF13, MF14, MF15**) are the same as the original ENDF-6 file. **Covariances data (MF31 MF33 MF34) are deleted** in random ENDF-6 files.

Methods

Flowchart of computing uncertainties based on NECP-SOUL



average value of the response R_0 can be written as

$$R_0 = \frac{1}{n}\sum_{i=1}^{n} R_i$$

Where R_i the i-th response (such as the multiplication factor k_{eff})

The uncertainty of the response R , σ_R can be written as:

$$\sigma_R = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(R_i - R_0)^2}$$

Our nuclear data processing code NECP-Atlas is used to generate random ACE libraries or multi-group libraries, and these random application libraries are used to calculate responses based on transport code.

Content

- Introduction
- Method
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Results

➢ V & V of NECP-SOUL

In order to test the correctness of our new code NECP-SOUL, we use NECP-SOUL to do the same calculation and compare the final results with another ENDF-6 formatted sampling code, SANDY , according to the benchmark questions and calculation conditions in the following article:

Fiorito, L., Dyrda, J., Fleming, M., 2019, JEFF-3.3 covariance application to ICSBEP using SANDY and NDAST. EPJ Web of Conferences 211, 07003. https://doi.org/10.1051/epjconf/201921107003.

Test uncertainties of Jezebel k_{eff} Reuslts:

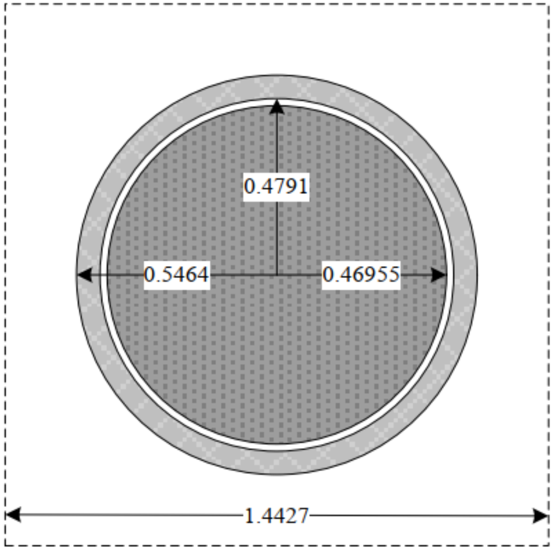
Nuclide	Nuclear Data	NECP-SOUL uncertainty	SANDY uncertainty
Pu-239	Fission neutron multiplicities	418 pcm	406 pcm
Pu-239	Corss sections	221 pcm	234 pcm
Pu-239	Prompt fission neutron spectrum	269 pcm	261 pcm

The results of NECP-SOUL agree well with those of SANDY, and prove the correctness of NECP-SOUL

Results

NECP ATLAS

- TMI-1 cell Benchmark(HFP)



Structure	Materials	Density/g • cm^{-3}	Temperature/K
Fuel Cylinder	UO_2	10.283	900
Gap	He	0.02685	900
Cladding	Zircaloy-4	6.55	600
Moderator	H_2O	0.7484	562

Transport code: NECP-MCX (Monte Carlo code)

Number of samples: 500

Compared Sampled Isotopes: H-1, Zr-90, U-235, U-238

Compared Sampled Data:

MF31 —— Average fission neutron multiplicities

MF33 —— Cross sections

MF34 —— angular distribution

MF35 —— fission spectrum

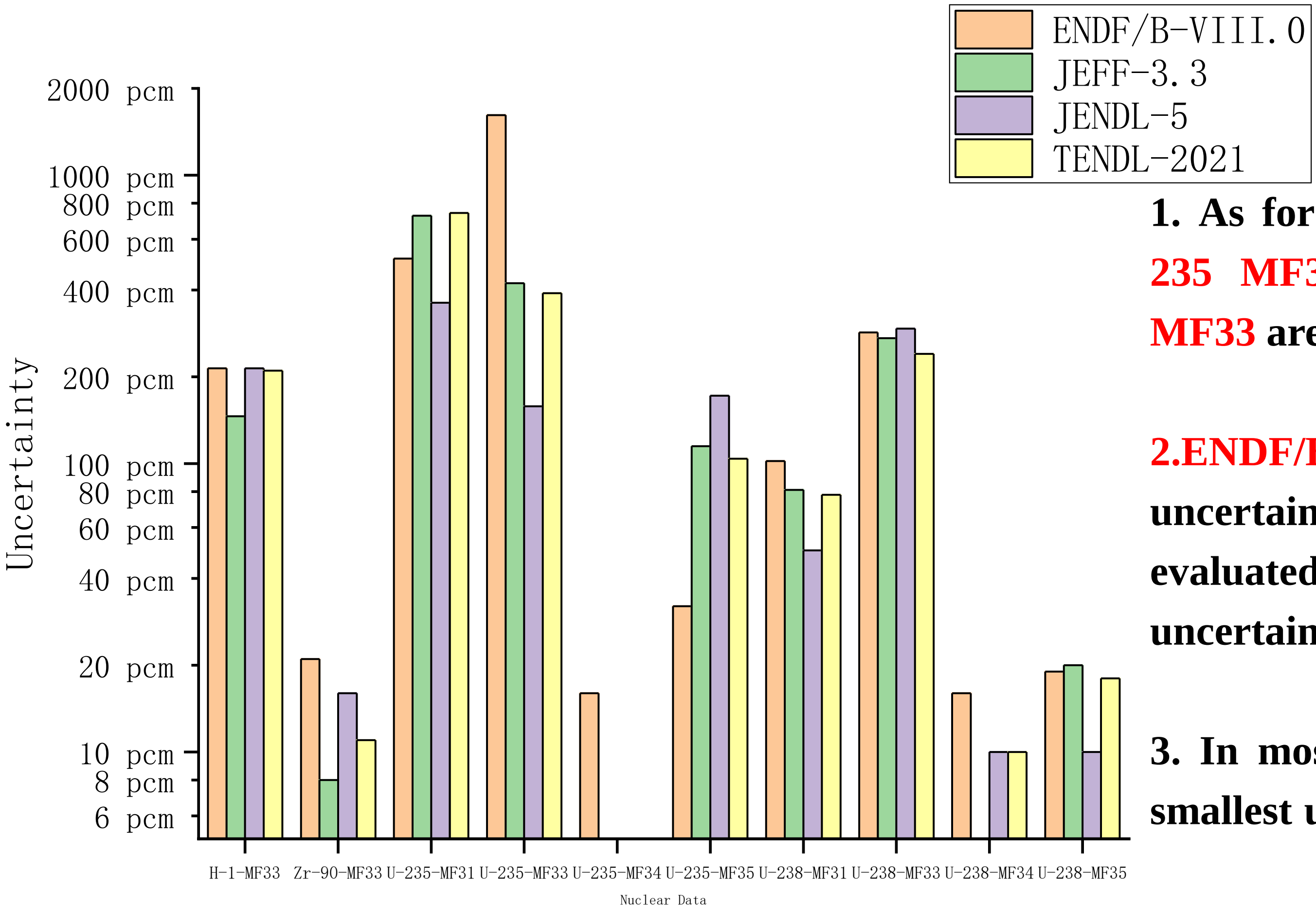
Compared Evaluated Libraries:

ENDF-B/VIII.0, JEFF-3.3, JENDL-5, TENDL-2021

Results

NECP ATLAS

➢ TMI-1 cell Benchmark(HFP)



1. As for all evaluated libraries, U-235 MF31、U-235 MF33、U-238 MF33 are among the top three

2.ENDF/B-VIII.0 has the Maximum uncertainty generally in these 4 evaluated libraries, the maximum uncertainties is U-235 MF33

3. In most cases, JENDL-5 has the smallest uncertainty results.

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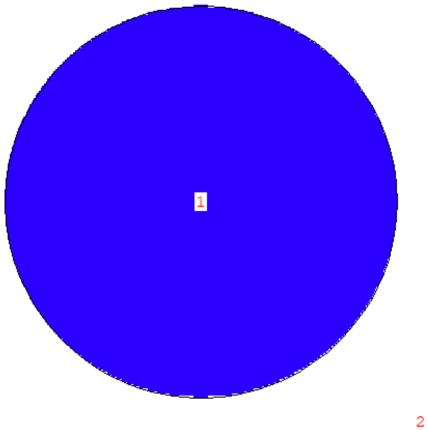
Godiva Benchmark

Cell	Sphere Radius/ cm	Temperature/K	Nuclide	density/10^{24} atom • cm^{-3}
			U-235	4.4994×10^{-2}
1	8.7407	300	U-234	4.9184×10^{-4}
			U-238	2.4984×10^{-3}



Transport code: NECP-MCX (Monte Carlo code)

Number of samples: 500

Compared Sampled Isotopes : U-235, U-238

Sampled Data:

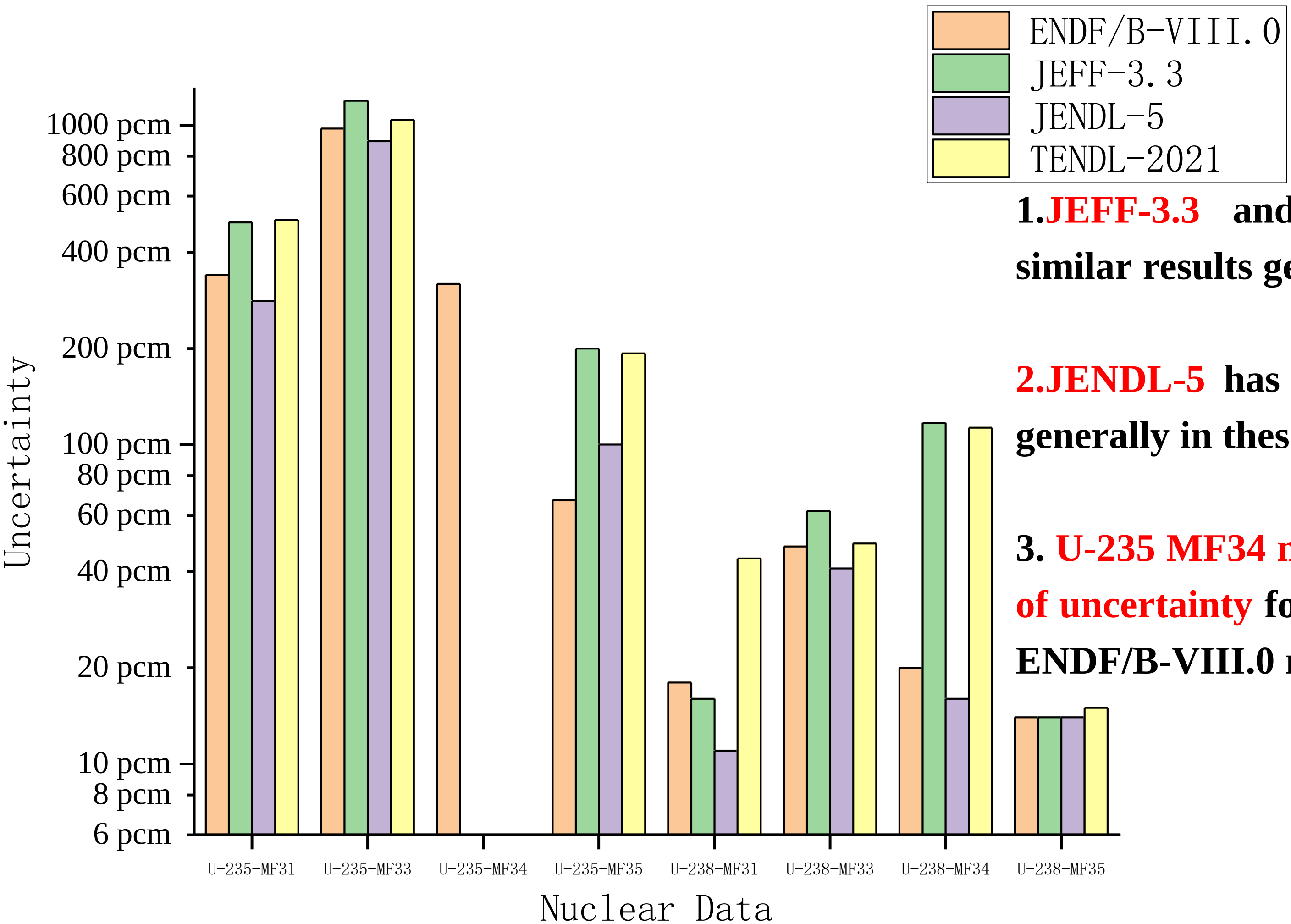
- **MF31 —— Average fission neutron multiplicities**
- **MF33 —— Cross sections**
- **MF34 —— angular distribution**
- **MF35 —— fission spectrum**

Evaluated Libraries:

ENDF-B/VIII.0, JEFF-3.3, JENDL-5, TENDL-2021

Results

- Godiva Benchmark



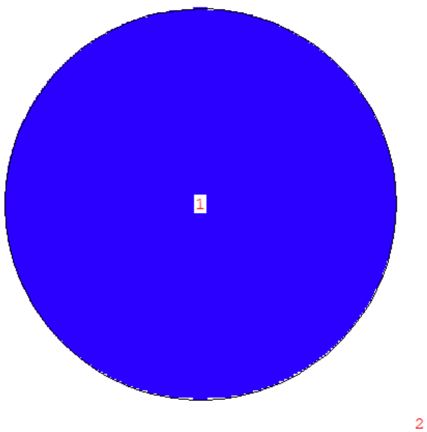
1.JEFF-3.3 and TENDL-2021 have the similar results generally

2.JENDL-5 has the Minimum uncertainty generally in these 4 evaluated libraries

3. U-235 MF34 may be an important source of uncertainty for this benchmark, but only ENDF/B-VIII.0 released the data.

➢ Jezebel Benchmark

Cell	Sphere Radius/ cm	Temperature/K	Nuclide	density/10^{24} atom • cm^{-3}
			Pu-239	3.7047×10^{-2}
1	6.38493	300	Pu-240	1.7512×10^{-4}
			Pu-241	1.1674×10^{-3}



Transport code: NECP-MCX (Monte Carlo code)

Number of samples: 500

Compared Sampled Isotopes : Pu-239

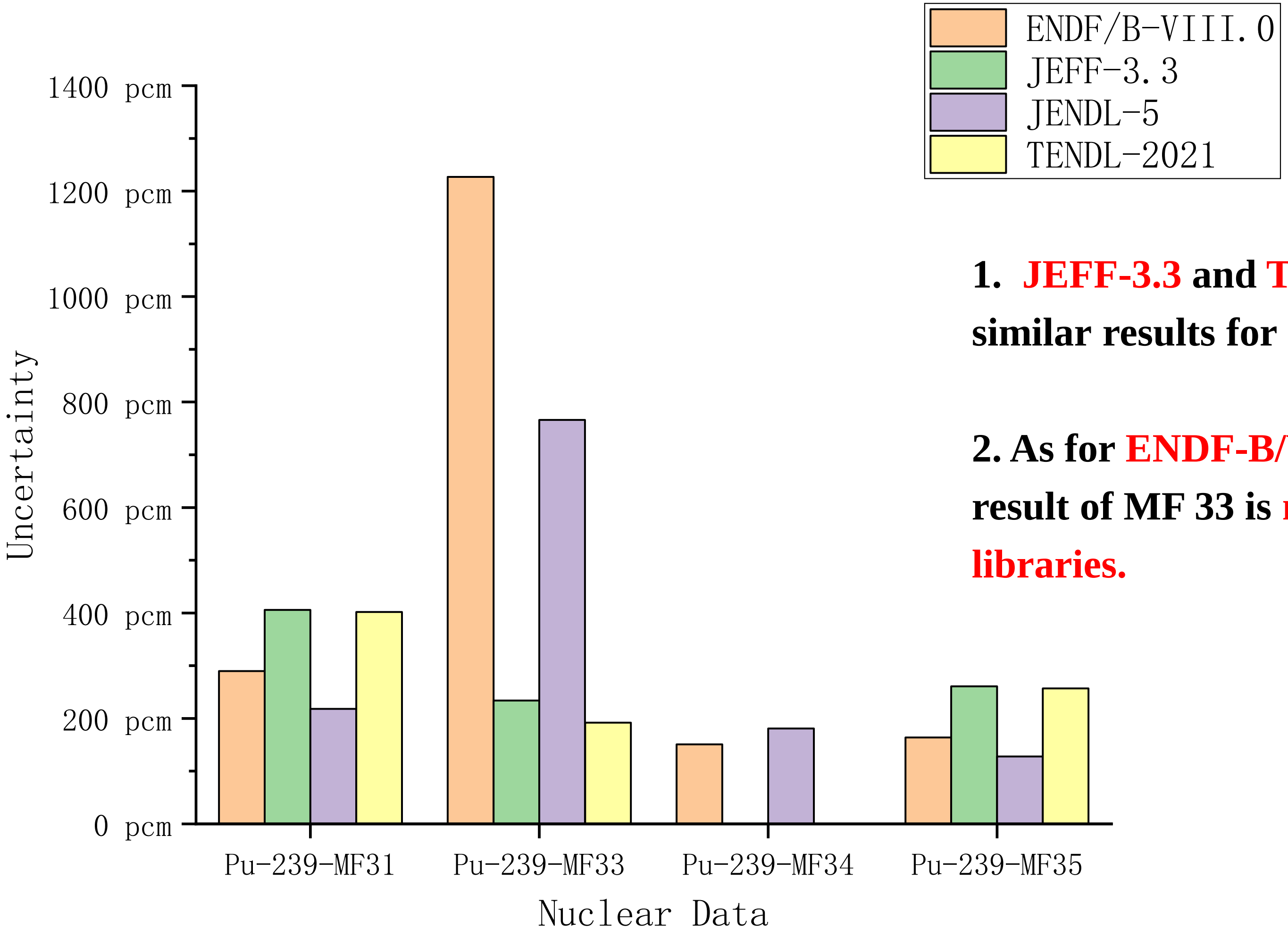
Sampled Data:

- **MF31 —— Average fission neutron multiplicities**
- **MF33 —— Cross sections**
- **MF34 —— angular distribution**
- **MF35 —— fission spectrum**

Evaluated Libraries:

ENDF-B/VIII.0, JEFF-3.3, JENDL-5, TENDL-2021

➢ Jezebel Benchmark



1. JEFF-3.3 and TENDL-2021 have the similar results for all nuclear data of Pu-239

2. As for ENDF-B/VIII.0, the uncertainty result of MF 33 is more large than other libraries.

Content

- Introduction
- Method
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Conclusions and Next Plan

➢ Conclusions

– A new code called NECP-SOUL is developed to generate random ENDF-6 files based on original ENDF-6 file and covariance data, these random ENDF-6 files have been used in uncertainty quantification based on nuclear data processing code NECP-Atlas and transport calculation code.

– ENDF/B-VIII.0, JEFF-3.3, JENDL-5, TENDL-2021 are used to calculate the uncertainties of three benchmarks. The results shows:

- In some cases, ENDF/B-VIII.0 may has more large uncertainties than other libraries.
- JEFF-3.3 and TENDL-2021 have the similar uncertainties results generally.
- Uncertainties calculated based on JENDL-5 are the smallest in most cases

Conclusions and Next Plan

➢ Next Plan

- Calculate the uncertainty results for **reactor assembly** and **reactor core** based on NECP-SOUL.

- Calculate the uncertainty results for shielding benchmarks, and analyze more data, such as **neutron flux** and **photon flux**.

- Develop code to **adjust data in ENDF-6 files** according to the uncertainty results

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