# FRENDY: A New Nuclear Data Processing Code being Developed at JAEA

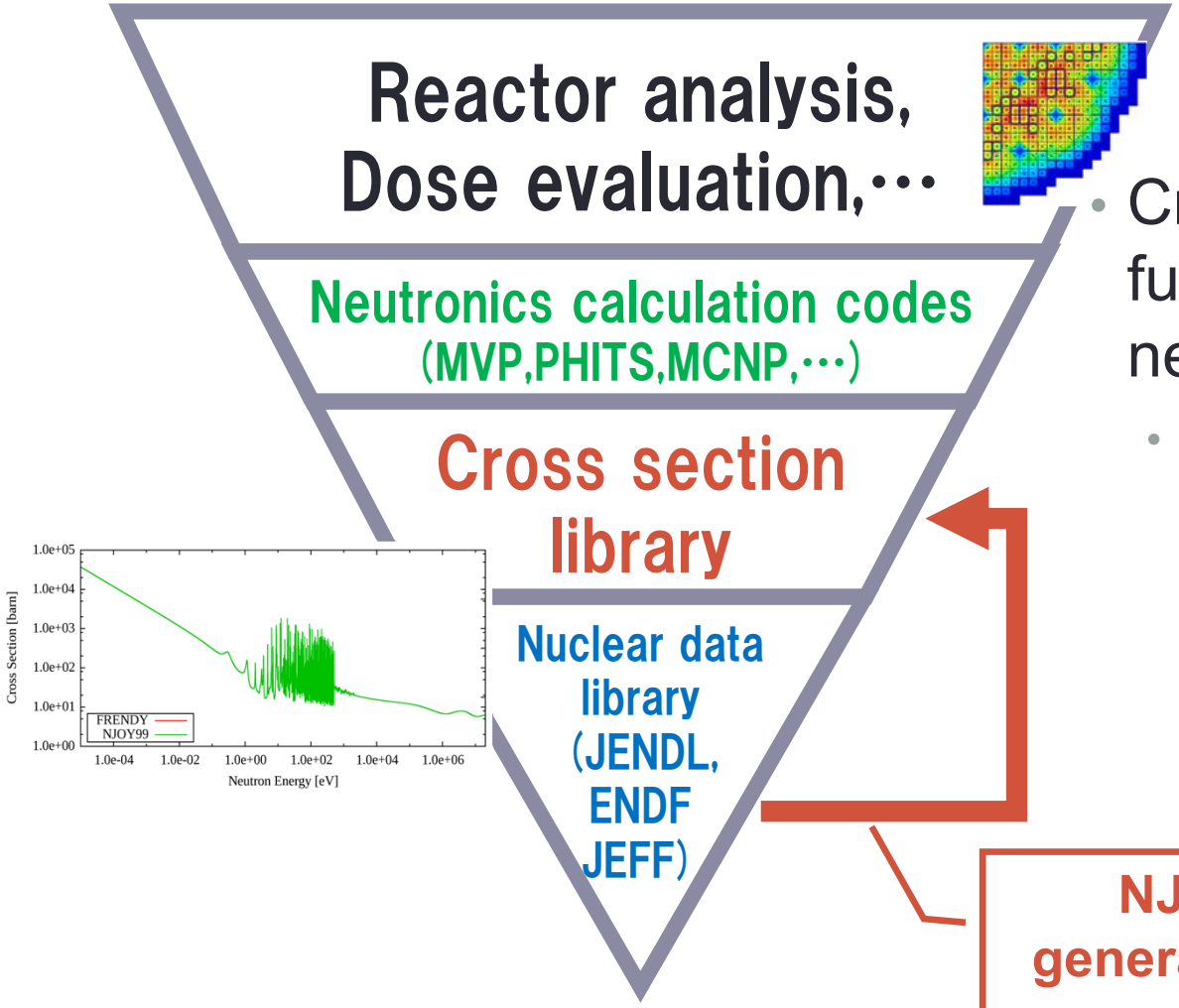
Japan Atomic Energy Agency (JAEA)
Kenichi Tada

# Outline

- Background
- Overview of FRENDY
- Comparison of processing results between FRENDY and NJOY
- Conclusions

# Overview of nuclear data processing and FRENDY

# Importance of nuclear data processing

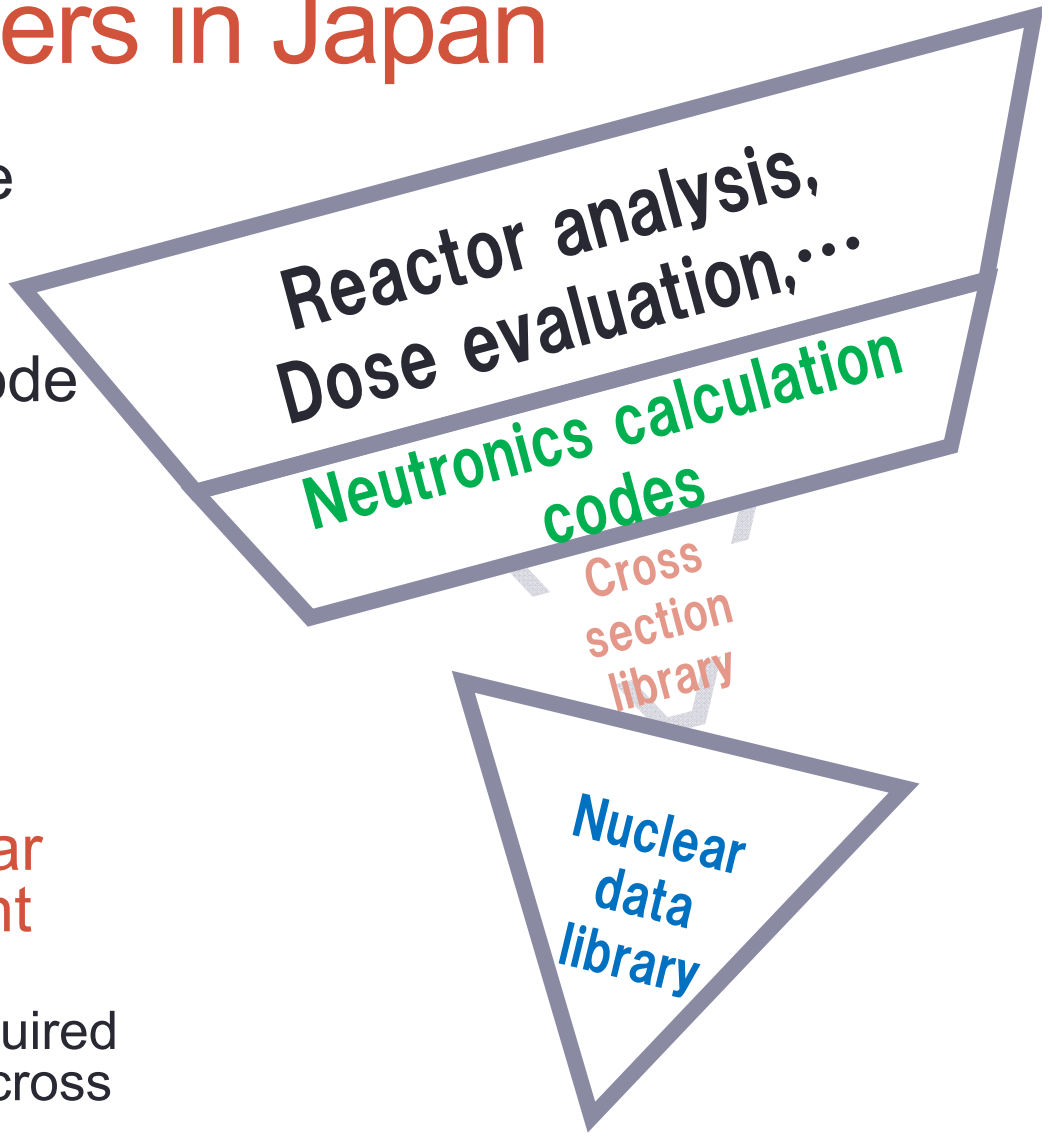



- Cross section library is the fundamental data for the neutronics calculations
  - Reliability of the cross section library has large impact on the neutronics calculation

**NJOY is widely used to generate cross section library in Japan**

# Number of engineers in Japan

- Neutronics calculation code users
  - More than 1,000
- Nuclear data processing code users
  - 1~2 in each company
  - Total : 20~30?
- Expert of nuclear data processing
  - Less than 10
- Technical tradition of nuclear data processing is important
  - Deeply understanding of the nuclear data processing is required to appropriately generate the cross section library

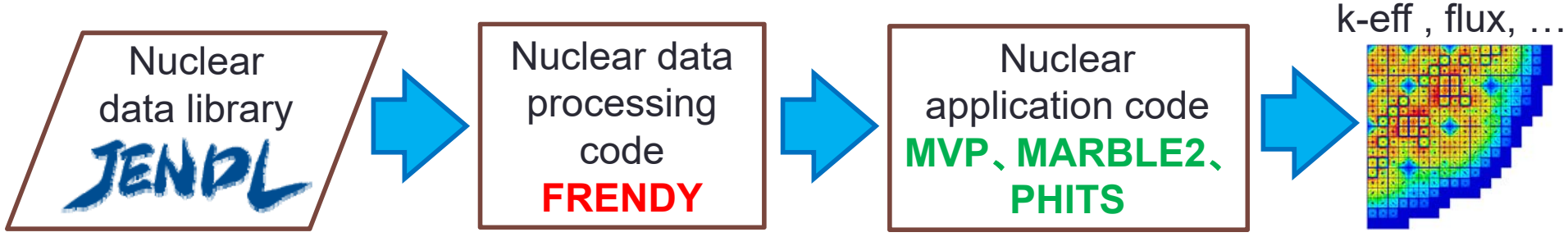


# Present situation of nuclear data processing in JAEA

- JAEA provides nuclear data library and many neutronics calculation codes
- The nuclear data processing code had not been developed
  - Imported nuclear data processing code are used
  - JAEA cannot release the nuclear data processing code for our neutronics calculation codes
- Development of domestic nuclear data processing code were desired

# 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 by JAEA's nuclear application codes users **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



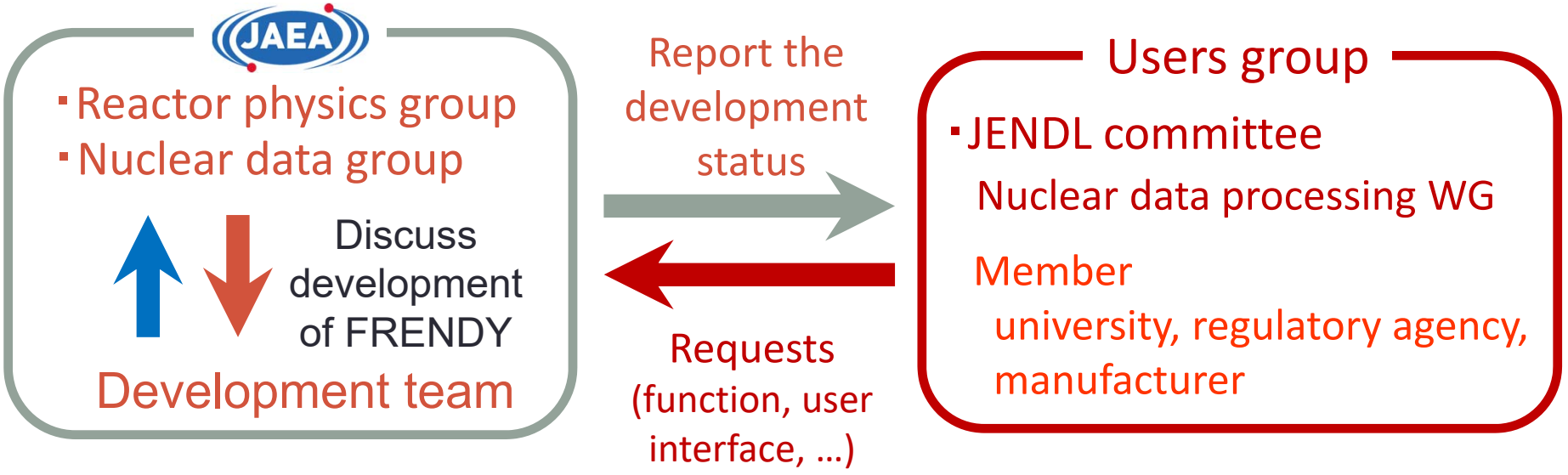
# Features of FRENDY

- 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
- Reflecting requests of nuclear data processing code users
  - 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)

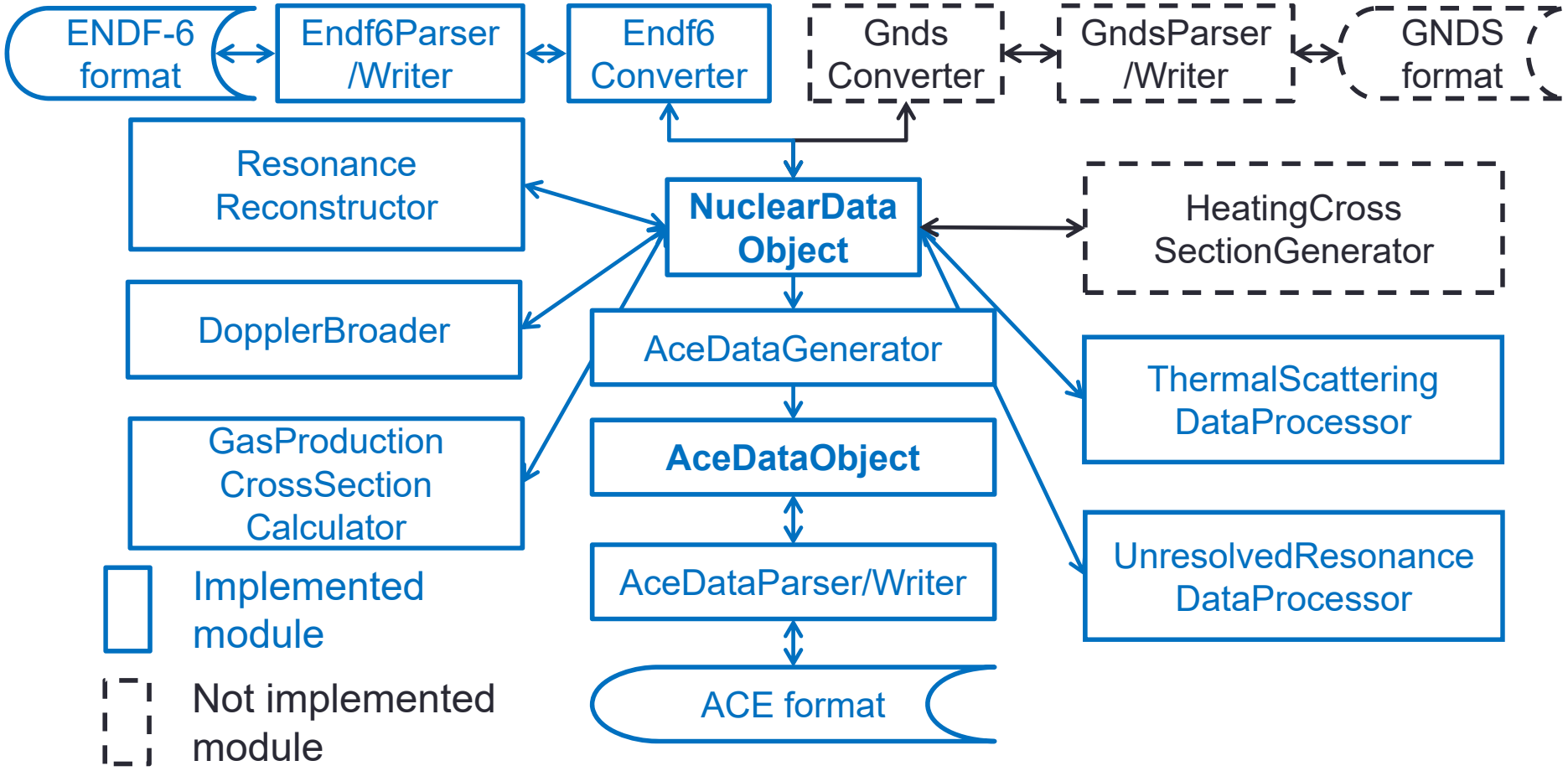
# Development system of FRENDY

- Development of FRENDY is supported many organization concerning to nuclear data processing in Japan
  - Reflecting request of nuclear data processing code users



# Structure of FRENDY

- Modularity is carefully considered
  - Modules of FRENDY can be used other calculation code by adding only a few lines



# GNDS format

- Developed by OECD/NEA/NSC/WPEC/SG38
  - Currently, maintained by WPEC/EGGNDS
- Completely different from ENDF-6 format
  - Utilizing Extensible Markup Language (XML)
  - It will be used not only for nuclear data file, but also other data file, e.g., cross section library and nuclear structure data file
- LLNL develops FUDGE code to convert ENDF-6 format to GNDS format
  - FUDGE code also processes nuclear data file to generate cross section library for LLNL's neutronics calculation codes

Ref. C. M. Mattoon, et al., "Generalized Nuclear Data: a New Structure (with Supporting Infrastructure) for Handling Nuclear Data," *Nucl. Data Sheets*, **113**, pp.3145-3171 (2012).
https://ndclx4.bnl.gov/gf/project/gnd/
https://www.oecd-nea.org/science/wpec/gnds/

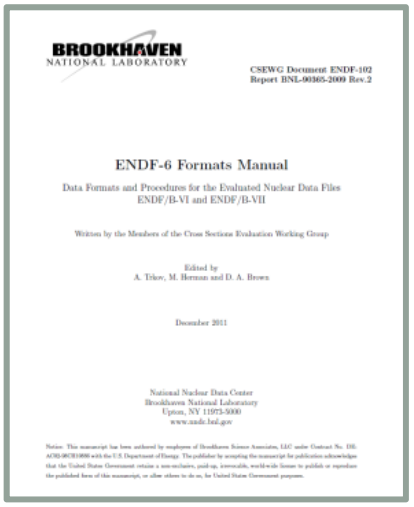
# Example of ENDF-6 format (MF=3)

## (n,2n) XS of Fe-56 from JENDL-4.0

| | | | | | | MAT | MF | MT | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 2.605600+4 | 5.545440+1 | 0 | 0 | 0 | 0 | 2631 | 3 | 16 | 1 | HEAD |
| -1.120270+7 | -1.120270+7 | 0 | 0 | 1 | 11 | 2631 | 3 | 16 | 2 | |
| 11 | 2 | 0 | 0 | 0 | 0 | 2631 | 3 | 16 | 3 | |
| 1.140470+7 | 0.000000+0 | 1.170000+7 | 1.622410-2 | 1.200000+7 | 4.800450-2 | 2631 | 3 | 16 | 4 | TAB1 |
| 1.300000+7 | 2.138200-1 | 1.400000+7 | 3.891650-1 | 1.500000+7 | 5.134000-1 | 2631 | 3 | 16 | 5 | |
| 1.600000+7 | 5.817500-1 | 1.700000+7 | 6.107500-1 | 1.800000+7 | 6.118000-1 | 2631 | 3 | 16 | 6 | |
| 1.900000+7 | 5.977000-1 | 2.000000+7 | 5.759000-1 | | | 2631 | 3 | 16 | 7 | |
| | | | | | | 2631 | 3 | | 99999 | SEND |

66 letters (11 data)

4 2 3 5 letters


BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-90365-2009 Rev.2

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI and ENDF/B-VII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

December 2011

National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973-5000
www.nndc.bnl.gov

[MAT, 3, MT/ ZA, AWR, 0, 0, 0, 0] HEAD
[MAT, 3, MT/ QM, QI, 0, LR, NR, NP/ Eint/ σ(E)] TAB1
[MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

ZA, AWR : 1000.0×Z+A, mass quantities for materials
QM : Mass-difference Q value (eV)
QI : Reaction Q value
LR : Complex or “breakup” reaction flag

# Example of GNDS format

(n,2n) cross section for Fe-56 from JENDL-4.0

(n, 2n) reaction

Reaction type

```
<reaction label="29" outputChannel="n[multiplicity:'2']
    + Fe55 + gamma" date="1987-03-01" ENDF_MT="16">
```

Cross Section

```
<crossSection nativeData="linear">
  <linear xData="XYs" length="11" accuracy="0.001">
    <axes>
      <axis index= "0"  label= "energy_in"  unit= "eV"
```

Interpolation

```
        interpolation="linear,linear" frame="lab"/>
      <axis index= "1"  label= "crossSection"  unit= "b"
        frame="lab"/></axes>
    <data> 1.14e7 0.00000 1.17e7 0.0162241 1.20e7 0.0480045
           1.30e7 0.21382 1.40e7 0.3891650 1.50e7 0.5134000
           1.60e7 0.58175 1.70e7 0.6107500 1.80e7 0.6118000
           1.90e7 0.59770 2.00e7 0.5759000 </data></linear>
</crossSection>
```

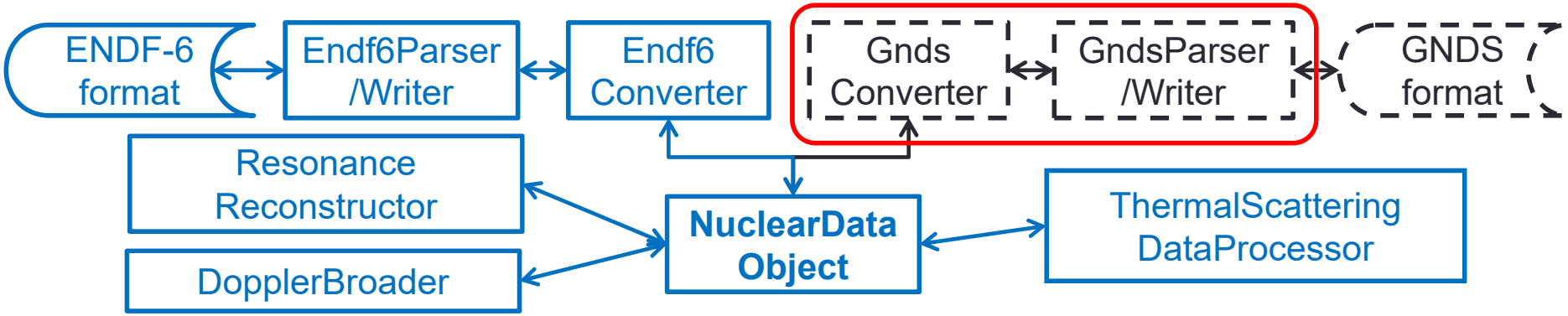
Cross section data

```
<outputChannel genre="NBody" Q="-11202700 eV">
  <product name="n" label="n" multiplicity="2"
    ENDFconversionFlag="MF6">
    <distributions nativeData="Legendre">
      <Legendre nativeData="LegendrePointwise">
```

Secondary energy and angular distribution

# Advantage for using the FRENDY's original nuclear data format

- FRENDY uses independent internal nuclear data format
  - NuclearDataObject class
- Minimizing the impact by the change of nuclear data format
  - Developer and users are not necessary to consider the nuclear data format
  - Consideration of a new data format GNDS
    - GNDS format can be addressed if another set of parser, writer and converter classes are implemented



# Input file of FRENDY

- FRENDY treats two types of the input format
  - FRENDY's original input format
  - NJOY compatible
- Simple input format
  - Nuclear data file name and processing mode are **only** required for the processing
    - FRENDY has recommended value in the source code
    - User can also change (override) parameters

# Input format of FRENDY and NJOY

- Input parameters of FRENDY consist of “input data name” and “input data”
  - Comment line is similar to C/C++
    - //~ or /* ~ */
- Input parameters of NJOY are hard to understand
  - This input format is so difficult for beginners

【Sample input of FRENDY】

```
ace_fast_mode  // Processing mode
  nucl_file_name   U235.dat
  ace_file_name    U235.ace
  temp              296.0
```

【Sample input of NJOY】

```
reconr                          / command
 20  21                         / input(tape20), output(tape21)
'pendf tape for JENDL-4 U235'   / identifier for PENDF
 9228                           / mat
 1.00e-03  0.00                 / err, temp
 0                              /
broadr                          / command
 20  21  22                     / endf, pendf(in), pendf(out)
 9228  1                       / mat, temp no
 1.00e-03  -5.0E+2              / err, thnmax
 296.0                          / temp
 0                              /
gaspr                           / command
 20  22  23                     / endf, pendf(in), pendf(out)
purr                            / command
 20  23  25                     / endf, pendf(in), pendf(out)
 9228  1  7  20  500            / mat, temp no, sig no, bin no, lad no
 296.0                          / temp
 1E10  1E4  1E3  300  100  30  10   / sig zero
 0                              /
acer                            / command
 20  25   0  30  31            / nendf, npend, ngend, nace, ndir
 1   1   1  0.30                / iopt(fast), iprint(max), itype, suffix
 'ACE file for JENDL-4 U235'  / descriptive character
 9228  296.0                   / mat, temp
 1  1                           / newfor(yes), iopp(yes)
 1  1  1                        / thin(1), thin(2), thin(3)
stop                            /
```

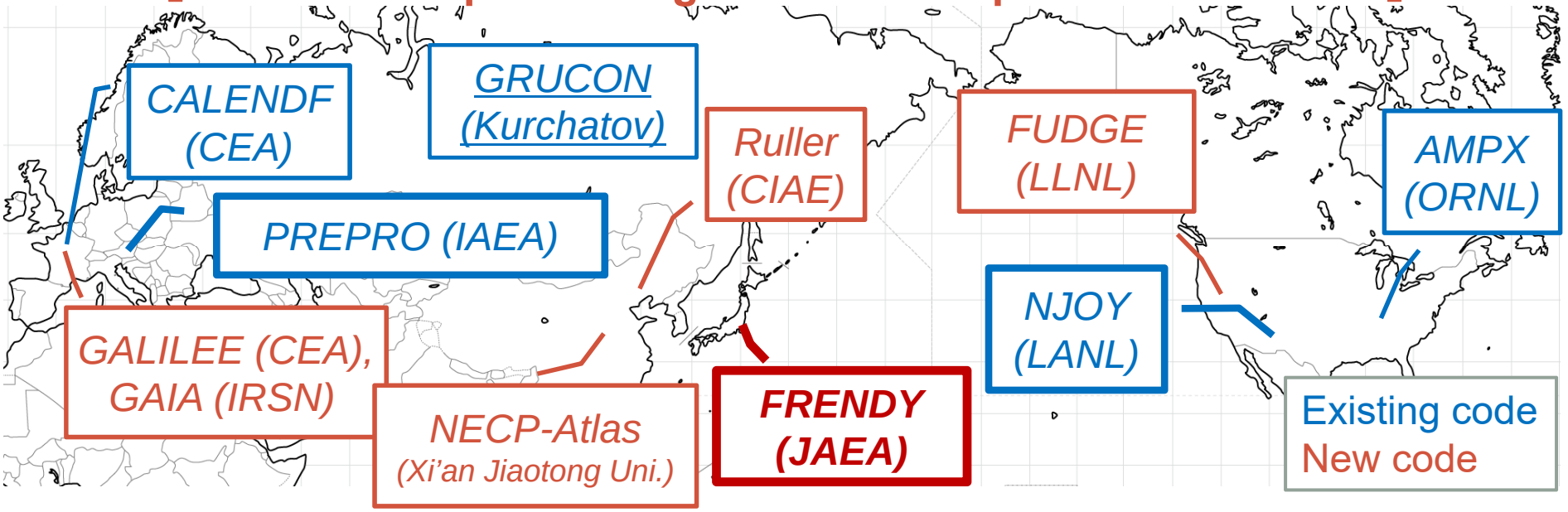
# Development schedule of FRENDY

- FRENDY ver.1 will be released in the next spring
  - Generation of ACE file
- Generation of multi-group cross-section library will be implemented in the near future
  - Processing covariance data and calculation of KERMA factor will also be implemented

# Present status of nuclear data processing code development

- 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*.

| Comparison of nuclear data processing code | | V&V | Close relationship with users and evaluators | Special focus on domestic utilization including nuclear regulators | Using latest programming technique | Treatment of new nuclear data format | Ease in use for beginners | NJOY compatible I/O | Continuing update and maintenance | Human resources |
|---|---|---|---|---|---|---|---|---|---|---|
| Existing code | NJOY2016 | △ | ○ | ○ | × | × | × | ○ | △ | 1.5 |
| | PREPRO | △ | ○ | △ | × | × | × | × | △ | 1 |
| New code | NJOY21 | ○ | ○ | △ | ○ | ○ | × | ○ | ○ | 2.5 |
| | FRENDY | ○ | ○ | ○ | ○ | ○ | ○ | ○ | ○ | 1.5 |

# Comparison of processing results between FRENDY and NJOY

# Comparison of processing results

- Processing results of FRENDY are compared to those of NJOY99.393 for verification
  - All nuclei in JENDL-3.3 and JENDL-4.0 are compared
  - We found several programming errors in NJOY
- Calculation conditions
  - Temperature : 296.0 K
  - Tolerance (error): 0.01%

# Comparison of processing time

- The processing time to generate ACE files is compared
  - Processing time of FRENDY is similar to that of NJOY
  - Adoption of the fixed energy grid affects the calculation time of the TLS data
- Cause of difference
  - Calculation method
  - Programming language
  - Adopting dynamic array

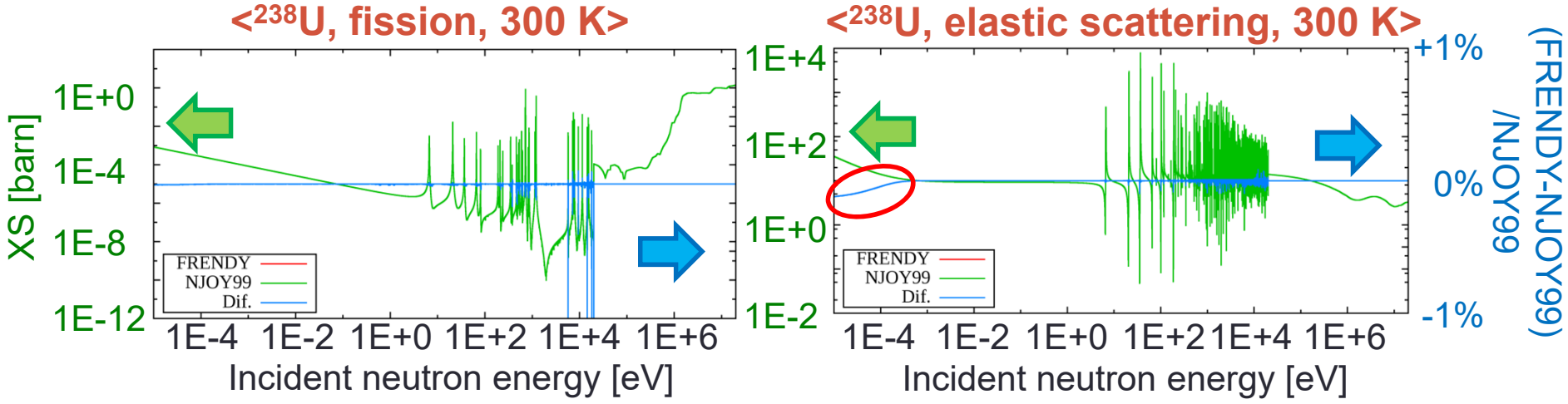
< Processing time [s] >

| | FRENDY | NJOY | F/N |
|---|---|---|---|
| $^{1}H$ | 0.1 | 0.2 | 0.5 |
| $^{16}O$ | 3.1 | 0.8 | 3.9 |
| $^{56}Fe$ | 18.7 | 9.1 | 2.1 |
| $^{235}U$ | 821.7 | 841.0 | 1.0 |
| $^{238}U$ | 507.5 | 709.1 | 0.7 |
| $^{239}Pu$ | 348.7 | 534.9 | 0.7 |
| $^{1}H$ in $H_2O$ | 213.8 | 14.8 | 14.4 |
| $^{1}H$ in ZrH | 101.7 | 58.6 | 1.7 |
| Graphite | 116.9 | 9.5 | 12.3 |

*Intel Xeon CPU E7-8857 v2 (3.00GHz, turbo 3.60GHz)

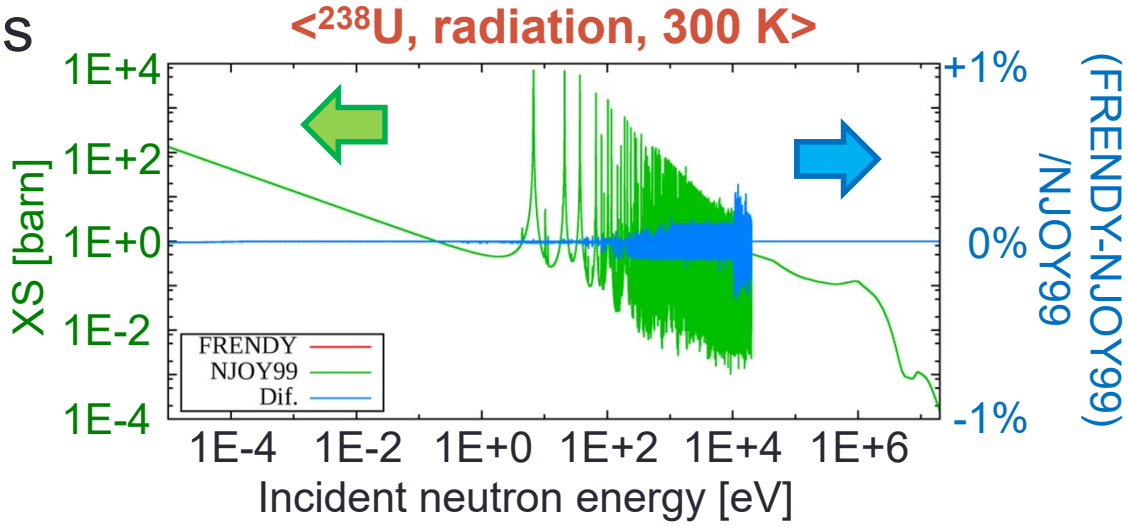
# Comparison of Doppler broadening

- The processing results of FRENDY are similar to those of NJOY99
  - The elastic scattering cross section shows the characteristics difference at the low energy region (less than $1.0 \times 10^{-3}$ eV)
    - The calculation of the cross section at 0.0 eV is different
  - Other nuclei also show similar difference



# Calculation of cross section at 0.0 eV

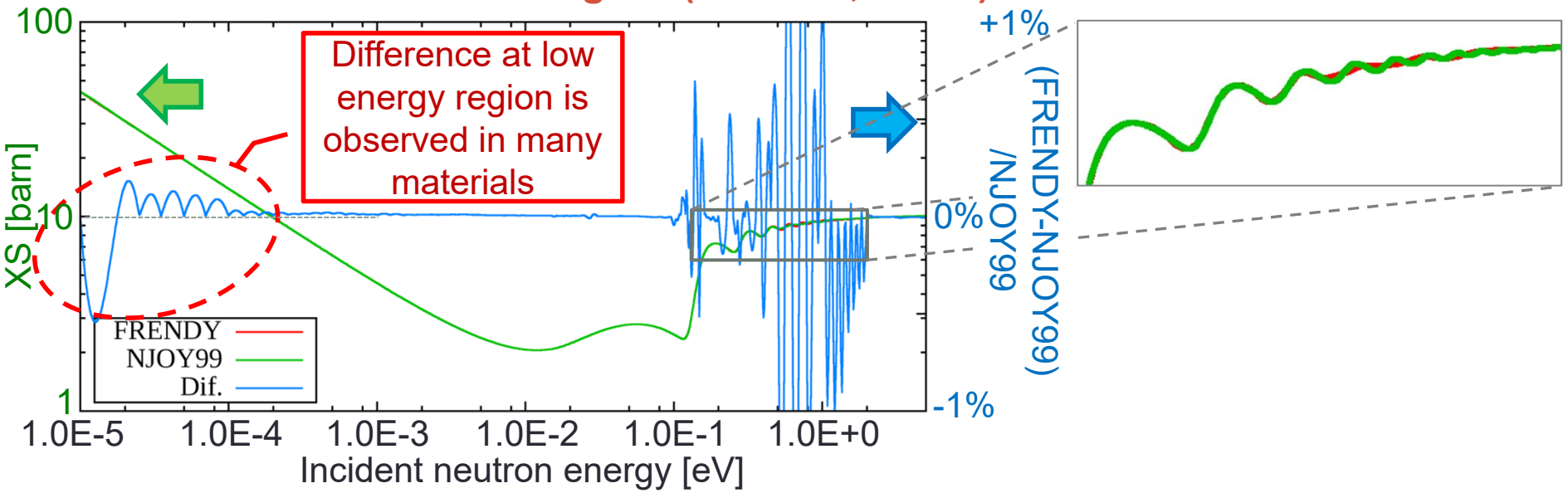
- The cross section at 0.0 eV is required to calculate the Doppler broadened cross section at low energy region
- NJOY approximates that the cross section follows the 1/v law
  - Since the elastic scattering cross section at the low energy region is constant, this approximation is not appropriate
- FRENDY uses linear extrapolation to calculate it
  - Linear extrapolation is appropriate for other reaction types which obey the 1/v law



# Difference of incoherent inelastic - Utilization of fixed energy grid -

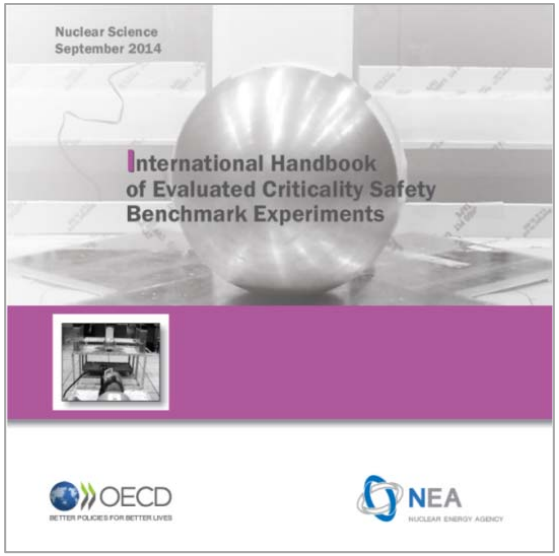
- NJOY only calculates the incoherent inelastic XS on 117 energy grids
  - Other energy grids are interpolated using the 5th order Lagrange interpolation
- The fixed energy grid is not appropriate for a material of which the cross section is oscillated
  - This difference may have impact on the TRIGA reactor

<Incoherent inelastic scattering XS (H in ZrH, 400 K)>



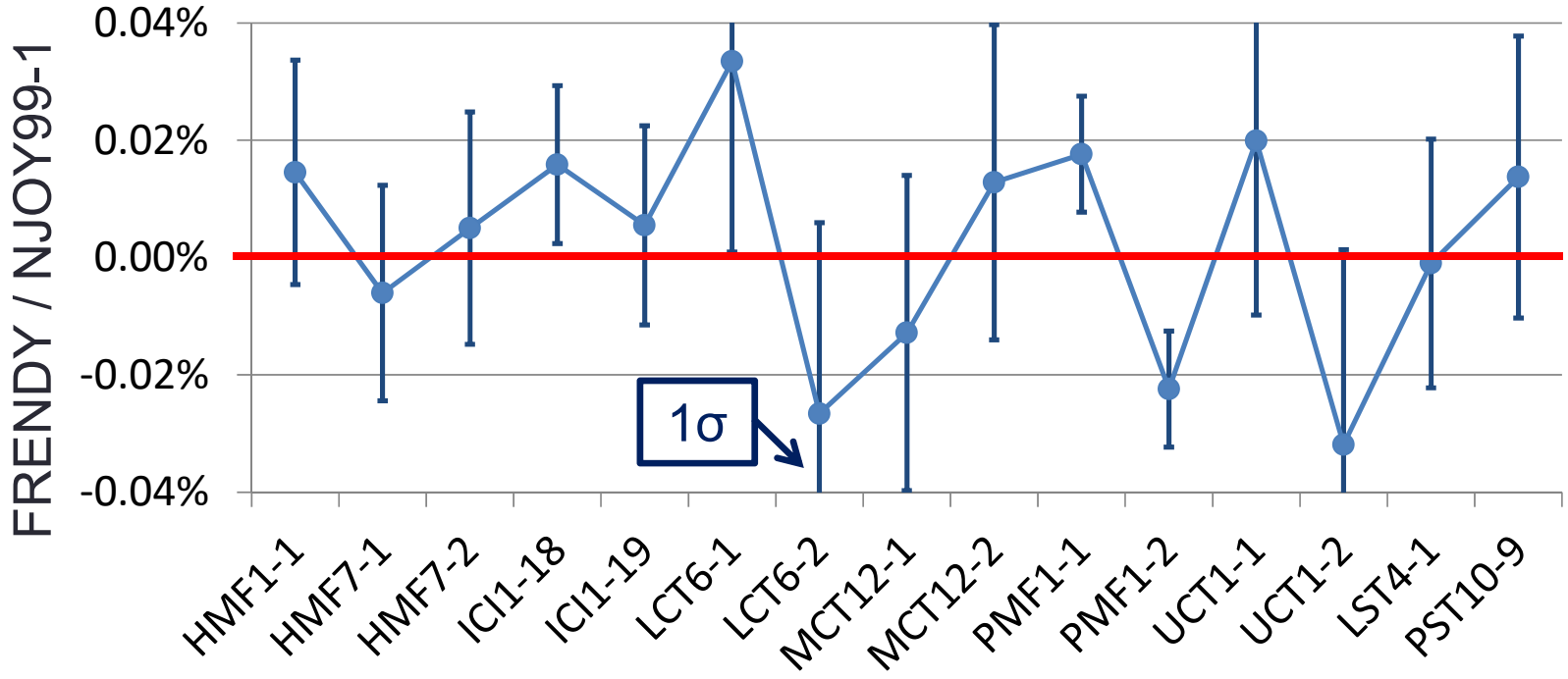
# Verification of ACE file generating function

- Comparison of $k_{eff}$ values of ICSBEP benchmark
  - MCNP sample input files in ICSBEP handbook
    - 79 benchmark experiments, 752 critical configurations
  - Calculation results are not compared to the experimental results
    - Many of sample input files were not intended to be used for the strict validation
- All processes to generate the ACE file are processed by FRENDY and NJOY99.393
  - **The processing methods of FRENDY are similar to those of NJOY**
    - The programming errors in NJOY is also implemented in FRENDY for the verification
- Processing condition
  - Nuclear data library : JENDL-4.0
  - Temperature : 296.0 K
  - Tolerance (error) : 0.1 %
  - Ladder number : 100



# Comparison for integral experiments

- $k_{eff}$ values of FRENDY are similar to those of NJOY99
  - Differences are not so varied with the neutron spectra and the major fissile materials
- FRENDY properly generates ACE files

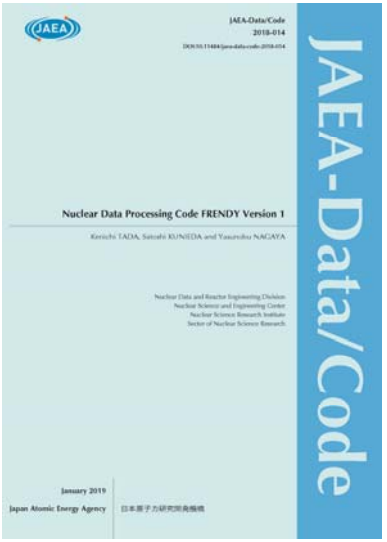


# Conclusions

- Overview of nuclear data processing
  - Nuclear data processing code is not just a converter
  - It performs many processes to generate cross section library
- Overview of FRENDY
  - Utilization of modern programming techniques
  - Simple input format
  - Reflecting requests of nuclear data processing code users
- Comparison of the processing results
  - Processing results of FRENDY are compatible to those of NJOY99.393/2012.08

# Release of FRENDY ver. 1

- FRENDY Ver.1 will is released
  - From our web site or NEA Data-Bank
    - https://rpg.jaea.go.jp/main/en/
  - FRENDY Ver.1 is only generates ACE files
    - Generation of multi-group cross section library will be implemented in the near future
  - 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